



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 10:13 AM UTC

PDB ID : 9Q85 / pdb_00009q85
EMDB ID : EMD-52886
Title : PAM-bound Cas9-Cas1-Cas2-Csn2 supercomplex in the locked conformation, Streptococcus thermophilus DGCC 7710 CRISPR3 system
Authors : Sasnauskas, G.; Gaizauskaite, U.; Tamulaitiene, G.
Deposited on : 2025-02-22
Resolution : 3.62 Å(reported)
Based on initial model : 9h2g

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

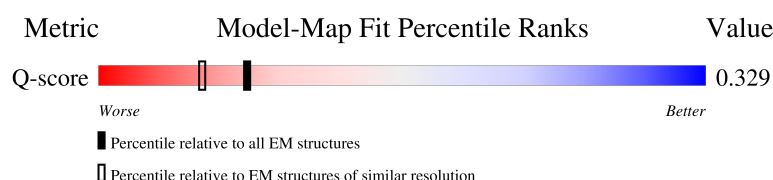
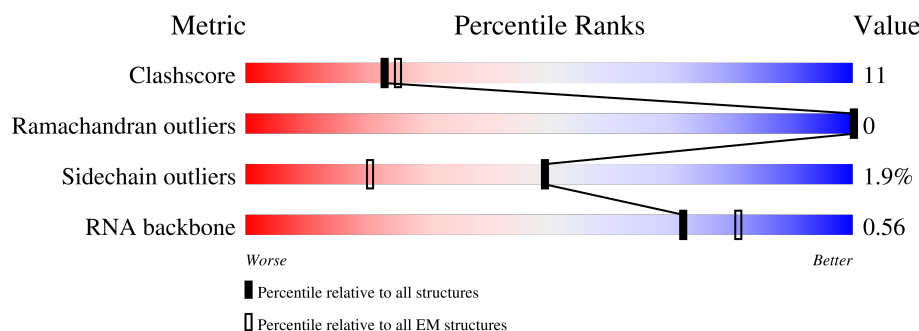
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.62 Å.

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11773 (3.12 - 4.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1397	
2	B	42	
3	C	75	

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Mol	Chain	Length	Quality of chain
4	D	49	
5	E	49	
6	F	297	
6	G	297	
7	I	114	
8	L	235	
8	M	235	
8	N	235	
8	O	235	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 23106 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 endonuclease Cas9.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1354	Total	C	N	O	S	0	0
			10096	6504	1788	1790	14		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1389	LEU	-	expression tag	UNP G3ECR1
A	1390	GLU	-	expression tag	UNP G3ECR1
A	1391	GLY	-	expression tag	UNP G3ECR1
A	1392	HIS	-	expression tag	UNP G3ECR1
A	1393	HIS	-	expression tag	UNP G3ECR1
A	1394	HIS	-	expression tag	UNP G3ECR1
A	1395	HIS	-	expression tag	UNP G3ECR1
A	1396	HIS	-	expression tag	UNP G3ECR1
A	1397	HIS	-	expression tag	UNP G3ECR1

- Molecule 2 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	29	Total	C	N	O	P	0	0
			624	278	111	206	29		

- Molecule 3 is a RNA chain called tracrRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	69	Total	C	N	O	P	0	0
			1474	660	269	476	69		

- Molecule 4 is a DNA chain called DNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	43	Total	C	N	O	P	0	0
			869	418	143	266	42		

- Molecule 5 is a DNA chain called DNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	43	Total	C	N	O	P	0	0
			888	421	179	246	42		

- Molecule 6 is a protein called CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	288	Total	C	N	O	S	0	0
			2035	1316	348	362	9		
6	G	288	Total	C	N	O	S	0	0
			2171	1412	373	376	10		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	289	MET	-	expression tag	UNP G3ECR2
F	290	SER	-	expression tag	UNP G3ECR2
F	291	GLY	-	expression tag	UNP G3ECR2
F	292	HIS	-	expression tag	UNP G3ECR2
F	293	HIS	-	expression tag	UNP G3ECR2
F	294	HIS	-	expression tag	UNP G3ECR2
F	295	HIS	-	expression tag	UNP G3ECR2
F	296	HIS	-	expression tag	UNP G3ECR2
F	297	HIS	-	expression tag	UNP G3ECR2
G	289	MET	-	expression tag	UNP G3ECR2
G	290	SER	-	expression tag	UNP G3ECR2
G	291	GLY	-	expression tag	UNP G3ECR2
G	292	HIS	-	expression tag	UNP G3ECR2
G	293	HIS	-	expression tag	UNP G3ECR2
G	294	HIS	-	expression tag	UNP G3ECR2
G	295	HIS	-	expression tag	UNP G3ECR2
G	296	HIS	-	expression tag	UNP G3ECR2
G	297	HIS	-	expression tag	UNP G3ECR2

- Molecule 7 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	I	10	Total	C	N	O	0	0
			73	50	10	13		

- Molecule 8 is a protein called CRISPR-associated protein Csn2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	218	Total 1487	C 971	N 233	O 278	S 5	0	0
8	L	219	Total 1605	C 1043	N 249	O 308	S 5	0	0
8	N	161	Total 818	C 494	N 162	O 162		0	0
8	M	164	Total 965	C 594	N 179	O 192		0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-15	MET	-	initiating methionine	UNP G3ECR4
O	-14	GLY	-	expression tag	UNP G3ECR4
O	-13	HIS	-	expression tag	UNP G3ECR4
O	-12	HIS	-	expression tag	UNP G3ECR4
O	-11	HIS	-	expression tag	UNP G3ECR4
O	-10	HIS	-	expression tag	UNP G3ECR4
O	-9	HIS	-	expression tag	UNP G3ECR4
O	-8	HIS	-	expression tag	UNP G3ECR4
O	-7	GLU	-	expression tag	UNP G3ECR4
O	-6	ASN	-	expression tag	UNP G3ECR4
O	-5	LEU	-	expression tag	UNP G3ECR4
O	-4	TYR	-	expression tag	UNP G3ECR4
O	-3	PHE	-	expression tag	UNP G3ECR4
O	-2	GLN	-	expression tag	UNP G3ECR4
O	-1	GLY	-	expression tag	UNP G3ECR4
O	0	GLY	-	expression tag	UNP G3ECR4
L	-15	MET	-	initiating methionine	UNP G3ECR4
L	-14	GLY	-	expression tag	UNP G3ECR4
L	-13	HIS	-	expression tag	UNP G3ECR4
L	-12	HIS	-	expression tag	UNP G3ECR4
L	-11	HIS	-	expression tag	UNP G3ECR4
L	-10	HIS	-	expression tag	UNP G3ECR4
L	-9	HIS	-	expression tag	UNP G3ECR4
L	-8	HIS	-	expression tag	UNP G3ECR4
L	-7	GLU	-	expression tag	UNP G3ECR4
L	-6	ASN	-	expression tag	UNP G3ECR4
L	-5	LEU	-	expression tag	UNP G3ECR4
L	-4	TYR	-	expression tag	UNP G3ECR4
L	-3	PHE	-	expression tag	UNP G3ECR4
L	-2	GLN	-	expression tag	UNP G3ECR4
L	-1	GLY	-	expression tag	UNP G3ECR4

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Chain	Residue	Modelled	Actual	Comment	Reference
L	0	GLY	-	expression tag	UNP G3ECR4
N	-15	MET	-	initiating methionine	UNP G3ECR4
N	-14	GLY	-	expression tag	UNP G3ECR4
N	-13	HIS	-	expression tag	UNP G3ECR4
N	-12	HIS	-	expression tag	UNP G3ECR4
N	-11	HIS	-	expression tag	UNP G3ECR4
N	-10	HIS	-	expression tag	UNP G3ECR4
N	-9	HIS	-	expression tag	UNP G3ECR4
N	-8	HIS	-	expression tag	UNP G3ECR4
N	-7	GLU	-	expression tag	UNP G3ECR4
N	-6	ASN	-	expression tag	UNP G3ECR4
N	-5	LEU	-	expression tag	UNP G3ECR4
N	-4	TYR	-	expression tag	UNP G3ECR4
N	-3	PHE	-	expression tag	UNP G3ECR4
N	-2	GLN	-	expression tag	UNP G3ECR4
N	-1	GLY	-	expression tag	UNP G3ECR4
N	0	GLY	-	expression tag	UNP G3ECR4
M	-15	MET	-	initiating methionine	UNP G3ECR4
M	-14	GLY	-	expression tag	UNP G3ECR4
M	-13	HIS	-	expression tag	UNP G3ECR4
M	-12	HIS	-	expression tag	UNP G3ECR4
M	-11	HIS	-	expression tag	UNP G3ECR4
M	-10	HIS	-	expression tag	UNP G3ECR4
M	-9	HIS	-	expression tag	UNP G3ECR4
M	-8	HIS	-	expression tag	UNP G3ECR4
M	-7	GLU	-	expression tag	UNP G3ECR4
M	-6	ASN	-	expression tag	UNP G3ECR4
M	-5	LEU	-	expression tag	UNP G3ECR4
M	-4	TYR	-	expression tag	UNP G3ECR4
M	-3	PHE	-	expression tag	UNP G3ECR4
M	-2	GLN	-	expression tag	UNP G3ECR4
M	-1	GLY	-	expression tag	UNP G3ECR4
M	0	GLY	-	expression tag	UNP G3ECR4

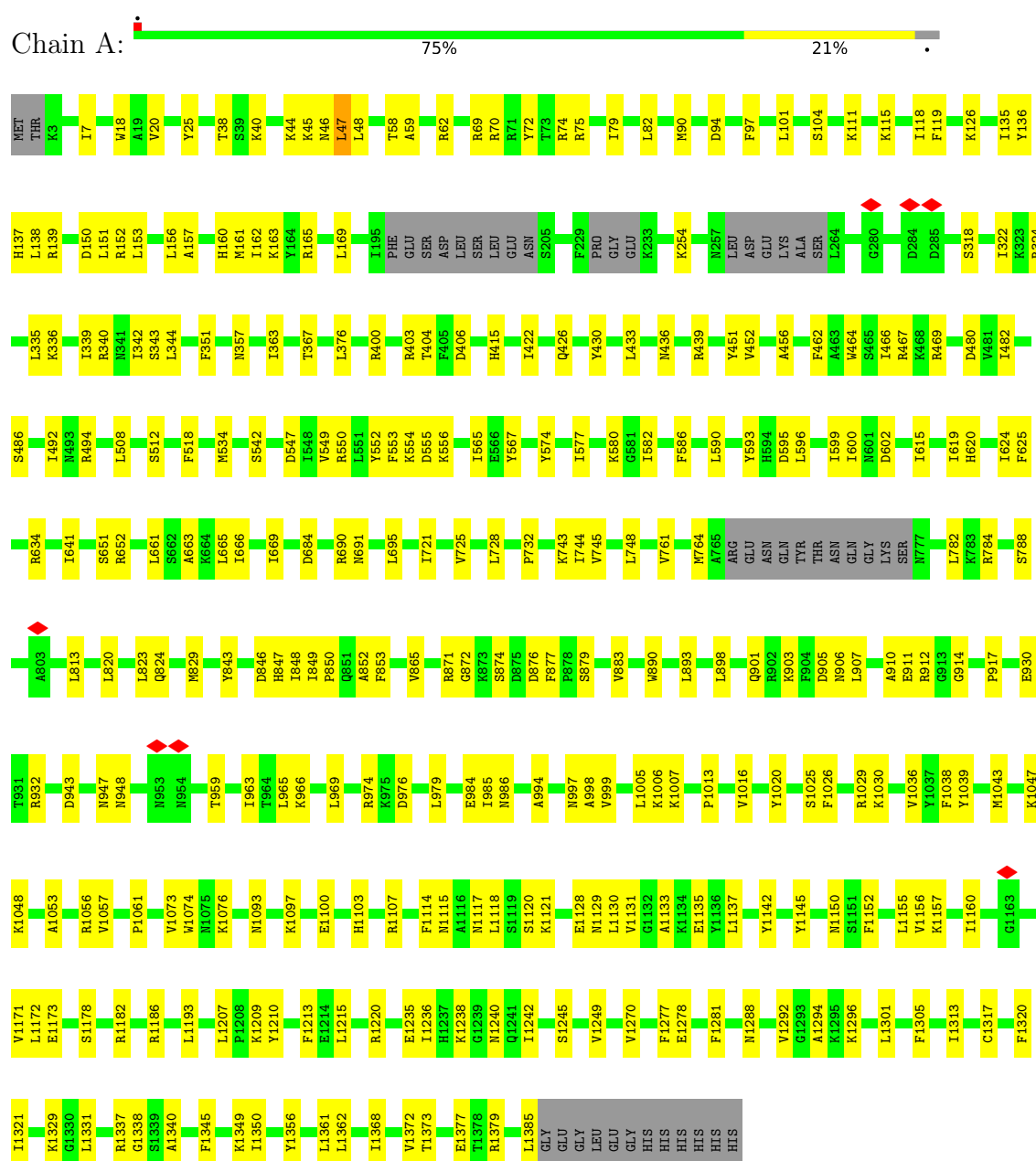
- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
9	C	1	Total Ca 1 1	0

