Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 02:41 AM UTC

PDB ID	:	9HP8 / pdb_00009hp8
EMDB ID	:	EMD-52320
Title	:	PAM-bound Cas9-Cas1-Cas2-Csn2 supercomplex in the docked conformation, Streptococcus thermophilus DGCC 7710 CRISPR3 system
Authors	:	Sasnauskas, G.; Gaizauskaite, U.; Tamulaitiene, G.
Deposited on	:	2024-12-12
Resolution	:	3.70 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:

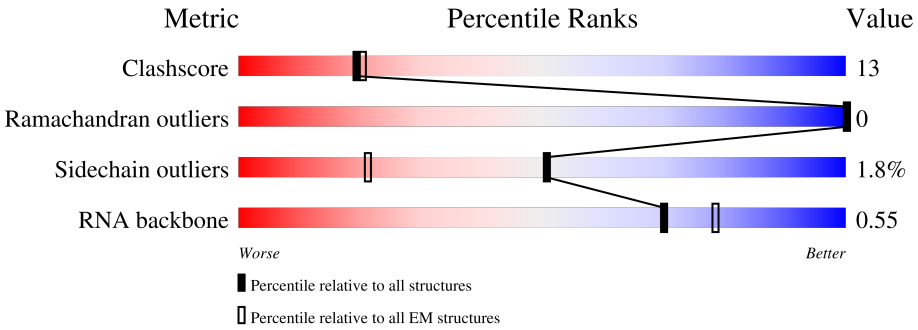
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

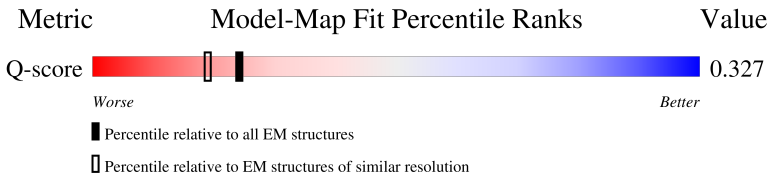
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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 <=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	77% 21%
2	B	42	26% 43% 31%
3	C	75	24% 64% 8%

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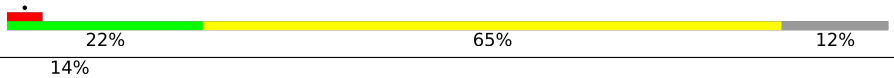
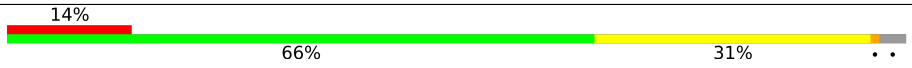
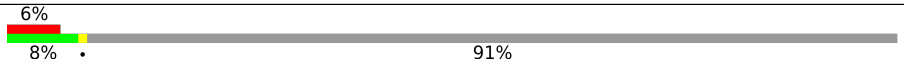
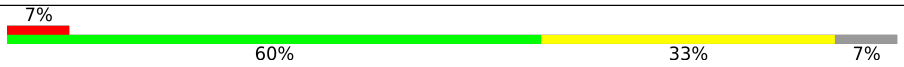
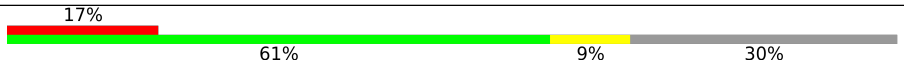
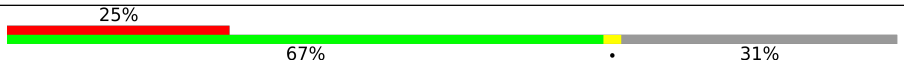
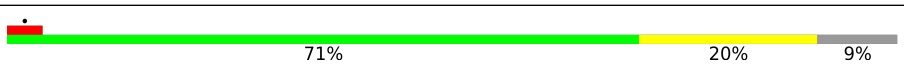
Mol	Chain	Length	Quality of chain
4	D	49	
5	E	49	
6	F	297	
6	G	297	
7	I	114	
8	L	235	
8	M	235	
8	N	235	
8	O	235	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 23089 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	1372	Total	C	N	O	S	0	0
			10325	6652	1811	1847	15		

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 Cas9 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 Cas9 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
			2021	1305	349	358	9		
6	G	288	Total	C	N	O	S	0	0
			2152	1403	371	369	9		

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	215	Total C N O S 1351 867 225 256 3	0	0
8	L	219	Total C N O S 1588 1034 250 299 5	0	0
8	N	161	Total C N O 815 491 162 162	0	0
8	M	164	Total C N O S 908 557 167 183 1	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).

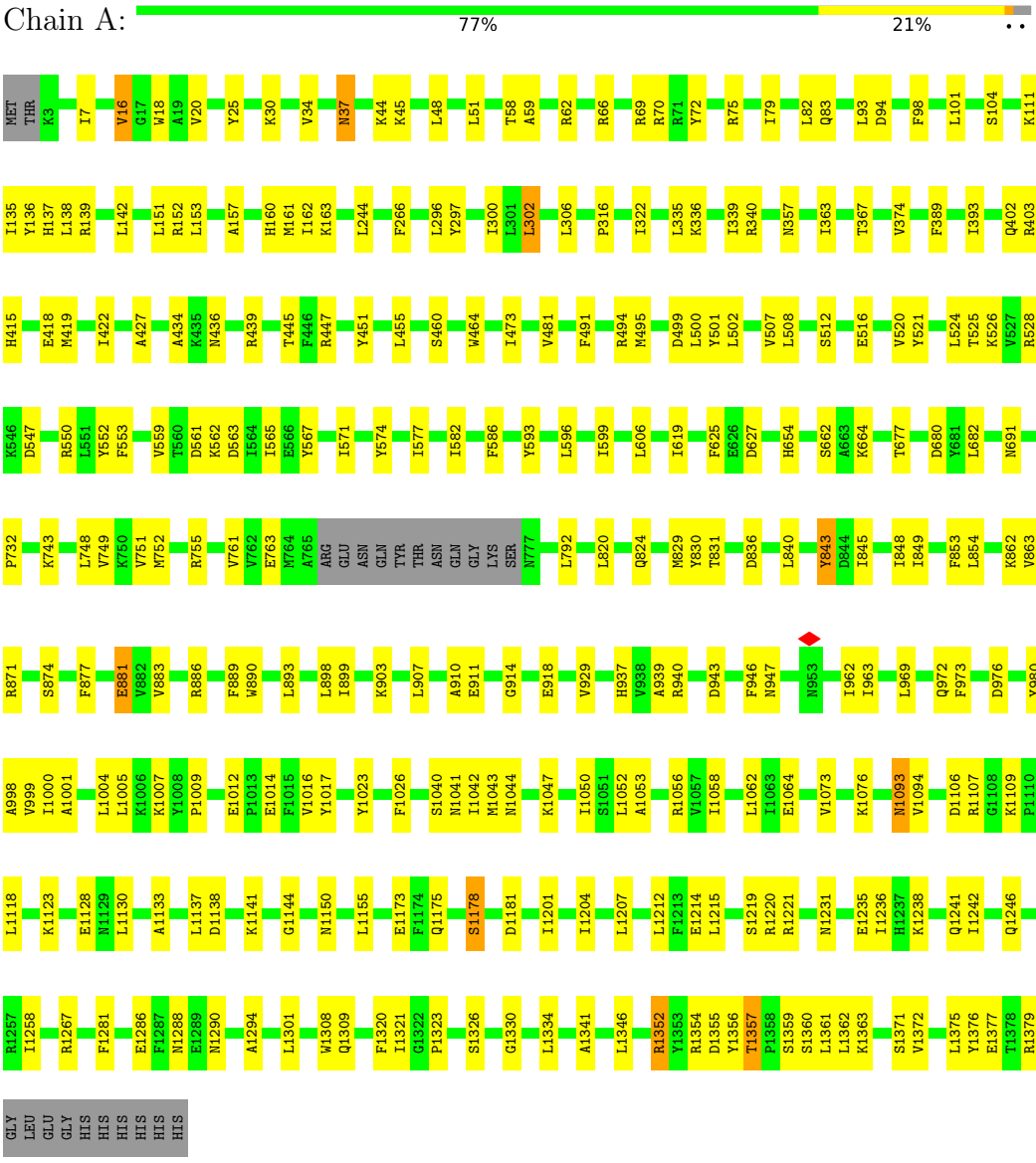
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
9	C	1	1	1	0

3 Residue-property plots (i)

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.

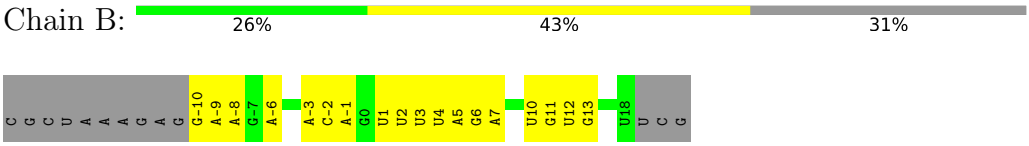
- Molecule 1: CRISPR-associated endonuclease Cas9

Chain A:



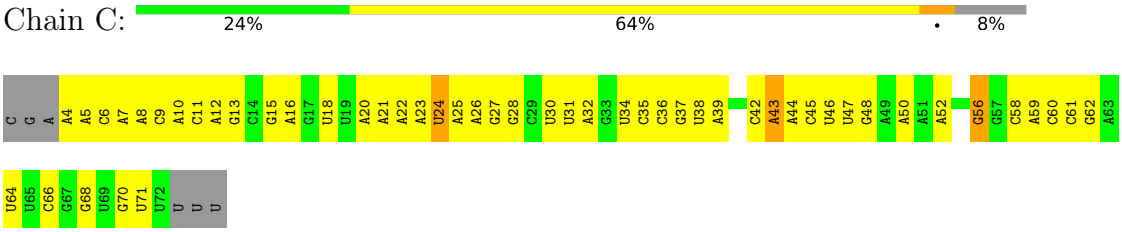
- Molecule 2: Cas9 crRNA

Chain B:



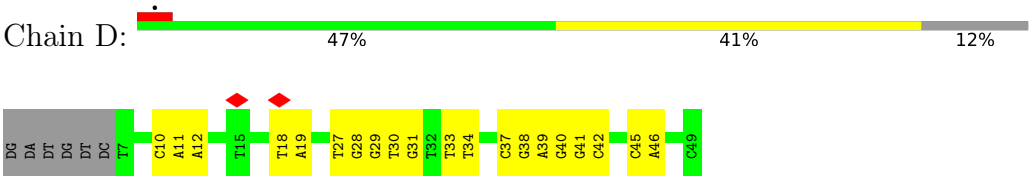
• Molecule 3: Cas9 tracrRNA

Chain C:



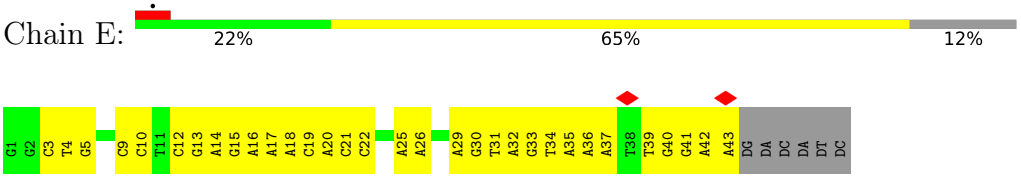
• Molecule 4: DNA (43-MER)

Chain D:



