



Full wwPDB EM Validation Report ⓘ

Dec 8, 2024 – 12:22 AM JST

PDB ID : 8JSG
EMDB ID : EMD-36619
Title : Structure of the 30S-IF3 complex from Escherichia coli
Authors : Uday, A.B.; Mishra, R.K.; Hussain, T.
Deposited on : 2023-06-20
Resolution : 4.60 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

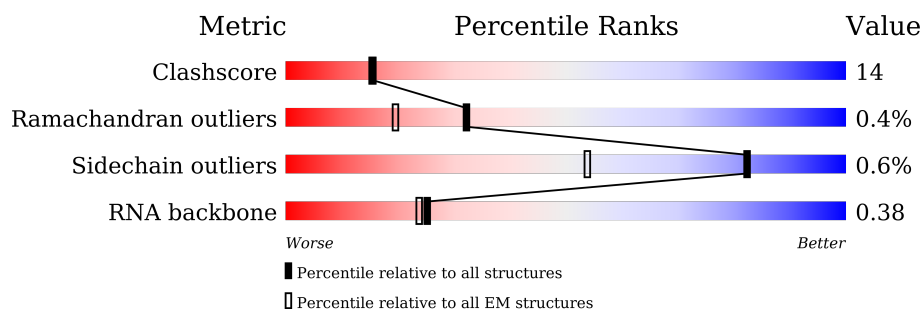
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	73	
2	2	53	
3	3	86	
4	A	180	
5	P	82	
6	g	1540	
7	k	158	

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Mol	Chain	Length	Quality of chain
8	l	205	 99% .
9	n	100	 98% .
10	p	129	 100%
11	q	128	 91% . 9%
12	t	123	 100%
13	u	88	 98% .
14	y	82	 100%
15	h	206	 99% .
16	m	151	 99% .
17	o	129	 97% . .
18	r	102	 93% . .
19	s	114	 100%
20	w	100	 96% .
21	z	80	 98% ..
22	j	225	 96% . .

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 52910 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 Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 2 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	51	Total	C	N	O	S	0	0
			426	265	86	74	1		

- Molecule 3 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 4 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	167	Total	C	N	O	S	0	0
			1342	843	241	252	6		

- Molecule 5 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	1539	Total	C	N	O	P	0	0
			33014	14726	6055	10695	1538		

- Molecule 7 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	150	Total	C	N	O	S	0	0
			1106	687	211	202	6		

- Molecule 8 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	l	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 9 is a protein called Small ribosomal subunit protein bS6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	n	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 10 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	p	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	q	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	u	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 14 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	y	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 15 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	h	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	m	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 17 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	o	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	w	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 21 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	z	79	Total 638	C 408	N 120	O 108	S 2	0	0

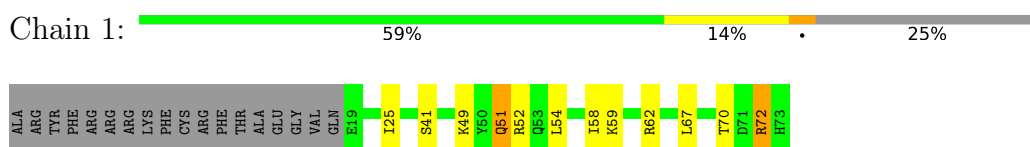
- Molecule 22 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	j	218	Total 1705	C 1081	N 305	O 312	S 7	0	0

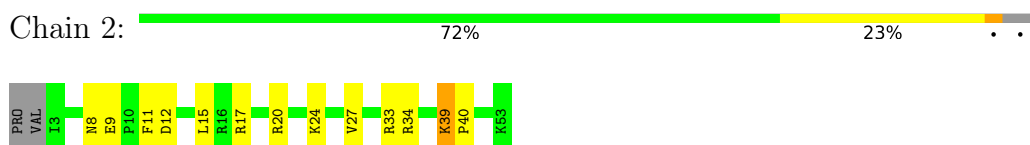
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

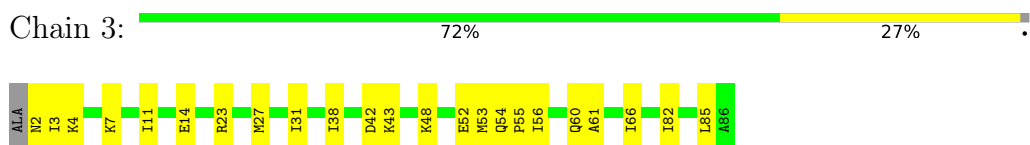
- Molecule 1: Small ribosomal subunit protein bS18