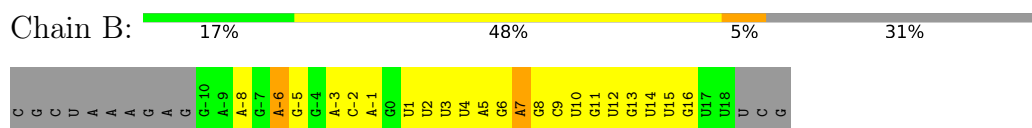
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

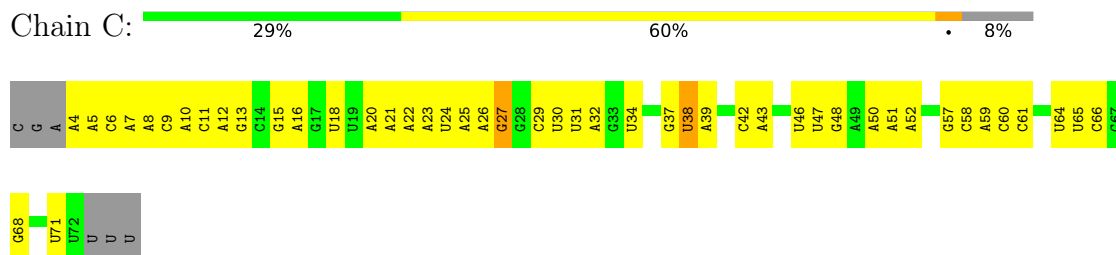
• Molecule 1: CRISPR-associated endonuclease Cas9



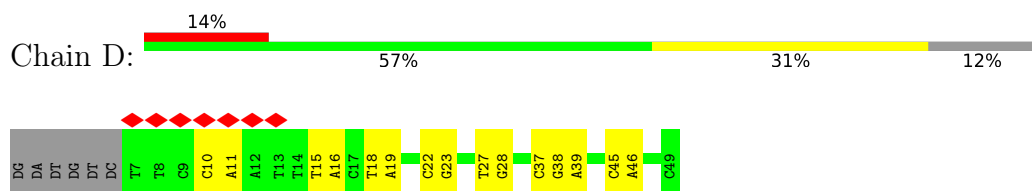
- Molecule 2: crRNA



- Molecule 3: tracrRNA



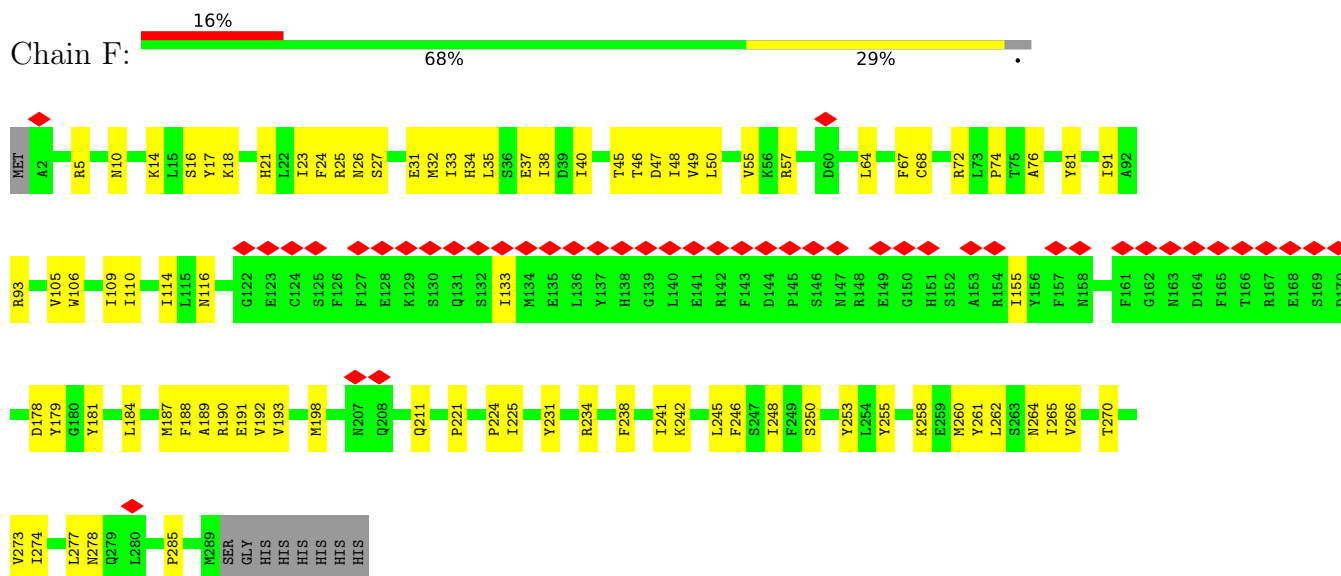
- Molecule 4: DNA (43-MER)



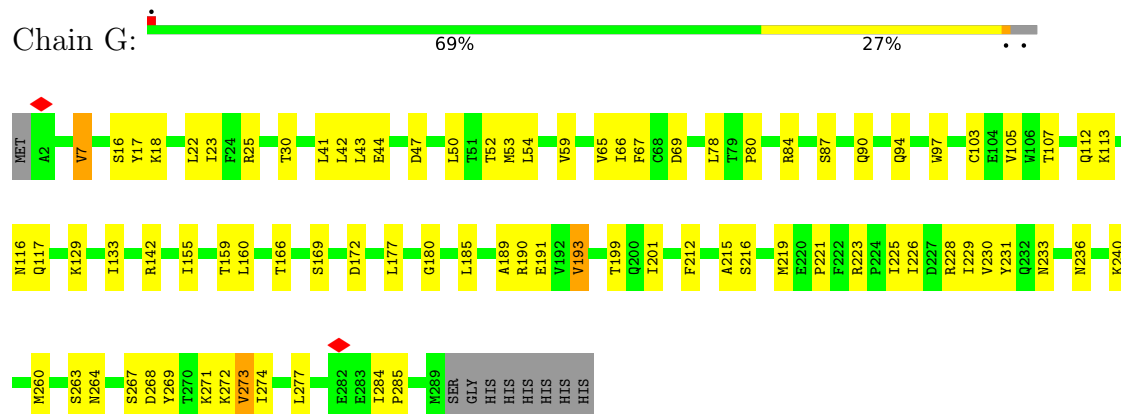
- Molecule 5: DNA (43-MER)



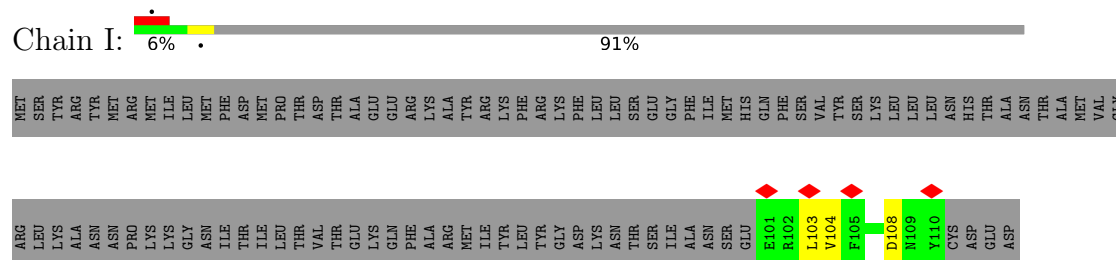
- Molecule 6: CRISPR-associated endonuclease Cas1



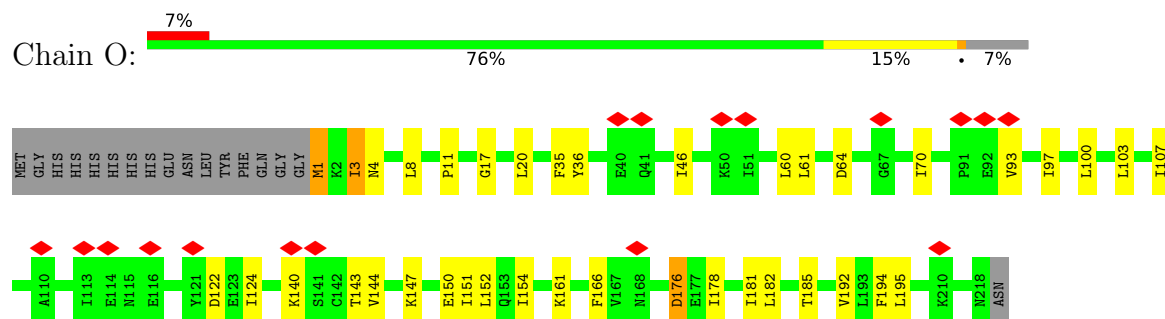
- Molecule 6: CRISPR-associated endonuclease Cas1



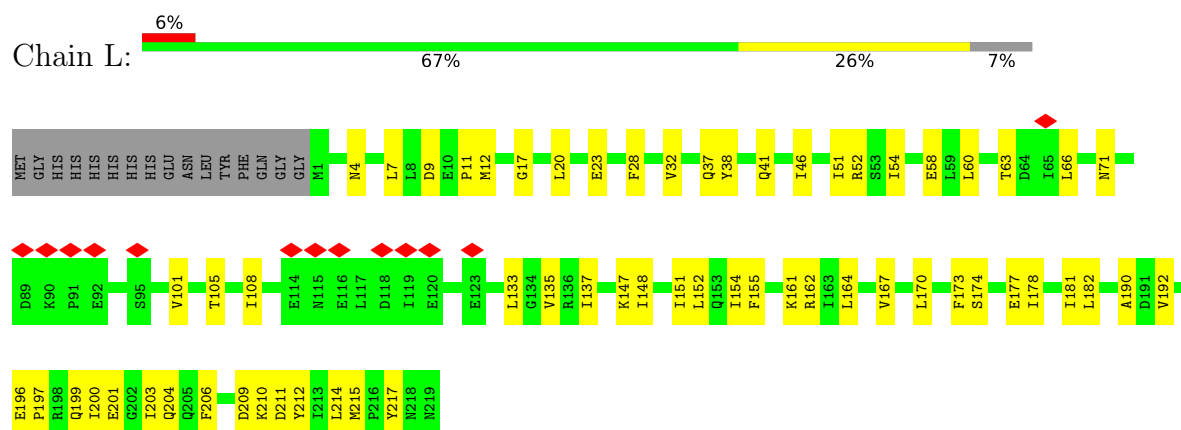
- Molecule 7: CRISPR-associated endoribonuclease Cas2



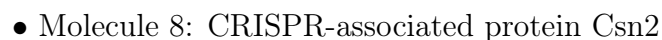
- Molecule 8: CRISPR-associated protein Csn2



- Molecule 8: CRISPR-associated protein Csn2



- Molecule 8: CRISPR-associated protein Csn2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24394	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	92000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	29.663	Depositor
Minimum map value	-7.642	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.008	Depositor
Recommended contour level	6	Depositor
Map size (\AA)	369.6, 369.6, 369.6	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/10284	0.37	0/13927
2	B	0.18	0/698	0.28	0/1087
3	C	0.16	0/1650	0.25	0/2569
4	D	0.22	0/969	0.48	0/1493
5	E	0.21	0/1001	0.42	0/1544
6	F	0.18	0/2071	0.46	0/2837
6	G	0.19	0/2214	0.43	0/3015
7	I	0.11	0/74	0.32	0/100
8	L	0.19	0/1627	0.49	0/2223
8	M	0.16	0/965	0.40	0/1332
8	N	0.10	0/817	0.25	0/1139
8	O	0.17	0/1508	0.42	0/2074
All	All	0.18	0/23878	0.39	0/33340

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	10096	0	9516	211	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	624	0	310	21	0
3	C	1474	0	744	42	0
4	D	869	0	491	10	0
5	E	888	0	481	21	0
6	F	2035	0	1841	64	0
6	G	2171	0	2069	61	0
7	I	73	0	61	4	0
8	L	1605	0	1473	53	0
8	M	965	0	679	12	0
8	N	818	0	371	2	0
8	O	1487	0	1283	34	0
9	C	1	0	0	0	0
All	All	23106	0	19319	472	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 11.

