Full wwPDB EM Validation Report

Jun 27, 2024 – 07:30 AM JST

PDB ID	:	7YHS
EMDB ID	:	EMD-33837
Title	:	Structure of Csy-AcrIF4-dsDNA
Authors	:	Feng, Y.; Zhang, L.X.
Deposited on	:	2022-07-14
Resolution	:	3.37 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:

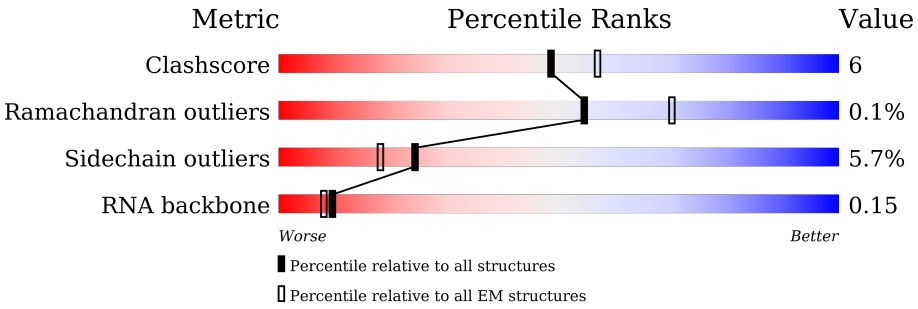
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.37 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	434	16% 86% 12% •
2	C	342	9% 69% 14% • 14%
2	D	342	9% 78% 16% • 5%
2	F	342	5% 80% 17% • •
2	G	342	• 82% 15% • •
2	H	342	• 80% 14% • 5%
2	I	342	6% 79% 16% • •

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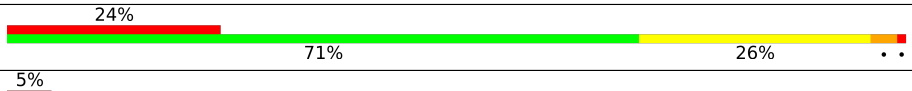
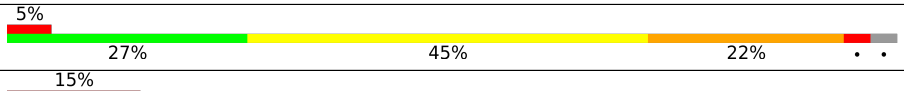
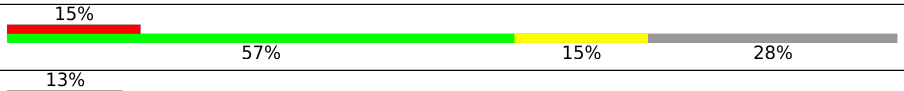
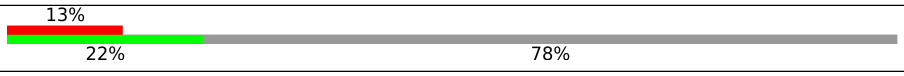
Mol	Chain	Length	Quality of chain
3	E	327	
4	J	100	
5	L	187	
6	M	60	
7	N	54	
8	O	54	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 24596 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 Type I-F CRISPR-associated protein Csy1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	423	3039	1916	574	547	2	0	0

- Molecule 2 is a protein called CRISPR-associated protein Csy3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	293	2240	1408	403	427	2	0	0
2	D	324	2425	1519	441	463	2	0	0
2	F	334	2548	1602	462	482	2	0	0
2	G	335	2529	1585	457	485	2	0	0
2	H	325	2490	1565	454	469	2	0	0
2	I	329	2514	1578	459	475	2	0	0

- Molecule 3 is a protein called CRISPR type I-F/YPEST-associated protein Csy2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	305	2373	1505	438	426	4	0	0

- Molecule 4 is a protein called AcrIF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	94	737	464	131	138	4	0	0

- Molecule 5 is a protein called Csy4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	187	Total	C	N	O	S	0	0
			1428	892	285	248	3		

- Molecule 6 is a RNA chain called RNA (58-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	58	Total	C	N	O	P	0	0
			1226	549	213	407	57		

- Molecule 7 is a DNA chain called DNA (39-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	39	Total	C	N	O	P	0	0
			803	378	156	230	39		

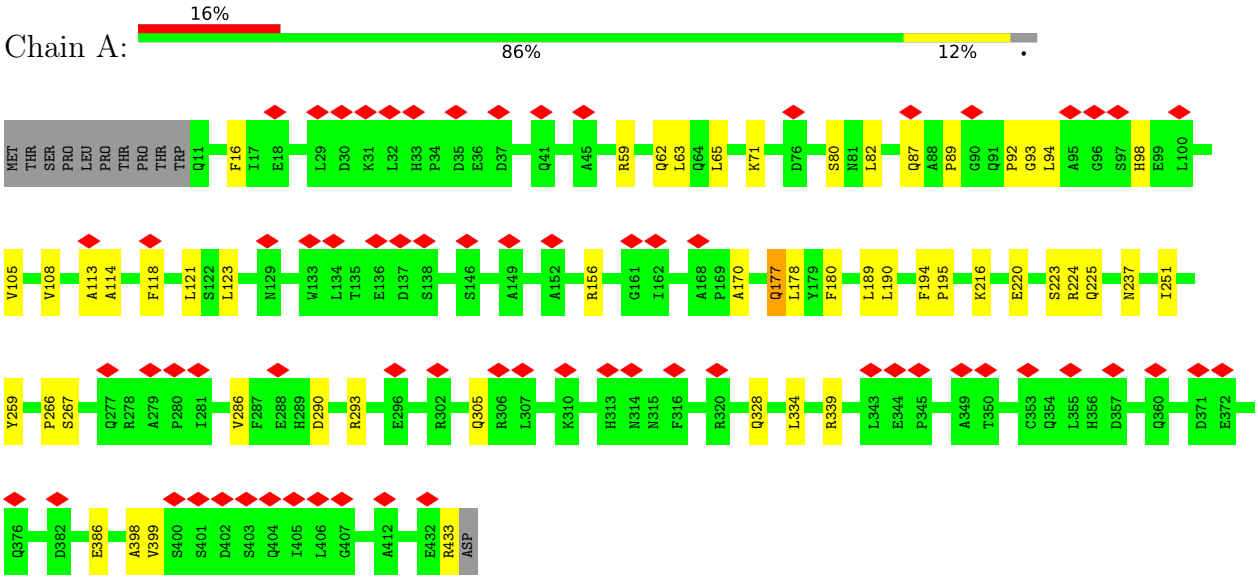
- Molecule 8 is a DNA chain called DNA (5'-D(P*AP*GP*CP*AP*GP*CP*TP*GP*CP*AP *CP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	12	Total	C	N	O	P	0	0
			244	115	47	70	12		

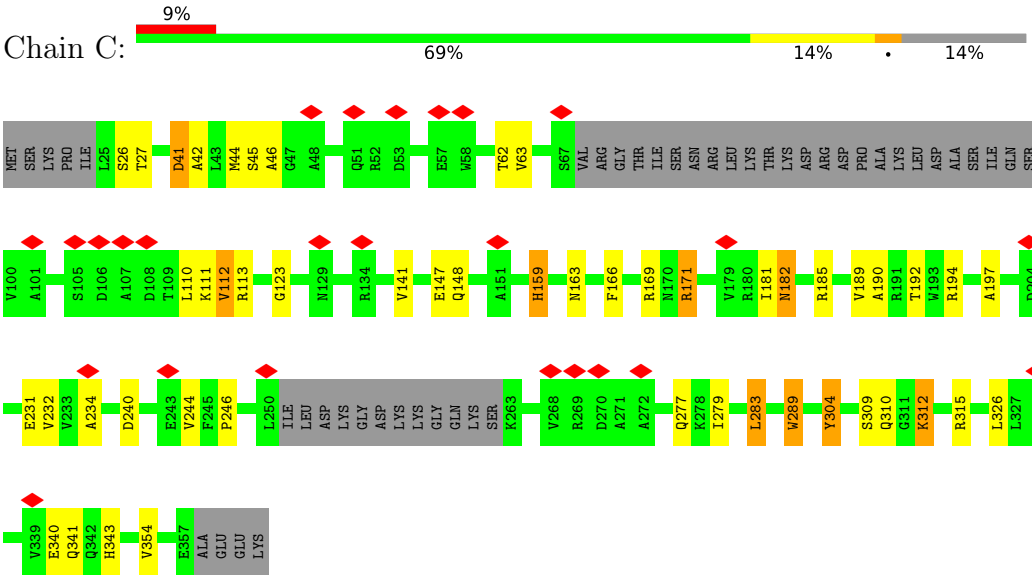
3 Residue-property plots (i)

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: Type I-F CRISPR-associated protein Csy1

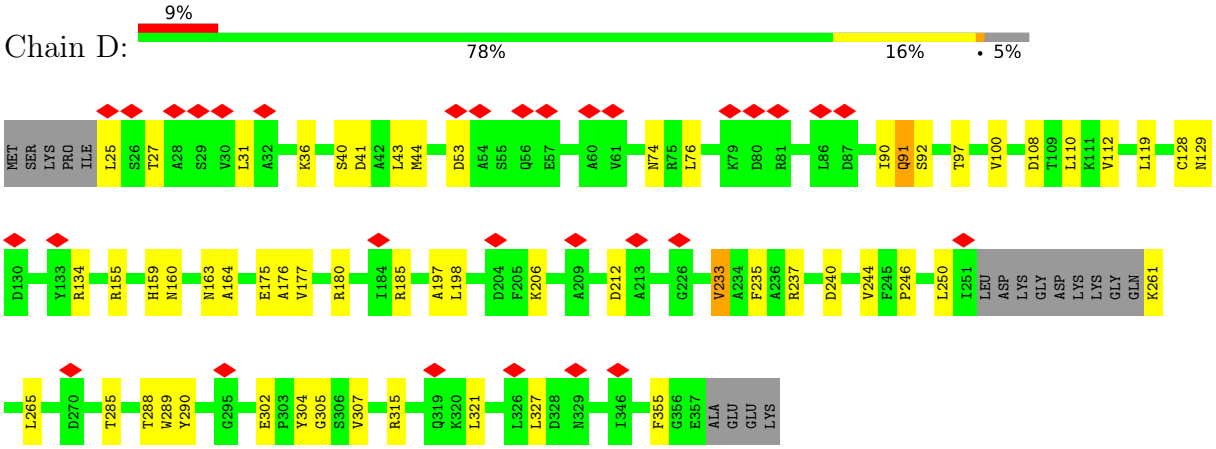


• Molecule 2: CRISPR-associated protein Csy3



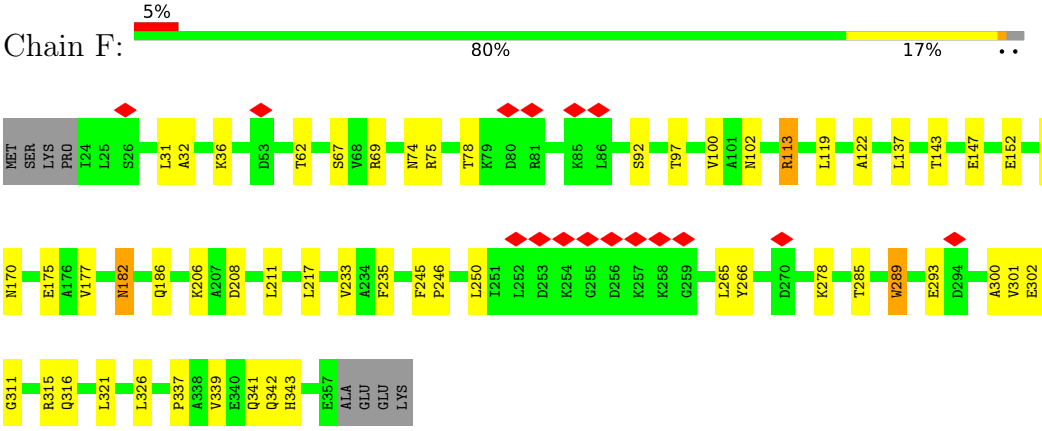
• Molecule 2: CRISPR-associated protein Csy3