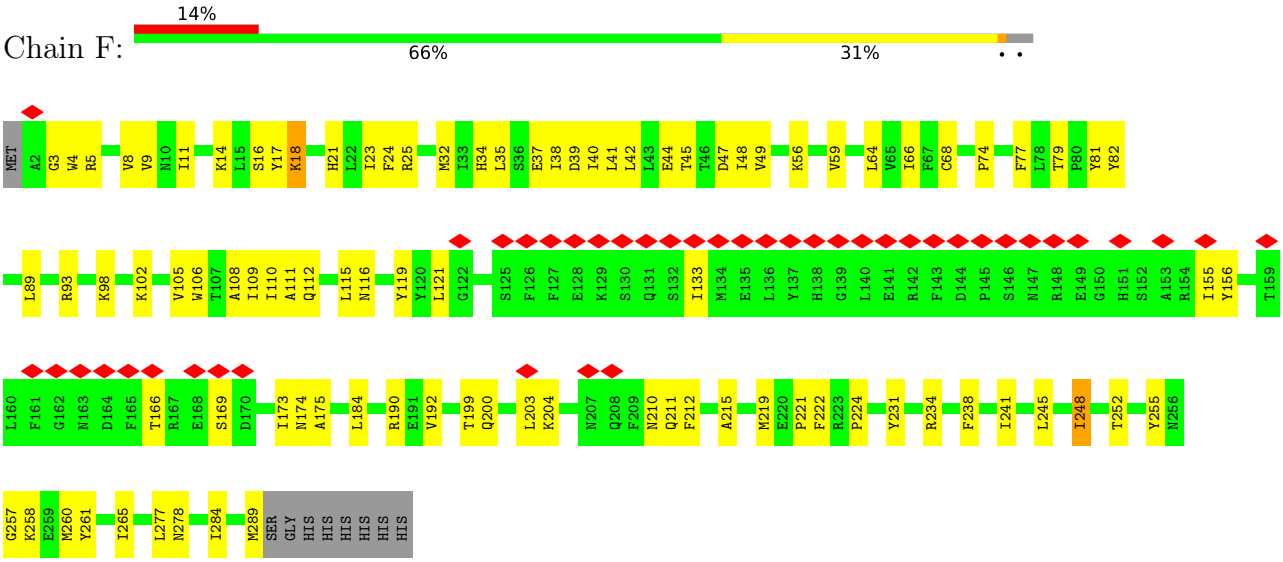
• Molecule 5: DNA (43-MER)

Chain E:



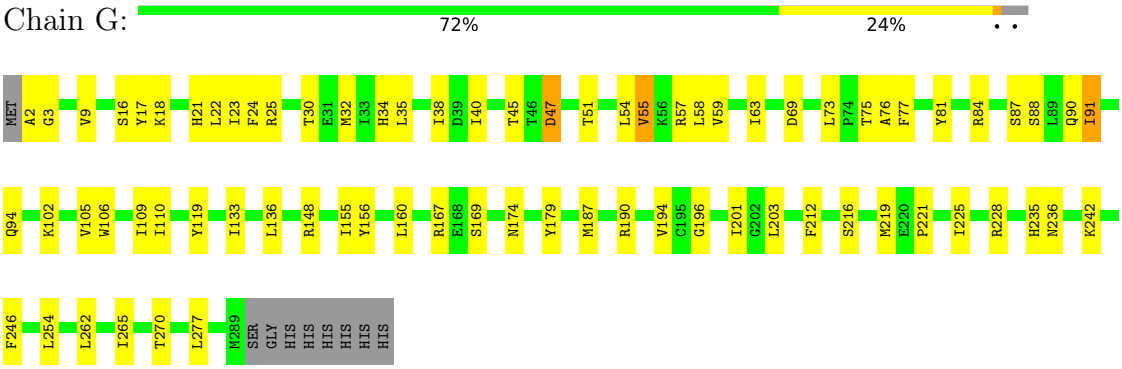
• Molecule 6: CRISPR-associated endonuclease Cas1

Chain F:



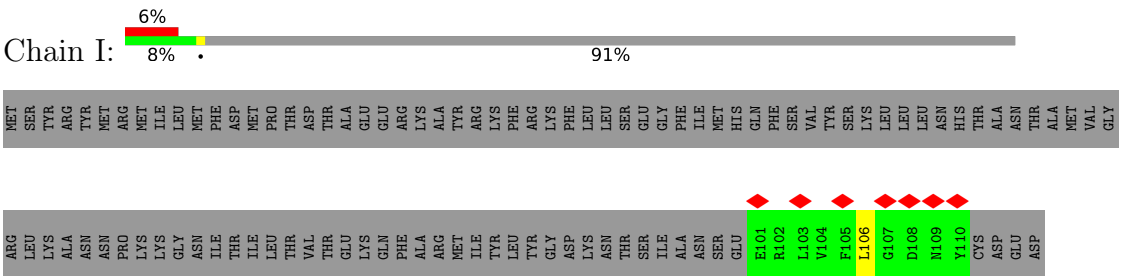
• Molecule 6: CRISPR-associated endonuclease Cas1

Chain G:



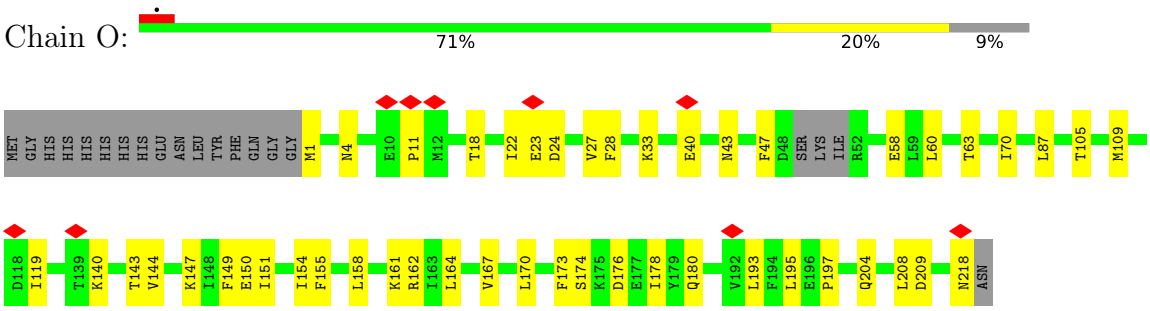
• Molecule 7: CRISPR-associated endoribonuclease Cas2

Chain I:



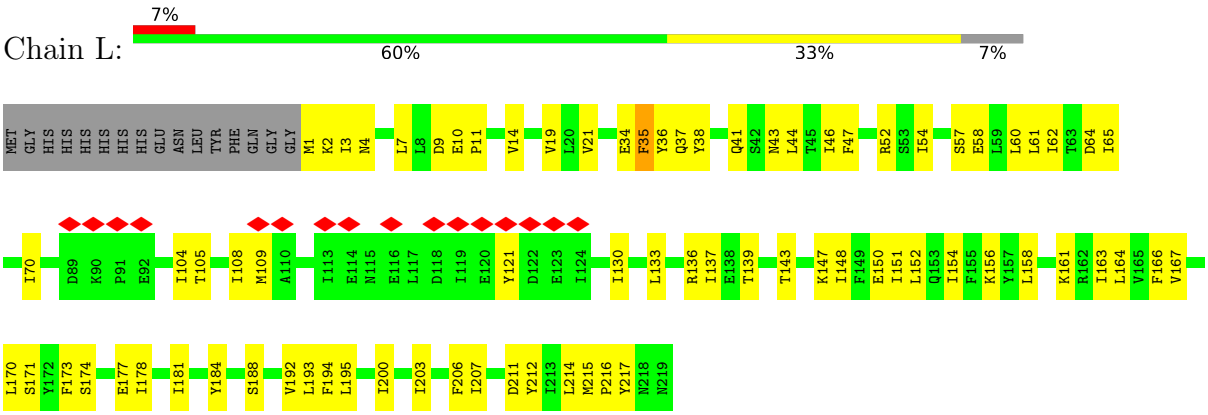
• Molecule 8: CRISPR-associated protein Csn2

Chain O:



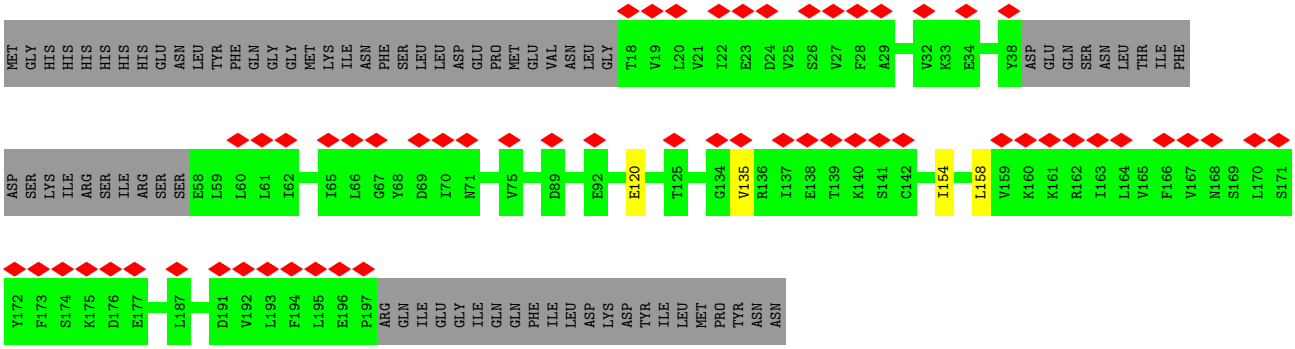
• Molecule 8: CRISPR-associated protein Csn2

Chain L:



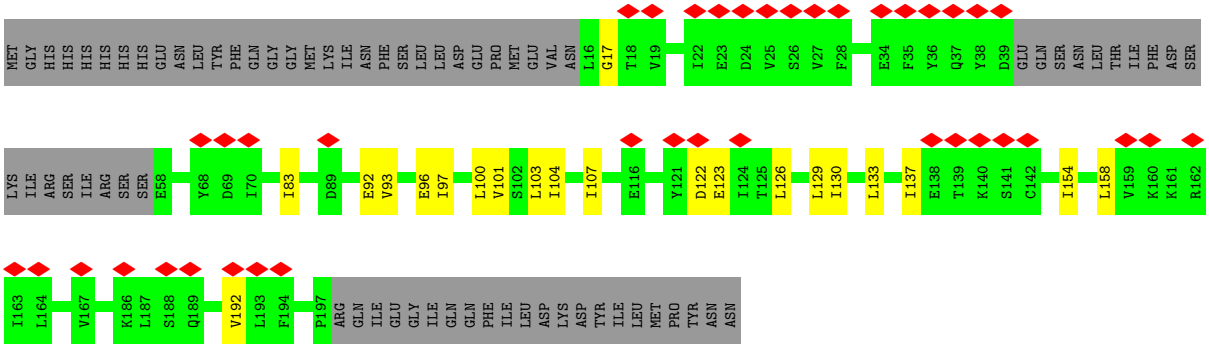
• Molecule 8: CRISPR-associated protein Csn2

Chain N:



• Molecule 8: CRISPR-associated protein Csn2

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26925	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 ($e^-/Å^2$)	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	30.655	Depositor
Minimum map value	-7.448	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.010	Depositor
Recommended contour level	6.31	Depositor
Map size (Å)	369.6, 369.6, 369.6	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.17	0/10522	0.39	0/14248
2	B	0.14	0/698	0.26	0/1087
3	C	0.12	0/1650	0.24	0/2569
4	D	0.20	0/969	0.45	0/1493
5	E	0.17	0/1001	0.39	0/1544
6	F	0.20	0/2056	0.50	0/2816
6	G	0.22	0/2195	0.51	0/2990
7	I	0.12	0/74	0.33	0/100
8	L	0.18	0/1609	0.49	0/2195
8	M	0.15	0/909	0.42	0/1263
8	N	0.11	0/814	0.31	0/1135
8	O	0.18	0/1366	0.43	1/1885 (0.1%)
All	All	0.17	0/23863	0.41	1/33325 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	O	40	GLU	CB-CA-C	-5.03	110.79	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	10325	0	9789	218	0
2	B	624	0	310	20	0
3	C	1474	0	744	46	0
4	D	869	0	491	16	0
5	E	888	0	481	24	0
6	F	2021	0	1814	93	0
6	G	2152	0	2041	65	0
7	I	73	0	61	1	0
8	L	1588	0	1457	66	0
8	M	908	0	539	11	0
8	N	815	0	362	3	0
8	O	1351	0	1041	31	0
9	C	1	0	0	0	0
All	All	23089	0	19130	530	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 13.