All (472) 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)
8:L:148:ILE:HD12	8:L:173:PHE:CZ	1.97	0.99
8:L:148:ILE:CD1	8:L:173:PHE:CZ	2.47	0.96
1:A:518:PHE:HE2	1:A:661:LEU:CD1	1.86	0.88
8:L:148:ILE:CD1	8:L:173:PHE:HZ	1.90	0.81
1:A:963:ILE:HD11	1:A:1005:LEU:HD22	1.62	0.81
8:O:64:ASP:OD1	8:L:63:THR:HG23	1.79	0.81
1:A:518:PHE:HE2	1:A:661:LEU:HD12	1.44	0.80
1:A:518:PHE:CE2	1:A:661:LEU:CD1	2.64	0.80
1:A:743:LYS:HG2	1:A:1372:VAL:HG11	1.66	0.77
1:A:574:TYR:HB3	1:A:577:ILE:HD11	1.68	0.76
1:A:596:LEU:HD11	1:A:619:ILE:HD11	1.67	0.76
6:G:191:GLU:HG2	6:G:267:SER:HA	1.67	0.75
6:G:272:LYS:HB2	6:G:285:PRO:HG3	1.69	0.74
8:L:17:GLY:HA2	8:L:192:VAL:O	1.88	0.74
6:G:273:VAL:HG23	6:G:285:PRO:HG2	1.70	0.74
1:A:138:LEU:HD11	1:A:153:LEU:HB3	1.69	0.73
8:L:148:ILE:HD11	8:L:173:PHE:HZ	1.54	0.72
1:A:70:ARG:NH2	2:B:-6:A:OP1	2.23	0.71
1:A:518:PHE:CE2	1:A:661:LEU:HD13	2.26	0.71
1:A:62:ARG:NH1	3:C:38:U:OP1	2.23	0.71
6:F:14:LYS:HE3	6:F:25:ARG:HH11	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:66:LEU:HA	8:L:147:LYS:HG2	1.73	0.70
2:B:6:G:N2	3:C:18:U:OP2	2.23	0.70
1:A:82:LEU:HD22	1:A:162:ILE:HD12	1.74	0.70
1:A:1155:LEU:CD2	1:A:1172:LEU:HD11	2.22	0.69
8:O:17:GLY:HA2	8:O:192:VAL:O	1.92	0.69
1:A:1157:LYS:HB2	1:A:1172:LEU:HD13	1.73	0.68
1:A:165:ARG:NH1	2:B:-3:A:OP1	2.26	0.68
1:A:126:LYS:NZ	2:B:7:A:OP2	2.26	0.68
1:A:451:TYR:O	1:A:464:TRP:NE1	2.27	0.68
3:C:57:G:H1	3:C:71:U:H3	1.40	0.68
8:L:148:ILE:HD11	8:L:173:PHE:CZ	2.29	0.68
6:G:105:VAL:HG11	6:G:277:LEU:HD11	1.76	0.67
6:F:255:TYR:H	6:F:258:LYS:HA	1.59	0.67
1:A:651:SER:OG	1:A:652:ARG:NH1	2.29	0.66
1:A:150:ASP:OD2	1:A:152:ARG:NH2	2.27	0.66
1:A:118:ILE:HG12	1:A:156:LEU:HD11	1.78	0.66
1:A:136:TYR:OH	1:A:403:ARG:NH1	2.30	0.65
8:L:209:ASP:OD1	8:L:210:LYS:N	2.30	0.65
6:F:26:ASN:OD1	6:F:27:SER:N	2.29	0.65
8:L:28:PHE:HE2	8:L:197:PRO:HG3	1.61	0.65
6:G:105:VAL:HG23	6:G:284:ILE:HD11	1.80	0.64
6:G:25:ARG:NH1	6:G:30:THR:HG21	2.13	0.64
1:A:943:ASP:OD1	1:A:947:ASN:ND2	2.31	0.64
8:L:170:LEU:HD13	8:L:178:ILE:HD12	1.80	0.64
6:F:34:HIS:HB3	6:F:37:GLU:HB2	1.80	0.63
1:A:1150:ASN:HA	1:A:1178:SER:HA	1.80	0.63
1:A:1220:ARG:NH2	3:C:65:U:O2'	2.32	0.62
1:A:44:LYS:NZ	3:C:68:G:O6	2.33	0.62
8:O:70:ILE:HD11	8:O:154:ILE:HG13	1.81	0.62
1:A:565:ILE:HG23	1:A:577:ILE:HB	1.82	0.62
1:A:160:HIS:HD2	3:C:20:A:H5''	1.65	0.62
6:F:116:ASN:HB3	6:F:224:PRO:HG2	1.82	0.61
8:O:107:ILE:HD13	8:M:97:ILE:HD13	1.82	0.61
1:A:69:ARG:NH2	3:C:38:U:OP2	2.33	0.61
8:M:97:ILE:O	8:M:101:VAL:HG23	1.99	0.61
6:G:43:LEU:CD1	6:G:67:PHE:CE1	2.84	0.61
6:F:24:PHE:HB3	6:F:31:GLU:HG2	1.81	0.61
6:G:87:SER:O	6:G:90:GLN:HB3	2.01	0.61
1:A:1317:CYS:O	1:A:1321:ILE:HG22	2.00	0.61
1:A:1025:SER:OG	1:A:1029:ARG:NH1	2.33	0.61
8:L:38:TYR:HA	8:L:41:GLN:HE21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:206:PHE:HB3	8:L:214:LEU:HD11	1.82	0.61
1:A:404:THR:HG23	1:A:406:ASP:H	1.66	0.60
1:A:874:SER:OG	1:A:1056:ARG:NH2	2.35	0.60
1:A:547:ASP:OD1	1:A:550:ARG:NH2	2.34	0.60
6:F:46:THR:OG1	6:G:53:MET:SD	2.59	0.60
1:A:318:SER:O	1:A:322:ILE:HG13	2.02	0.59
1:A:1281:PHE:HZ	1:A:1301:LEU:HB3	1.66	0.59
6:F:105:VAL:HG11	6:F:277:LEU:HD21	1.85	0.59
1:A:58:THR:HG22	1:A:732:PRO:HD2	1.84	0.59
6:G:41:LEU:HB3	6:G:65:VAL:HG12	1.85	0.59
1:A:1155:LEU:HD21	1:A:1172:LEU:HD11	1.85	0.59
8:O:140:LYS:O	8:L:37:GLN:NE2	2.36	0.59
8:L:4:ASN:HD22	8:L:11:PRO:HG3	1.68	0.59
1:A:163:LYS:NZ	3:C:22:A:OP2	2.34	0.58
6:F:109:ILE:HG23	6:F:221:PRO:HD3	1.85	0.58
1:A:48:LEU:O	1:A:1093:ASN:ND2	2.37	0.58
1:A:624:ILE:HG22	1:A:625:PHE:CD1	2.39	0.57
1:A:1288:ASN:ND2	1:A:1294:ALA:O	2.28	0.57
1:A:456:ALA:O	1:A:467:ARG:NH2	2.37	0.57
1:A:994:ALA:O	1:A:997:ASN:HB2	2.04	0.57
6:F:250:SER:HB3	7:I:103:LEU:HD23	1.87	0.57
6:G:65:VAL:HG22	6:G:78:LEU:HB2	1.87	0.57
1:A:1133:ALA:HB3	1:A:1137:LEU:HD12	1.86	0.56
8:L:28:PHE:CE2	8:L:197:PRO:HG3	2.38	0.56
6:G:229:ILE:O	6:G:233:ASN:ND2	2.32	0.56
8:L:12:MET:HE3	8:L:20:LEU:HD12	1.87	0.56
1:A:466:ILE:HD12	1:A:486:SER:HB2	1.85	0.56
1:A:469:ARG:NH1	1:A:480:ASP:O	2.37	0.56
6:F:76:ALA:HB2	6:G:59:VAL:HG21	1.88	0.56
1:A:7:ILE:HG12	1:A:20:VAL:HG22	1.88	0.56
8:O:176:ASP:OD1	8:O:176:ASP:N	2.35	0.56
1:A:324:ARG:HD3	1:A:400:ARG:HG3	1.88	0.56
8:O:100:LEU:HD21	8:M:103:LEU:HD23	1.87	0.55
1:A:400:ARG:HH21	1:A:404:THR:HG21	1.71	0.55
1:A:1349:LYS:HZ3	1:A:1350:ILE:H	1.54	0.55
1:A:75:ARG:NH2	3:C:24:U:O4	2.39	0.55
1:A:339:ILE:HA	1:A:342:ILE:HG22	1.88	0.55
2:B:3:U:H2'	2:B:4:U:C6	2.42	0.55
1:A:464:TRP:HE3	1:A:494:ARG:HD2	1.72	0.55
1:A:1107:ARG:HB3	4:D:39:DA:C2	2.41	0.55
1:A:1007:LYS:HE3	1:A:1036:VAL:HG13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:267:SER:O	6:G:271:LYS:HG2	2.07	0.55
8:L:203:ILE:HD12	8:L:204:GLN:H	1.72	0.54
1:A:59:ALA:N	2:B:-8:A:OP1	2.33	0.54
6:G:22:LEU:HD12	6:G:54:LEU:HD11	1.90	0.54
1:A:744:ILE:HG12	1:A:1373:THR:HG22	1.89	0.54
1:A:849:ILE:HD11	1:A:906:ASN:ND2	2.23	0.54
6:F:93:ARG:HD2	6:F:278:ASN:HB2	1.88	0.54
6:F:25:ARG:NH1	8:L:9:ASP:OD1	2.34	0.54
1:A:1320:PHE:O	1:A:1331:LEU:N	2.33	0.54
8:O:35:PHE:HB3	8:O:61:LEU:HD21	1.89	0.54
1:A:969:LEU:HD22	1:A:1043:MET:HE2	1.90	0.54
6:G:212:PHE:HB3	6:G:215:ALA:HB3	1.89	0.54
1:A:963:ILE:HG12	1:A:1016:VAL:HG22	1.89	0.54
1:A:1160:ILE:HD13	1:A:1171:VAL:HG11	1.89	0.53
1:A:1238:LYS:HZ1	1:A:1340:ALA:HB2	1.72	0.53
1:A:903:LYS:O	1:A:907:LEU:HG	2.08	0.53
8:M:130:ILE:HA	8:M:133:LEU:HG	1.90	0.53
1:A:1156:VAL:HG21	1:A:1193:LEU:HD22	1.90	0.53
3:C:48:G:N2	3:C:51:A:OP2	2.41	0.53
8:L:151:ILE:HA	8:L:154:ILE:HG22	1.91	0.53
6:F:178:ASP:HA	6:F:181:TYR:HD2	1.73	0.53
6:G:155:ILE:O	6:G:159:THR:HG23	2.08	0.53
6:F:262:LEU:O	6:F:265:ILE:HG22	2.08	0.53
1:A:403:ARG:NE	2:B:-1:A:OP1	2.39	0.53
1:A:72:TYR:OH	2:B:-1:A:N6	2.41	0.53
8:L:155:PHE:HE2	8:L:190:ALA:HB1	1.74	0.53
8:O:124:ILE:HG12	8:M:133:LEU:HD23	1.91	0.53
1:A:340:ARG:HH12	1:A:344:LEU:HA	1.73	0.53
1:A:1142:TYR:O	2:B:2:U:O2'	2.27	0.53
8:L:66:LEU:HA	8:L:147:LYS:HE3	1.91	0.52
1:A:254:LYS:HZ3	4:D:22:DC:H2'	1.74	0.52
1:A:1173:GLU:HA	1:A:1362:LEU:HD21	1.90	0.52
1:A:1296:LYS:NZ	5:E:7:DC:OP1	2.43	0.52
1:A:25:TYR:HB3	1:A:999:VAL:HG22	1.91	0.52
1:A:930:GLU:HB2	1:A:966:LYS:HG2	1.91	0.52
1:A:1100:GLU:OE1	1:A:1186:ARG:NH2	2.43	0.52
6:F:231:TYR:HA	6:F:234:ARG:HE	1.75	0.52
6:G:43:LEU:HD12	6:G:67:PHE:CE1	2.45	0.52
6:G:260:MET:HE2	6:G:264:ASN:HB3	1.92	0.52
1:A:1061:PRO:O	1:A:1076:LYS:NZ	2.39	0.52
5:E:17:DA:H2''	5:E:18:DA:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:PHE:CD2	1:A:1039:TYR:CE1	2.98	0.52
2:B:7:A:N1	3:C:15:G:O2'	2.33	0.52
8:L:60:LEU:HD22	8:L:161:LYS:HD2	1.92	0.52
1:A:254:LYS:NZ	4:D:22:DC:H2'	2.25	0.52
6:F:40:ILE:HD11	6:F:187:MET:HE2	1.92	0.52
8:L:108:ILE:HD12	8:N:133:LEU:HD13	1.91	0.52
6:F:188:PHE:HE1	6:F:266:VAL:HG22	1.75	0.51
1:A:1155:LEU:CD2	1:A:1172:LEU:CD1	2.88	0.51
8:O:143:THR:OG1	8:O:144:VAL:N	2.43	0.51
1:A:1281:PHE:HB2	1:A:1320:PHE:HZ	1.76	0.51
8:L:101:VAL:O	8:L:105:THR:OG1	2.23	0.51
1:A:160:HIS:CD2	3:C:20:A:H5''	2.45	0.51
6:G:7:VAL:HB	6:G:41:LEU:HD12	1.92	0.51
1:A:104:SER:OG	3:C:21:A:N3	2.42	0.51