Chain D:



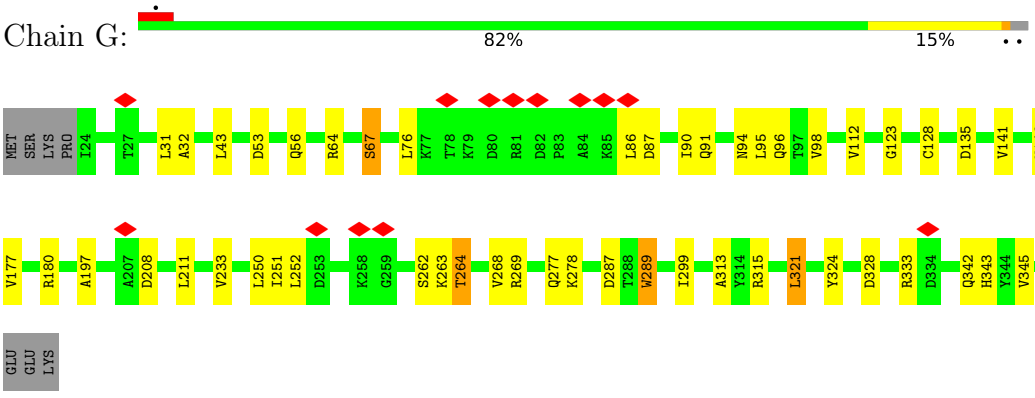
• Molecule 2: CRISPR-associated protein Csy3

Chain F:



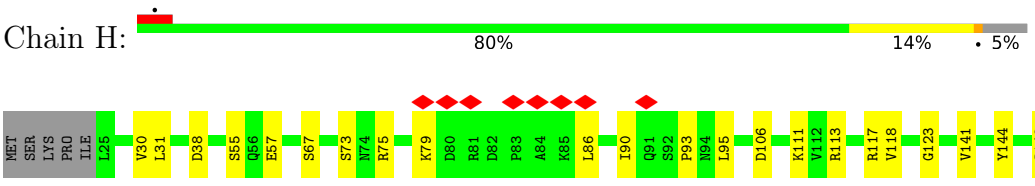
• Molecule 2: CRISPR-associated protein Csy3

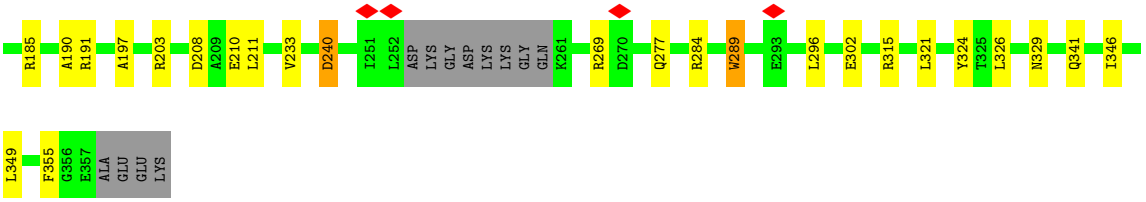
Chain G:



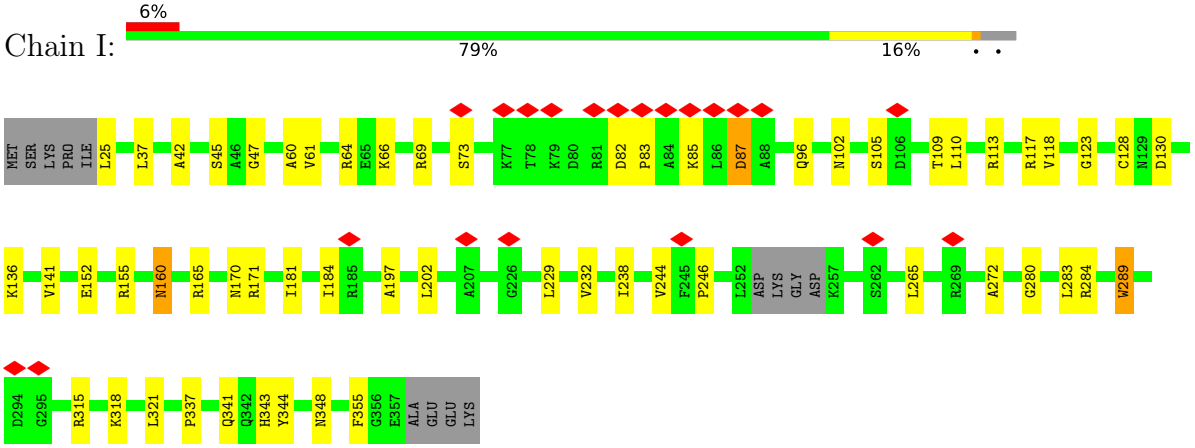
• Molecule 2: CRISPR-associated protein Csy3

Chain H:

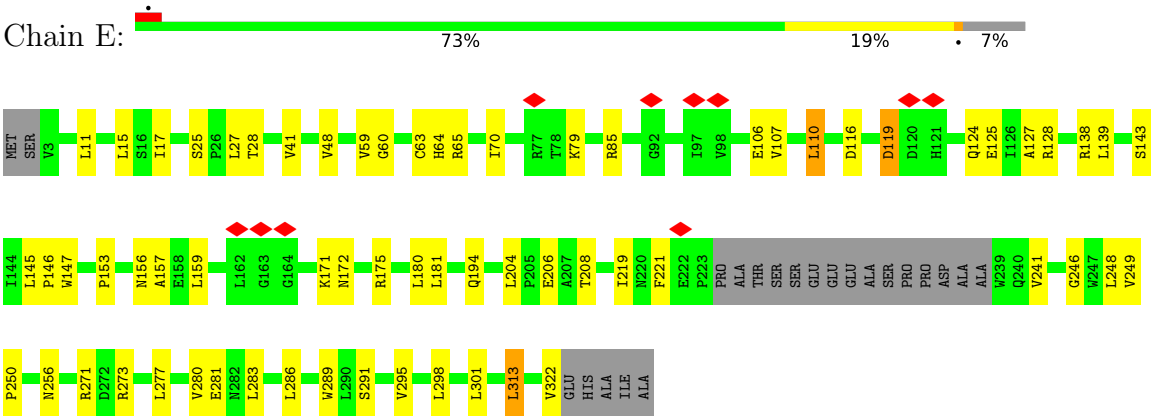




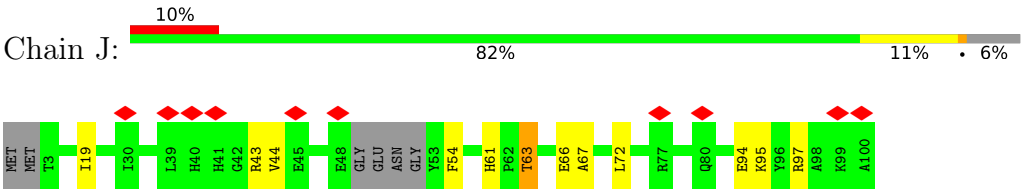
• Molecule 2: CRISPR-associated protein Csy3



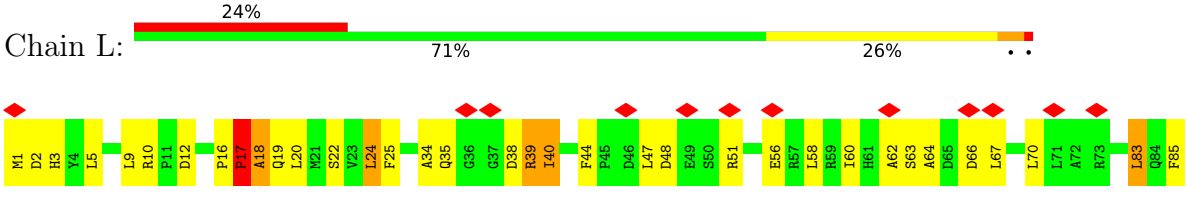
• Molecule 3: CRISPR type I-F/YPEST-associated protein Csy2

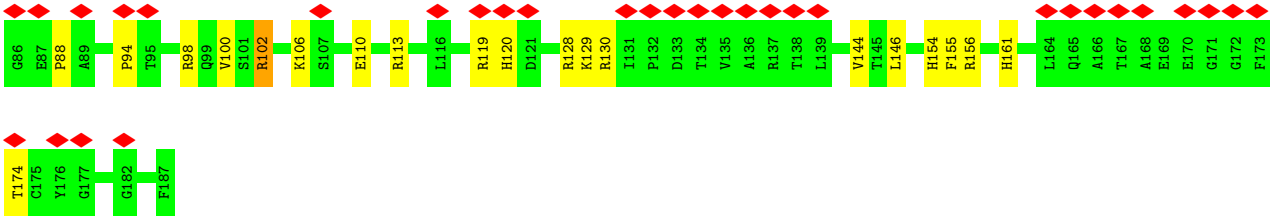


• Molecule 4: AcrIF4

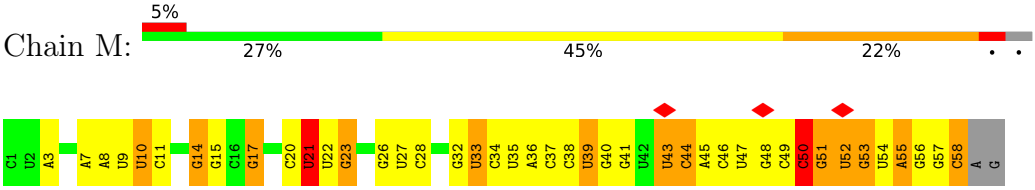


• Molecule 5: Csy4

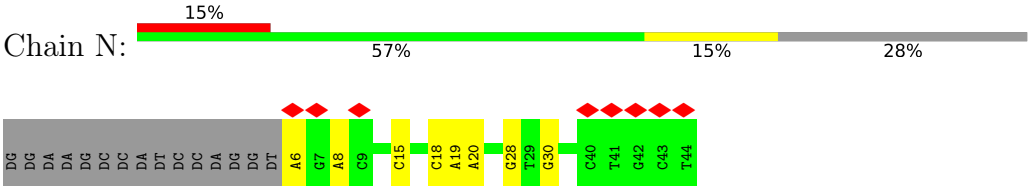




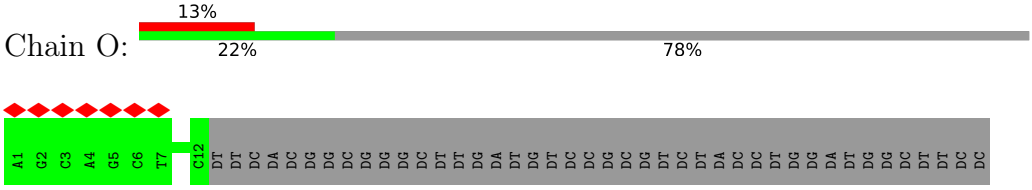
• Molecule 6: RNA (58-MER)



• Molecule 7: DNA (39-MER)



• Molecule 8: DNA (5'-D(P*AP*GP*CP*AP*GP*CP*TP*GP*CP*AP*CP*C)-3')



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117510	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.392	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	232.8, 232.8, 232.8	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