All (530) 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)
6:F:56:LYS:HD2	6:G:69:ASP:CB	1.75	1.16
6:F:56:LYS:HD3	6:G:69:ASP:HA	1.20	1.16
6:F:56:LYS:HD2	6:G:69:ASP:HB2	1.11	1.09
1:A:1346:LEU:HD23	1:A:1346:LEU:O	1.59	1.01
6:F:252:THR:HG22	6:F:261:TYR:HD1	1.29	0.97
6:F:56:LYS:CD	6:G:69:ASP:HB2	1.96	0.95
1:A:1004:LEU:HD11	1:A:1042:ILE:HD12	1.49	0.94
6:F:56:LYS:CD	6:G:69:ASP:CB	2.48	0.91
1:A:1042:ILE:HG13	1:A:1043:MET:HE2	1.54	0.89
6:F:56:LYS:HD3	6:G:69:ASP:CA	2.02	0.89
6:F:252:THR:HG22	6:F:261:TYR:CD1	2.09	0.88
6:F:56:LYS:CD	6:G:69:ASP:HA	2.05	0.84
6:F:184:LEU:HD21	6:F:222:PHE:HB3	1.60	0.84
6:G:87:SER:O	6:G:90:GLN:HB3	1.84	0.78
8:O:149:PHE:HZ	8:O:180:GLN:HE21	1.30	0.77
6:F:252:THR:CG2	6:F:261:TYR:CD1	2.69	0.76
1:A:677:THR:HG23	1:A:680:ASP:H	1.50	0.76
1:A:1150:ASN:HA	1:A:1178:SER:HA	1.68	0.75
1:A:943:ASP:OD1	1:A:947:ASN:ND2	2.20	0.75
1:A:451:TYR:O	1:A:464:TRP:NE1	2.20	0.74
8:L:4:ASN:HD22	8:L:11:PRO:HG3	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:17:GLY:HA2	8:M:192:VAL:H	1.53	0.73
1:A:565:ILE:HG23	1:A:577:ILE:HB	1.71	0.72
1:A:1246:GLN:HA	1:A:1249:VAL:HG12	1.70	0.72
6:F:45:THR:HG22	6:F:47:ASP:H	1.54	0.72
6:F:200:GLN:HA	6:F:211:GLN:HA	1.74	0.70
6:F:252:THR:CG2	6:F:261:TYR:HD1	2.03	0.69
6:F:192:VAL:CG1	6:F:199:THR:HG22	2.23	0.69
1:A:70:ARG:NH2	2:B:-6:A:OP1	2.26	0.69
1:A:160:HIS:HD2	3:C:20:A:H5"	1.58	0.68
1:A:82:LEU:HD22	1:A:162:ILE:HD12	1.74	0.68
1:A:1133:ALA:HB3	1:A:1137:LEU:HD12	1.76	0.67
1:A:1256:LYS:HB2	1:A:1321:ILE:HD13	1.77	0.67
6:F:56:LYS:CD	6:G:69:ASP:CA	2.67	0.67
6:F:116:ASN:HB3	6:F:224:PRO:HG3	1.77	0.66
1:A:1341:ALA:HA	1:A:1352:ARG:HD2	1.77	0.65
1:A:883:VAL:HG11	1:A:911:GLU:HB2	1.78	0.65
1:A:1044:ASN:HD22	1:A:1050:ILE:HD12	1.60	0.65
8:L:130:ILE:HA	8:L:133:LEU:HB3	1.78	0.65
1:A:79:ILE:HD11	1:A:163:LYS:HB2	1.79	0.65
1:A:910:ALA:HA	1:A:914:GLY:HA2	1.79	0.65
6:F:255:TYR:H	6:F:258:LYS:HA	1.62	0.64
6:F:192:VAL:HG13	6:F:199:THR:HG22	1.80	0.64
1:A:37:ASN:OD1	1:A:37:ASN:N	2.31	0.64
1:A:44:LYS:NZ	3:C:68:G:O6	2.29	0.64
1:A:34:VAL:HG11	1:A:1379:ARG:HD2	1.80	0.64
8:O:33:LYS:NZ	8:L:143:THR:OG1	2.29	0.64
8:L:35:PHE:HB3	8:L:61:LEU:HD11	1.79	0.64
8:M:126:LEU:HA	8:M:129:LEU:HD23	1.80	0.63
1:A:138:LEU:HD11	1:A:153:LEU:HB3	1.81	0.63
1:A:728:LEU:HD22	1:A:937:HIS:HB3	1.79	0.63
6:F:79:THR:CG2	6:G:77:PHE:CE1	2.82	0.63
8:O:70:ILE:HD12	8:O:154:ILE:HD12	1.79	0.63
1:A:1004:LEU:CD1	1:A:1042:ILE:HD12	2.28	0.62
1:A:412:TYR:HE2	1:A:445:THR:HG22	1.64	0.62
6:F:166:THR:O	6:F:174:ASN:ND2	2.32	0.62
1:A:969:LEU:HD22	1:A:1043:MET:HE3	1.81	0.62
8:M:97:ILE:O	8:M:101:VAL:HG23	2.00	0.62
1:A:1004:LEU:HD11	1:A:1042:ILE:CD1	2.27	0.61
1:A:72:TYR:OH	2:B:-1:A:N6	2.31	0.61
1:A:104:SER:OG	3:C:21:A:N3	2.32	0.61
6:F:260:MET:HB2	6:F:265:ILE:HG12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:37:DC:O2	5:E:13:DG:N1	2.31	0.61
6:F:18:LYS:O	6:F:21:HIS:HB2	2.00	0.61
6:G:169:SER:O	6:G:174:ASN:ND2	2.34	0.60
6:G:2:ALA:N	6:G:34:HIS:O	2.35	0.60
8:L:60:LEU:HD22	8:L:164:LEU:HG	1.83	0.60
1:A:552:TYR:HB3	1:A:559:VAL:HG21	1.83	0.60
1:A:25:TYR:HB3	1:A:999:VAL:HG22	1.84	0.60
1:A:521:TYR:HB3	1:A:682:LEU:HB3	1.82	0.60
1:A:1128:GLU:HG2	1:A:1130:LEU:HG	1.84	0.60
1:A:567:TYR:CE1	1:A:571:ILE:HD12	2.37	0.60
6:G:225:ILE:HD12	6:G:228:ARG:HD2	1.83	0.60
6:F:184:LEU:HD23	6:F:219:MET:SD	2.42	0.60
1:A:843:TYR:HB3	1:A:866:SER:HA	1.83	0.59
1:A:508:LEU:HB3	1:A:512:SER:OG	2.02	0.59
6:G:55:VAL:O	6:G:59:VAL:HG23	2.01	0.59
6:F:169:SER:CB	6:F:174:ASN:ND2	2.65	0.59
1:A:1281:PHE:HZ	1:A:1301:LEU:HB3	1.67	0.59
6:G:109:ILE:HG23	6:G:221:PRO:HD3	1.84	0.59
1:A:524:LEU:HG	1:A:545:LYS:HG2	1.85	0.59
8:O:63:THR:HB	8:L:64:ASP:HB3	1.84	0.59
8:O:140:LYS:O	8:L:37:GLN:NE2	2.34	0.59
6:G:25:ARG:HH22	8:L:217:TYR:HB2	1.68	0.59
1:A:899:ILE:HB	1:A:903:LYS:HD3	1.84	0.58
1:A:1246:GLN:HA	1:A:1249:VAL:CG1	2.33	0.58
6:F:211:GLN:HG2	6:G:84:ARG:HH12	1.69	0.58
6:F:211:GLN:HG2	6:G:84:ARG:NH1	2.18	0.58
8:L:60:LEU:HB2	8:L:161:LYS:HD2	1.85	0.58
1:A:1354:ARG:HG3	1:A:1355:ASP:H	1.68	0.58
6:G:40:ILE:HG21	6:G:194:VAL:HG13	1.83	0.58
1:A:160:HIS:CD2	3:C:20:A:H5"	2.37	0.58
1:A:1009:PRO:O	1:A:1012:GLU:HB3	2.04	0.58
1:A:1346:LEU:O	1:A:1346:LEU:CD2	2.44	0.58
1:A:499:ASP:OD1	1:A:502:LEU:N	2.31	0.58
1:A:507:VAL:HA	1:A:662:SER:HA	1.86	0.58
1:A:139:ARG:NH1	1:A:418:GLU:OE2	2.37	0.57
8:L:36:TYR:CZ	8:L:61:LEU:HD22	2.39	0.57
8:L:215:MET:HE3	8:L:216:PRO:HD2	1.86	0.57
6:F:38:ILE:HD11	6:F:41:LEU:HB2	1.86	0.57
2:B:4:U:H2'	2:B:5:A:H8	1.68	0.57
1:A:75:ARG:NH2	3:C:24:U:O4	2.35	0.57
5:E:12:DC:H1'	5:E:13:DG:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:39:ASP:OD1	6:F:190:ARG:NH1	2.37	0.57
1:A:528:ARG:HB3	1:A:537:TYR:HB3	1.87	0.56
1:A:625:PHE:O	1:A:654:HIS:NE2	2.33	0.56
8:L:105:THR:O	8:L:109:MET:HG3	2.04	0.56
1:A:1107:ARG:HH22	4:D:38:DG:H21	1.53	0.56
6:F:192:VAL:HG13	6:F:199:THR:CG2	2.34	0.56
1:A:59:ALA:HB2	3:C:39:A:H1'	1.87	0.56
1:A:357:ASN:HA	1:A:367:THR:HG21	1.88	0.56
1:A:883:VAL:HA	1:A:890:TRP:HZ3	1.69	0.56
6:F:66:ILE:HG12	6:F:77:PHE:HB3	1.87	0.56
1:A:1106:ASP:HB2	1:A:1111:LYS:HD3	1.88	0.56
8:L:46:ILE:HD13	8:L:163:ILE:HD13	1.87	0.56
1:A:48:LEU:O	1:A:1093:ASN:ND2	2.39	0.56
1:A:849:ILE:HG21	1:A:854:LEU:HB3	1.88	0.56
6:F:173:ILE:HG21	6:F:234:ARG:HG3	1.86	0.56
6:F:121:LEU:HD21	6:F:156:TYR:HA	1.87	0.56
6:F:231:TYR:HA	6:F:234:ARG:HE	1.71	0.55
6:G:25:ARG:HG2	6:G:30:THR:HG23	1.87	0.55
1:A:526:LYS:HD3	1:A:691:ASN:HB3	1.88	0.55
2:B:-10:G:H2'	2:B:-9:A:H8	1.69	0.55
5:E:34:DT:H2"	5:E:35:DA:C8	2.42	0.55
6:F:79:THR:HG21	6:G:77:PHE:CE1	2.42	0.55
1:A:157:ALA:O	1:A:161:MET:HG3	2.06	0.55
1:A:1235:GLU:OE1	1:A:1354:ARG:NH2	2.39	0.55
8:N:154:ILE:O	8:N:158:LEU:N	2.36	0.55
1:A:58:THR:HG22	1:A:732:PRO:HD2	1.88	0.55
2:B:6:G:N2	3:C:18:U:OP2	2.39	0.55
1:A:137:HIS:HA	1:A:322:ILE:HD11	1.89	0.55
1:A:677:THR:HG22	1:A:680:ASP:HB2	1.88	0.55
5:E:31:DT:H2"	5:E:32:DA:C8	2.42	0.55
6:F:68:CYS:HA	6:F:74:PRO:HA	1.89	0.55
8:O:58:GLU:O	8:O:162:ARG:N	2.38	0.55
8:L:70:ILE:HG23	8:L:154:ILE:HD11	1.89	0.55
1:A:567:TYR:HE1	1:A:571:ILE:HD12	1.71	0.54
1:A:336:LYS:NZ	3:C:16:A:OP2	2.39	0.54
6:F:9:VAL:HG12	7:I:106:LEU:HD12	1.89	0.54
8:L:65:ILE:HG21	8:L:148:ILE:HG12	1.89	0.54
8:O:105:THR:O	8:O:109:MET:HG2	2.06	0.54
6:G:216:SER:HA	6:G:219:MET:HE2	1.89	0.54
1:A:763:GLU:OE1	1:A:997:ASN:ND2	2.37	0.54
1:A:1238:LYS:NZ	1:A:1334:LEU:O	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:48:ILE:HD12	6:F:48:ILE:H	1.71	0.54
1:A:136:TYR:OH	1:A:403:ARG:NH1	2.36	0.54
3:C:20:A:H2'	3:C:21:A:C8	2.42	0.54
8:O:23:GLU:HB2	8:O:209:ASP:HA	1.89	0.54
8:M:83:ILE:HG21	8:M:130:ILE:HG21	1.90	0.54
1:A:93:LEU:HD13	1:A:151:LEU:HB2	1.88	0.54
1:A:464:TRP:HE3	1:A:494:ARG:HD2	1.72	0.54
8:L:167:VAL:HG22	8:L:195:LEU:HD23	1.90	0.54
1:A:743:LYS:NZ	3:C:43:A:OP1	2.41	0.53
8:O:4:ASN:HB2	8:O:11:PRO:HG3	1.90	0.53
3:C:9:C:H2'	3:C:10:A:C8	2.43	0.53
3:C:58:C:H2'	3:C:59:A:H8	1.73	0.53
8:O:147:LYS:HE2	8:O:151:ILE:HD11	1.91	0.53
1:A:524:LEU:HD21	1:A:545:LYS:HA	1.91	0.53
1:A:976:ASP:OD2	1:A:1047:LYS:NZ	2.40	0.53
6:F:49:VAL:HG21	8:L:211:ASP:HB3	1.91	0.53
1:A:903:LYS:O	1:A:907:LEU:HG	2.09	0.53
1:A:45:LYS:NZ	1:A:1377:GLU:OE1	2.38	0.53
3:C:58:C:H2'	3:C:59:A:C8	2.44	0.53
6:F:192:VAL:HG11	6:F:199:THR:HG22	1.90	0.53
6:G:133:ILE:HG22	6:G:155:ILE:HD11	1.90	0.53
5:E:21:DC:H2"	5:E:22:DC:C5	2.44	0.53
8:O:119:ILE:HA	8:M:137:ILE:HA	1.90	0.53
8:O:170:LEU:HG	8:O:178:ILE:HD12	1.91	0.53
8:L:60:LEU:HD21	8:L:62:ILE:HD12	1.91	0.53
1:A:677:THR:CG2	1:A:680:ASP:H	2.21	0.52
1:A:973:PHE:HB2	1:A:1000:ILE:HD11	1.91	0.52
8:L:1:MET:HA	8:L:47:PHE:O	2.10	0.52
1:A:306:LEU:HD22	1:A:316:PRO:HB2	1.91	0.52
1:A:1246:GLN:CA	1:A:1249:VAL:HG12	2.37	0.52
8:O:150:GLU:O	8:O:154:ILE:HG13	2.10	0.52
1:A:427:ALA:HB1	1:A:434:ALA:HB2	1.90	0.52
6:G:87:SER:HB2	6:G:196:GLY:HA3	1.91	0.52
8:O:147:LYS:O	8:O:151:ILE:HG12	2.09	0.52
1:A:824:GLN:NE2	1:A:864:LEU:H	2.07	0.52
1:A:969:LEU:CD1	1:A:1042:ILE:HD11	2.39	0.52
2:B:3:U:H2'	2:B:4:U:C6	2.45	0.52
5:E:3:DC:H2'	5:E:4:DT:C6	2.45	0.52
1:A:918:GLU:HG2	1:A:1026:PHE:HZ	1.75	0.52
1:A:963:ILE:HD11	1:A:1005:LEU:HD22	1.91	0.51
8:O:158:LEU:HD22	8:O:161:LYS:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:34:HIS:HB3	6:F:37:GLU:HG3	1.91	0.51
8:L:136:ARG:O	8:N:120:GLU:N	2.36	0.51
2:B:-2:C:H2'	2:B:-1:A:O4'	2.10	0.51
3:C:12:A:H2'	3:C:13:G:H8	1.75	0.51
1:A:111:LYS:NZ	1:A:115:LYS:O	2.43	0.51
3:C:15:G:H2'	3:C:16:A:H8	1.76	0.51
6:F:210:ASN:O	6:G:84:ARG:NH2	2.41	0.51
8:O:143:THR:OG1	8:O:144:VAL:N	2.43	0.51
1:A:1052:LEU:HD13	1:A:1056:ARG:HE	1.74	0.51
1:A:1173:GLU:HA	1:A:1362:LEU:HD11	1.91	0.51
1:A:1371:SER:HA	3:C:43:A:C8	2.46	0.51
1:A:69:ARG:NH2	3:C:38:U:OP2	2.44	0.51
6:G:22:LEU:HD12	6:G:54:LEU:HD11	1.93	0.51
8:O:176:ASP:N	8:O:176:ASP:OD1	2.43	0.51
3:C:9:C:H2'	3:C:10:A:H8	1.76	0.51
8:L:177:GLU:O	8:L:181:ILE:HG12	2.11	0.51
3:C:12:A:H2'	3:C:13:G:C8	2.46	0.51
6:F:203:LEU:HD21	6:F:277:LEU:HD11	1.92	0.50
6:F:252:THR:CG2	6:F:261:TYR:CE1	2.94	0.50
1:A:824:GLN:HE22	1:A:829:MET:HB2	1.76	0.50
1:A:1155:LEU:HB2	1:A:1207:LEU:HD11	1.94	0.50
6:F:184:LEU:HB3	6:F:219:MET:HE1	1.92	0.50
1:A:972:GLN:O	1:A:976:ASP:HB2	2.12	0.50
8:L:1:MET:HG3	8:L:14:VAL:HG23	1.94	0.50
8:L:2:LYS:HB2	8:L:47:PHE:CE1	2.47	0.50
1:A:831:THR:HA	1:A:886:ARG:HH21	1.76	0.50
1:A:848:ILE:HD11	1:A:903:LYS:HE3	1.93	0.50
6:F:212:PHE:HB3	6:F:215:ALA:HB3	1.94	0.50
8:L:121:TYR:HA	8:N:135:VAL:HA	1.93	0.50
8:L:148:ILE:O	8:L:152:LEU:HG	2.11	0.50
1:A:59:ALA:N	2:B:-8:A:OP1	2.42	0.50
6:F:59:VAL:HG11	6:G:76:ALA:HB2	1.94	0.50
1:A:1214:GLU:OE1	1:A:1379:ARG:NH2	2.45	0.49
3:C:4:A:H2'	3:C:5:A:H8	1.76	0.49
5:E:9:DC:H1'	5:E:10:DC:H5'	1.95	0.49
6:F:5:ARG:O	6:F:38:ILE:HA	2.12	0.49
1:A:1258:ILE:HD11	1:A:1267:ARG:HD3	1.93	0.49
6:F:111:ALA:O	6:F:115:LEU:HG	2.11	0.49
1:A:502:LEU:HD22	1:A:664:LYS:HE3	1.94	0.49
8:L:158:LEU:HD23	8:L:161:LYS:HE3	1.93	0.49
1:A:1118:LEU:O	2:B:1:U:O2'	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:35:LEU:HD12	6:G:35:LEU:O	2.13	0.49
8:L:14:VAL:HG11	8:L:193:LEU:HB2	1.95	0.49
8:L:130:ILE:HG22	8:L:133:LEU:HD23	1.93	0.49
8:L:200:ILE:HD11	8:L:203:ILE:HD11	1.94	0.49
1:A:1215:LEU:HD21	1:A:1361:LEU:HD23	1.95	0.49
6:F:184:LEU:HD23	6:F:219:MET:HE1	1.95	0.49
5:E:19:DC:H2"	5:E:20:DA:C8	2.48	0.49
6:F:98:LYS:O	6:F:102:LYS:HG3	2.13	0.49
1:A:94:ASP:OD2	1:A:152:ARG:NH1	2.45	0.49
6:F:106:TRP:O	6:F:110:ILE:HG12	2.13	0.49
6:G:58:LEU:HD22	6:G:63:ILE:HG21	1.94	0.49
1:A:51:LEU:HD12	1:A:1372:VAL:O	2.13	0.48
8:L:64:ASP:OD1	8:L:64:ASP:N	2.44	0.48
1:A:969:LEU:HD13	1:A:1042:ILE:HD11	1.95	0.48
1:A:562:LYS:HA	1:A:565:ILE:HD12	1.96	0.48
6:F:184:LEU:HD21	6:F:222:PHE:CB	2.38	0.48
6:G:88:SER:O	6:G:91:ILE:HG12	2.13	0.48
1:A:984:GLU:N	1:A:984:GLU:OE1	2.46	0.48
3:C:11:C:H2'	3:C:12:A:C8	2.48	0.48
6:G:16:SER:OG	6:G:17:TYR:N	2.45	0.48
1:A:58:THR:HA	1:A:732:PRO:HG2	1.95	0.48
1:A:824:GLN:NE2	1:A:829:MET:HB2	2.29	0.48
8:L:34:GLU:OE2	8:L:43:ASN:ND2	2.39	0.48
2:B:4:U:H2'	2:B:5:A:C8	2.48	0.48
6:F:23:ILE:HG22	6:F:25:ARG:HG3	1.96	0.48
1:A:30:LYS:NZ	3:C:58:C:OP1	2.45	0.48
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.76	0.48
1:A:1014:GLU:OE1	1:A:1023:TYR:OH	2.28	0.48
1:A:1118:LEU:HD21	1:A:1133:ALA:HB2	1.96	0.48
8:L:104:ILE:O	8:L:108:ILE:HG23	2.13	0.48
3:C:4:A:H2'	3:C:5:A:C8	2.49	0.47
6:G:179:TYR:CE2	6:G:242:LYS:HG3	2.48	0.47
6:G:190:ARG:O	6:G:194:VAL:HG23	2.13	0.47
8:O:149:PHE:HZ	8:O:180:GLN:NE2	2.05	0.47
8:O:197:PRO:HG3	8:L:171:SER:HB3	1.96	0.47
1:A:1219:SER:OG	1:A:1221:ARG:NH1	2.48	0.47
1:A:820:LEU:HD23	1:A:864:LEU:HB2	1.96	0.47
2:B:-10:G:H2'	2:B:-9:A:C8	2.48	0.47
5:E:16:DA:H2"	5:E:17:DA:C8	2.49	0.47
1:A:845:ILE:HD13	1:A:862:LYS:NZ	2.30	0.47
1:A:1212:LEU:HD11	1:A:1220:ARG:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1288:ASN:HD22	1:A:1334:LEU:HD21	1.80	0.47
6:G:254:LEU:H	6:G:254:LEU:HD23	1.80	0.47
8:L:38:TYR:OH	8:L:46:ILE:N	2.45	0.47
1:A:664:LYS:HB3	1:A:664:LYS:HE2	1.68	0.47
3:C:15:G:H2'	3:C:16:A:C8	2.50	0.47
1:A:830:TYR:CD2	1:A:865:VAL:HG11	2.49	0.47