6:F:191:GLU:HG2	6:F:266:VAL:HG12	1.93	0.51
6:G:42:LEU:HD21	6:G:190:ARG:HG2	1.92	0.51
6:F:81:TYR:CZ	6:G:193:VAL:HG11	2.45	0.51
1:A:1038:PHE:HD2	1:A:1039:TYR:CE1	2.29	0.51
1:A:508:LEU:HD21	1:A:663:ALA:HB2	1.92	0.50
1:A:1207:LEU:HD13	1:A:1213:PHE:HZ	1.77	0.50
8:L:54:ILE:HG23	8:L:58:GLU:HB3	1.92	0.50
1:A:1278:GLU:HA	1:A:1305:PHE:HZ	1.76	0.50
1:A:111:LYS:NZ	1:A:115:LYS:O	2.43	0.50
1:A:930:GLU:OE1	1:A:932:ARG:NH1	2.45	0.50
3:C:15:G:H2'	3:C:16:A:H8	1.77	0.50
5:E:34:DT:H2''	5:E:35:DA:C8	2.47	0.50
1:A:910:ALA:HA	1:A:914:GLY:HA2	1.94	0.50
1:A:1128:GLU:HB3	1:A:1130:LEU:HG	1.94	0.50
4:D:45:DC:H2''	4:D:46:DA:C8	2.47	0.50
8:O:103:LEU:O	8:O:107:ILE:HG22	2.12	0.50
6:F:16:SER:OG	6:F:17:TYR:N	2.44	0.49
6:F:191:GLU:HG3	6:F:270:THR:HB	1.94	0.49
1:A:976:ASP:OD2	1:A:1047:LYS:NZ	2.39	0.49
5:E:25:DA:H2''	5:E:26:DA:C8	2.47	0.49
6:G:112:GLN:O	6:G:116:ASN:ND2	2.45	0.49
8:O:147:LYS:O	8:O:151:ILE:HG12	2.12	0.49
3:C:7:A:H2'	3:C:8:A:C8	2.47	0.49
6:F:68:CYS:HA	6:F:74:PRO:HA	1.95	0.49
8:M:101:VAL:HG13	8:M:124:ILE:HG23	1.95	0.49
6:G:25:ARG:HH12	8:L:217:TYR:HD2	1.61	0.49
1:A:20:VAL:HB	1:A:47:LEU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:C:H2'	3:C:7:A:H8	1.78	0.49
3:C:11:C:H2'	3:C:12:A:C8	2.47	0.49
5:E:9:DC:H1'	5:E:10:DC:H5'	1.94	0.48
6:G:65:VAL:C	6:G:66:ILE:HD13	2.38	0.48
8:O:64:ASP:OD1	8:O:64:ASP:N	2.44	0.48
1:A:595:ASP:O	1:A:599:ILE:HG12	2.13	0.48
1:A:743:LYS:NZ	3:C:42:C:OP1	2.40	0.48
3:C:58:C:H2'	3:C:59:A:C8	2.48	0.48
8:O:1:MET:SD	8:O:1:MET:N	2.86	0.48
8:O:4:ASN:HB2	8:O:11:PRO:HB3	1.95	0.48
1:A:90:MET:O	1:A:94:ASP:N	2.43	0.48
8:O:182:LEU:HA	8:O:185:THR:HG22	1.95	0.48
6:G:177:LEU:HD23	6:G:230:VAL:HG21	1.96	0.48
1:A:157:ALA:O	1:A:161:MET:HG3	2.14	0.48
6:F:33:ILE:HB	6:F:38:ILE:HD11	1.96	0.48
6:F:179:TYR:HE2	6:F:242:LYS:HG2	1.78	0.48
1:A:46:ASN:N	1:A:46:ASN:HD22	2.10	0.48
3:C:58:C:H2'	3:C:59:A:H8	1.78	0.48
8:O:36:TYR:CE1	8:O:61:LEU:HG	2.48	0.48
1:A:580:LYS:NZ	1:A:905:ASP:OD2	2.35	0.48
6:F:48:ILE:O	6:G:52:THR:OG1	2.28	0.48
6:F:211:GLN:HG2	6:G:84:ARG:HD2	1.96	0.48
1:A:784:ARG:O	1:A:788:SER:OG	2.23	0.48
3:C:11:C:H2'	3:C:12:A:H8	1.79	0.48
6:G:59:VAL:HG13	6:G:80:PRO:HB3	1.96	0.48
1:A:45:LYS:NZ	1:A:1377:GLU:OE1	2.46	0.47
1:A:872:GLY:HA3	1:A:879:SER:HB2	1.95	0.47
6:F:17:TYR:OH	6:F:57:ARG:NH1	2.46	0.47
8:L:174:SER:O	8:L:178:ILE:HG12	2.14	0.47
1:A:137:HIS:CE1	1:A:322:ILE:HG23	2.50	0.47
8:L:148:ILE:HD12	8:L:173:PHE:CE2	2.44	0.47
1:A:552:TYR:CE2	1:A:567:TYR:HB2	2.50	0.47
1:A:846:ASP:OD1	1:A:847:HIS:N	2.48	0.47
6:F:189:ALA:O	6:F:193:VAL:HG23	2.14	0.47
6:G:268:ASP:O	6:G:272:LYS:HG3	2.14	0.47
1:A:136:TYR:O	1:A:318:SER:OG	2.31	0.47
1:A:625:PHE:CE2	1:A:634:ARG:HD2	2.49	0.47
1:A:848:ILE:O	1:A:871:ARG:NH2	2.47	0.47
1:A:1120:SER:OG	1:A:1121:LYS:N	2.48	0.47
6:F:14:LYS:NZ	8:L:7:LEU:O	2.38	0.47
6:F:23:ILE:HD13	6:F:32:MET:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:228:ARG:HD2	6:G:229:ILE:HD13	1.96	0.47
6:G:236:ASN:HD22	6:G:240:LYS:HG2	1.80	0.47
1:A:600:ILE:HG22	1:A:602:ASP:HB3	1.96	0.47
1:A:782:LEU:HA	1:A:813:LEU:HD12	1.97	0.47
1:A:1118:LEU:O	2:B:1:U:O2'	2.32	0.47
1:A:1270:VAL:HG12	1:A:1313:ILE:HD11	1.97	0.47
4:D:18:DT:H2''	4:D:19:DA:C8	2.50	0.47
1:A:165:ARG:HG2	1:A:165:ARG:HH11	1.80	0.47
1:A:492:ILE:HD13	1:A:624:ILE:HG21	1.97	0.47
1:A:1115:ASN:ND2	5:E:11:DT:H4'	2.29	0.47
1:A:850:PRO:HD2	1:A:853:PHE:HD2	1.80	0.46
6:F:45:THR:HG22	6:F:47:ASP:H	1.80	0.46
6:G:25:ARG:HG2	6:G:30:THR:CG2	2.45	0.46
6:G:94:GLN:HG2	6:G:201:ILE:HD12	1.97	0.46
8:O:1:MET:HB3	8:O:46:ILE:HD11	1.97	0.46
1:A:1155:LEU:HD22	1:A:1172:LEU:HD11	1.98	0.46
8:L:148:ILE:O	8:L:152:LEU:HG	2.15	0.46
1:A:761:VAL:HG21	1:A:998:ALA:HA	1.98	0.46
5:E:3:DC:H2'	5:E:4:DT:H71	1.97	0.46
8:O:20:LEU:HB3	8:O:195:LEU:HD12	1.98	0.46
1:A:1013:PRO:HB3	1:A:1020:TYR:CD1	2.50	0.46
6:G:166:THR:O	6:G:169:SER:OG	2.29	0.46
1:A:843:TYR:HB2	1:A:865:VAL:O	2.16	0.46
8:O:64:ASP:OD1	8:L:63:THR:CG2	2.59	0.46
8:O:122:ASP:HB3	8:M:133:LEU:O	2.16	0.46
8:L:133:LEU:HD11	8:L:135:VAL:HG23	1.98	0.46
8:L:148:ILE:O	8:L:151:ILE:HG22	2.15	0.46
1:A:343:SER:OG	1:A:344:LEU:N	2.48	0.46
1:A:1385:LEU:HD23	1:A:1385:LEU:HA	1.81	0.46
1:A:553:PHE:HB3	1:A:590:LEU:HD12	1.98	0.46
3:C:46:U:H2'	3:C:47:U:H6	1.80	0.46
4:D:37:DC:H2''	4:D:38:DG:C8	2.51	0.46
1:A:74:ARG:NH1	2:B:-5:G:OP1	2.41	0.46
2:B:10:U:H2'	2:B:11:G:C8	2.51	0.46
6:G:107:THR:HG21	6:G:142:ARG:HA	1.98	0.45
1:A:336:LYS:HA	1:A:351:PHE:HE2	1.81	0.45
1:A:984:GLU:HG3	1:A:1329:LYS:HG2	1.98	0.45
1:A:1117:ASN:ND2	5:E:12:DC:OP2	2.49	0.45
6:G:216:SER:HA	6:G:219:MET:HE2	1.97	0.45
8:L:148:ILE:HA	8:L:151:ILE:HG22	1.98	0.45
1:A:1281:PHE:CZ	1:A:1301:LEU:HB3	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:G:H2'	3:C:16:A:C8	2.50	0.45
5:E:24:DG:H2''	5:E:25:DA:C8	2.51	0.45
6:F:184:LEU:HD23	6:F:184:LEU:HA	1.73	0.45
6:G:221:PRO:HG2	6:G:269:TYR:OH	2.17	0.45
5:E:12:DC:H2''	5:E:13:DG:C8	2.51	0.45
6:F:64:LEU:HD13	6:F:190:ARG:HD2	1.98	0.45
6:G:42:LEU:HD12	6:G:66:ILE:HB	1.99	0.45
1:A:690:ARG:HB2	1:A:695:LEU:HD23	1.98	0.45
3:C:4:A:H2'	3:C:5:A:C8	2.52	0.45
5:E:4:DT:H2''	5:E:5:DG:C8	2.52	0.45
6:F:114:ILE:HG23	6:F:133:ILE:HG22	1.98	0.45
8:L:182:LEU:HD12	8:L:203:ILE:HG12	1.99	0.45
2:B:-2:C:H2'	2:B:-1:A:O4'	2.17	0.45
6:F:262:LEU:O	6:F:266:VAL:HG23	2.16	0.45
8:O:140:LYS:C	8:L:37:GLN:HE22	2.23	0.45
1:A:871:ARG:NH1	1:A:876:ASP:O	2.41	0.45
1:A:905:ASP:OD1	1:A:912:ARG:NH1	2.49	0.45
1:A:985:ILE:HG13	1:A:986:ASN:N	2.31	0.45
3:C:23:A:H2'	3:C:24:U:O4'	2.17	0.45
5:E:31:DT:H2''	5:E:32:DA:C8	2.51	0.45
6:G:112:GLN:NE2	6:G:285:PRO:O	2.49	0.45
1:A:79:ILE:HD11	1:A:163:LYS:HB2	1.98	0.45
1:A:725:VAL:HA	1:A:728:LEU:HG	1.99	0.45
1:A:721:ILE:O	1:A:725:VAL:HG23	2.17	0.45
6:G:25:ARG:HG2	6:G:30:THR:HG22	1.98	0.45
1:A:97:PHE:CE1	1:A:152:ARG:HG2	2.52	0.44
1:A:849:ILE:HG13	1:A:877:PHE:HE1	1.81	0.44
4:D:10:DC:H2''	4:D:11:DA:C8	2.51	0.44
1:A:38:THR:HG22	1:A:40:LYS:H	1.82	0.44
6:F:10:ASN:HB2	6:F:72:ARG:NH2	2.32	0.44
8:L:38:TYR:OH	8:L:46:ILE:N	2.47	0.44
1:A:582:ILE:HD12	1:A:582:ILE:HA	1.82	0.44
1:A:1209:LYS:NZ	1:A:1210:TYR:OH	2.47	0.44
1:A:18:TRP:CE3	1:A:748:LEU:HD11	2.52	0.44
1:A:118:ILE:HG22	1:A:119:PHE:CD1	2.52	0.44
1:A:335:LEU:HG	1:A:351:PHE:HZ	1.81	0.44
1:A:823:LEU:HD22	1:A:898:LEU:HB3	1.99	0.44
1:A:893:LEU:HD22	1:A:898:LEU:HB2	1.98	0.44
1:A:1235:GLU:O	1:A:1236:ILE:HD13	2.18	0.44
5:E:29:DA:H2''	5:E:30:DG:C8	2.51	0.44
6:F:187:MET:HG3	6:F:266:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:113:LYS:O	6:G:117:GLN:HG2	2.18	0.44
6:G:225:ILE:O	6:G:229:ILE:HG12	2.18	0.44
8:L:170:LEU:HB2	8:L:196:GLU:CD	2.43	0.44
8:L:177:GLU:O	8:L:181:ILE:HG13	2.17	0.44
1:A:436:ASN:OD1	1:A:439:ARG:NE	2.30	0.44
1:A:549:VAL:HA	1:A:553:PHE:HD2	1.83	0.44
1:A:1100:GLU:HG3	1:A:1152:PHE:HD2	1.82	0.44
2:B:1:U:H2'	2:B:2:U:C6	2.53	0.44
5:E:41:DG:H2''	5:E:42:DA:C8	2.52	0.44
1:A:1215:LEU:HD21	1:A:1361:LEU:HD23	2.00	0.44
6:F:14:LYS:HE3	6:F:25:ARG:NH1	2.30	0.44
6:G:25:ARG:HH21	8:L:215:MET:HB2	1.82	0.44
8:L:23:GLU:OE2	8:L:210:LYS:N	2.51	0.44