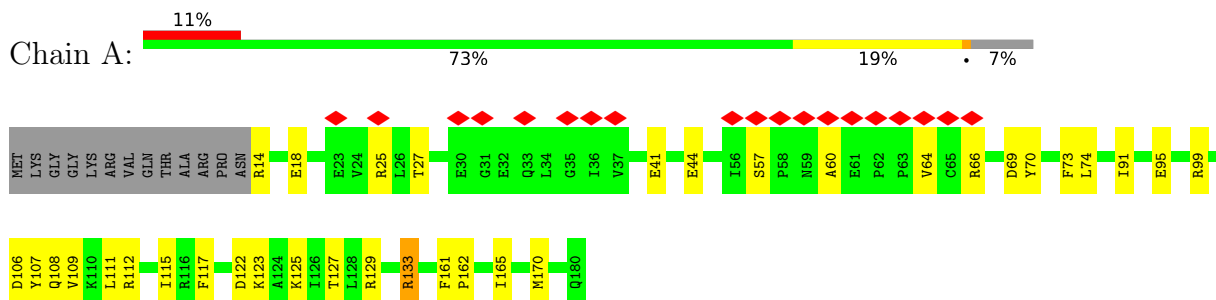
- Molecule 2: Small ribosomal subunit protein bS21



- Molecule 3: Small ribosomal subunit protein bS20



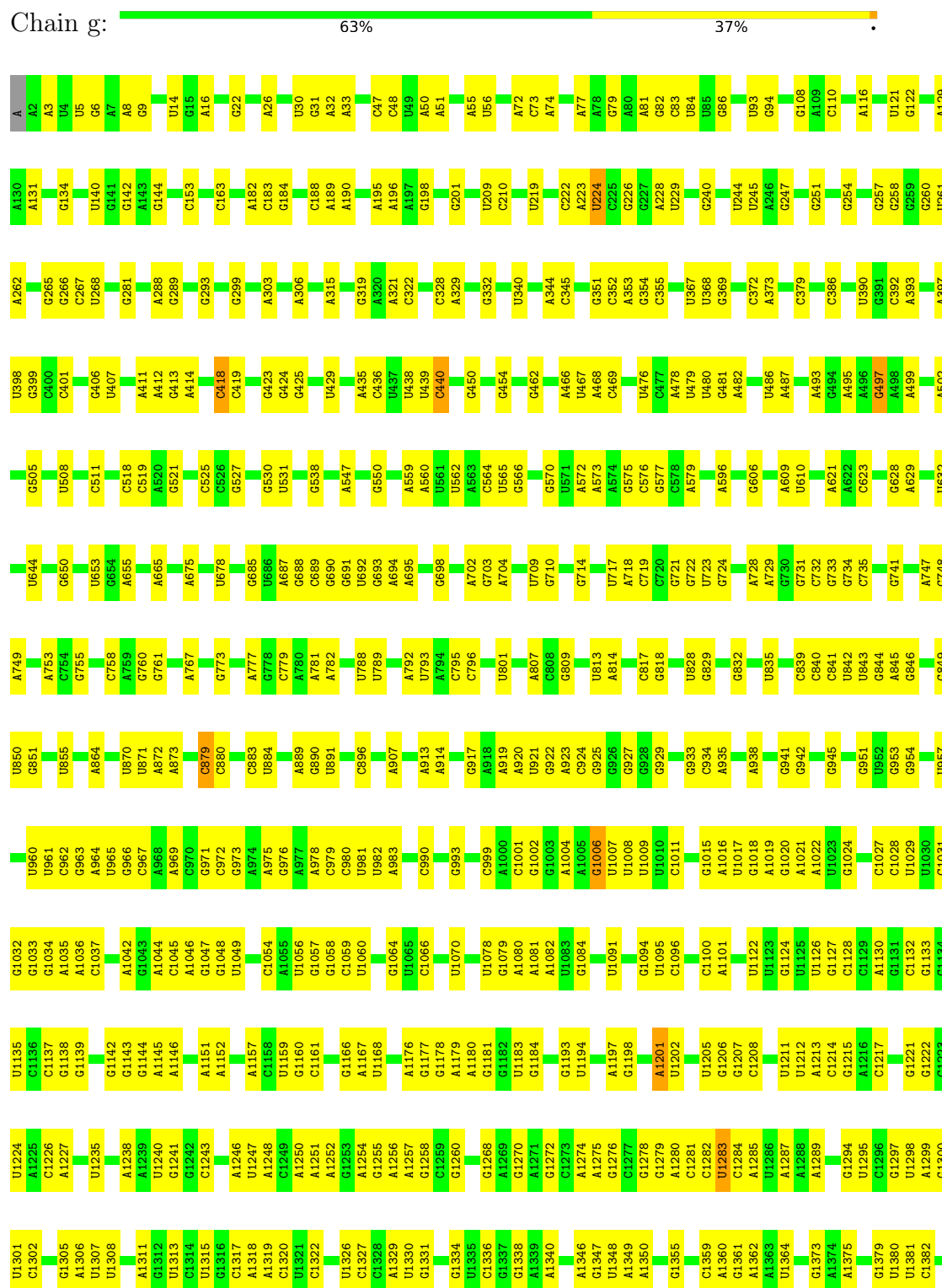
- Molecule 4: Translation initiation factor IF-3