1:A:1376:TYR:HB3	3:C:56:G:N1	2.30	0.47
6:G:18:LYS:O	6:G:21:HIS:HB2	2.15	0.47
6:G:94:GLN:HG3	6:G:201:ILE:HD12	1.96	0.47
8:L:151:ILE:HA	8:L:154:ILE:HG13	1.95	0.47
6:F:11:ILE:HD11	6:F:24:PHE:HZ	1.80	0.47
6:F:16:SER:OG	6:F:17:TYR:N	2.46	0.47
6:F:81:TYR:CZ	6:G:77:PHE:HD2	2.33	0.47
1:A:266:PHE:HB3	1:A:297:TYR:CE2	2.49	0.47
3:C:44:A:H2'	3:C:45:C:C6	2.50	0.47
6:G:45:THR:OG1	6:G:47:ASP:OD2	2.30	0.47
3:C:60:C:H2'	3:C:61:C:C6	2.50	0.46
3:C:70:G:H2'	3:C:71:U:C6	2.51	0.46
6:F:56:LYS:HD2	6:G:69:ASP:HB3	1.86	0.46
1:A:335:LEU:O	1:A:339:ILE:HG22	2.15	0.46
1:A:1352:ARG:HH22	4:D:39:DA:H2'	1.80	0.46
6:F:8:VAL:HG13	6:F:42:LEU:HB3	1.96	0.46
1:A:521:TYR:O	1:A:525:THR:HG23	2.16	0.46
1:A:963:ILE:HG12	1:A:1016:VAL:HG22	1.97	0.46
3:C:27:G:H2'	3:C:28:G:H8	1.81	0.46
8:O:167:VAL:HG13	8:O:195:LEU:HD23	1.96	0.46
8:M:92:GLU:O	8:M:96:GLU:HG2	2.15	0.46
5:E:35:DA:H2"	5:E:36:DA:C8	2.51	0.46
5:E:40:DG:H2"	5:E:41:DG:C8	2.51	0.46
8:L:148:ILE:HG13	8:L:173:PHE:CZ	2.51	0.46
8:L:150:GLU:O	8:L:154:ILE:HG13	2.15	0.46
8:M:122:ASP:OD1	8:M:123:GLU:N	2.46	0.46
1:A:163:LYS:NZ	3:C:22:A:OP2	2.39	0.46
6:F:169:SER:H	6:F:174:ASN:ND2	2.14	0.46
8:L:62:ILE:O	8:L:166:PHE:HA	2.15	0.46
8:L:174:SER:O	8:L:178:ILE:HG13	2.16	0.46
1:A:1308:TRP:CE2	1:A:1309:GLN:HG3	2.50	0.46
3:C:23:A:H2'	3:C:24:U:O4'	2.16	0.46
6:F:261:TYR:O	6:F:265:ILE:HG13	2.16	0.46
8:L:60:LEU:HD13	8:L:164:LEU:HD12	1.97	0.46
1:A:582:ILE:HD11	1:A:586:PHE:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:30:DT:H2"	4:D:31:DG:C8	2.51	0.46
6:F:14:LYS:NZ	6:F:25:ARG:HE	2.14	0.46
8:O:204:GLN:HA	8:O:218:ASN:HA	1.98	0.46
1:A:1138:ASP:HB2	1:A:1141:LYS:HB2	1.98	0.46
4:D:18:DT:H2"	4:D:19:DA:C8	2.51	0.46
6:F:49:VAL:HA	6:G:51:THR:HA	1.97	0.46
1:A:16:VAL:HG13	1:A:51:LEU:HB3	1.98	0.46
1:A:1106:ASP:O	1:A:1109:LYS:HB2	2.16	0.45
6:F:245:LEU:O	6:F:248:ILE:HG12	2.16	0.45
8:O:60:LEU:HD22	8:O:161:LYS:HG3	1.99	0.45
8:L:9:ASP:OD1	8:L:10:GLU:N	2.47	0.45
8:L:70:ILE:HG22	8:L:137:ILE:HD13	1.98	0.45
1:A:414:ILE:O	1:A:418:GLU:HG3	2.17	0.45
6:F:93:ARG:HE	6:F:278:ASN:HB2	1.80	0.45
1:A:296:LEU:O	1:A:300:ILE:HG12	2.17	0.45
8:L:41:GLN:HE22	8:L:44:LEU:HB3	1.82	0.45
4:D:28:DG:H2"	4:D:29:DG:N7	2.32	0.45
1:A:139:ARG:HH22	1:A:415:HIS:HE1	1.65	0.45
1:A:436:ASN:ND2	1:A:439:ARG:HH21	2.14	0.45
1:A:829:MET:HG3	1:A:890:TRP:HE1	1.81	0.45
1:A:1175:GLN:OE1	1:A:1231:ASN:ND2	2.49	0.45
4:D:27:DT:H2"	4:D:28:DG:C8	2.52	0.45
6:F:133:ILE:HG12	6:F:155:ILE:HD11	1.98	0.45
1:A:62:ARG:HD3	1:A:66:ARG:NH1	2.32	0.45
1:A:101:LEU:O	3:C:21:A:O2'	2.33	0.45
6:F:4:TRP:N	6:F:37:GLU:O	2.42	0.45
6:F:210:ASN:C	6:G:84:ARG:HH12	2.23	0.45
6:G:119:TYR:HE2	6:G:228:ARG:HH22	1.65	0.45
1:A:244:LEU:HG	1:A:266:PHE:CE2	2.52	0.45
1:A:547:ASP:OD1	1:A:550:ARG:NH2	2.49	0.45
5:E:15:DG:H2"	5:E:16:DA:C8	2.52	0.45
6:F:81:TYR:HD2	6:G:75:THR:C	2.24	0.45
8:L:105:THR:O	8:L:108:ILE:HG12	2.16	0.45
8:M:154:ILE:O	8:M:158:LEU:N	2.50	0.45
3:C:7:A:H2'	3:C:8:A:H8	1.82	0.45
3:C:46:U:H2'	3:C:47:U:H6	1.82	0.45
5:E:17:DA:H2"	5:E:18:DA:C8	2.52	0.45
6:G:102:LYS:HD3	6:G:203:LEU:HA	1.98	0.45
8:O:174:SER:O	8:O:178:ILE:HG12	2.17	0.45
1:A:516:GLU:O	1:A:520:VAL:HG12	2.16	0.45
1:A:1118:LEU:HD23	1:A:1144:GLY:HA2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:ILE:HG23	6:F:221:PRO:HD3	1.99	0.44
1:A:1058:ILE:HD12	1:A:1058:ILE:HA	1.83	0.44
3:C:6:C:H2'	3:C:7:A:H8	1.81	0.44
3:C:46:U:H2'	3:C:47:U:C6	2.52	0.44
1:A:460:SER:OG	3:C:36:C:OP1	2.34	0.44
2:B:-3:A:H2'	2:B:-2:C:H6	1.83	0.44
6:F:74:PRO:HB2	6:G:81:TYR:HE2	1.83	0.44
1:A:473:ILE:HG12	1:A:481:VAL:HG11	1.99	0.44
1:A:500:LEU:HD21	2:B:-10:G:N1	2.32	0.44
1:A:824:GLN:OE1	1:A:829:MET:N	2.50	0.44
6:F:79:THR:HG21	6:G:77:PHE:HE1	1.83	0.44
8:O:24:ASP:HB3	8:O:27:VAL:HG22	1.99	0.44
1:A:340:ARG:O	1:A:340:ARG:NH1	2.51	0.44
1:A:929:VAL:HG23	1:A:1014:GLU:HG3	1.99	0.44
6:F:39:ASP:O	6:F:190:ARG:NH1	2.51	0.44
8:L:21:VAL:HB	8:L:207:ILE:HD13	1.99	0.44
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.90	0.44
2:B:-3:A:H2'	2:B:-2:C:C6	2.52	0.44
2:B:10:U:H2'	2:B:11:G:C8	2.53	0.44
6:G:235:HIS:O	6:G:236:ASN:ND2	2.51	0.44
1:A:749:VAL:HG21	1:A:946:PHE:CE1	2.52	0.44
3:C:11:C:H2'	3:C:12:A:H8	1.82	0.44
6:F:106:TRP:CZ3	6:F:204:LYS:HA	2.52	0.44
6:F:257:GLY:HA3	6:F:260:MET:HE2	2.00	0.44
1:A:524:LEU:CD2	1:A:545:LYS:HG2	2.47	0.44
1:A:845:ILE:HG21	1:A:862:LYS:HZ2	1.82	0.44
1:A:939:ALA:HA	1:A:962:ILE:HG21	2.00	0.44
3:C:44:A:H2'	3:C:45:C:H6	1.82	0.44
5:E:39:DT:H2"	5:E:40:DG:C8	2.52	0.44
6:G:262:LEU:HA	6:G:265:ILE:HG22	1.99	0.44
1:A:512:SER:HA	1:A:619:ILE:HG21	2.00	0.43
1:A:561:ASP:O	1:A:565:ILE:HG13	2.17	0.43
1:A:840:LEU:HD23	1:A:843:TYR:HE1	1.82	0.43
1:A:1359:SER:O	1:A:1363:LYS:NZ	2.44	0.43
1:A:451:TYR:HE2	1:A:627:ASP:OD2	2.02	0.43
1:A:464:TRP:CE3	1:A:494:ARG:HD2	2.52	0.43
1:A:845:ILE:HD13	1:A:862:LYS:HZ2	1.83	0.43
3:C:22:A:H2'	3:C:23:A:C8	2.53	0.43
5:E:41:DG:H2"	5:E:42:DA:C8	2.53	0.43
8:O:70:ILE:HD13	8:O:70:ILE:HA	1.85	0.43
1:A:491:PHE:CE1	1:A:495:MET:HE3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:TYR:HB3	1:A:577:ILE:HD11	2.00	0.43
1:A:1323:PRO:HB2	1:A:1326:SER:HB3	2.00	0.43
4:D:11:DA:H2"	4:D:12:DA:C8	2.53	0.43
1:A:571:ILE:HG23	8:L:11:PRO:HG2	2.01	0.43
1:A:1201:ILE:HD12	1:A:1204:ILE:HD11	1.99	0.43
6:F:119:TYR:CD2	6:F:289:MET:HB3	2.52	0.43
6:F:231:TYR:HA	6:F:234:ARG:NE	2.33	0.43
6:F:238:PHE:HA	6:F:241:ILE:HD12	2.00	0.43
8:L:156:LYS:HE2	8:L:156:LYS:HB3	1.80	0.43
1:A:1288:ASN:HD21	1:A:1294:ALA:HB3	1.84	0.43
6:F:89:LEU:O	6:F:93:ARG:HG3	2.18	0.43
8:L:70:ILE:HD11	8:L:147:LYS:HE3	2.00	0.43
1:A:559:VAL:HG13	1:A:563:ASP:HB2	2.01	0.43
1:A:761:VAL:HG21	1:A:998:ALA:HA	2.00	0.43
1:A:1352:ARG:HH22	4:D:39:DA:C2'	2.32	0.43
1:A:1352:ARG:HH12	4:D:39:DA:H2'	1.84	0.43
6:F:79:THR:HG23	6:G:77:PHE:CE1	2.54	0.43
6:F:173:ILE:HD13	6:F:234:ARG:HD2	2.01	0.43
6:G:90:GLN:O	6:G:94:GLN:N	2.49	0.43
1:A:18:TRP:HE3	1:A:748:LEU:HD11	1.83	0.43
1:A:1281:PHE:HB2	1:A:1320:PHE:CZ	2.54	0.43
6:F:44:GLU:HA	6:F:68:CYS:SG	2.59	0.43
6:G:106:TRP:O	6:G:110:ILE:HG12	2.19	0.43
8:L:54:ILE:HG23	8:L:58:GLU:HB2	2.01	0.43
1:A:501:TYR:HA	1:A:711:GLN:HE21	1.83	0.42
3:C:7:A:H2'	3:C:8:A:C8	2.54	0.42
6:G:21:HIS:ND1	6:G:32:MET:HE3	2.34	0.42
8:L:58:GLU:HA	8:L:161:LYS:HA	2.01	0.42
6:G:105:VAL:HG21	6:G:277:LEU:HD11	2.00	0.42
8:O:155:PHE:CD1	8:O:164:LEU:HD13	2.54	0.42
1:A:1246:GLN:C	1:A:1249:VAL:HG12	2.44	0.42
8:L:58:GLU:OE1	8:L:58:GLU:N	2.47	0.42
1:A:136:TYR:HH	1:A:403:ARG:HH11	1.64	0.42
1:A:1286:GLU:O	1:A:1290:ASN:HB2	2.19	0.42
8:M:103:LEU:O	8:M:107:ILE:HG12	2.19	0.42
6:G:136:LEU:HA	6:G:148:ARG:HH11	1.85	0.42
6:G:156:TYR:CZ	6:G:160:LEU:HD11	2.55	0.42
1:A:7:ILE:HG12	1:A:20:VAL:HG22	2.02	0.42
1:A:752:MET:O	1:A:755:ARG:NH2	2.41	0.42
1:A:830:TYR:CE2	1:A:871:ARG:HB3	2.55	0.42
1:A:830:TYR:O	1:A:886:ARG:NE	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1359:SER:OG	5:E:4:DT:OP1	2.36	0.42
4:D:10:DC:H2"	4:D:11:DA:C8	2.54	0.42
6:G:187:MET:HE1	6:G:262:LEU:HD23	2.01	0.42
8:L:52:ARG:HA	8:L:52:ARG:HD3	1.71	0.42
8:L:148:ILE:HA	8:L:151:ILE:HG22	2.01	0.42
1:A:596:LEU:HA	1:A:599:ILE:HD12	2.02	0.42
1:A:848:ILE:HG22	1:A:877:PHE:HD1	1.85	0.42
1:A:853:PHE:HA	1:A:1040:SER:H	1.84	0.42
1:A:1041:ASN:HB3	1:A:1044:ASN:OD1	2.20	0.42
2:B:2:U:H2'	2:B:3:U:C6	2.55	0.42
5:E:42:DA:H2"	5:E:43:DA:C8	2.54	0.42
6:F:105:VAL:HG13	6:F:284:ILE:HD12	2.02	0.42
1:A:389:PHE:O	1:A:393:ILE:HG12	2.19	0.42
1:A:403:ARG:HB3	2:B:-1:A:OP1	2.19	0.42
1:A:874:SER:HB2	1:A:1053:ALA:HB3	2.00	0.42
6:F:169:SER:CA	6:F:174:ASN:HD22	2.33	0.42
6:G:17:TYR:CE2	6:G:57:ARG:HG3	2.55	0.42
1:A:363:ILE:HG23	3:C:18:U:H5'	2.00	0.42
1:A:403:ARG:HH21	2:B:-1:A:P	2.43	0.42
5:E:29:DA:H2"	5:E:30:DG:C8	2.55	0.42
6:F:169:SER:N	6:F:174:ASN:ND2	2.68	0.42
8:L:41:GLN:NE2	8:L:44:LEU:HB3	2.34	0.42
1:A:455:LEU:HB3	1:A:473:ILE:HD12	2.01	0.42
1:A:881:GLU:H	1:A:881:GLU:HG3	1.68	0.42
1:A:1357:THR:O	1:A:1360:SER:OG	2.33	0.42
8:M:100:LEU:O	8:M:104:ILE:HG22	2.19	0.42
1:A:134:THR:HG21	1:A:402:GLN:HE21	1.83	0.41
1:A:142:LEU:HD12	1:A:422:ILE:HD11	2.01	0.41
3:C:6:C:H2'	3:C:7:A:C8	2.55	0.41
4:D:45:DC:H2"	4:D:46:DA:C8	2.55	0.41
6:F:3:GLY:C	6:F:39:ASP:HB2	2.45	0.41
6:G:167:ARG:NH1	6:G:174:ASN:OD1	2.42	0.41
8:L:139:THR:O	8:L:139:THR:OG1	2.31	0.41
8:L:164:LEU:HD22	8:L:192:VAL:HG22	2.02	0.41
8:L:170:LEU:HD21	8:L:194:PHE:CG	2.55	0.41
1:A:889:PHE:O	1:A:893:LEU:HG	2.20	0.41
4:D:37:DC:O2	5:E:13:DG:C2	2.73	0.41
5:E:25:DA:H2"	5:E:26:DA:C8	2.55	0.41
8:O:1:MET:HA	8:O:47:PHE:O	2.20	0.41
8:L:7:LEU:HD12	8:L:212:TYR:HB3	2.02	0.41
8:L:57:SER:OG	8:L:58:GLU:OE1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:169:SER:CB	6:F:174:ASN:HD21	2.32	0.41
1:A:792:LEU:HD22	1:A:898:LEU:HD11	2.02	0.41
1:A:1007:LYS:NZ	1:A:1064:GLU:OE1	2.45	0.41
6:F:119:TYR:CE2	6:F:289:MET:HB3	2.56	0.41
6:G:3:GLY:O	6:G:38:ILE:HA	2.20	0.41
8:O:22:ILE:HB	8:O:28:PHE:HB2	2.01	0.41
1:A:836:ASP:O	1:A:843:TYR:OH	2.24	0.41
1:A:980:TYR:HD2	1:A:1250:LYS:HG2	1.86	0.41
4:D:40:DG:H2"	4:D:41:DG:C8	2.56	0.41
8:L:215:MET:HE3	8:L:215:MET:HA	2.03	0.41
1:A:1321:ILE:C	1:A:1330:GLY:H	2.28	0.41
5:E:36:DA:H2"	5:E:37:DA:C8	2.56	0.41
1:A:83:GLN:HG2	1:A:98:PHE:CE1	2.55	0.41
3:C:26:A:OP2	3:C:37:G:N2	2.52	0.41
8:L:206:PHE:HD2	8:L:214:LEU:HD11	1.85	0.41
1:A:940:ARG:HG3	1:A:1017:TYR:OH	2.21	0.41
1:A:1094:VAL:HG11	1:A:1241:GLN:NE2	2.35	0.41
2:B:11:G:H2'	2:B:12:U:C6	2.56	0.41
6:G:18:LYS:HB2	6:G:23:ILE:HD11	2.02	0.41
1:A:161:MET:HE1	1:A:419:MET:HA	2.03	0.41
1:A:553:PHE:CE1	1:A:559:VAL:HB	2.55	0.41
1:A:593:TYR:CE1	1:A:606:LEU:HB3	2.56	0.41
1:A:820:LEU:HD21	1:A:863:VAL:C	2.46	0.41
1:A:1178:SER:OG	1:A:1181:ASP:OD2	2.39	0.41
1:A:1236:ILE:HB	1:A:1356:TYR:HB3	2.02	0.41
4:D:41:DG:C6	4:D:42:DC:C4	3.09	0.41
5:E:14:DA:H2"	5:E:15:DG:C8	2.55	0.41
6:F:40:ILE:HG12	6:F:64:LEU:HB3	2.03	0.41
6:F:108:ALA:O	6:F:112:GLN:HG3	2.21	0.41
6:F:175:ALA:HB3	6:F:238:PHE:HE2	1.86	0.41
8:O:18:THR:O	8:O:193:LEU:HA	2.21	0.41
8:O:164:LEU:HD12	8:O:164:LEU:HA	1.96	0.41
8:M:129:LEU:O	8:M:133:LEU:HD22	2.21	0.41
1:A:340:ARG:HD2	1:A:340:ARG:HA	1.82	0.41
1:A:963:ILE:HG21	1:A:1001:ALA:HB1	2.02	0.41
1:A:1123:LYS:HE3	1:A:1123:LYS:HB2	1.95	0.41
4:D:33:DT:H2"	4:D:34:DT:C6	2.56	0.41
5:E:32:DA:H2"	5:E:33:DG:C8	2.56	0.41
6:F:21:HIS:ND1	6:F:32:MET:HG2	2.36	0.41
8:L:137:ILE:H	8:L:137:ILE:HD12	1.85	0.41
8:L:184:TYR:O	8:L:188:SER:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:LEU:O	1:A:1076:LYS:HG3	2.20	0.40
3:C:48:G:O2'	3:C:50:A:N7	2.43	0.40
6:G:58:LEU:HD23	6:G:58:LEU:HA	1.96	0.40
6:G:179:TYR:HE2	6:G:242:LYS:HG3	1.86	0.40
6:G:262:LEU:O	6:G:265:ILE:HG22	2.20	0.40
5:E:4:DT:H2"	5:E:5:DG:C8	2.56	0.40
6:F:106:TRP:HE1	6:F:110:ILE:HD11	1.86	0.40
6:G:9:VAL:HG12	6:G:24:PHE:CZ	2.56	0.40
2:B:-10:G:C2	2:B:-9:A:C5	3.09	0.40
3:C:59:A:N6	3:C:70:G:O6	2.54	0.40
6:G:73:LEU:HD13	6:G:212:PHE:CZ	2.56	0.40
1:A:751:VAL:HG21	1:A:1375:LEU:HD12	2.03	0.40
8:O:208:LEU:HD13	8:O:208:LEU:HA	1.95	0.40
8:L:19:VAL:HG22	8:L:194:PHE:HB2	2.03	0.40
1:A:135:ILE:HG21	1:A:160:HIS:CD2	2.56	0.40
8:L:60:LEU:HD12	8:L:161:LYS:NZ	2.36	0.40
8:L:166:PHE:HD2	8:L:194:PHE:HE1	1.69	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	1368/1397 (98%)	1334 (98%)	34 (2%)	0	100	100
6	F	286/297 (96%)	275 (96%)	11 (4%)	0	100	100
6	G	286/297 (96%)	280 (98%)	6 (2%)	0	100	100
7	I	8/114 (7%)	8 (100%)	0	0	100	100
8	L	217/235 (92%)	211 (97%)	6 (3%)	0	100	100
8	M	160/235 (68%)	157 (98%)	3 (2%)	0	100	100
8	N	157/235 (67%)	156 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	O	211/235 (90%)	205 (97%)	6 (3%)	0	100	100
All	All	2693/3045 (88%)	2626 (98%)	67 (2%)	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	965/1260 (77%)	951 (98%)	14 (2%)	57	68
6	F	173/272 (64%)	169 (98%)	4 (2%)	44	62
6	G	201/272 (74%)	196 (98%)	5 (2%)	42	61
7	I	6/102 (6%)	6 (100%)	0	100	100
8	L	148/224 (66%)	146 (99%)	2 (1%)	59	70
8	M	32/224 (14%)	31 (97%)	1 (3%)	35	57
8	N	4/224 (2%)	4 (100%)	0	100	100
8	O	91/224 (41%)	88 (97%)	3 (3%)	33	55
All	All	1620/2802 (58%)	1591 (98%)	29 (2%)	51	67