8:L:199:GLN:C	8:L:200:ILE:HD13	2.43	0.44
1:A:917:PRO:HB2	1:A:1030:LYS:NZ	2.32	0.44
1:A:1301:LEU:HD23	1:A:1301:LEU:HA	1.76	0.44
1:A:883:VAL:HG22	1:A:890:TRP:HZ3	1.83	0.44
1:A:1103:HIS:ND1	3:C:39:A:OP1	2.50	0.44
6:F:245:LEU:O	6:F:248:ILE:HG12	2.17	0.44
1:A:542:SER:HB2	1:A:684:ASP:HA	1.99	0.44
1:A:661:LEU:HD22	1:A:665:LEU:HD23	2.00	0.44
1:A:1155:LEU:HD21	1:A:1172:LEU:CD1	2.47	0.44
2:B:10:U:H2'	2:B:11:G:H8	1.83	0.44
4:D:15:DT:H2''	4:D:16:DA:C8	2.53	0.44
1:A:1236:ILE:HB	1:A:1356:TYR:HB3	2.00	0.43
5:E:39:DT:H2''	5:E:40:DG:C8	2.53	0.43
8:O:93:VAL:O	8:O:97:ILE:HG23	2.17	0.43
1:A:974:ARG:NH1	1:A:979:LEU:O	2.51	0.43
6:F:188:PHE:CE1	6:F:266:VAL:HG22	2.52	0.43
6:F:238:PHE:HA	6:F:241:ILE:HD12	1.99	0.43
6:G:103:CYS:O	6:G:107:THR:HG23	2.17	0.43
8:N:130:ILE:HA	8:N:133:LEU:HG	1.99	0.43
1:A:615:ILE:O	1:A:619:ILE:HG12	2.18	0.43
2:B:4:U:H2'	2:B:5:A:H8	1.82	0.43
6:G:44:GLU:N	6:G:44:GLU:OE1	2.51	0.43
1:A:47:LEU:HD13	1:A:47:LEU:HA	1.87	0.43
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.85	0.43
4:D:22:DC:H2''	4:D:23:DG:C8	2.54	0.43
6:F:17:TYR:CE1	6:F:57:ARG:HG2	2.53	0.43
6:F:260:MET:HG2	6:F:264:ASN:HB2	2.01	0.43
6:G:185:LEU:HD11	6:G:212:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ALA:HB2	3:C:39:A:H1'	2.00	0.43
3:C:4:A:H2'	3:C:5:A:H8	1.83	0.43
1:A:743:LYS:HB2	1:A:743:LYS:HE3	1.81	0.43
6:F:273:VAL:HG23	6:F:285:PRO:HG2	1.99	0.43
8:L:164:LEU:HB3	8:L:192:VAL:HG22	1.99	0.43
1:A:1135:GLU:N	3:C:27:G:OP1	2.45	0.43
3:C:9:C:H2'	3:C:10:A:C8	2.54	0.43
6:G:44:GLU:HB3	6:G:190:ARG:HD3	2.01	0.43
8:M:70:ILE:HB	8:M:139:THR:HG21	2.00	0.43
6:G:129:LYS:HE2	6:G:159:THR:HG22	2.01	0.43
8:O:3:ILE:HD12	8:O:3:ILE:HA	1.88	0.43
1:A:582:ILE:HD11	1:A:586:PHE:HA	2.00	0.43
4:D:27:DT:H2''	4:D:28:DG:C8	2.54	0.43
6:G:16:SER:OG	6:G:17:TYR:N	2.52	0.43
6:G:160:LEU:HD22	6:G:231:TYR:CD1	2.53	0.43
1:A:422:ILE:O	1:A:426:GLN:HG2	2.18	0.42
1:A:1074:TRP:NE1	1:A:1076:LYS:HA	2.34	0.42
6:F:188:PHE:O	6:F:192:VAL:HG12	2.19	0.42
1:A:550:ARG:HA	1:A:554:LYS:HG3	2.00	0.42
6:G:18:LYS:HG2	6:G:23:ILE:HG13	2.01	0.42
8:O:36:TYR:HE1	8:O:61:LEU:HG	1.83	0.42
8:O:60:LEU:HB2	8:O:161:LYS:HG3	2.01	0.42
1:A:850:PRO:HB3	1:A:1053:ALA:HB2	2.02	0.42
2:B:1:U:H2'	2:B:2:U:H6	1.85	0.42
5:E:4:DT:H2''	5:E:5:DG:H8	1.85	0.42
5:E:19:DC:H2''	5:E:20:DA:C8	2.55	0.42
6:F:14:LYS:NZ	8:L:212:TYR:O	2.29	0.42
6:F:91:ILE:HD13	6:F:91:ILE:HA	1.82	0.42
6:G:69:ASP:OD1	6:G:69:ASP:N	2.39	0.42
8:M:109:MET:O	8:M:113:ILE:HG12	2.18	0.42
1:A:139:ARG:HH22	1:A:415:HIS:HE1	1.68	0.42
1:A:357:ASN:HA	1:A:367:THR:HG21	2.01	0.42
1:A:363:ILE:HG23	3:C:18:U:H5'	2.01	0.42
3:C:12:A:H2'	3:C:13:G:H8	1.85	0.42
3:C:46:U:H2'	3:C:47:U:C6	2.54	0.42
8:L:32:VAL:HG23	8:L:167:VAL:HG21	2.02	0.42
1:A:555:ASP:OD1	1:A:556:LYS:N	2.51	0.42
1:A:1245:SER:O	1:A:1249:VAL:HG23	2.19	0.42
2:B:11:G:H2'	2:B:12:U:C6	2.55	0.42
3:C:48:G:O2'	3:C:50:A:N7	2.49	0.42
5:E:42:DA:H2''	5:E:43:DA:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:ILE:H	1:A:849:ILE:HD12	1.83	0.42
1:A:1026:PHE:CZ	1:A:1030:LYS:HD2	2.55	0.42
6:F:246:PHE:HB3	7:I:103:LEU:HD11	2.01	0.42
1:A:169:LEU:HD23	1:A:169:LEU:HA	1.88	0.42
1:A:764:MET:HE3	1:A:764:MET:HB3	1.93	0.42
6:F:5:ARG:HD3	7:I:104:VAL:HG21	2.01	0.42
6:F:225:ILE:HD11	6:F:253:TYR:CE1	2.55	0.42
8:O:8:LEU:HD12	8:O:8:LEU:HA	1.93	0.42
8:O:147:LYS:HE2	8:O:151:ILE:HD11	2.01	0.42
3:C:60:C:H2'	3:C:61:C:C6	2.55	0.42
1:A:580:LYS:HG3	1:A:901:GLN:HG2	2.02	0.42
1:A:691:ASN:O	1:A:695:LEU:HG	2.19	0.42
3:C:6:C:H2'	3:C:7:A:C8	2.53	0.42
8:L:170:LEU:HB2	8:L:196:GLU:OE2	2.19	0.42
1:A:534:MET:HG2	6:F:21:HIS:NE2	2.35	0.41
1:A:666:ILE:HD13	1:A:666:ILE:HA	1.87	0.41
1:A:948:ASN:OD1	1:A:948:ASN:N	2.52	0.41
1:A:1157:LYS:HB2	1:A:1172:LEU:CD1	2.47	0.41
1:A:1331:LEU:HD22	1:A:1345:PHE:HE2	1.84	0.41
1:A:1368:ILE:HG12	1:A:1379:ARG:HG2	2.02	0.41
1:A:1048:LYS:HE3	1:A:1048:LYS:HB3	1.89	0.41
6:F:50:LEU:N	6:G:50:LEU:O	2.54	0.41
6:F:255:TYR:HB2	6:F:265:ILE:HD12	2.01	0.41
1:A:62:ARG:NH2	1:A:462:PHE:HZ	2.18	0.41
1:A:160:HIS:NE2	3:C:20:A:OP1	2.42	0.41
1:A:1337:ARG:HG2	1:A:1338:GLY:N	2.35	0.41
8:O:150:GLU:OE1	8:M:117:LEU:HD12	2.20	0.41
8:O:152:LEU:HA	8:O:152:LEU:HD23	1.75	0.41
8:L:215:MET:HE3	8:L:215:MET:HA	2.03	0.41
5:E:14:DA:H2''	5:E:15:DG:H8	1.85	0.41
6:F:10:ASN:ND2	7:I:108:ASP:O	2.53	0.41
6:F:18:LYS:HB2	6:F:23:ILE:HD11	2.03	0.41
8:O:166:PHE:HB2	8:O:194:PHE:HD1	1.84	0.41
1:A:433:LEU:HD23	1:A:433:LEU:HA	1.93	0.41
1:A:893:LEU:HD23	1:A:893:LEU:HA	1.91	0.41
2:B:15:U:H2'	2:B:16:G:C8	2.55	0.41
1:A:135:ILE:HG12	1:A:160:HIS:CD2	2.56	0.41
3:C:26:A:OP2	3:C:37:G:N2	2.48	0.41
8:O:152:LEU:HD21	8:O:192:VAL:HG21	2.02	0.41
1:A:492:ILE:HD12	1:A:620:HIS:NE2	2.36	0.41
2:B:8:G:H2'	2:B:9:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:23:DA:H2''	5:E:24:DG:C8	2.56	0.41
6:F:198:MET:HE2	6:F:198:MET:HB3	1.68	0.41
6:G:103:CYS:HB3	6:G:142:ARG:HD2	2.03	0.41
8:L:162:ARG:HA	8:L:162:ARG:HD2	1.87	0.41
1:A:824:GLN:NE2	1:A:829:MET:SD	2.93	0.41
1:A:1100:GLU:OE2	1:A:1182:ARG:NH1	2.53	0.41
6:F:187:MET:HG2	6:F:266:VAL:HG21	2.03	0.41
6:G:180:GLY:HA3	6:G:226:ILE:HG21	2.02	0.41
8:L:51:ILE:O	8:L:52:ARG:NE	2.54	0.41
1:A:452:VAL:C	1:A:464:TRP:HE1	2.29	0.41
1:A:482:ILE:HD12	1:A:482:ILE:HA	1.92	0.41
1:A:512:SER:HA	1:A:619:ILE:HG21	2.03	0.41
1:A:820:LEU:O	1:A:824:GLN:HG3	2.21	0.41
1:A:852:ALA:HB1	1:A:1039:TYR:HD2	1.86	0.41
1:A:1006:LYS:HB3	1:A:1073:VAL:HG23	2.03	0.41
1:A:1097:LYS:NZ	3:C:42:C:OP2	2.42	0.41
1:A:1131:VAL:O	1:A:1145:TYR:N	2.54	0.41
6:G:274:ILE:HD13	6:G:274:ILE:HA	1.97	0.41
8:L:161:LYS:HE2	8:L:161:LYS:HB2	1.84	0.41
3:C:9:C:H2'	3:C:10:A:H8	1.86	0.41
5:E:14:DA:H2''	5:E:15:DG:C8	2.56	0.41
6:G:97:TRP:CH2	6:G:277:LEU:HD23	2.56	0.41
1:A:101:LEU:O	3:C:21:A:O2'	2.33	0.40
1:A:1292:VAL:O	1:A:1356:TYR:OH	2.24	0.40
6:F:248:ILE:HB	6:F:262:LEU:HD13	2.02	0.40
6:G:189:ALA:O	6:G:193:VAL:HG23	2.21	0.40
8:L:71:ASN:ND2	8:L:137:ILE:O	2.51	0.40
1:A:336:LYS:NZ	3:C:16:A:OP2	2.42	0.40
6:F:49:VAL:HG21	8:L:211:ASP:HB3	2.03	0.40
6:F:106:TRP:O	6:F:110:ILE:HG12	2.21	0.40
8:O:166:PHE:HD2	8:O:194:PHE:HE1	1.69	0.40
1:A:554:LYS:HB3	1:A:593:TYR:HE2	1.86	0.40
1:A:1349:LYS:NZ	1:A:1350:ILE:H	2.20	0.40
6:F:133:ILE:HG12	6:F:155:ILE:HD11	2.03	0.40
6:G:219:MET:HE3	6:G:223:ARG:NE	2.37	0.40
8:O:178:ILE:O	8:O:181:ILE:HG22	2.20	0.40
8:M:90:LYS:HD3	8:M:93:VAL:HG21	2.03	0.40
1:A:430:TYR:HB2	1:A:433:LEU:HB2	2.03	0.40
6:F:67:PHE:HD2	6:G:52:THR:HG23	1.86	0.40
6:F:274:ILE:HD13	6:F:274:ILE:HA	1.93	0.40
8:M:154:ILE:O	8:M:158:LEU:N	2.54	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	1344/1397 (96%)	1303 (97%)	41 (3%)	0	100	100
6	F	286/297 (96%)	272 (95%)	14 (5%)	0	100	100
6	G	286/297 (96%)	279 (98%)	7 (2%)	0	100	100
7	I	8/114 (7%)	8 (100%)	0	0	100	100
8	L	217/235 (92%)	212 (98%)	5 (2%)	0	100	100
8	M	160/235 (68%)	156 (98%)	4 (2%)	0	100	100
8	N	157/235 (67%)	155 (99%)	2 (1%)	0	100	100
8	O	216/235 (92%)	207 (96%)	9 (4%)	0	100	100
All	All	2674/3045 (88%)	2592 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

