Full wwPDB EM Validation Report

Jul 28, 2024 – 12:46 AM JST

PDB ID	:	8YB6
EMDB ID	:	EMD-39110
Title	:	Type I-EHNH Cascade complex
Authors	:	Li, Z.
Deposited on	:	2024-02-11
Resolution	:	3.06 Å(reported)

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:

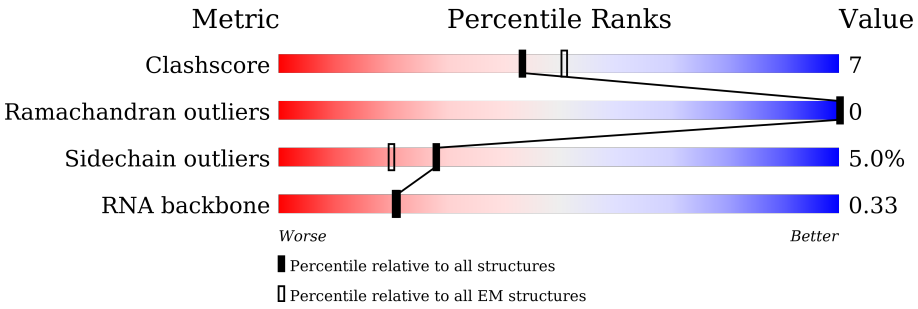
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.06 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	388	5% 73% 15% • 10%
2	B	272	7% 77% 19% • •
3	C	61	7% 41% 39% 20%
4	D	378	23% 74% 23% • •
4	E	378	15% 75% 22% • •
4	F	378	13% 81% 17% •
4	G	378	11% 82% 16% •

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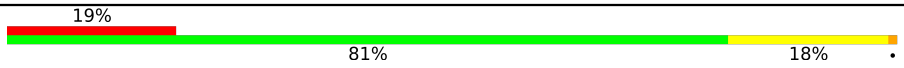
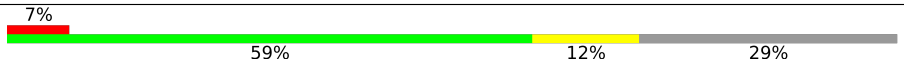
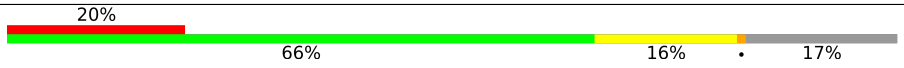
Mol	Chain	Length	Quality of chain
4	H	378	
4	I	378	
5	J	535	
6	K	174	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27758 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 system Cascade subunit CasD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	350	Total	C	N	O	S	0	0
			2768	1746	514	490	18		

- Molecule 2 is a protein called CRISPR-associated endoribonuclease Cse3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	267	Total	C	N	O	S	0	0
			2166	1392	387	383	4		

- Molecule 3 is a RNA chain called 61-nt crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	61	Total	C	N	O	P	0	0
			1303	584	239	420	60		

- Molecule 4 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	372	Total	C	N	O	S	0	0
			2897	1830	506	549	12		
4	E	370	Total	C	N	O	S	0	0
			2882	1821	503	546	12		
4	F	374	Total	C	N	O	S	0	0
			2911	1839	509	551	12		
4	G	377	Total	C	N	O	S	0	0
			2935	1856	512	555	12		
4	H	377	Total	C	N	O	S	0	0
			2935	1856	512	555	12		
4	I	268	Total	C	N	O	S	0	0
			2072	1319	358	387	8		

- Molecule 5 is a protein called CRISPR-associated protein Cse1 (CRISPR_cse1).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	J	443	Total	C	N	O	S	0	0
			3531	2266	605	641	19		

- Molecule 6 is a protein called CRISPR-associated protein Cse2 (CRISPR_cse2).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	165	Total	C	N	O	S	0	0
			1356	878	239	233	6		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

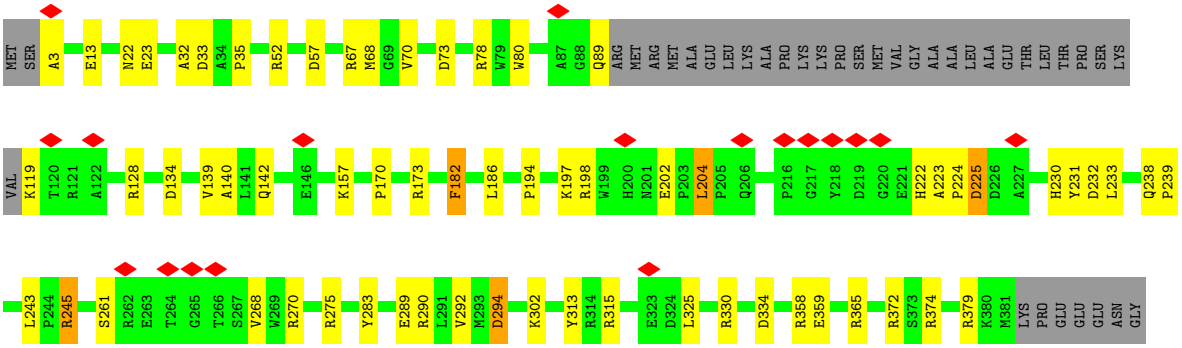
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Zn	0
			1	1	
7	J	1	Total	Zn	0
			1	1	

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.

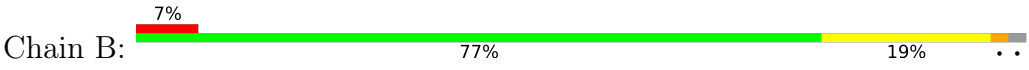
• Molecule 1: CRISPR system Cascade subunit CasD

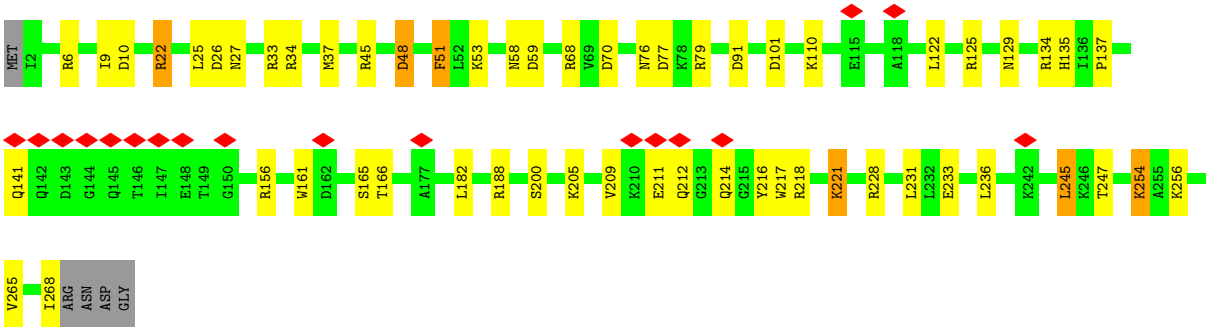
Chain A:



• Molecule 2: CRISPR-associated endoribonuclease Cse3

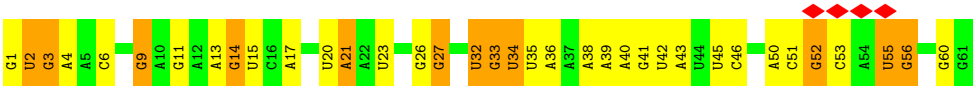
Chain B:





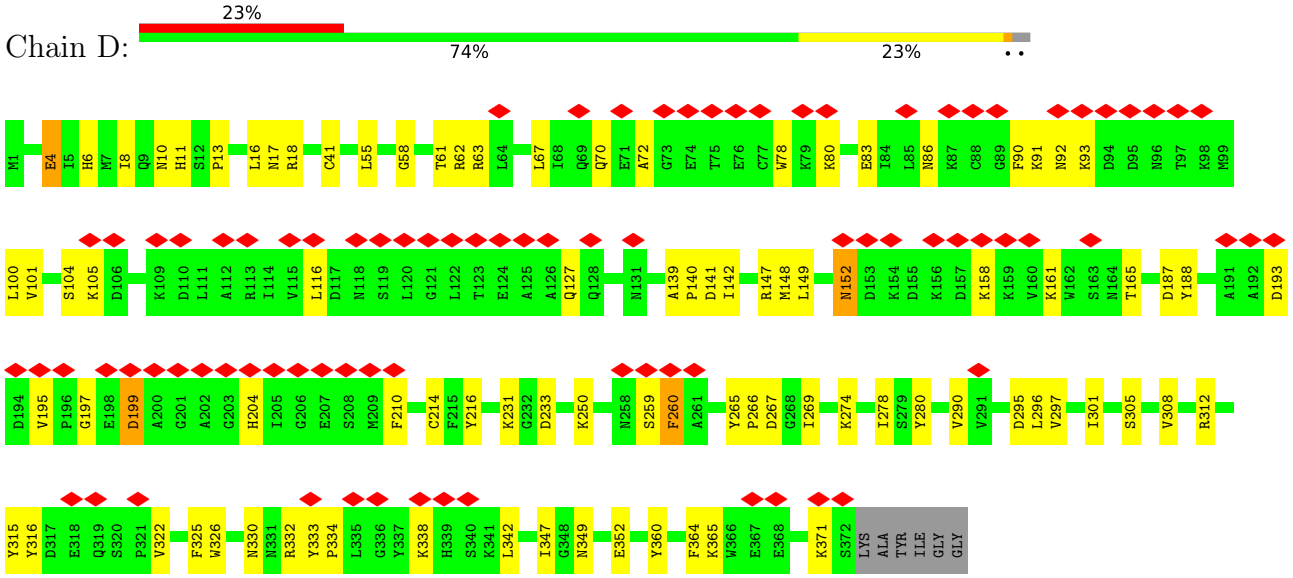
• Molecule 3: 61-nt crRNA

Chain C:



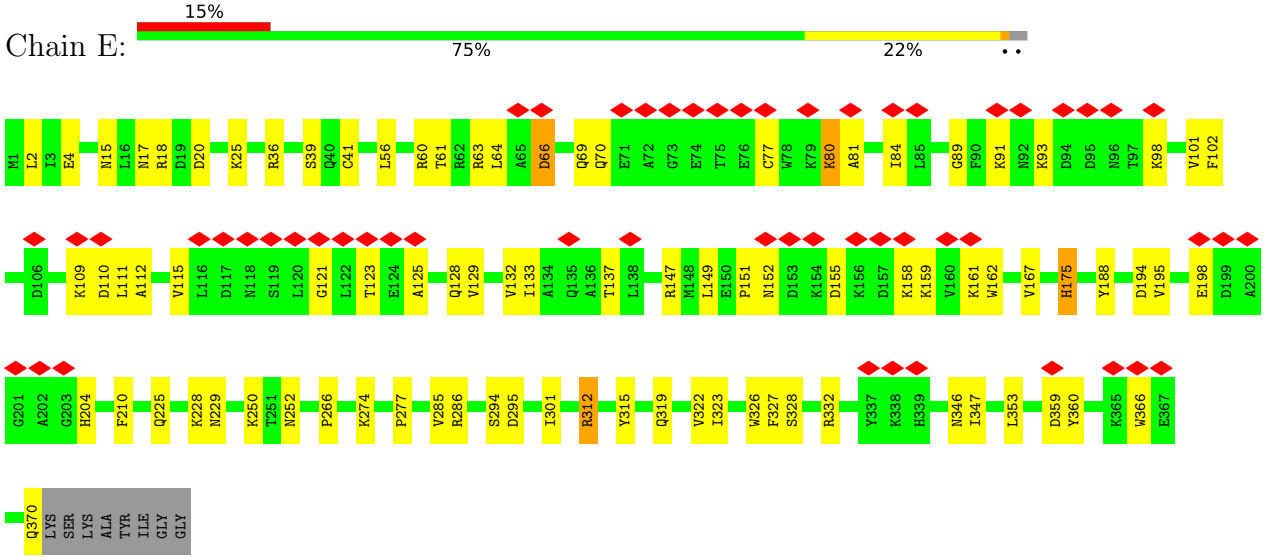
• Molecule 4: CRISPR system Cascade subunit CasC

Chain D:



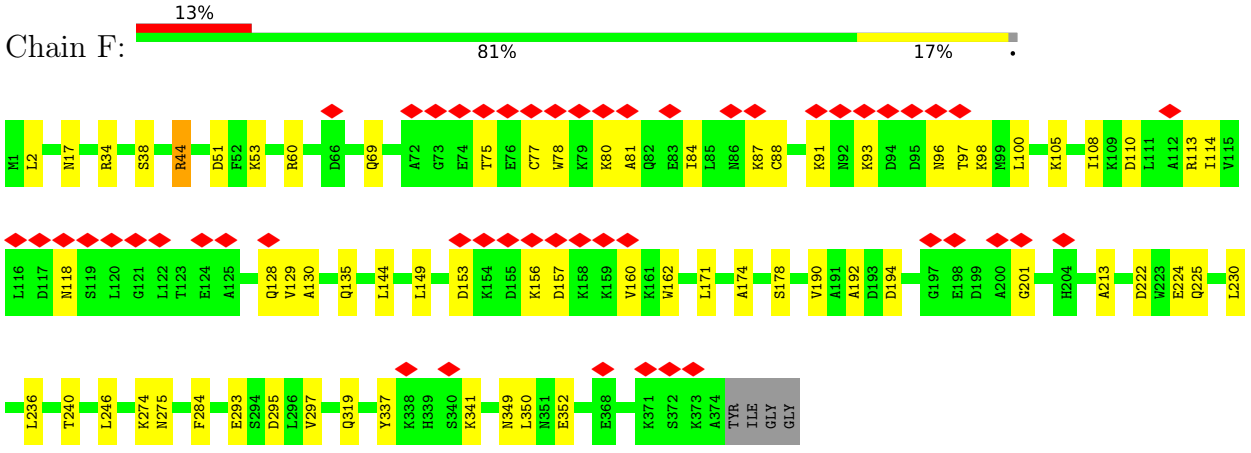
• Molecule 4: CRISPR system Cascade subunit CasC

Chain E:



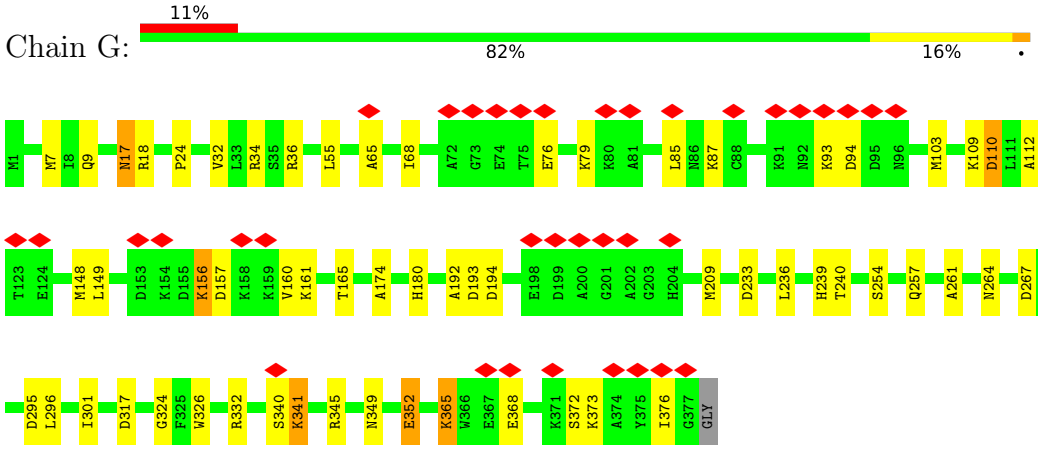
• Molecule 4: CRISPR system Cascade subunit CasC

Chain F:



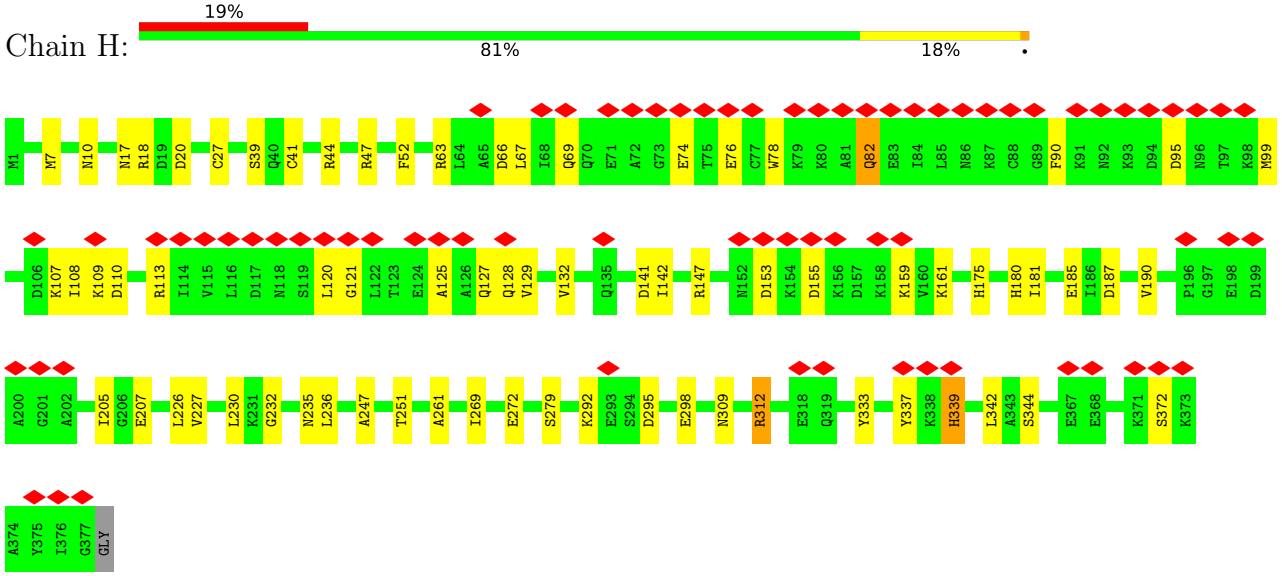
• Molecule 4: CRISPR system Cascade subunit CasC

Chain G:



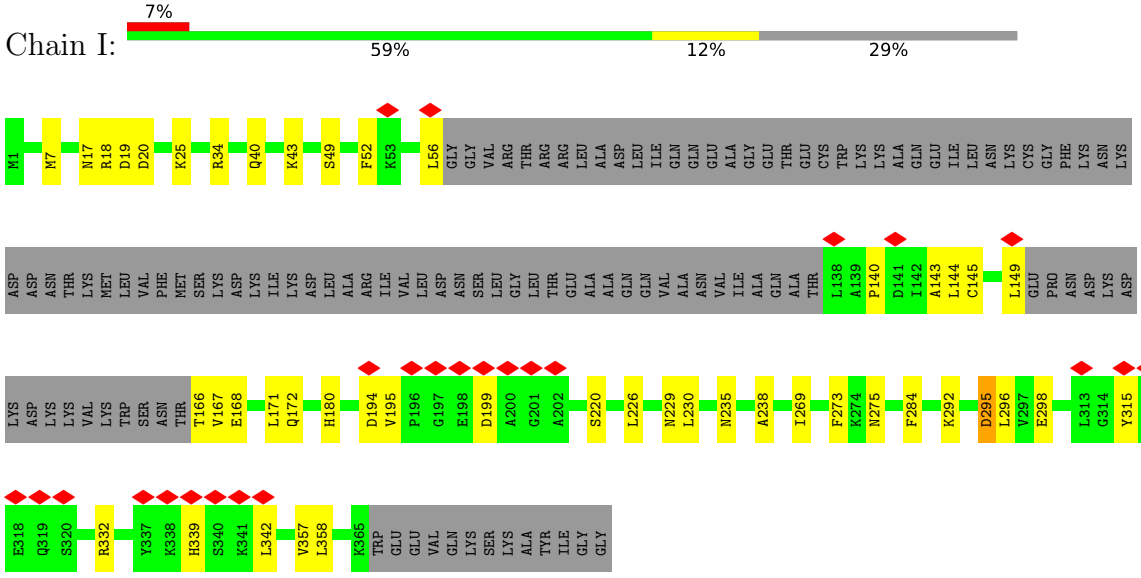
• Molecule 4: CRISPR system Cascade subunit CasC

Chain H:



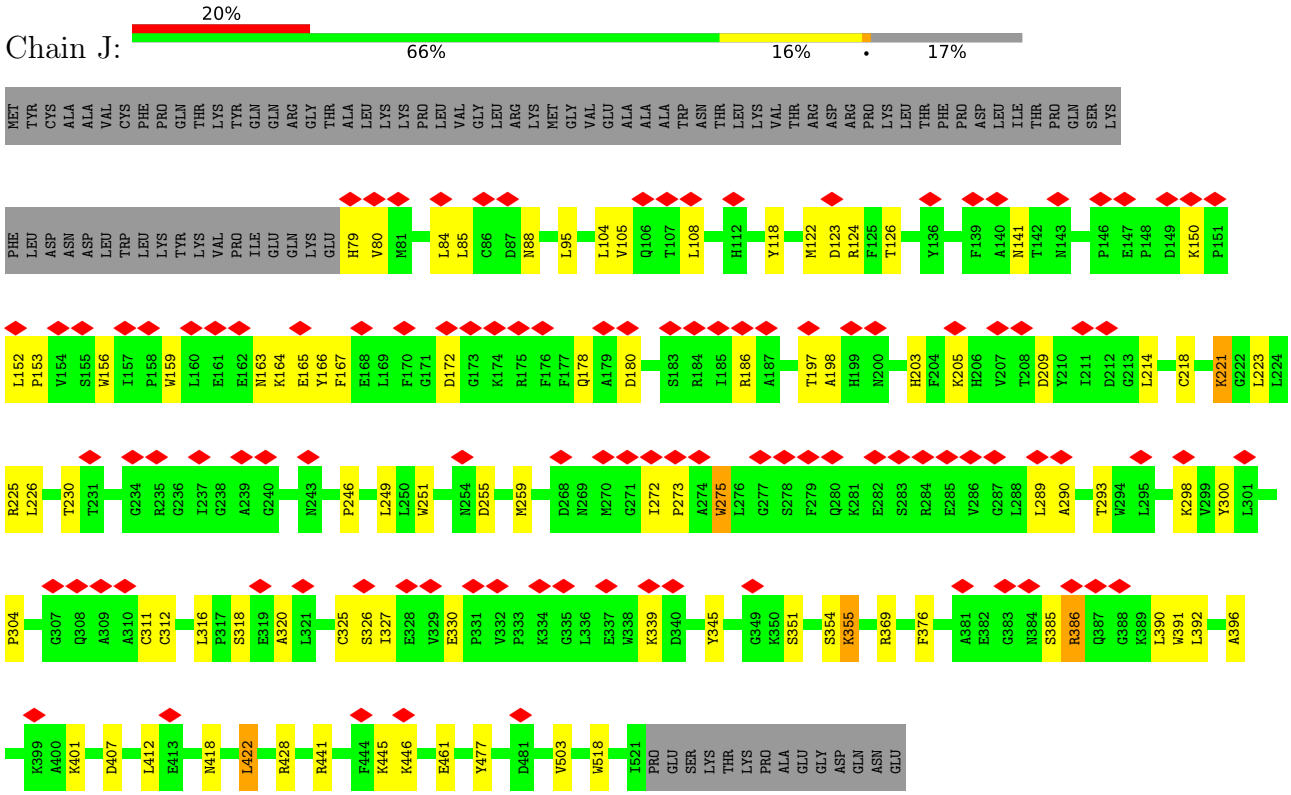
• Molecule 4: CRISPR system Cascade subunit CasC

Chain I:



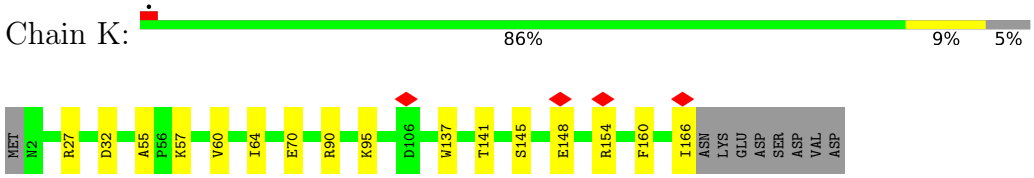
• Molecule 5: CRISPR-associated protein Cse1 (CRISPR_cse1)

Chain J:



• Molecule 6: CRISPR-associated protein Cse2 (CRISPR_cse2)

Chain K:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	291872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.600	Depositor
Minimum map value	-1.568	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.080	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	272.0, 272.0, 272.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/2837	0.55	0/3848
2	B	0.25	0/2224	0.52	0/3012
3	C	0.30	0/1459	0.88	0/2273
4	D	0.26	0/2954	0.51	0/3995
4	E	0.28	0/2939	0.51	0/3976
4	F	0.28	0/2968	0.49	0/4013
4	G	0.27	0/2993	0.50	0/4047
4	H	0.28	0/2993	0.48	0/4047
4	I	0.27	0/2118	0.49	0/2870
5	J	0.26	0/3632	0.51	0/4942
6	K	0.26	0/1386	0.53	0/1866
All	All	0.27	0/28503	0.54	0/38889

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

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	2768	0	2765	43	0
2	B	2166	0	2177	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1303	0	659	35	0
4	D	2897	0	2878	48	0
4	E	2882	0	2860	51	0
4	F	2911	0	2896	48	0
4	G	2935	0	2919	37	0
4	H	2935	0	2919	49	0
4	I	2072	0	2036	27	0
5	J	3531	0	3460	54	0
6	K	1356	0	1398	10	0
7	A	1	0	0	0	0
7	J	1	0	0	0	0
All	All	27758	0	26967	385	0

