CellPress

TABLE FOR AUTHOR TO COMPLETE

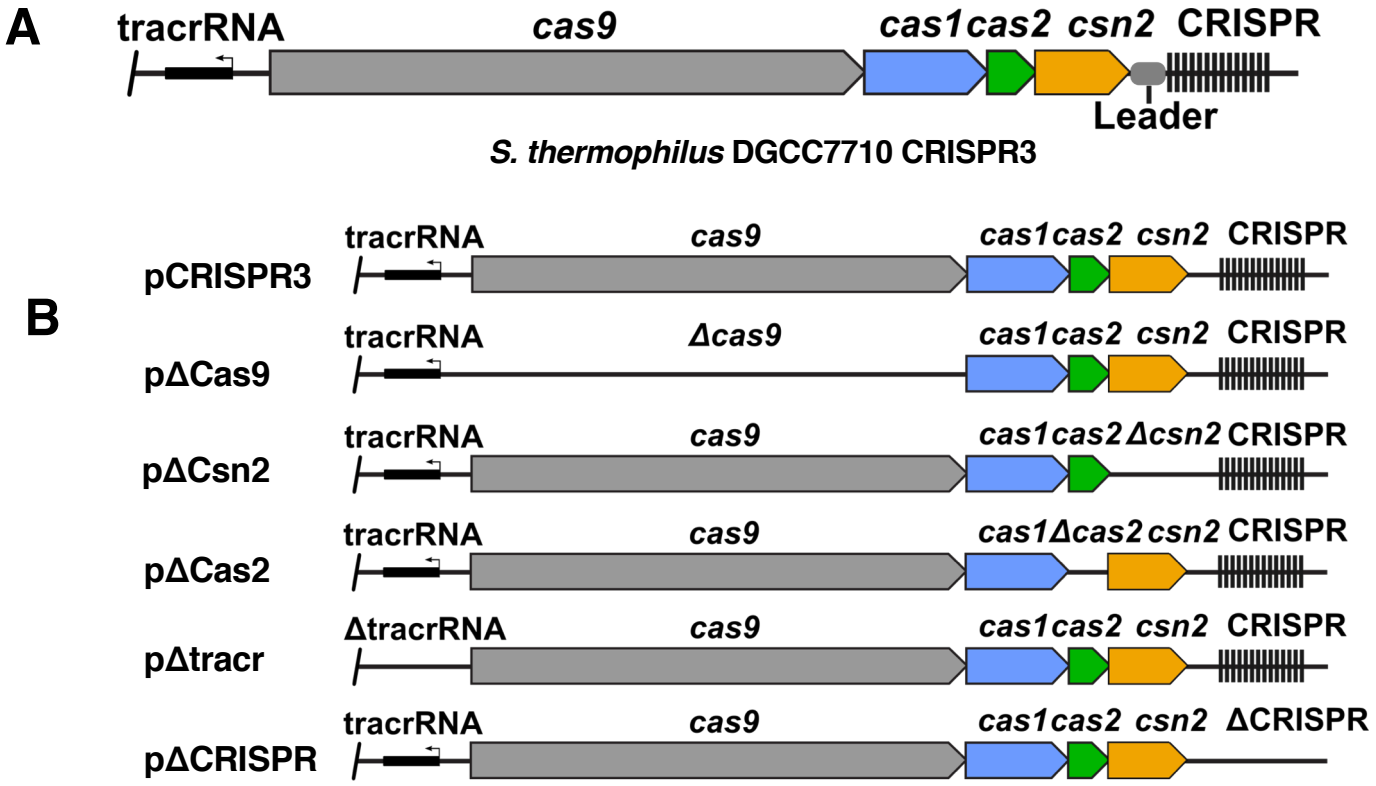
Please upload the completed table as a separate document. ***Please do not add subheadings to the Key Resources Table.*** *If you wish to make an entry that does not fall into one of the subheadings below, please contact your handling editor. (**NOTE:** For authors publishing in Current Biology, please note that references within the KRT should be in numbered style, rather than Harvard.)*

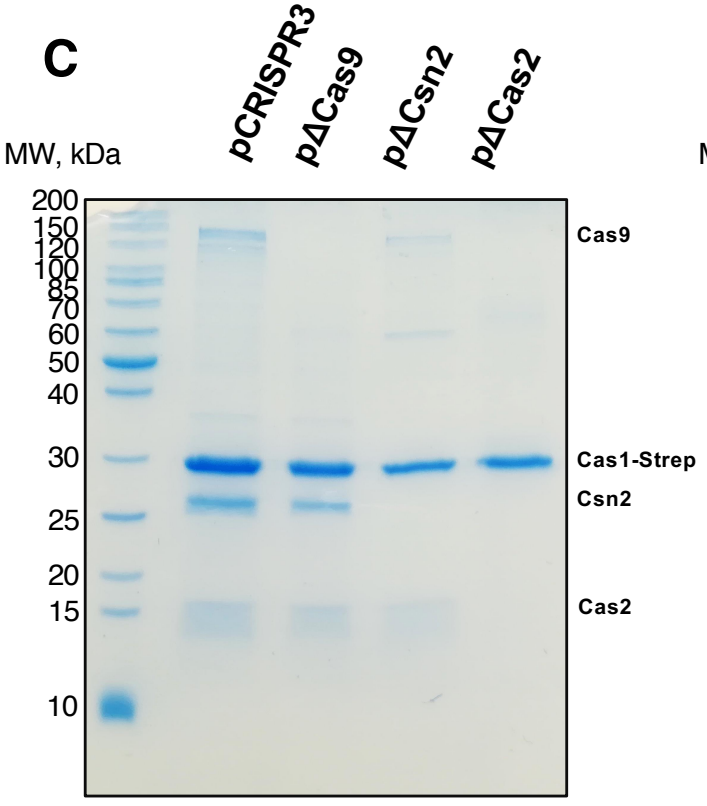
KEY RESOURCES TABLE

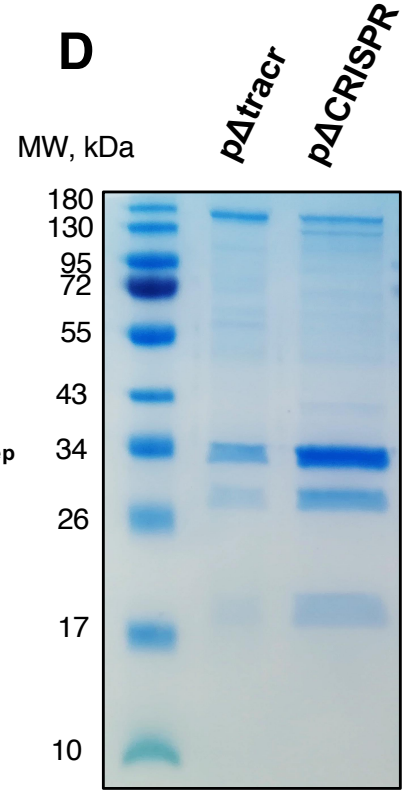
REAGENT or RESOURCE	SOURCE	IDENTIFIER
Bacterial and Virus Strains		
E. coli BL21(DE3)	Novagen	69450
Chemicals, Peptides, and Recombinant Proteins		
Recombinant DNaseI (RNase free)	Roche	03539121103
T4 PNK	Thermofisher	EK0031
Graphene Oxide	Sigma-Aldrich	763705-25ML
IPTG	Thermofisher	R0392
Critical Commercial Assays		
NEBNext® Ultra™ II DNA Library Prep Kit for Illumina®	NEB	E7645S
Deposited Data		
Cas1Cas2Csn2 single complex bound to DNA	This work	PDB: 6QXF, EMD: 4668
Cas1Cas2Csn2 dimer complex bound to DNA	This work	PDB:, EMD:
Cas1Cas2Csn2 filament complex bound to DNA	This work	PDB:, EMD:
Oligonucleotides		
acgaggagctattggcacaacttaca (Prospacer duplex forward)	Macrogen	N/A
agttgtgccaatagctcctcgtcatt (prospacer duplex reverse)	Metabion	
agatatcctacgaggttttagagctgtgttgtttcgaatggttccaaaacaaatt ctaaacgctaaagaggaag (CRISPR3 Leader-Repeat-Spacer duplex for in vitro integration reaction forward)	Metabion	
cttcctctttagcgtttagaatttgttttggaaccattcgaaacaacacagctcta aaacctcgtaggatatct (CRISPR3 Leader-Repeat-Spacer duplex for in vitro integration reaction forward reverse)	Metabion	
Recombinant DNA		
pCRISPR3 (expressing full S. thermophiles CRISPR3 loci)	Sapranauskas et al., 2011	N/A
pCas9- (Cas9 delete, containing the rest of the CRISPR3 loci)	Sapranauskas et al., 2011	N/A
pCas2- (Cas2 delete, containing the rest of the CRISPR3 loci)	Sapranauskas et al., 2011	N/A
pCsn2- (Csn2 delete, containing the rest of the CRISPR3 loci)	Sapranauskas et al., 2011	N/A
pCas1Strep (expressing C-Term Strep-tagged Cas1)	This work	N/A
pCR3ΔCRISPR (CRISPR region deleted, containing the rest of CRISPR3 loci)	This work	N/A
pCR3Δtracr (tracrRNA deleted, contain the rest of CRISPR3 locus)	Karvelis et al., 2013	N/A
Software and Algorithms		
Phyre2 webserver	Kelley et al., 2015	http://www.sbg.bio.ic.ac.uk/~phyre2/html/page.cgi?id=index

Chimera	Goddard et al., 2007	https://www.cgl.ucsf.edu/chimera/
COOT	Emsley et al., 2010	https://www2.mrc-lmb.cam.ac.uk/personal/pemsley/coot/
Refmac jelly-body refinement script	Murshudov et al., 1997	https://www2.mrc-lmb.cam.ac.uk/groups/murshudov/content/em_fitting/em_fitting.html
PHENIX real space refine	Afonine et al., 2018	https://www.phenix-online.org/documentation/reference/real_space_refine.html
Motioncorr	Li et al., 2013	http://cryoem.ucsf.edu/software/driftcorr.html
Motioncor2	Zheng et al., 2017	http://msg.ucsf.edu/em/software/motioncor2.html
Gctf	Zhang, 2016	https://www.mrc-lmb.cam.ac.uk/kzhang/
Gautomatch	N/A	https://www.mrc-lmb.cam.ac.uk/kzhang/
IMAGIC	van Heel & Keegstra, 1981	https://download.image-science.de/index.html
RELION3	Zivanov et al., 2018	https://www2.mrc-lmb.cam.ac.uk/relion/index.php?title=Main_Page
cryoSPARC	Punjani et al., 2017	https://guide.cryosparc.com/install.html
GraphPad Prism 8	N/A	https://www.graphpad.com/scientific-software/prism/

Figure 1


A
tracrRNA
cas9
cas1cas2 csn2 CRISPR
Leader
S. thermophilus DGCC7710 CRISPR3
B
pCRISPR3
tracrRNA
cas9
cas1cas2 csn2 CRISPR
pΔCas9
tracrRNA
Δcas9
cas1cas2 csn2 CRISPR
pΔCsn2
tracrRNA
cas9
cas1cas2Δcsn2 CRISPR
pΔCas2
tracrRNA
cas9
cas1Δcas2 csn2 CRISPR
pΔtracr
ΔtracrRNA
cas9
cas1cas2 csn2 CRISPR
pΔCRISPR
tracrRNA
cas9
cas1cas2 csn2 ΔCRISPR


C
pCRISPR3
pΔCas9
pΔCsn2
pΔCas2
MW, kDa
200
150
120
100
85
70
60
50
40
30
25
20
15
10
Cas9
Cas1-Strep
Csn2
Cas2


D
pΔtracr
pΔCRISPR
MW, kDa
180
130
95
72
55
43
34
26
17
10

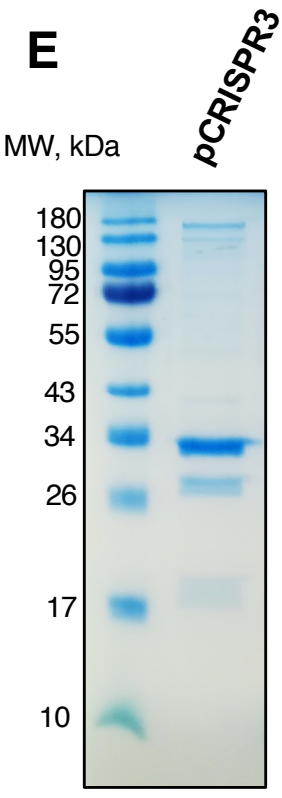

E
pCRISPR3
MW, kDa
180
130
95
72
55
43
34
26
17
10

Figure 2

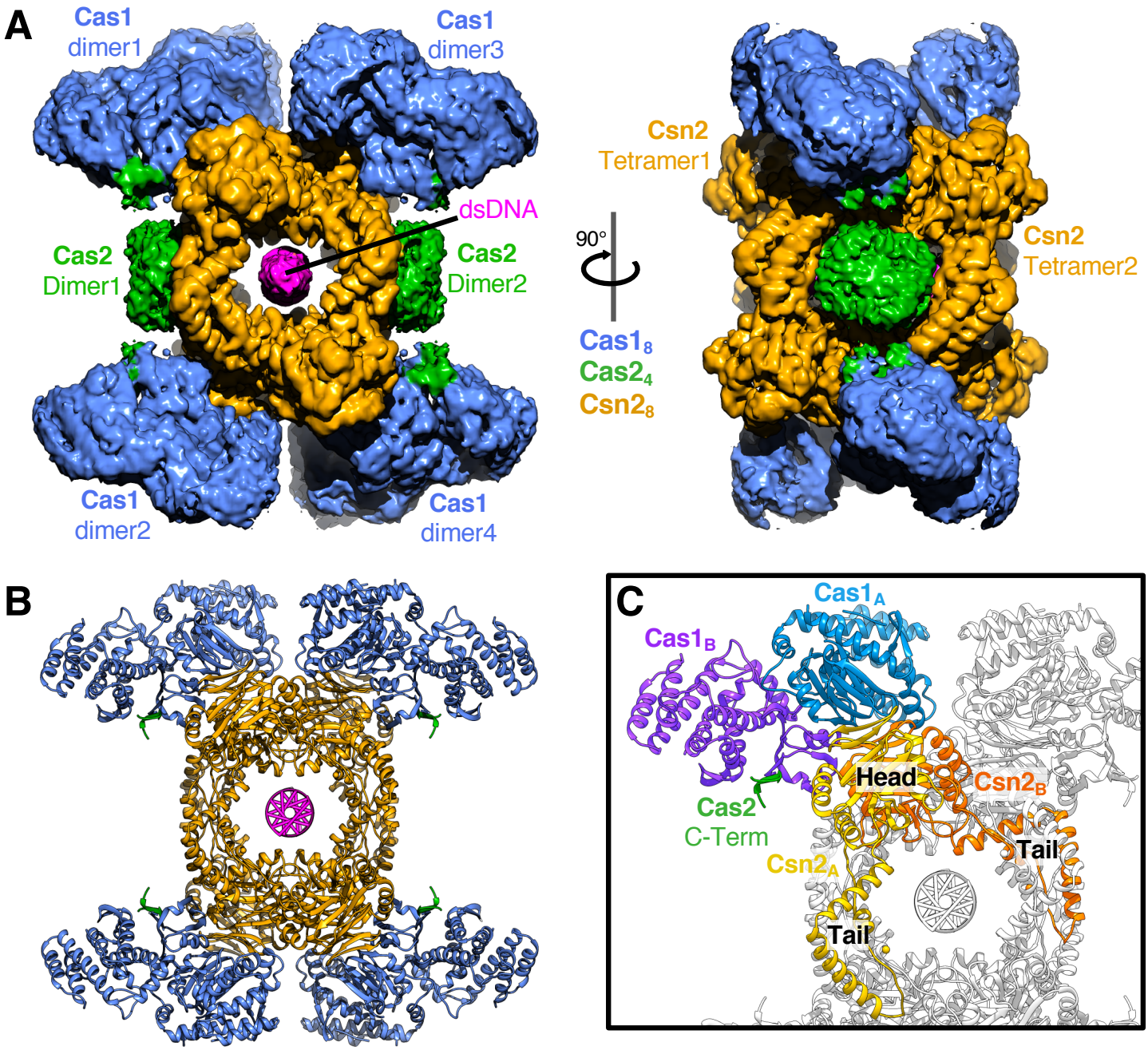

A
Cas1
dimer1
Cas1
dimer3
dsDNA
Cas2
Dimer1
Cas2
Dimer2
Cas1
dimer2
Cas1
dimer4
Csn2
Tetramer1
90°
Cas1$_8$
Cas2$_4$
Csn2$_8$
Csn2
Tetramer2
B
C
Cas1$_A$
Cas1$_B$
Head
Csn2$_B$
Cas2
C-Term
Tail
Csn2$_A$
Tail

Figure 3

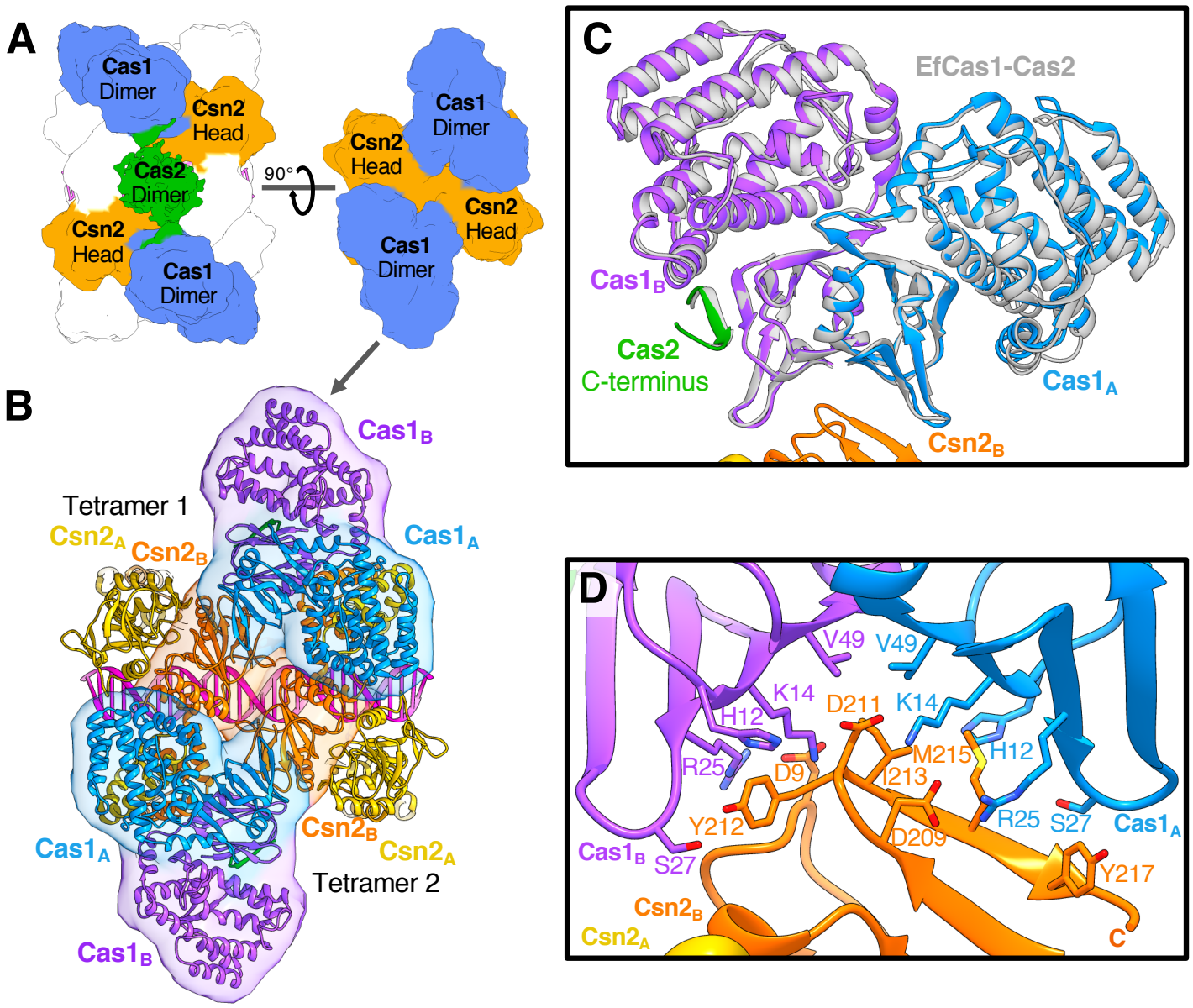

A
Cas1
Dimer
Csn2
Head
Cas2
Dimer
Csn2
Head
Cas1
Dimer
90°
Cas1
Dimer
Csn2
Head
Csn2
Head
Cas1
Dimer
B
Cas1B
Tetramer 1
Csn2A
Csn2B
Cas1A
Cas1A
Csn2B
Csn2A
Tetramer 2
Cas1B
C
EfCas1-Cas2
Cas1B
Cas2
C-terminus
Cas1A
Csn2B
D
V49
V49
K14
D211
K14
H12
R25
D9
M215
H12
I213
Y212
R25
S27
Cas1A
D209
Cas1B
S27
Y217
Csn2B
Csn2A
C

Figure 4

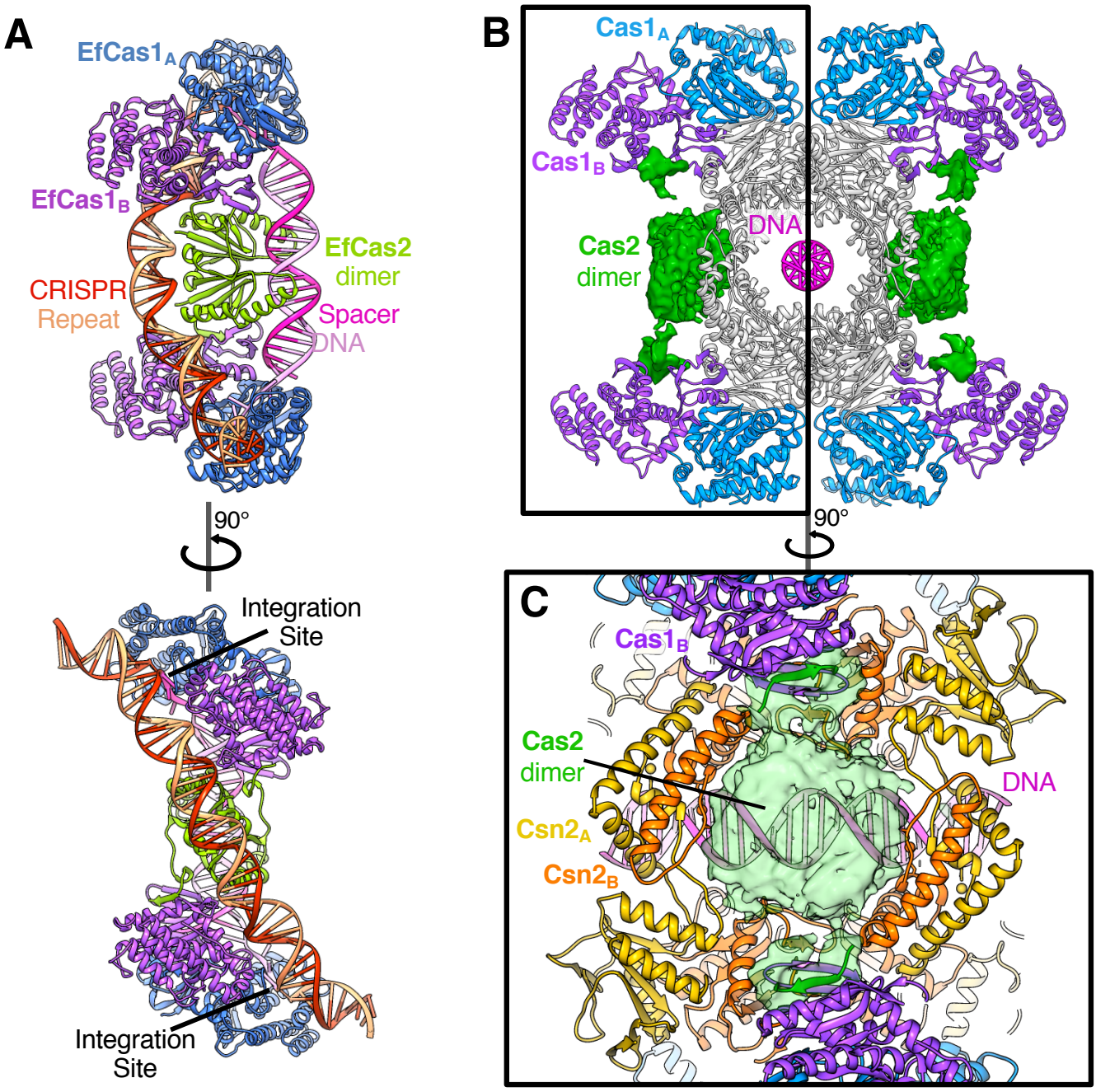

A
EfCas1A
EfCas1B
EfCas2
dimer
CRISPR
Repeat
Spacer
DNA
90°
Integration
Site
Integration
Site
B
Cas1A
Cas1B
DNA
Cas2
dimer
90°
C
Cas1B
Cas2
dimer
DNA
Csn2A
Csn2B

Figure 5

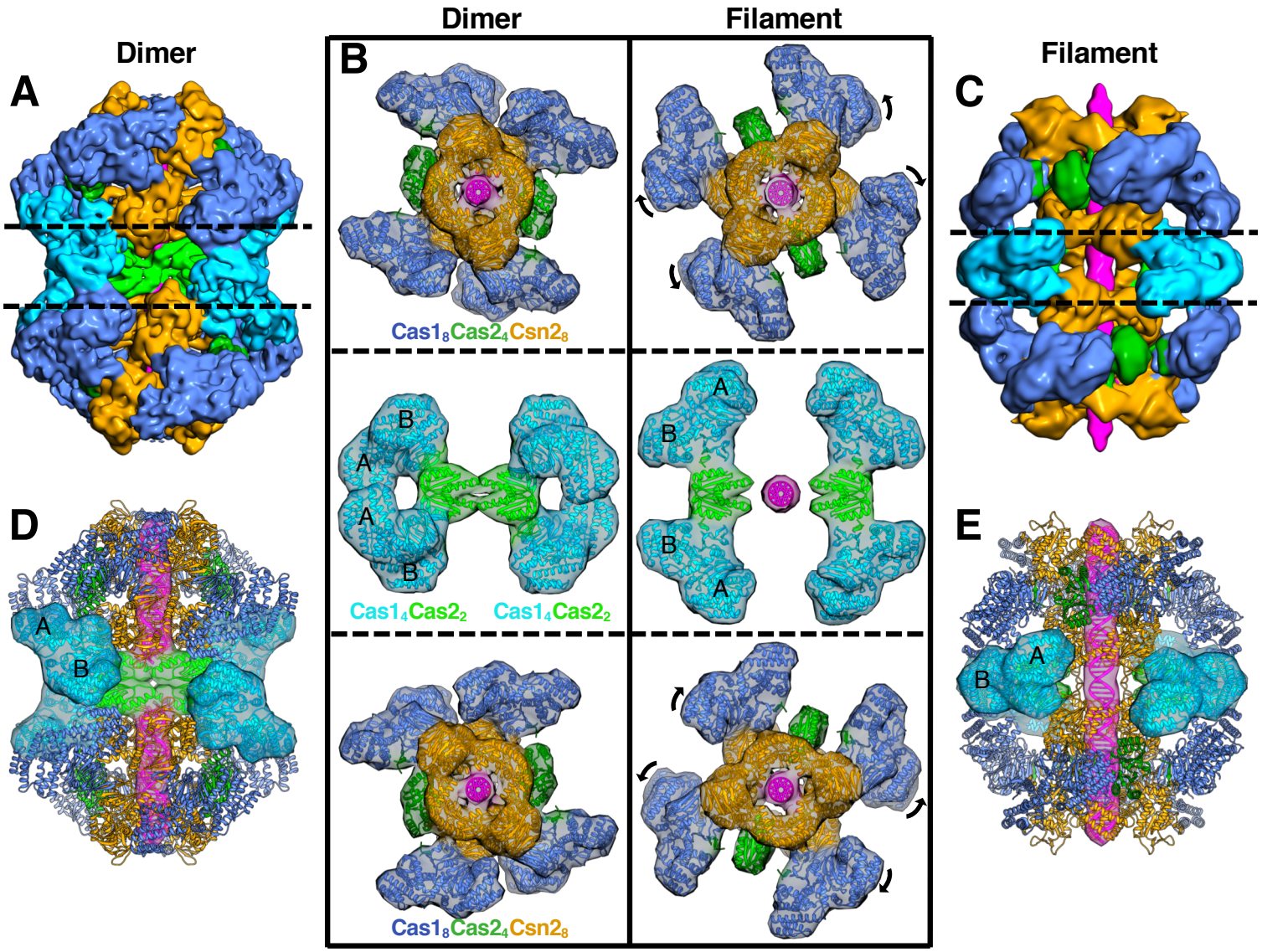

Dimer
A
B
Dimer
Filament
Filament
C
D
E
Cas1$_8$Cas2$_4$Csn2$_8$
Cas1$_4$Cas2$_2$
Cas1$_4$Cas2$_2$
Cas1$_8$Cas2$_4$Csn2$_8$

Figure 6

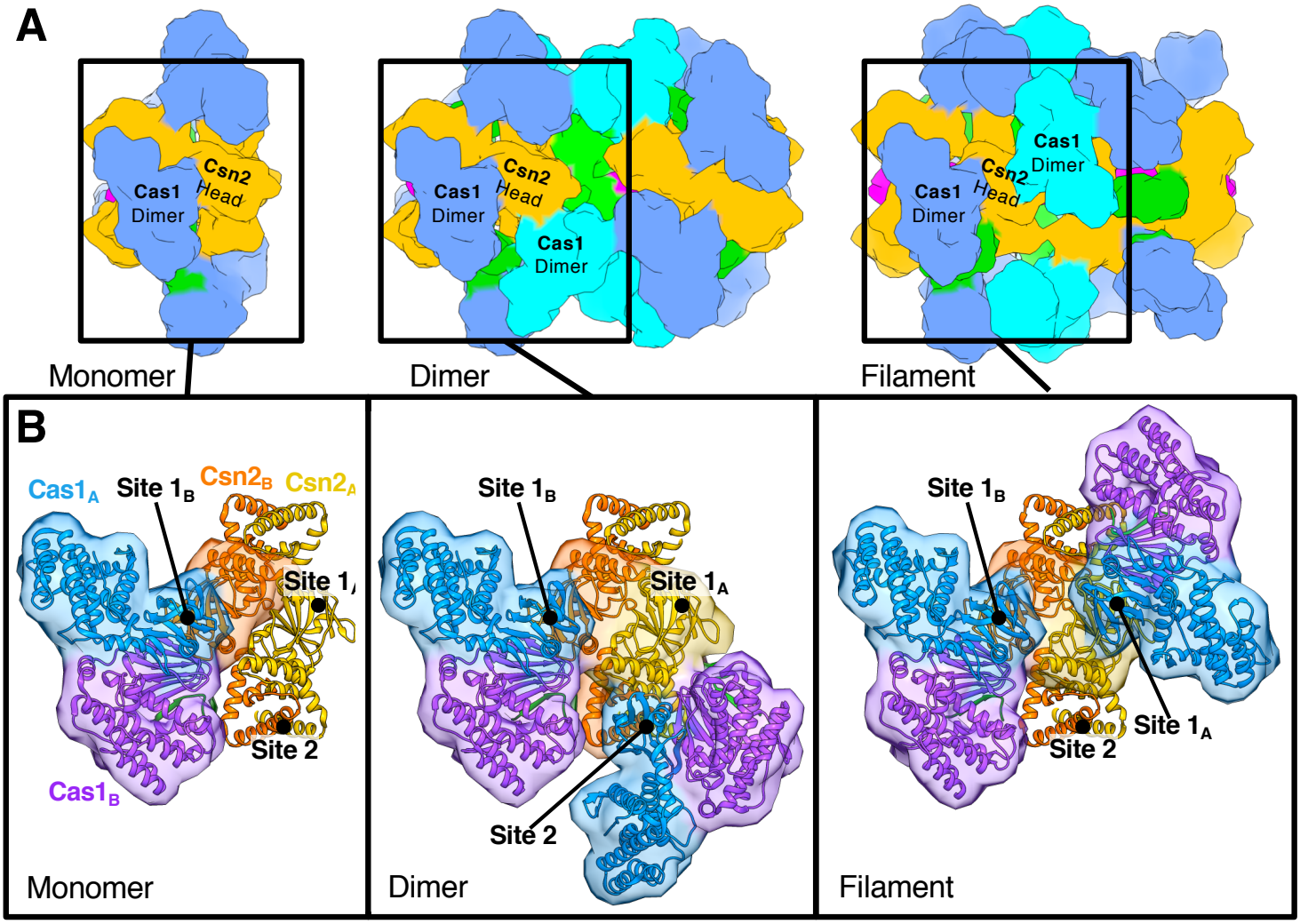
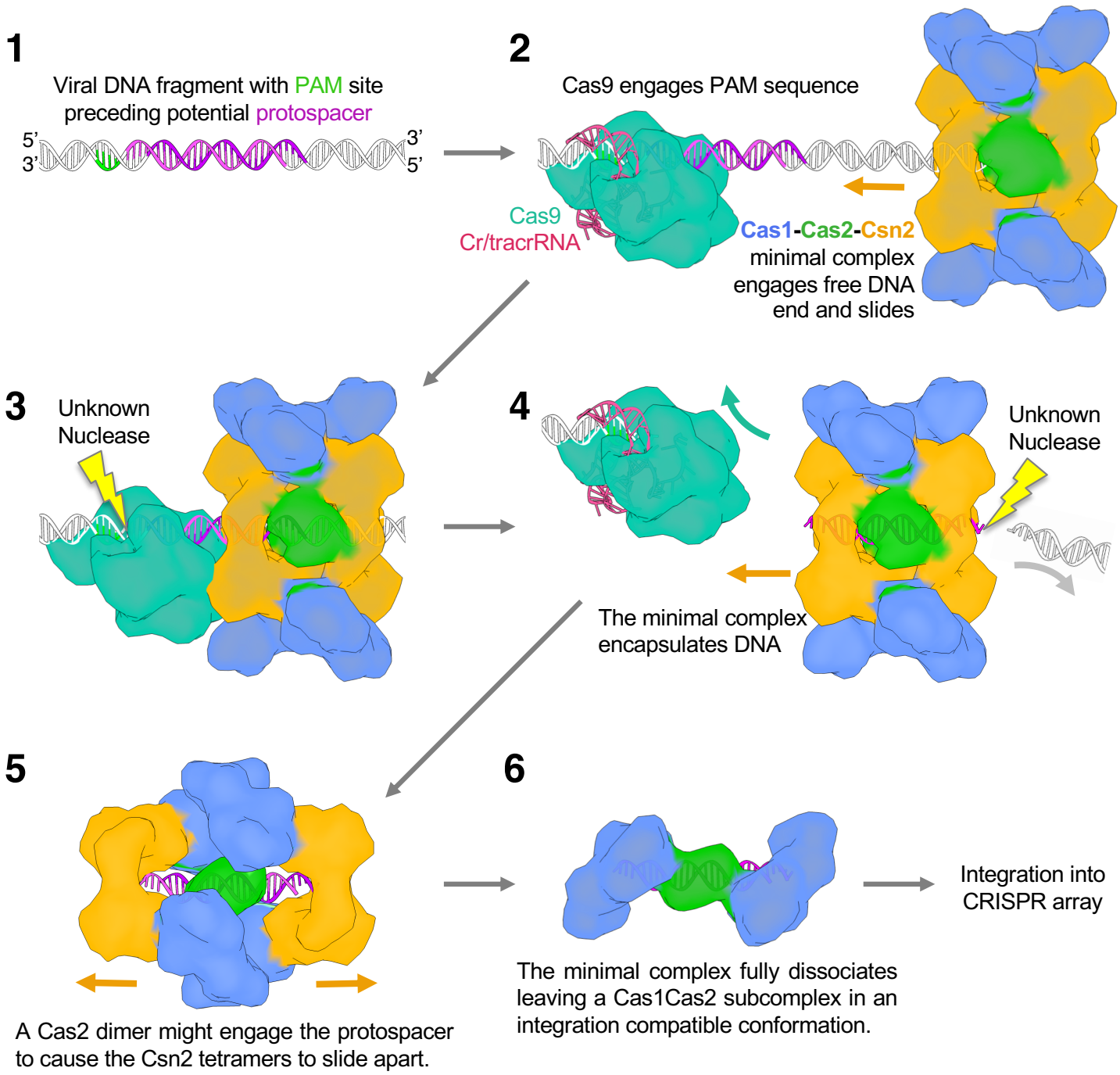

A
Cas1
Dimer
Csn2
Head
Monomer
Dimer
Filament
B
Cas1A
Site 1B
Csn2B
Csn2A
Site 1A
Site 2
Cas1B
Monomer
Dimer
Filament

Figure 7


1
Viral DNA fragment with PAM site preceding potential protospacer
5'
3'
3'
5'
2
Cas9 engages PAM sequence
Cas9
Cr/tracrRNA
Cas1-Cas2-Csn2
minimal complex
engages free DNA
end and slides
3
Unknown
Nuclease
4
Unknown
Nuclease
The minimal complex
encapsulates DNA
5
A Cas2 dimer might engage the protospacer
to cause the Csn2 tetramers to slide apart.
6
The minimal complex fully dissociates
leaving a Cas1Cas2 subcomplex in an
integration compatible conformation.
Integration into
CRISPR array

Molecular Cell Volume 74

Supplemental Information

Structure of the DNA-bound spacer capture complex of a Type II CRISPR-Cas system

Martin Wilkinson, Gediminas Drabavicius, Arunas Silanskas, Giedrius Gasiunas, Virginijus Siksnys and Dale B. Wigley

Figure S1: Cryo-EM images of the mixture. Related to Figure 1, Figure 2 and Figure 5.