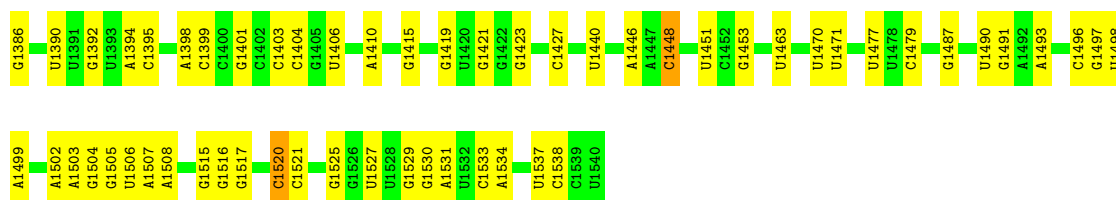


- Molecule 5: Small ribosomal subunit protein uS17



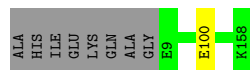
- Molecule 6: 16S ribosomal RNA





- Molecule 7: Small ribosomal subunit protein uS5

Chain k: 94% 5%



- Molecule 8: Small ribosomal subunit protein uS4

Chain l: 99%



- Molecule 9: Small ribosomal subunit protein bS6, non-modified isoform

Chain n: 98%



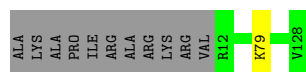
- Molecule 10: Small ribosomal subunit protein uS8

Chain p: 100%

There are no outlier residues recorded for this chain.

- Molecule 11: Small ribosomal subunit protein uS11

Chain q: 91% 9%



- Molecule 12: Small ribosomal subunit protein uS12

Chain t: 100%

There are no outlier residues recorded for this chain.

- Molecule 13: Small ribosomal subunit protein uS15

Chain u: 98%



- Molecule 14: 30S ribosomal protein S16

Chain y: 100%

There are no outlier residues recorded for this chain.

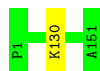
- Molecule 15: Small ribosomal subunit protein uS3

Chain h: 99%



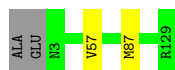
- Molecule 16: Small ribosomal subunit protein uS7

Chain m: 99%



- Molecule 17: Small ribosomal subunit protein uS9

Chain o: 97%



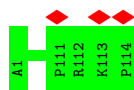
- Molecule 18: Small ribosomal subunit protein uS10