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

All (385) 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)
4:H:247:ALA:O	4:H:251:THR:HG22	1.33	1.23
2:B:182:LEU:HD23	2:B:247:THR:HG23	1.40	1.02
4:F:114:ILE:HG21	4:F:129:VAL:HG23	1.52	0.91
4:F:105:LYS:O	4:F:108:ILE:HB	1.77	0.83
4:H:247:ALA:O	4:H:251:THR:CG2	2.24	0.82
4:H:337:TYR:CE1	4:H:339:HIS:HB3	2.18	0.79
4:I:226:LEU:O	4:I:230:LEU:HD22	1.85	0.76
4:E:4:GLU:OE2	4:E:277:PRO:HA	1.86	0.74
4:F:114:ILE:CG2	4:F:129:VAL:HG23	2.16	0.74
4:E:137:THR:HG21	4:E:167:VAL:HG21	1.72	0.71
3:C:26:G:H2'	3:C:26:G:N3	2.06	0.71
2:B:135:HIS:ND1	3:C:55:U:OP1	2.23	0.70
4:D:326:TRP:HE1	4:D:334:PRO:HB3	1.56	0.70
4:H:78:TRP:CE2	4:H:82:GLN:NE2	2.59	0.70
4:F:69:GLN:HB2	4:F:78:TRP:HB2	1.76	0.68
4:F:114:ILE:CD1	4:F:128:GLN:HB3	2.23	0.68
4:E:159:LYS:HE3	4:E:161:LYS:HD3	1.76	0.67
4:D:55:LEU:HB3	4:D:140:PRO:HG2	1.76	0.66
4:E:66:ASP:O	4:E:70:GLN:HB2	1.95	0.66
4:F:2:LEU:HB2	4:F:274:LYS:O	1.95	0.65
4:I:292:LYS:HE3	6:K:148:GLU:HB2	1.77	0.65
4:D:195:VAL:HG22	4:D:197:GLY:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:340:SER:OG	4:G:341:LYS:N	2.31	0.63
4:F:174:ALA:HB2	4:G:261:ALA:HB3	1.81	0.63
4:D:312:ARG:NH2	4:D:322:VAL:O	2.29	0.62
4:E:327:PHE:HB2	4:E:353:LEU:HD13	1.81	0.62
1:A:379:ARG:NH1	4:E:20:ASP:OD1	2.33	0.61
4:F:114:ILE:HD13	4:F:128:GLN:CB	2.30	0.61
5:J:186:ARG:NH2	5:J:327:ILE:O	2.33	0.61
4:H:128:GLN:O	4:H:132:VAL:HG12	2.00	0.61
1:A:334:ASP:OD2	1:A:372:ARG:NH2	2.34	0.61
5:J:354:SER:HB3	5:J:396:ALA:HB2	1.83	0.61
4:E:2:LEU:HB2	4:E:274:LYS:O	2.01	0.60
3:C:35:U:OP2	4:E:18:ARG:NH2	2.33	0.60
4:F:130:ALA:HB1	4:F:162:TRP:CZ3	2.37	0.60
2:B:135:HIS:CE1	3:C:55:U:OP2	2.54	0.60
4:F:114:ILE:HD13	4:F:128:GLN:HB3	1.81	0.60
1:A:52:ARG:HG3	3:C:1:G:H1'	1.83	0.60
4:G:295:ASP:OD1	4:G:295:ASP:N	2.35	0.60
3:C:11:G:OP2	4:I:18:ARG:NH2	2.35	0.60
4:H:337:TYR:HE1	4:H:339:HIS:HB3	1.63	0.60
4:H:90:PHE:HA	4:H:99:MET:HE3	1.84	0.60
3:C:33:G:OP1	4:E:25:LYS:NZ	2.35	0.59
4:H:74:GLU:HG2	4:H:76:GLU:H	1.66	0.59
5:J:445:LYS:CG	5:J:446:LYS:N	2.64	0.59
1:A:32:ALA:O	1:A:78:ARG:NH2	2.36	0.59
3:C:6:C:N3	5:J:203:HIS:NE2	2.47	0.59
1:A:68:MET:HA	1:A:140:ALA:O	2.01	0.59
4:F:44:ARG:NH1	4:G:194:ASP:OD1	2.36	0.59
4:H:17:ASN:ND2	4:H:41:CYS:SG	2.76	0.59
4:E:64:LEU:HD22	4:E:101:VAL:HG11	1.84	0.58
4:I:166:THR:OG1	4:I:167:VAL:N	2.36	0.58
4:I:226:LEU:O	4:I:230:LEU:CD2	2.51	0.58
4:E:225:GLN:NE2	4:E:229:ASN:OD1	2.36	0.58
2:B:182:LEU:HD23	2:B:247:THR:CG2	2.24	0.58
4:H:142:ILE:HD11	4:H:147:ARG:HD3	1.86	0.58
4:D:13:PRO:HA	4:D:16:LEU:HD12	1.85	0.58
1:A:57:ASP:OD1	1:A:57:ASP:N	2.33	0.57
4:D:297:VAL:O	4:D:301:ILE:HG12	2.03	0.57
4:D:312:ARG:HE	4:D:342:LEU:HD21	1.69	0.57
3:C:17:A:OP2	4:H:18:ARG:NH2	2.38	0.57
4:F:295:ASP:OD1	4:F:295:ASP:N	2.38	0.57
4:G:9:GLN:NE2	4:G:264:ASN:O	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:HIS:NE2	3:C:56:G:O4'	2.37	0.57
2:B:122:LEU:HD22	2:B:265:VAL:HB	1.86	0.56
1:A:365:ARG:NH2	2:B:101:ASP:OD1	2.38	0.56
4:D:91:LYS:HG3	4:D:152:ASN:HB2	1.87	0.56
4:I:295:ASP:OD1	4:I:295:ASP:N	2.37	0.56
2:B:45:ARG:NH2	2:B:91:ASP:OD2	2.37	0.56
4:D:127:GLN:NE2	4:D:161:LYS:O	2.37	0.56
4:F:114:ILE:HD11	4:F:128:GLN:HB3	1.88	0.56
4:F:110:ASP:HA	4:F:113:ARG:HD3	1.88	0.56
4:D:58:GLY:HA2	4:D:104:SER:HA	1.88	0.56
4:G:7:MET:HG2	4:G:269:ILE:HG12	1.87	0.56
4:D:141:ASP:OD1	4:D:141:ASP:N	2.39	0.55
4:H:20:ASP:OD1	5:J:441:ARG:NH1	2.38	0.55
1:A:358:ARG:NH1	1:A:359:GLU:OE2	2.40	0.55
4:E:295:ASP:OD1	4:E:295:ASP:N	2.38	0.55
4:E:128:GLN:O	4:E:132:VAL:HG23	2.06	0.55
4:G:156:LYS:NZ	4:G:160:VAL:O	2.35	0.55
4:F:194:ASP:N	4:F:194:ASP:OD1	2.40	0.55
4:F:153:ASP:O	4:F:156:LYS:NZ	2.40	0.54
4:H:292:LYS:NZ	6:K:32:ASP:OD2	2.39	0.54
5:J:445:LYS:HG3	5:J:446:LYS:N	2.21	0.54
4:E:89:GLY:HA2	4:E:155:ASP:HB3	1.89	0.54
4:D:101:VAL:HG13	4:D:149:LEU:HD22	1.90	0.54
4:F:75:THR:O	4:F:78:TRP:HB3	2.08	0.54
4:E:286:ARG:NH1	4:F:293:GLU:O	2.40	0.54
4:F:144:LEU:HD22	4:F:171:LEU:HB2	1.90	0.54
4:H:309:ASN:HB2	4:H:342:LEU:HD11	1.90	0.54
2:B:22:ARG:NH1	4:E:188:TYR:OH	2.41	0.54
6:K:90:ARG:NH1	6:K:166:ILE:O	2.42	0.53
5:J:445:LYS:CG	5:J:446:LYS:H	2.21	0.53
4:E:93:LYS:HD3	4:E:98:LYS:HB2	1.90	0.53
4:F:77:CYS:HA	4:F:80:LYS:HE3	1.91	0.53
4:F:91:LYS:HD2	4:F:98:LYS:HB3	1.91	0.53
5:J:339:LYS:HE2	5:J:345:TYR:HE2	1.74	0.53
4:D:83:GLU:OE1	4:D:86:ASN:ND2	2.40	0.53
5:J:325:CYS:SG	5:J:326:SER:N	2.81	0.53
3:C:36:A:H5'	4:D:148:MET:HB3	1.91	0.53
4:D:6:HIS:ND1	4:D:216:TYR:OH	2.38	0.53
1:A:302:LYS:O	2:B:34:ARG:NH2	2.42	0.53
4:F:77:CYS:O	4:F:81:ALA:N	2.42	0.53
4:E:36:ARG:HD2	4:E:175:HIS:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:385:SER:OG	5:J:386:ARG:N	2.43	0.52
4:G:32:VAL:HG21	4:G:287:PRO:HG3	1.92	0.52
4:G:87:LYS:HG3	4:G:122:LEU:HD21	1.90	0.52
3:C:26:G:C2	4:G:192:ALA:HB2	2.44	0.52
2:B:134:ARG:HB2	2:B:137:PRO:HB3	1.91	0.52
2:B:33:ARG:O	2:B:37:MET:HG3	2.09	0.52
5:J:226:LEU:O	5:J:230:THR:OG1	2.27	0.52
5:J:272:ILE:HG13	5:J:273:PRO:HD2	1.92	0.52
2:B:68:ARG:NH1	2:B:70:ASP:OD2	2.43	0.52
4:F:17:ASN:HD22	4:F:38:SER:H	1.58	0.52
1:A:197:LYS:HD2	1:A:202:GLU:HB3	1.91	0.51
1:A:35:PRO:HD2	1:A:70:VAL:HG11	1.93	0.51
4:E:39:SER:OG	4:E:175:HIS:ND1	2.40	0.51
4:G:109:LYS:O	4:G:112:ALA:HB3	2.10	0.51
4:E:91:LYS:HB3	4:E:93:LYS:HG3	1.91	0.51
1:A:23:GLU:OE1	5:J:369:ARG:NH2	2.43	0.51
1:A:290:ARG:NE	1:A:294:ASP:OD1	2.44	0.51
1:A:275:ARG:NH2	6:K:55:ALA:O	2.42	0.51
3:C:32:U:H5”	4:F:190:VAL:O	2.11	0.51
4:G:317:ASP:N	4:G:317:ASP:OD1	2.42	0.51
4:I:143:ALA:HB1	4:I:229:ASN:HB3	1.92	0.51
5:J:118:TYR:HB2	5:J:124:ARG:HB3	1.93	0.50
5:J:503:VAL:HG21	6:K:160:PHE:HD2	1.76	0.50
6:K:60:VAL:O	6:K:64:ILE:HG12	2.11	0.50
1:A:67:ARG:HG3	1:A:142:GLN:HB3	1.94	0.50
6:K:137:TRP:O	6:K:141:THR:OG1	2.28	0.50
5:J:197:THR:HG22	5:J:198:ALA:H	1.77	0.50
3:C:20:U:H6	3:C:21:A:H4’	1.75	0.50
4:D:80:LYS:HA	4:D:83:GLU:HB2	1.93	0.50
4:H:155:ASP:OD1	4:H:155:ASP:N	2.45	0.50
4:G:373:LYS:HD3	4:G:376:ILE:HD13	1.94	0.50
4:F:87:LYS:NZ	4:F:157:ASP:OD2	2.45	0.50
4:H:120:LEU:CD1	4:H:125:ALA:HB2	2.41	0.50
5:J:167:PHE:HE1	5:J:275:TRP:HE1	1.59	0.50
4:H:110:ASP:HA	4:H:113:ARG:HD3	1.94	0.49
1:A:70:VAL:HG22	1:A:139:VAL:HG22	1.95	0.49
2:B:212:GLN:NE2	2:B:214:GLN:OE1	2.44	0.49
4:F:130:ALA:HB1	4:F:162:TRP:CH2	2.47	0.49
2:B:209:VAL:HG22	2:B:216:TYR:HA	1.93	0.49
4:F:84:ILE:O	4:F:88:CYS:N	2.45	0.49
4:F:97:THR:OG1	4:F:98:LYS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:349:ASN:HB3	4:G:352:GLU:HB2	1.95	0.49
4:H:337:TYR:CE1	4:H:339:HIS:CB	2.92	0.49
4:E:61:THR:HG22	4:E:63:ARG:H	1.77	0.49
4:E:301:ILE:HD12	4:E:326:TRP:HH2	1.77	0.49
4:E:315:TYR:HD2	4:F:350:LEU:HD22	1.76	0.49
4:I:238:ALA:HB1	4:I:358:LEU:HD22	1.93	0.49
4:H:69:GLN:HA	4:H:76:GLU:HG3	1.94	0.49
4:H:295:ASP:HB2	4:H:298:GLU:HB3	1.95	0.49
4:I:172:GLN:HB3	4:I:220:SER:HB2	1.93	0.49
1:A:292:VAL:HG11	2:B:218:ARG:HB3	1.94	0.48
4:D:250:LYS:HD2	4:D:265:TYR:HE1	1.77	0.48
4:I:56:LEU:HD12	4:I:140:PRO:HG2	1.95	0.48
1:A:3:ALA:HB1	1:A:182:PHE:HD2	1.77	0.48
4:H:236:LEU:HD12	4:H:372:SER:HB3	1.94	0.48
4:E:77:CYS:HA	4:E:80:LYS:HB3	1.95	0.48
1:A:232:ASP:OD1	1:A:245:ARG:NE	2.40	0.48
4:D:347:ILE:HG22	4:D:349:ASN:H	1.78	0.48
4:H:63:ARG:NH2	4:I:199:ASP:O	2.46	0.48
4:I:7:MET:HG2	4:I:269:ILE:HG12	1.95	0.48
5:J:428:ARG:NH1	5:J:461:GLU:OE2	2.46	0.48
3:C:32:U:O4	3:C:34:U:H1'	2.13	0.48
4:E:129:VAL:O	4:E:133:ILE:HG12	2.13	0.48
4:E:133:ILE:O	4:E:147:ARG:NH2	2.43	0.48
4:E:285:VAL:HG12	4:F:295:ASP:HB2	1.96	0.48
4:G:24:PRO:HD3	4:G:209:MET:HB3	1.95	0.48
1:A:22:ASN:HD22	1:A:231:TYR:HB2	1.79	0.48
4:H:230:LEU:HD22	4:H:236:LEU:HD23	1.95	0.48
4:I:20:ASP:N	4:I:20:ASP:OD1	2.38	0.48
2:B:48:ASP:OD2	2:B:53:LYS:HB2	2.13	0.48
4:F:78:TRP:O	4:F:81:ALA:HB3	2.13	0.48
2:B:256:LYS:NZ	3:C:60:G:OP2	2.41	0.48
4:I:43:LYS:NZ	4:I:145:CYS:O	2.45	0.48
5:J:123:ASP:OD1	5:J:225:ARG:NH2	2.42	0.48
4:D:338:LYS:HZ2	4:D:342:LEU:H	1.61	0.47
6:K:27:ARG:HD3	6:K:70:GLU:OE1	2.14	0.47
1:A:170:PRO:HB3	4:I:172:GLN:HE21	1.79	0.47
2:B:236:LEU:HD12	2:B:236:LEU:O	2.15	0.47
3:C:26:G:C8	4:F:44:ARG:HG2	2.50	0.47
4:E:123:THR:OG1	4:E:158:LYS:NZ	2.38	0.47
4:F:275:ASN:ND2	4:F:319:GLN:OE1	2.47	0.47
4:G:79:LYS:HB3	4:G:79:LYS:HE3	1.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:149:LEU:O	4:G:165:THR:OG1	2.32	0.47
4:D:61:THR:HG22	4:E:195:VAL:HG22	1.96	0.47
4:H:125:ALA:O	4:H:129:VAL:HG12	2.14	0.47
5:J:84:LEU:HB3	5:J:104:LEU:HD12	1.96	0.47
5:J:85:LEU:HB3	5:J:105:VAL:HG13	1.96	0.47
5:J:249:LEU:HD11	5:J:392:LEU:HD23	1.96	0.47
4:F:118:ASN:OD1	4:F:118:ASN:N	2.47	0.47
1:A:33:ASP:OD1	1:A:78:ARG:NH2	2.38	0.47
1:A:233:LEU:HB3	1:A:243:LEU:HB2	1.95	0.47
4:D:139:ALA:HB3	4:D:142:ILE:HB	1.96	0.47
5:J:445:LYS:HE2	5:J:446:LYS:HG2	1.95	0.47
5:J:178:GLN:NE2	5:J:223:LEU:HD11	2.29	0.47
4:D:315:TYR:OH	4:E:266:PRO:O	2.29	0.47
4:E:112:ALA:O	4:E:115:VAL:HB	2.14	0.47
4:F:17:ASN:ND2	4:F:38:SER:H	2.12	0.47
4:H:295:ASP:OD2	4:H:333:TYR:OH	2.33	0.47
4:I:17:ASN:HB3	4:I:25:LYS:HD2	1.97	0.47
5:J:246:PRO:HB3	5:J:351:SER:HB3	1.96	0.47
4:G:365:LYS:HB2	4:G:368:GLU:HG3	1.95	0.47