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.

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	924/1260 (73%)	910 (98%)	14 (2%)	57	66
6	F	178/272 (65%)	175 (98%)	3 (2%)	53	65
6	G	207/272 (76%)	199 (96%)	8 (4%)	28	51
7	I	6/102 (6%)	6 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	L	155/224 (69%)	154 (99%)	1 (1%)	78	77
8	M	51/224 (23%)	49 (96%)	2 (4%)	28	51
8	N	5/224 (2%)	5 (100%)	0	100	100
8	O	125/224 (56%)	122 (98%)	3 (2%)	43	60
All	All	1651/2802 (59%)	1620 (98%)	31 (2%)	49	64

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	376	LEU
1	A	641	ILE
1	A	669	ILE
1	A	745	VAL
1	A	911	GLU
1	A	959	THR
1	A	965	LEU
1	A	1057	VAL
1	A	1114	PHE
1	A	1129	ASN
1	A	1240	ASN
1	A	1242	ILE
1	A	1277	PHE
6	F	35	LEU
6	F	55	VAL
6	F	261	TYR
6	G	7	VAL
6	G	47	ASP
6	G	133	ILE
6	G	172	ASP
6	G	193	VAL
6	G	199	THR
6	G	263	SER
6	G	273	VAL
8	O	1	MET
8	O	3	ILE
8	O	176	ASP
8	L	201	GLU
8	M	103	LEU
8	M	117	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	77	ASN
1	A	368	ASN
1	A	369	GLN
1	A	538	GLN
1	A	740	GLN
1	A	847	HIS
1	A	1044	ASN
1	A	1066	ASN
1	A	1230	ASN
6	G	117	GLN
6	G	200	GLN
6	G	235	HIS
8	L	37	GLN
8	L	41	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	28/42 (66%)	4 (14%)	0
3	C	68/75 (90%)	12 (17%)	0
All	All	96/117 (82%)	16 (16%)	0

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-6	A
2	B	7	A
2	B	13	G
2	B	14	U
3	C	25	A
3	C	27	G
3	C	29	C
3	C	30	U
3	C	31	U
3	C	32	A
3	C	34	U
3	C	38	U
3	C	43	A
3	C	52	A

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Mol	Chain	Res	Type
3	C	64	U
3	C	66	C

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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](#)

There are no chain breaks in this entry.

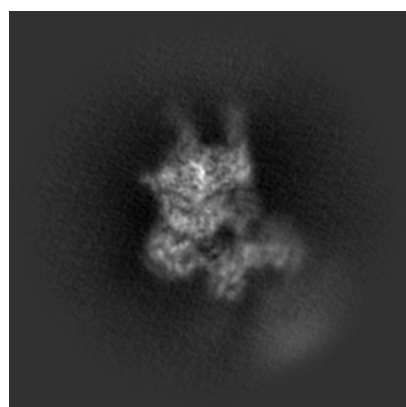
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52886. These allow visual inspection of the internal detail of the map and identification of artifacts.

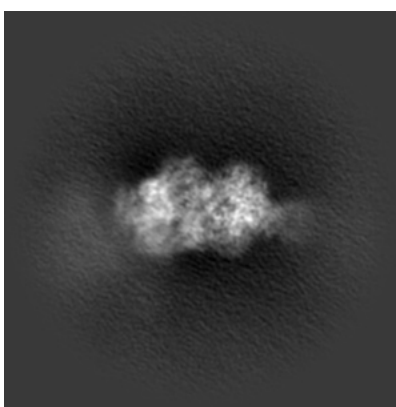
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

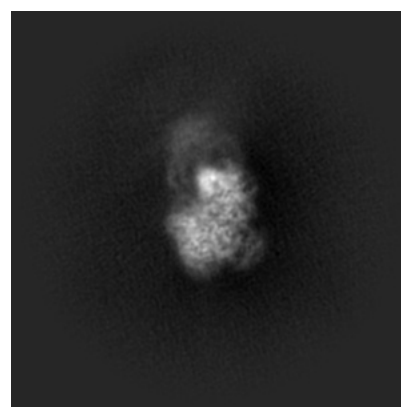
6.1.1 Primary map



X



Y

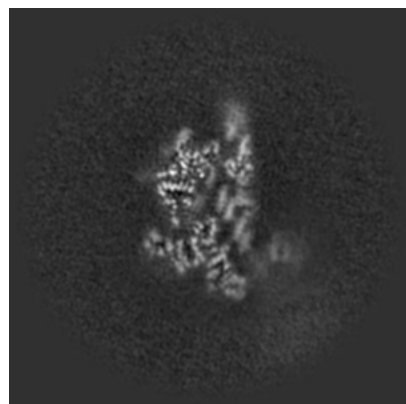


Z

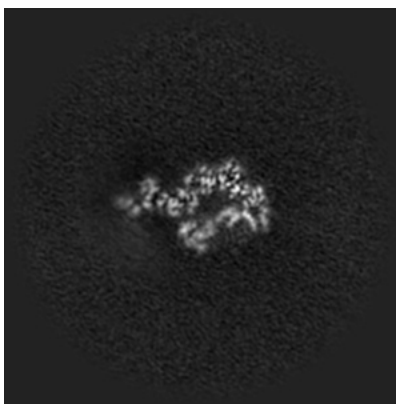
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

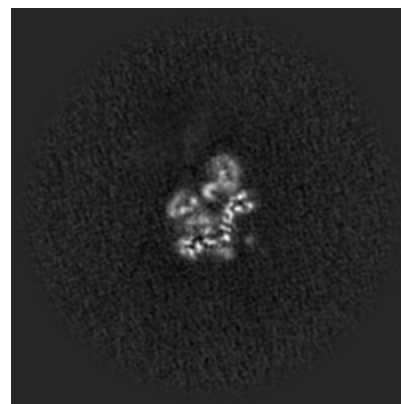
6.2.1 Primary map



X Index: 168



Y Index: 168

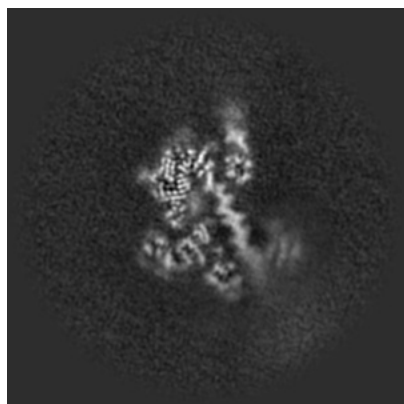


Z Index: 168

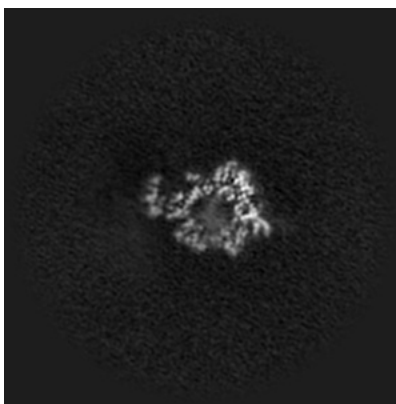
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