Chain r: 93%



- Molecule 19: Small ribosomal subunit protein uS13

Chain s: 100%

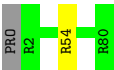


- Molecule 20: Small ribosomal subunit protein uS14

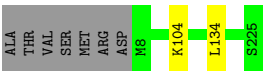
Chain w: 96%



- Molecule 21: Small ribosomal subunit protein uS19



- Molecule 22: Small ribosomal subunit protein uS2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145664	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	45000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.024	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00126	Depositor
Map size (Å)	384.0, 384.0, 384.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1	0.28	0/463	0.64	0/621
2	2	0.25	0/431	0.64	0/570
3	3	0.37	0/671	0.60	0/888
4	A	0.25	0/1356	0.53	0/1807
5	P	0.28	0/658	0.58	0/881
6	g	0.37	0/36966	0.89	31/57667 (0.1%)
7	k	0.31	0/1119	0.60	0/1504
8	l	0.29	0/1665	0.55	0/2227
9	n	0.31	0/836	0.68	1/1128 (0.1%)
10	p	0.31	0/989	0.55	0/1326
11	q	0.28	0/893	0.61	0/1205
12	t	0.30	0/969	0.62	0/1300
13	u	0.28	0/722	0.59	0/964
14	y	0.31	0/659	0.60	0/884
15	h	0.26	0/1652	0.56	1/2225 (0.0%)
16	m	0.27	0/1196	0.59	0/1602
17	o	0.30	0/1034	0.65	1/1375 (0.1%)
18	r	0.25	0/797	0.59	0/1077
19	s	0.24	0/893	0.61	0/1193
20	w	0.25	0/785	0.58	0/1043
21	z	0.25	0/653	0.54	0/877
22	j	0.26	0/1736	0.54	1/2338 (0.0%)
All	All	0.34	0/57143	0.81	35/84702 (0.0%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	g	1520	C	N1-C2-O2	9.38	124.53	118.90
6	g	1520	C	N3-C2-O2	-9.20	115.46	121.90
6	g	1521	C	N3-C2-O2	-8.78	115.75	121.90
6	g	419	C	N3-C2-O2	-7.83	116.42	121.90
6	g	440	C	N1-C2-O2	7.64	123.49	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	g	1515	G	N1-C2-N2	-7.47	109.47	116.20
6	g	436	C	N3-C2-O2	-6.94	117.04	121.90
6	g	440	C	N3-C2-O2	-6.85	117.10	121.90
6	g	1283	U	C2-N1-C1'	6.68	125.72	117.70
6	g	222	C	N3-C2-O2	-6.36	117.45	121.90
6	g	418	C	N1-C2-O2	6.20	122.62	118.90
6	g	1448	C	C2-N1-C1'	6.06	125.47	118.80
6	g	497	G	N1-C2-N2	-6.00	110.80	116.20
17	o	87	MET	CB-CG-SD	-5.90	94.70	112.40
15	h	133	MET	CA-CB-CG	5.82	123.19	113.30
6	g	879	C	N1-C2-O2	5.79	122.38	118.90
6	g	379	C	N1-C2-O2	5.79	122.37	118.90
6	g	1006	G	OP1-P-O3'	5.76	117.86	105.20
6	g	1515	G	N3-C2-N2	5.74	123.92	119.90
6	g	419	C	C6-N1-C2	-5.71	118.01	120.30
6	g	425	G	N1-C2-N2	-5.69	111.08	116.20
6	g	1066	C	C2-N1-C1'	5.48	124.83	118.80
6	g	1283	U	C6-N1-C1'	-5.35	113.71	121.20
6	g	418	C	C2-N1-C1'	5.32	124.65	118.80
6	g	1006	G	P-O3'-C3'	5.31	126.07	119.70
6	g	1521	C	N1-C2-N3	5.31	122.92	119.20
6	g	224	U	C2-N1-C1'	5.30	124.06	117.70
6	g	1066	C	N1-C2-O2	5.30	122.08	118.90
6	g	1201	A	P-O3'-C3'	5.29	126.05	119.70
22	j	134	LEU	CB-CG-CD1	-5.11	102.32	111.00
6	g	1521	C	C6-N1-C2	-5.10	118.26	120.30
6	g	883	C	N3-C2-O2	-5.07	118.35	121.90
6	g	879	C	N3-C2-O2	-5.06	118.36	121.90
9	n	21	MET	CA-CB-CG	5.04	121.87	113.30
6	g	896	C	C2-N1-C1'	5.03	124.33	118.80

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	1	456	0	478	9	0
2	2	426	0	449	8	0
3	3	665	0	714	16	0
4	A	1342	0	1404	22	0
5	P	649	0	691	13	0
6	g	33014	0	16619	0	0
7	k	1106	0	1148	0	0
8	l	1643	0	1710	0	0
9	n	818	0	808	0	0
10	p	979	0	1034	0	0
11	q	877	0	887	0	0
12	t	955	0	1019	0	0
13	u	714	0	737	0	0
14	y	649	0	666	0	0
15	h	1625	0	1699	0	0
16	m	1182	0	1240	0	0
17	o	1022	0	1070	0	0
18	r	787	0	828	0	0
19	s	884	0	944	0	0
20	w	774	0	827	0	0
21	z	638	0	665	0	0
22	j	1705	0	1732	0	0
All	All	52910	0	37369	68	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 14.