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	37	ASN
1	A	302	LEU
1	A	374	VAL
1	A	447	ARG
1	A	843	TYR
1	A	881	GLU
1	A	1073	VAL
1	A	1093	ASN
1	A	1114	PHE

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Mol	Chain	Res	Type
1	A	1178	SER
1	A	1242	ILE
1	A	1352	ARG
1	A	1357	THR
6	F	18	LYS
6	F	35	LEU
6	F	82	TYR
6	F	248	ILE
6	G	47	ASP
6	G	55	VAL
6	G	91	ILE
6	G	246	PHE
6	G	270	THR
8	O	43	ASN
8	O	87	LEU
8	O	173	PHE
8	L	3	ILE
8	L	35	PHE
8	M	93	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	426	GLN
1	A	436	ASN
1	A	544	GLN
1	A	689	ASN
1	A	933	GLN
1	A	1241	GLN
1	A	1288	ASN
6	F	10	ASN
6	F	174	ASN
6	G	21	HIS
6	G	90	GLN
6	G	211	GLN
6	G	256	ASN
8	O	4	ASN
8	O	71	ASN
8	O	180	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	28/42 (66%)	2 (7%)	0
3	C	68/75 (90%)	14 (20%)	0
All	All	96/117 (82%)	16 (16%)	0