Figure S2: EM processing for the Cas1Cas2Csn2 monomer complex. Related to Figure 2.

Figure S3: EM processing for the Cas1Cas2Csn2 dimer complex. Related to Figure 5.

Figure S4: DNA binds within a positive channel through the Csn2 tetramers. Related to Figure 2.

Figure S5: Deep-sequencing analysis of DNA captured by Cas1- Cas2-Csn2-Cas9 complex and integration assays. Related to Figure 1, Figure 2 and Figure 5.

Figure S6: *In vitro* interactions of CRISPR3-Cas proteins. Related to Figure 1.

Figure S7: EM processing for the Cas1Cas2Csn2 filament complex. Related to Figure 5.

Figure S1. Related to Figure 1, Figure 2 and Figure 5.

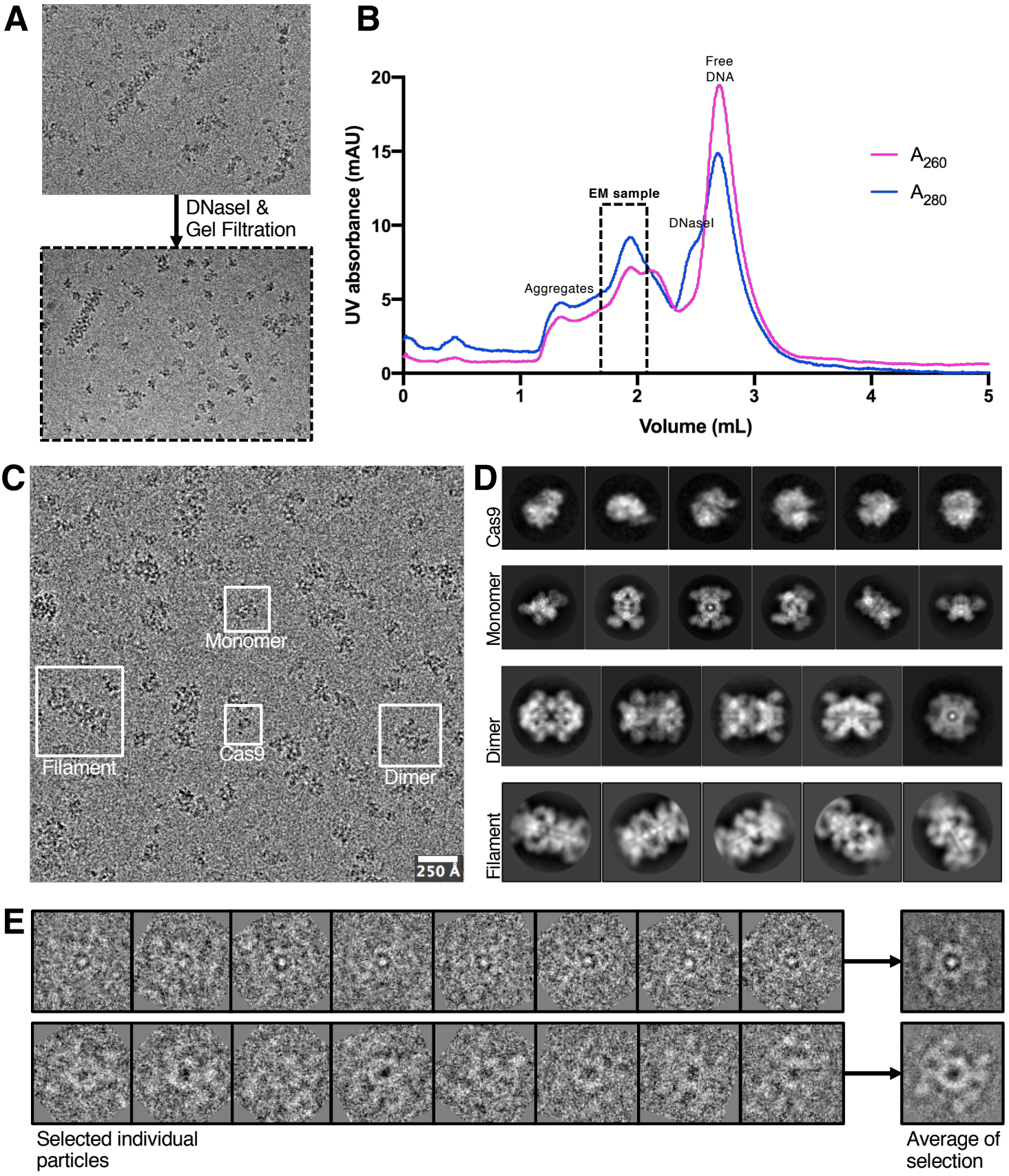


Figure S1. Cryo-EM images of the mixture. Related to Figure 1, Figure 2 and Figure 5.

(A) Initial cryo image of the sample showing long threads of DNA.

(B) Cryo image after DNaseI treatment. Both images were taken on a Technai T12 microscope with CCD detector.

(C) Section of a micrograph from the Krios-Falcon III dataset. An example of each of the different particle populations is boxed.

(D) Representative 2D classes generated in RELION from the Krios-Falcon III dataset showing different views for each of the four particle populations.

(E) A selection of particles from a subset of the Krios-Falcon III dataset that represented just the front view of the monomer complex. The particles could be separated into two species: 98.6 % were DNA bound (top row) and 1.4 % were fully assembled without DNA (bottom row). Particles and class averages were generated and displayed using Relion.

Figure S2. Related to Figure 2.

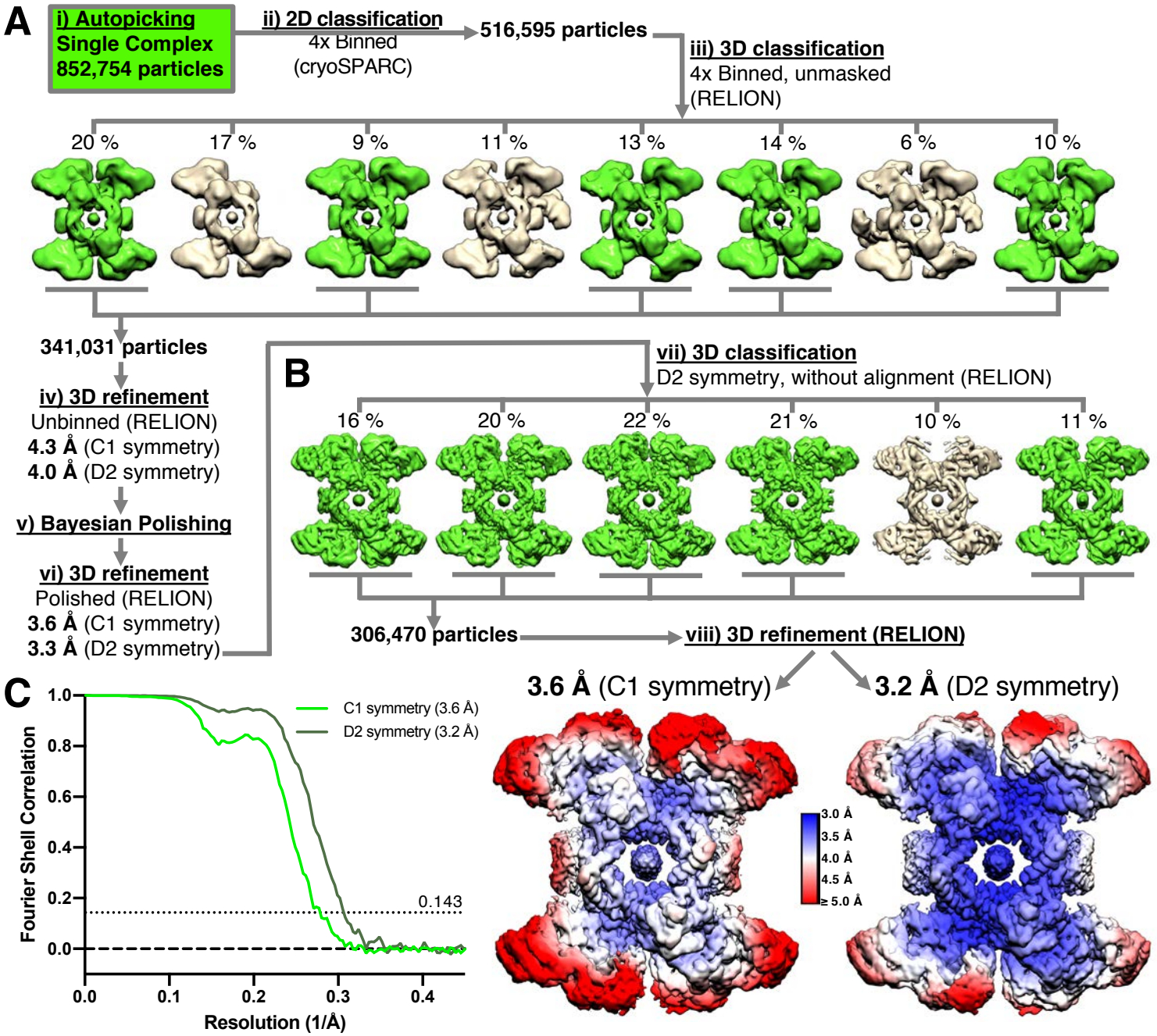


Figure S2. EM processing for the Cas1Cas2Csn2 monomer complex. Related to Figure 2.

(A) Scheme overview of the initial processing steps for the monomer particle set.

(B) The 3D classes from the final classification step are shown. The classes show flexibility in the orientation of the Cas1 dimers relative to the rest of the complex.

(C) FSC plot for the final monomer maps (left). The deposited C1 and supplemental D2-symmetrised maps are shown coloured by local resolution (calculated using RELION) (right).

(D) The deposited 3.6 Å monomer map is shown as a transparent surface with the coordinates underneath. Both are coloured similarly to Figure 2.

(E) A section of the 3.2 Å D2-symmetrised map displayed as grey mesh showing ordered side-chain density for the selected region within Csn2.

(F) A section of the 3.2 Å D2-symmetrised map displayed as grey mesh showing the fit of the contact regions between the C-terminus of Cas2, the Cas1 NTD and the Csn2 head domain.

Figure S3. Related to Figure 5.

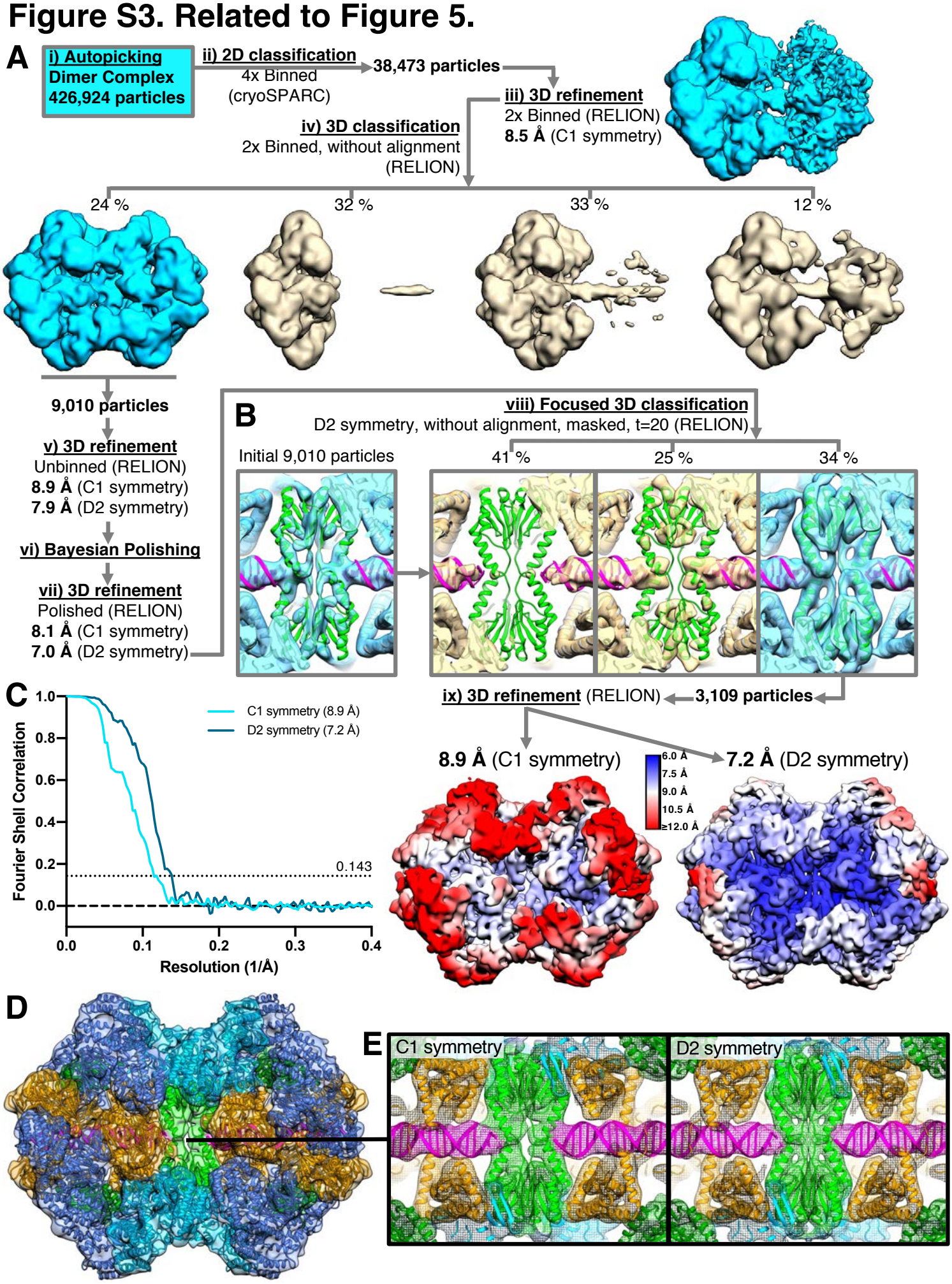


Figure S3. EM processing for the Cas1Cas2Csn2 dimer complex. Related to Figure 5.

(A) Scheme overview of the initial processing steps for the dimer particle set.

(B) A section around the middle Cas2 dimer,s which cap the DNA fragment ends, are shown for each of the 3D classes from the final focused classification step as well as for the initial map before classification. The classes show flexibility in the orientation of the Cas1 dimers relative to the rest of the complex. A homogeneous class with strong density for the region was selected for the final refinement.

(C) FSC plot for the final dimer maps (left). The deposited C1 and supplemental D2-symmetrised maps are shown coloured by local resolution (calculated using RELION) (right).

(D) The deposited 8.9 Å dimer map is shown as a transparent surface with the coordinates underneath. Both are coloured similarly to Figure 5.

(E) A section of both the C1 and D2-symmetrised maps is displayed as coloured mesh showing the fit of the ordered Cas2 dimers capping the end of the DNA fragments. There is no free density to suggest that the DNA ends are joined.

Figure S4. Related to Figure 2.

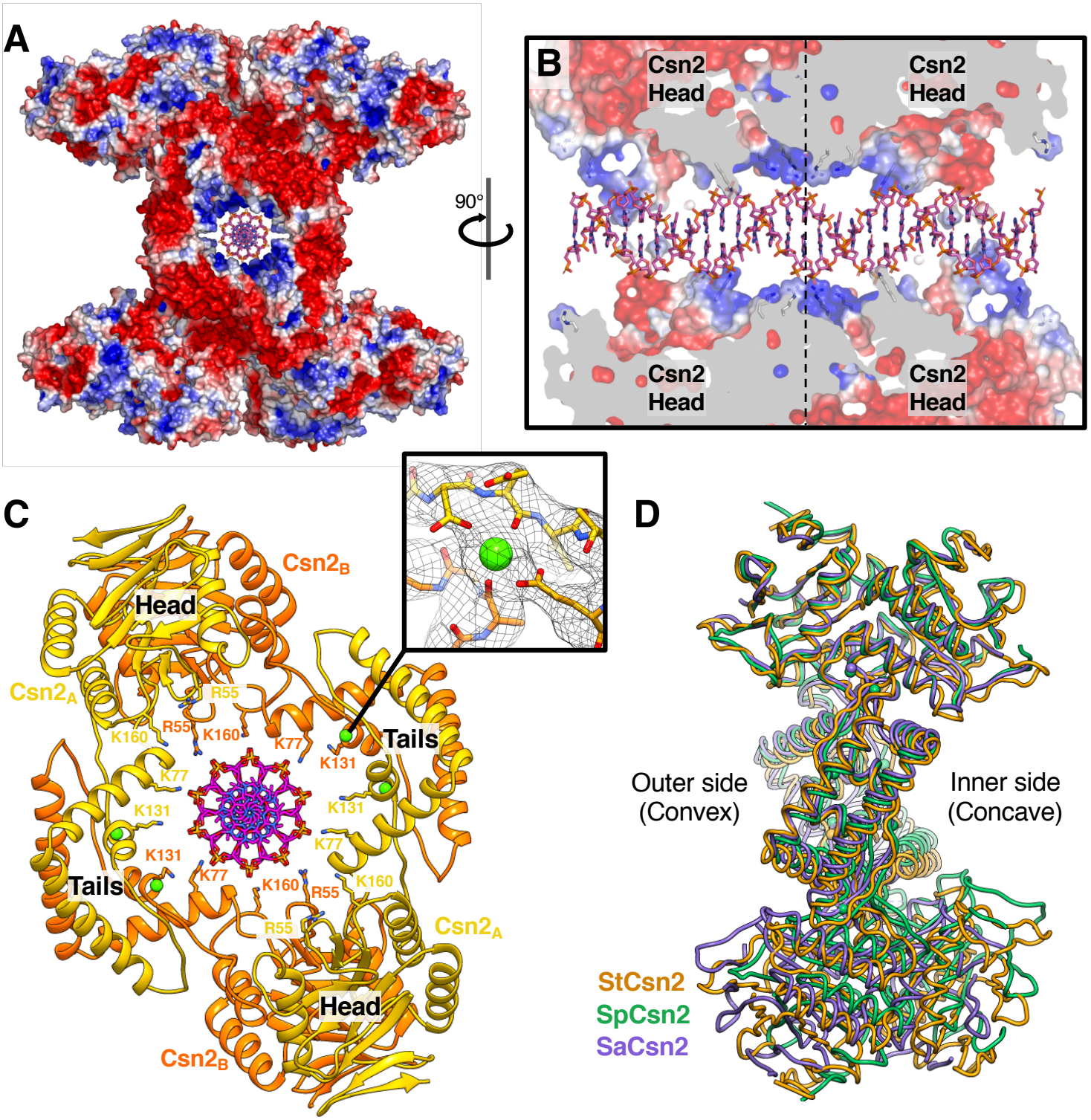


Figure S4. DNA binds within a positive channel through the Csn2 tetramers. Related to Figure 2.

(A) Overall charge distribution on the surface of the monomer structure calculated by APBS displaying a range from -3 (red) to +3 (blue) kT/e. The bound DNA was deleted from the charge calculation but overlaid for reference.

(B) Cutaway showing the charge distribution along the central channel through the two Csn2 tetramers, which are divided here by a dotted line. Due to the concave nature of the interacting Csn2 tetramer surfaces, more DNA contacts are found in the centre of the channel than in the peripheries.

(C) A single Csn2 tetramer is displayed as cartoon coloured by chain showing the conserved residues positioned to bind non-specifically to the DNA backbone. Bound Ca2+ ions are shown as green spheres.

(D) Side view with the crystal structures of different Csn2 tetramers (Koo et al., 2012; PDB 3TOC and Ellinger et al., 2012; PDB 3QHQ) aligned to the top head domain of a Csn2 tetramer from the complexes described in this work. The concave side formed by different conformations of the Csn2A and Csn2B chains is conserved in all three structures but with varying degrees of rotation.

Figure S5. Related to Figure 1, Figure 2 and Figure 5

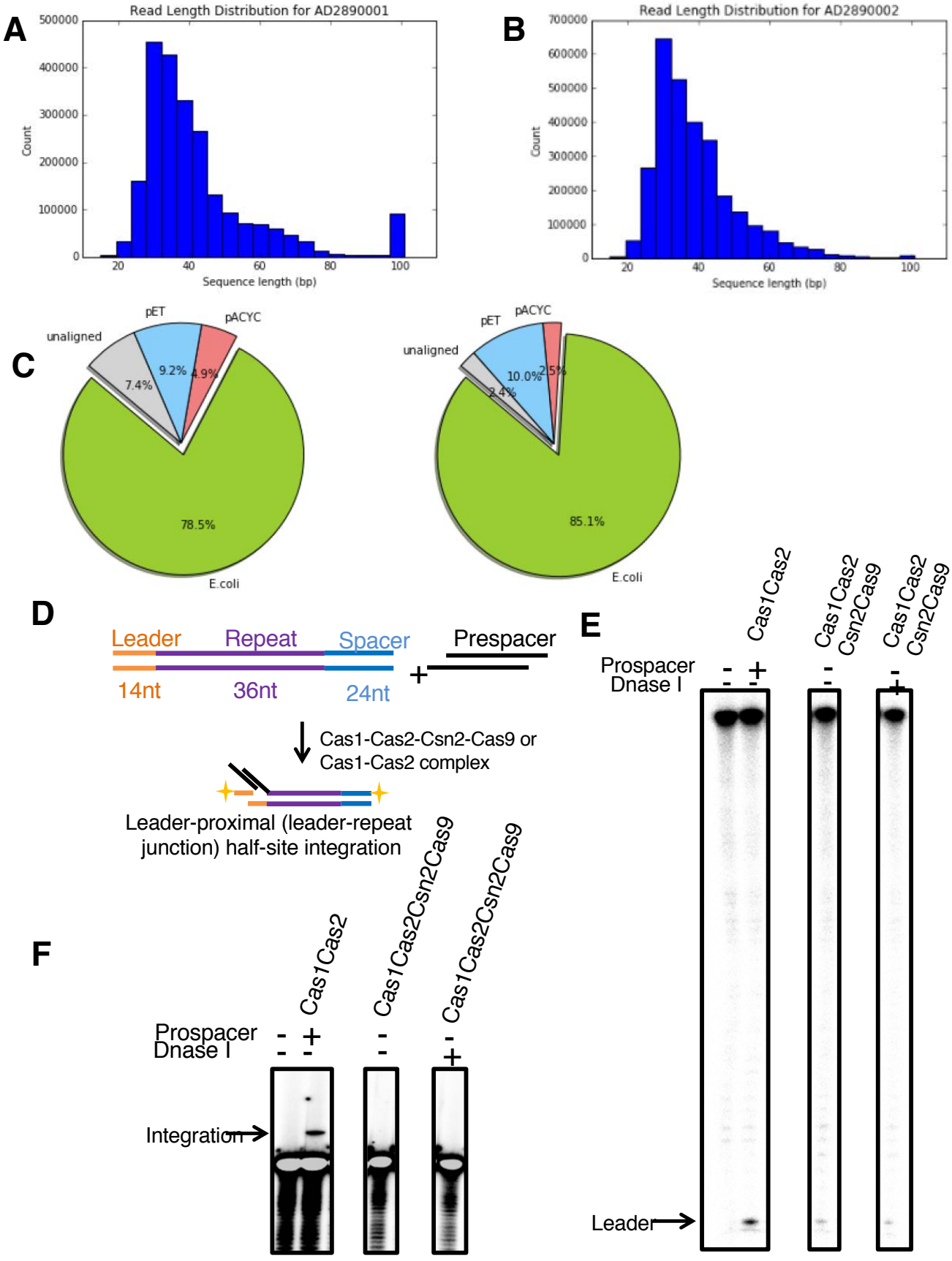


Figure S5. Deep-sequencing analysis of DNA captured by Cas1- Cas2-Csn2-Cas9 complex and integration assays. Related to Figure 1, Figure 2 and Figure 5.

(A) DNA captured by Cas1-Cas2-Csn2-Cas9 length distribution before DNAse I treatment. Many reads of 100 or more bp are evident. They are the likely filamentous structures seen in initial negative stain EM.

(B) DNA captured by Cas1-Cas2-Csn2-Cas9 length distribution after DNAse I treatment. The number of reads of 100+ length is decreased dramatically and the main distribution is more streamlined. This is consistent with the homogenization of DNA in the sample.

(C) Maps of the DNA captured by Cas1-Cas2-Csn2-Cas9 complexes onto *E. coli* genome and plasmids encoding CRISPR3-Cas system. As expected, DNA distribution closely matched expected DNA concentrations in the cell. No enrichment near PAM sequences was detected.

(D) Schematic representation of the integration assay. Prespacer was not added in case of Cas1-Cas2-Csn2-Cas9, as it was assumed that DNA bound by the complex may serve as one. 28

(E) Integration assay into substrates with labelled 5' end. Both complexes catalyse the nicking at the Leader-Repeat junction as evidenced by the release 14nt Leader fragment indicative of integration.

(F) Integration assay into substrates with labelled 3' ends. Only Cas1-Cas2 complex, but not the full complex exhibited permanent integrations resulting in the elongation of the initial substrate strand.

Figure S6. Related to Figure 1.

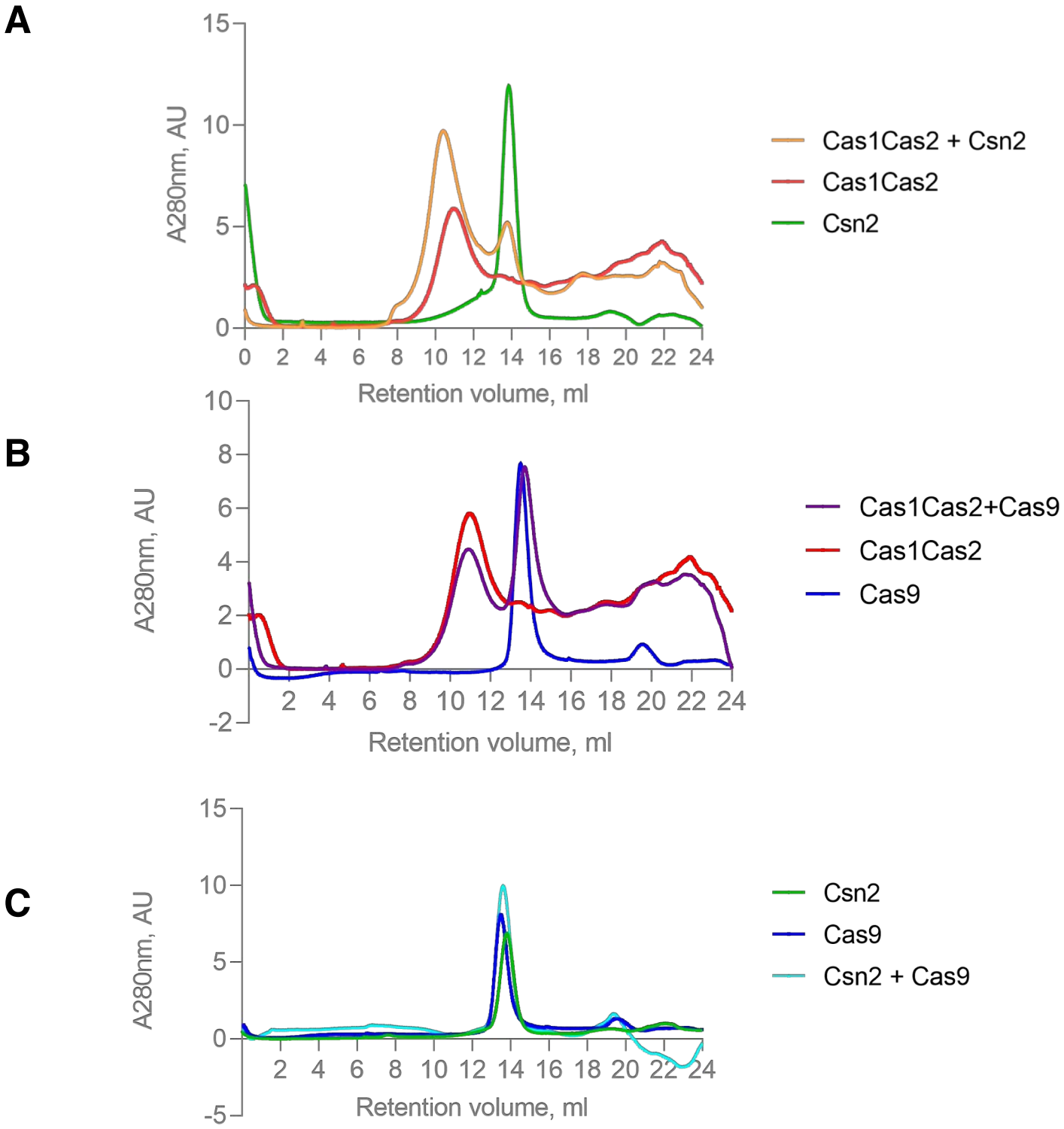


Figure S6. *In vitro* interactions of CRISPR3-Cas proteins. Related to Figure 1.
(A) Cas1-Cas2 interacts with Csn2 directly. Cas1-Cas2 eluted in the void volume, because they Had bound nucleic acids. However, upon mixing it with excess Csn2, a portion of Csn2 moved to the void volume as well.
(B) Cas1-Cas2 does not directly interact with Cas9. Cas9 peak neither decreased in size not moved to the left, therefore Cas9 did not interact with Cas1-Cas2.
(C) Csn2 does not interact with Cas9 directly, as the retention volume of the combined proteins did not shift left. Cas9 used for these experiments was complexed with tracr:crRNA duplex.