All (68) 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)
3:3:31:ILE:HD13	3:3:53:MET:CE	2.13	0.78
3:3:23:ARG:HH21	3:3:60:GLN:HE22	1.32	0.78
3:3:31:ILE:HD13	3:3:53:MET:HE1	1.64	0.77
5:P:63:CYS:SG	5:P:64:ARG:N	2.62	0.72
3:3:82:ILE:HD12	3:3:85:LEU:HD21	1.73	0.70
1:1:41:SER:HB3	1:1:51:GLN:HG3	1.75	0.68
4:A:106:ASP:HA	4:A:109:VAL:HG22	1.76	0.66
5:P:18:LYS:HZ2	5:P:48:GLU:HA	1.63	0.63
5:P:14:ASP:OD1	5:P:15:LYS:N	2.34	0.60
4:A:27:THR:HB	4:A:66:ARG:HA	1.84	0.59
1:1:54:LEU:O	1:1:58:ILE:HG23	2.03	0.59
4:A:95:GLU:OE2	4:A:127:THR:OG1	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:16:MET:HB2	5:P:19:SER:HB3	1.86	0.57
2:2:17:ARG:HA	2:2:20:ARG:HE	1.69	0.57
3:3:38:ILE:HG12	3:3:82:ILE:HD13	1.87	0.56
4:A:70:TYR:O	4:A:74:LEU:HB2	2.05	0.56
3:3:2:ASN:O	3:3:7:LYS:NZ	2.28	0.55
2:2:33:ARG:HG2	2:2:34:ARG:HD3	1.88	0.55
5:P:78:VAL:HG12	5:P:79:GLU:OE1	2.06	0.55
5:P:46:HIS:HB2	5:P:70:LYS:HD3	1.88	0.54
4:A:14:ARG:N	4:A:18:GLU:OE1	2.41	0.54
1:1:49:LYS:HZ3	1:1:52:ARG:HH12	1.57	0.53
3:3:11:ILE:O	3:3:14:GLU:HG3	2.09	0.52
4:A:133:ARG:H	4:A:133:ARG:HD3	1.74	0.52
3:3:61:ALA:HA	3:3:66:ILE:HG22	1.92	0.52
4:A:112:ARG:HA	4:A:115:ILE:HD12	1.91	0.52
4:A:170:MET:SD	4:A:170:MET:N	2.84	0.51
4:A:91:ILE:HB	4:A:123:LYS:HE3	1.92	0.51
2:2:11:PHE:CG	2:2:12:ASP:N	2.79	0.51
3:3:2:ASN:OD1	3:3:3:ILE:N	2.43	0.51
5:P:17:GLU:OE1	5:P:17:GLU:N	2.45	0.49
2:2:11:PHE:HB2	2:2:15:LEU:HD12	1.93	0.48
3:3:42:ASP:OD1	3:3:43:LYS:N	2.47	0.47
5:P:27:PHE:HE1	5:P:38:LYS:HG2	1.78	0.47
4:A:108:GLN:O	4:A:112:ARG:HG3	2.15	0.46
1:1:70:THR:HG23	1:1:72:ARG:H	1.81	0.46
3:3:3:ILE:O	3:3:4:LYS:NZ	2.27	0.46
5:P:11:VAL:HG11	5:P:15:LYS:HZ1	1.81	0.46
5:P:80:LYS:HE3	5:P:81:ALA:HB2	1.99	0.45
2:2:8:ASN:OD1	2:2:9:GLU:N	2.42	0.44
5:P:68:LYS:HG2	5:P:69:THR:HG23	1.99	0.44
4:A:99:ARG:HH21	4:A:129:ARG:HG3	1.82	0.44
3:3:7:LYS:O	3:3:11:ILE:HG12	2.17	0.44
3:3:27:MET:HE1	3:3:56:ILE:HG23	1.99	0.44
4:A:165:ILE:HG12	4:A:170:MET:SD	2.58	0.44
2:2:39:LYS:N	2:2:40:PRO:HD2	2.33	0.44
3:3:52:GLU:OE1	3:3:52:GLU:N	2.45	0.44
4:A:107:TYR:CZ	4:A:111:LEU:HD11	2.52	0.44
5:P:11:VAL:O	5:P:13:SER:OG	2.36	0.44
4:A:95:GLU:HG3	4:A:125:LYS:O	2.19	0.43
2:2:39:LYS:H	2:2:40:PRO:HD2	1.84	0.43
1:1:58:ILE:HG13	1:1:59:LYS:N	2.34	0.43
4:A:117:PHE:HB3	4:A:122:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:49:LYS:NZ	1:1:52:ARG:HH12	2.17	0.42
3:3:48:LYS:O	3:3:52:GLU:OE1	2.36	0.42
4:A:111:LEU:O	4:A:115:ILE:HG13	2.19	0.42
4:A:57:SER:HB3	4:A:60:ALA:HB2	2.02	0.42
4:A:69:ASP:O	4:A:73:PHE:HB3	2.19	0.42
5:P:60:ILE:HD12	5:P:60:ILE:HA	1.88	0.42
1:1:59:LYS:HA	1:1:62:ARG:HD2	2.02	0.41
4:A:161:PHE:CG	4:A:162:PRO:HD2	2.55	0.41
2:2:24:LYS:O	2:2:27:VAL:HG22	2.20	0.41
3:3:54:GLN:N	3:3:55:PRO:HD2	2.35	0.41
4:A:25:ARG:HD2	4:A:64:VAL:HG22	2.02	0.41
4:A:99:ARG:HH21	4:A:129:ARG:CG	2.34	0.41
1:1:25:ILE:HG23	1:1:67:LEU:HD21	2.02	0.40
1:1:51:GLN:HE21	1:1:51:GLN:HB3	1.73	0.40
4:A:41:GLU:O	4:A:44:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1	53/73 (73%)	51 (96%)	2 (4%)	0	100	100
2	2	49/53 (92%)	36 (74%)	12 (24%)	1 (2%)	6	32
3	3	83/86 (96%)	79 (95%)	4 (5%)	0	100	100
4	A	165/180 (92%)	158 (96%)	7 (4%)	0	100	100
5	P	78/82 (95%)	69 (88%)	8 (10%)	1 (1%)	10	42
7	k	148/158 (94%)	132 (89%)	15 (10%)	1 (1%)	19	56
8	l	203/205 (99%)	186 (92%)	17 (8%)	0	100	100
9	n	98/100 (98%)	82 (84%)	16 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	p	127/129 (98%)	121 (95%)	6 (5%)	0	100	100
11	q	115/128 (90%)	106 (92%)	9 (8%)	0	100	100
12	t	121/123 (98%)	104 (86%)	17 (14%)	0	100	100
13	u	86/88 (98%)	80 (93%)	4 (5%)	2 (2%)	5	29
14	y	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
15	h	204/206 (99%)	190 (93%)	13 (6%)	1 (0%)	25	64
16	m	149/151 (99%)	141 (95%)	8 (5%)	0	100	100
17	o	125/129 (97%)	114 (91%)	10 (8%)	1 (1%)	16	54
18	r	96/102 (94%)	87 (91%)	6 (6%)	3 (3%)	3	22
19	s	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
20	w	92/100 (92%)	85 (92%)	7 (8%)	0	100	100
21	z	77/80 (96%)	71 (92%)	6 (8%)	0	100	100
22	j	216/225 (96%)	198 (92%)	18 (8%)	0	100	100
All	All	2477/2594 (96%)	2268 (92%)	199 (8%)	10 (0%)	32	68