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	7	A
2	B	13	G
3	C	24	U
3	C	25	A
3	C	30	U
3	C	31	U
3	C	32	A
3	C	34	U
3	C	35	C
3	C	42	C
3	C	43	A
3	C	52	A
3	C	56	G
3	C	62	G
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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

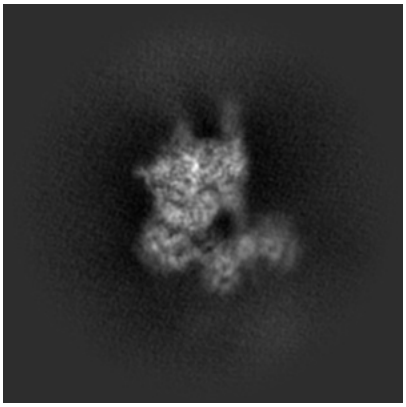
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52320. These allow visual inspection of the internal detail of the map and identification of artifacts.

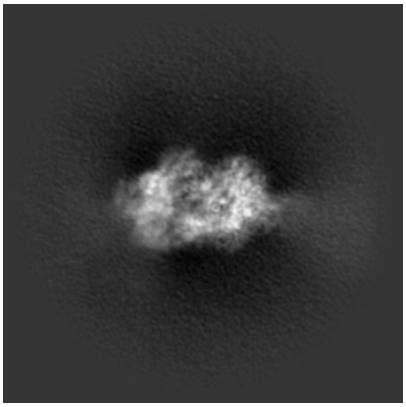
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

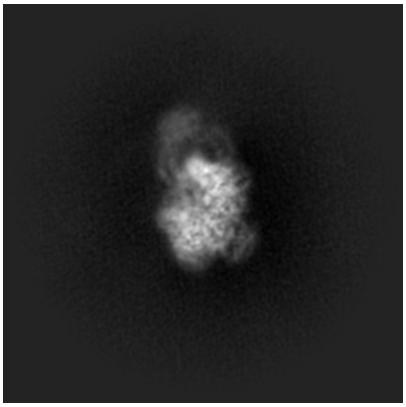
6.1.1 Primary map



X



Y

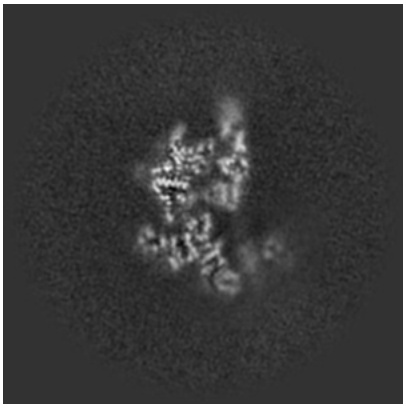


Z

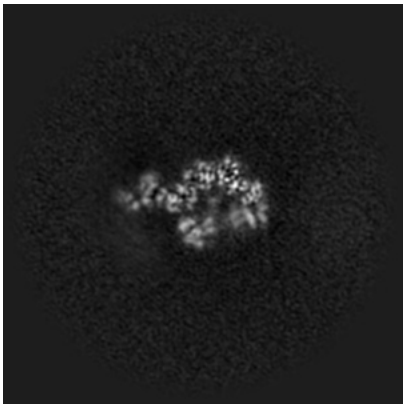
The images above show the map projected in three orthogonal directions.