5 Model quality

5.1 Standard geometry

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	0.31	0/3107	0.52	0/4241
2	C	0.30	0/2280	0.54	0/3097
2	D	0.28	0/2466	0.52	0/3354
2	F	0.31	0/2594	0.54	0/3525
2	G	0.31	0/2573	0.54	1/3497 (0.0%)
2	H	0.29	0/2533	0.52	1/3438 (0.0%)
2	I	0.30	0/2559	0.54	0/3474
3	E	0.30	0/2430	0.58	1/3311 (0.0%)
4	J	0.28	0/752	0.49	0/1018
5	L	0.35	0/1459	0.74	1/1973 (0.1%)
6	M	0.51	0/1368	1.33	20/2128 (0.9%)
7	N	0.78	0/902	1.02	0/1390
8	O	0.56	0/273	0.83	0/418
All	All	0.35	0/25296	0.65	24/34864 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	21	U	N1-C2-O2	12.14	131.30	122.80
6	M	21	U	C2-N1-C1'	11.41	131.39	117.70
6	M	21	U	N3-C2-O2	-11.20	114.36	122.20
6	M	38	C	N1-C2-O2	8.53	124.02	118.90
6	M	17	G	O4'-C1'-N9	8.11	114.69	108.20
6	M	21	U	C6-N1-C1'	-7.64	110.50	121.20
6	M	50	C	C6-N1-C2	-7.37	117.35	120.30
6	M	38	C	N3-C2-O2	-7.26	116.82	121.90
6	M	38	C	C2-N1-C1'	7.24	126.77	118.80
5	L	17	PRO	N-CA-C	6.63	129.35	112.10
6	M	37	C	C2-N1-C1'	6.40	125.84	118.80
6	M	37	C	N1-C2-O2	6.22	122.63	118.90
6	M	33	U	P-O3'-C3'	6.14	127.07	119.70
6	M	10	U	C5-C6-N1	5.99	125.70	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	20	C	N1-C2-O2	5.95	122.47	118.90
6	M	55	A	P-O3'-C3'	5.76	126.62	119.70
6	M	50	C	N1-C2-O2	5.65	122.29	118.90
2	G	135	ASP	CB-CG-OD1	5.56	123.31	118.30
3	E	110	LEU	CA-CB-CG	5.55	128.06	115.30
6	M	44	C	P-O3'-C3'	5.51	126.31	119.70
6	M	50	C	N3-C2-O2	-5.19	118.27	121.90
2	H	86	LEU	CA-CB-CG	5.18	127.22	115.30
6	M	21	U	C5-C6-N1	5.04	125.22	122.70
6	M	50	C	C5-C6-N1	5.00	123.50	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3039	0	2716	30	0
2	C	2240	0	2179	31	0
2	D	2425	0	2333	26	0
2	F	2548	0	2499	35	0
2	G	2529	0	2474	32	0
2	H	2490	0	2465	30	0
2	I	2514	0	2465	34	0
3	E	2373	0	2356	39	0
4	J	737	0	710	8	0
5	L	1428	0	1366	59	0
6	M	1226	0	625	15	0
7	N	803	0	435	7	0
8	O	244	0	134	0	0
All	All	24596	0	22757	294	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 6.