2:B:70:ASP:OD1	2:B:70:ASP:N	2.47	0.46
2:B:161:TRP:O	3:C:43:A:N6	2.48	0.46
4:D:8:ILE:HD12	4:D:301:ILE:HD13	1.97	0.46
4:E:285:VAL:HG11	4:F:297:VAL:HG23	1.97	0.46
4:H:120:LEU:HD11	4:H:125:ALA:HB2	1.96	0.46
2:B:125:ARG:HG3	2:B:233:GLU:HG2	1.97	0.46
3:C:51:C:H2'	3:C:52:G:C5	2.50	0.46
4:G:36:ARG:NH1	4:H:187:ASP:OD1	2.39	0.46
5:J:152:LEU:HD22	5:J:153:PRO:HD2	1.97	0.46
4:E:225:GLN:HA	4:E:228:LYS:HB3	1.96	0.46
4:G:65:ALA:HB2	4:G:85:LEU:HD21	1.96	0.46
4:H:207:GLU:OE2	4:H:207:GLU:HA	2.16	0.46
5:J:376:PHE:HA	5:J:422:LEU:HD21	1.97	0.46
6:K:141:THR:O	6:K:145:SER:OG	2.30	0.46
4:H:78:TRP:NE1	4:H:82:GLN:NE2	2.62	0.46
4:I:292:LYS:HB3	6:K:148:GLU:HG3	1.97	0.46
4:D:149:LEU:O	4:D:165:THR:OG1	2.26	0.46
4:F:60:ARG:HG2	4:F:100:LEU:HD22	1.96	0.46
4:E:323:ILE:HG21	4:E:360:TYR:CE2	2.51	0.46
4:G:282:ASN:OD1	4:H:10:ASN:ND2	2.44	0.46
1:A:197:LYS:HD3	1:A:204:LEU:HD21	1.98	0.46
1:A:223:ALA:HB3	5:J:95:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:109:LYS:O	4:E:112:ALA:HB3	2.16	0.46
3:C:51:C:H2'	3:C:52:G:C4	2.51	0.46
5:J:289:LEU:O	5:J:293:THR:OG1	2.34	0.46
2:B:48:ASP:OD2	2:B:53:LYS:N	2.28	0.45
3:C:3:G:H4'	3:C:4:A:C8	2.51	0.45
1:A:194:PRO:HB2	1:A:261:SER:HB2	1.98	0.45
4:D:4:GLU:OE2	4:D:6:HIS:NE2	2.49	0.45
4:E:111:LEU:HD22	4:E:129:VAL:HG22	1.98	0.45
4:F:53:LYS:HD3	4:F:53:LYS:HA	1.64	0.45
5:J:255:ASP:O	5:J:259:MET:N	2.48	0.45
4:G:301:ILE:HD12	4:G:326:TRP:HH2	1.81	0.45
1:A:186:LEU:HD12	1:A:186:LEU:H	1.82	0.45
1:A:238:GLN:HB3	1:A:239:PRO:HD3	1.98	0.45
4:D:349:ASN:HB3	4:D:352:GLU:HB3	1.98	0.45
1:A:128:ARG:NH2	4:I:20:ASP:OD2	2.50	0.45
4:D:17:ASN:ND2	4:D:41:CYS:SG	2.90	0.45
4:H:180:HIS:ND1	4:H:181:ILE:O	2.50	0.45
4:H:120:LEU:HD12	4:H:121:GLY:O	2.16	0.44
5:J:391:TRP:HE1	5:J:407:ASP:HB2	1.82	0.44
4:E:250:LYS:HE3	4:E:250:LYS:HB2	1.81	0.44
4:E:312:ARG:HD2	4:E:322:VAL:HG11	1.99	0.44
4:G:174:ALA:HB2	4:H:261:ALA:HB3	1.99	0.44
5:J:221:LYS:HB3	5:J:221:LYS:HE2	1.67	0.44
4:E:366:TRP:O	4:E:370:GLN:NE2	2.50	0.44
2:B:165:SER:OG	2:B:166:THR:N	2.51	0.44
4:G:32:VAL:HG23	4:G:34:ARG:HE	1.82	0.44
5:J:122:MET:O	5:J:126:THR:HG23	2.18	0.44
5:J:272:ILE:HG22	5:J:290:ALA:HB2	1.99	0.44
5:J:412:LEU:HD23	5:J:412:LEU:HA	1.89	0.44
1:A:22:ASN:HA	3:C:3:G:N7	2.33	0.44
3:C:14:G:O2'	4:H:41:CYS:SG	2.70	0.44
4:F:96:ASN:HB3	4:F:97:THR:H	1.65	0.44
1:A:73:ASP:N	1:A:73:ASP:OD1	2.51	0.44
2:B:48:ASP:OD1	2:B:53:LYS:HG3	2.18	0.44
4:G:68:ILE:HD11	4:G:112:ALA:HB2	1.98	0.44
4:D:274:LYS:HE2	4:D:278:ILE:HD12	2.00	0.44
5:J:304:PRO:HB3	5:J:320:ALA:HB1	1.99	0.44
4:H:127:GLN:HE21	4:H:161:LYS:HB3	1.83	0.44
2:B:268:ILE:HD13	4:D:204:HIS:HB2	1.99	0.43
4:D:312:ARG:HG3	4:D:342:LEU:HD21	1.99	0.43
4:E:91:LYS:HD2	4:E:152:ASN:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:121:GLY:HA2	4:E:125:ALA:HB2	1.99	0.43
5:J:153:PRO:HB2	5:J:156:TRP:NE1	2.32	0.43
4:H:107:LYS:HD2	4:H:107:LYS:HA	1.83	0.43
4:H:226:LEU:HD12	4:H:226:LEU:HA	1.88	0.43
5:J:205:LYS:HA	5:J:205:LYS:HD2	1.75	0.43
2:B:9:ILE:HD12	2:B:25:LEU:HD11	2.00	0.43
4:F:349:ASN:HB3	4:F:352:GLU:HG3	2.00	0.43
4:E:347:ILE:HG21	4:E:353:LEU:HB2	2.01	0.43
4:F:178:SER:HB2	4:F:213:ALA:HB1	2.00	0.43
5:J:164:LYS:HE2	5:J:164:LYS:HB2	1.79	0.43
5:J:249:LEU:HD23	5:J:390:LEU:HD21	2.00	0.43
3:C:1:G:H4'	3:C:2:U:OP2	2.18	0.43
4:E:15:ASN:HB2	4:E:210:PHE:HA	2.01	0.43
4:G:236:LEU:O	4:G:240:THR:OG1	2.31	0.43
5:J:355:LYS:H	5:J:355:LYS:HG2	1.62	0.43
5:J:369:ARG:HA	5:J:369:ARG:HD3	1.87	0.43
2:B:245:LEU:HD23	2:B:245:LEU:HA	1.88	0.43
3:C:26:G:N3	3:C:26:G:C2'	2.79	0.43
3:C:32:U:C2	4:F:192:ALA:HB2	2.54	0.43
4:E:225:GLN:HA	4:E:228:LYS:HE2	1.99	0.43
3:C:3:G:H4'	3:C:4:A:H8	1.83	0.43
5:J:214:LEU:HA	5:J:311:CYS:HB2	2.01	0.43
5:J:316:LEU:HD12	5:J:316:LEU:HA	1.92	0.43
4:I:180:HIS:CD2	4:I:296:LEU:HD21	2.54	0.43
4:E:39:SER:H	4:E:175:HIS:CE1	2.36	0.43
4:H:109:LYS:H	4:H:109:LYS:HG2	1.55	0.43
1:A:157:LYS:HE2	4:I:275:ASN:HB3	2.01	0.42
2:B:37:MET:HE3	2:B:51:PHE:HE2	1.84	0.42
4:D:63:ARG:HD2	4:E:198:GLU:HA	2.00	0.42
1:A:268:VAL:HB	1:A:270:ARG:NH2	2.34	0.42
2:B:135:HIS:ND1	3:C:55:U:P	2.92	0.42
4:D:93:LYS:HD2	4:D:93:LYS:HA	1.73	0.42
4:D:295:ASP:OD1	4:D:295:ASP:N	2.46	0.42
4:H:67:LEU:HD23	4:H:108:ILE:HD13	2.02	0.42
5:J:418:ASN:OD1	5:J:418:ASN:N	2.52	0.42
4:E:147:ARG:HH21	4:E:149:LEU:HD23	1.84	0.42
4:I:339:HIS:HB2	4:I:342:LEU:HD22	2.00	0.42
2:B:135:HIS:CD2	3:C:56:G:H8	2.37	0.42
2:B:156:ARG:HE	2:B:254:LYS:HD2	1.85	0.42
4:D:290:VAL:HG11	4:D:296:LEU:HB2	2.02	0.42
4:D:325:PHE:HZ	4:D:360:TYR:HD2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:338:LYS:HZ1	4:D:342:LEU:HD13	1.85	0.42
4:H:272:GLU:OE2	4:H:312:ARG:NH2	2.42	0.42
2:B:110:LYS:HA	2:B:110:LYS:HD3	1.74	0.42
4:G:17:ASN:HD22	4:G:17:ASN:HA	1.66	0.42
4:H:7:MET:HG2	4:H:269:ILE:HG12	2.02	0.42
5:J:218:CYS:HA	5:J:221:LYS:HB2	2.01	0.42
5:J:163:ASN:HB2	5:J:166:TYR:HD2	1.84	0.42
1:A:283:TYR:HE1	1:A:325:LEU:HD21	1.85	0.42
2:B:129:ASN:ND2	2:B:228:ARG:O	2.48	0.42
4:G:68:ILE:HD12	4:G:68:ILE:HA	1.87	0.42
4:G:180:HIS:CD2	4:G:296:LEU:HD21	2.55	0.42
5:J:141:ASN:HB3	5:J:159:TRP:CH2	2.55	0.42
4:E:147:ARG:HE	4:E:149:LEU:HD23	1.85	0.42
4:F:246:LEU:HD23	4:F:246:LEU:HA	1.88	0.42
4:G:372:SER:O	4:G:372:SER:OG	2.31	0.42
4:H:78:TRP:CZ2	4:H:82:GLN:NE2	2.88	0.42
1:A:89:GLN:H	1:A:89:GLN:HG3	1.62	0.42
5:J:84:LEU:HD12	5:J:167:PHE:HB3	2.00	0.42
2:B:165:SER:O	3:C:41:G:N2	2.51	0.41
3:C:23:U:OP2	4:G:18:ARG:NH1	2.53	0.41
4:D:67:LEU:O	4:D:70:GLN:NE2	2.53	0.41
4:F:222:ASP:HB3	4:F:225:GLN:HB3	2.02	0.41
4:I:273:PHE:HZ	4:I:357:VAL:HG13	1.85	0.41
4:D:10:ASN:O	4:D:11:HIS:ND1	2.53	0.41
4:D:62:ARG:HG3	4:D:100:LEU:HG	2.02	0.41
4:D:187:ASP:OD1	4:D:188:TYR:N	2.53	0.41
4:D:330:ASN:HA	4:D:334:PRO:HG2	2.02	0.41
2:B:27:ASN:HD21	2:B:200:SER:HB2	1.85	0.41
4:F:160:VAL:HG22	4:F:162:TRP:HB2	2.03	0.41
4:G:271:VAL:O	4:G:324:GLY:HA2	2.20	0.41
4:H:66:ASP:OD1	4:H:66:ASP:N	2.53	0.41
1:A:289:GLU:OE1	2:B:218:ARG:NH2	2.53	0.41
1:A:290:ARG:HA	1:A:290:ARG:HD2	1.85	0.41
3:C:33:G:N1	4:F:201:GLY:O	2.37	0.41
4:E:151:PRO:HG3	4:E:162:TRP:CD1	2.55	0.41
4:F:236:LEU:O	4:F:240:THR:OG1	2.28	0.41
4:G:55:LEU:HD21	4:G:239:HIS:CE1	2.55	0.41
2:B:10:ASP:OD1	2:B:79:ARG:NE	2.53	0.41
3:C:26:G:O2'	3:C:27:G:H4'	2.21	0.41
4:G:254:SER:HA	4:G:257:GLN:HG3	2.03	0.41
4:I:171:LEU:HD23	4:I:171:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:66:ASP:HA	4:E:69:GLN:HE21	1.85	0.41
4:F:230:LEU:HD13	4:F:236:LEU:HB3	2.03	0.41
1:A:223:ALA:HA	1:A:224:PRO:HD3	1.95	0.41
2:B:135:HIS:CD2	3:C:56:G:H5"	2.55	0.41
4:D:72:ALA:HB1	4:D:116:LEU:HD21	2.03	0.41
4:D:280:TYR:CZ	4:D:308:VAL:HG23	2.56	0.41
4:H:159:LYS:HA	4:H:159:LYS:HD3	1.93	0.41
5:J:150:LYS:HD2	5:J:150:LYS:HA	1.67	0.41
5:J:390:LEU:HB2	5:J:412:LEU:HD12	2.03	0.41
1:A:225:ASP:OD1	1:A:225:ASP:N	2.54	0.41
2:B:205:LYS:HE2	2:B:221:LYS:HG3	2.02	0.41
3:C:9:G:OP2	4:I:40:GLN:NE2	2.54	0.41
4:D:92:ASN:OD1	4:D:92:ASN:N	2.52	0.41
4:D:259:SER:OG	4:D:260:PHE:N	2.53	0.41
4:D:266:PRO:HG2	4:D:269:ILE:HD11	2.03	0.41
4:E:81:ALA:O	4:E:84:ILE:HB	2.21	0.41
4:H:39:SER:HB3	4:H:175:HIS:CD2	2.56	0.41
4:H:141:ASP:OD1	4:H:141:ASP:N	2.54	0.41
4:H:190:VAL:HG23	4:H:205:ILE:HD13	2.03	0.41
5:J:79:HIS:HB2	5:J:80:VAL:H	1.73	0.41
1:A:13:GLU:OE1	1:A:173:ARG:NE	2.48	0.41
4:H:67:LEU:HD11	4:I:195:VAL:HG21	2.03	0.41
1:A:198:ARG:HE	1:A:198:ARG:HB2	1.67	0.40
2:B:211:GLU:H	2:B:211:GLU:HG3	1.68	0.40
4:H:227:VAL:HG13	4:H:232:GLY:HA2	2.03	0.40
5:J:298:LYS:NZ	5:J:330:GLU:HG3	2.36	0.40
4:G:93:LYS:NZ	4:G:94:ASP:OD2	2.48	0.40
4:I:149:LEU:HD12	4:I:149:LEU:HA	1.87	0.40
1:A:52:ARG:NH2	4:I:168:GLU:OE2	2.45	0.40
4:G:110:ASP:HA	4:G:113:ARG:HG2	2.03	0.40
4:G:112:ALA:HA	4:G:115:VAL:HG22	2.03	0.40
1:A:80:TRP:CE3	1:A:128:ARG:HB3	2.55	0.40
4:D:199:ASP:HA	4:D:204:HIS:HB3	2.03	0.40
4:D:231:LYS:HE2	4:D:231:LYS:HB3	1.73	0.40
5:J:445:LYS:HG2	5:J:446:LYS:H	1.86	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	346/388 (89%)	314 (91%)	32 (9%)	0	100	100
2	B	265/272 (97%)	250 (94%)	15 (6%)	0	100	100
4	D	370/378 (98%)	334 (90%)	36 (10%)	0	100	100
4	E	368/378 (97%)	331 (90%)	37 (10%)	0	100	100
4	F	372/378 (98%)	341 (92%)	31 (8%)	0	100	100
4	G	375/378 (99%)	340 (91%)	35 (9%)	0	100	100
4	H	375/378 (99%)	352 (94%)	23 (6%)	0	100	100
4	I	262/378 (69%)	236 (90%)	26 (10%)	0	100	100
5	J	441/535 (82%)	397 (90%)	44 (10%)	0	100	100
6	K	163/174 (94%)	153 (94%)	10 (6%)	0	100	100
All	All	3337/3637 (92%)	3048 (91%)	289 (9%)	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	290/322 (90%)	277 (96%)	13 (4%)	27	58
2	B	234/238 (98%)	218 (93%)	16 (7%)	16	42
4	D	310/313 (99%)	288 (93%)	22 (7%)	14	41
4	E	308/313 (98%)	289 (94%)	19 (6%)	18	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	311/313 (99%)	301 (97%)	10 (3%)	39	68
4	G	313/313 (100%)	297 (95%)	16 (5%)	24	53
4	H	313/313 (100%)	300 (96%)	13 (4%)	30	60
4	I	220/313 (70%)	208 (94%)	12 (6%)	21	50
5	J	378/459 (82%)	360 (95%)	18 (5%)	25	55
6	K	144/153 (94%)	141 (98%)	3 (2%)	53	77
All	All	2821/3050 (92%)	2679 (95%)	142 (5%)	28	54