6.2 Central slices

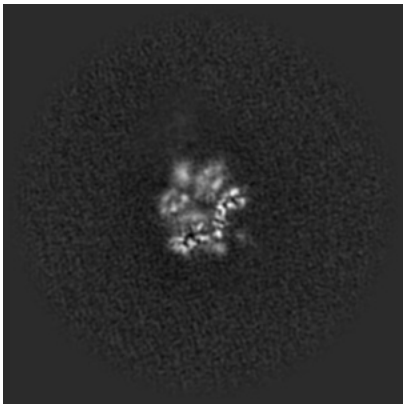
6.2.1 Primary map



X Index: 168



Y Index: 168

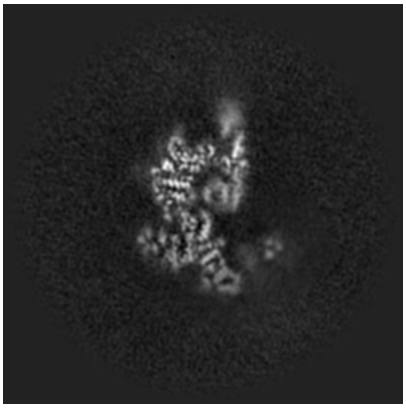


Z Index: 168

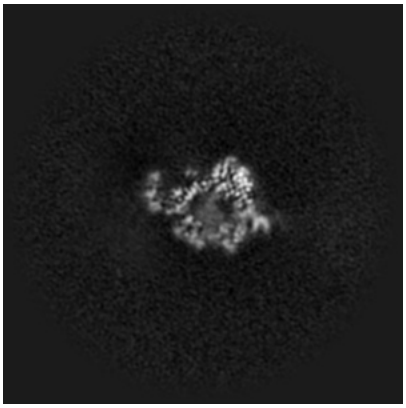
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

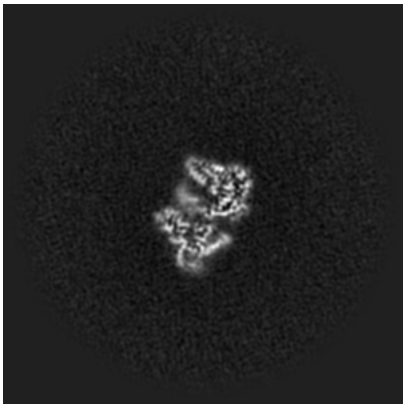
6.3.1 Primary map



X Index: 170



Y Index: 161

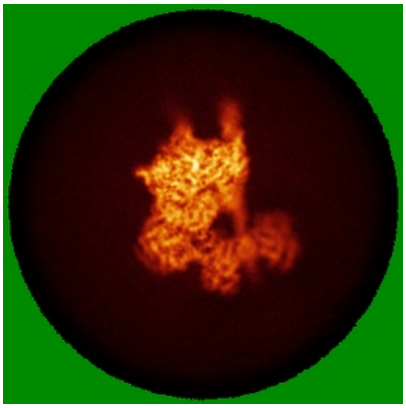


Z Index: 196

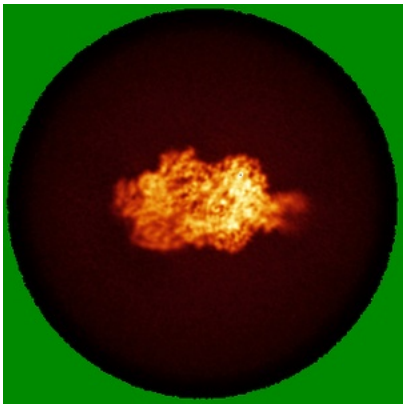
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

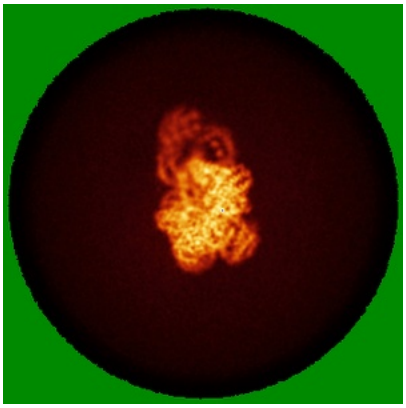
6.4.1 Primary map



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 6.31. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

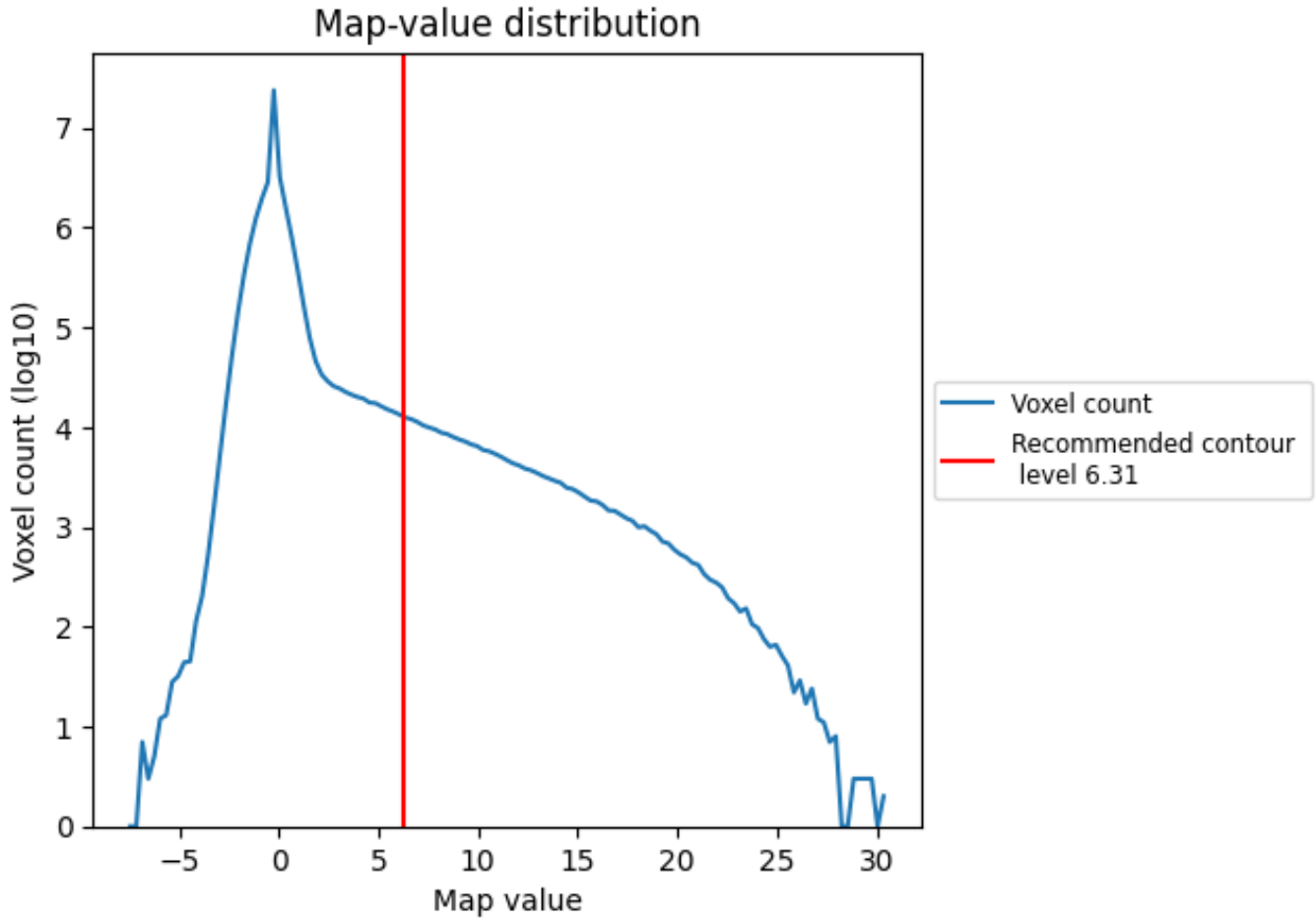
6.6 Mask visualisation (i)

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

7 Map analysis

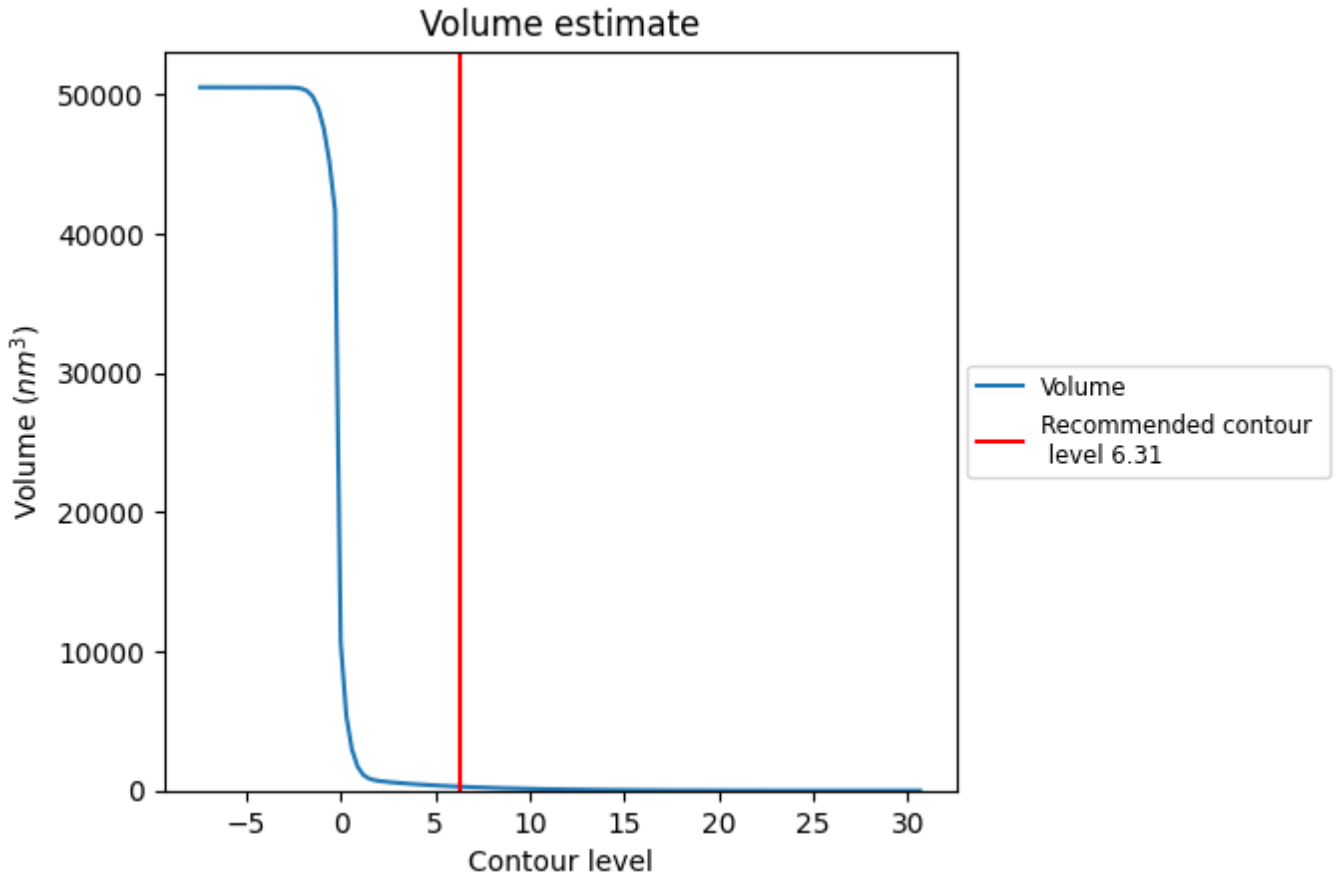
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