All (294) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:40:ILE:CG2	5:L:62:ALA:HB2	1.75	1.14
5:L:40:ILE:HG21	5:L:62:ALA:HB2	1.28	1.06
5:L:40:ILE:HG21	5:L:62:ALA:CB	1.87	1.04
5:L:35:GLN:NE2	5:L:70:LEU:CG	2.31	0.94
5:L:35:GLN:HE21	5:L:70:LEU:HD12	1.33	0.93
5:L:35:GLN:NE2	5:L:70:LEU:HD12	1.85	0.91
5:L:40:ILE:CG2	5:L:62:ALA:CB	2.47	0.88
5:L:35:GLN:NE2	5:L:70:LEU:HG	1.89	0.86
5:L:35:GLN:NE2	5:L:70:LEU:CD1	2.40	0.85
5:L:40:ILE:CG2	5:L:62:ALA:CA	2.56	0.82
5:L:35:GLN:HE22	5:L:70:LEU:HG	1.45	0.81
5:L:17:PRO:O	5:L:19:GLN:N	2.13	0.81
5:L:39:ARG:CD	5:L:39:ARG:H	1.94	0.80
5:L:40:ILE:HG21	5:L:62:ALA:N	1.96	0.80
5:L:39:ARG:H	5:L:39:ARG:HD2	1.46	0.80
5:L:40:ILE:HG23	5:L:62:ALA:HB2	1.63	0.79
5:L:40:ILE:HG21	5:L:62:ALA:CA	2.13	0.79
5:L:40:ILE:CG2	5:L:62:ALA:N	2.48	0.76
1:A:225:GLN:OE1	4:J:19:ILE:CD1	2.34	0.75
2:H:31:LEU:HB3	2:H:355:PHE:O	1.87	0.74
2:I:280:GLY:O	2:I:284:ARG:HB2	1.88	0.73
2:D:31:LEU:HB3	2:D:355:PHE:O	1.91	0.71
2:I:47:GLY:O	2:I:109:THR:HB	1.92	0.70
5:L:128:ARG:HG3	5:L:129:LYS:HG2	1.75	0.69
5:L:38:ASP:N	5:L:38:ASP:OD2	2.26	0.68
2:D:302:GLU:HB3	2:D:305:GLY:HA2	1.76	0.68
5:L:35:GLN:HE22	5:L:70:LEU:CG	2.00	0.66
2:D:128:CYS:HB3	2:D:134:ARG:HD3	1.76	0.66
6:M:35:U:N3	7:N:6:DA:N1	2.46	0.64
5:L:17:PRO:O	5:L:18:ALA:C	2.37	0.63
5:L:5:LEU:HB3	5:L:60:ILE:HB	1.82	0.61
2:F:250:LEU:HB3	2:G:67:SER:HB3	1.83	0.60
5:L:1:MET:HA	5:L:63:SER:HB3	1.83	0.60
2:F:250:LEU:HD21	2:G:95:LEU:HB3	1.83	0.59
3:E:159:LEU:HD11	3:E:175:ARG:HH22	1.66	0.59
2:G:208:ASP:HB3	2:G:211:LEU:HB2	1.84	0.59
2:I:289:TRP:O	2:I:315:ARG:NH2	2.36	0.59
2:C:289:TRP:HB3	2:C:340:GLU:HB3	1.86	0.58
5:L:35:GLN:HE22	5:L:70:LEU:CB	2.16	0.58
2:G:159:HIS:O	2:G:163:ASN:ND2	2.36	0.58
5:L:25:PHE:HB3	5:L:146:LEU:HD21	1.85	0.58
2:D:155:ARG:O	2:D:159:HIS:ND1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:113:ARG:HG3	2:H:233:VAL:HG12	1.85	0.57
2:C:309:SER:HB2	5:L:16:PRO:HB3	1.85	0.57
2:D:27:THR:HG21	2:F:75:ARG:HH12	1.70	0.57
2:F:289:TRP:O	2:F:315:ARG:NH2	2.38	0.57
5:L:35:GLN:NE2	5:L:70:LEU:CB	2.67	0.57
2:H:171:ARG:NH2	2:H:197:ALA:O	2.38	0.57
5:L:48:ASP:HB3	5:L:51:ARG:HH22	1.69	0.57
2:H:277:GLN:OE1	2:I:66:LYS:NZ	2.37	0.57
2:F:69:ARG:NH1	6:M:32:G:O2'	2.37	0.57
2:F:316:GLN:NE2	2:G:87:ASP:OD1	2.37	0.57
3:E:25:SER:HB2	3:E:28:THR:H	1.68	0.57
3:E:119:ASP:OD1	3:E:119:ASP:N	2.34	0.57
2:F:302:GLU:HB3	2:F:305:GLY:HA2	1.87	0.56
2:F:250:LEU:HD11	2:G:95:LEU:HD13	1.87	0.56
3:E:147:TRP:HE1	3:E:153:PRO:HA	1.70	0.56
2:H:269:ARG:HH12	2:I:105:SER:H	1.51	0.56
5:L:40:ILE:HG23	5:L:62:ALA:CB	2.28	0.56
1:A:62:GLN:NE2	1:A:114:ALA:O	2.38	0.56
2:G:315:ARG:NH1	2:G:321:LEU:O	2.38	0.56
1:A:225:GLN:OE1	4:J:19:ILE:HD12	2.05	0.56
5:L:94:PRO:O	5:L:98:ARG:NH2	2.38	0.56
3:E:70:ILE:HD12	3:E:79:LYS:HD3	1.87	0.56
2:I:96:GLN:NE2	7:N:28:DG:OP2	2.36	0.55
3:E:65:ARG:HG2	3:E:106:GLU:HB3	1.87	0.55
2:H:55:SER:O	2:H:111:LYS:NZ	2.38	0.55
2:I:181:ILE:HG12	2:I:232:VAL:HG13	1.88	0.55
2:H:315:ARG:NH1	2:H:321:LEU:O	2.39	0.55
2:D:97:THR:O	2:D:261:LYS:N	2.40	0.55
2:C:326:LEU:HD21	2:C:341:GLN:HB3	1.89	0.55
2:H:93:PRO:HD2	7:N:20:DA:H1'	1.88	0.55
2:G:289:TRP:O	2:G:315:ARG:NH2	2.39	0.55
2:I:82:ASP:HB2	2:I:85:LYS:HE3	1.89	0.55
2:F:337:PRO:O	2:F:342:GLN:NE2	2.40	0.55
2:G:250:LEU:HD21	2:H:95:LEU:HD22	1.89	0.54
2:G:98:VAL:HG23	2:G:263:LYS:HB3	1.89	0.54
5:L:9:LEU:HB2	5:L:56:GLU:HB2	1.89	0.54
3:E:85:ARG:HB3	6:M:8:A:H3'	1.90	0.54
2:G:94:ASN:HB2	7:N:15:DC:H4'	1.89	0.54
2:C:185:ARG:HB2	2:C:190:ALA:HB2	1.90	0.54
5:L:102:ARG:NH1	6:M:58:C:OP1	2.40	0.54
2:F:113:ARG:HB2	2:F:233:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:180:ARG:HB3	2:G:233:VAL:HG12	1.90	0.54
2:G:313:ALA:HB2	2:H:90:ILE:HA	1.90	0.54
2:D:40:SER:OG	2:D:41:ASP:N	2.41	0.54
3:E:63:CYS:H	3:E:107:VAL:HG23	1.72	0.54
2:C:147:GLU:OE1	2:C:148:GLN:NE2	2.40	0.54
2:I:123:GLY:HA3	2:I:141:VAL:HG11	1.90	0.53
5:L:17:PRO:O	5:L:20:LEU:N	2.35	0.53
2:F:159:HIS:NE2	2:F:206:LYS:O	2.41	0.53
1:A:63:LEU:HD23	1:A:65:LEU:HD11	1.90	0.53
2:C:289:TRP:O	2:C:315:ARG:NH2	2.40	0.53
2:C:244:VAL:HG13	2:C:246:PRO:HD3	1.90	0.53
3:E:273:ARG:NH1	2:I:130:ASP:OD1	2.42	0.53
2:F:177:VAL:HA	2:F:235:PHE:O	2.09	0.53
2:F:266:TYR:OH	2:G:64:ARG:NH2	2.41	0.53
3:E:15:LEU:O	3:E:106:GLU:HA	2.08	0.53
5:L:12:ASP:OD2	5:L:12:ASP:N	2.42	0.53
2:C:171:ARG:NH2	2:C:197:ALA:O	2.42	0.53
2:D:185:ARG:NH2	2:F:175:GLU:OE2	2.39	0.52
2:C:123:GLY:HA3	2:C:141:VAL:HG21	1.91	0.52
3:E:15:LEU:HB2	3:E:107:VAL:O	2.08	0.52
2:F:92:SER:HB2	7:N:8:DA:H4'	1.91	0.52
2:F:170:ASN:HD21	2:F:245:PHE:H	1.56	0.52
2:F:309:SER:OG	2:F:310:GLN:N	2.43	0.52
1:A:216:LYS:HG2	4:J:97:ARG:HH12	1.75	0.52
2:F:36:LYS:HG3	2:F:119:LEU:HB2	1.91	0.52
1:A:93:GLY:H	3:E:194:GLN:HE21	1.58	0.52
2:C:304:TYR:HA	2:C:315:ARG:HB2	1.92	0.52
2:D:155:ARG:NH1	2:D:212:ASP:OD1	2.43	0.52
2:G:278:LYS:NZ	6:M:22:U:OP1	2.37	0.52
5:L:144:VAL:O	5:L:156:ARG:NH1	2.42	0.52
2:H:284:ARG:NH2	2:H:302:GLU:OE2	2.43	0.51
2:I:37:LEU:HG	2:I:118:VAL:HG12	1.92	0.51
2:G:277:GLN:NE2	6:M:21:U:OP2	2.44	0.51
2:I:344:TYR:O	2:I:348:ASN:ND2	2.40	0.51
1:A:180:PHE:HB2	1:A:190:LEU:HD22	1.92	0.51
5:L:10:ARG:NH1	5:L:83:LEU:O	2.44	0.51
1:A:189:LEU:HD23	3:E:277:LEU:HD12	1.93	0.50
3:E:295:VAL:HG11	3:E:301:LEU:HD21	1.92	0.50
1:A:177:GLN:HG3	3:E:271:ARG:HB2	1.94	0.50
2:C:159:HIS:O	2:C:163:ASN:ND2	2.45	0.50
2:D:159:HIS:O	2:D:163:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:11:LEU:HB3	3:E:157:ALA:HB3	1.93	0.50
2:I:184:ILE:HB	2:I:229:LEU:HD22	1.94	0.50
2:D:246:PRO:HG2	2:D:265:LEU:HD13	1.93	0.50
2:F:32:ALA:HB1	6:M:23:G:H1'	1.92	0.50
2:I:315:ARG:NH1	2:I:321:LEU:O	2.45	0.50
5:L:24:LEU:HG	5:L:58:LEU:HD12	1.93	0.49
2:F:337:PRO:HG2	2:F:342:GLN:HG3	1.94	0.49
2:H:191:ARG:NH2	2:H:210:GLU:OE1	2.46	0.49
3:E:116:ASP:OD1	3:E:116:ASP:N	2.43	0.49
2:D:129:ASN:HA	2:F:311:GLY:HA3	1.94	0.49
3:E:125:GLU:HG3	3:E:128:ARG:HH12	1.77	0.49
2:G:164:ALA:H	2:G:197:ALA:HB1	1.78	0.49
5:L:40:ILE:HG21	5:L:62:ALA:H	1.77	0.49
1:A:305:GLN:HE21	1:A:398:ALA:HA	1.78	0.49
2:C:44:MET:HB2	2:C:110:LEU:HD11	1.95	0.49
5:L:47:LEU:HD13	5:L:56:GLU:H	1.78	0.49
1:A:98:HIS:HD1	1:A:98:HIS:H	1.61	0.49
2:F:36:LYS:HE3	2:F:122:ALA:HA	1.95	0.48
3:E:127:ALA:HB1	3:E:156:ASN:HD22	1.77	0.48
2:F:67:SER:HA	2:F:97:THR:HA	1.96	0.48
2:D:315:ARG:NE	2:D:321:LEU:O	2.47	0.48
6:M:50:C:O2'	6:M:52:U:OP1	2.24	0.48
2:D:36:LYS:HG2	2:D:119:LEU:HB2	1.94	0.48
2:G:342:GLN:HA	2:G:345:VAL:HG22	1.95	0.48
1:A:190:LEU:HG	3:E:280:VAL:HG11	1.96	0.48
1:A:89:PRO:HB3	3:E:313:LEU:HD21	1.95	0.48
2:G:252:LEU:HD21	2:H:95:LEU:HD13	1.95	0.48
5:L:5:LEU:HD11	5:L:85:PHE:HD2	1.79	0.48
2:H:31:LEU:CB	2:H:355:PHE:O	2.58	0.48
5:L:40:ILE:CG2	5:L:62:ALA:HA	2.44	0.48
2:I:170:ASN:HB3	2:I:238:ILE:HD11	1.96	0.47
2:C:112:VAL:HG23	2:C:234:ALA:HB3	1.95	0.47
2:H:289:TRP:O	2:H:315:ARG:NH2	2.35	0.47
2:H:326:LEU:HD13	2:H:341:GLN:HB3	1.96	0.47
2:I:171:ARG:NH2	2:I:197:ALA:O	2.46	0.47
5:L:40:ILE:HG22	5:L:62:ALA:N	2.28	0.47
2:C:277:GLN:NE2	6:M:39:U:OP1	2.47	0.47
5:L:17:PRO:HA	5:L:20:LEU:HD12	1.96	0.47
5:L:39:ARG:CD	5:L:39:ARG:N	2.73	0.47
2:G:287:ASP:HB3	2:G:299:ILE:HG13	1.96	0.47
2:C:62:THR:OG1	2:C:63:VAL:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:321:LEU:HD21	2:F:341:GLN:HE22	1.80	0.47
2:H:208:ASP:HB3	2:H:211:LEU:HB2	1.96	0.47
5:L:110:GLU:HA	5:L:113:ARG:HG2	1.96	0.47
2:I:42:ALA:HA	2:I:113:ARG:O	2.15	0.46
2:I:45:SER:HA	2:I:60:ALA:HA	1.97	0.46
3:E:219:ILE:HG22	3:E:241:VAL:HB	1.96	0.46
2:G:324:TYR:OH	2:H:73:SER:O	2.28	0.46
1:A:290:ASP:HA	1:A:293:ARG:HB2	1.97	0.46
2:I:64:ARG:HH22	2:I:102:ASN:HD21	1.63	0.46
3:E:143:SER:HB3	2:I:117:ARG:HH22	1.81	0.46
5:L:2:ASP:OD1	5:L:2:ASP:N	2.43	0.46
2:F:316:GLN:HE22	2:G:90:ILE:HD11	1.81	0.46
6:M:51:G:N3	6:M:53:G:O2'	2.47	0.46
2:C:111:LYS:HE3	2:C:111:LYS:HB2	1.72	0.45
1:A:16:PHE:HE2	1:A:123:LEU:HB3	1.82	0.45
2:F:143:THR:O	2:F:147:GLU:HB2	2.15	0.45
2:G:94:ASN:HD22	2:G:96:GLN:HE21	1.64	0.45
2:H:177:VAL:HB	2:H:197:ALA:HB3	1.98	0.45
2:C:330:TRP:HB2	2:C:336:ALA:HB2	1.98	0.45
2:I:337:PRO:HB2	2:I:341:GLN:HB2	1.98	0.45
2:C:283:LEU:H	2:C:283:LEU:HG	1.66	0.45
5:L:17:PRO:O	5:L:20:LEU:HB2	2.16	0.45
2:F:246:PRO:HG2	2:F:265:LEU:HD13	1.98	0.45
2:G:32:ALA:HB1	6:M:17:G:H1'	1.98	0.45
2:I:69:ARG:NE	6:M:14:G:O2'	2.38	0.45
5:L:39:ARG:HG3	5:L:66:ASP:OD1	2.17	0.45
1:A:92:PRO:HB2	3:E:194:GLN:HG3	1.98	0.45
5:L:39:ARG:HA	5:L:174:THR:CB	2.47	0.45
2:I:83:PRO:O	2:I:87:ASP:HB2	2.17	0.44
5:L:34:ALA:HB3	5:L:35:GLN:OE1	2.17	0.44
1:A:194:PHE:HA	1:A:195:PRO:HD3	1.81	0.44
3:E:41:VAL:HG21	3:E:59:VAL:HB	2.00	0.44
2:F:159:HIS:O	2:F:163:ASN:ND2	2.50	0.44
5:L:100:VAL:HG23	5:L:161:HIS:HA	1.99	0.44
2:D:176:ALA:HA	2:D:198:LEU:HD11	2.00	0.44
2:G:123:GLY:HA3	2:G:141:VAL:HG11	1.99	0.44
1:A:189:LEU:HB3	3:E:277:LEU:HA	1.98	0.44
3:E:17:ILE:HD11	3:E:139:LEU:HD23	2.00	0.44
2:H:30:VAL:HG13	7:N:30:DG:H21	1.83	0.44
2:H:180:ARG:HB3	2:H:233:VAL:HG22	2.00	0.44
2:C:26:SER:OG	2:C:27:THR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:164:ALA:H	2:D:197:ALA:HB1	1.82	0.43
2:F:285:THR:HA	2:F:300:ALA:HA	1.99	0.43
2:I:152:GLU:HG2	2:I:155:ARG:HH21	1.82	0.43
7:N:18:DC:H2"	7:N:19:DA:C8	2.53	0.43
2:D:177:VAL:HA	2:D:235:PHE:O	2.18	0.43
2:G:177:VAL:HB	2:G:197:ALA:HB3	2.00	0.43
2:F:326:LEU:HD22	2:F:337:PRO:HB3	2.01	0.43
2:I:246:PRO:HG2	2:I:265:LEU:HD22	1.99	0.43
3:E:171:LYS:HE3	3:E:171:LYS:HB3	1.73	0.43
3:E:172:ASN:OD1	3:E:175:ARG:NH1	2.52	0.43
2:G:31:LEU:HB2	2:G:355:PHE:O	2.18	0.43
2:I:318:LYS:HD3	2:I:318:LYS:HA	1.88	0.43
1:A:225:GLN:OE1	4:J:19:ILE:HD11	2.17	0.43
3:E:85:ARG:O	6:M:7:A:O2'	2.34	0.43
3:E:248:LEU:HD22	3:E:286:LEU:HD23	1.99	0.43
4:J:95:LYS:HE2	4:J:95:LYS:HB2	1.80	0.43
1:A:71:LYS:HB2	1:A:251:ILE:HG23	2.00	0.43
2:D:180:ARG:HB2	2:D:233:VAL:HG13	2.00	0.43
5:L:154:HIS:HB2	6:M:43:U:H4'	2.01	0.43
2:D:160:ASN:HD22	2:D:160:ASN:HA	1.72	0.43
2:D:91:GLN:H	2:D:91:GLN:HG2	1.56	0.43
2:I:160:ASN:HB3	2:I:283:LEU:HA	2.01	0.43
2:C:41:ASP:OD1	2:C:41:ASP:N	2.52	0.43
2:F:315:ARG:NH1	2:F:321:LEU:O	2.45	0.43
2:H:324:TYR:OH	2:I:73:SER:O	2.31	0.43
2:I:110:LEU:HD13	2:I:244:VAL:HG11	2.00	0.43
5:L:67:LEU:HD22	5:L:88:PRO:HG3	2.01	0.43
5:L:3:HIS:CE1	5:L:64:ALA:HB2	2.53	0.42
1:A:80:SER:HB2	1:A:170:ALA:H	1.84	0.42
1:A:334:LEU:HG	3:E:181:LEU:HD21	2.01	0.42
3:E:64:HIS:N	3:E:106:GLU:O	2.52	0.42
1:A:267:SER:OG	3:E:250:PRO:O	2.38	0.42
2:H:269:ARG:NH1	2:I:105:SER:H	2.16	0.42
1:A:220:GLU:O	1:A:224:ARG:HG3	2.20	0.42
2:C:182:ASN:HB3	2:C:189:VAL:HG23	2.01	0.42
2:C:182:ASN:HD22	2:C:231:GLU:HB3	1.85	0.42
4:J:63:THR:HB	4:J:66:GLU:HG3	2.02	0.42
2:F:307:VAL:HG12	2:F:310:GLN:H	1.85	0.42
1:A:118:PHE:HA	1:A:121:LEU:HD12	2.02	0.42
1:A:237:ASN:HB2	1:A:266:PRO:HG3	2.02	0.42
2:D:110:LEU:HD13	2:D:244:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:152:GLU:HG2	2:F:343:HIS:CD2	2.54	0.42
2:H:203:ARG:NH1	2:H:296:LEU:O	2.41	0.42
2:H:123:GLY:HA3	2:H:141:VAL:HG11	2.01	0.42
2:H:144:TYR:O	2:H:148:GLN:N	2.51	0.42
2:H:346:ILE:HD13	2:H:349:LEU:HD12	2.02	0.42
2:C:166:PHE:HB2	2:C:279:ILE:HD12	2.00	0.42
2:G:251:ILE:HD11	2:G:264:THR:HG21	2.02	0.42
2:I:25:LEU:N	2:I:136:LYS:HZ1	2.17	0.42
2:C:211:LEU:HD23	2:C:211:LEU:HA	1.90	0.41
3:E:60:GLY:N	3:E:110:LEU:O	2.41	0.41
2:H:185:ARG:HB2	2:H:190:ALA:HB2	2.02	0.41
2:D:43:LEU:O	2:D:112:VAL:HA	2.20	0.41
2:C:45:SER:OG	2:C:46:ALA:N	2.54	0.41
3:E:249:VAL:HG21	3:E:289:TRP:HE1	1.86	0.41
1:A:87:GLN:H	1:A:87:GLN:HG3	1.73	0.41
1:A:328:GLN:HE22	3:E:246:GLY:H	1.68	0.41
2:C:208:ASP:OD1	2:C:209:ALA:N	2.54	0.41
4:J:61:HIS:HB2	4:J:67:ALA:HB2	2.02	0.41
2:C:44:MET:HA	2:C:111:LYS:O	2.21	0.41
2:H:240:ASP:OD1	2:H:240:ASP:N	2.53	0.41
5:L:119:ARG:O	5:L:120:HIS:ND1	2.54	0.41
2:D:90:ILE:H	2:D:90:ILE:HG13	1.58	0.41
2:D:206:LYS:HE3	2:D:206:LYS:HB2	1.89	0.41
2:G:53:ASP:OD1	2:G:53:ASP:N	2.53	0.41
2:G:76:LEU:HD22	2:G:86:LEU:HG	2.03	0.41
1:A:59:ARG:NH1	1:A:113:ALA:O	2.53	0.41
2:C:42:ALA:HA	2:C:113:ARG:O	2.20	0.41
2:C:310:GLN:NE2	5:L:12:ASP:O	2.54	0.41
2:D:25:LEU:HD23	2:D:25:LEU:HA	1.94	0.41
2:D:175:GLU:OE2	2:D:237:ARG:NE	2.41	0.41
2:F:182:ASN:OD1	2:F:182:ASN:N	2.54	0.41
2:I:165:ARG:NH2	2:I:202:LEU:O	2.54	0.41
2:I:265:LEU:HD23	2:I:265:LEU:HA	1.93	0.41
2:G:328:ASP:O	2:G:333:ARG:NH1	2.54	0.40
4:J:43:ARG:NH1	4:J:44:VAL:O	2.54	0.40
1:A:290:ASP:H	1:A:293:ARG:HD2	1.86	0.40
5:L:39:ARG:HD2	5:L:39:ARG:N	2.25	0.40
2:H:79:LYS:HA	2:H:79:LYS:HD3	1.95	0.40
6:M:52:U:O2'	6:M:53:G:N2	2.54	0.40
2:C:181:ILE:HG12	2:C:232:VAL:HG13	2.04	0.40
2:C:312:LYS:HA	2:C:312:LYS:HD2	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:162:ALA:HB2	2:F:211:LEU:HD21	2.03	0.40
2:G:43:LEU:O	2:G:112:VAL:HA	2.21	0.40
5:L:22:SER:HB2	5:L:146:LEU:H	1.87	0.40
3:E:145:LEU:HA	3:E:146:PRO:HD3	1.92	0.40
3:E:256:ASN:HB2	3:E:283:LEU:HD21	2.03	0.40
2:I:61:VAL:HG23	2:I:272:ALA:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	421/434 (97%)	378 (90%)	43 (10%)	0	100	100
2	C	287/342 (84%)	267 (93%)	20 (7%)	0	100	100
2	D	320/342 (94%)	304 (95%)	16 (5%)	0	100	100
2	F	332/342 (97%)	302 (91%)	30 (9%)	0	100	100
2	G	333/342 (97%)	313 (94%)	20 (6%)	0	100	100
2	H	321/342 (94%)	302 (94%)	19 (6%)	0	100	100
2	I	325/342 (95%)	307 (94%)	18 (6%)	0	100	100
3	E	301/327 (92%)	270 (90%)	31 (10%)	0	100	100
4	J	90/100 (90%)	88 (98%)	2 (2%)	0	100	100
5	L	185/187 (99%)	150 (81%)	33 (18%)	2 (1%)	14	46
All	All	2915/3100 (94%)	2681 (92%)	232 (8%)	2 (0%)	54	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	17	PRO