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LYS
1	A	134	ASP
1	A	182	PHE
1	A	204	LEU
1	A	222	HIS
1	A	225	ASP
1	A	230	HIS
1	A	245	ARG
1	A	294	ASP
1	A	313	TYR
1	A	315	ARG
1	A	330	ARG
1	A	374	ARG
2	B	6	ARG
2	B	22	ARG
2	B	26	ASP
2	B	48	ASP
2	B	51	PHE
2	B	58	ASN
2	B	59	ASP
2	B	76	ASN
2	B	77	ASP
2	B	141	GLN
2	B	188	ARG
2	B	217	TRP
2	B	221	LYS
2	B	231	LEU
2	B	245	LEU
2	B	254	LYS

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Mol	Chain	Res	Type
4	D	4	GLU
4	D	18	ARG
4	D	78	TRP
4	D	90	PHE
4	D	105	LYS
4	D	147	ARG
4	D	152	ASN
4	D	158	LYS
4	D	193	ASP
4	D	199	ASP
4	D	210	PHE
4	D	214	CYS
4	D	233	ASP
4	D	260	PHE
4	D	267	ASP
4	D	305	SER
4	D	316	TYR
4	D	332	ARG
4	D	333	TYR
4	D	364	PHE
4	D	365	LYS
4	D	371	LYS
4	E	17	ASN
4	E	41	CYS
4	E	56	LEU
4	E	60	ARG
4	E	66	ASP
4	E	80	LYS
4	E	102	PHE
4	E	110	ASP
4	E	175	HIS
4	E	194	ASP
4	E	204	HIS
4	E	252	ASN
4	E	294	SER
4	E	312	ARG
4	E	319	GLN
4	E	328	SER
4	E	332	ARG
4	E	346	ASN
4	E	359	ASP
4	F	34	ARG

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Mol	Chain	Res	Type
4	F	44	ARG
4	F	51	ASP
4	F	93	LYS
4	F	135	GLN
4	F	149	LEU
4	F	224	GLU
4	F	284	PHE
4	F	337	TYR
4	F	341	LYS
4	G	17	ASN
4	G	76	GLU
4	G	103	MET
4	G	110	ASP
4	G	148	MET
4	G	156	LYS
4	G	157	ASP
4	G	161	LYS
4	G	193	ASP
4	G	233	ASP
4	G	267	ASP
4	G	332	ARG
4	G	341	LYS
4	G	345	ARG
4	G	352	GLU
4	G	365	LYS
4	H	27	CYS
4	H	44	ARG
4	H	47	ARG
4	H	52	PHE
4	H	82	GLN
4	H	95	ASP
4	H	153	ASP
4	H	185	GLU
4	H	235	ASN
4	H	279	SER
4	H	312	ARG
4	H	339	HIS
4	H	344	SER
4	I	19	ASP
4	I	34	ARG
4	I	49	SER
4	I	52	PHE

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Mol	Chain	Res	Type
4	I	144	LEU
4	I	194	ASP
4	I	235	ASN
4	I	284	PHE
4	I	295	ASP
4	I	298	GLU
4	I	315	TYR
4	I	332	ARG
5	J	88	ASN
5	J	108	LEU
5	J	165	GLU
5	J	172	ASP
5	J	180	ASP
5	J	209	ASP
5	J	221	LYS
5	J	251	TRP
5	J	275	TRP
5	J	300	TYR
5	J	312	CYS
5	J	318	SER
5	J	355	LYS
5	J	386	ARG
5	J	401	LYS
5	J	422	LEU
5	J	477	TYR
5	J	518	TRP
6	K	57	LYS
6	K	95	LYS
6	K	154	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	86	ASN
4	F	275	ASN
4	F	319	GLN
4	G	225	GLN
4	H	131	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	60/61 (98%)	22 (36%)	1 (1%)

All (22) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	2	U
3	C	3	G
3	C	9	G
3	C	13	A
3	C	14	G
3	C	15	U
3	C	21	A
3	C	27	G
3	C	32	U
3	C	33	G
3	C	34	U
3	C	38	A
3	C	39	A
3	C	40	A
3	C	42	U
3	C	45	U
3	C	46	C
3	C	50	A
3	C	52	G
3	C	53	C
3	C	55	U
3	C	56	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	2	U

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

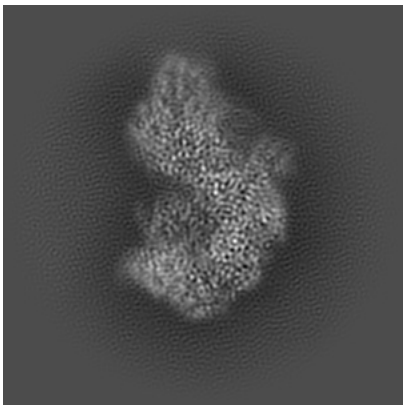
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39110. These allow visual inspection of the internal detail of the map and identification of artifacts.