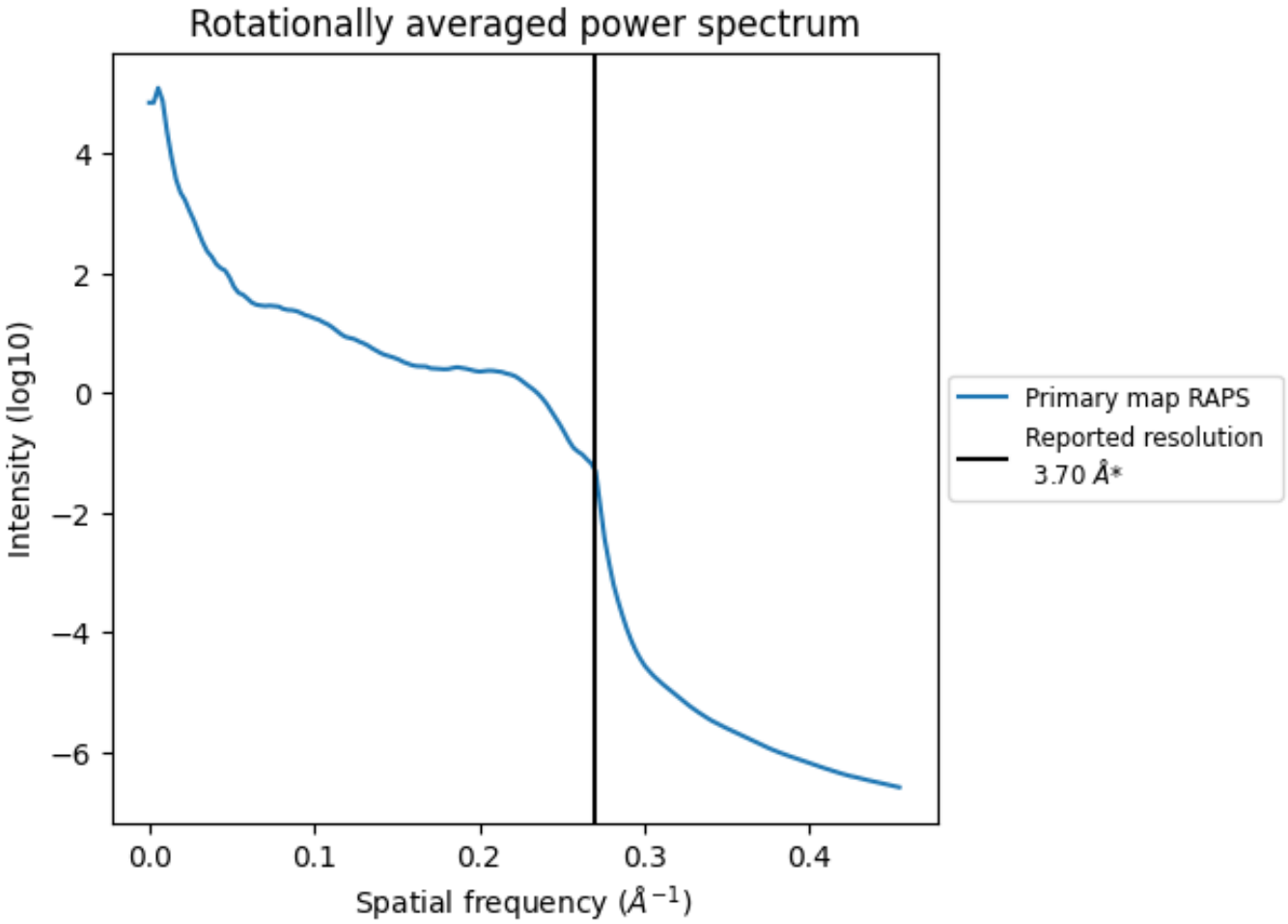
7.2 Volume estimate



The volume at the recommended contour level is 280 nm^3; this corresponds to an approximate mass of 253 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 (i)



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

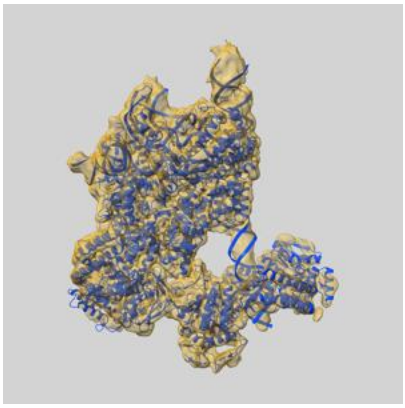
8 Fourier-Shell correlation (i)

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

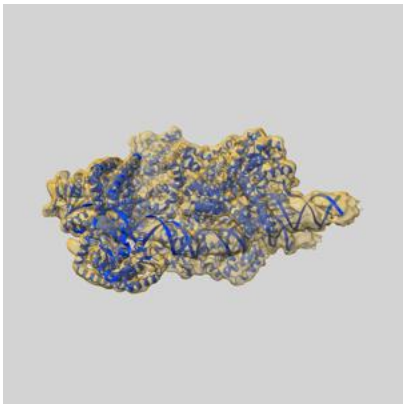
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52320 and PDB model 9HP8. Per-residue inclusion information can be found in section 3 on page 8.

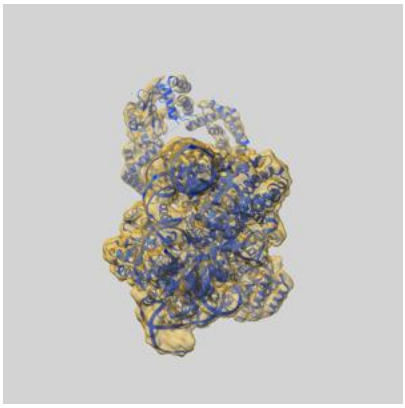
9.1 Map-model overlay



X



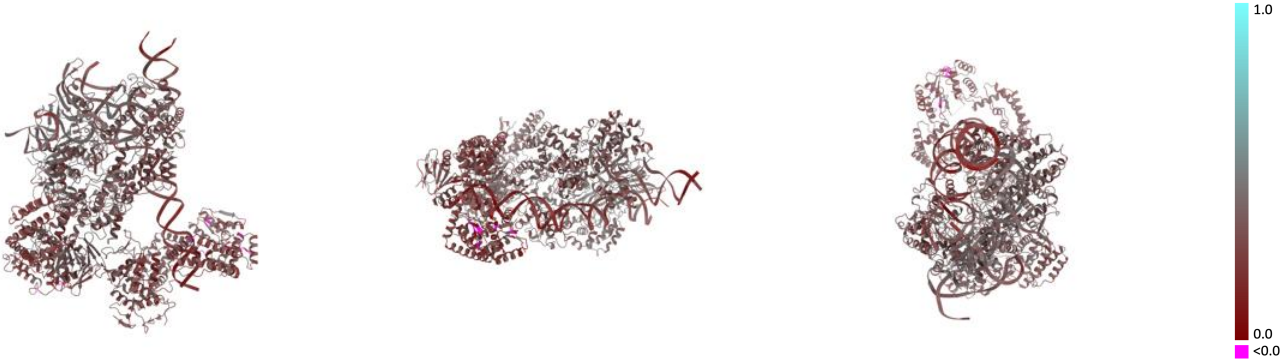
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.31 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.

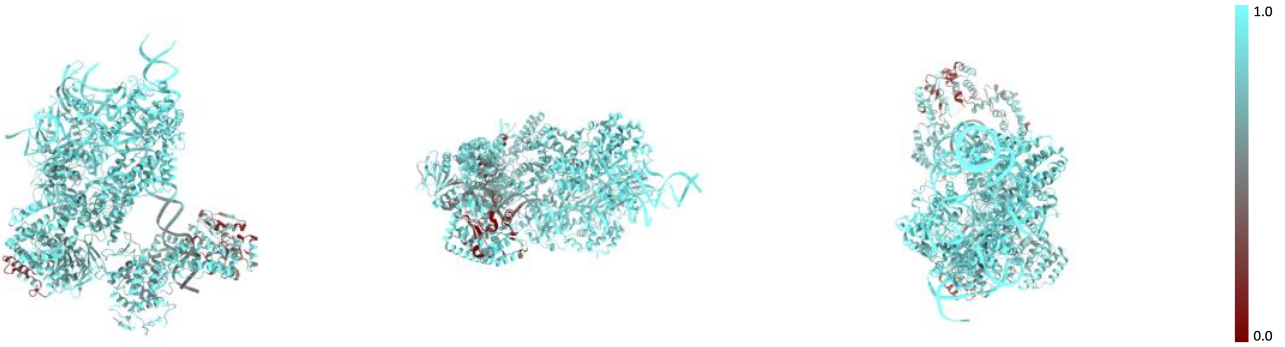
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

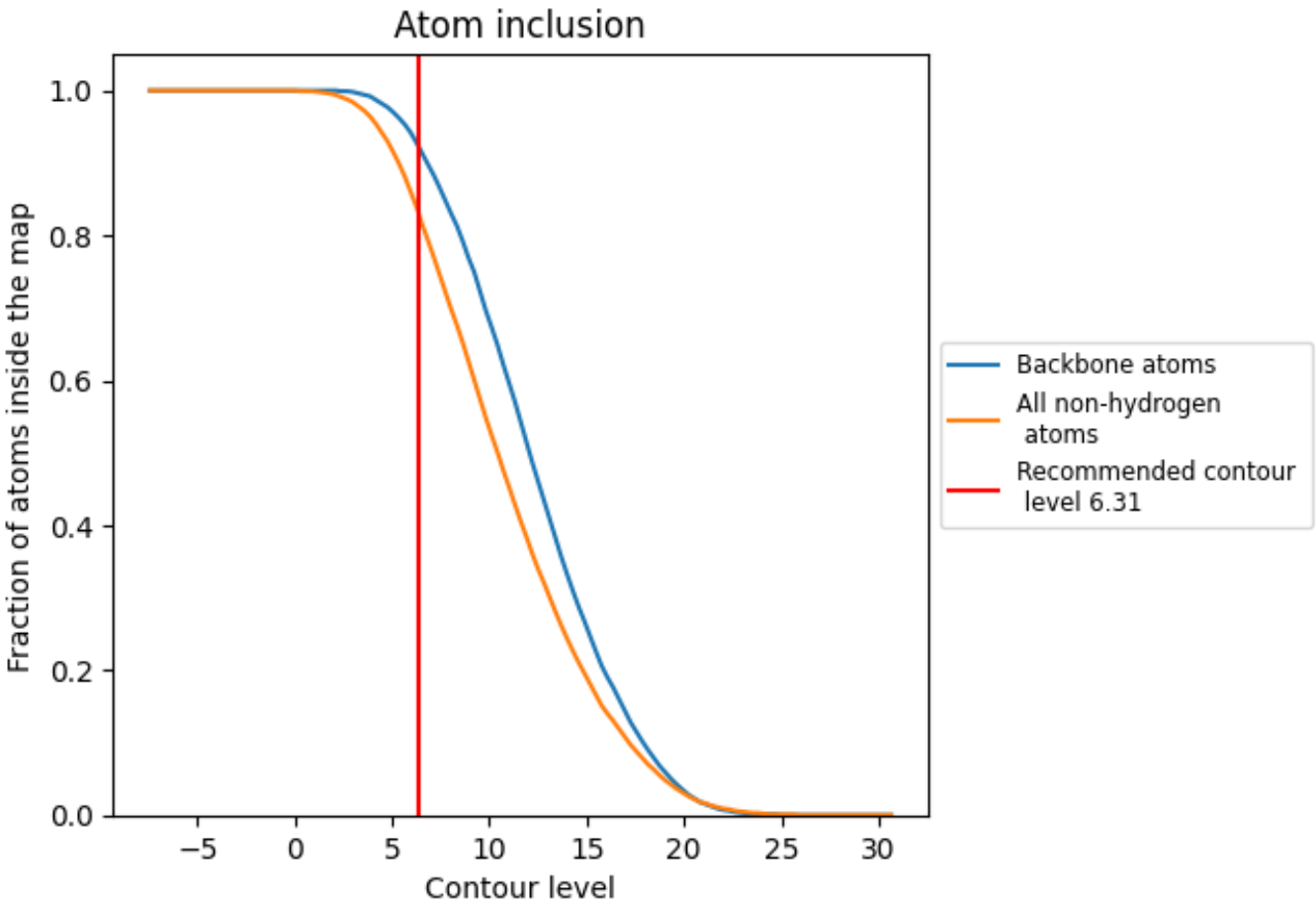
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (6.31).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (6.31) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.3270
A	0.9030	0.3700
B	0.9840	0.3360
C	0.9850	0.3580
D	0.7820	0.1980
E	0.7950	0.2090
F	0.6900	0.2970
G	0.8440	0.3240
I	0.2780	0.2530
L	0.7350	0.2950
M	0.6540	0.2550
N	0.5630	0.2520
O	0.7870	0.2970