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Mol	Chain	Res	Type
5	L	18	ALA

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	255/365 (70%)	241 (94%)	14 (6%)	21 53
2	C	223/274 (81%)	207 (93%)	16 (7%)	14 44
2	D	235/274 (86%)	217 (92%)	18 (8%)	13 41
2	F	254/274 (93%)	236 (93%)	18 (7%)	14 44
2	G	252/274 (92%)	239 (95%)	13 (5%)	23 54
2	H	251/274 (92%)	241 (96%)	10 (4%)	31 61
2	I	251/274 (92%)	245 (98%)	6 (2%)	49 74
3	E	246/270 (91%)	231 (94%)	15 (6%)	18 49
4	J	73/77 (95%)	69 (94%)	4 (6%)	21 53
5	L	136/160 (85%)	126 (93%)	10 (7%)	13 42
All	All	2176/2516 (86%)	2052 (94%)	124 (6%)	24 52

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	A	94	LEU
1	A	105	VAL
1	A	108	VAL
1	A	156	ARG
1	A	177	GLN
1	A	178	LEU
1	A	223	SER
1	A	259	TYR
1	A	286	VAL
1	A	339	ARG
1	A	386	GLU

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Mol	Chain	Res	Type
1	A	399	VAL
1	A	433	ARG
2	C	41	ASP
2	C	112	VAL
2	C	159	HIS
2	C	169	ARG
2	C	171	ARG
2	C	182	ASN
2	C	192	THR
2	C	194	ARG
2	C	228	VAL
2	C	240	ASP
2	C	283	LEU
2	C	289	TRP
2	C	304	TYR
2	C	312	LYS
2	C	343	HIS
2	C	354	VAL
2	D	44	MET
2	D	53	ASP
2	D	74	ASN
2	D	76	LEU
2	D	91	GLN
2	D	92	SER
2	D	100	VAL
2	D	108	ASP
2	D	233	VAL
2	D	240	ASP
2	D	250	LEU
2	D	285	THR
2	D	288	THR
2	D	289	TRP
2	D	290	TYR
2	D	304	TYR
2	D	307	VAL
2	D	327	LEU
3	E	27	LEU
3	E	48	VAL
3	E	119	ASP
3	E	124	GLN
3	E	138	ARG
3	E	180	LEU

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Mol	Chain	Res	Type
3	E	204	LEU
3	E	206	GLU
3	E	208	THR
3	E	221	PHE
3	E	281	GLU
3	E	291	SER
3	E	298	LEU
3	E	313	LEU
3	E	322	VAL
2	F	31	LEU
2	F	62	THR
2	F	74	ASN
2	F	78	THR
2	F	100	VAL
2	F	102	ASN
2	F	113	ARG
2	F	137	LEU
2	F	169	ARG
2	F	182	ASN
2	F	186	GLN
2	F	208	ASP
2	F	217	LEU
2	F	278	LYS
2	F	289	TRP
2	F	293	GLU
2	F	301	VAL
2	F	339	VAL
2	G	56	GLN
2	G	67	SER
2	G	91	GLN
2	G	128	CYS
2	G	146	ASN
2	G	262	SER
2	G	264	THR
2	G	268	VAL
2	G	269	ARG
2	G	289	TRP
2	G	321	LEU
2	G	343	HIS
2	G	351	ARG
2	H	38	ASP
2	H	57	GLU

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Mol	Chain	Res	Type
2	H	67	SER
2	H	75	ARG
2	H	106	ASP
2	H	117	ARG
2	H	118	VAL
2	H	240	ASP
2	H	289	TRP
2	H	329	ASN
2	I	87	ASP
2	I	128	CYS
2	I	160	ASN
2	I	289	TRP
2	I	343	HIS
2	I	355	PHE
4	J	54	PHE
4	J	63	THR
4	J	72	LEU
4	J	94	GLU
5	L	17	PRO
5	L	24	LEU
5	L	39	ARG
5	L	40	ILE
5	L	44	PHE
5	L	83	LEU
5	L	102	ARG
5	L	106	LYS
5	L	130	ARG
5	L	155	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	HIS
1	A	305	GLN
2	C	159	HIS
2	C	183	HIS
2	C	186	GLN
2	C	341	GLN
2	C	348	ASN
2	D	163	ASN
3	E	82	ASN
3	E	129	GLN

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Mol	Chain	Res	Type
3	E	168	GLN
3	E	194	GLN
3	E	195	GLN
3	E	293	HIS
2	F	102	ASN
2	F	163	ASN
2	F	170	ASN
2	F	242	GLN
2	F	281	ASN
2	F	316	GLN
2	F	319	GLN
2	F	343	HIS
2	G	56	GLN
2	G	94	ASN
2	H	129	ASN
2	H	163	ASN
2	H	242	GLN
2	H	329	ASN
2	I	91	GLN
4	J	27	GLN
5	L	61	HIS
5	L	99	GLN
5	L	104	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	M	57/60 (95%)	33 (57%)	3 (5%)

All (33) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	M	3	A
6	M	9	U
6	M	10	U
6	M	11	C
6	M	14	G
6	M	15	G
6	M	21	U
6	M	23	G
6	M	26	G

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Mol	Chain	Res	Type
6	M	27	U
6	M	28	C
6	M	33	U
6	M	34	C
6	M	36	A
6	M	39	U
6	M	40	G
6	M	41	G
6	M	43	U
6	M	44	C
6	M	45	A
6	M	46	C
6	M	47	U
6	M	48	G
6	M	49	C
6	M	50	C
6	M	51	G
6	M	52	U
6	M	53	G
6	M	54	U
6	M	55	A
6	M	56	G
6	M	57	G
6	M	58	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	M	33	U
6	M	44	C
6	M	47	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)

There are no ligands in this entry.

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.

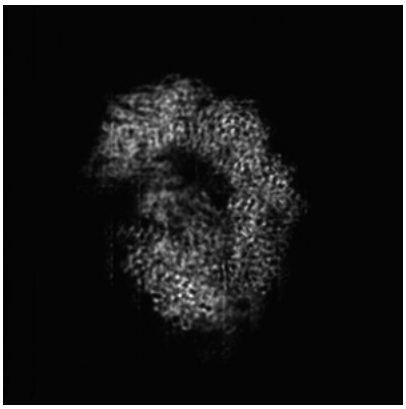
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-33837. These allow visual inspection of the internal detail of the map and identification of artifacts.