Figure S7. Related to Figure 5.

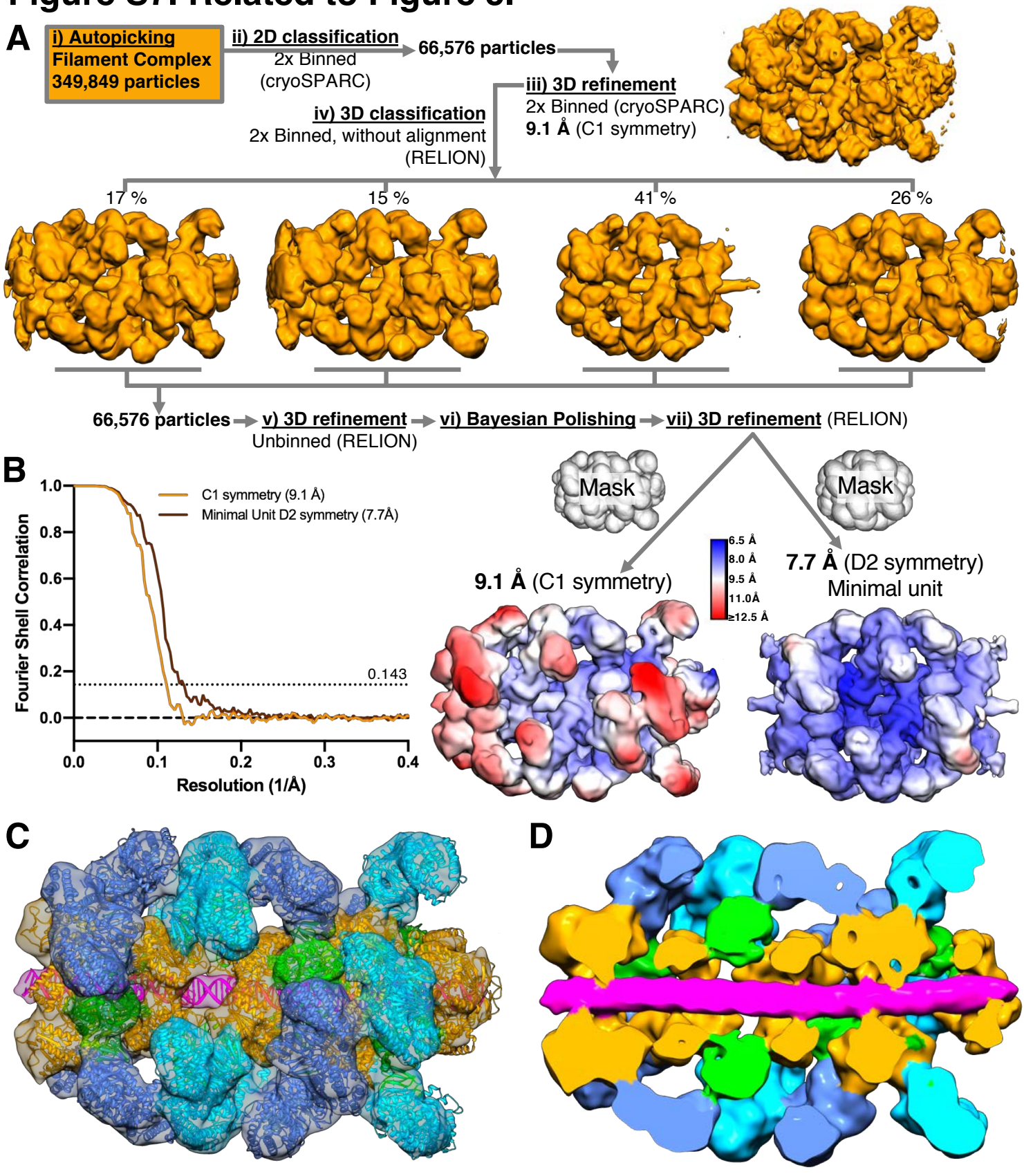


Figure S7. EM processing for the Cas1Cas2Csn2 filament complex. Related to Figure 5.

(A) Scheme overview of the initail processing steps for the filament particle set.

(B) FSC plot for the final filament maps (left). The deposited C1 and supplemental D2-symmetrised maps, coloured by local resolution (calculated using RELION), are displayed along with the corresponding masks used during refinement (right).

(C) The deposited 9.1 Å filament map is shown as a transparent surface with the coordinates underneath. Both are coloured similarly to Figure 5.

(D) Similar view to S7C of the deposited filament map, which is sliced in half to show the continuous density for dsDNA (magenta) through the entire filament.

Supplementary Video 1

Click here to access/download

Supplemental Videos and Spreadsheets

Supplementary movie S1.mp4

Supplementary Video 2

Click here to access/download

Supplemental Videos and Spreadsheets

Supplementary movie S2.mp4

Supplementary Video 3

Click here to access/download

Supplemental Videos and Spreadsheets

Supplementary movie S3.mp4

PDB Validation Report monomer
Click here to access/download;PDB Validation Report;D_1292101067_val-report-full_monomer.pdf

Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Mar 26, 2019 – 08:09 pm GMT

Deposition ID : D_1292101067
PDB ID : *(not yet assigned)*

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

PRELIMINARY VALIDATION REPORT

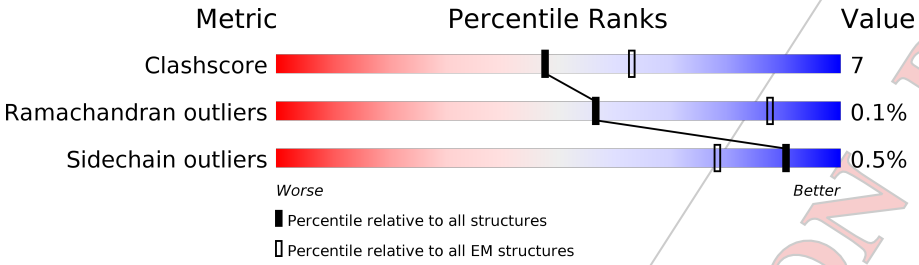
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	219	83% 17%
1	B	219	80% 20%
1	C	219	82% 18%
1	D	219	81% 19%
1	E	219	82% 17%
1	F	219	82% 18%
1	G	219	82% 17%
1	H	219	80% 20%
2	I	302	80% 15% 5%

Continued on next page...

PRELIMINARY VALIDATION REPORT

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	302	75% 20% 5%
2	L	302	80% 15% 5%
2	M	302	75% 20% 5%
2	O	302	79% 16% 5%
2	P	302	75% 21% 5%
2	R	302	80% 15% 5%
2	S	302	76% 19% 5%
3	K	114	7% 90%
3	N	114	8% 90%
3	Q	114	7% 90%
3	T	114	8% 90%
4	X	25	100%
5	Y	25	96%

PRELIMINARY VALIDATION REPORT

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 34693 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CRISPR-associated protein Csn2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total 1787	C 1162	N 271	O 348	S 6	0	0
1	B	219	Total 1795	C 1166	N 273	O 350	S 6	0	0
1	C	218	Total 1787	C 1162	N 271	O 348	S 6	0	0
1	D	219	Total 1795	C 1166	N 273	O 350	S 6	0	0
1	E	218	Total 1787	C 1162	N 271	O 348	S 6	0	0
1	F	219	Total 1795	C 1166	N 273	O 350	S 6	0	0
1	G	218	Total 1787	C 1162	N 271	O 348	S 6	0	0
1	H	219	Total 1795	C 1166	N 273	O 350	S 6	0	0

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	287	Total 2369	C 1523	N 399	O 435	S 12	0	0
2	J	287	Total 2369	C 1523	N 399	O 435	S 12	0	0
2	L	287	Total 2369	C 1523	N 399	O 435	S 12	0	0
2	M	287	Total 2369	C 1523	N 399	O 435	S 12	0	0
2	O	287	Total 2369	C 1523	N 399	O 435	S 12	0	0
2	P	287	Total 2369	C 1523	N 399	O 435	S 12	0	0
2	R	287	Total 2369	C 1523	N 399	O 435	S 12	0	0

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	287	Total	C	N	O	S	0	0
			2369	1523	399	435	12		

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	205	ALA	HIS	conflict	UNP G3ECR2
I	290	LEU	-	expression tag	UNP G3ECR2
I	291	GLU	-	expression tag	UNP G3ECR2
I	292	SER	-	expression tag	UNP G3ECR2
I	293	GLY	-	expression tag	UNP G3ECR2
I	294	TRP	-	expression tag	UNP G3ECR2
I	295	SER	-	expression tag	UNP G3ECR2
I	296	HIS	-	expression tag	UNP G3ECR2
I	297	PRO	-	expression tag	UNP G3ECR2
I	298	GLN	-	expression tag	UNP G3ECR2
I	299	PHE	-	expression tag	UNP G3ECR2
I	300	GLU	-	expression tag	UNP G3ECR2
I	301	LYS	-	expression tag	UNP G3ECR2
I	302	ALA	-	expression tag	UNP G3ECR2
J	205	ALA	HIS	conflict	UNP G3ECR2
J	290	LEU	-	expression tag	UNP G3ECR2
J	291	GLU	-	expression tag	UNP G3ECR2
J	292	SER	-	expression tag	UNP G3ECR2
J	293	GLY	-	expression tag	UNP G3ECR2
J	294	TRP	-	expression tag	UNP G3ECR2
J	295	SER	-	expression tag	UNP G3ECR2
J	296	HIS	-	expression tag	UNP G3ECR2
J	297	PRO	-	expression tag	UNP G3ECR2
J	298	GLN	-	expression tag	UNP G3ECR2
J	299	PHE	-	expression tag	UNP G3ECR2
J	300	GLU	-	expression tag	UNP G3ECR2
J	301	LYS	-	expression tag	UNP G3ECR2
J	302	ALA	-	expression tag	UNP G3ECR2
L	205	ALA	HIS	conflict	UNP G3ECR2
L	290	LEU	-	expression tag	UNP G3ECR2
L	291	GLU	-	expression tag	UNP G3ECR2
L	292	SER	-	expression tag	UNP G3ECR2
L	293	GLY	-	expression tag	UNP G3ECR2
L	294	TRP	-	expression tag	UNP G3ECR2
L	295	SER	-	expression tag	UNP G3ECR2
L	296	HIS	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

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Chain	Residue	Modelled	Actual	Comment	Reference
L	297	PRO	-	expression tag	UNP G3ECR2
L	298	GLN	-	expression tag	UNP G3ECR2
L	299	PHE	-	expression tag	UNP G3ECR2
L	300	GLU	-	expression tag	UNP G3ECR2
L	301	LYS	-	expression tag	UNP G3ECR2
L	302	ALA	-	expression tag	UNP G3ECR2
M	205	ALA	HIS	conflict	UNP G3ECR2
M	290	LEU	-	expression tag	UNP G3ECR2
M	291	GLU	-	expression tag	UNP G3ECR2
M	292	SER	-	expression tag	UNP G3ECR2
M	293	GLY	-	expression tag	UNP G3ECR2
M	294	TRP	-	expression tag	UNP G3ECR2
M	295	SER	-	expression tag	UNP G3ECR2
M	296	HIS	-	expression tag	UNP G3ECR2
M	297	PRO	-	expression tag	UNP G3ECR2
M	298	GLN	-	expression tag	UNP G3ECR2
M	299	PHE	-	expression tag	UNP G3ECR2
M	300	GLU	-	expression tag	UNP G3ECR2
M	301	LYS	-	expression tag	UNP G3ECR2
M	302	ALA	-	expression tag	UNP G3ECR2
O	205	ALA	HIS	conflict	UNP G3ECR2
O	290	LEU	-	expression tag	UNP G3ECR2
O	291	GLU	-	expression tag	UNP G3ECR2
O	292	SER	-	expression tag	UNP G3ECR2
O	293	GLY	-	expression tag	UNP G3ECR2
O	294	TRP	-	expression tag	UNP G3ECR2
O	295	SER	-	expression tag	UNP G3ECR2
O	296	HIS	-	expression tag	UNP G3ECR2
O	297	PRO	-	expression tag	UNP G3ECR2
O	298	GLN	-	expression tag	UNP G3ECR2
O	299	PHE	-	expression tag	UNP G3ECR2
O	300	GLU	-	expression tag	UNP G3ECR2
O	301	LYS	-	expression tag	UNP G3ECR2
O	302	ALA	-	expression tag	UNP G3ECR2
P	205	ALA	HIS	conflict	UNP G3ECR2
P	290	LEU	-	expression tag	UNP G3ECR2
P	291	GLU	-	expression tag	UNP G3ECR2
P	292	SER	-	expression tag	UNP G3ECR2
P	293	GLY	-	expression tag	UNP G3ECR2
P	294	TRP	-	expression tag	UNP G3ECR2
P	295	SER	-	expression tag	UNP G3ECR2
P	296	HIS	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

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Chain	Residue	Modelled	Actual	Comment	Reference
P	297	PRO	-	expression tag	UNP G3ECR2
P	298	GLN	-	expression tag	UNP G3ECR2
P	299	PHE	-	expression tag	UNP G3ECR2
P	300	GLU	-	expression tag	UNP G3ECR2
P	301	LYS	-	expression tag	UNP G3ECR2
P	302	ALA	-	expression tag	UNP G3ECR2
R	205	ALA	HIS	conflict	UNP G3ECR2
R	290	LEU	-	expression tag	UNP G3ECR2
R	291	GLU	-	expression tag	UNP G3ECR2
R	292	SER	-	expression tag	UNP G3ECR2
R	293	GLY	-	expression tag	UNP G3ECR2
R	294	TRP	-	expression tag	UNP G3ECR2
R	295	SER	-	expression tag	UNP G3ECR2
R	296	HIS	-	expression tag	UNP G3ECR2
R	297	PRO	-	expression tag	UNP G3ECR2
R	298	GLN	-	expression tag	UNP G3ECR2
R	299	PHE	-	expression tag	UNP G3ECR2
R	300	GLU	-	expression tag	UNP G3ECR2
R	301	LYS	-	expression tag	UNP G3ECR2
R	302	ALA	-	expression tag	UNP G3ECR2
S	205	ALA	HIS	conflict	UNP G3ECR2
S	290	LEU	-	expression tag	UNP G3ECR2
S	291	GLU	-	expression tag	UNP G3ECR2
S	292	SER	-	expression tag	UNP G3ECR2
S	293	GLY	-	expression tag	UNP G3ECR2
S	294	TRP	-	expression tag	UNP G3ECR2
S	295	SER	-	expression tag	UNP G3ECR2
S	296	HIS	-	expression tag	UNP G3ECR2
S	297	PRO	-	expression tag	UNP G3ECR2
S	298	GLN	-	expression tag	UNP G3ECR2
S	299	PHE	-	expression tag	UNP G3ECR2
S	300	GLU	-	expression tag	UNP G3ECR2
S	301	LYS	-	expression tag	UNP G3ECR2
S	302	ALA	-	expression tag	UNP G3ECR2

- Molecule 3 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	11	Total	C	N	O	0	0
			95	61	15	19		
3	N	11	Total	C	N	O	0	0
			95	61	15	19		

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Residues	Atoms	AltConf	Trace
3	Q	11	Total C N O 95 61 15 19	0	0
3	T	11	Total C N O 95 61 15 19	0	0

- Molecule 4 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms	AltConf	Trace
4	X	25	Total C N O P 500 250 50 175 25	0	0

- Molecule 5 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms	AltConf	Trace
5	Y	25	Total C N O P 525 250 125 125 25	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Ca 1 1	0
6	B	1	Total Ca 1 1	0
6	C	1	Total Ca 1 1	0
6	D	1	Total Ca 1 1	0
6	E	1	Total Ca 1 1	0
6	F	1	Total Ca 1 1	0
6	G	1	Total Ca 1 1	0
6	H	1	Total Ca 1 1	0

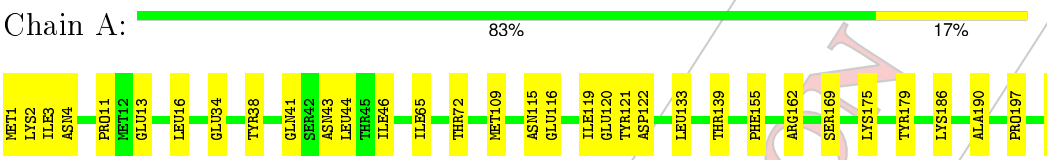
PRELIMINARY VALIDATION REPORT

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

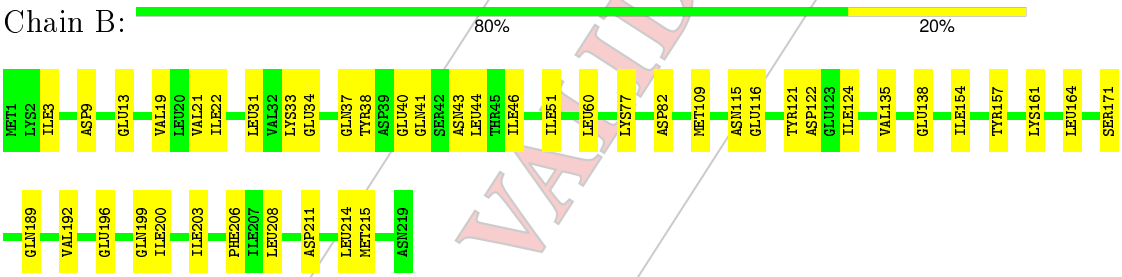
- Molecule 1: CRISPR-associated protein Csn2

Chain A:



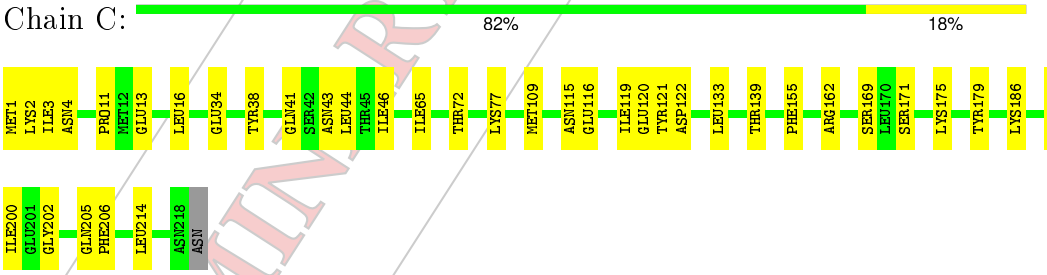
- Molecule 1: CRISPR-associated protein Csn2

Chain B:



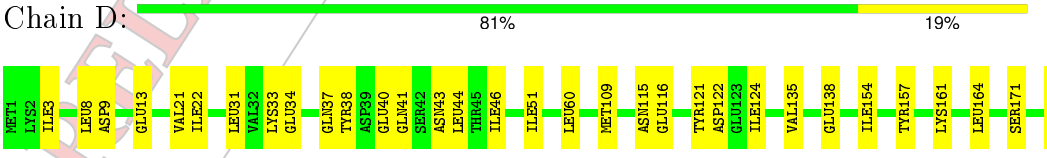
- Molecule 1: CRISPR-associated protein Csn2

Chain C:

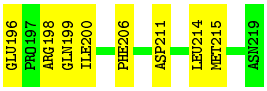


- Molecule 1: CRISPR-associated protein Csn2

Chain D:



PRELIMINARY VALIDATION REPORT

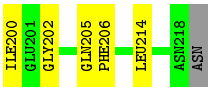


- Molecule 1: CRISPR-associated protein Csn2

Chain E:



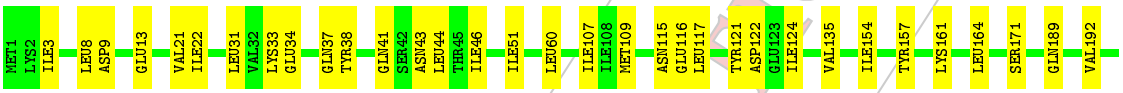


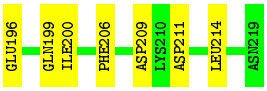


- Molecule 1: CRISPR-associated protein Csn2

Chain F:



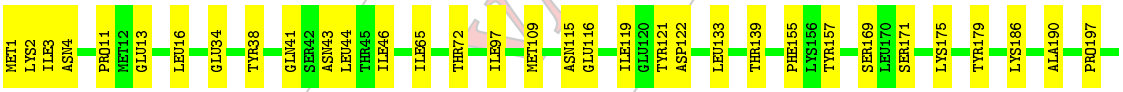


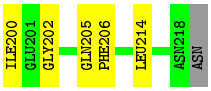


- Molecule 1: CRISPR-associated protein Csn2

Chain G:



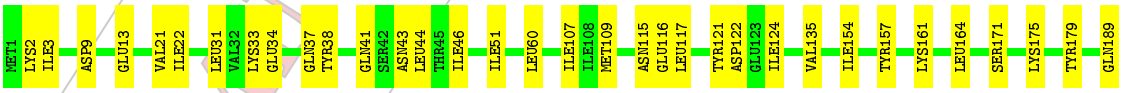




- Molecule 1: CRISPR-associated protein Csn2

Chain H:





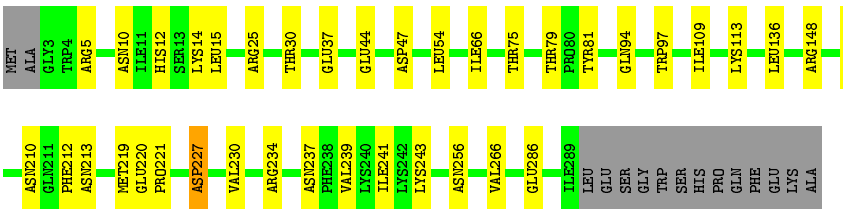


- Molecule 2: CRISPR-associated endonuclease Cas1

Chain I:



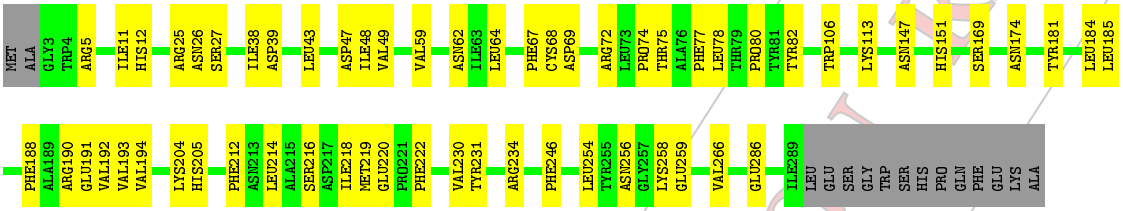
PRELIMINARY VALIDATION REPORT



- Molecule 2: CRISPR-associated endonuclease Cas1

Chain J:

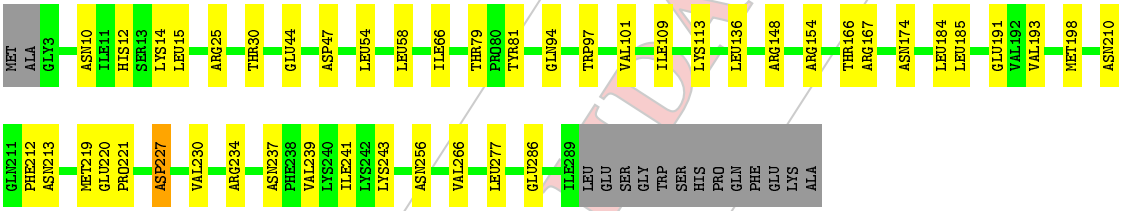




- Molecule 2: CRISPR-associated endonuclease Cas1

Chain L:

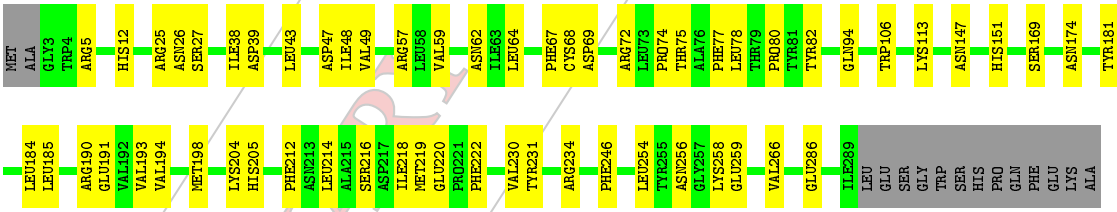




- Molecule 2: CRISPR-associated endonuclease Cas1

Chain M:

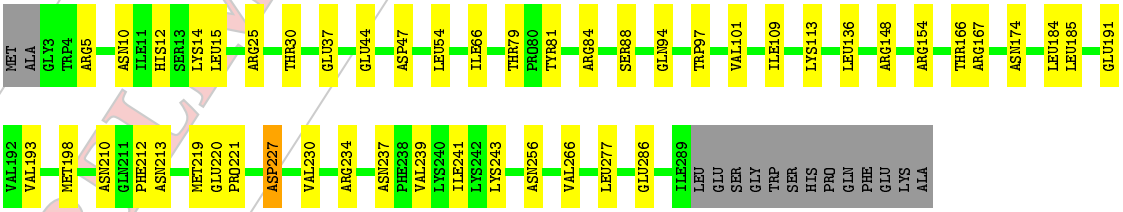




- Molecule 2: CRISPR-associated endonuclease Cas1

Chain O:

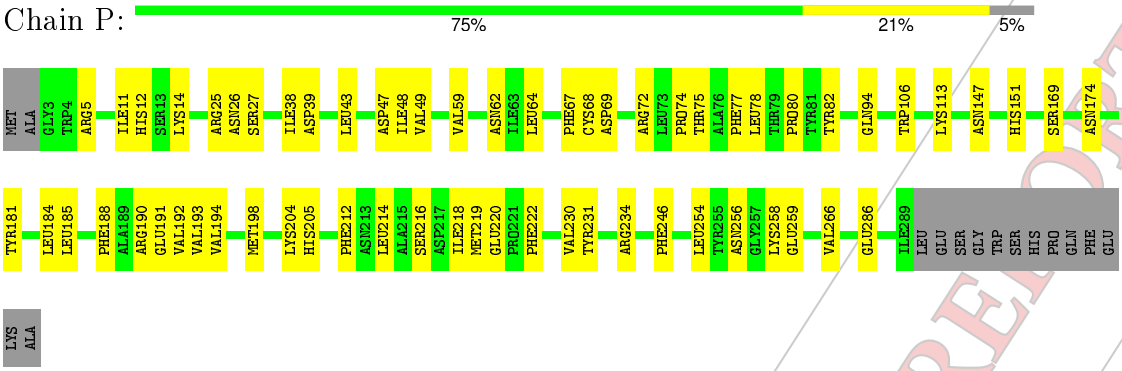




- Molecule 2: CRISPR-associated endonuclease Cas1

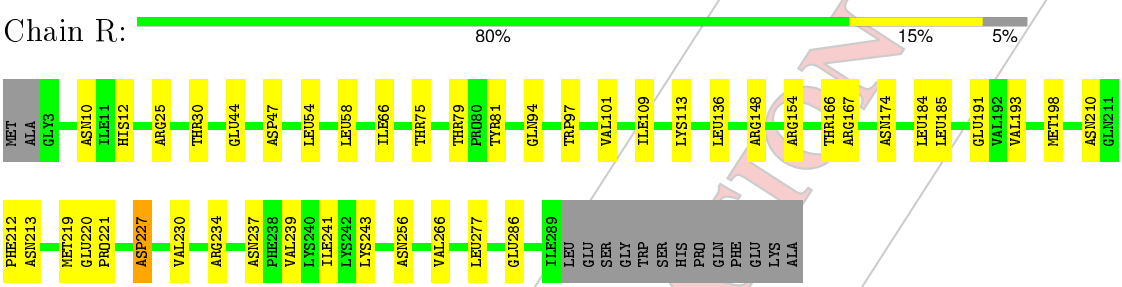
PRELIMINARY VALIDATION REPORT

Chain P:



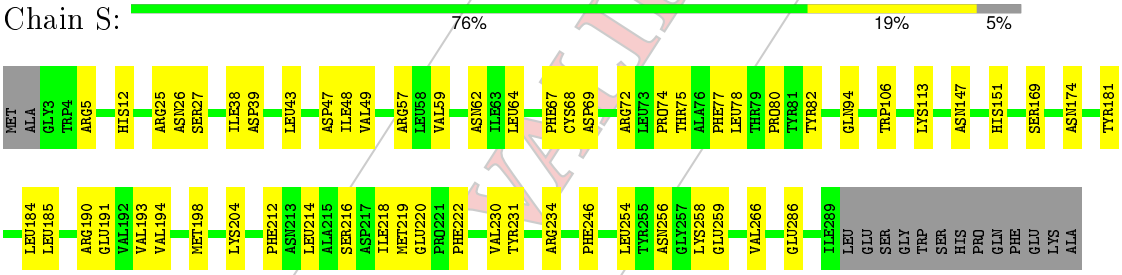
- Molecule 2: CRISPR-associated endonuclease Cas1

Chain R:



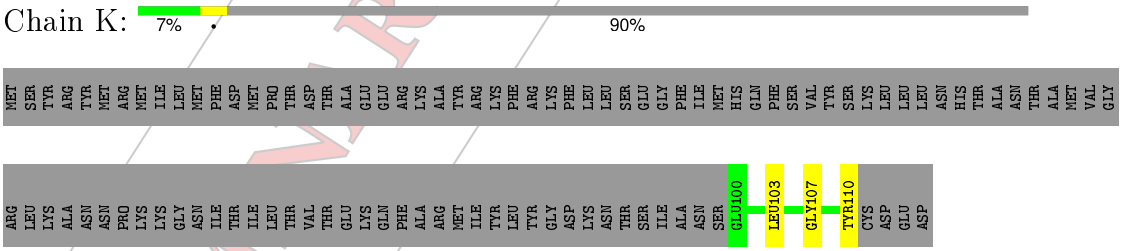
- Molecule 2: CRISPR-associated endonuclease Cas1

Chain S:



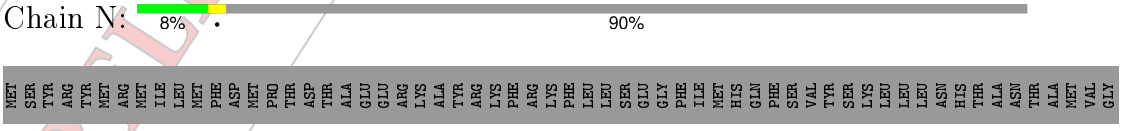
- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain K:

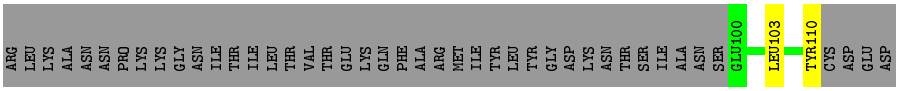


- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain N:



PRELIMINARY VALIDATION REPORT

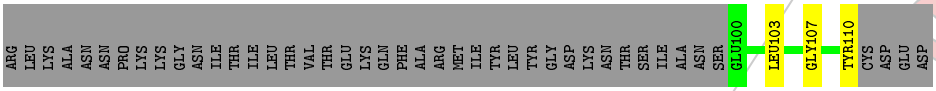


• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain Q:





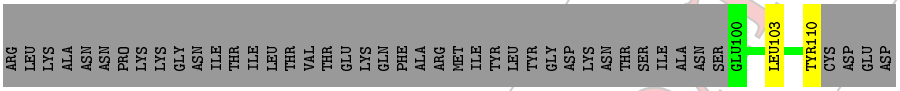


• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain T:

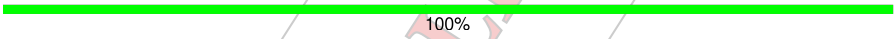






• Molecule 4: DNA (25-MER)

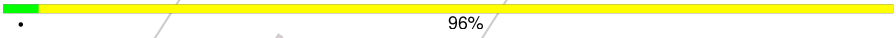
Chain X:



There are no outlier residues recorded for this chain.