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	39	LYS
18	r	57	VAL
13	u	46	LYS
17	o	57	VAL
18	r	36	VAL
7	k	100	GLU
13	u	87	ARG
15	h	65	VAL
5	P	12	VAL
18	r	6	ILE

5.3.2 Protein sidechains ⓘ

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	1	48/63 (76%)	46 (96%)	2 (4%)	25	47
2	2	44/46 (96%)	44 (100%)	0	100	100
3	3	65/65 (100%)	65 (100%)	0	100	100
4	A	146/156 (94%)	145 (99%)	1 (1%)	81	87
5	P	74/76 (97%)	73 (99%)	1 (1%)	62	75
7	k	113/118 (96%)	113 (100%)	0	100	100
8	l	172/172 (100%)	169 (98%)	3 (2%)	56	72
9	n	87/87 (100%)	86 (99%)	1 (1%)	70	80
10	p	104/104 (100%)	104 (100%)	0	100	100
11	q	90/98 (92%)	89 (99%)	1 (1%)	70	80
12	t	103/103 (100%)	103 (100%)	0	100	100
13	u	76/76 (100%)	76 (100%)	0	100	100
14	y	65/65 (100%)	65 (100%)	0	100	100
15	h	170/170 (100%)	169 (99%)	1 (1%)	84	88
16	m	124/124 (100%)	123 (99%)	1 (1%)	79	84
17	o	105/106 (99%)	105 (100%)	0	100	100
18	r	86/90 (96%)	86 (100%)	0	100	100
19	s	92/92 (100%)	92 (100%)	0	100	100
20	w	79/83 (95%)	79 (100%)	0	100	100
21	z	70/71 (99%)	69 (99%)	1 (1%)	62	75
22	j	180/186 (97%)	179 (99%)	1 (1%)	84	88
All	All	2093/2151 (97%)	2080 (99%)	13 (1%)	82	88