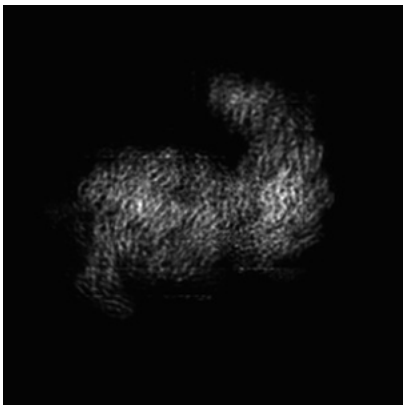
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

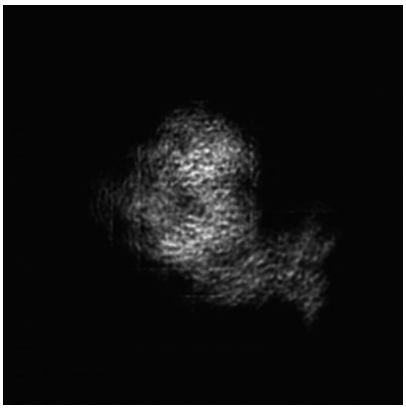
6.1.1 Primary map



X

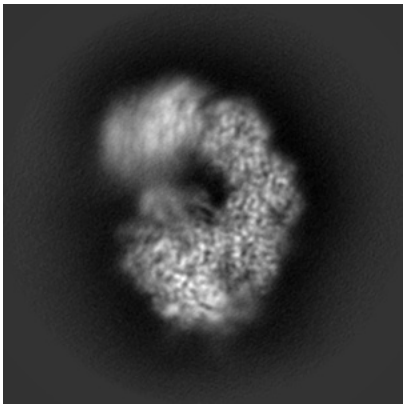


Y

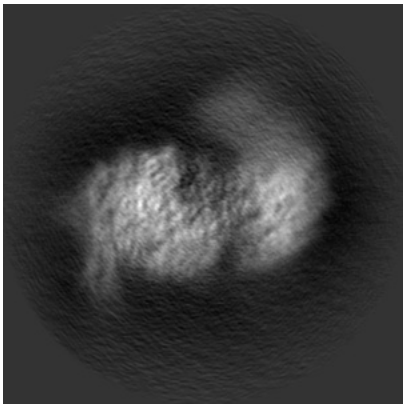


Z

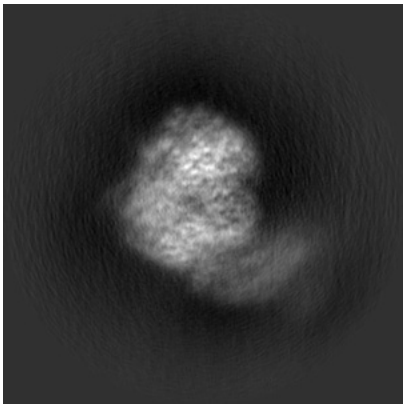
6.1.2 Raw map



X



Y



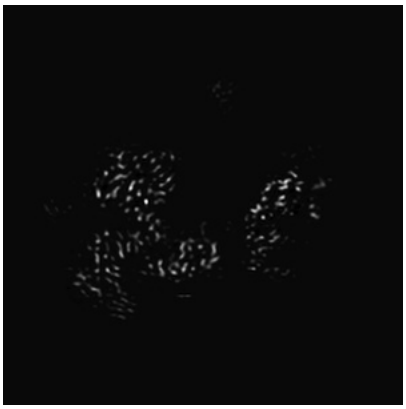
Z

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

6.2 Central slices (i)

6.2.1 Primary map

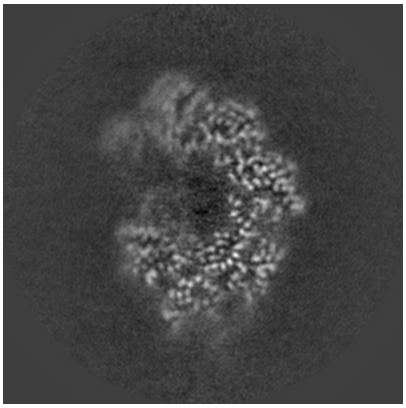
X Index: 120



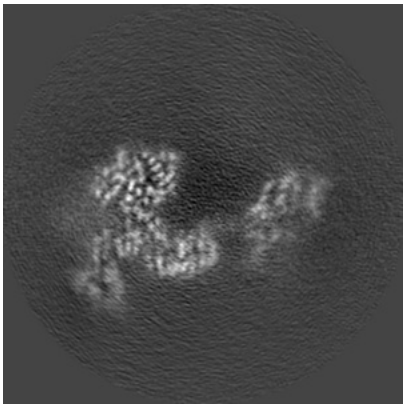
Y Index: 120

Z Index: 120

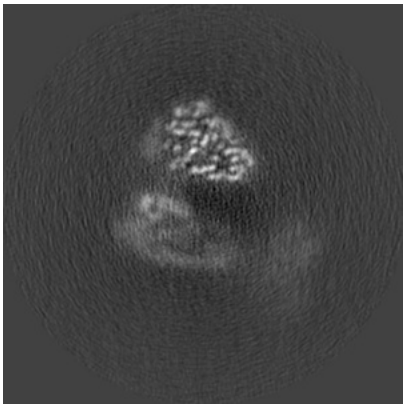
6.2.2 Raw map



X Index: 120



Y Index: 120



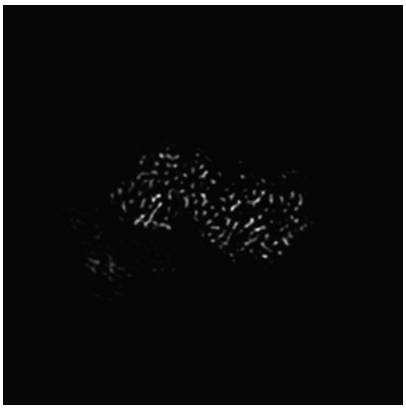
Z Index: 120

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

6.3 Largest variance slices (i)

6.3.1 Primary map

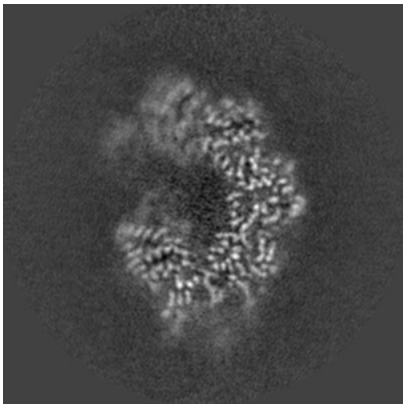
X Index: 121



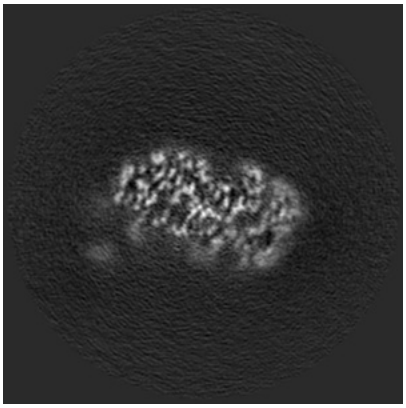
Y Index: 141

Z Index: 165

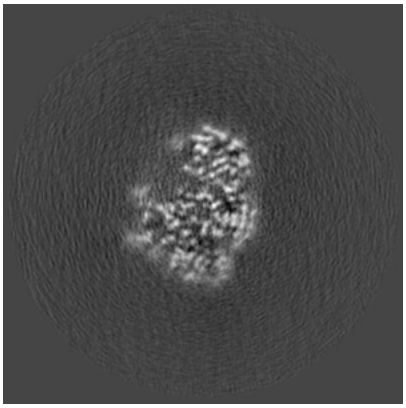
6.3.2 Raw map



X Index: 118



Y Index: 151

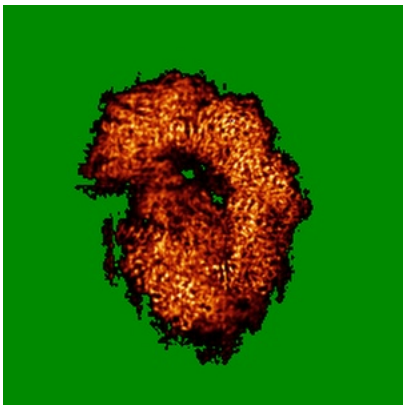


Z Index: 87

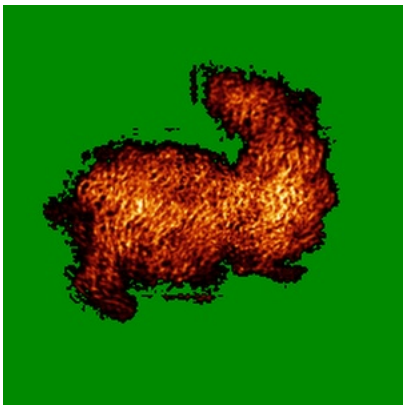
The images above show the largest variance slices of the map in three orthogonal directions.

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

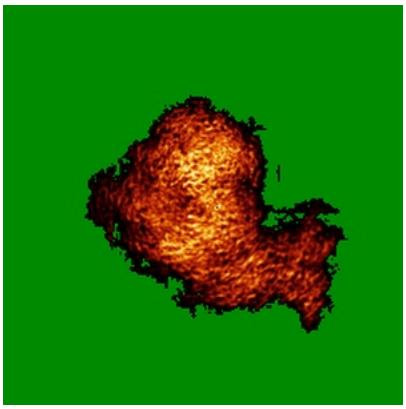
6.4.1 Primary map



X

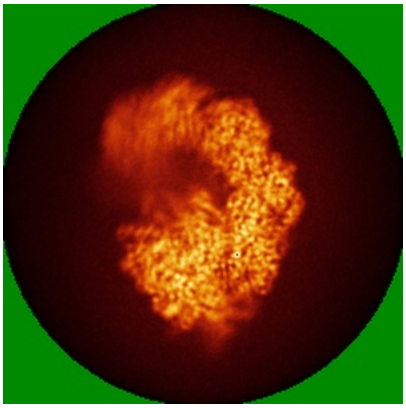


Y

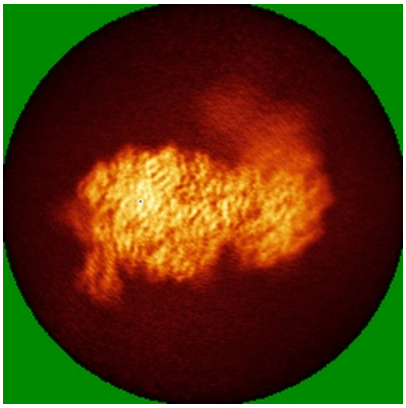


Z

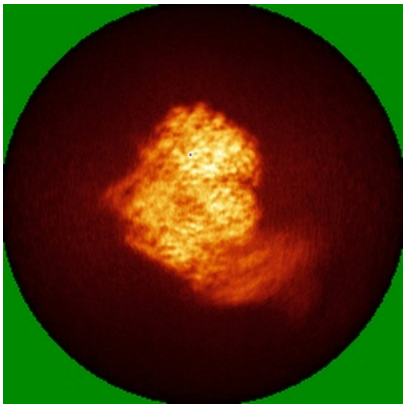
6.4.2 Raw map



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 0.06. 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.