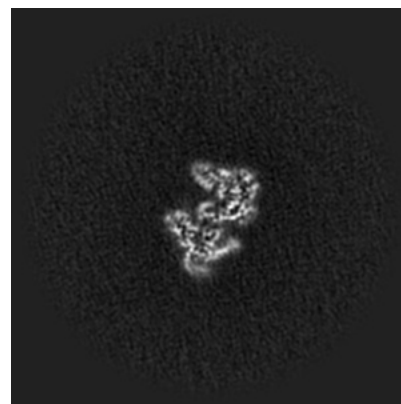
6.3.1 Primary map



X Index: 163



Y Index: 162

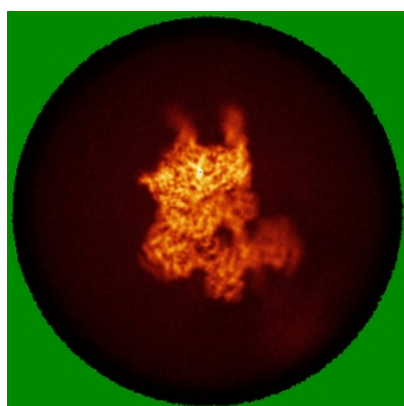


Z Index: 196

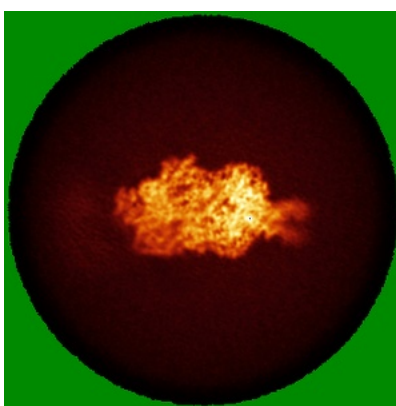
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

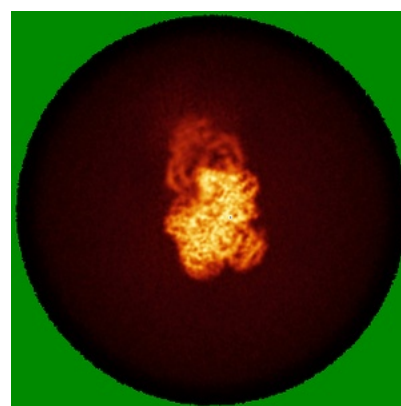
6.4.1 Primary map



X



Y

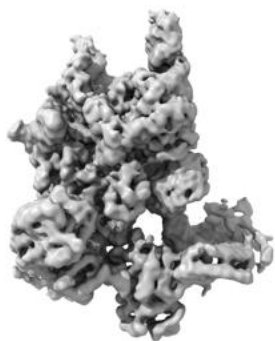


Z

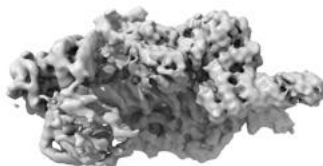
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

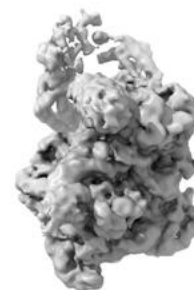
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

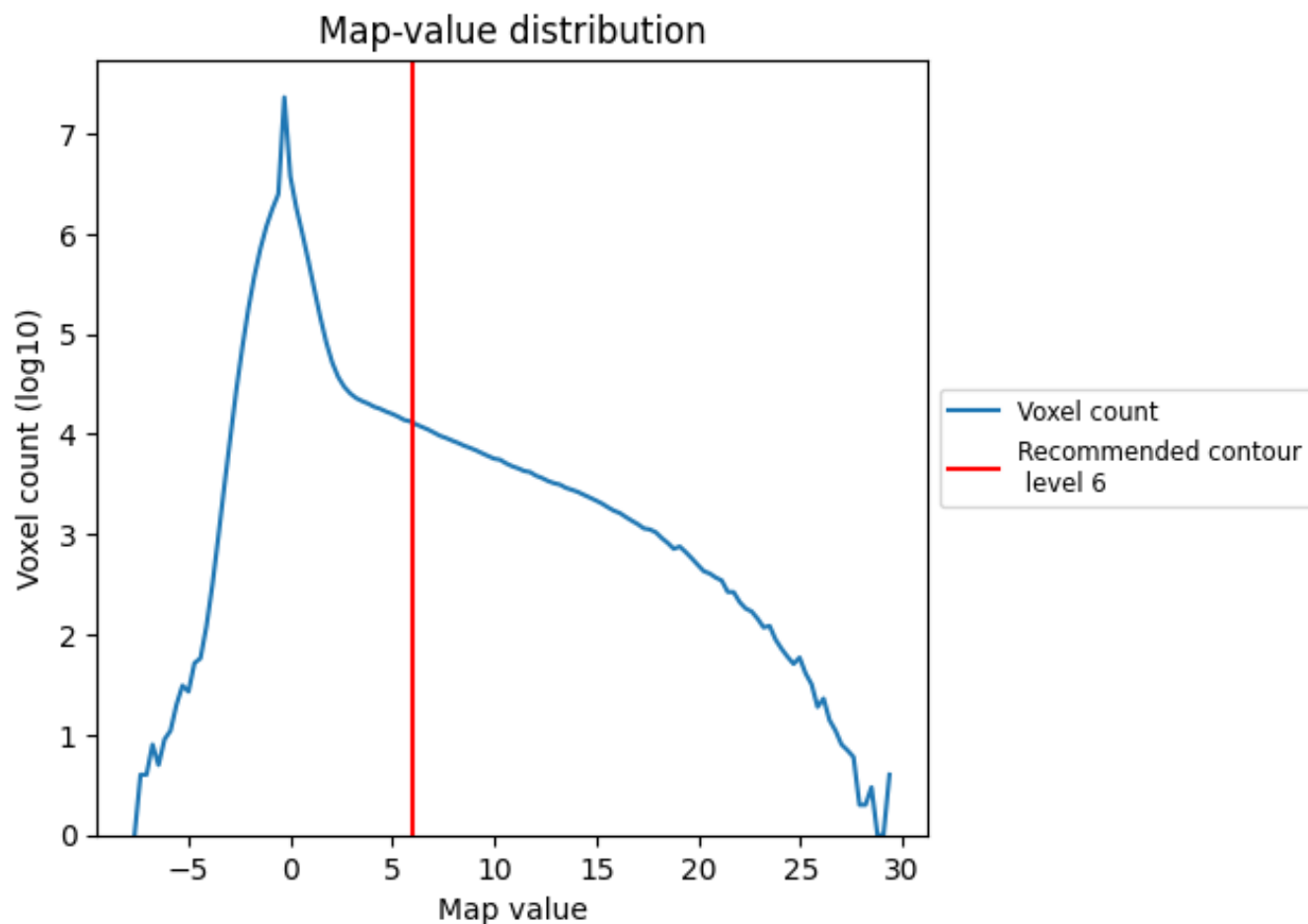
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

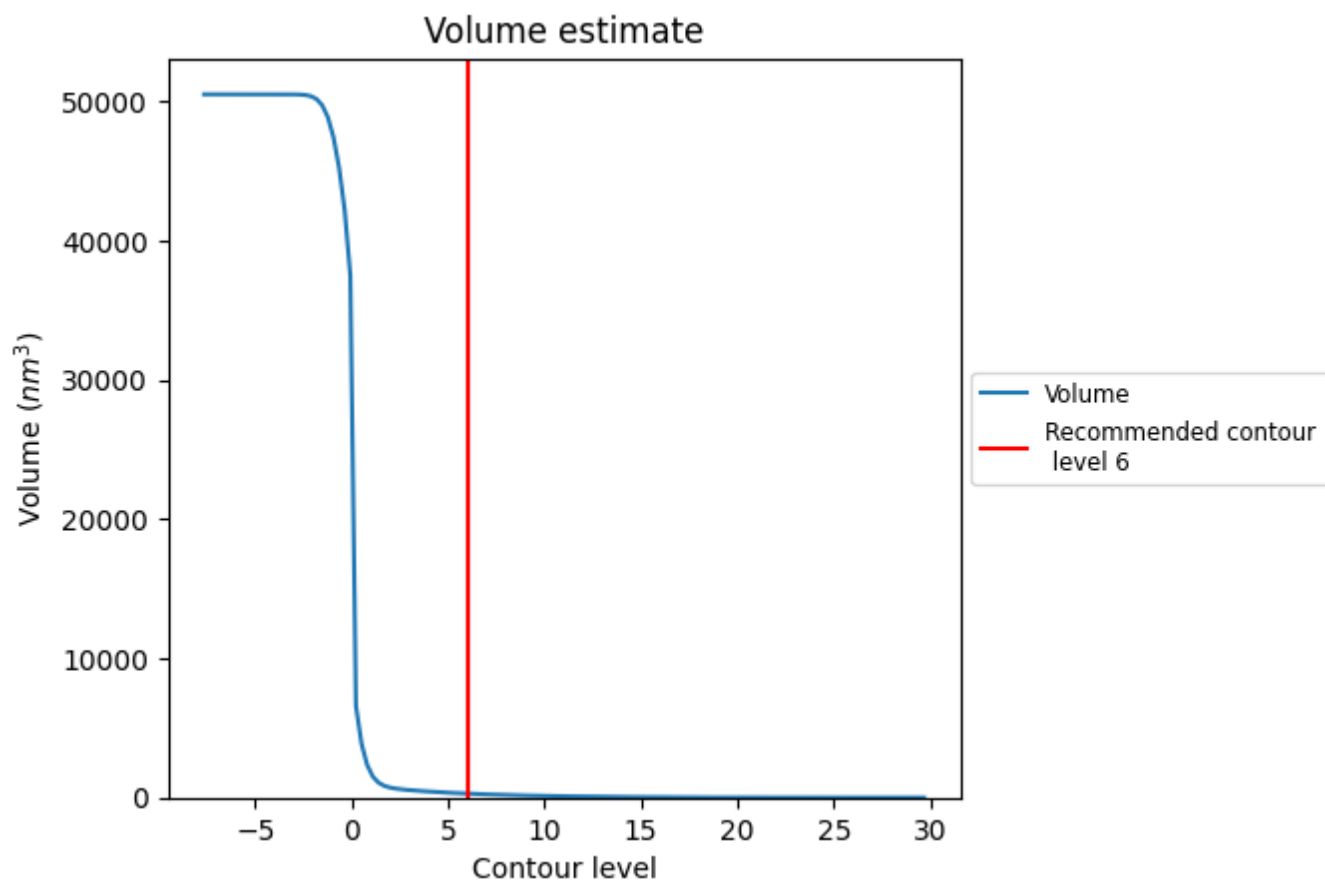
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