• Molecule 5: DNA (25-MER)

Chain Y:





PRELIMINARY VALIDATION REPORT

4 Experimental information (i)

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

PRELIMINARY VALIDATION REPORT

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.24	0/1812	0.38	0/2451
1	B	0.24	0/1820	0.38	0/2462
1	C	0.24	0/1812	0.38	0/2451
1	D	0.24	0/1820	0.38	0/2462
1	E	0.24	0/1812	0.38	0/2451
1	F	0.24	0/1820	0.38	0/2462
1	G	0.24	0/1812	0.38	0/2451
1	H	0.24	0/1820	0.38	0/2462
2	I	0.24	0/2420	0.39	0/3271
2	J	0.24	0/2420	0.38	0/3271
2	L	0.24	0/2420	0.39	0/3271
2	M	0.24	0/2420	0.38	0/3271
2	O	0.24	0/2420	0.38	0/3271
2	P	0.24	0/2420	0.38	0/3271
2	R	0.24	0/2420	0.39	0/3271
2	S	0.24	0/2420	0.38	0/3271
3	K	0.25	0/96	0.41	0/128
3	N	0.26	0/96	0.41	0/128
3	Q	0.26	0/96	0.41	0/128
3	T	0.26	0/96	0.41	0/128
4	X	0.59	0/549	1.29	0/846
5	Y	0.49	0/599	0.74	0/921
All	All	0.25	0/35420	0.42	0/48099

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

PRELIMINARY VALIDATION REPORT

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1787	0	1838	23	0
1	B	1795	0	1844	31	0
1	C	1787	0	1838	25	0
1	D	1795	0	1844	29	0
1	E	1787	0	1838	25	0
1	F	1795	0	1844	27	0
1	G	1787	0	1838	26	0
1	H	1795	0	1844	30	0
2	I	2369	0	2356	31	0
2	J	2369	0	2356	43	0
2	L	2369	0	2356	33	0
2	M	2369	0	2356	39	0
2	O	2369	0	2356	31	0
2	P	2369	0	2356	41	0
2	R	2369	0	2356	31	0
2	S	2369	0	2356	41	0
3	K	95	0	86	3	0
3	N	95	0	86	2	0
3	Q	95	0	86	3	0
3	T	95	0	86	2	0
4	X	500	0	301	0	0
5	Y	525	0	276	24	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
All	All	34693	0	34497	479	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (479) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

PRELIMINARY VALIDATION REPORT

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:41:GLN:HE22	1:H:44:LEU:HB3	1.51	0.75
1:F:41:GLN:HE22	1:F:44:LEU:HB3	1.52	0.75
1:B:41:GLN:HE22	1:B:44:LEU:HB3	1.51	0.74
1:D:41:GLN:HE22	1:D:44:LEU:HB3	1.51	0.73
2:J:5:ARG:O	2:J:39:ASP:N	2.20	0.72
2:P:5:ARG:O	2:P:39:ASP:N	2.20	0.72
2:S:5:ARG:O	2:S:39:ASP:N	2.20	0.71
2:M:5:ARG:O	2:M:39:ASP:N	2.20	0.70
2:I:12:HIS:HD2	2:I:47:ASP:HB2	1.59	0.68
2:O:12:HIS:HD2	2:O:47:ASP:HB2	1.59	0.68
2:L:12:HIS:HD2	2:L:47:ASP:HB2	1.59	0.68
2:R:12:HIS:HD2	2:R:47:ASP:HB2	1.59	0.67
2:S:62:ASN:HD21	2:S:194:VAL:HG22	1.59	0.67
2:J:62:ASN:HD21	2:J:194:VAL:HG22	1.59	0.67
2:P:62:ASN:HD21	2:P:194:VAL:HG22	1.59	0.67
2:I:256:ASN:ND2	2:I:286:GLU:O	2.28	0.67
2:R:256:ASN:ND2	2:R:286:GLU:O	2.28	0.67
2:J:216:SER:HA	2:J:219:MET:HG2	1.77	0.67
2:L:256:ASN:ND2	2:L:286:GLU:O	2.28	0.67
2:M:62:ASN:HD21	2:M:194:VAL:HG22	1.59	0.66
2:O:256:ASN:ND2	2:O:286:GLU:O	2.28	0.66
1:G:139:THR:HG22	1:G:139:THR:O	1.95	0.66
2:P:216:SER:HA	2:P:219:MET:HG2	1.77	0.66
1:B:9:ASP:OD1	2:J:25:ARG:NH1	2.28	0.66
2:M:216:SER:HA	2:M:219:MET:HG2	1.77	0.66
2:S:216:SER:HA	2:S:219:MET:HG2	1.77	0.66
1:E:139:THR:HG22	1:E:139:THR:O	1.95	0.66
1:A:139:THR:O	1:A:139:THR:HG22	1.95	0.64
1:C:139:THR:O	1:C:139:THR:HG22	1.95	0.64
1:B:206:PHE:HB3	1:B:214:LEU:HD11	1.78	0.64
2:I:25:ARG:HG3	2:I:30:THR:HG22	1.78	0.63
1:H:206:PHE:HB3	1:H:214:LEU:HD11	1.79	0.63
2:L:25:ARG:HG3	2:L:30:THR:HG22	1.80	0.63
2:O:25:ARG:HG3	2:O:30:THR:HG22	1.80	0.63
2:R:25:ARG:HG3	2:R:30:THR:HG22	1.79	0.63
2:M:169:SER:OG	2:M:174:ASN:ND2	2.33	0.62
2:S:169:SER:OG	2:S:174:ASN:ND2	2.33	0.62
1:A:41:GLN:HE22	1:A:44:LEU:HB3	1.65	0.62
1:C:41:GLN:HE22	1:C:44:LEU:HB3	1.65	0.62
1:F:206:PHE:HB3	1:F:214:LEU:HD11	1.80	0.62
2:J:169:SER:OG	2:J:174:ASN:ND2	2.33	0.62
2:P:169:SER:OG	2:P:174:ASN:ND2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:TYR:HA	1:F:41:GLN:HE21	1.65	0.62
2:M:256:ASN:ND2	2:M:286:GLU:O	2.33	0.62
2:S:256:ASN:ND2	2:S:286:GLU:O	2.33	0.62
1:D:206:PHE:HB3	1:D:214:LEU:HD11	1.80	0.61
1:G:41:GLN:HE22	1:G:44:LEU:HB3	1.65	0.61
1:H:38:TYR:HA	1:H:41:GLN:HE21	1.64	0.61
2:R:113:LYS:HD3	2:R:220:GLU:HB3	1.81	0.61
2:L:113:LYS:HD3	2:L:220:GLU:HB3	1.81	0.61
2:P:256:ASN:ND2	2:P:286:GLU:O	2.33	0.61
1:E:41:GLN:HE22	1:E:44:LEU:HB3	1.65	0.61
2:J:256:ASN:ND2	2:J:286:GLU:O	2.33	0.61
1:D:38:TYR:HA	1:D:41:GLN:HE21	1.65	0.61
1:B:38:TYR:HA	1:B:41:GLN:HE21	1.64	0.60
1:C:77:LYS:NZ	5:Y:25:DA:OP1	2.34	0.60
1:C:4:ASN:HB2	1:C:11:PRO:HB3	1.84	0.60
2:I:113:LYS:HD3	2:I:220:GLU:HB3	1.81	0.60
1:G:4:ASN:HB2	1:G:11:PRO:HB3	1.84	0.60
1:E:4:ASN:HB2	1:E:11:PRO:HB3	1.84	0.60
2:J:231:TYR:O	2:J:234:ARG:NH1	2.35	0.60
1:A:4:ASN:HB2	1:A:11:PRO:HB3	1.84	0.60
1:D:189:GLN:NE2	1:H:13:GLU:OE1	2.35	0.59
2:O:113:LYS:HD3	2:O:220:GLU:HB3	1.82	0.59
2:P:231:TYR:O	2:P:234:ARG:NH1	2.35	0.59
1:B:189:GLN:NE2	1:F:13:GLU:OE1	2.36	0.59
1:D:13:GLU:OE1	1:H:189:GLN:NE2	2.36	0.59
2:R:210:ASN:O	2:R:213:ASN:ND2	2.36	0.59
1:E:206:PHE:HB3	1:E:214:LEU:HD11	1.85	0.59
2:M:231:TYR:O	2:M:234:ARG:NH1	2.35	0.59
1:A:120:GLU:HB2	1:D:138:GLU:HB3	1.85	0.59
2:L:210:ASN:O	2:L:213:ASN:ND2	2.36	0.59
1:G:206:PHE:HB3	1:G:214:LEU:HD11	1.85	0.58
2:S:231:TYR:O	2:S:234:ARG:NH1	2.35	0.58
1:C:206:PHE:HB3	1:C:214:LEU:HD11	1.85	0.58
2:O:94:GLN:NE2	2:O:198:MET:O	2.33	0.58
1:A:206:PHE:HB3	1:A:214:LEU:HD11	1.85	0.58
1:B:13:GLU:OE1	1:F:189:GLN:NE2	2.36	0.58
2:M:191:GLU:HG3	2:M:266:VAL:HG12	1.86	0.58
2:S:191:GLU:HG3	2:S:266:VAL:HG12	1.86	0.57
2:I:210:ASN:O	2:I:213:ASN:ND2	2.37	0.57
2:O:210:ASN:O	2:O:213:ASN:ND2	2.36	0.57
2:P:191:GLU:HG3	2:P:266:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:191:GLU:HG3	2:J:266:VAL:HG12	1.86	0.57
2:R:191:GLU:HG3	2:R:266:VAL:HG12	1.87	0.57
2:L:191:GLU:HG3	2:L:266:VAL:HG12	1.88	0.56
2:I:94:GLN:NE2	2:I:198:MET:O	2.35	0.56
2:I:191:GLU:HG3	2:I:266:VAL:HG12	1.88	0.56
2:O:191:GLU:HG3	2:O:266:VAL:HG12	1.88	0.56
1:G:65:ILE:HD11	1:G:169:SER:HB3	1.88	0.56
2:J:184:LEU:HB3	2:J:219:MET:HE3	1.88	0.55
2:M:64:LEU:HB2	2:M:190:ARG:HG3	1.88	0.55
2:P:184:LEU:HB3	2:P:219:MET:HE3	1.88	0.55
1:A:65:ILE:HD11	1:A:169:SER:HB3	1.88	0.55
1:B:138:GLU:HB3	1:C:120:GLU:HB2	1.88	0.55
2:S:64:LEU:HB2	2:S:190:ARG:HG3	1.89	0.55
1:E:65:ILE:HD11	1:E:169:SER:HB3	1.88	0.55
2:L:94:GLN:NE2	2:L:198:MET:O	2.33	0.55
2:M:147:ASN:O	2:M:151:HIS:ND1	2.36	0.55
2:J:64:LEU:HB2	2:J:190:ARG:HG3	1.89	0.55
1:C:65:ILE:HD11	1:C:169:SER:HB3	1.88	0.55
2:P:68:CYS:HA	2:P:74:PRO:HA	1.89	0.55
2:P:64:LEU:HB2	2:P:190:ARG:HG3	1.89	0.54
2:J:68:CYS:HA	2:J:74:PRO:HA	1.89	0.54
2:M:68:CYS:HA	2:M:74:PRO:HA	1.89	0.54
1:A:133:LEU:HD13	1:D:124:ILE:HG13	1.89	0.54
2:S:147:ASN:O	2:S:151:HIS:ND1	2.36	0.54
2:S:68:CYS:HA	2:S:74:PRO:HA	1.89	0.54
1:D:34:GLU:OE2	1:D:43:ASN:ND2	2.37	0.54
2:R:94:GLN:NE2	2:R:198:MET:O	2.33	0.53
2:M:184:LEU:HB3	2:M:219:MET:HE3	1.90	0.53
2:L:109:ILE:HG23	2:L:221:PRO:HD3	1.91	0.53
2:I:109:ILE:HG23	2:I:221:PRO:HD3	1.91	0.53
2:R:109:ILE:HG23	2:R:221:PRO:HD3	1.91	0.53
1:H:21:VAL:HG21	1:H:199:GLN:HA	1.91	0.53
5:Y:14:DA:H2"	5:Y:15:DA:C8	2.45	0.52
2:S:184:LEU:HB3	2:S:219:MET:HE3	1.91	0.52
2:P:147:ASN:O	2:P:151:HIS:ND1	2.36	0.52
5:Y:10:DA:H2"	5:Y:11:DA:C8	2.45	0.52
1:G:175:LYS:HE3	1:G:202:GLY:HA3	1.91	0.52
2:M:204:LYS:HG3	2:M:205:HIS:N	2.25	0.52
5:Y:15:DA:H2"	5:Y:16:DA:C8	2.45	0.52
5:Y:19:DA:H2"	5:Y:20:DA:C8	2.45	0.52
5:Y:5:DA:H2"	5:Y:6:DA:C8	2.45	0.52

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PRELIMINARY VALIDATION REPORT

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:MET:SD	1:E:121:TYR:OH	2.65	0.52
1:G:109:MET:SD	1:G:121:TYR:OH	2.64	0.52
5:Y:9:DA:H2"	5:Y:10:DA:C8	2.45	0.52
5:Y:18:DA:H2"	5:Y:19:DA:C8	2.45	0.52
1:B:34:GLU:OE2	1:B:43:ASN:ND2	2.37	0.52
1:E:175:LYS:HE3	1:E:202:GLY:HA3	1.91	0.52
2:J:147:ASN:O	2:J:151:HIS:ND1	2.36	0.52
5:Y:8:DA:H2"	5:Y:9:DA:C8	2.45	0.52
2:O:154:ARG:NH2	2:O:166:THR:OG1	2.43	0.52
5:Y:20:DA:H2"	5:Y:21:DA:C8	2.45	0.52
1:D:21:VAL:HG21	1:D:199:GLN:HA	1.91	0.52
1:H:34:GLU:OE2	1:H:43:ASN:ND2	2.37	0.52
2:J:113:LYS:HD3	2:J:220:GLU:HB3	1.92	0.52
5:Y:11:DA:H2"	5:Y:12:DA:C8	2.45	0.52
5:Y:13:DA:H2"	5:Y:14:DA:C8	2.45	0.52
5:Y:16:DA:H2"	5:Y:17:DA:C8	2.45	0.51
5:Y:4:DA:H2"	5:Y:5:DA:C8	2.46	0.51
5:Y:6:DA:H2"	5:Y:7:DA:C8	2.45	0.51
2:O:167:ARG:HA	2:O:174:ASN:HD21	1.75	0.51
5:Y:7:DA:H2"	5:Y:8:DA:C8	2.45	0.51
2:P:113:LYS:HD3	2:P:220:GLU:HB3	1.92	0.51
5:Y:12:DA:H2"	5:Y:13:DA:C8	2.45	0.51
2:I:154:ARG:NH2	2:I:166:THR:OG1	2.44	0.51
2:R:167:ARG:HA	2:R:174:ASN:HD21	1.75	0.51
5:Y:17:DA:H2"	5:Y:18:DA:C8	2.45	0.51
1:A:175:LYS:HE3	1:A:202:GLY:HA3	1.91	0.51
2:O:109:ILE:HG23	2:O:221:PRO:HD3	1.92	0.51
2:I:167:ARG:HA	2:I:174:ASN:HD21	1.75	0.51
2:J:26:ASN:OD1	2:J:27:SER:N	2.43	0.51
2:P:26:ASN:OD1	2:P:27:SER:N	2.43	0.51
1:F:3:ILE:HG22	1:F:46:ILE:HG23	1.93	0.51
1:B:124:ILE:HG13	1:C:133:LEU:HD13	1.93	0.51
1:B:21:VAL:HG21	1:B:199:GLN:HA	1.92	0.51
1:C:175:LYS:HE3	1:C:202:GLY:HA3	1.91	0.51
1:F:21:VAL:HG21	1:F:199:GLN:HA	1.92	0.50
2:M:113:LYS:HD3	2:M:220:GLU:HB3	1.92	0.50
2:S:113:LYS:HD3	2:S:220:GLU:HB3	1.92	0.50
1:G:34:GLU:OE2	1:G:43:ASN:ND2	2.44	0.50
2:O:136:LEU:HB3	2:O:148:ARG:HB3	1.94	0.50
2:R:154:ARG:NH2	2:R:166:THR:OG1	2.43	0.50
5:Y:21:DA:H2"	5:Y:22:DA:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLU:OE2	1:A:43:ASN:ND2	2.44	0.50
1:F:34:GLU:OE2	1:F:43:ASN:ND2	2.38	0.50
2:I:136:LEU:HB3	2:I:148:ARG:HB3	1.93	0.50
2:L:154:ARG:NH2	2:L:166:THR:OG1	2.43	0.50
2:L:167:ARG:HA	2:L:174:ASN:HD21	1.76	0.50
1:H:3:ILE:HG22	1:H:46:ILE:HG23	1.94	0.50
2:O:84:ARG:HH21	2:O:88:SER:HG	1.59	0.50
1:D:9:ASP:HA	2:P:25:ARG:HH12	1.76	0.50
5:Y:3:DA:H2"	5:Y:4:DA:C8	2.46	0.50
2:I:79:THR:OG1	2:J:77:PHE:O	2.30	0.50
1:E:34:GLU:OE2	1:E:43:ASN:ND2	2.44	0.50
1:E:119:ILE:HG23	1:H:135:VAL:HG13	1.94	0.50
2:S:94:GLN:OE1	2:S:198:MET:N	2.38	0.50
2:J:67:PHE:HE1	2:J:78:LEU:HG	1.77	0.49
1:B:164:LEU:O	1:B:192:VAL:HA	2.13	0.49
2:M:67:PHE:HE1	2:M:78:LEU:HG	1.78	0.49
2:M:94:GLN:OE1	2:M:198:MET:N	2.38	0.49
1:F:164:LEU:O	1:F:192:VAL:HA	2.13	0.49
2:S:67:PHE:HE1	2:S:78:LEU:HG	1.78	0.49
1:C:34:GLU:OE2	1:C:43:ASN:ND2	2.44	0.49
1:D:3:ILE:HG22	1:D:46:ILE:HG23	1.93	0.49
1:D:164:LEU:O	1:D:192:VAL:HA	2.13	0.49
1:H:164:LEU:O	1:H:192:VAL:HA	2.13	0.49
2:P:67:PHE:HE1	2:P:78:LEU:HG	1.78	0.49
1:F:135:VAL:HG13	1:G:119:ILE:HG23	1.95	0.49
2:J:5:ARG:HB2	2:J:38:ILE:HA	1.95	0.49
5:Y:22:DA:H2"	5:Y:23:DA:C8	2.47	0.49
1:B:211:ASP:HB3	2:J:49:VAL:HG21	1.94	0.49
1:F:115:ASN:OD1	1:F:116:GLU:N	2.46	0.49
1:G:3:ILE:HG22	1:G:46:ILE:HG12	1.95	0.49
1:H:115:ASN:OD1	1:H:116:GLU:N	2.46	0.49
1:E:3:ILE:HG22	1:E:46:ILE:HG12	1.95	0.48
2:I:185:LEU:HD11	2:I:212:PHE:HB3	1.94	0.48
2:P:5:ARG:HB2	2:P:38:ILE:HA	1.95	0.48
2:L:136:LEU:HB3	2:L:148:ARG:HB3	1.94	0.48
2:R:136:LEU:HB3	2:R:148:ARG:HB3	1.94	0.48
2:R:184:LEU:HB2	2:R:219:MET:HE3	1.94	0.48
2:S:26:ASN:OD1	2:S:27:SER:N	2.43	0.48
2:L:185:LEU:HD11	2:L:212:PHE:HB3	1.95	0.48
2:S:5:ARG:HB2	2:S:38:ILE:HA	1.95	0.48
2:M:26:ASN:OD1	2:M:27:SER:N	2.43	0.48

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PRELIMINARY VALIDATION REPORT

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:79:THR:OG1	2:M:77:PHE:O	2.30	0.48
1:G:139:THR:O	1:G:139:THR:CG2	2.62	0.48
2:I:75:THR:HB	2:J:59:VAL:HG11	1.94	0.48
2:M:5:ARG:HB2	2:M:38:ILE:HA	1.95	0.48
2:I:81:TYR:HA	2:J:212:PHE:HE2	1.79	0.48
1:B:9:ASP:HA	2:J:25:ARG:HH12	1.77	0.48
2:L:184:LEU:HB2	2:L:219:MET:HE3	1.95	0.48
2:R:79:THR:OG1	2:S:77:PHE:O	2.28	0.48
1:B:115:ASN:OD1	1:B:116:GLU:N	2.46	0.47
5:Y:23:DA:H2"	5:Y:24:DA:C8	2.49	0.47
1:A:109:MET:SD	1:A:121:TYR:OH	2.64	0.47
1:D:115:ASN:OD1	1:D:116:GLU:N	2.46	0.47
2:O:185:LEU:HD11	2:O:212:PHE:HB3	1.95	0.47
5:Y:2:DA:H2"	5:Y:3:DA:C8	2.48	0.47
1:B:109:MET:SD	1:B:121:TYR:OH	2.73	0.47
2:I:227:ASP:OD1	2:I:227:ASP:N	2.48	0.47
2:J:254:LEU:HA	2:J:259:GLU:HA	1.96	0.47
2:O:227:ASP:OD1	2:O:227:ASP:N	2.48	0.47
2:R:185:LEU:HD11	2:R:212:PHE:HB3	1.95	0.47
1:E:139:THR:CG2	1:E:139:THR:O	2.62	0.47
1:A:3:ILE:HG22	1:A:46:ILE:HG12	1.95	0.47
1:C:109:MET:SD	1:C:121:TYR:OH	2.65	0.47
1:B:135:VAL:HG13	1:C:119:ILE:HG23	1.97	0.47
2:I:184:LEU:HB2	2:I:219:MET:HE3	1.95	0.47
2:P:254:LEU:HA	2:P:259:GLU:HA	1.96	0.47
1:H:109:MET:SD	1:H:121:TYR:OH	2.72	0.47
2:R:227:ASP:OD1	2:R:227:ASP:N	2.47	0.47
1:C:3:ILE:HG22	1:C:46:ILE:HG12	1.95	0.47
2:R:239:VAL:HG12	2:R:243:LYS:HE3	1.97	0.47
1:D:109:MET:SD	1:D:121:TYR:OH	2.73	0.47
2:J:69:ASP:HB2	2:J:75:THR:HG23	1.97	0.47
2:L:227:ASP:N	2:L:227:ASP:OD1	2.47	0.47
2:L:230:VAL:O	2:L:234:ARG:HB3	2.15	0.47
2:L:239:VAL:HG12	2:L:243:LYS:HE3	1.97	0.47
2:O:184:LEU:HB2	2:O:219:MET:HE3	1.96	0.47
2:M:258:LYS:HG2	2:M:259:GLU:H	1.80	0.46
2:M:254:LEU:HA	2:M:259:GLU:HA	1.96	0.46
2:R:230:VAL:O	2:R:234:ARG:HB3	2.15	0.46
2:S:258:LYS:HG2	2:S:259:GLU:H	1.80	0.46
1:A:119:ILE:HG23	1:D:135:VAL:HG13	1.97	0.46
1:E:1:MET:HE1	1:E:162:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:MET:SD	1:F:121:TYR:OH	2.73	0.46
2:M:69:ASP:HB2	2:M:75:THR:HG23	1.97	0.46
2:P:69:ASP:HB2	2:P:75:THR:HG23	1.97	0.46
1:B:3:ILE:HG22	1:B:46:ILE:HG23	1.96	0.46
2:L:210:ASN:HD21	2:L:212:PHE:HB2	1.81	0.46
1:E:133:LEU:HD13	1:H:124:ILE:HG13	1.98	0.46
2:S:69:ASP:HB2	2:S:75:THR:HG23	1.97	0.46
2:S:72:ARG:NH2	3:T:110:TYR:OH	2.48	0.46
2:S:254:LEU:HA	2:S:259:GLU:HA	1.96	0.46
1:F:196:GLU:HG3	1:F:200:ILE:HD11	1.98	0.46
2:O:210:ASN:HD21	2:O:212:PHE:HB2	1.81	0.46
2:P:72:ARG:NH2	3:Q:110:TYR:OH	2.48	0.46
2:J:72:ARG:NH2	3:K:110:TYR:OH	2.48	0.46
2:O:239:VAL:HG12	2:O:243:LYS:HE3	1.98	0.46
1:G:115:ASN:OD1	1:G:116:GLU:N	2.49	0.46
2:J:204:LYS:HG3	2:J:205:HIS:CD2	2.50	0.46
2:M:72:ARG:NH2	3:N:110:TYR:OH	2.48	0.46
1:D:196:GLU:HG3	1:D:200:ILE:HD11	1.98	0.46
1:F:9:ASP:HA	2:S:25:ARG:HH12	1.81	0.46
2:I:167:ARG:HA	2:I:174:ASN:ND2	2.32	0.45
1:H:196:GLU:HG3	1:H:200:ILE:HD11	1.98	0.45
2:I:239:VAL:HG12	2:I:243:LYS:HE3	1.98	0.45
2:O:136:LEU:HD23	2:O:148:ARG:HH11	1.81	0.45
2:P:258:LYS:HG2	2:P:259:GLU:H	1.80	0.45
1:C:139:THR:O	1:C:139:THR:CG2	2.62	0.45
1:F:60:LEU:HD22	1:F:161:LYS:HG3	1.98	0.45
1:H:33:LYS:O	1:H:37:GLN:HG2	2.17	0.45
1:H:9:ASP:HA	2:M:25:ARG:HH12	1.82	0.45
2:I:230:VAL:O	2:I:234:ARG:HB3	2.15	0.45
2:O:167:ARG:HA	2:O:174:ASN:ND2	2.32	0.45
2:O:81:TYR:HA	2:P:212:PHE:HE2	1.82	0.45
2:R:210:ASN:HD21	2:R:212:PHE:HB2	1.82	0.45
1:B:60:LEU:HD22	1:B:161:LYS:HG3	1.99	0.45
1:E:115:ASN:OD1	1:E:116:GLU:N	2.49	0.45
2:O:230:VAL:O	2:O:234:ARG:HB3	2.16	0.45
1:A:139:THR:O	1:A:139:THR:CG2	2.62	0.45
1:F:33:LYS:O	1:F:37:GLN:HG2	2.17	0.45
2:I:136:LEU:HD23	2:I:148:ARG:HH11	1.82	0.45
2:J:258:LYS:HG2	2:J:259:GLU:H	1.80	0.45
2:L:167:ARG:HA	2:L:174:ASN:ND2	2.32	0.45
1:C:115:ASN:OD1	1:C:116:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:PRO:HG2	1:D:171:SER:HB3	1.98	0.45
1:B:196:GLU:HG3	1:B:200:ILE:HD11	1.98	0.45
1:B:33:LYS:O	1:B:37:GLN:HG2	2.17	0.45
2:I:210:ASN:HD21	2:I:212:PHE:HB2	1.82	0.45
2:R:136:LEU:HD23	2:R:148:ARG:HH11	1.82	0.45
2:R:167:ARG:HA	2:R:174:ASN:ND2	2.32	0.45
1:A:115:ASN:OD1	1:A:116:GLU:N	2.49	0.45
1:C:171:SER:OG	1:D:198:ARG:NH2	2.50	0.45
1:H:215:MET:HE3	2:L:14:LYS:HB2	1.98	0.45
2:M:185:LEU:HD11	2:M:212:PHE:HB3	1.99	0.45
2:S:185:LEU:HD11	2:S:212:PHE:HB3	1.99	0.45
1:D:60:LEU:HD22	1:D:161:LYS:HG3	1.99	0.44
1:D:60:LEU:HB2	1:D:161:LYS:HD2	1.99	0.44
1:H:154:ILE:HA	1:H:157:TYR:HD2	1.82	0.44
2:L:136:LEU:HD23	2:L:148:ARG:HH11	1.82	0.44
1:B:154:ILE:HA	1:B:157:TYR:HD2	1.82	0.44
1:B:215:MET:HE3	2:I:14:LYS:HB2	2.00	0.44
1:G:197:PRO:HG2	1:H:171:SER:HB3	2.00	0.44
1:A:197:PRO:HG2	1:B:171:SER:HB3	1.98	0.44
1:D:211:ASP:HB3	2:P:49:VAL:HG21	1.98	0.44
1:E:155:PHE:HE2	1:E:190:ALA:HB1	1.82	0.44
2:J:12:HIS:HD2	2:J:47:ASP:HB2	1.83	0.44
2:S:181:TYR:O	2:S:185:LEU:HB2	2.17	0.44
1:C:155:PHE:HE2	1:C:190:ALA:HB1	1.82	0.44
1:C:16:LEU:HD23	1:C:186:LYS:HG2	2.00	0.44
1:D:154:ILE:HA	1:D:157:TYR:HD2	1.82	0.44
1:F:154:ILE:HA	1:F:157:TYR:HD2	1.83	0.44
1:G:16:LEU:HD23	1:G:186:LYS:HG2	2.00	0.44
1:H:60:LEU:HB2	1:H:161:LYS:HD2	2.00	0.44
2:P:12:HIS:HD2	2:P:47:ASP:HB2	1.83	0.44
1:A:16:LEU:HD23	1:A:186:LYS:HG2	2.00	0.44
1:D:33:LYS:O	1:D:37:GLN:HG2	2.17	0.44
1:E:16:LEU:HD23	1:E:186:LYS:HG2	2.00	0.44
1:G:155:PHE:HE2	1:G:190:ALA:HB1	1.82	0.44
2:O:94:GLN:HA	2:O:97:TRP:CE2	2.53	0.44
1:A:155:PHE:HE2	1:A:190:ALA:HB1	1.82	0.44
2:M:181:TYR:O	2:M:185:LEU:HB2	2.17	0.44
2:P:181:TYR:O	2:P:185:LEU:HB2	2.17	0.44
2:I:94:GLN:HA	2:I:97:TRP:CE2	2.53	0.44
2:J:185:LEU:HD11	2:J:212:PHE:HB3	1.99	0.44
1:E:34:GLU:O	1:E:41:GLN:NE2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:15:LEU:HB3	2:I:54:LEU:HD22	2.00	0.43
2:J:214:LEU:O	2:J:218:ILE:HG13	2.18	0.43
2:P:185:LEU:HD11	2:P:212:PHE:HB3	1.99	0.43
5:Y:24:DA:H2"	5:Y:25:DA:C8	2.52	0.43
1:A:200:ILE:O	1:A:205:GLN:NE2	2.52	0.43
1:F:124:ILE:HG13	1:G:133:LEU:HD13	2.00	0.43
2:J:181:TYR:O	2:J:185:LEU:HB2	2.17	0.43
1:H:60:LEU:HD22	1:H:161:LYS:HG3	1.99	0.43
2:R:81:TYR:HA	2:S:212:PHE:HE2	1.83	0.43
1:A:38:TYR:HA	1:A:41:GLN:HE21	1.83	0.43
1:C:200:ILE:O	1:C:205:GLN:NE2	2.52	0.43
1:F:22:ILE:HD11	1:F:31:LEU:HD23	2.01	0.43
1:G:200:ILE:O	1:G:205:GLN:NE2	2.52	0.43
2:L:237:ASN:O	2:L:241:ILE:HG13	2.19	0.43
2:P:214:LEU:O	2:P:218:ILE:HG13	2.18	0.43
2:R:75:THR:HB	2:S:59:VAL:HG11	2.00	0.43
1:C:38:TYR:HA	1:C:41:GLN:HE21	1.83	0.43
1:G:34:GLU:O	1:G:41:GLN:NE2	2.49	0.43
1:G:38:TYR:HA	1:G:41:GLN:HE21	1.83	0.43
1:E:200:ILE:O	1:E:205:GLN:NE2	2.52	0.43
1:E:38:TYR:HA	1:E:41:GLN:HE21	1.83	0.43
1:C:179:TYR:OH	1:C:202:GLY:O	2.28	0.43
2:R:237:ASN:O	2:R:241:ILE:HG13	2.19	0.43
2:S:12:HIS:HD2	2:S:47:ASP:HB2	1.83	0.43
1:A:179:TYR:OH	1:A:202:GLY:O	2.28	0.43
1:F:60:LEU:HB2	1:F:161:LYS:HD2	2.02	0.42
1:A:1:MET:HE1	1:A:162:ARG:HB3	2.01	0.42
1:C:34:GLU:O	1:C:41:GLN:NE2	2.49	0.42
2:J:106:TRP:CD1	2:J:204:LYS:HB3	2.54	0.42
2:L:81:TYR:HA	2:M:212:PHE:HE2	1.84	0.42
2:M:12:HIS:HD2	2:M:47:ASP:HB2	1.83	0.42
2:M:214:LEU:O	2:M:218:ILE:HG13	2.18	0.42
2:S:106:TRP:CD1	2:S:204:LYS:HB3	2.54	0.42
2:M:246:PHE:HB3	3:N:103:LEU:HD21	2.01	0.42
2:S:214:LEU:O	2:S:218:ILE:HG13	2.18	0.42
1:E:97:ILE:HD11	1:H:107:ILE:HG21	2.00	0.42
1:H:22:ILE:HD11	1:H:31:LEU:HD23	2.02	0.42
2:R:94:GLN:HA	2:R:97:TRP:CE2	2.54	0.42
1:F:211:ASP:HB3	2:S:49:VAL:HG21	2.00	0.42
1:B:22:ILE:HG23	1:B:208:LEU:HD23	2.01	0.42
1:B:77:LYS:HE3	1:B:77:LYS:HB2	1.88	0.42