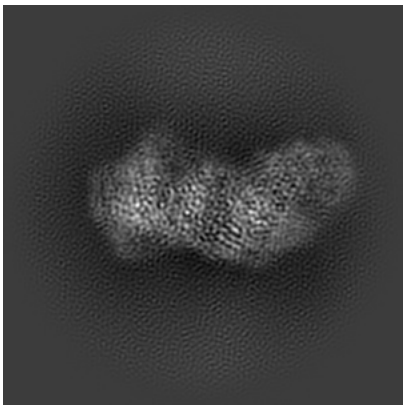
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

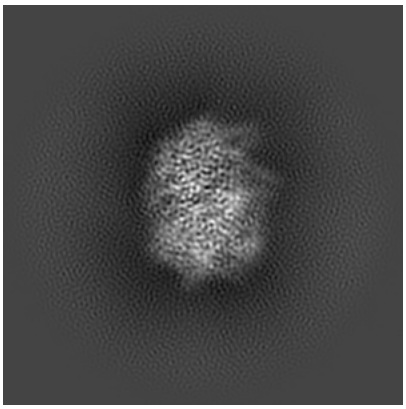
6.1.1 Primary map



X

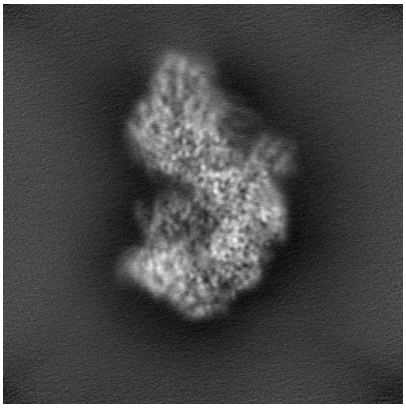


Y

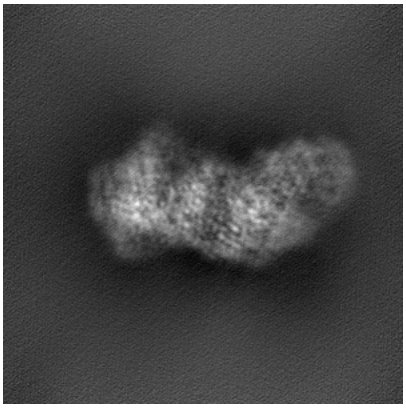


Z

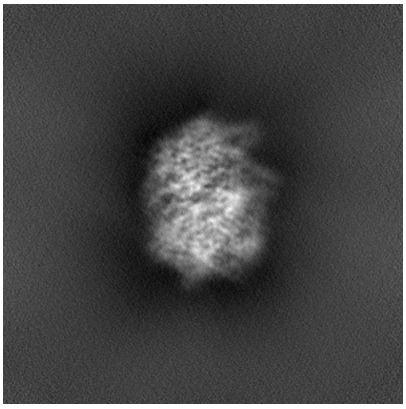
6.1.2 Raw map



X



Y

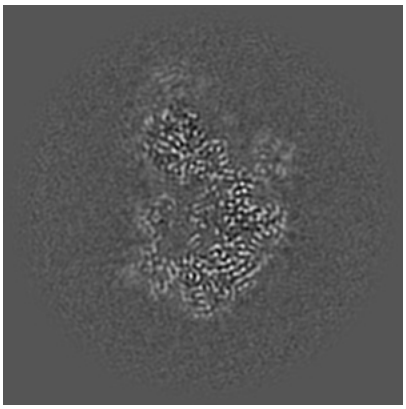


Z

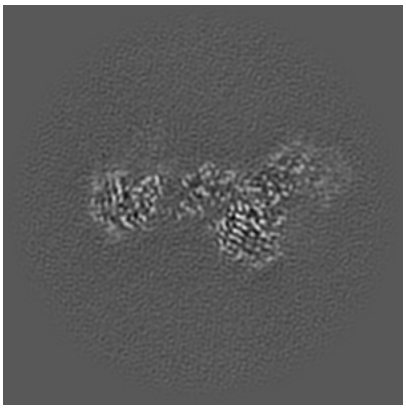
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

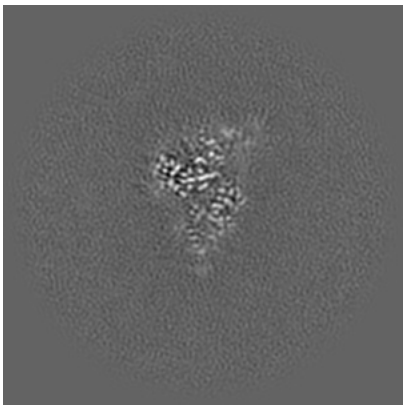
6.2.1 Primary map



X Index: 160

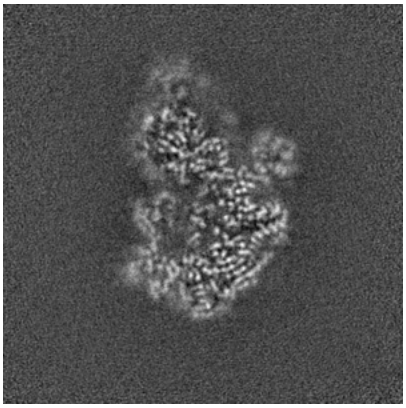


Y Index: 160

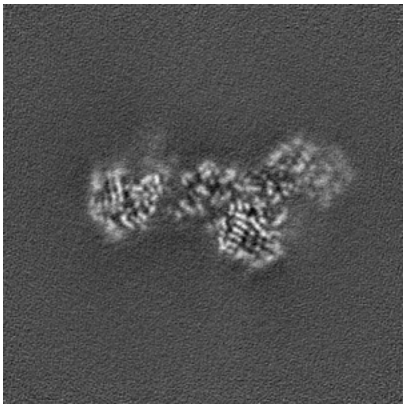


Z Index: 160

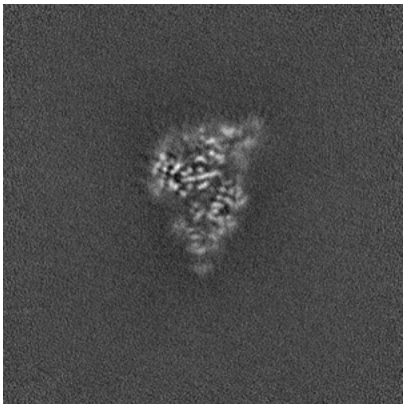
6.2.2 Raw map



X Index: 160



Y Index: 160

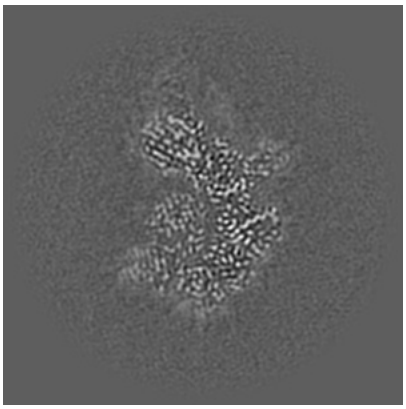


Z Index: 160

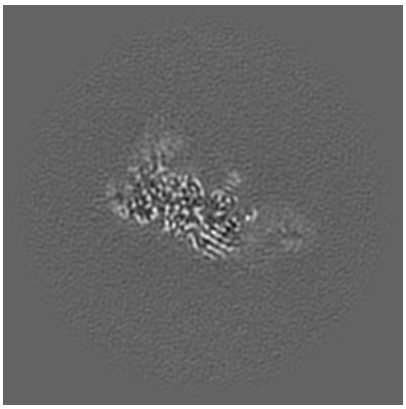
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

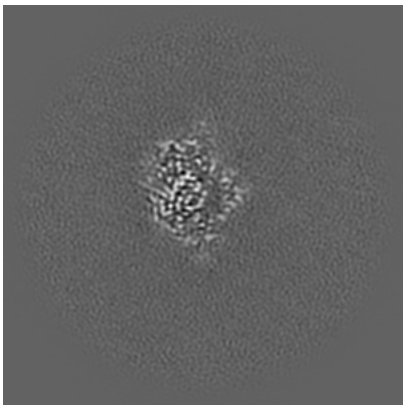
6.3.1 Primary map



X Index: 153

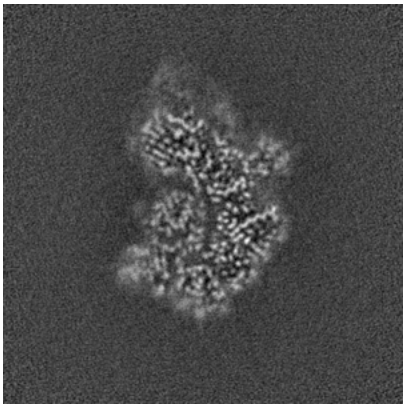


Y Index: 185

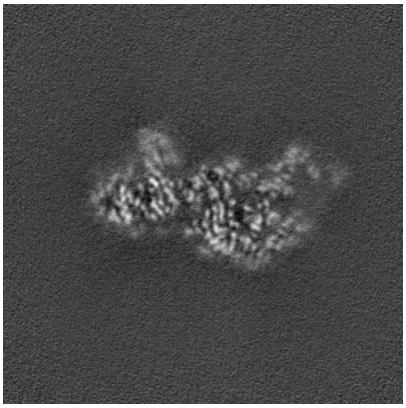


Z Index: 184

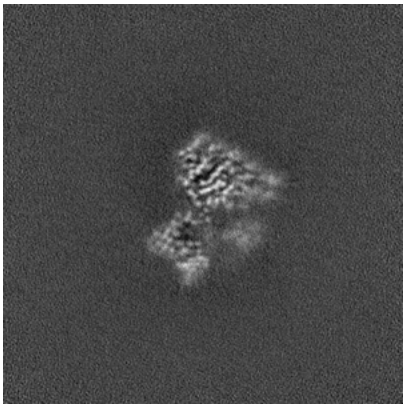
6.3.2 Raw map



X Index: 153



Y Index: 169

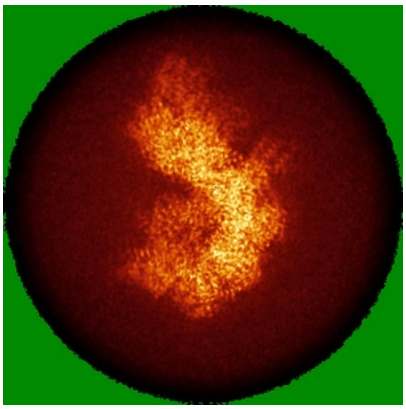


Z Index: 120

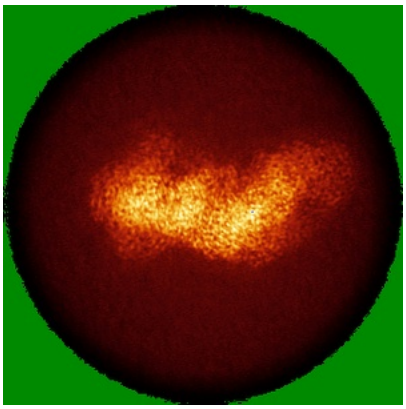
The images above show the largest variance slices of the map in three orthogonal directions.

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

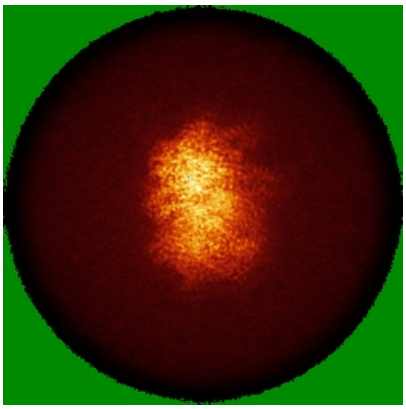
6.4.1 Primary map



X

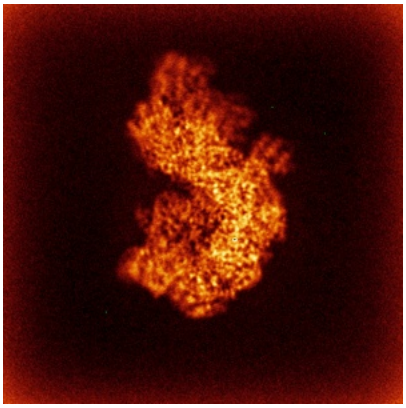


Y

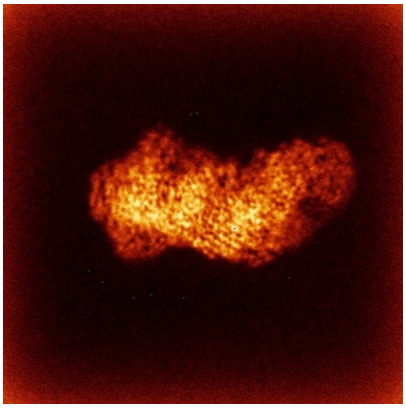


Z

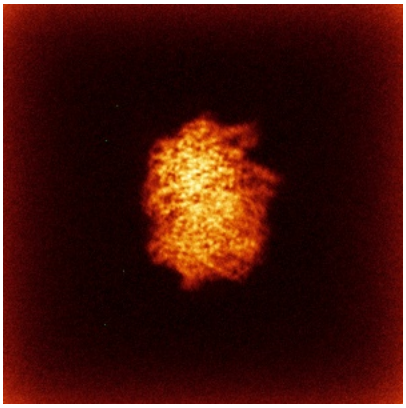
6.4.2 Raw map



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.