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	51	GLN
1	1	72	ARG
4	A	133	ARG
5	P	26	ARG
8	l	62	ARG
8	l	150	LYS
8	l	164	ARG
9	n	38	ARG
11	q	79	LYS
15	h	168	ARG

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Mol	Chain	Res	Type
16	m	130	LYS
21	z	54	ARG
22	j	104	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	3	60	GLN
8	l	58	GLN
8	l	88	ASN
9	n	63	ASN
11	q	37	GLN
11	q	39	ASN
21	z	51	HIS
21	z	56	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	g	1538/1540 (99%)	563 (36%)	0

All (563) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	g	3	A
6	g	5	U
6	g	6	G
6	g	8	A
6	g	9	G
6	g	14	U
6	g	16	A
6	g	22	G
6	g	26	A
6	g	30	U
6	g	31	G
6	g	32	A
6	g	33	A
6	g	47	C
6	g	48	C
6	g	50	A

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Mol	Chain	Res	Type
6	g	51	A
6	g	55	A
6	g	56	U
6	g	72	A
6	g	73	C
6	g	74	A
6	g	77	A
6	g	79	G
6	g	81	A
6	g	82	G
6	g	83	C
6	g	84	U
6	g	86	G
6	g	93	U
6	g	94	G
6	g	108	G
6	g	110	C
6	g	116	A
6	g	121	U
6	g	122	G
6	g	129	A
6	g	131	A
6	g	134	G
6	g	140	U
6	g	142	G
6	g	144	G
6	g	153	C
6	g	163	C
6	g	182	A
6	g	183	C
6	g	184	G
6	g	188	C
6	g	189	A
6	g	190	A
6	g	195	A
6	g	196	A
6	g	198	G
6	g	201	G
6	g	209	U
6	g	210	C
6	g	219	U
6	g	223	A

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Mol	Chain	Res	Type
6	g	224	U
6	g	226	G
6	g	228	A
6	g	229	U
6	g	240	G
6	g	244	U
6	g	245	U
6	g	247	G
6	g	251	G
6	g	254	G
6	g	257	G
6	g	258	G
6	g	260	G
6	g	261	U
6	g	262	A
6	g	265	G
6	g	266	G
6	g	267	C
6	g	268	U
6	g	281	G
6	g	288	A
6	g	289	G
6	g	293	G
6	g	299	G
6	g	303	A
6	g	306	A
6	g	315	A
6	g	319	G
6	g	321	A
6	g	322	C
6	g	328	C
6	g	329	A
6	g	332	G
6	g	340	U
6	g	344	A
6	g	345	C
6	g	351	G
6	g	352	C
6	g	353	A
6	g	354	G
6	g	355	C
6	g	367	U

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Mol	Chain	Res	Type
6	g	368	U
6	g	369	G
6	g	372	C
6	g	373	A
6	g	386	C
6	g	390	U
6	g	392	C
6	g	393	A
6	g	397	A
6	g	398	U
6	g	399	G
6	g	401	C
6	g	406	G
6	g	407	U
6	g	411	A
6	g	412	A
6	g	413	G
6	g	414	A
6	g	418	C
6	g	423	G
6	g	424	G
6	g	429	U
6	g	435	A
6	g	438	U
6	g	439	U
6	g	440	C
6	g	450	G
6	g	454	G
6	g	462	G
6	g	466	A
6	g	467	U
6	g	468	A
6	g	469	C
6	g	476	U
6	g	478	A
6	g	479	U
6	g	480	U
6	g	481	G
6	g	482	A
6	g	486	U
6	g	487	A
6	g	493	A

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Mol	Chain	Res	Type
6	g	495	A
6	g	497	G
6	g	499	A
6	g	502	A
6	g	505	G
6	g	508	U
6	g	511	C
6	g	518	C
6	g	519	C
6	g	521	G
6	g	525	C
6	g	527	G
6	g	530	G
6	g	531	U
6	g	538	G
6	g	547	A
6	g	550	G
6	g	559	A
6	g	560	A
6	g	562	U
6	g	564	C
6	g	565	U
6	g	566	G
6	g	570	G
6	g	572	A
6	g	573	A
6	g	575	G
6	g	576	C
6	g	577	G
6	g	579	A
6	g	596	A
6	g	606	G
6	g	609	A
6	g	610	U
6	g	621	A
6	g	623	C
6	g	628	G
6	g	629	A
6	g	632	U
6	g	644	U
6	g	650	G
6	g	653	U