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PRELIMINARY VALIDATION REPORT

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HE1	1:C:162:ARG:HB3	2.01	0.42
1:D:22:ILE:HD11	1:D:31:LEU:HD23	2.01	0.42
2:L:94:GLN:HA	2:L:97:TRP:CE2	2.54	0.42
2:M:184:LEU:HD21	2:M:222:PHE:HB2	2.02	0.42
2:S:246:PHE:HB3	3:T:103:LEU:HD21	2.01	0.42
2:S:184:LEU:HD21	2:S:222:PHE:HB2	2.02	0.42
1:E:157:TYR:CG	1:H:117:LEU:HD11	2.55	0.42
2:P:106:TRP:CD1	2:P:204:LYS:HB3	2.54	0.42
1:B:82:ASP:OD2	1:B:157:TYR:OH	2.37	0.42
2:J:246:PHE:HB3	3:K:103:LEU:HD21	2.01	0.42
1:D:215:MET:HE3	2:O:14:LYS:HB2	2.01	0.42
2:P:246:PHE:HB3	3:Q:103:LEU:HD21	2.01	0.42
1:A:2:LYS:HG2	1:A:13:GLU:HA	2.02	0.42
1:A:34:GLU:O	1:A:41:GLN:NE2	2.49	0.42
1:C:2:LYS:HG2	1:C:13:GLU:HA	2.02	0.42
1:D:21:VAL:HA	1:D:196:GLU:O	2.20	0.42
2:O:15:LEU:HB3	2:O:54:LEU:HD22	2.02	0.42
2:P:11:ILE:HB	3:Q:107:GLY:HA2	2.02	0.42
1:E:2:LYS:HG2	1:E:13:GLU:HA	2.02	0.41
1:F:209:ASP:OD2	2:R:25:ARG:NH1	2.53	0.41
2:I:94:GLN:HG3	2:I:97:TRP:CZ3	2.55	0.41
2:S:43:LEU:HB3	2:S:48:ILE:HD12	2.02	0.41
1:D:8:LEU:HD22	1:D:214:LEU:HD22	2.03	0.41
1:F:117:LEU:HD11	1:G:157:TYR:CG	2.55	0.41
1:H:211:ASP:HB3	2:M:49:VAL:HG21	2.01	0.41
2:I:237:ASN:O	2:I:241:ILE:HG13	2.19	0.41
2:J:216:SER:O	2:J:220:GLU:HG2	2.20	0.41
2:P:230:VAL:O	2:P:234:ARG:HB3	2.21	0.41
2:R:101:VAL:HG12	2:R:277:LEU:HD23	2.02	0.41
2:S:216:SER:O	2:S:220:GLU:HG2	2.20	0.41
2:J:11:ILE:HB	3:K:107:GLY:HA2	2.02	0.41
2:J:230:VAL:O	2:J:234:ARG:HB3	2.21	0.41
2:L:101:VAL:HG12	2:L:277:LEU:HD23	2.02	0.41
2:R:54:LEU:O	2:R:58:LEU:HG	2.21	0.41
1:B:60:LEU:HB2	1:B:161:LYS:HD2	2.02	0.41
1:G:2:LYS:HG2	1:G:13:GLU:HA	2.02	0.41
1:F:107:ILE:HG21	1:G:97:ILE:HD11	2.02	0.41
2:I:66:ILE:HD13	2:I:193:VAL:HG12	2.02	0.41
2:L:54:LEU:O	2:L:58:LEU:HG	2.21	0.41
2:O:237:ASN:O	2:O:241:ILE:HG13	2.19	0.41
2:P:43:LEU:HB3	2:P:48:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:94:GLN:HG3	2:R:97:TRP:CZ3	2.56	0.41
1:B:37:GLN:O	1:B:40:GLU:N	2.49	0.41
1:F:8:LEU:HD22	1:F:214:LEU:HD22	2.02	0.41
2:L:94:GLN:HG3	2:L:97:TRP:CZ3	2.56	0.41
2:M:216:SER:O	2:M:220:GLU:HG2	2.19	0.41
2:M:43:LEU:HB3	2:M:48:ILE:HD12	2.01	0.41
2:O:94:GLN:HG3	2:O:97:TRP:CZ3	2.55	0.41
2:P:80:PRO:HD2	2:P:193:VAL:HG11	2.03	0.41
1:D:9:ASP:OD1	2:P:14:LYS:NZ	2.46	0.41
1:G:179:TYR:OH	1:G:202:GLY:O	2.28	0.41
2:J:43:LEU:HB3	2:J:48:ILE:HD12	2.02	0.41
2:P:94:GLN:OE1	2:P:198:MET:N	2.38	0.41
2:S:59:VAL:HG13	2:S:80:PRO:HB3	2.03	0.41
1:D:37:GLN:O	1:D:40:GLU:N	2.49	0.41
1:H:209:ASP:OD2	2:L:25:ARG:NH1	2.53	0.41
2:I:10:ASN:HA	2:I:44:GLU:HB2	2.02	0.41
2:R:66:ILE:HD13	2:R:193:VAL:HG12	2.03	0.41
2:R:10:ASN:HA	2:R:44:GLU:HB2	2.02	0.41
1:E:197:PRO:HG2	1:F:171:SER:HB3	2.03	0.41
1:F:21:VAL:HA	1:F:196:GLU:O	2.20	0.41
2:J:184:LEU:HD21	2:J:222:PHE:HB2	2.02	0.41
2:J:80:PRO:HD2	2:J:193:VAL:HG11	2.03	0.41
2:L:12:HIS:CD2	2:L:47:ASP:HB2	2.47	0.41
2:P:216:SER:O	2:P:220:GLU:HG2	2.20	0.41
1:B:21:VAL:HA	1:B:196:GLU:O	2.21	0.41
2:P:184:LEU:HD21	2:P:222:PHE:HB2	2.02	0.41
1:E:179:TYR:OH	1:E:202:GLY:O	2.28	0.41
2:I:5:ARG:NH2	2:I:37:GLU:OE1	2.54	0.41
2:L:10:ASN:HA	2:L:44:GLU:HB2	2.02	0.41
2:L:66:ILE:HD13	2:L:193:VAL:HG12	2.03	0.41
2:M:59:VAL:HG13	2:M:80:PRO:HB3	2.03	0.41
2:P:188:PHE:O	2:P:192:VAL:HG23	2.21	0.41
1:B:19:VAL:HG21	1:B:203:ILE:HD12	2.03	0.41
1:H:175:LYS:HE2	1:H:179:TYR:HE2	1.86	0.41
1:H:21:VAL:HA	1:H:196:GLU:O	2.20	0.41
2:J:188:PHE:O	2:J:192:VAL:HG23	2.21	0.41
2:J:59:VAL:HG13	2:J:80:PRO:HB3	2.03	0.41
2:M:106:TRP:CD1	2:M:204:LYS:HB3	2.56	0.41
2:M:67:PHE:O	2:M:75:THR:OG1	2.34	0.41
2:O:79:THR:OG1	2:P:77:PHE:O	2.32	0.41
2:S:230:VAL:O	2:S:234:ARG:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:67:PHE:O	2:S:75:THR:OG1	2.34	0.41
2:L:15:LEU:HB3	2:L:54:LEU:HD22	2.02	0.40
2:M:57:ARG:HA	2:M:57:ARG:HH11	1.86	0.40
2:M:80:PRO:HD2	2:M:193:VAL:HG11	2.03	0.40
2:P:59:VAL:HG13	2:P:80:PRO:HB3	2.03	0.40
2:S:106:TRP:CE2	2:S:204:LYS:HB3	2.56	0.40
1:H:2:LYS:HG2	1:H:13:GLU:HA	2.04	0.40
2:O:5:ARG:NH2	2:O:37:GLU:OE1	2.54	0.40
2:S:57:ARG:HA	2:S:57:ARG:HH11	1.86	0.40
1:G:171:SER:OG	1:H:198:ARG:NH2	2.55	0.40
2:J:204:LYS:HG3	2:J:205:HIS:HD2	1.87	0.40
2:L:210:ASN:HB3	2:L:213:ASN:OD1	2.21	0.40
2:M:230:VAL:O	2:M:234:ARG:HB3	2.21	0.40
2:O:10:ASN:HA	2:O:44:GLU:HB2	2.02	0.40
2:P:204:LYS:HG3	2:P:205:HIS:N	2.36	0.40
2:R:210:ASN:HB3	2:R:213:ASN:OD1	2.21	0.40
2:P:12:HIS:CD2	2:P:47:ASP:HB2	2.57	0.40
2:S:80:PRO:HD2	2:S:193:VAL:HG11	2.03	0.40
1:B:22:ILE:HD11	1:B:31:LEU:HD23	2.03	0.40
1:E:155:PHE:CE2	1:E:190:ALA:HB1	2.57	0.40
1:G:155:PHE:CE2	1:G:190:ALA:HB1	2.56	0.40
1:G:1:MET:HB2	1:G:1:MET:HE2	1.95	0.40
2:I:81:TYR:HA	2:J:212:PHE:CE2	2.56	0.40
2:J:12:HIS:CD2	2:J:47:ASP:HB2	2.57	0.40
2:O:101:VAL:HG12	2:O:277:LEU:HD23	2.02	0.40
2:O:66:ILE:HD13	2:O:193:VAL:HG12	2.03	0.40
2:S:12:HIS:CD2	2:S:47:ASP:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

PRELIMINARY VALIDATION REPORT

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
1	B	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	C	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
1	D	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	E	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
1	F	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	G	216/219 (99%)	210 (97%)	6 (3%)	0	100	100
1	H	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
2	I	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	J	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	L	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	M	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	O	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	P	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	R	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	S	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
3	K	9/114 (8%)	9 (100%)	0	0	100	100
3	N	9/114 (8%)	9 (100%)	0	0	100	100
3	Q	9/114 (8%)	9 (100%)	0	0	100	100
3	T	9/114 (8%)	9 (100%)	0	0	100	100
All	All	4048/4624 (88%)	3956 (98%)	88 (2%)	4 (0%)	56	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	ILE
1	D	51	ILE
1	F	51	ILE
1	H	51	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

PRELIMINARY VALIDATION REPORT

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	210/211 (100%)	208 (99%)	2 (1%)	78 78
1	B	211/211 (100%)	210 (100%)	1 (0%)	90 90
1	C	210/211 (100%)	208 (99%)	2 (1%)	78 78
1	D	211/211 (100%)	210 (100%)	1 (0%)	90 90
1	E	210/211 (100%)	208 (99%)	2 (1%)	78 78
1	F	211/211 (100%)	210 (100%)	1 (0%)	90 90
1	G	210/211 (100%)	208 (99%)	2 (1%)	78 78
1	H	211/211 (100%)	210 (100%)	1 (0%)	90 90
2	I	264/276 (96%)	263 (100%)	1 (0%)	92 92
2	J	264/276 (96%)	263 (100%)	1 (0%)	92 92
2	L	264/276 (96%)	263 (100%)	1 (0%)	92 92
2	M	264/276 (96%)	263 (100%)	1 (0%)	92 92
2	O	264/276 (96%)	263 (100%)	1 (0%)	92 92
2	P	264/276 (96%)	263 (100%)	1 (0%)	92 92
2	R	264/276 (96%)	263 (100%)	1 (0%)	92 92
2	S	264/276 (96%)	263 (100%)	1 (0%)	92 92
3	K	10/102 (10%)	10 (100%)	0	100 100
3	N	10/102 (10%)	10 (100%)	0	100 100
3	Q	10/102 (10%)	10 (100%)	0	100 100
3	T	10/102 (10%)	10 (100%)	0	100 100
All	All	3836/4304 (89%)	3816 (100%)	20 (0%)	90 90

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	THR
1	A	122	ASP
1	B	122	ASP
1	C	72	THR
1	C	122	ASP
1	D	122	ASP
1	E	72	THR
1	E	122	ASP

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Res	Type
1	F	122	ASP
1	G	72	THR
1	G	122	ASP
1	H	122	ASP
2	I	227	ASP
2	J	82	TYR
2	L	227	ASP
2	M	82	TYR
2	O	227	ASP
2	P	82	TYR
2	R	227	ASP
2	S	82	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	GLN
1	A	153	GLN
1	B	180	GLN
1	C	86	GLN
1	C	153	GLN
1	D	180	GLN
1	E	86	GLN
1	E	153	GLN
1	F	86	GLN
1	F	180	GLN
1	G	86	GLN
1	G	153	GLN
1	H	86	GLN
1	H	180	GLN
2	I	12	HIS
2	I	174	ASN
2	I	211	GLN
2	J	12	HIS
2	J	62	ASN
2	J	174	ASN
2	J	205	HIS
2	J	233	ASN
2	J	236	ASN
2	L	12	HIS
2	L	174	ASN
2	L	211	GLN

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Res	Type
2	M	12	HIS
2	M	62	ASN
2	M	174	ASN
2	M	233	ASN
2	M	236	ASN
2	O	12	HIS
2	O	174	ASN
2	O	211	GLN
2	P	12	HIS
2	P	62	ASN
2	P	174	ASN
2	P	233	ASN
2	P	236	ASN
2	R	12	HIS
2	R	174	ASN
2	R	211	GLN
2	R	233	ASN
2	S	12	HIS
2	S	62	ASN
2	S	174	ASN
2	S	233	ASN
2	S	236	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

PRELIMINARY VALIDATION REPORT

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

PRELIMINARY VALIDATION REPORT

Click here to access/download;PDB Validation Report;D_1292101120_val-report-full_dimer.pdf

Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Mar 28, 2019 – 02:06 pm GMT

Deposition ID : D_1292101120
PDB ID : *(not yet assigned)*

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

PRELIMINARY VALIDATION REPORT

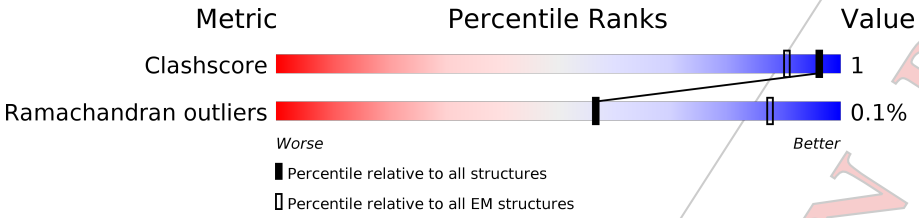
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	219	100%
1	B	219	100%
1	C	219	100%
1	D	219	99%
1	E	219	100%
1	F	219	100%
1	G	219	100%
1	H	219	100%
1	a	219	100%
1	b	219	100%
1	c	219	100%

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Length	Quality of chain
1	d	219	100%
1	e	219	100%
1	f	219	100%
1	g	219	100%
1	h	219	100%
2	I	302	93% • 5%
2	J	302	94% • 5%
2	L	302	95% 5%
2	M	302	93% • 5%
2	O	302	95% 5%
2	P	302	94% • 5%
2	R	302	95% 5%
2	S	302	94% • 5%
2	U	302	95% 5%
2	V	302	92% • 5%
2	Y	302	95% 5%
2	Z	302	94% • 5%
2	i	302	95% 5%
2	j	302	95% 5%
2	l	302	95% 5%
2	m	302	95% 5%
2	o	302	95% 5%
2	p	302	95% 5%
2	r	302	95% 5%
2	s	302	95% 5%

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Length	Quality of chain
2	u	302	95% 5%
2	v	302	95% 5%
2	y	302	95% 5%
2	z	302	95% 5%
3	K	114	79% 5% 16%
3	N	114	78% 6% 16%
3	Q	114	80% 16%
3	T	114	78% 6% 16%
3	W	114	80% 11% 10%
3	X	114	81% 10% 10%
3	k	114	84% 16%
3	n	114	84% 16%
3	q	114	84% 16%
3	t	114	84% 16%
3	w	114	90% 10%
3	x	114	90% 10%
4	1	64	81% 16%
5	2	64	25% 59% 16%

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2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 59686 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CRISPR-associated protein Csn2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	218	Total 1086	C 650	N 218	O 218	0	0
1	B	219	Total 1091	C 653	N 219	O 219	0	0
1	C	218	Total 1086	C 650	N 218	O 218	0	0
1	D	219	Total 1091	C 653	N 219	O 219	0	0
1	E	218	Total 1086	C 650	N 218	O 218	0	0
1	F	219	Total 1091	C 653	N 219	O 219	0	0
1	G	218	Total 1086	C 650	N 218	O 218	0	0
1	H	219	Total 1091	C 653	N 219	O 219	0	0
1	a	218	Total 1086	C 650	N 218	O 218	0	0
1	b	219	Total 1091	C 653	N 219	O 219	0	0
1	c	218	Total 1086	C 650	N 218	O 218	0	0
1	d	219	Total 1091	C 653	N 219	O 219	0	0
1	e	218	Total 1086	C 650	N 218	O 218	0	0
1	f	219	Total 1091	C 653	N 219	O 219	0	0
1	g	218	Total 1086	C 650	N 218	O 218	0	0
1	h	219	Total 1091	C 653	N 219	O 219	0	0

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas1.

PRELIMINARY VALIDATION REPORT

Mol	Chain	Residues	Atoms				AltConf	Trace
2	I	287	Total	C	N	O	0	0
			1425	851	287	287		
2	J	287	Total	C	N	O	0	0
			1425	851	287	287		
2	L	287	Total	C	N	O	0	0
			1425	851	287	287		
2	M	287	Total	C	N	O	0	0
			1425	851	287	287		
2	O	287	Total	C	N	O	0	0
			1425	851	287	287		
2	P	287	Total	C	N	O	0	0
			1425	851	287	287		
2	R	287	Total	C	N	O	0	0
			1425	851	287	287		
2	S	287	Total	C	N	O	0	0
			1425	851	287	287		
2	U	287	Total	C	N	O	0	0
			1425	851	287	287		
2	V	287	Total	C	N	O	0	0
			1425	851	287	287		
2	Y	287	Total	C	N	O	0	0
			1425	851	287	287		
2	Z	287	Total	C	N	O	0	0
			1425	851	287	287		
2	i	287	Total	C	N	O	0	0
			1425	851	287	287		
2	j	287	Total	C	N	O	0	0
			1425	851	287	287		
2	l	287	Total	C	N	O	0	0
			1425	851	287	287		
2	m	287	Total	C	N	O	0	0
			1425	851	287	287		
2	o	287	Total	C	N	O	0	0
			1425	851	287	287		
2	p	287	Total	C	N	O	0	0
			1425	851	287	287		
2	r	287	Total	C	N	O	0	0
			1425	851	287	287		
2	s	287	Total	C	N	O	0	0
			1425	851	287	287		
2	u	287	Total	C	N	O	0	0
			1425	851	287	287		
2	v	287	Total	C	N	O	0	0
			1425	851	287	287		

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	y	287	Total	C	N	O	0	0
			1425	851	287	287		
2	z	287	Total	C	N	O	0	0
			1425	851	287	287		

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	205	ALA	HIS	conflict	UNP G3ECR2
I	290	LEU	-	expression tag	UNP G3ECR2
I	291	GLU	-	expression tag	UNP G3ECR2
I	292	SER	-	expression tag	UNP G3ECR2
I	293	GLY	-	expression tag	UNP G3ECR2
I	294	TRP	-	expression tag	UNP G3ECR2
I	295	SER	-	expression tag	UNP G3ECR2
I	296	HIS	-	expression tag	UNP G3ECR2
I	297	PRO	-	expression tag	UNP G3ECR2
I	298	GLN	-	expression tag	UNP G3ECR2
I	299	PHE	-	expression tag	UNP G3ECR2
I	300	GLU	-	expression tag	UNP G3ECR2
I	301	LYS	-	expression tag	UNP G3ECR2
I	302	ALA	-	expression tag	UNP G3ECR2
J	205	ALA	HIS	conflict	UNP G3ECR2
J	290	LEU	-	expression tag	UNP G3ECR2
J	291	GLU	-	expression tag	UNP G3ECR2
J	292	SER	-	expression tag	UNP G3ECR2
J	293	GLY	-	expression tag	UNP G3ECR2
J	294	TRP	-	expression tag	UNP G3ECR2
J	295	SER	-	expression tag	UNP G3ECR2
J	296	HIS	-	expression tag	UNP G3ECR2
J	297	PRO	-	expression tag	UNP G3ECR2
J	298	GLN	-	expression tag	UNP G3ECR2
J	299	PHE	-	expression tag	UNP G3ECR2
J	300	GLU	-	expression tag	UNP G3ECR2
J	301	LYS	-	expression tag	UNP G3ECR2
J	302	ALA	-	expression tag	UNP G3ECR2
L	205	ALA	HIS	conflict	UNP G3ECR2
L	290	LEU	-	expression tag	UNP G3ECR2
L	291	GLU	-	expression tag	UNP G3ECR2
L	292	SER	-	expression tag	UNP G3ECR2
L	293	GLY	-	expression tag	UNP G3ECR2
L	294	TRP	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

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Chain	Residue	Modelled	Actual	Comment	Reference
L	295	SER	-	expression tag	UNP G3ECR2
L	296	HIS	-	expression tag	UNP G3ECR2
L	297	PRO	-	expression tag	UNP G3ECR2
L	298	GLN	-	expression tag	UNP G3ECR2
L	299	PHE	-	expression tag	UNP G3ECR2
L	300	GLU	-	expression tag	UNP G3ECR2
L	301	LYS	-	expression tag	UNP G3ECR2
L	302	ALA	-	expression tag	UNP G3ECR2
M	205	ALA	HIS	conflict	UNP G3ECR2
M	290	LEU	-	expression tag	UNP G3ECR2
M	291	GLU	-	expression tag	UNP G3ECR2
M	292	SER	-	expression tag	UNP G3ECR2
M	293	GLY	-	expression tag	UNP G3ECR2
M	294	TRP	-	expression tag	UNP G3ECR2
M	295	SER	-	expression tag	UNP G3ECR2
M	296	HIS	-	expression tag	UNP G3ECR2
M	297	PRO	-	expression tag	UNP G3ECR2
M	298	GLN	-	expression tag	UNP G3ECR2
M	299	PHE	-	expression tag	UNP G3ECR2
M	300	GLU	-	expression tag	UNP G3ECR2
M	301	LYS	-	expression tag	UNP G3ECR2
M	302	ALA	-	expression tag	UNP G3ECR2
O	205	ALA	HIS	conflict	UNP G3ECR2
O	290	LEU	-	expression tag	UNP G3ECR2
O	291	GLU	-	expression tag	UNP G3ECR2
O	292	SER	-	expression tag	UNP G3ECR2
O	293	GLY	-	expression tag	UNP G3ECR2
O	294	TRP	-	expression tag	UNP G3ECR2
O	295	SER	-	expression tag	UNP G3ECR2
O	296	HIS	-	expression tag	UNP G3ECR2
O	297	PRO	-	expression tag	UNP G3ECR2
O	298	GLN	-	expression tag	UNP G3ECR2
O	299	PHE	-	expression tag	UNP G3ECR2
O	300	GLU	-	expression tag	UNP G3ECR2
O	301	LYS	-	expression tag	UNP G3ECR2
O	302	ALA	-	expression tag	UNP G3ECR2
P	205	ALA	HIS	conflict	UNP G3ECR2
P	290	LEU	-	expression tag	UNP G3ECR2
P	291	GLU	-	expression tag	UNP G3ECR2
P	292	SER	-	expression tag	UNP G3ECR2
P	293	GLY	-	expression tag	UNP G3ECR2
P	294	TRP	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

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Chain	Residue	Modelled	Actual	Comment	Reference
P	295	SER	-	expression tag	UNP G3ECR2
P	296	HIS	-	expression tag	UNP G3ECR2
P	297	PRO	-	expression tag	UNP G3ECR2
P	298	GLN	-	expression tag	UNP G3ECR2
P	299	PHE	-	expression tag	UNP G3ECR2
P	300	GLU	-	expression tag	UNP G3ECR2
P	301	LYS	-	expression tag	UNP G3ECR2
P	302	ALA	-	expression tag	UNP G3ECR2
R	205	ALA	HIS	conflict	UNP G3ECR2
R	290	LEU	-	expression tag	UNP G3ECR2
R	291	GLU	-	expression tag	UNP G3ECR2
R	292	SER	-	expression tag	UNP G3ECR2
R	293	GLY	-	expression tag	UNP G3ECR2
R	294	TRP	-	expression tag	UNP G3ECR2
R	295	SER	-	expression tag	UNP G3ECR2
R	296	HIS	-	expression tag	UNP G3ECR2
R	297	PRO	-	expression tag	UNP G3ECR2
R	298	GLN	-	expression tag	UNP G3ECR2
R	299	PHE	-	expression tag	UNP G3ECR2
R	300	GLU	-	expression tag	UNP G3ECR2
R	301	LYS	-	expression tag	UNP G3ECR2
R	302	ALA	-	expression tag	UNP G3ECR2
S	205	ALA	HIS	conflict	UNP G3ECR2
S	290	LEU	-	expression tag	UNP G3ECR2
S	291	GLU	-	expression tag	UNP G3ECR2
S	292	SER	-	expression tag	UNP G3ECR2
S	293	GLY	-	expression tag	UNP G3ECR2
S	294	TRP	-	expression tag	UNP G3ECR2
S	295	SER	-	expression tag	UNP G3ECR2
S	296	HIS	-	expression tag	UNP G3ECR2
S	297	PRO	-	expression tag	UNP G3ECR2
S	298	GLN	-	expression tag	UNP G3ECR2
S	299	PHE	-	expression tag	UNP G3ECR2
S	300	GLU	-	expression tag	UNP G3ECR2
S	301	LYS	-	expression tag	UNP G3ECR2
S	302	ALA	-	expression tag	UNP G3ECR2
U	205	ALA	HIS	conflict	UNP G3ECR2
U	290	LEU	-	expression tag	UNP G3ECR2
U	291	GLU	-	expression tag	UNP G3ECR2
U	292	SER	-	expression tag	UNP G3ECR2
U	293	GLY	-	expression tag	UNP G3ECR2
U	294	TRP	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

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Chain	Residue	Modelled	Actual	Comment	Reference
U	295	SER	-	expression tag	UNP G3ECR2
U	296	HIS	-	expression tag	UNP G3ECR2
U	297	PRO	-	expression tag	UNP G3ECR2
U	298	GLN	-	expression tag	UNP G3ECR2
U	299	PHE	-	expression tag	UNP G3ECR2
U	300	GLU	-	expression tag	UNP G3ECR2
U	301	LYS	-	expression tag	UNP G3ECR2
U	302	ALA	-	expression tag	UNP G3ECR2
V	205	ALA	HIS	conflict	UNP G3ECR2
V	290	LEU	-	expression tag	UNP G3ECR2
V	291	GLU	-	expression tag	UNP G3ECR2
V	292	SER	-	expression tag	UNP G3ECR2
V	293	GLY	-	expression tag	UNP G3ECR2
V	294	TRP	-	expression tag	UNP G3ECR2
V	295	SER	-	expression tag	UNP G3ECR2
V	296	HIS	-	expression tag	UNP G3ECR2
V	297	PRO	-	expression tag	UNP G3ECR2
V	298	GLN	-	expression tag	UNP G3ECR2
V	299	PHE	-	expression tag	UNP G3ECR2
V	300	GLU	-	expression tag	UNP G3ECR2
V	301	LYS	-	expression tag	UNP G3ECR2
V	302	ALA	-	expression tag	UNP G3ECR2
Y	205	ALA	HIS	conflict	UNP G3ECR2
Y	290	LEU	-	expression tag	UNP G3ECR2
Y	291	GLU	-	expression tag	UNP G3ECR2
Y	292	SER	-	expression tag	UNP G3ECR2
Y	293	GLY	-	expression tag	UNP G3ECR2
Y	294	TRP	-	expression tag	UNP G3ECR2
Y	295	SER	-	expression tag	UNP G3ECR2
Y	296	HIS	-	expression tag	UNP G3ECR2
Y	297	PRO	-	expression tag	UNP G3ECR2
Y	298	GLN	-	expression tag	UNP G3ECR2
Y	299	PHE	-	expression tag	UNP G3ECR2
Y	300	GLU	-	expression tag	UNP G3ECR2
Y	301	LYS	-	expression tag	UNP G3ECR2
Y	302	ALA	-	expression tag	UNP G3ECR2
Z	205	ALA	HIS	conflict	UNP G3ECR2
Z	290	LEU	-	expression tag	UNP G3ECR2
Z	291	GLU	-	expression tag	UNP G3ECR2
Z	292	SER	-	expression tag	UNP G3ECR2
Z	293	GLY	-	expression tag	UNP G3ECR2
Z	294	TRP	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	295	SER	-	expression tag	UNP G3ECR2
Z	296	HIS	-	expression tag	UNP G3ECR2
Z	297	PRO	-	expression tag	UNP G3ECR2
Z	298	GLN	-	expression tag	UNP G3ECR2
Z	299	PHE	-	expression tag	UNP G3ECR2
Z	300	GLU	-	expression tag	UNP G3ECR2
Z	301	LYS	-	expression tag	UNP G3ECR2
Z	302	ALA	-	expression tag	UNP G3ECR2
i	205	ALA	HIS	conflict	UNP G3ECR2
i	290	LEU	-	expression tag	UNP G3ECR2
i	291	GLU	-	expression tag	UNP G3ECR2
i	292	SER	-	expression tag	UNP G3ECR2
i	293	GLY	-	expression tag	UNP G3ECR2
i	294	TRP	-	expression tag	UNP G3ECR2
i	295	SER	-	expression tag	UNP G3ECR2
i	296	HIS	-	expression tag	UNP G3ECR2
i	297	PRO	-	expression tag	UNP G3ECR2
i	298	GLN	-	expression tag	UNP G3ECR2
i	299	PHE	-	expression tag	UNP G3ECR2
i	300	GLU	-	expression tag	UNP G3ECR2
i	301	LYS	-	expression tag	UNP G3ECR2
i	302	ALA	-	expression tag	UNP G3ECR2
j	205	ALA	HIS	conflict	UNP G3ECR2
j	290	LEU	-	expression tag	UNP G3ECR2
j	291	GLU	-	expression tag	UNP G3ECR2
j	292	SER	-	expression tag	UNP G3ECR2
j	293	GLY	-	expression tag	UNP G3ECR2
j	294	TRP	-	expression tag	UNP G3ECR2
j	295	SER	-	expression tag	UNP G3ECR2
j	296	HIS	-	expression tag	UNP G3ECR2
j	297	PRO	-	expression tag	UNP G3ECR2
j	298	GLN	-	expression tag	UNP G3ECR2
j	299	PHE	-	expression tag	UNP G3ECR2
j	300	GLU	-	expression tag	UNP G3ECR2
j	301	LYS	-	expression tag	UNP G3ECR2
j	302	ALA	-	expression tag	UNP G3ECR2
l	205	ALA	HIS	conflict	UNP G3ECR2
l	290	LEU	-	expression tag	UNP G3ECR2
l	291	GLU	-	expression tag	UNP G3ECR2
l	292	SER	-	expression tag	UNP G3ECR2
l	293	GLY	-	expression tag	UNP G3ECR2
l	294	TRP	-	expression tag	UNP G3ECR2

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Chain	Residue	Modelled	Actual	Comment	Reference
l	295	SER	-	expression tag	UNP G3ECR2
l	296	HIS	-	expression tag	UNP G3ECR2
l	297	PRO	-	expression tag	UNP G3ECR2
l	298	GLN	-	expression tag	UNP G3ECR2
l	299	PHE	-	expression tag	UNP G3ECR2
l	300	GLU	-	expression tag	UNP G3ECR2
l	301	LYS	-	expression tag	UNP G3ECR2
l	302	ALA	-	expression tag	UNP G3ECR2
m	205	ALA	HIS	conflict	UNP G3ECR2
m	290	LEU	-	expression tag	UNP G3ECR2
m	291	GLU	-	expression tag	UNP G3ECR2
m	292	SER	-	expression tag	UNP G3ECR2
m	293	GLY	-	expression tag	UNP G3ECR2
m	294	TRP	-	expression tag	UNP G3ECR2
m	295	SER	-	expression tag	UNP G3ECR2
m	296	HIS	-	expression tag	UNP G3ECR2
m	297	PRO	-	expression tag	UNP G3ECR2
m	298	GLN	-	expression tag	UNP G3ECR2
m	299	PHE	-	expression tag	UNP G3ECR2
m	300	GLU	-	expression tag	UNP G3ECR2
m	301	LYS	-	expression tag	UNP G3ECR2
m	302	ALA	-	expression tag	UNP G3ECR2
o	205	ALA	HIS	conflict	UNP G3ECR2
o	290	LEU	-	expression tag	UNP G3ECR2
o	291	GLU	-	expression tag	UNP G3ECR2
o	292	SER	-	expression tag	UNP G3ECR2
o	293	GLY	-	expression tag	UNP G3ECR2
o	294	TRP	-	expression tag	UNP G3ECR2
o	295	SER	-	expression tag	UNP G3ECR2
o	296	HIS	-	expression tag	UNP G3ECR2
o	297	PRO	-	expression tag	UNP G3ECR2
o	298	GLN	-	expression tag	UNP G3ECR2
o	299	PHE	-	expression tag	UNP G3ECR2
o	300	GLU	-	expression tag	UNP G3ECR2
o	301	LYS	-	expression tag	UNP G3ECR2
o	302	ALA	-	expression tag	UNP G3ECR2
p	205	ALA	HIS	conflict	UNP G3ECR2
p	290	LEU	-	expression tag	UNP G3ECR2
p	291	GLU	-	expression tag	UNP G3ECR2
p	292	SER	-	expression tag	UNP G3ECR2
p	293	GLY	-	expression tag	UNP G3ECR2
p	294	TRP	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