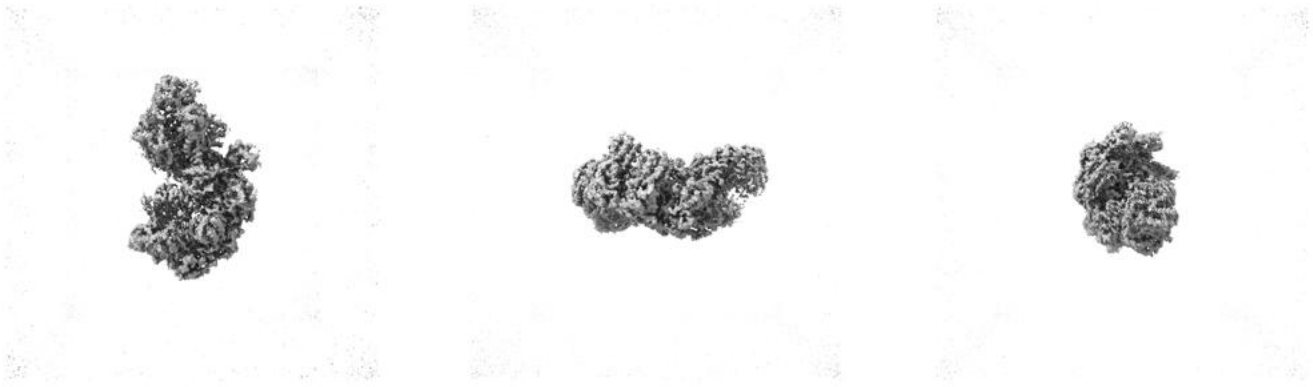
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

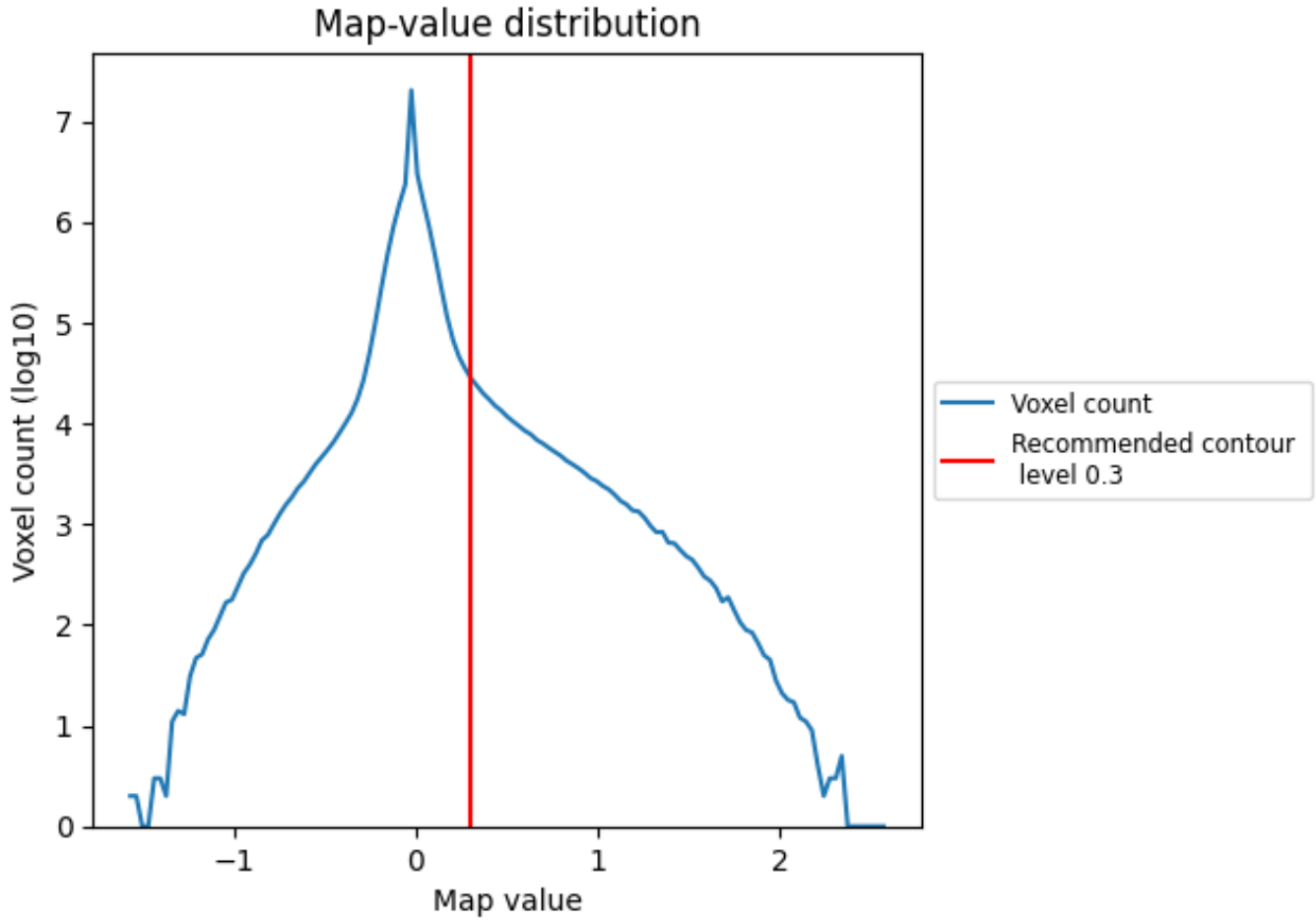
6.6 Mask visualisation (i)

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

7 Map analysis

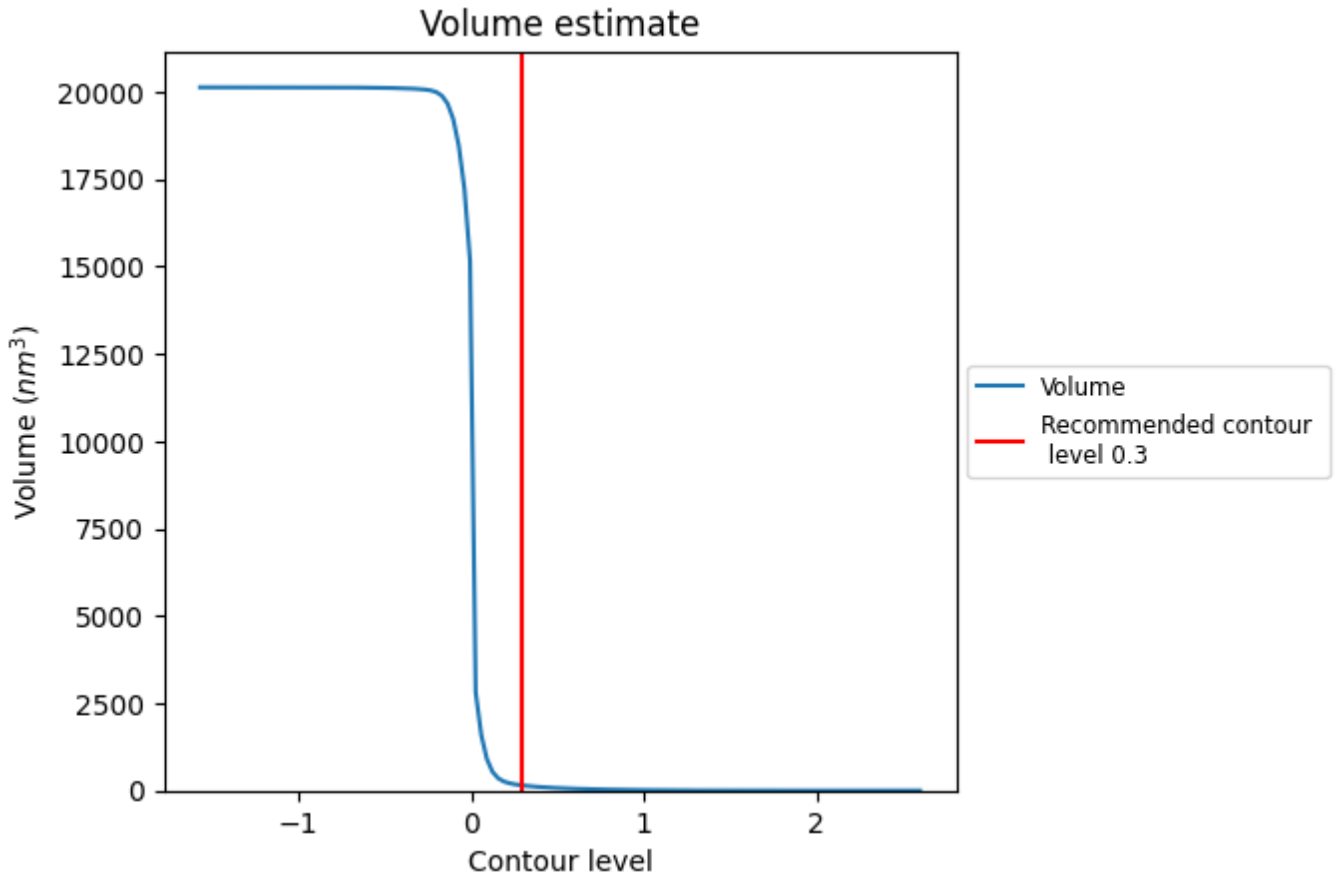
This section contains the results of statistical analysis of the map.

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.

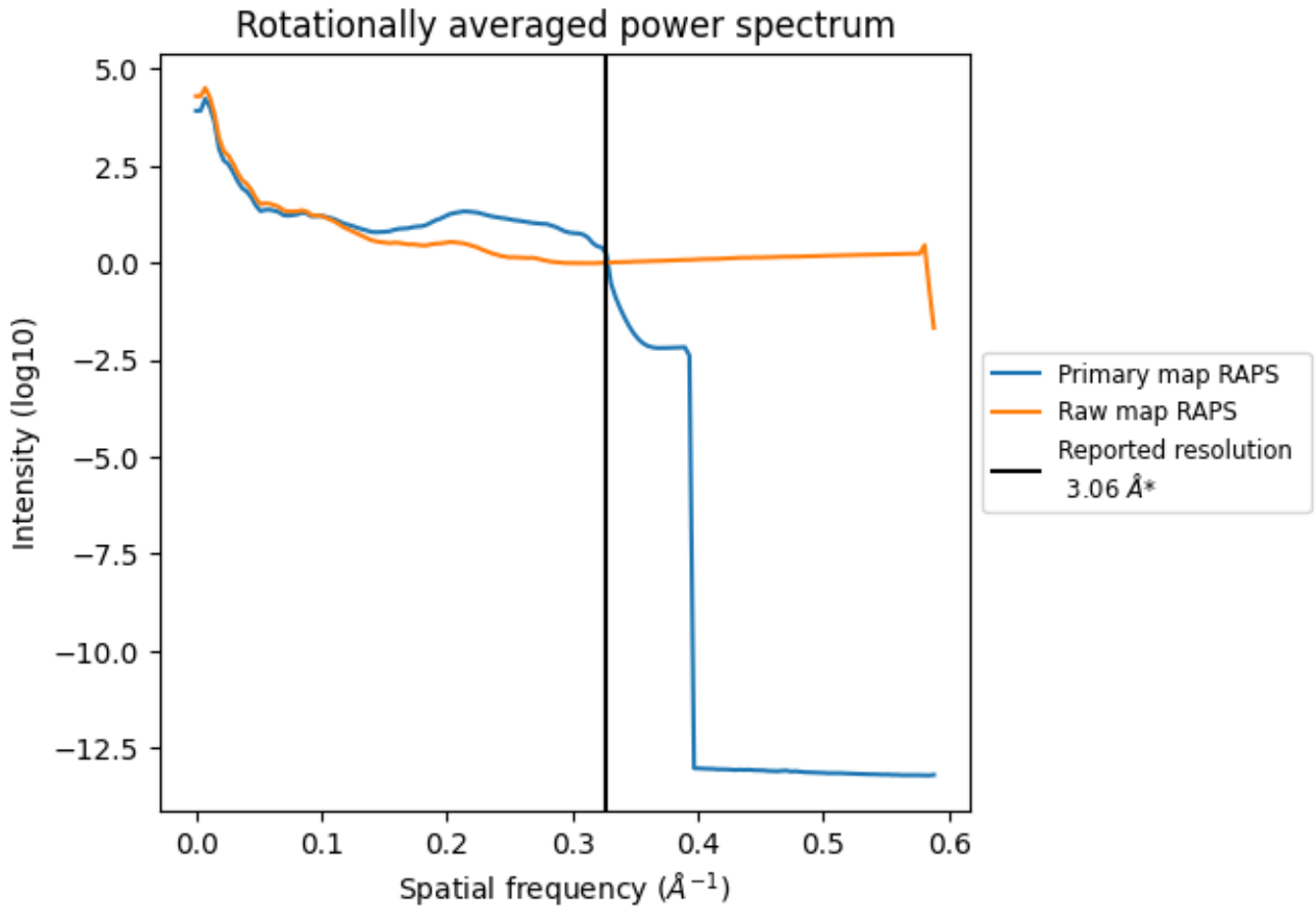
7.2 Volume estimate



The volume at the recommended contour level is 147 nm^3; this corresponds to an approximate mass of 133 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)