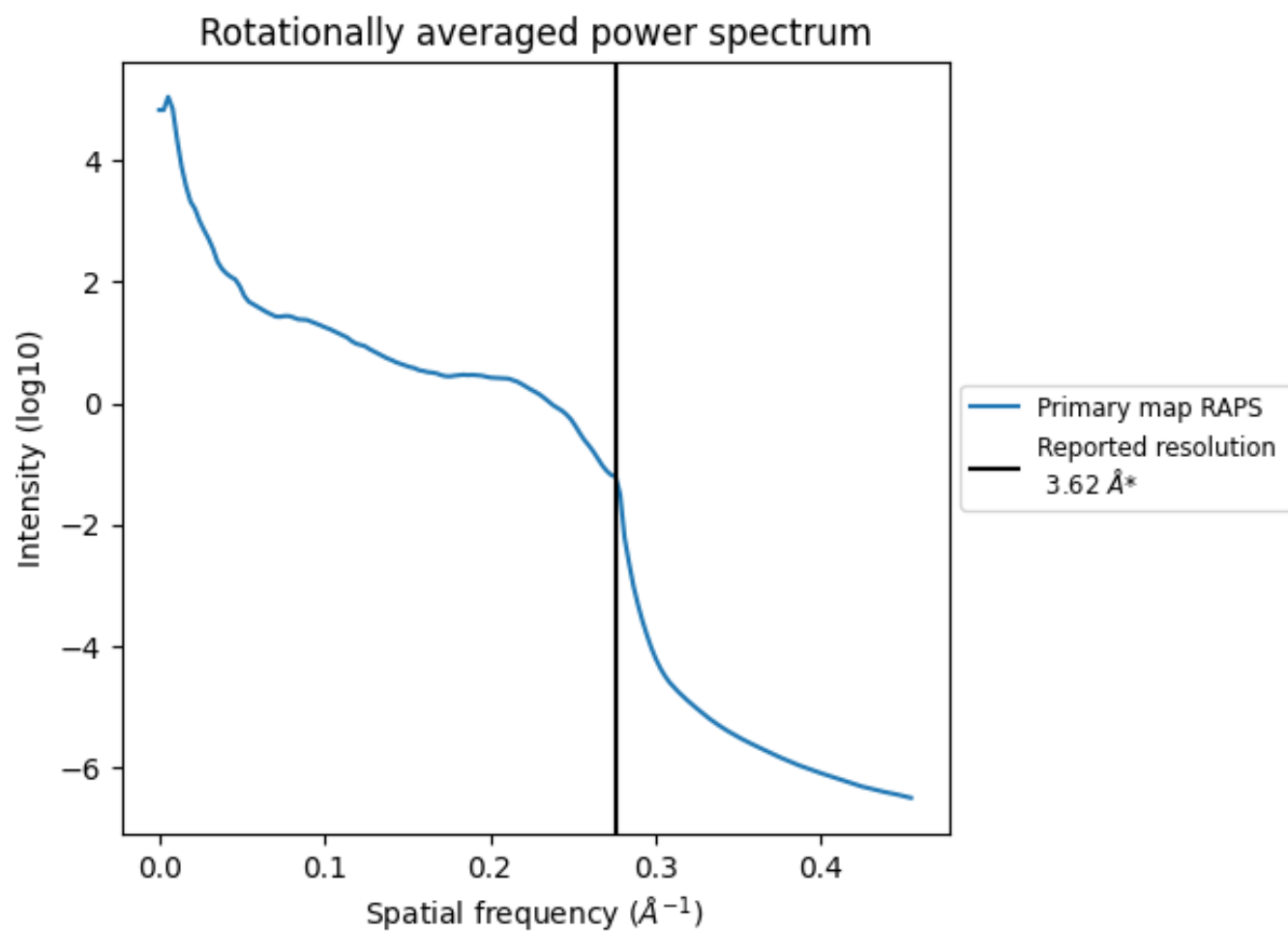
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 284 nm^3 ; this corresponds to an approximate mass of 256 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.276 \AA^{-1}

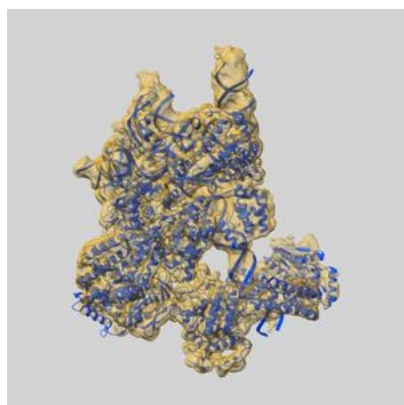
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

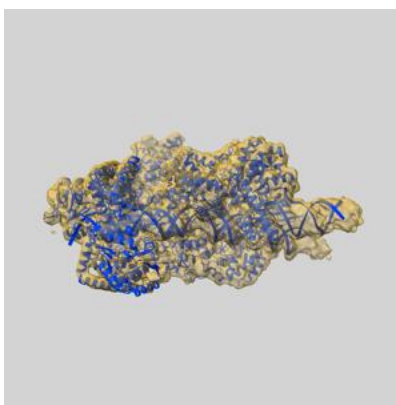
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52886 and PDB model 9Q85. Per-residue inclusion information can be found in section [3](#) on page [8](#).

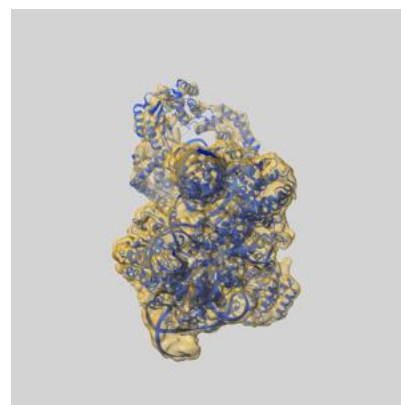
9.1 Map-model overlay [i](#)



X



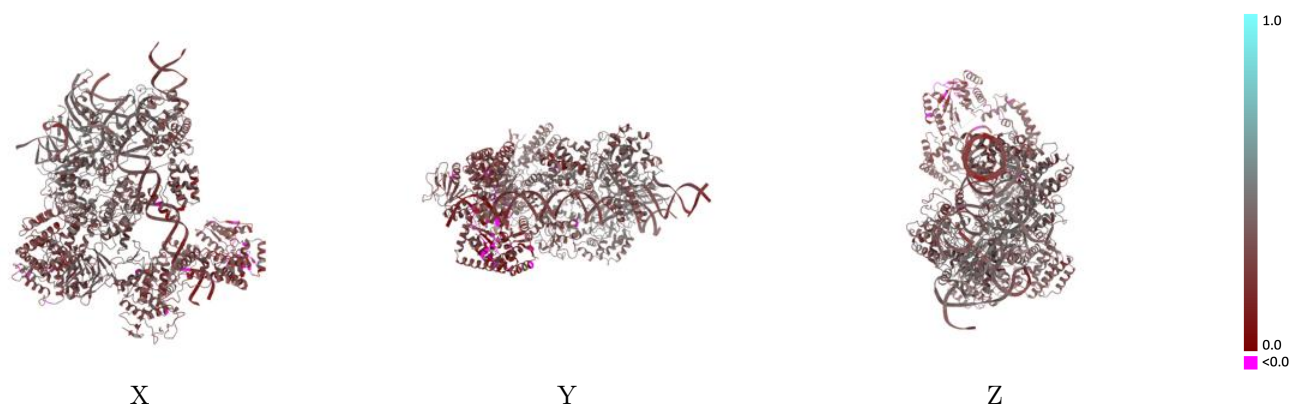
Y



Z

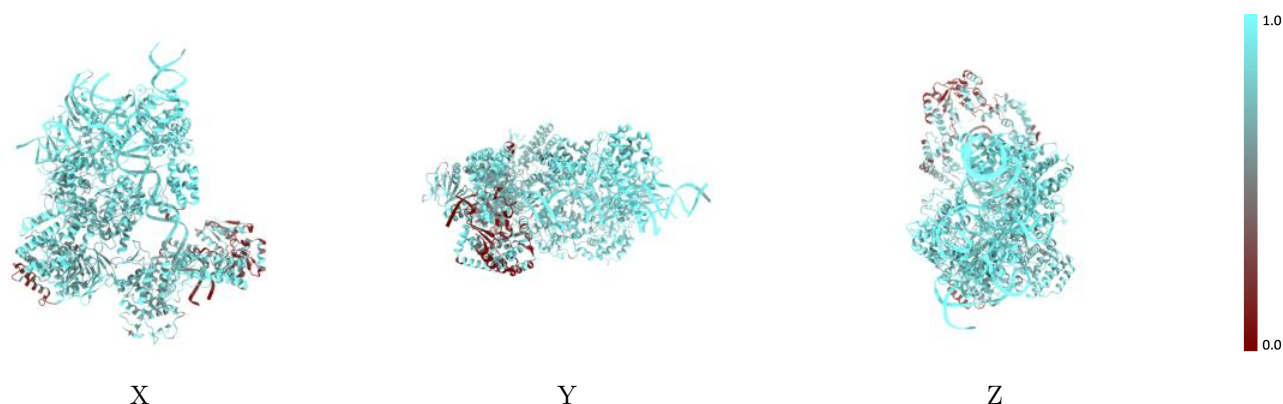
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



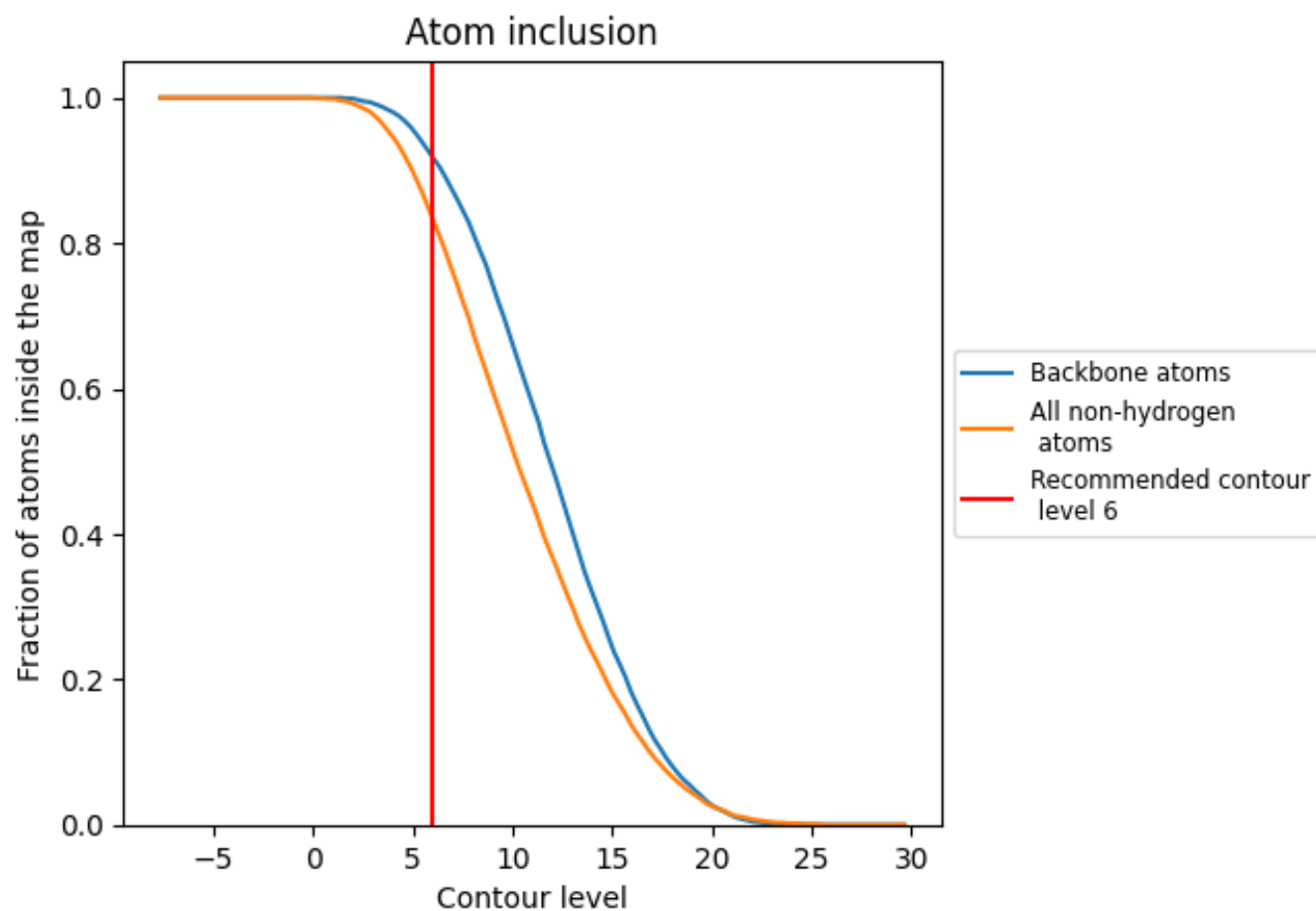
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8340	<div></div> 0.3290
A	<div></div> 0.9040	<div></div> 0.3760
B	<div></div> 0.9920	<div></div> 0.3430
C	<div></div> 0.9820	<div></div> 0.3650
D	<div></div> 0.8210	<div></div> 0.2640
E	<div></div> 0.8480	<div></div> 0.2540
F	<div></div> 0.6990	<div></div> 0.2920
G	<div></div> 0.8450	<div></div> 0.3280
I	<div></div> 0.4860	<div></div> 0.2490
L	<div></div> 0.7640	<div></div> 0.3070
M	<div></div> 0.6040	<div></div> 0.2100
N	<div></div> 0.4900	<div></div> 0.1980
O	<div></div> 0.7520	<div></div> 0.2840