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Chain	Residue	Modelled	Actual	Comment	Reference
p	295	SER	-	expression tag	UNP G3ECR2
p	296	HIS	-	expression tag	UNP G3ECR2
p	297	PRO	-	expression tag	UNP G3ECR2
p	298	GLN	-	expression tag	UNP G3ECR2
p	299	PHE	-	expression tag	UNP G3ECR2
p	300	GLU	-	expression tag	UNP G3ECR2
p	301	LYS	-	expression tag	UNP G3ECR2
p	302	ALA	-	expression tag	UNP G3ECR2
r	205	ALA	HIS	conflict	UNP G3ECR2
r	290	LEU	-	expression tag	UNP G3ECR2
r	291	GLU	-	expression tag	UNP G3ECR2
r	292	SER	-	expression tag	UNP G3ECR2
r	293	GLY	-	expression tag	UNP G3ECR2
r	294	TRP	-	expression tag	UNP G3ECR2
r	295	SER	-	expression tag	UNP G3ECR2
r	296	HIS	-	expression tag	UNP G3ECR2
r	297	PRO	-	expression tag	UNP G3ECR2
r	298	GLN	-	expression tag	UNP G3ECR2
r	299	PHE	-	expression tag	UNP G3ECR2
r	300	GLU	-	expression tag	UNP G3ECR2
r	301	LYS	-	expression tag	UNP G3ECR2
r	302	ALA	-	expression tag	UNP G3ECR2
s	205	ALA	HIS	conflict	UNP G3ECR2
s	290	LEU	-	expression tag	UNP G3ECR2
s	291	GLU	-	expression tag	UNP G3ECR2
s	292	SER	-	expression tag	UNP G3ECR2
s	293	GLY	-	expression tag	UNP G3ECR2
s	294	TRP	-	expression tag	UNP G3ECR2
s	295	SER	-	expression tag	UNP G3ECR2
s	296	HIS	-	expression tag	UNP G3ECR2
s	297	PRO	-	expression tag	UNP G3ECR2
s	298	GLN	-	expression tag	UNP G3ECR2
s	299	PHE	-	expression tag	UNP G3ECR2
s	300	GLU	-	expression tag	UNP G3ECR2
s	301	LYS	-	expression tag	UNP G3ECR2
s	302	ALA	-	expression tag	UNP G3ECR2
u	205	ALA	HIS	conflict	UNP G3ECR2
u	290	LEU	-	expression tag	UNP G3ECR2
u	291	GLU	-	expression tag	UNP G3ECR2
u	292	SER	-	expression tag	UNP G3ECR2
u	293	GLY	-	expression tag	UNP G3ECR2
u	294	TRP	-	expression tag	UNP G3ECR2

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Chain	Residue	Modelled	Actual	Comment	Reference
u	295	SER	-	expression tag	UNP G3ECR2
u	296	HIS	-	expression tag	UNP G3ECR2
u	297	PRO	-	expression tag	UNP G3ECR2
u	298	GLN	-	expression tag	UNP G3ECR2
u	299	PHE	-	expression tag	UNP G3ECR2
u	300	GLU	-	expression tag	UNP G3ECR2
u	301	LYS	-	expression tag	UNP G3ECR2
u	302	ALA	-	expression tag	UNP G3ECR2
v	205	ALA	HIS	conflict	UNP G3ECR2
v	290	LEU	-	expression tag	UNP G3ECR2
v	291	GLU	-	expression tag	UNP G3ECR2
v	292	SER	-	expression tag	UNP G3ECR2
v	293	GLY	-	expression tag	UNP G3ECR2
v	294	TRP	-	expression tag	UNP G3ECR2
v	295	SER	-	expression tag	UNP G3ECR2
v	296	HIS	-	expression tag	UNP G3ECR2
v	297	PRO	-	expression tag	UNP G3ECR2
v	298	GLN	-	expression tag	UNP G3ECR2
v	299	PHE	-	expression tag	UNP G3ECR2
v	300	GLU	-	expression tag	UNP G3ECR2
v	301	LYS	-	expression tag	UNP G3ECR2
v	302	ALA	-	expression tag	UNP G3ECR2
y	205	ALA	HIS	conflict	UNP G3ECR2
y	290	LEU	-	expression tag	UNP G3ECR2
y	291	GLU	-	expression tag	UNP G3ECR2
y	292	SER	-	expression tag	UNP G3ECR2
y	293	GLY	-	expression tag	UNP G3ECR2
y	294	TRP	-	expression tag	UNP G3ECR2
y	295	SER	-	expression tag	UNP G3ECR2
y	296	HIS	-	expression tag	UNP G3ECR2
y	297	PRO	-	expression tag	UNP G3ECR2
y	298	GLN	-	expression tag	UNP G3ECR2
y	299	PHE	-	expression tag	UNP G3ECR2
y	300	GLU	-	expression tag	UNP G3ECR2
y	301	LYS	-	expression tag	UNP G3ECR2
y	302	ALA	-	expression tag	UNP G3ECR2
z	205	ALA	HIS	conflict	UNP G3ECR2
z	290	LEU	-	expression tag	UNP G3ECR2
z	291	GLU	-	expression tag	UNP G3ECR2
z	292	SER	-	expression tag	UNP G3ECR2
z	293	GLY	-	expression tag	UNP G3ECR2
z	294	TRP	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

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Chain	Residue	Modelled	Actual	Comment	Reference
z	295	SER	-	expression tag	UNP G3ECR2
z	296	HIS	-	expression tag	UNP G3ECR2
z	297	PRO	-	expression tag	UNP G3ECR2
z	298	GLN	-	expression tag	UNP G3ECR2
z	299	PHE	-	expression tag	UNP G3ECR2
z	300	GLU	-	expression tag	UNP G3ECR2
z	301	LYS	-	expression tag	UNP G3ECR2
z	302	ALA	-	expression tag	UNP G3ECR2

- Molecule 3 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	96	Total 475	C 283	N 96	O 96	0	0
3	N	96	Total 475	C 283	N 96	O 96	0	0
3	Q	96	Total 475	C 283	N 96	O 96	0	0
3	T	96	Total 475	C 283	N 96	O 96	0	0
3	W	103	Total 510	C 304	N 103	O 103	0	0
3	X	103	Total 510	C 304	N 103	O 103	0	0
3	k	96	Total 475	C 283	N 96	O 96	0	0
3	n	96	Total 475	C 283	N 96	O 96	0	0
3	q	96	Total 475	C 283	N 96	O 96	0	0
3	t	96	Total 475	C 283	N 96	O 96	0	0
3	w	103	Total 510	C 304	N 103	O 103	0	0
3	x	103	Total 510	C 304	N 103	O 103	0	0

- Molecule 4 is a DNA chain called DNA (64-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	54	Total 1080	C 540	N 108	O 378	P 54	0	0

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- Molecule 5 is a DNA chain called DNA (64-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	54	Total	C	N	O	P	0	0
			1134	540	270	270	54		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	
6	F	1	Total	Ca	0
			1	1	
6	G	1	Total	Ca	0
			1	1	
6	H	1	Total	Ca	0
			1	1	
6	a	1	Total	Ca	0
			1	1	
6	b	1	Total	Ca	0
			1	1	
6	c	1	Total	Ca	0
			1	1	
6	d	1	Total	Ca	0
			1	1	
6	e	1	Total	Ca	0
			1	1	
6	f	1	Total	Ca	0
			1	1	
6	g	1	Total	Ca	0
			1	1	
6	h	1	Total	Ca	0
			1	1	

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3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: CRISPR-associated protein Csn2

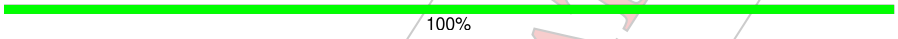
Chain A:





- Molecule 1: CRISPR-associated protein Csn2

Chain B:





- Molecule 1: CRISPR-associated protein Csn2

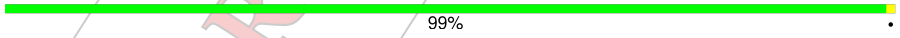
Chain C:

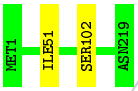




- Molecule 1: CRISPR-associated protein Csn2

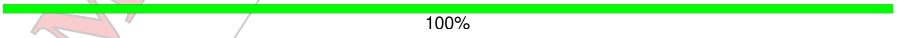
Chain D:





- Molecule 1: CRISPR-associated protein Csn2

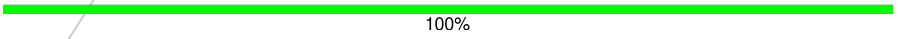
Chain E:





- Molecule 1: CRISPR-associated protein Csn2

Chain F:

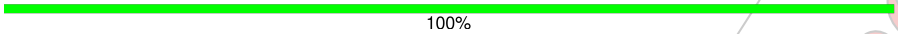


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- Molecule 1: CRISPR-associated protein Csn2

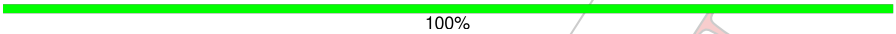
Chain G:





- Molecule 1: CRISPR-associated protein Csn2

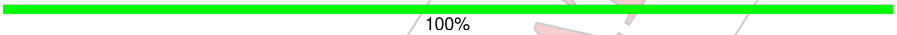
Chain H:





- Molecule 1: CRISPR-associated protein Csn2

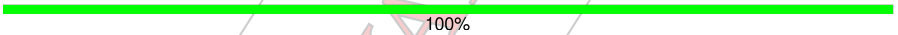
Chain a:





- Molecule 1: CRISPR-associated protein Csn2

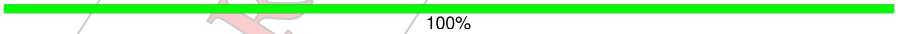
Chain b:





- Molecule 1: CRISPR-associated protein Csn2

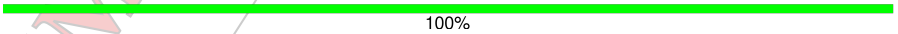
Chain c:





- Molecule 1: CRISPR-associated protein Csn2

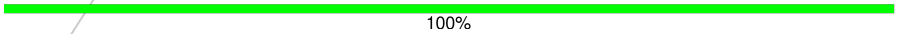
Chain d:





- Molecule 1: CRISPR-associated protein Csn2

Chain e:

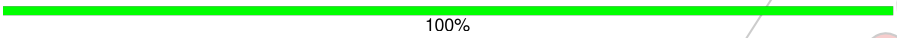


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• Molecule 1: CRISPR-associated protein Csn2

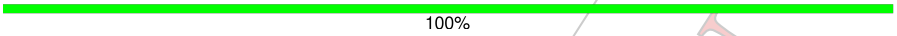
Chain f:





• Molecule 1: CRISPR-associated protein Csn2

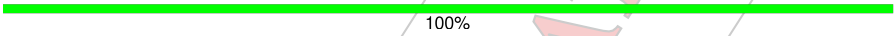
Chain g:





• Molecule 1: CRISPR-associated protein Csn2

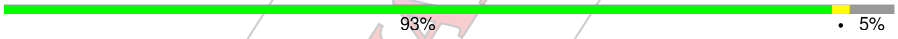
Chain h:

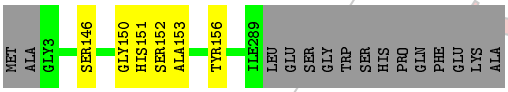




• Molecule 2: CRISPR-associated endonuclease Cas1

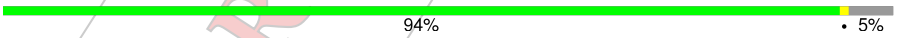
Chain I:

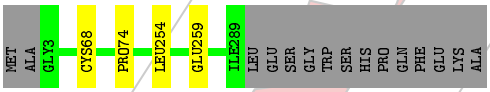




• Molecule 2: CRISPR-associated endonuclease Cas1

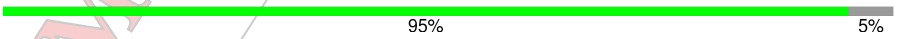
Chain J:





• Molecule 2: CRISPR-associated endonuclease Cas1

Chain L:



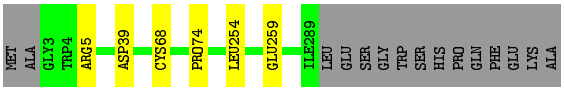


• Molecule 2: CRISPR-associated endonuclease Cas1

Chain M:

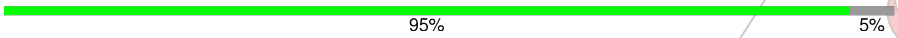


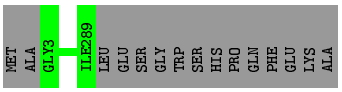
PRELIMINARY VALIDATION REPORT



- Molecule 2: CRISPR-associated endonuclease Cas1

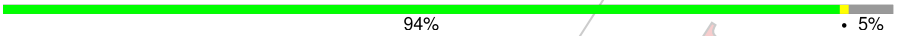
Chain O:

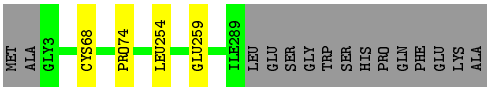




- Molecule 2: CRISPR-associated endonuclease Cas1

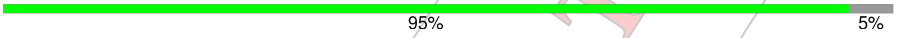
Chain P:

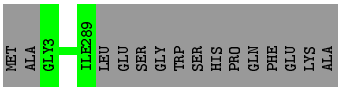




- Molecule 2: CRISPR-associated endonuclease Cas1

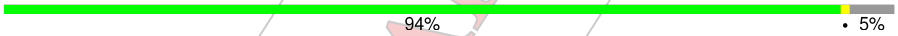
Chain R:

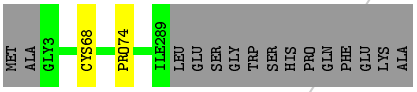




- Molecule 2: CRISPR-associated endonuclease Cas1

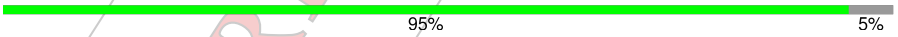
Chain S:

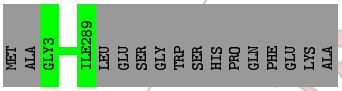




- Molecule 2: CRISPR-associated endonuclease Cas1

Chain U:

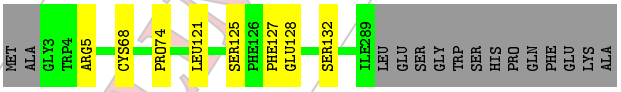




- Molecule 2: CRISPR-associated endonuclease Cas1

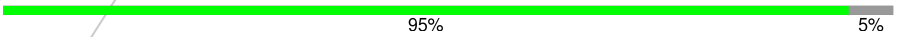
Chain V:



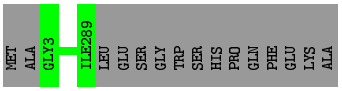


- Molecule 2: CRISPR-associated endonuclease Cas1

Chain Y:

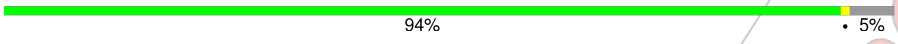


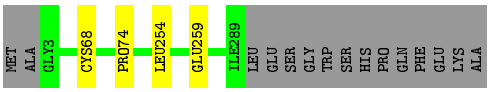
PRELIMINARY VALIDATION REPORT



- Molecule 2: CRISPR-associated endonuclease Cas1

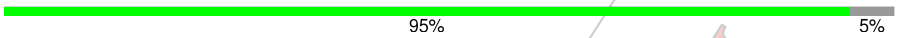
Chain Z:

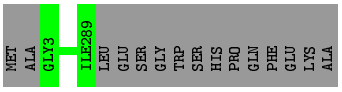




- Molecule 2: CRISPR-associated endonuclease Cas1

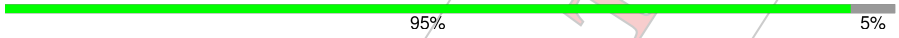
Chain i:

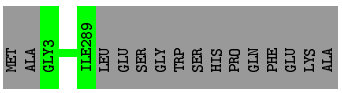




- Molecule 2: CRISPR-associated endonuclease Cas1

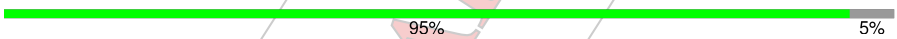
Chain j:

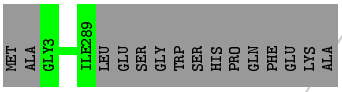




- Molecule 2: CRISPR-associated endonuclease Cas1

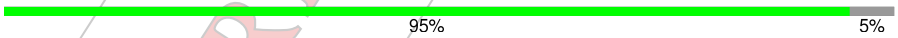
Chain l:

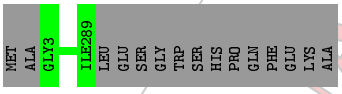




- Molecule 2: CRISPR-associated endonuclease Cas1

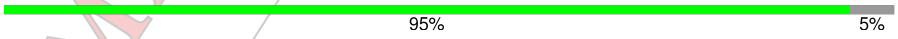
Chain m:

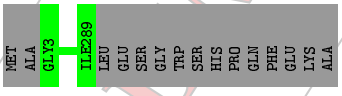




- Molecule 2: CRISPR-associated endonuclease Cas1

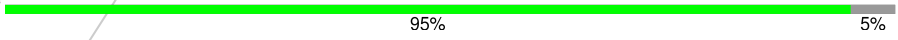
Chain o:



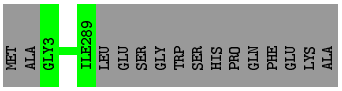


- Molecule 2: CRISPR-associated endonuclease Cas1

Chain p:

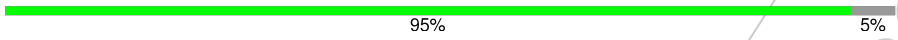


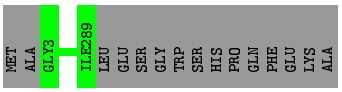
PRELIMINARY VALIDATION REPORT



- Molecule 2: CRISPR-associated endonuclease Cas1

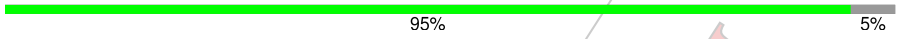
Chain r:

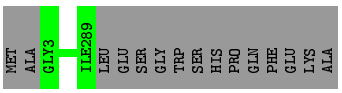




- Molecule 2: CRISPR-associated endonuclease Cas1

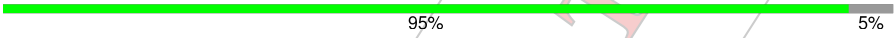
Chain s:

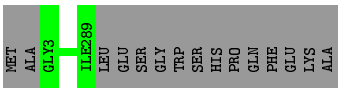




- Molecule 2: CRISPR-associated endonuclease Cas1

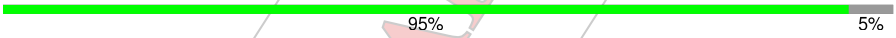
Chain u:

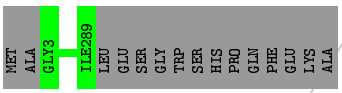




- Molecule 2: CRISPR-associated endonuclease Cas1

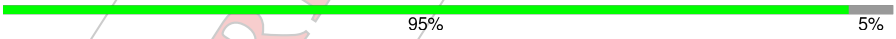
Chain v:

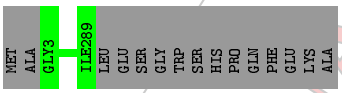




- Molecule 2: CRISPR-associated endonuclease Cas1

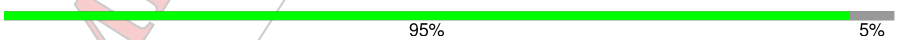
Chain y:

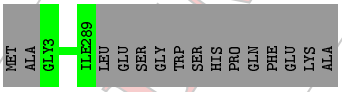




- Molecule 2: CRISPR-associated endonuclease Cas1

Chain z:



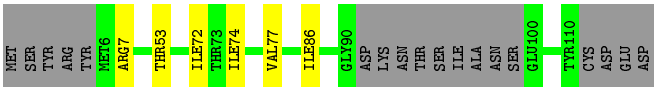


- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain K:



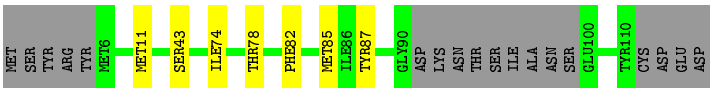
PRELIMINARY VALIDATION REPORT



- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain N:

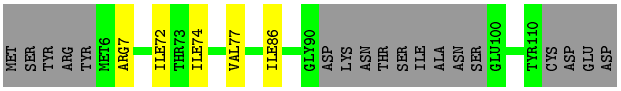




- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain Q:

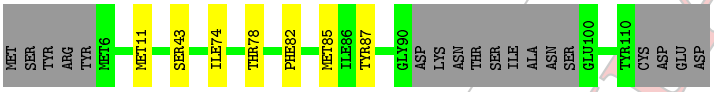




- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain T:

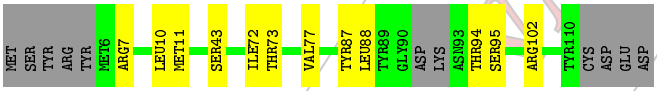




- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain W:

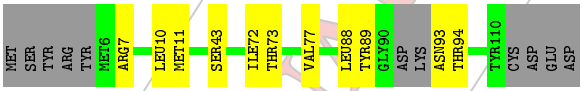




- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain X:

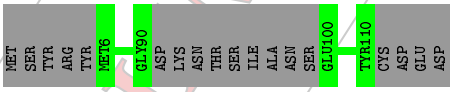




- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain k:



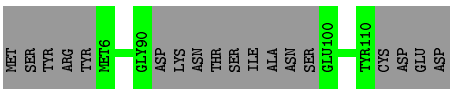


- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain n:



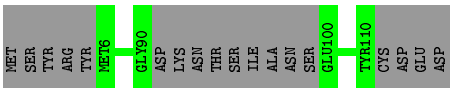
PRELIMINARY VALIDATION REPORT



- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain q:

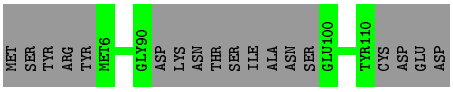




- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain t:

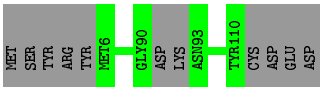




- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain w:

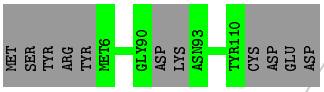




- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain x:





- Molecule 4: DNA (64-MER)

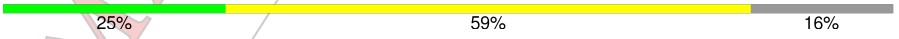
Chain 1:





- Molecule 5: DNA (64-MER)

Chain 2:





PRELIMINARY VALIDATION REPORT

4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

PRELIMINARY VALIDATION REPORT

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.23	0/1085	0.41	0/1515
1	B	0.23	0/1090	0.40	0/1522
1	C	0.23	0/1085	0.41	0/1515
1	D	0.23	0/1090	0.40	0/1522
1	E	0.23	0/1085	0.41	0/1515
1	F	0.23	0/1090	0.40	0/1522
1	G	0.23	0/1085	0.41	0/1515
1	H	0.23	0/1090	0.40	0/1522
1	a	0.23	0/1085	0.41	0/1515
1	b	0.23	0/1090	0.40	0/1522
1	c	0.23	0/1085	0.41	0/1515
1	d	0.23	0/1090	0.40	0/1522
1	e	0.23	0/1085	0.41	0/1515
1	f	0.23	0/1090	0.40	0/1522
1	g	0.23	0/1085	0.41	0/1515
1	h	0.23	0/1090	0.40	0/1522
2	I	0.24	0/1424	0.41	0/1986
2	J	0.23	0/1424	0.40	0/1986
2	L	0.23	0/1424	0.40	0/1986
2	M	0.23	0/1424	0.40	0/1986
2	O	0.23	0/1424	0.40	0/1986
2	P	0.23	0/1424	0.40	0/1986
2	R	0.23	0/1424	0.40	0/1986
2	S	0.23	0/1424	0.40	0/1986
2	U	0.23	0/1424	0.40	0/1986
2	V	0.25	0/1424	0.42	0/1986
2	Y	0.23	0/1424	0.40	0/1986
2	Z	0.23	0/1424	0.40	0/1986
2	i	0.24	0/1424	0.43	0/1986
2	j	0.23	0/1424	0.40	0/1986
2	l	0.23	0/1424	0.40	0/1986
2	m	0.23	0/1424	0.40	0/1986

PRELIMINARY VALIDATION REPORT

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
2	o	0.23	0/1424	0.40	0/1986
2	p	0.23	0/1424	0.40	0/1986
2	r	0.23	0/1424	0.40	0/1986
2	s	0.23	0/1424	0.40	0/1986
2	u	0.23	0/1424	0.40	0/1986
2	v	0.23	0/1424	0.40	0/1986
2	y	0.23	0/1424	0.40	0/1986
2	z	0.23	0/1424	0.40	0/1986
3	K	0.24	0/473	0.42	0/656
3	N	0.24	0/473	0.41	0/656
3	Q	0.24	0/473	0.42	0/656
3	T	0.24	0/473	0.41	0/656
3	W	0.23	0/508	0.42	0/705
3	X	0.23	0/508	0.42	0/705
3	k	0.24	0/473	0.42	0/656
3	n	0.24	0/473	0.41	0/656
3	q	0.24	0/473	0.42	0/656
3	t	0.24	0/473	0.43	0/656
3	w	0.23	0/508	0.42	0/705
3	x	0.23	0/508	0.42	0/705
4	1	0.60	0/1186	1.35	0/1828
5	2	0.57	0/1294	0.80	0/1990
All	All	0.26	0/59872	0.46	0/83846

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1086	0	450	0	0
1	B	1091	0	452	0	0
1	C	1086	0	450	0	0

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1091	0	452	1	0
1	E	1086	0	450	0	0
1	F	1091	0	452	0	0
1	G	1086	0	450	0	0
1	H	1091	0	452	0	0
1	a	1086	0	450	0	0
1	b	1091	0	452	0	0
1	c	1086	0	450	0	0
1	d	1091	0	452	0	0
1	e	1086	0	450	0	0
1	f	1091	0	452	0	0
1	g	1086	0	450	0	0
1	h	1091	0	452	0	0
2	I	1425	0	616	5	0
2	J	1425	0	616	2	0
2	L	1425	0	616	0	0
2	M	1425	0	616	3	0
2	O	1425	0	616	0	0
2	P	1425	0	616	2	0
2	R	1425	0	616	0	0
2	S	1425	0	616	1	0
2	U	1425	0	616	0	0
2	V	1425	0	616	7	0
2	Y	1425	0	616	0	0
2	Z	1425	0	616	2	0
2	i	1425	0	616	0	0
2	j	1425	0	616	0	0
2	l	1425	0	616	0	0
2	m	1425	0	616	0	0
2	o	1425	0	619	0	0
2	p	1425	0	616	0	0
2	r	1425	0	616	0	0
2	s	1425	0	616	0	0
2	u	1425	0	616	0	0
2	v	1425	0	616	0	0
2	y	1425	0	616	0	0
2	z	1425	0	616	0	0
3	K	475	0	211	5	0
3	N	475	0	211	5	0
3	Q	475	0	211	4	0
3	T	475	0	211	5	0
3	W	510	0	228	7	0

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	510	0	228	6	0
3	k	475	0	211	0	0
3	n	475	0	211	0	0
3	q	475	0	211	0	0
3	t	475	0	211	0	0
3	w	510	0	228	0	0
3	x	510	0	228	0	0
4	1	1080	0	650	2	0
5	2	1134	0	596	35	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	a	1	0	0	0	0
6	b	1	0	0	0	0
6	c	1	0	0	0	0
6	d	1	0	0	0	0
6	e	1	0	0	0	0
6	f	1	0	0	0	0
6	g	1	0	0	0	0
6	h	1	0	0	0	0
All	All	59686	0	25849	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:128:GLU:O	2:V:132:SER:CB	2.23	0.87
3:Q:74:ILE:O	3:T:85:MET:HA	1.85	0.77
3:K:74:ILE:O	3:N:85:MET:HA	1.85	0.76
3:K:72:ILE:O	3:N:87:TYR:HA	1.92	0.70
3:Q:72:ILE:O	3:T:87:TYR:HA	1.92	0.69
2:V:5:ARG:HA	3:W:102:ARG:O	1.95	0.67
5:2:12:DA:H2"	5:2:13:DA:C8	2.35	0.62
3:W:88:LEU:HA	3:W:94:THR:HA	1.91	0.61

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PRELIMINARY VALIDATION REPORT

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:48:DA:H2"	5:2:49:DA:C8	2.35	0.61
2:I:150:GLY:HA3	2:V:125:SER:CB	81.77	0.60
2:I:150:GLY:HA2	2:I:153:ALA:HB3	3.24	0.59
5:2:43:DA:H2"	5:2:44:DA:C8	2.37	0.59
5:2:13:DA:H2"	5:2:14:DA:C8	2.38	0.58
5:2:42:DA:H2"	5:2:43:DA:C8	2.38	0.58
5:2:47:DA:H2"	5:2:48:DA:C8	2.38	0.58
5:2:15:DA:H2"	5:2:16:DA:C8	2.39	0.57
5:2:19:DA:H2"	5:2:20:DA:C8	2.40	0.57
5:2:39:DA:H2"	5:2:40:DA:C8	2.40	0.57
3:X:89:TYR:O	3:X:93:ASN:N	2.37	0.57
2:I:146:SER:O	2:V:127:PHE:HA	89.09	0.56
5:2:18:DA:H2"	5:2:19:DA:C8	2.41	0.55
5:2:41:DA:H2"	5:2:42:DA:C8	2.42	0.55
5:2:40:DA:H2"	5:2:41:DA:C8	2.42	0.54
5:2:16:DA:H2"	5:2:17:DA:C8	2.43	0.54
5:2:20:DA:H2"	5:2:21:DA:C8	2.44	0.53
5:2:5:DA:H2"	5:2:6:DA:C8	2.43	0.53
5:2:44:DA:H2"	5:2:45:DA:C8	2.43	0.52
5:2:38:DA:H2"	5:2:39:DA:C8	2.45	0.52
5:2:54:DA:H2"	5:2:55:DA:C8	2.44	0.52
3:X:11:MET:O	3:X:72:ILE:HA	2.17	0.52
3:N:78:THR:O	3:N:82:PHE:N	2.41	0.51
5:2:17:DA:H2"	5:2:18:DA:C8	2.46	0.51
3:K:86:ILE:O	3:N:74:ILE:CB	2.59	0.51
3:Q:86:ILE:O	3:T:74:ILE:CB	2.59	0.51
2:I:151:HIS:H	2:V:127:PHE:CB	83.51	0.50
5:2:14:DA:H2"	5:2:15:DA:C8	2.45	0.50
3:T:78:THR:O	3:T:82:PHE:N	2.41	0.50
2:M:5:ARG:O	2:M:39:ASP:N	2.29	0.50
5:2:10:DA:H2"	5:2:11:DA:C8	2.47	0.50
5:2:9:DA:H2"	5:2:10:DA:C8	2.49	0.48
1:D:102:SER:CB	3:K:53:THR:HA	2.44	0.48
3:Q:7:ARG:CB	3:Q:77:VAL:O	2.62	0.47
3:K:7:ARG:CB	3:K:77:VAL:O	2.62	0.47
3:W:7:ARG:CB	3:W:77:VAL:O	2.63	0.47
3:X:7:ARG:CB	3:X:77:VAL:O	2.63	0.47
5:2:46:DA:H2"	5:2:47:DA:C8	2.49	0.46
3:X:10:LEU:HA	3:X:73:THR:O	2.19	0.46
5:2:24:DA:H2"	5:2:25:DA:C8	2.50	0.46
5:2:57:DA:H2"	5:2:58:DA:C8	2.51	0.46

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PRELIMINARY VALIDATION REPORT