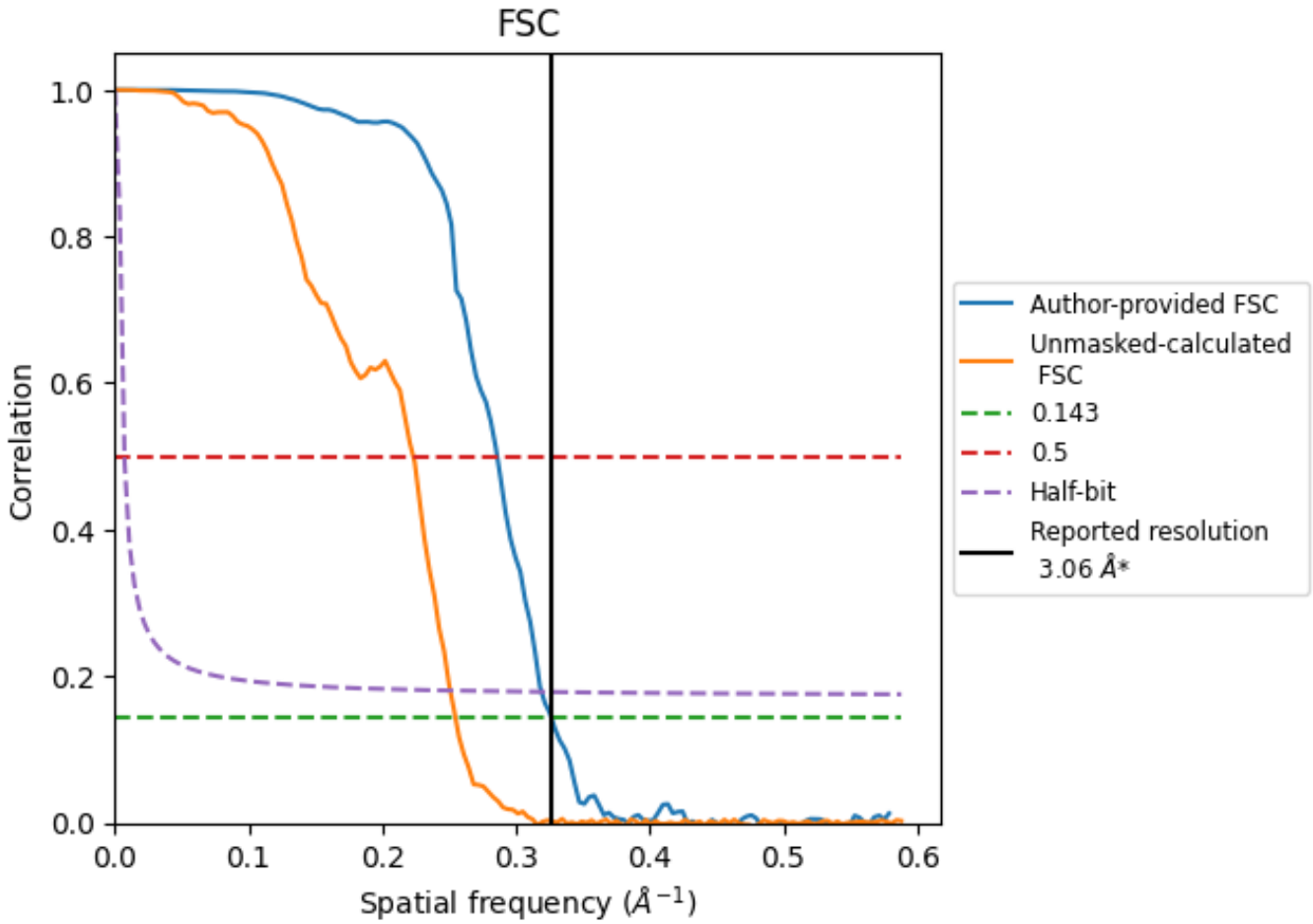


*Reported resolution corresponds to spatial frequency of 0.327 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.327 Å^{-1}

8.2 Resolution estimates (i)

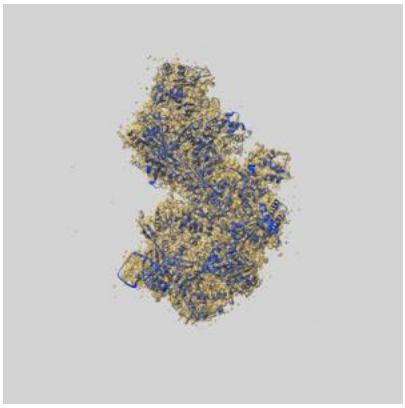
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.06	-	-
Author-provided FSC curve	3.06	3.50	3.13
Unmasked-calculated*	3.92	4.48	3.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.92 differs from the reported value 3.06 by more than 10 %

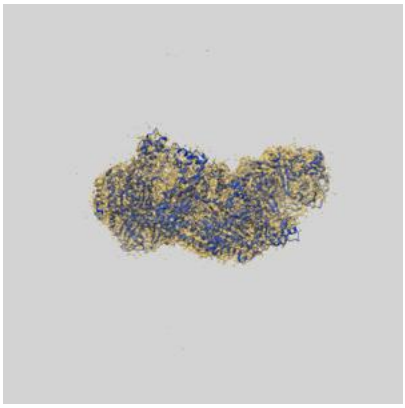
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39110 and PDB model 8YB6. Per-residue inclusion information can be found in section 3 on page 6.

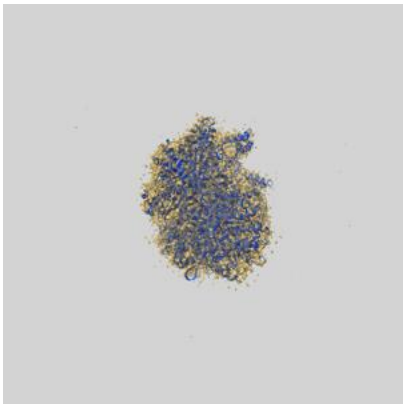
9.1 Map-model overlay



X



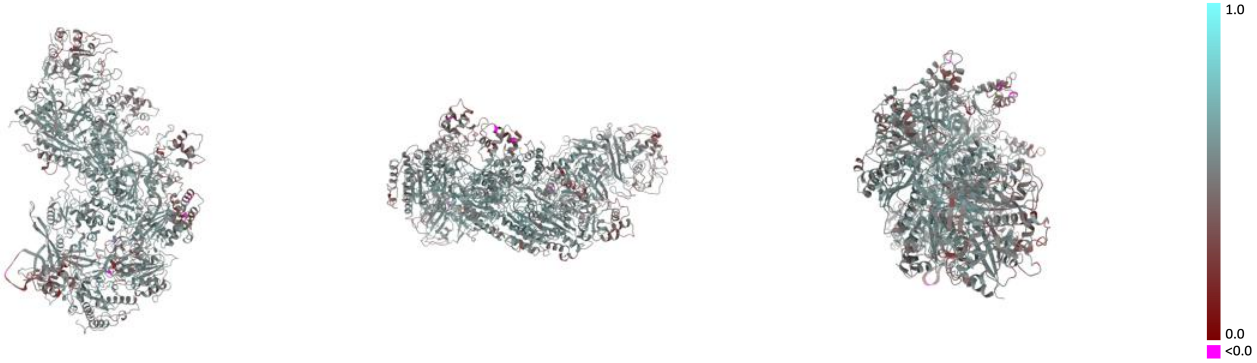
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

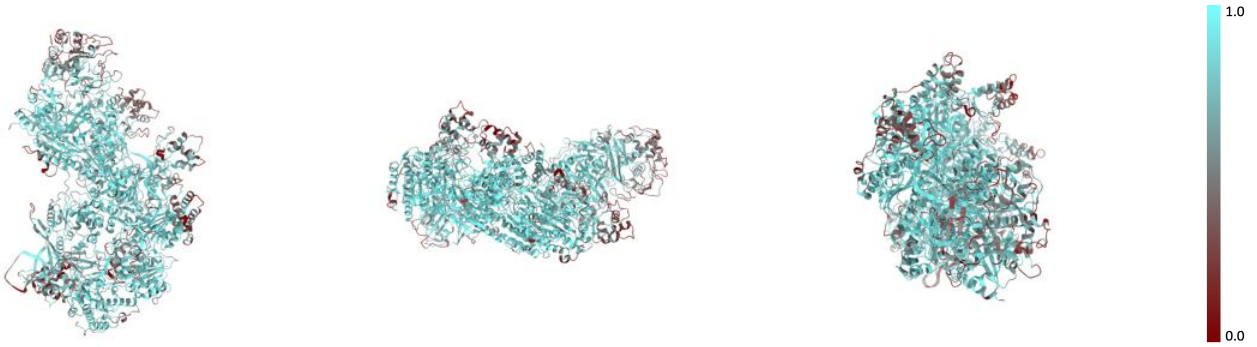
9.2 Q-score mapped to coordinate model (i)



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.

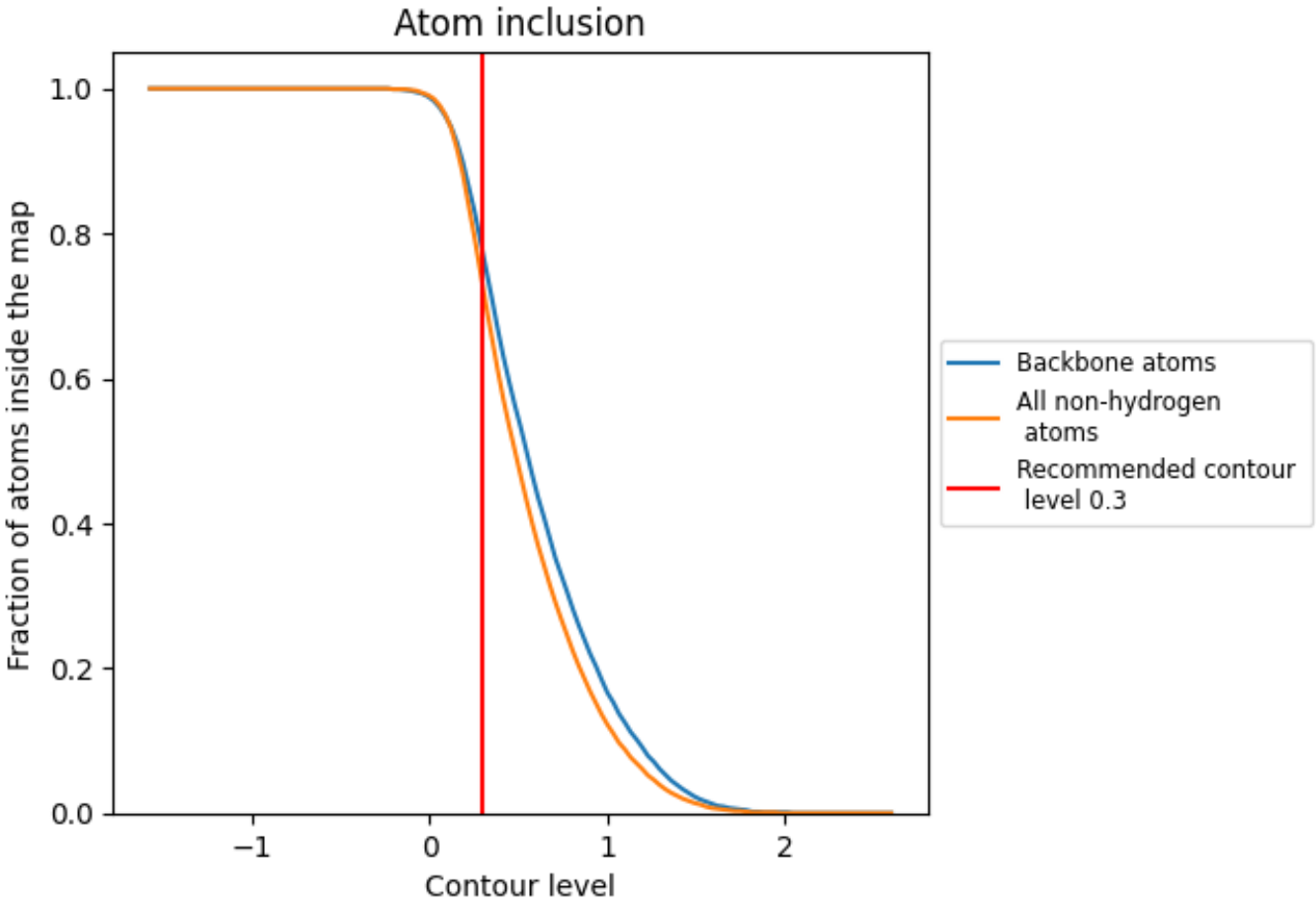
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 73% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7310	0.5120
A	0.7740	0.5330
B	0.7500	0.5170
C	0.8240	0.4940
D	0.6620	0.4770
E	0.7470	0.5100
F	0.7650	0.5190
G	0.7660	0.5300
H	0.7120	0.5180
I	0.7680	0.5260
J	0.6030	0.4780
K	0.8040	0.5520