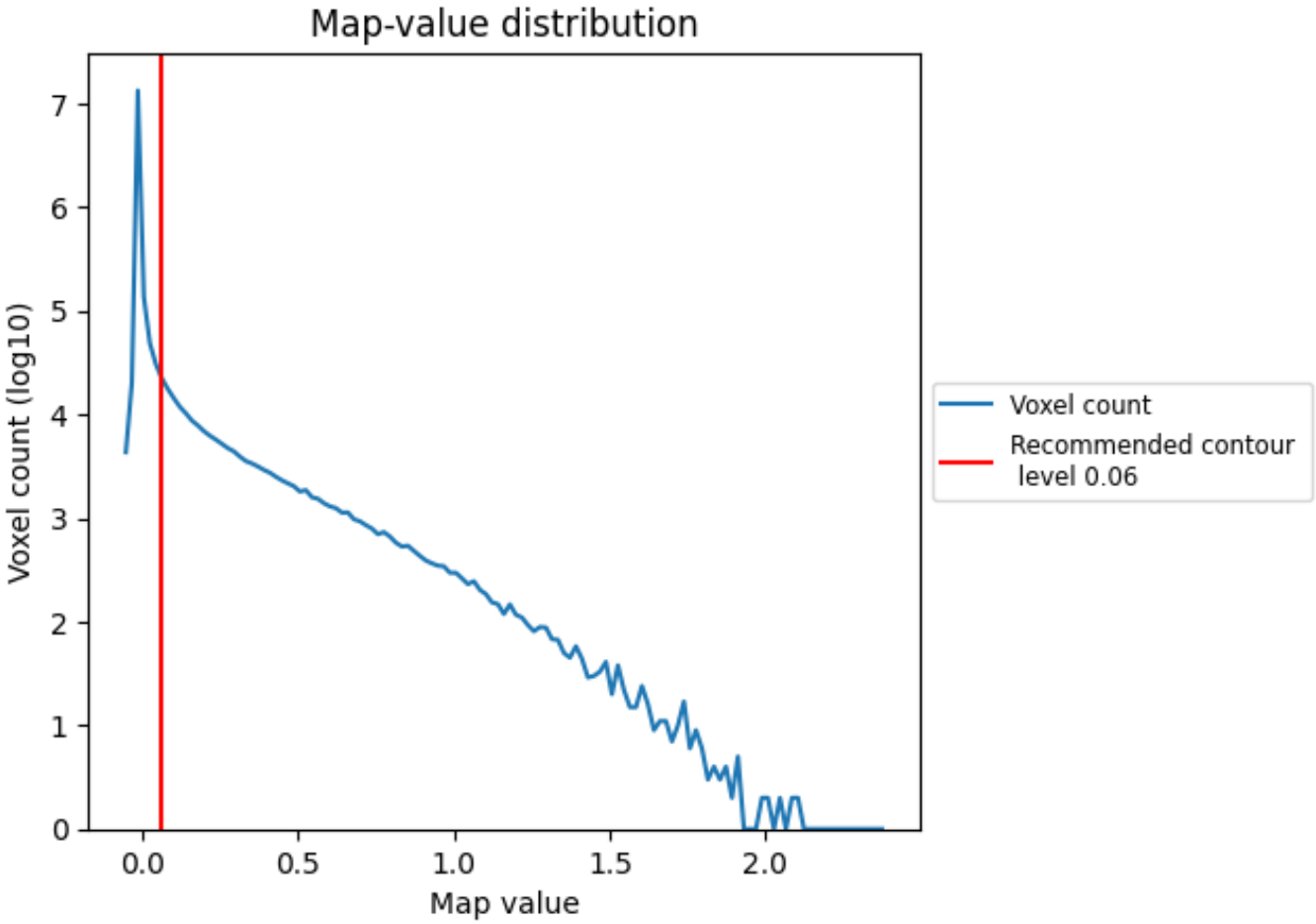
6.6 Mask visualisation (i)

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

7 Map analysis

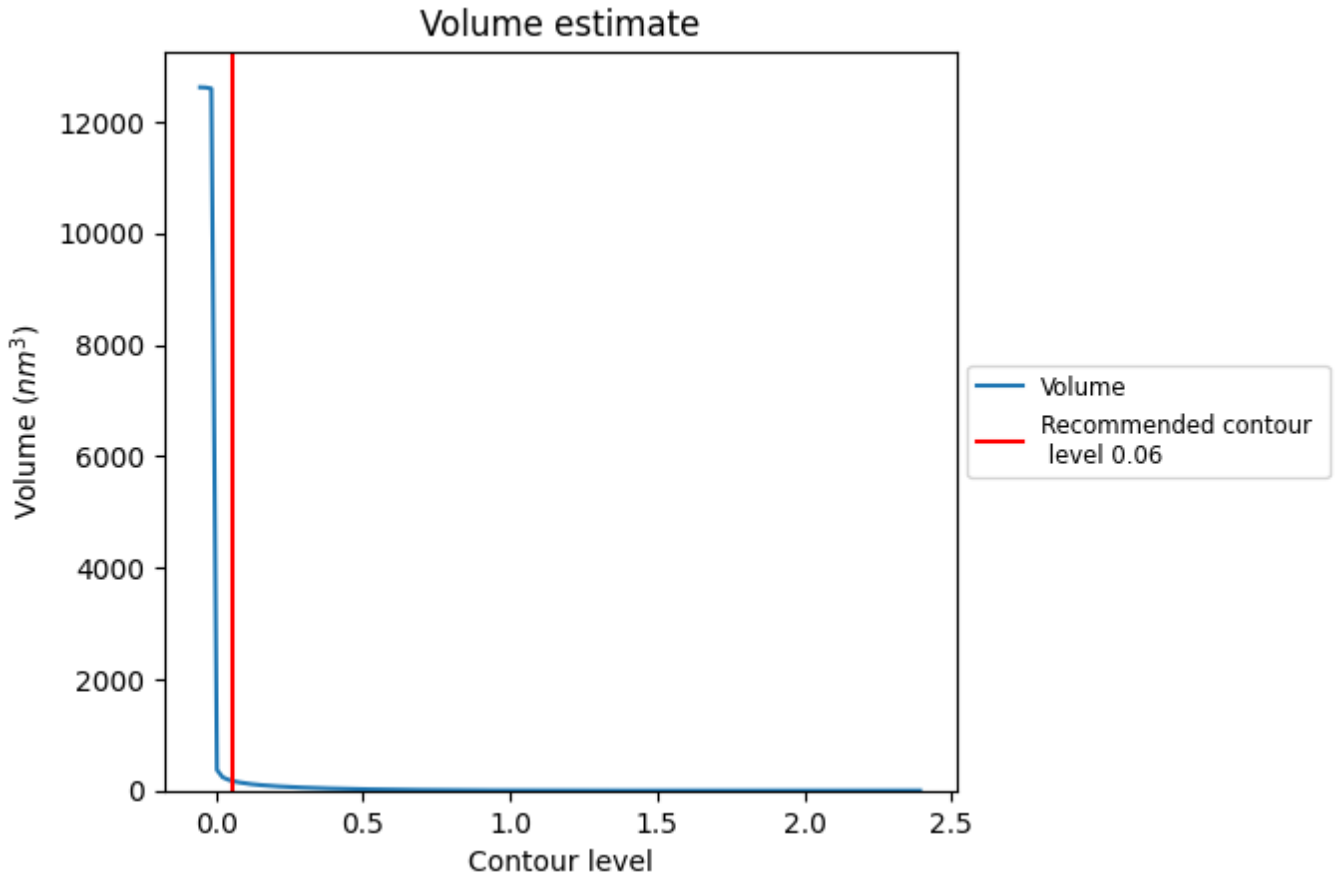
This section contains the results of statistical analysis of the map.

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.

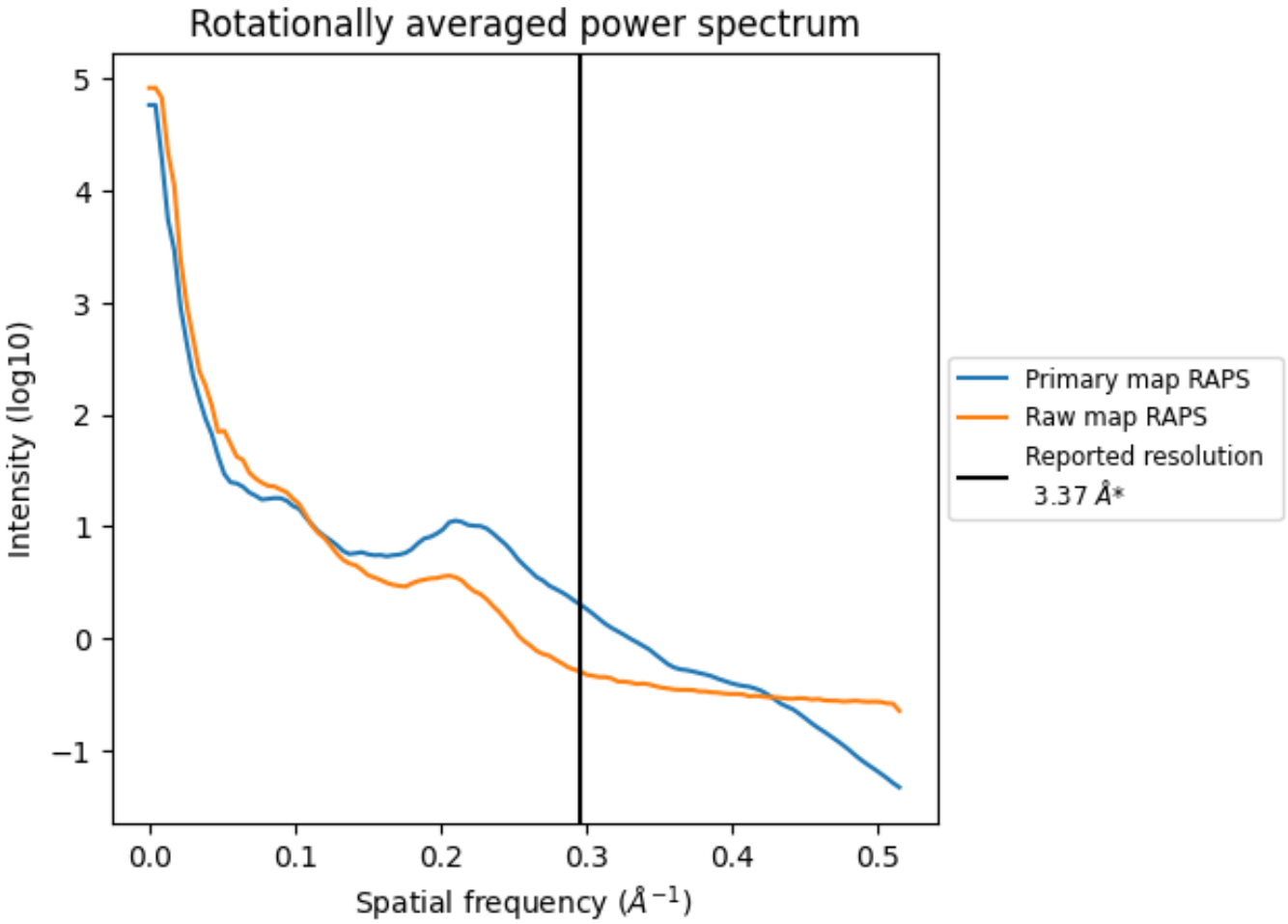
7.2 Volume estimate



The volume at the recommended contour level is 169 nm^3; this corresponds to an approximate mass of 153 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)