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:68:CYS:HA	2:J:74:PRO:HA	1.99	0.45
2:P:68:CYS:HA	2:P:74:PRO:HA	1.99	0.45
2:S:68:CYS:HA	2:S:74:PRO:HA	1.99	0.45
3:X:11:MET:HA	3:X:43:SER:O	2.16	0.45
2:V:121:LEU:O	2:V:125:SER:N	2.50	0.44
2:M:68:CYS:HA	2:M:74:PRO:HA	1.99	0.44
2:V:68:CYS:HA	2:V:74:PRO:HA	1.99	0.44
3:W:11:MET:HA	3:W:43:SER:O	2.18	0.44
2:Z:68:CYS:HA	2:Z:74:PRO:HA	1.99	0.44
5:2:21:DA:H2"	5:2:22:DA:C8	2.53	0.43
3:N:11:MET:HA	3:N:43:SER:O	2.19	0.43
3:W:87:TYR:H	3:W:95:SER:CB	2.34	0.43
5:2:56:DA:H2"	5:2:57:DA:C8	2.54	0.43
3:T:11:MET:HA	3:T:43:SER:O	2.19	0.42
5:2:49:DA:H2"	5:2:50:DA:C8	2.54	0.42
2:I:152:SER:O	2:I:156:TYR:CB	3.22	0.42
3:W:11:MET:O	3:W:72:ILE:HA	2.21	0.42
5:2:11:DA:H2"	5:2:12:DA:C8	2.55	0.42
5:2:45:DA:H2"	5:2:46:DA:C8	2.55	0.42
5:2:4:DA:H2"	5:2:5:DA:C8	2.56	0.41
3:X:88:LEU:HA	3:X:94:THR:HA	2.25	0.41
4:1:16:DT:O4	5:2:48:DA:N6	2.53	0.41
3:W:10:LEU:HA	3:W:73:THR:O	2.21	0.41
4:1:45:DT:O4	5:2:19:DA:N6	2.54	0.41
2:M:254:LEU:HA	2:M:259:GLU:HA	2.04	0.40
2:P:254:LEU:HA	2:P:259:GLU:HA	2.04	0.40
2:Z:254:LEU:HA	2:Z:259:GLU:HA	2.04	0.40
5:2:12:DA:H2"	5:2:13:DA:H8	1.84	0.40
5:2:23:DA:H2"	5:2:24:DA:C8	2.57	0.40
2:J:254:LEU:HA	2:J:259:GLU:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

PRELIMINARY VALIDATION REPORT

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	B	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	C	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	D	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	E	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	F	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	G	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	H	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	a	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	b	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	c	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	d	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	e	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	f	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	g	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	h	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
2	I	285/302 (94%)	276 (97%)	9 (3%)	0	100	100
2	J	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	L	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	M	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	O	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	P	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	R	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	S	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	U	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	V	285/302 (94%)	276 (97%)	9 (3%)	0	100	100
2	Y	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	Z	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	i	285/302 (94%)	275 (96%)	10 (4%)	0	100	100
2	j	285/302 (94%)	280 (98%)	5 (2%)	0	100	100

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	l	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	m	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	o	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	p	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	r	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	s	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	u	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	v	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	y	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	z	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
3	K	92/114 (81%)	89 (97%)	3 (3%)	0	100	100
3	N	92/114 (81%)	89 (97%)	3 (3%)	0	100	100
3	Q	92/114 (81%)	90 (98%)	2 (2%)	0	100	100
3	T	92/114 (81%)	89 (97%)	3 (3%)	0	100	100
3	W	99/114 (87%)	97 (98%)	2 (2%)	0	100	100
3	X	99/114 (87%)	97 (98%)	2 (2%)	0	100	100
3	k	92/114 (81%)	90 (98%)	2 (2%)	0	100	100
3	n	92/114 (81%)	89 (97%)	3 (3%)	0	100	100
3	q	92/114 (81%)	90 (98%)	2 (2%)	0	100	100
3	t	92/114 (81%)	89 (97%)	3 (3%)	0	100	100
3	w	99/114 (87%)	98 (99%)	1 (1%)	0	100	100
3	x	99/114 (87%)	97 (98%)	2 (2%)	0	100	100
All	All	11436/12120 (94%)	11157 (98%)	271 (2%)	8 (0%)	56	53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	ILE
1	D	51	ILE
1	F	51	ILE
1	H	51	ILE
1	b	51	ILE
1	d	51	ILE
1	f	51	ILE

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Res	Type
1	h	51	ILE

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

PRELIMINARY VALIDATION REPORT

Mol	Chain	Number of breaks
5	2	1
4	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	27:DT	O3'	38:DT	P	30.67
1	2	27:DA	O3'	38:DA	P	29.94

PRELIMINARY VALIDATION REPORT

PDB Validation Report filament
Click here to access/download;PDB Validation Report;D_1292101122_val-report-full_filament.pdf

Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Mar 28, 2019 – 01:44 pm GMT

Deposition ID : D_1292101122
PDB ID : *(not yet assigned)*

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

PRELIMINARY VALIDATION REPORT

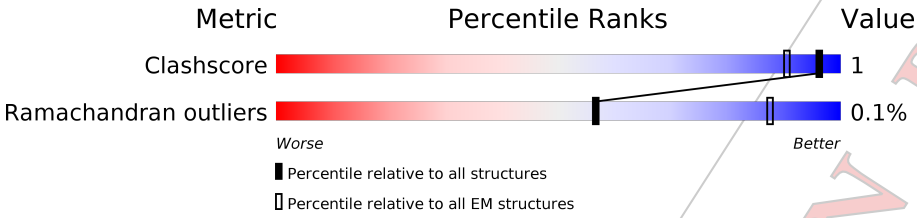
MolProbity	:	4.02b-467
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	219	100%
1	B	219	100%
1	C	219	100%
1	D	219	100%
1	E	219	100%
1	F	219	100%
1	G	219	99%
1	H	219	100%
1	a	219	100%
1	b	219	100%
1	c	219	100%

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Length	Quality of chain
1	d	219	100%
1	e	219	100%
1	f	219	100%
1	g	219	100%
1	h	219	100%
2	I	302	95% 5%
2	J	302	95% 5%
2	L	302	95% 5%
2	M	302	94% • 5%
2	O	302	95% 5%
2	P	302	94% • 5%
2	R	302	95% 5%
2	S	302	95% 5%
2	U	302	95% 5%
2	V	302	94% • 5%
2	Y	302	95% 5%
2	Z	302	94% • 5%
2	i	302	95% 5%
2	j	302	95% 5%
2	l	302	95% 5%
2	m	302	95% 5%
2	o	302	95% 5%
2	p	302	95% 5%
2	r	302	95% 5%
2	s	302	95% 5%

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Length	Quality of chain
2	u	302	95% 5%
2	v	302	95% 5%
2	y	302	95% 5%
2	z	302	95% 5%
3	K	114	10% 90%
3	N	114	10% 90%
3	Q	114	10% 90%
3	T	114	10% 90%
3	W	114	10% 90%
3	X	114	10% 90%
3	k	114	10% 90%
3	n	114	10% 90%
3	q	114	10% 90%
3	t	114	10% 90%
3	w	114	10% 90%
3	x	114	10% 90%
4	1	66	100%
5	2	66	100%

PRELIMINARY VALIDATION REPORT

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 54986 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CRISPR-associated protein Csn2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	218	Total 1086	C 650	N 218	O 218	0	0
1	B	219	Total 1091	C 653	N 219	O 219	0	0
1	C	218	Total 1086	C 650	N 218	O 218	0	0
1	D	219	Total 1091	C 653	N 219	O 219	0	0
1	E	218	Total 1086	C 650	N 218	O 218	0	0
1	F	219	Total 1091	C 653	N 219	O 219	0	0
1	G	218	Total 1086	C 650	N 218	O 218	0	0
1	H	219	Total 1091	C 653	N 219	O 219	0	0
1	a	218	Total 1086	C 650	N 218	O 218	0	0
1	b	219	Total 1091	C 653	N 219	O 219	0	0
1	c	218	Total 1086	C 650	N 218	O 218	0	0
1	d	219	Total 1091	C 653	N 219	O 219	0	0
1	e	218	Total 1086	C 650	N 218	O 218	0	0
1	f	219	Total 1091	C 653	N 219	O 219	0	0
1	g	218	Total 1086	C 650	N 218	O 218	0	0
1	h	219	Total 1091	C 653	N 219	O 219	0	0

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas1.

PRELIMINARY VALIDATION REPORT

Mol	Chain	Residues	Atoms				AltConf	Trace
2	I	287	Total	C	N	O	0	0
			1425	851	287	287		
2	J	287	Total	C	N	O	0	0
			1425	851	287	287		
2	L	287	Total	C	N	O	0	0
			1425	851	287	287		
2	M	287	Total	C	N	O	0	0
			1425	851	287	287		
2	O	287	Total	C	N	O	0	0
			1425	851	287	287		
2	P	287	Total	C	N	O	0	0
			1425	851	287	287		
2	R	287	Total	C	N	O	0	0
			1425	851	287	287		
2	S	287	Total	C	N	O	0	0
			1425	851	287	287		
2	U	287	Total	C	N	O	0	0
			1425	851	287	287		
2	V	287	Total	C	N	O	0	0
			1425	851	287	287		
2	Y	287	Total	C	N	O	0	0
			1425	851	287	287		
2	Z	287	Total	C	N	O	0	0
			1425	851	287	287		
2	i	287	Total	C	N	O	0	0
			1425	851	287	287		
2	j	287	Total	C	N	O	0	0
			1425	851	287	287		
2	l	287	Total	C	N	O	0	0
			1425	851	287	287		
2	m	287	Total	C	N	O	0	0
			1425	851	287	287		
2	o	287	Total	C	N	O	0	0
			1425	851	287	287		
2	p	287	Total	C	N	O	0	0
			1425	851	287	287		
2	r	287	Total	C	N	O	0	0
			1425	851	287	287		
2	s	287	Total	C	N	O	0	0
			1425	851	287	287		
2	u	287	Total	C	N	O	0	0
			1425	851	287	287		
2	v	287	Total	C	N	O	0	0
			1425	851	287	287		

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Residues	Atoms				AltConf	Trace
2	y	287	Total	C	N	O	0	0
			1425	851	287	287		
2	z	287	Total	C	N	O	0	0
			1425	851	287	287		

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	205	ALA	HIS	conflict	UNP G3ECR2
I	290	LEU	-	expression tag	UNP G3ECR2
I	291	GLU	-	expression tag	UNP G3ECR2
I	292	SER	-	expression tag	UNP G3ECR2
I	293	GLY	-	expression tag	UNP G3ECR2
I	294	TRP	-	expression tag	UNP G3ECR2
I	295	SER	-	expression tag	UNP G3ECR2
I	296	HIS	-	expression tag	UNP G3ECR2
I	297	PRO	-	expression tag	UNP G3ECR2
I	298	GLN	-	expression tag	UNP G3ECR2
I	299	PHE	-	expression tag	UNP G3ECR2
I	300	GLU	-	expression tag	UNP G3ECR2
I	301	LYS	-	expression tag	UNP G3ECR2
I	302	ALA	-	expression tag	UNP G3ECR2
J	205	ALA	HIS	conflict	UNP G3ECR2
J	290	LEU	-	expression tag	UNP G3ECR2
J	291	GLU	-	expression tag	UNP G3ECR2
J	292	SER	-	expression tag	UNP G3ECR2
J	293	GLY	-	expression tag	UNP G3ECR2
J	294	TRP	-	expression tag	UNP G3ECR2
J	295	SER	-	expression tag	UNP G3ECR2
J	296	HIS	-	expression tag	UNP G3ECR2
J	297	PRO	-	expression tag	UNP G3ECR2
J	298	GLN	-	expression tag	UNP G3ECR2
J	299	PHE	-	expression tag	UNP G3ECR2
J	300	GLU	-	expression tag	UNP G3ECR2
J	301	LYS	-	expression tag	UNP G3ECR2
J	302	ALA	-	expression tag	UNP G3ECR2
L	205	ALA	HIS	conflict	UNP G3ECR2
L	290	LEU	-	expression tag	UNP G3ECR2
L	291	GLU	-	expression tag	UNP G3ECR2
L	292	SER	-	expression tag	UNP G3ECR2
L	293	GLY	-	expression tag	UNP G3ECR2
L	294	TRP	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

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Chain	Residue	Modelled	Actual	Comment	Reference
L	295	SER	-	expression tag	UNP G3ECR2
L	296	HIS	-	expression tag	UNP G3ECR2
L	297	PRO	-	expression tag	UNP G3ECR2
L	298	GLN	-	expression tag	UNP G3ECR2
L	299	PHE	-	expression tag	UNP G3ECR2
L	300	GLU	-	expression tag	UNP G3ECR2
L	301	LYS	-	expression tag	UNP G3ECR2
L	302	ALA	-	expression tag	UNP G3ECR2
M	205	ALA	HIS	conflict	UNP G3ECR2
M	290	LEU	-	expression tag	UNP G3ECR2
M	291	GLU	-	expression tag	UNP G3ECR2
M	292	SER	-	expression tag	UNP G3ECR2
M	293	GLY	-	expression tag	UNP G3ECR2
M	294	TRP	-	expression tag	UNP G3ECR2
M	295	SER	-	expression tag	UNP G3ECR2
M	296	HIS	-	expression tag	UNP G3ECR2
M	297	PRO	-	expression tag	UNP G3ECR2
M	298	GLN	-	expression tag	UNP G3ECR2
M	299	PHE	-	expression tag	UNP G3ECR2
M	300	GLU	-	expression tag	UNP G3ECR2
M	301	LYS	-	expression tag	UNP G3ECR2
M	302	ALA	-	expression tag	UNP G3ECR2
O	205	ALA	HIS	conflict	UNP G3ECR2
O	290	LEU	-	expression tag	UNP G3ECR2
O	291	GLU	-	expression tag	UNP G3ECR2
O	292	SER	-	expression tag	UNP G3ECR2
O	293	GLY	-	expression tag	UNP G3ECR2
O	294	TRP	-	expression tag	UNP G3ECR2
O	295	SER	-	expression tag	UNP G3ECR2
O	296	HIS	-	expression tag	UNP G3ECR2
O	297	PRO	-	expression tag	UNP G3ECR2
O	298	GLN	-	expression tag	UNP G3ECR2
O	299	PHE	-	expression tag	UNP G3ECR2
O	300	GLU	-	expression tag	UNP G3ECR2
O	301	LYS	-	expression tag	UNP G3ECR2
O	302	ALA	-	expression tag	UNP G3ECR2
P	205	ALA	HIS	conflict	UNP G3ECR2
P	290	LEU	-	expression tag	UNP G3ECR2
P	291	GLU	-	expression tag	UNP G3ECR2
P	292	SER	-	expression tag	UNP G3ECR2
P	293	GLY	-	expression tag	UNP G3ECR2
P	294	TRP	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

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Chain	Residue	Modelled	Actual	Comment	Reference
P	295	SER	-	expression tag	UNP G3ECR2
P	296	HIS	-	expression tag	UNP G3ECR2
P	297	PRO	-	expression tag	UNP G3ECR2
P	298	GLN	-	expression tag	UNP G3ECR2
P	299	PHE	-	expression tag	UNP G3ECR2
P	300	GLU	-	expression tag	UNP G3ECR2
P	301	LYS	-	expression tag	UNP G3ECR2
P	302	ALA	-	expression tag	UNP G3ECR2
R	205	ALA	HIS	conflict	UNP G3ECR2
R	290	LEU	-	expression tag	UNP G3ECR2
R	291	GLU	-	expression tag	UNP G3ECR2
R	292	SER	-	expression tag	UNP G3ECR2
R	293	GLY	-	expression tag	UNP G3ECR2
R	294	TRP	-	expression tag	UNP G3ECR2
R	295	SER	-	expression tag	UNP G3ECR2
R	296	HIS	-	expression tag	UNP G3ECR2
R	297	PRO	-	expression tag	UNP G3ECR2
R	298	GLN	-	expression tag	UNP G3ECR2
R	299	PHE	-	expression tag	UNP G3ECR2
R	300	GLU	-	expression tag	UNP G3ECR2
R	301	LYS	-	expression tag	UNP G3ECR2
R	302	ALA	-	expression tag	UNP G3ECR2
S	205	ALA	HIS	conflict	UNP G3ECR2
S	290	LEU	-	expression tag	UNP G3ECR2
S	291	GLU	-	expression tag	UNP G3ECR2
S	292	SER	-	expression tag	UNP G3ECR2
S	293	GLY	-	expression tag	UNP G3ECR2
S	294	TRP	-	expression tag	UNP G3ECR2
S	295	SER	-	expression tag	UNP G3ECR2
S	296	HIS	-	expression tag	UNP G3ECR2
S	297	PRO	-	expression tag	UNP G3ECR2
S	298	GLN	-	expression tag	UNP G3ECR2
S	299	PHE	-	expression tag	UNP G3ECR2
S	300	GLU	-	expression tag	UNP G3ECR2
S	301	LYS	-	expression tag	UNP G3ECR2
S	302	ALA	-	expression tag	UNP G3ECR2
U	205	ALA	HIS	conflict	UNP G3ECR2
U	290	LEU	-	expression tag	UNP G3ECR2
U	291	GLU	-	expression tag	UNP G3ECR2
U	292	SER	-	expression tag	UNP G3ECR2
U	293	GLY	-	expression tag	UNP G3ECR2
U	294	TRP	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

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Chain	Residue	Modelled	Actual	Comment	Reference
U	295	SER	-	expression tag	UNP G3ECR2
U	296	HIS	-	expression tag	UNP G3ECR2
U	297	PRO	-	expression tag	UNP G3ECR2
U	298	GLN	-	expression tag	UNP G3ECR2
U	299	PHE	-	expression tag	UNP G3ECR2
U	300	GLU	-	expression tag	UNP G3ECR2
U	301	LYS	-	expression tag	UNP G3ECR2
U	302	ALA	-	expression tag	UNP G3ECR2
V	205	ALA	HIS	conflict	UNP G3ECR2
V	290	LEU	-	expression tag	UNP G3ECR2
V	291	GLU	-	expression tag	UNP G3ECR2
V	292	SER	-	expression tag	UNP G3ECR2
V	293	GLY	-	expression tag	UNP G3ECR2
V	294	TRP	-	expression tag	UNP G3ECR2
V	295	SER	-	expression tag	UNP G3ECR2
V	296	HIS	-	expression tag	UNP G3ECR2
V	297	PRO	-	expression tag	UNP G3ECR2
V	298	GLN	-	expression tag	UNP G3ECR2
V	299	PHE	-	expression tag	UNP G3ECR2
V	300	GLU	-	expression tag	UNP G3ECR2
V	301	LYS	-	expression tag	UNP G3ECR2
V	302	ALA	-	expression tag	UNP G3ECR2
Y	205	ALA	HIS	conflict	UNP G3ECR2
Y	290	LEU	-	expression tag	UNP G3ECR2
Y	291	GLU	-	expression tag	UNP G3ECR2
Y	292	SER	-	expression tag	UNP G3ECR2
Y	293	GLY	-	expression tag	UNP G3ECR2
Y	294	TRP	-	expression tag	UNP G3ECR2
Y	295	SER	-	expression tag	UNP G3ECR2
Y	296	HIS	-	expression tag	UNP G3ECR2
Y	297	PRO	-	expression tag	UNP G3ECR2
Y	298	GLN	-	expression tag	UNP G3ECR2
Y	299	PHE	-	expression tag	UNP G3ECR2
Y	300	GLU	-	expression tag	UNP G3ECR2
Y	301	LYS	-	expression tag	UNP G3ECR2
Y	302	ALA	-	expression tag	UNP G3ECR2
Z	205	ALA	HIS	conflict	UNP G3ECR2
Z	290	LEU	-	expression tag	UNP G3ECR2
Z	291	GLU	-	expression tag	UNP G3ECR2
Z	292	SER	-	expression tag	UNP G3ECR2
Z	293	GLY	-	expression tag	UNP G3ECR2
Z	294	TRP	-	expression tag	UNP G3ECR2

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	295	SER	-	expression tag	UNP G3ECR2
Z	296	HIS	-	expression tag	UNP G3ECR2
Z	297	PRO	-	expression tag	UNP G3ECR2
Z	298	GLN	-	expression tag	UNP G3ECR2
Z	299	PHE	-	expression tag	UNP G3ECR2
Z	300	GLU	-	expression tag	UNP G3ECR2
Z	301	LYS	-	expression tag	UNP G3ECR2
Z	302	ALA	-	expression tag	UNP G3ECR2
i	205	ALA	HIS	conflict	UNP G3ECR2
i	290	LEU	-	expression tag	UNP G3ECR2
i	291	GLU	-	expression tag	UNP G3ECR2
i	292	SER	-	expression tag	UNP G3ECR2
i	293	GLY	-	expression tag	UNP G3ECR2
i	294	TRP	-	expression tag	UNP G3ECR2
i	295	SER	-	expression tag	UNP G3ECR2
i	296	HIS	-	expression tag	UNP G3ECR2
i	297	PRO	-	expression tag	UNP G3ECR2
i	298	GLN	-	expression tag	UNP G3ECR2
i	299	PHE	-	expression tag	UNP G3ECR2
i	300	GLU	-	expression tag	UNP G3ECR2
i	301	LYS	-	expression tag	UNP G3ECR2
i	302	ALA	-	expression tag	UNP G3ECR2
j	205	ALA	HIS	conflict	UNP G3ECR2
j	290	LEU	-	expression tag	UNP G3ECR2
j	291	GLU	-	expression tag	UNP G3ECR2
j	292	SER	-	expression tag	UNP G3ECR2
j	293	GLY	-	expression tag	UNP G3ECR2
j	294	TRP	-	expression tag	UNP G3ECR2
j	295	SER	-	expression tag	UNP G3ECR2
j	296	HIS	-	expression tag	UNP G3ECR2
j	297	PRO	-	expression tag	UNP G3ECR2
j	298	GLN	-	expression tag	UNP G3ECR2
j	299	PHE	-	expression tag	UNP G3ECR2
j	300	GLU	-	expression tag	UNP G3ECR2
j	301	LYS	-	expression tag	UNP G3ECR2
j	302	ALA	-	expression tag	UNP G3ECR2
l	205	ALA	HIS	conflict	UNP G3ECR2
l	290	LEU	-	expression tag	UNP G3ECR2
l	291	GLU	-	expression tag	UNP G3ECR2
l	292	SER	-	expression tag	UNP G3ECR2
l	293	GLY	-	expression tag	UNP G3ECR2
l	294	TRP	-	expression tag	UNP G3ECR2

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Chain	Residue	Modelled	Actual	Comment	Reference
l	295	SER	-	expression tag	UNP G3ECR2
l	296	HIS	-	expression tag	UNP G3ECR2
l	297	PRO	-	expression tag	UNP G3ECR2
l	298	GLN	-	expression tag	UNP G3ECR2
l	299	PHE	-	expression tag	UNP G3ECR2
l	300	GLU	-	expression tag	UNP G3ECR2
l	301	LYS	-	expression tag	UNP G3ECR2
l	302	ALA	-	expression tag	UNP G3ECR2
m	205	ALA	HIS	conflict	UNP G3ECR2
m	290	LEU	-	expression tag	UNP G3ECR2
m	291	GLU	-	expression tag	UNP G3ECR2
m	292	SER	-	expression tag	UNP G3ECR2
m	293	GLY	-	expression tag	UNP G3ECR2
m	294	TRP	-	expression tag	UNP G3ECR2
m	295	SER	-	expression tag	UNP G3ECR2
m	296	HIS	-	expression tag	UNP G3ECR2
m	297	PRO	-	expression tag	UNP G3ECR2
m	298	GLN	-	expression tag	UNP G3ECR2
m	299	PHE	-	expression tag	UNP G3ECR2
m	300	GLU	-	expression tag	UNP G3ECR2
m	301	LYS	-	expression tag	UNP G3ECR2
m	302	ALA	-	expression tag	UNP G3ECR2
o	205	ALA	HIS	conflict	UNP G3ECR2
o	290	LEU	-	expression tag	UNP G3ECR2
o	291	GLU	-	expression tag	UNP G3ECR2
o	292	SER	-	expression tag	UNP G3ECR2
o	293	GLY	-	expression tag	UNP G3ECR2
o	294	TRP	-	expression tag	UNP G3ECR2
o	295	SER	-	expression tag	UNP G3ECR2
o	296	HIS	-	expression tag	UNP G3ECR2
o	297	PRO	-	expression tag	UNP G3ECR2
o	298	GLN	-	expression tag	UNP G3ECR2
o	299	PHE	-	expression tag	UNP G3ECR2
o	300	GLU	-	expression tag	UNP G3ECR2
o	301	LYS	-	expression tag	UNP G3ECR2
o	302	ALA	-	expression tag	UNP G3ECR2
p	205	ALA	HIS	conflict	UNP G3ECR2
p	290	LEU	-	expression tag	UNP G3ECR2
p	291	GLU	-	expression tag	UNP G3ECR2
p	292	SER	-	expression tag	UNP G3ECR2
p	293	GLY	-	expression tag	UNP G3ECR2
p	294	TRP	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
p	295	SER	-	expression tag	UNP G3ECR2
p	296	HIS	-	expression tag	UNP G3ECR2
p	297	PRO	-	expression tag	UNP G3ECR2
p	298	GLN	-	expression tag	UNP G3ECR2
p	299	PHE	-	expression tag	UNP G3ECR2
p	300	GLU	-	expression tag	UNP G3ECR2
p	301	LYS	-	expression tag	UNP G3ECR2
p	302	ALA	-	expression tag	UNP G3ECR2
r	205	ALA	HIS	conflict	UNP G3ECR2
r	290	LEU	-	expression tag	UNP G3ECR2
r	291	GLU	-	expression tag	UNP G3ECR2
r	292	SER	-	expression tag	UNP G3ECR2
r	293	GLY	-	expression tag	UNP G3ECR2
r	294	TRP	-	expression tag	UNP G3ECR2
r	295	SER	-	expression tag	UNP G3ECR2
r	296	HIS	-	expression tag	UNP G3ECR2
r	297	PRO	-	expression tag	UNP G3ECR2
r	298	GLN	-	expression tag	UNP G3ECR2
r	299	PHE	-	expression tag	UNP G3ECR2
r	300	GLU	-	expression tag	UNP G3ECR2
r	301	LYS	-	expression tag	UNP G3ECR2
r	302	ALA	-	expression tag	UNP G3ECR2
s	205	ALA	HIS	conflict	UNP G3ECR2
s	290	LEU	-	expression tag	UNP G3ECR2
s	291	GLU	-	expression tag	UNP G3ECR2
s	292	SER	-	expression tag	UNP G3ECR2
s	293	GLY	-	expression tag	UNP G3ECR2
s	294	TRP	-	expression tag	UNP G3ECR2
s	295	SER	-	expression tag	UNP G3ECR2
s	296	HIS	-	expression tag	UNP G3ECR2
s	297	PRO	-	expression tag	UNP G3ECR2
s	298	GLN	-	expression tag	UNP G3ECR2
s	299	PHE	-	expression tag	UNP G3ECR2
s	300	GLU	-	expression tag	UNP G3ECR2
s	301	LYS	-	expression tag	UNP G3ECR2
s	302	ALA	-	expression tag	UNP G3ECR2
u	205	ALA	HIS	conflict	UNP G3ECR2
u	290	LEU	-	expression tag	UNP G3ECR2
u	291	GLU	-	expression tag	UNP G3ECR2
u	292	SER	-	expression tag	UNP G3ECR2
u	293	GLY	-	expression tag	UNP G3ECR2
u	294	TRP	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
u	295	SER	-	expression tag	UNP G3ECR2
u	296	HIS	-	expression tag	UNP G3ECR2
u	297	PRO	-	expression tag	UNP G3ECR2
u	298	GLN	-	expression tag	UNP G3ECR2
u	299	PHE	-	expression tag	UNP G3ECR2
u	300	GLU	-	expression tag	UNP G3ECR2
u	301	LYS	-	expression tag	UNP G3ECR2
u	302	ALA	-	expression tag	UNP G3ECR2
v	205	ALA	HIS	conflict	UNP G3ECR2
v	290	LEU	-	expression tag	UNP G3ECR2
v	291	GLU	-	expression tag	UNP G3ECR2
v	292	SER	-	expression tag	UNP G3ECR2
v	293	GLY	-	expression tag	UNP G3ECR2
v	294	TRP	-	expression tag	UNP G3ECR2
v	295	SER	-	expression tag	UNP G3ECR2
v	296	HIS	-	expression tag	UNP G3ECR2
v	297	PRO	-	expression tag	UNP G3ECR2
v	298	GLN	-	expression tag	UNP G3ECR2
v	299	PHE	-	expression tag	UNP G3ECR2
v	300	GLU	-	expression tag	UNP G3ECR2
v	301	LYS	-	expression tag	UNP G3ECR2
v	302	ALA	-	expression tag	UNP G3ECR2
y	205	ALA	HIS	conflict	UNP G3ECR2
y	290	LEU	-	expression tag	UNP G3ECR2
y	291	GLU	-	expression tag	UNP G3ECR2
y	292	SER	-	expression tag	UNP G3ECR2
y	293	GLY	-	expression tag	UNP G3ECR2
y	294	TRP	-	expression tag	UNP G3ECR2
y	295	SER	-	expression tag	UNP G3ECR2
y	296	HIS	-	expression tag	UNP G3ECR2
y	297	PRO	-	expression tag	UNP G3ECR2
y	298	GLN	-	expression tag	UNP G3ECR2
y	299	PHE	-	expression tag	UNP G3ECR2
y	300	GLU	-	expression tag	UNP G3ECR2
y	301	LYS	-	expression tag	UNP G3ECR2
y	302	ALA	-	expression tag	UNP G3ECR2
z	205	ALA	HIS	conflict	UNP G3ECR2
z	290	LEU	-	expression tag	UNP G3ECR2
z	291	GLU	-	expression tag	UNP G3ECR2
z	292	SER	-	expression tag	UNP G3ECR2
z	293	GLY	-	expression tag	UNP G3ECR2
z	294	TRP	-	expression tag	UNP G3ECR2

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PRELIMINARY VALIDATION REPORT

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
z	295	SER	-	expression tag	UNP G3ECR2
z	296	HIS	-	expression tag	UNP G3ECR2
z	297	PRO	-	expression tag	UNP G3ECR2
z	298	GLN	-	expression tag	UNP G3ECR2
z	299	PHE	-	expression tag	UNP G3ECR2
z	300	GLU	-	expression tag	UNP G3ECR2
z	301	LYS	-	expression tag	UNP G3ECR2
z	302	ALA	-	expression tag	UNP G3ECR2

- Molecule 3 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	K	11	Total	C	N	O	0	0
			54	32	11	11		
3	N	11	Total	C	N	O	0	0
			54	32	11	11		
3	Q	11	Total	C	N	O	0	0
			54	32	11	11		
3	T	11	Total	C	N	O	0	0
			54	32	11	11		
3	W	11	Total	C	N	O	0	0
			54	32	11	11		
3	X	11	Total	C	N	O	0	0
			54	32	11	11		
3	k	11	Total	C	N	O	0	0
			54	32	11	11		
3	n	11	Total	C	N	O	0	0
			54	32	11	11		
3	q	11	Total	C	N	O	0	0
			54	32	11	11		
3	t	11	Total	C	N	O	0	0
			54	32	11	11		
3	w	11	Total	C	N	O	0	0
			54	32	11	11		
3	x	11	Total	C	N	O	0	0
			54	32	11	11		

- Molecule 4 is a DNA chain called DNA (66-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	66	Total	C	N	O	P	0	0
			1320	660	132	462	66		

PRELIMINARY VALIDATION REPORT

- Molecule 5 is a DNA chain called DNA (66-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	2	66	Total	C	N	O	P	0	0
			1386	660	330	330	66		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	
6	E	1	Total	Ca	0
			1	1	
6	F	1	Total	Ca	0
			1	1	
6	G	1	Total	Ca	0
			1	1	
6	H	1	Total	Ca	0
			1	1	
6	a	1	Total	Ca	0
			1	1	
6	b	1	Total	Ca	0
			1	1	
6	c	1	Total	Ca	0
			1	1	
6	d	1	Total	Ca	0
			1	1	
6	e	1	Total	Ca	0
			1	1	
6	f	1	Total	Ca	0
			1	1	
6	g	1	Total	Ca	0
			1	1	
6	h	1	Total	Ca	0
			1	1	

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3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: CRISPR-associated protein Csn2

Chain A:





- Molecule 1: CRISPR-associated protein Csn2

Chain B:





- Molecule 1: CRISPR-associated protein Csn2

Chain C:





- Molecule 1: CRISPR-associated protein Csn2

Chain D:





- Molecule 1: CRISPR-associated protein Csn2

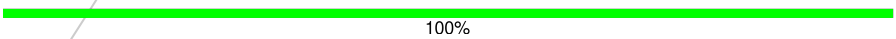
Chain E:





- Molecule 1: CRISPR-associated protein Csn2

Chain F:

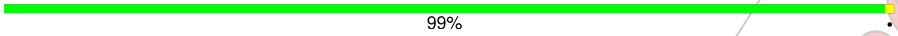


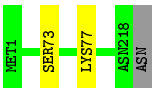
PRELIMINARY VALIDATION REPORT



- Molecule 1: CRISPR-associated protein Csn2

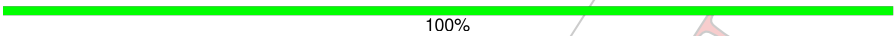
Chain G:





- Molecule 1: CRISPR-associated protein Csn2

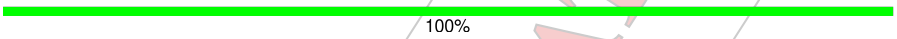
Chain H:





- Molecule 1: CRISPR-associated protein Csn2

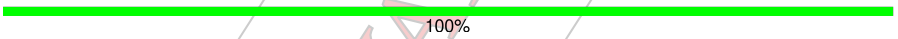
Chain a:





- Molecule 1: CRISPR-associated protein Csn2

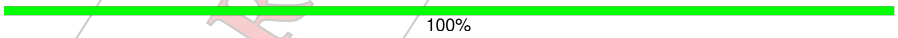
Chain b:





- Molecule 1: CRISPR-associated protein Csn2

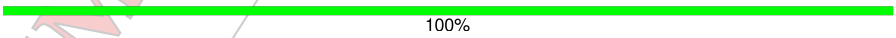
Chain c:





- Molecule 1: CRISPR-associated protein Csn2

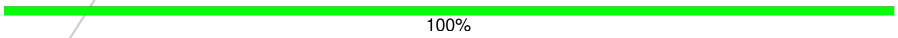
Chain d:





- Molecule 1: CRISPR-associated protein Csn2

Chain e:

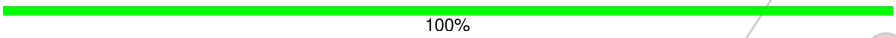


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- Molecule 1: CRISPR-associated protein Csn2

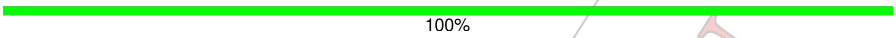
Chain f:





- Molecule 1: CRISPR-associated protein Csn2

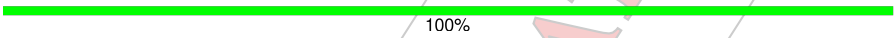
Chain g:





- Molecule 1: CRISPR-associated protein Csn2

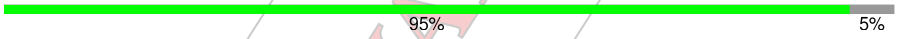
Chain h:

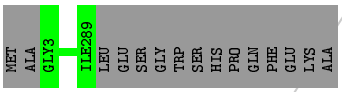




- Molecule 2: CRISPR-associated endonuclease Cas1

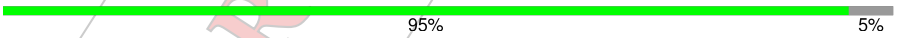
Chain I:

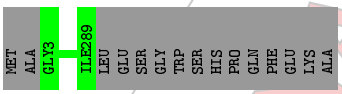




- Molecule 2: CRISPR-associated endonuclease Cas1

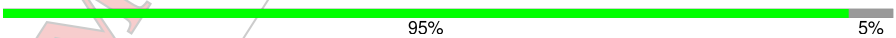
Chain J:

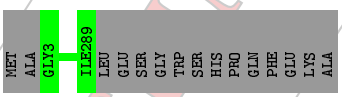




- Molecule 2: CRISPR-associated endonuclease Cas1

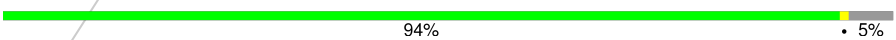
Chain L:



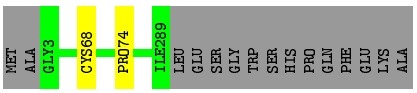


- Molecule 2: CRISPR-associated endonuclease Cas1

Chain M:

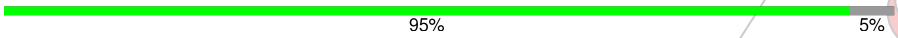


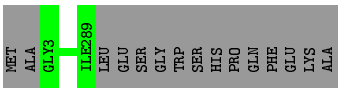
PRELIMINARY VALIDATION REPORT



- Molecule 2: CRISPR-associated endonuclease Cas1

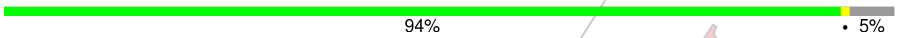
Chain O:

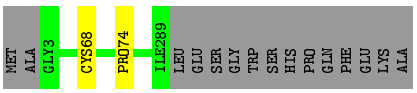




- Molecule 2: CRISPR-associated endonuclease Cas1

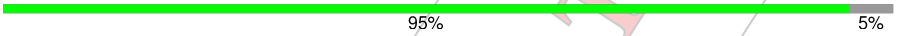
Chain P:

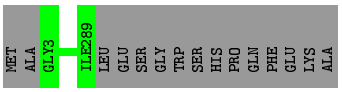




- Molecule 2: CRISPR-associated endonuclease Cas1

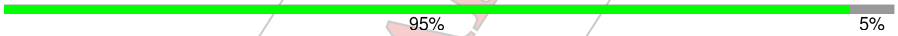
Chain R:

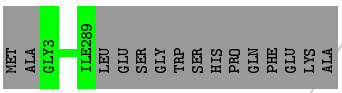




- Molecule 2: CRISPR-associated endonuclease Cas1

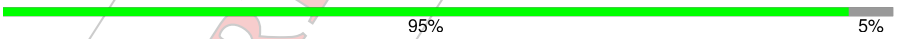
Chain S:

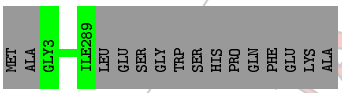




- Molecule 2: CRISPR-associated endonuclease Cas1

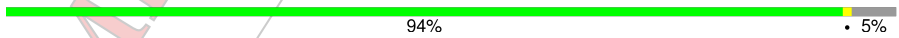
Chain U:

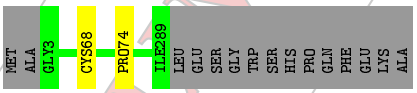




- Molecule 2: CRISPR-associated endonuclease Cas1

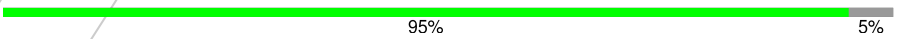
Chain V:



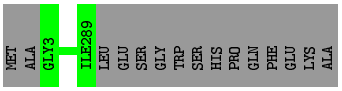


- Molecule 2: CRISPR-associated endonuclease Cas1

Chain Y:

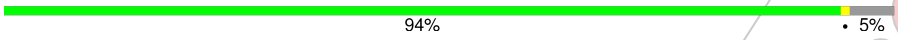


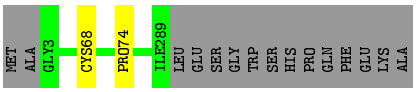
PRELIMINARY VALIDATION REPORT



- Molecule 2: CRISPR-associated endonuclease Cas1

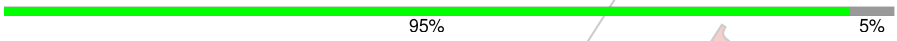
Chain Z:

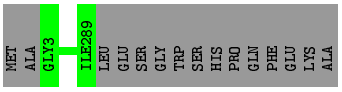




- Molecule 2: CRISPR-associated endonuclease Cas1

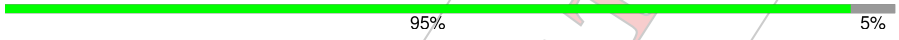
Chain i:

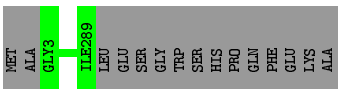




- Molecule 2: CRISPR-associated endonuclease Cas1

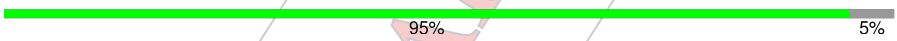
Chain j:

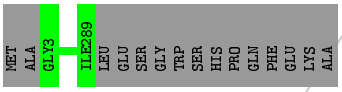




- Molecule 2: CRISPR-associated endonuclease Cas1

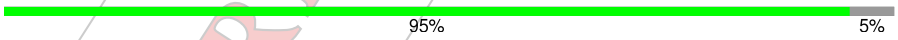
Chain l:

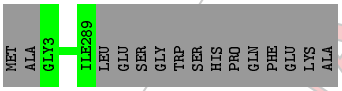




- Molecule 2: CRISPR-associated endonuclease Cas1

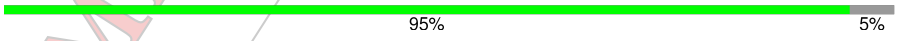
Chain m:

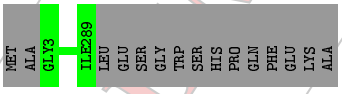




- Molecule 2: CRISPR-associated endonuclease Cas1

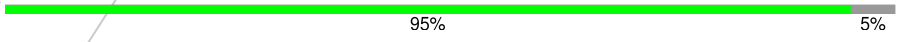
Chain o:



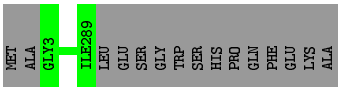


- Molecule 2: CRISPR-associated endonuclease Cas1

Chain p:

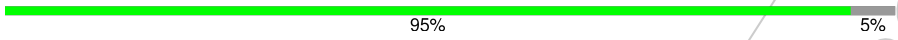


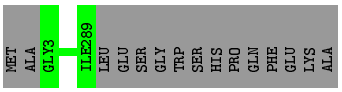
PRELIMINARY VALIDATION REPORT



- Molecule 2: CRISPR-associated endonuclease Cas1

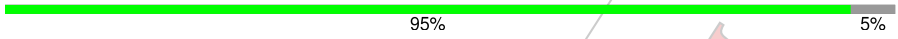
Chain r:

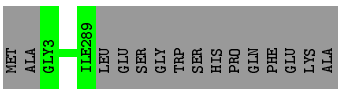




- Molecule 2: CRISPR-associated endonuclease Cas1

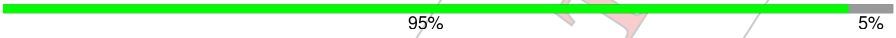
Chain s:

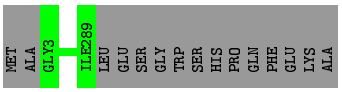




- Molecule 2: CRISPR-associated endonuclease Cas1

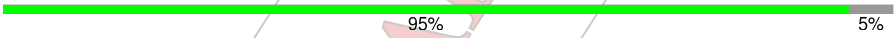
Chain u:

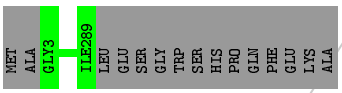




- Molecule 2: CRISPR-associated endonuclease Cas1

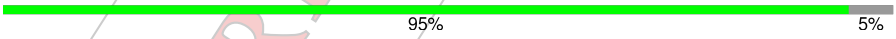
Chain v:

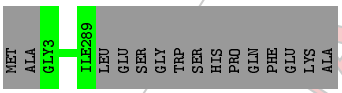




- Molecule 2: CRISPR-associated endonuclease Cas1

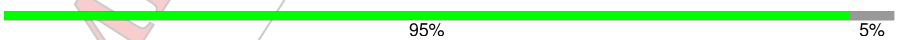
Chain y:

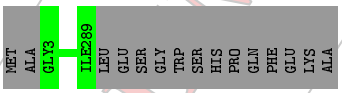




- Molecule 2: CRISPR-associated endonuclease Cas1

Chain z:



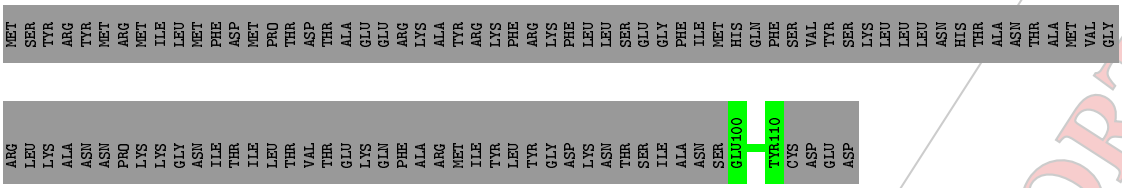


- Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain K:



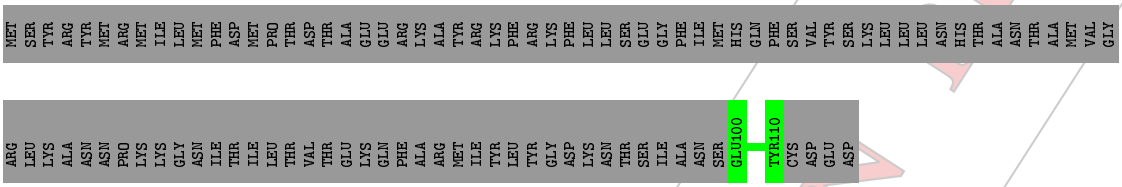
PRELIMINARY VALIDATION REPORT



• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain N:

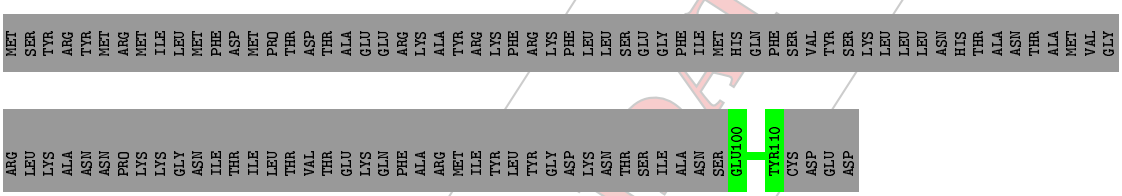




• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain Q:

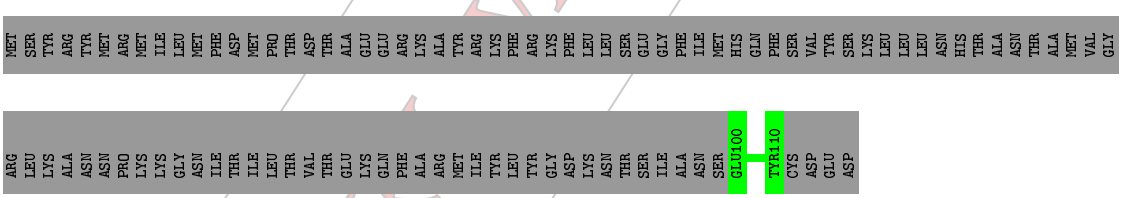




• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain T:

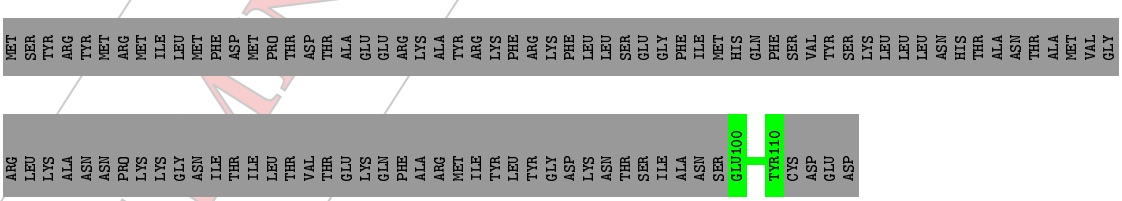




• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain W:



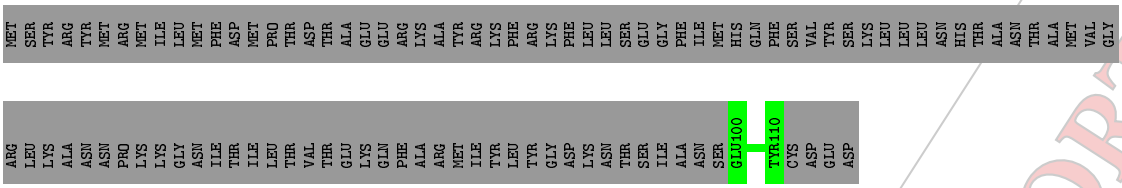


• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain X:



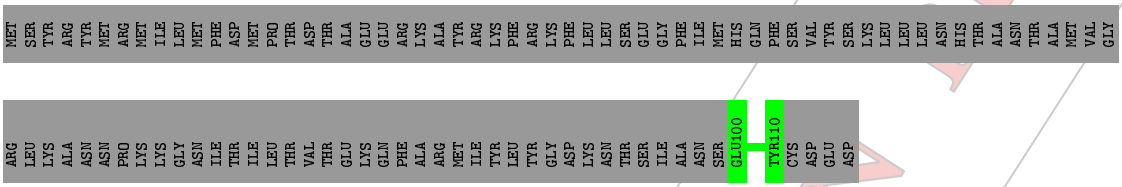
PRELIMINARY VALIDATION REPORT



• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain k:

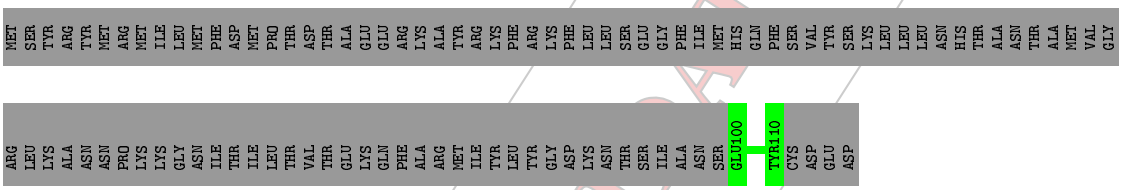




• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain n:

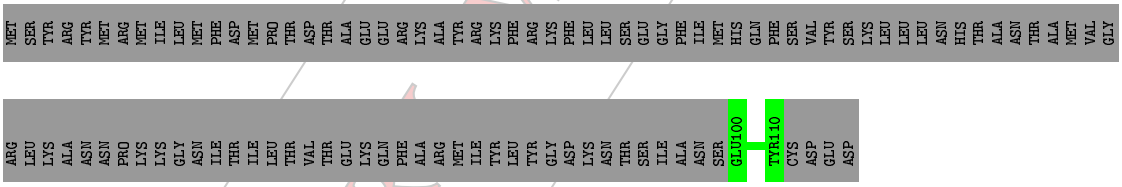




• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain q:

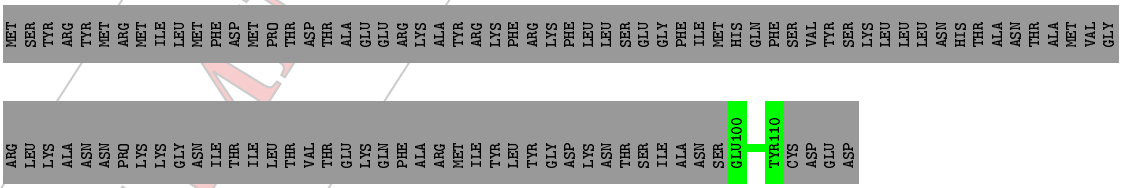




• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain t:



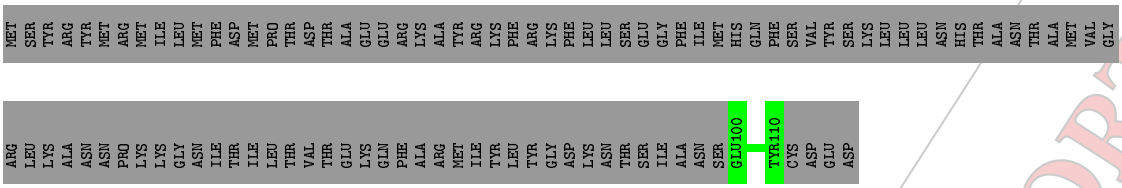


• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain w:

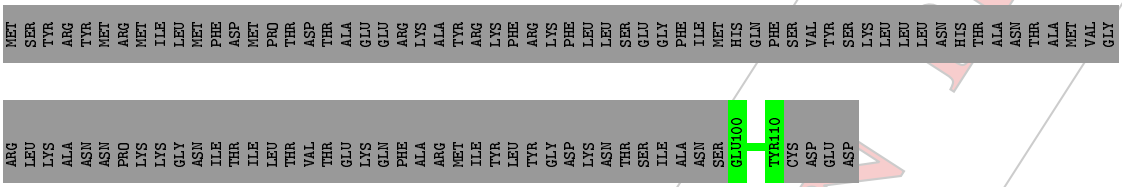


PRELIMINARY VALIDATION REPORT



• Molecule 3: CRISPR-associated endoribonuclease Cas2

Chain x: 10% 90%



• Molecule 4: DNA (66-MER)

Chain 1: 100%

There are no outlier residues recorded for this chain.

• Molecule 5: DNA (66-MER)

Chain 2: 100%



PRELIMINARY VALIDATION REPORT

4 Experimental information (i)

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

PRELIMINARY VALIDATION REPORT

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.23	0/1085	0.41	0/1515
1	B	0.23	0/1090	0.40	0/1522
1	C	0.23	0/1085	0.41	0/1515
1	D	0.23	0/1090	0.40	0/1522
1	E	0.23	0/1085	0.41	0/1515
1	F	0.23	0/1090	0.40	0/1522
1	G	0.25	0/1085	0.42	0/1515
1	H	0.23	0/1090	0.40	0/1522
1	a	0.23	0/1085	0.41	0/1515
1	b	0.23	0/1090	0.40	0/1522
1	c	0.23	0/1085	0.41	0/1515
1	d	0.23	0/1090	0.40	0/1522
1	e	0.23	0/1085	0.41	0/1515
1	f	0.23	0/1090	0.40	0/1522
1	g	0.23	0/1085	0.41	0/1515
1	h	0.23	0/1090	0.40	0/1522
2	I	0.23	0/1424	0.40	0/1986
2	J	0.23	0/1424	0.40	0/1986
2	L	0.23	0/1424	0.40	0/1986
2	M	0.23	0/1424	0.40	0/1986
2	O	0.23	0/1424	0.40	0/1986
2	P	0.23	0/1424	0.40	0/1986
2	R	0.23	0/1424	0.40	0/1986
2	S	0.23	0/1424	0.40	0/1986
2	U	0.23	0/1424	0.40	0/1986
2	V	0.23	0/1424	0.40	0/1986
2	Y	0.23	0/1424	0.40	0/1986
2	Z	0.23	0/1424	0.40	0/1986
2	i	0.23	0/1424	0.40	0/1986
2	j	0.23	0/1424	0.40	0/1986
2	l	0.23	0/1424	0.40	0/1986
2	m	0.23	0/1424	0.40	0/1986

PRELIMINARY VALIDATION REPORT

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
2	o	0.23	0/1424	0.40	0/1986
2	p	0.23	0/1424	0.40	0/1986
2	r	0.23	0/1424	0.40	0/1986
2	s	0.23	0/1424	0.40	0/1986
2	u	0.23	0/1424	0.40	0/1986
2	v	0.23	0/1424	0.40	0/1986
2	y	0.23	0/1424	0.40	0/1986
2	z	0.23	0/1424	0.40	0/1986
3	K	0.25	0/53	0.45	0/72
3	N	0.24	0/53	0.45	0/72
3	Q	0.24	0/53	0.45	0/72
3	T	0.24	0/53	0.45	0/72
3	W	0.24	0/53	0.45	0/72
3	X	0.25	0/53	0.45	0/72
3	k	0.25	0/53	0.45	0/72
3	n	0.24	0/53	0.45	0/72
3	q	0.24	0/53	0.45	0/72
3	t	0.24	0/53	0.45	0/72
3	w	0.25	0/53	0.45	0/72
3	x	0.24	0/53	0.45	0/72
4	1	0.69	0/1451	1.36	0/2240
5	2	0.57	0/1583	0.84	0/2438
All	All	0.27	0/55246	0.48	0/77502

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1086	0	450	0	0
1	B	1091	0	452	0	0
1	C	1086	0	450	0	0

Continued on next page...

PRELIMINARY VALIDATION REPORT

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1091	0	452	0	0
1	E	1086	0	450	0	0
1	F	1091	0	452	0	0
1	G	1086	0	450	1	0
1	H	1091	0	452	0	0
1	a	1086	0	450	0	0
1	b	1091	0	452	0	0
1	c	1086	0	450	0	0
1	d	1091	0	452	0	0
1	e	1086	0	450	0	0
1	f	1091	0	452	0	0
1	g	1086	0	450	0	0
1	h	1091	0	452	0	0
2	I	1425	0	616	0	0
2	J	1425	0	616	0	0
2	L	1425	0	616	0	0
2	M	1425	0	616	1	0
2	O	1425	0	616	0	0
2	P	1425	0	616	1	0
2	R	1425	0	616	0	0
2	S	1425	0	616	0	0
2	U	1425	0	616	0	0
2	V	1425	0	616	1	0
2	Y	1425	0	616	0	0
2	Z	1425	0	616	1	0
2	i	1425	0	616	0	0
2	j	1425	0	616	0	0
2	l	1425	0	616	0	0
2	m	1425	0	616	0	0
2	o	1425	0	616	0	0
2	p	1425	0	616	0	0
2	r	1425	0	616	0	0
2	s	1425	0	616	0	0
2	u	1425	0	616	0	0
2	v	1425	0	616	0	0
2	y	1425	0	616	0	0
2	z	1425	0	616	0	0
3	K	54	0	22	0	0
3	N	54	0	22	0	0
3	Q	54	0	22	0	0
3	T	54	0	22	0	0
3	W	54	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	X	54	0	22	0	0
3	k	54	0	22	0	0
3	n	54	0	22	0	0
3	q	54	0	22	0	0
3	t	54	0	22	0	0
3	w	54	0	22	0	0
3	x	54	0	22	0	0
4	1	1320	0	793	0	0
5	2	1386	0	727	65	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	a	1	0	0	0	0
6	b	1	0	0	0	0
6	c	1	0	0	0	0
6	d	1	0	0	0	0
6	e	1	0	0	0	0
6	f	1	0	0	0	0
6	g	1	0	0	0	0
6	h	1	0	0	0	0
All	All	54986	0	23784	70	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:35:DA:H2"	5:2:36:DA:C8	2.36	0.61
5:2:15:DA:H2"	5:2:16:DA:C8	2.37	0.60
5:2:34:DA:H2"	5:2:35:DA:C8	2.37	0.59
5:2:44:DA:H2"	5:2:45:DA:C8	2.38	0.59
5:2:45:DA:H2"	5:2:46:DA:C8	2.39	0.58
5:2:27:DA:H2"	5:2:28:DA:C8	2.38	0.57
5:2:24:DA:H2"	5:2:25:DA:C8	2.39	0.57
5:2:25:DA:H2"	5:2:26:DA:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:32:DA:H2"	5:2:33:DA:C8	2.40	0.56
5:2:33:DA:H2"	5:2:34:DA:C8	2.39	0.56
5:2:11:DA:H2"	5:2:12:DA:C8	2.40	0.56
5:2:28:DA:H2"	5:2:29:DA:C8	2.39	0.56
5:2:43:DA:H2"	5:2:44:DA:C8	2.41	0.56
5:2:56:DA:H2"	5:2:57:DA:C8	2.41	0.56
5:2:8:DA:H2"	5:2:9:DA:C8	2.41	0.56
5:2:52:DA:H2"	5:2:53:DA:C8	2.40	0.56
5:2:7:DA:H2"	5:2:8:DA:C8	2.41	0.56
5:2:9:DA:H2"	5:2:10:DA:C8	2.41	0.56
5:2:57:DA:H2"	5:2:58:DA:C8	2.41	0.56
5:2:61:DA:H2"	5:2:62:DA:C8	2.41	0.56
5:2:51:DA:H2"	5:2:52:DA:C8	2.41	0.56
5:2:38:DA:H2"	5:2:39:DA:C8	2.40	0.55
5:2:10:DA:H2"	5:2:11:DA:C8	2.42	0.55
5:2:39:DA:H2"	5:2:40:DA:C8	2.41	0.55
5:2:49:DA:H2"	5:2:50:DA:C8	2.41	0.55
5:2:29:DA:H2"	5:2:30:DA:C8	2.41	0.55
5:2:40:DA:H2"	5:2:41:DA:C8	2.41	0.55
5:2:18:DA:H2"	5:2:19:DA:C8	2.41	0.55
5:2:21:DA:H2"	5:2:22:DA:C8	2.41	0.55
5:2:31:DA:H2"	5:2:32:DA:C8	2.41	0.55
5:2:50:DA:H2"	5:2:51:DA:C8	2.42	0.55
5:2:53:DA:H2"	5:2:54:DA:C8	2.41	0.55
5:2:60:DA:H2"	5:2:61:DA:C8	2.41	0.55
5:2:59:DA:H2"	5:2:60:DA:C8	2.42	0.55
5:2:22:DA:H2"	5:2:23:DA:C8	2.41	0.54
5:2:23:DA:H2"	5:2:24:DA:C8	2.42	0.54
5:2:5:DA:H2"	5:2:6:DA:C8	2.42	0.54
5:2:4:DA:H2"	5:2:5:DA:C8	2.42	0.54
5:2:58:DA:H2"	5:2:59:DA:C8	2.42	0.54
5:2:54:DA:H2"	5:2:55:DA:C8	2.42	0.54
5:2:55:DA:H2"	5:2:56:DA:C8	2.43	0.54
5:2:62:DA:H2"	5:2:63:DA:C8	2.42	0.54
5:2:6:DA:H2"	5:2:7:DA:C8	2.42	0.54
5:2:3:DA:H2"	5:2:4:DA:C8	2.43	0.54
5:2:19:DA:H2"	5:2:20:DA:C8	2.43	0.54
5:2:30:DA:H2"	5:2:31:DA:C8	2.42	0.54
5:2:20:DA:H2"	5:2:21:DA:C8	2.43	0.54
5:2:12:DA:H2"	5:2:13:DA:C8	2.43	0.54
5:2:48:DA:H2"	5:2:49:DA:C8	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:2:41:DA:H2"	5:2:42:DA:C8	2.43	0.53
5:2:42:DA:H2"	5:2:43:DA:C8	2.44	0.52
5:2:2:DA:H2"	5:2:3:DA:C8	2.45	0.52
5:2:37:DA:H2"	5:2:38:DA:C8	2.45	0.51
5:2:46:DA:H2"	5:2:47:DA:C8	2.45	0.51
5:2:13:DA:H2"	5:2:14:DA:C8	2.46	0.51
5:2:36:DA:H2"	5:2:37:DA:C8	2.47	0.50
5:2:14:DA:H2"	5:2:15:DA:C8	2.46	0.50
5:2:47:DA:H2"	5:2:48:DA:C8	2.47	0.50
5:2:63:DA:H2"	5:2:64:DA:C8	2.47	0.49
5:2:26:DA:H2"	5:2:27:DA:C8	2.48	0.49
5:2:65:DA:H2"	5:2:66:DA:C8	2.49	0.47
5:2:1:DA:H2"	5:2:2:DA:C8	2.50	0.47
5:2:64:DA:H2"	5:2:65:DA:C8	2.50	0.46
5:2:16:DA:H2"	5:2:17:DA:C8	2.50	0.46
5:2:17:DA:H2"	5:2:18:DA:C8	2.54	0.43
1:G:73:SER:O	1:G:77:LYS:CB	2.69	0.41
2:M:68:CYS:HA	2:M:74:PRO:HA	2.03	0.41
2:Z:68:CYS:HA	2:Z:74:PRO:HA	2.03	0.40
2:V:68:CYS:HA	2:V:74:PRO:HA	2.03	0.40
2:P:68:CYS:HA	2:P:74:PRO:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	216/219 (99%)	209 (97%)	7 (3%)	0	100 100
1	B	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31 31
1	C	216/219 (99%)	209 (97%)	7 (3%)	0	100 100
1	D	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31 31

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	F	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	G	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	H	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	a	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	b	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	c	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	d	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	e	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	f	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
1	g	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
1	h	217/219 (99%)	212 (98%)	4 (2%)	1 (0%)	31	31
2	I	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	J	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
2	L	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	M	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	O	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	P	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	R	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	S	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	U	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	V	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
2	Y	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	Z	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	i	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	j	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	l	285/302 (94%)	277 (97%)	8 (3%)	0	100	100
2	m	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	o	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	p	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
2	r	285/302 (94%)	278 (98%)	7 (2%)	0	100	100

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PRELIMINARY VALIDATION REPORT

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	s	285/302 (94%)	280 (98%)	5 (2%)	0	100	100
2	u	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	v	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
2	y	285/302 (94%)	278 (98%)	7 (2%)	0	100	100
2	z	285/302 (94%)	279 (98%)	6 (2%)	0	100	100
3	K	9/114 (8%)	9 (100%)	0	0	100	100
3	N	9/114 (8%)	9 (100%)	0	0	100	100
3	Q	9/114 (8%)	9 (100%)	0	0	100	100
3	T	9/114 (8%)	9 (100%)	0	0	100	100
3	W	9/114 (8%)	9 (100%)	0	0	100	100
3	X	9/114 (8%)	9 (100%)	0	0	100	100
3	k	9/114 (8%)	9 (100%)	0	0	100	100
3	n	9/114 (8%)	9 (100%)	0	0	100	100
3	q	9/114 (8%)	9 (100%)	0	0	100	100
3	t	9/114 (8%)	9 (100%)	0	0	100	100
3	w	9/114 (8%)	9 (100%)	0	0	100	100
3	x	9/114 (8%)	9 (100%)	0	0	100	100
All	All	10412/12120 (86%)	10162 (98%)	242 (2%)	8 (0%)	56	53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	51	ILE
1	D	51	ILE
1	F	51	ILE
1	H	51	ILE
1	b	51	ILE
1	d	51	ILE
1	f	51	ILE
1	h	51	ILE

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

PRELIMINARY VALIDATION REPORT

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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