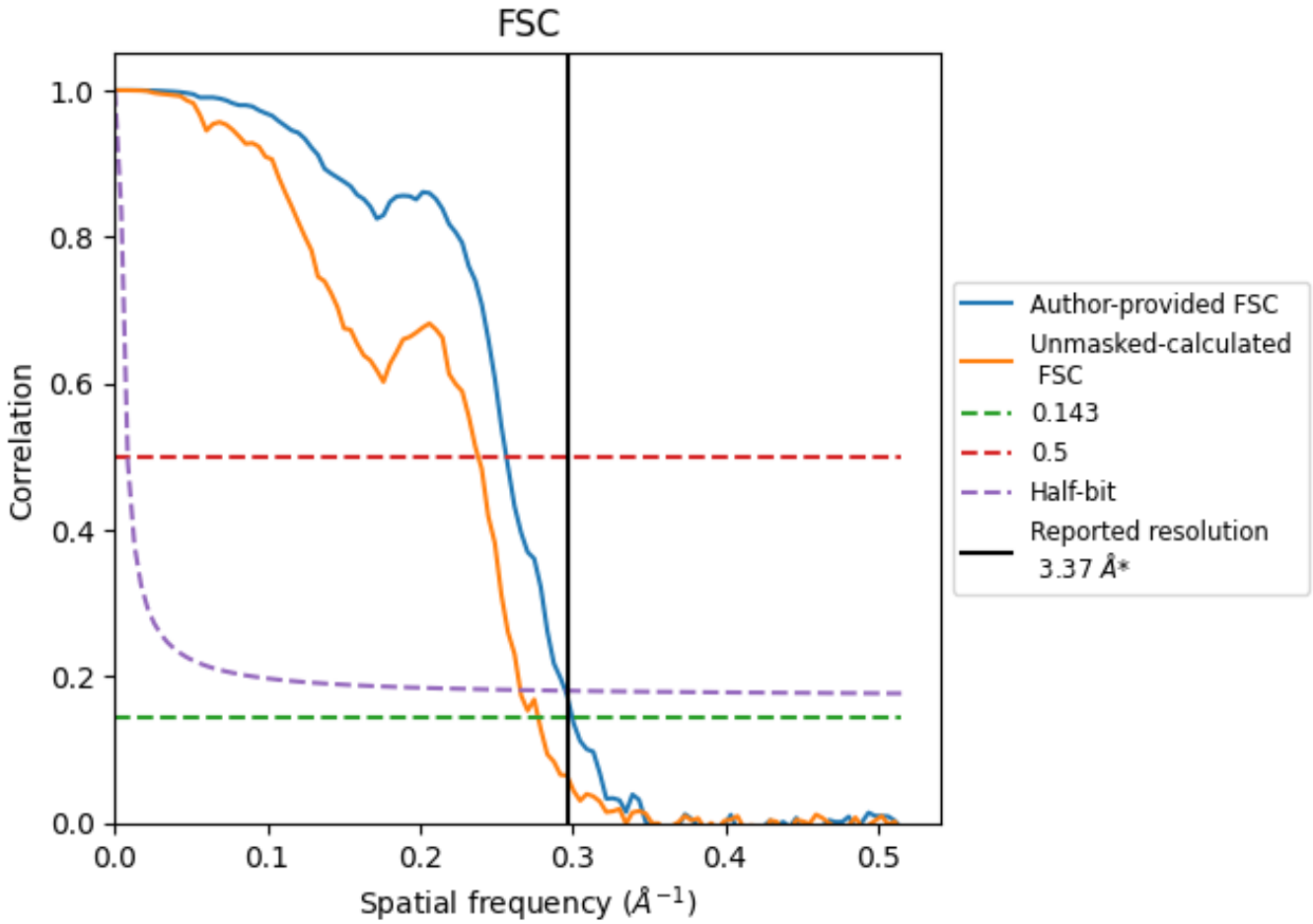


*Reported resolution corresponds to spatial frequency of 0.297 $Å^{-1}$

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 0.297 Å^{-1}

8.2 Resolution estimates (i)

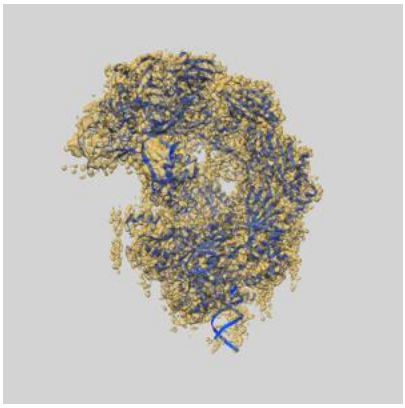
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.37	-	-
Author-provided FSC curve	3.33	3.90	3.39
Unmasked-calculated*	3.60	4.20	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

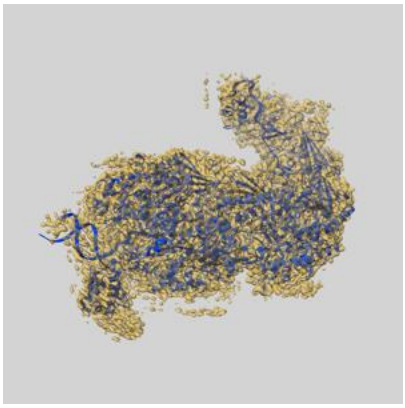
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-33837 and PDB model 7YHS. Per-residue inclusion information can be found in section 3 on page 6.

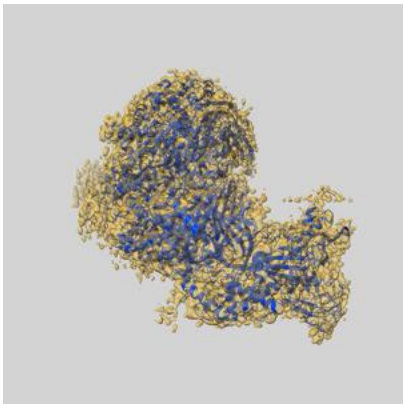
9.1 Map-model overlay



X



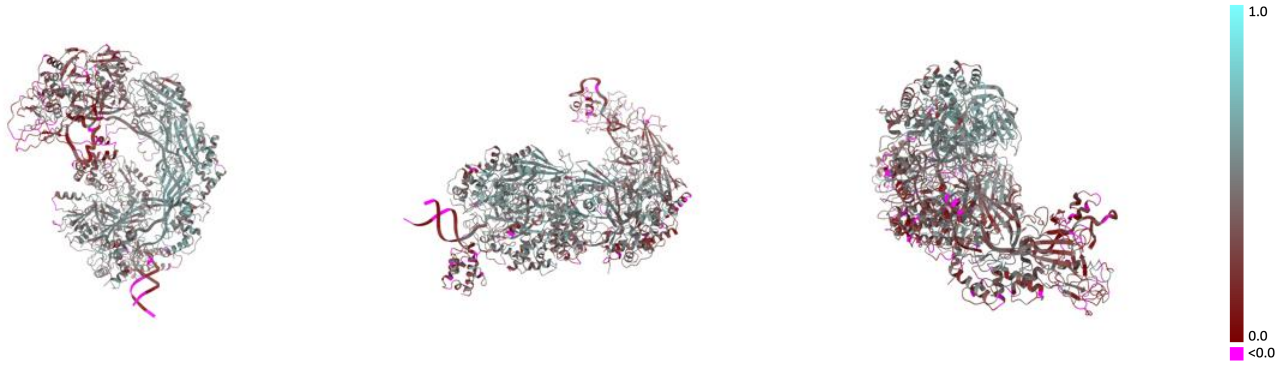
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06 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.

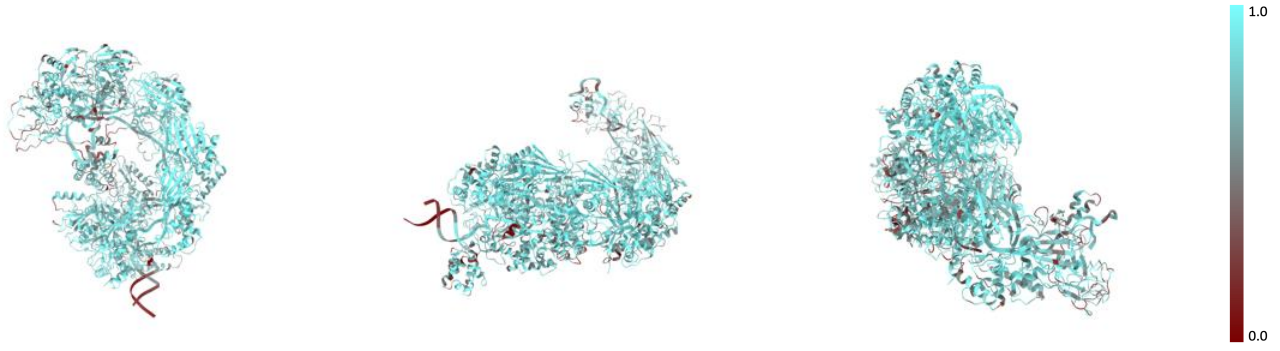
9.2 Q-score mapped to coordinate model (i)



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.

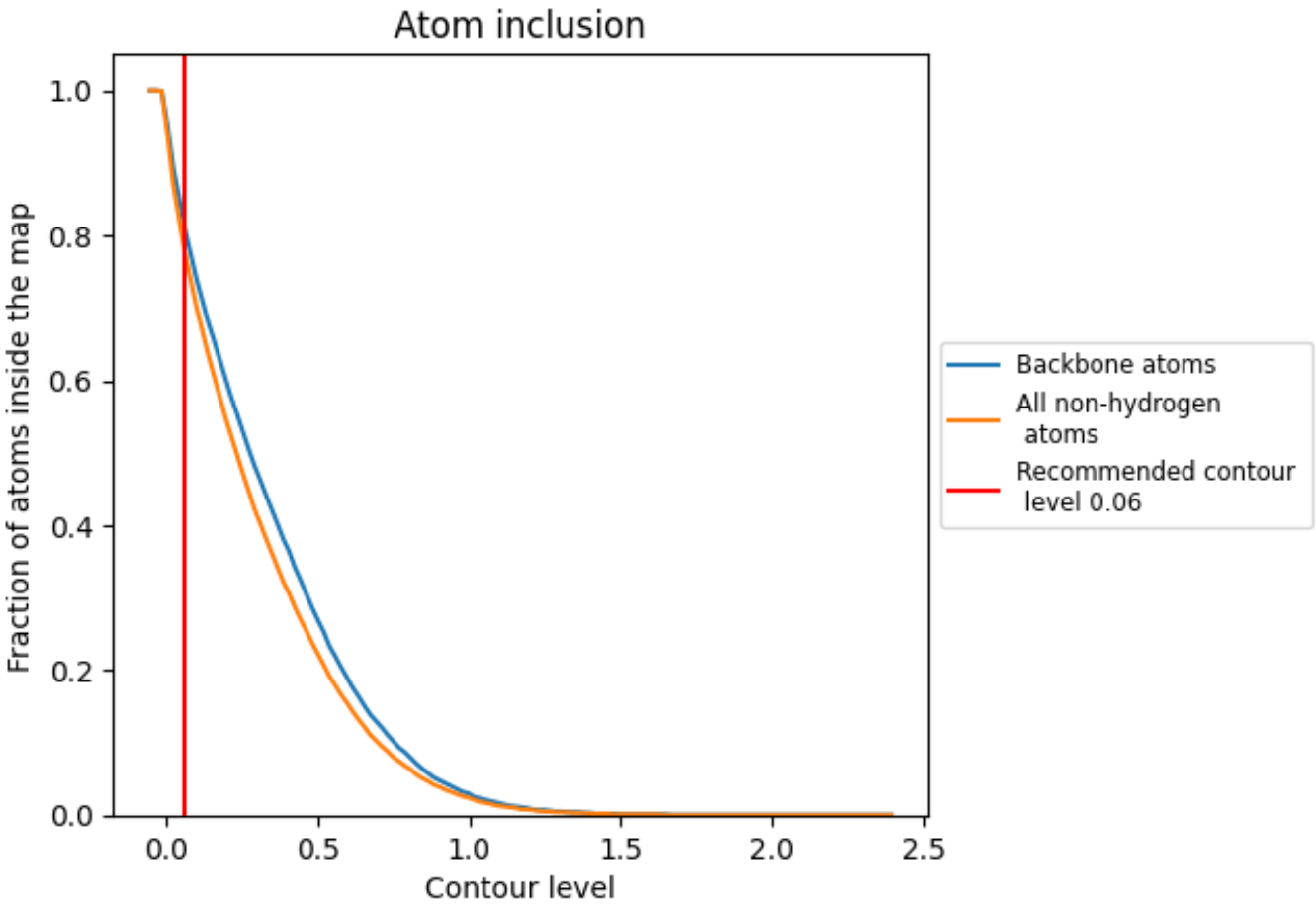
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.06).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 78% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7790	0.4040
A	0.7270	0.3580
C	0.7410	0.3300
D	0.7230	0.3220
E	0.8320	0.4440
F	0.8270	0.4300
G	0.8590	0.5070
H	0.8680	0.5290
I	0.7910	0.4550
J	0.7180	0.4060
L	0.6630	0.2500
M	0.8300	0.3930
N	0.6950	0.3470
O	0.3400	0.0900