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Mol	Chain	Res	Type
6	g	655	A
6	g	665	A
6	g	675	A
6	g	678	U
6	g	685	G
6	g	687	A
6	g	688	G
6	g	689	C
6	g	690	G
6	g	691	G
6	g	692	U
6	g	693	G
6	g	694	A
6	g	695	A
6	g	698	G
6	g	702	A
6	g	703	G
6	g	704	A
6	g	709	U
6	g	710	G
6	g	714	G
6	g	717	U
6	g	718	A
6	g	719	C
6	g	721	G
6	g	722	G
6	g	723	U
6	g	724	G
6	g	728	A
6	g	729	A
6	g	731	G
6	g	732	C
6	g	733	G
6	g	734	G
6	g	735	C
6	g	741	G
6	g	747	A
6	g	748	G
6	g	749	A
6	g	753	A
6	g	755	G
6	g	758	C

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Mol	Chain	Res	Type
6	g	760	G
6	g	761	G
6	g	767	A
6	g	773	G
6	g	777	A
6	g	779	C
6	g	781	A
6	g	782	A
6	g	788	U
6	g	789	U
6	g	792	A
6	g	793	U
6	g	795	C
6	g	796	C
6	g	801	U
6	g	807	A
6	g	809	G
6	g	813	U
6	g	814	A
6	g	817	C
6	g	818	G
6	g	828	U
6	g	829	G
6	g	832	G
6	g	835	U
6	g	839	C
6	g	840	C
6	g	841	C
6	g	842	U
6	g	843	U
6	g	844	G
6	g	845	A
6	g	846	G
6	g	849	G
6	g	850	U
6	g	851	G
6	g	855	U
6	g	864	A
6	g	870	U
6	g	871	U
6	g	872	A
6	g	873	A

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Mol	Chain	Res	Type
6	g	879	C
6	g	880	C
6	g	884	U
6	g	889	A
6	g	890	G
6	g	891	U
6	g	907	A
6	g	913	A
6	g	914	A
6	g	917	G
6	g	919	A
6	g	920	A
6	g	921	U
6	g	922	G
6	g	923	A
6	g	924	C
6	g	925	G
6	g	927	G
6	g	929	G
6	g	933	G
6	g	934	C
6	g	935	A
6	g	938	A
6	g	941	G
6	g	942	G
6	g	945	G
6	g	951	G
6	g	953	G
6	g	954	G
6	g	957	U
6	g	960	U
6	g	961	U
6	g	962	C
6	g	963	G
6	g	964	A
6	g	965	U
6	g	966	G
6	g	967	C
6	g	969	A
6	g	971	G
6	g	972	C
6	g	973	G

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Mol	Chain	Res	Type
6	g	975	A
6	g	976	G
6	g	978	A
6	g	979	C
6	g	980	C
6	g	981	U
6	g	982	U
6	g	983	A
6	g	990	C
6	g	993	G
6	g	999	C
6	g	1001	C
6	g	1002	G
6	g	1004	A
6	g	1006	G
6	g	1007	U
6	g	1008	U
6	g	1009	U
6	g	1011	C
6	g	1015	G
6	g	1016	A
6	g	1017	U
6	g	1018	G
6	g	1019	A
6	g	1020	G
6	g	1021	A
6	g	1022	A
6	g	1024	G
6	g	1027	C
6	g	1028	C
6	g	1029	U
6	g	1031	C
6	g	1032	G
6	g	1033	G
6	g	1034	G
6	g	1035	A
6	g	1036	A
6	g	1037	C
6	g	1042	A
6	g	1044	A
6	g	1045	C
6	g	1046	A

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Mol	Chain	Res	Type
6	g	1047	G
6	g	1048	G
6	g	1049	U
6	g	1054	C
6	g	1056	U
6	g	1057	G
6	g	1058	G
6	g	1059	C
6	g	1060	U
6	g	1064	G
6	g	1070	U
6	g	1078	U
6	g	1079	G
6	g	1080	A
6	g	1081	A
6	g	1082	A
6	g	1084	G
6	g	1091	U
6	g	1094	G
6	g	1095	U
6	g	1096	C
6	g	1100	C
6	g	1101	A
6	g	1122	U
6	g	1124	G
6	g	1126	U
6	g	1127	G
6	g	1128	C
6	g	1130	A
6	g	1132	C
6	g	1133	G
6	g	1135	U
6	g	1137	C
6	g	1138	G
6	g	1139	G
6	g	1142	G
6	g	1143	G
6	g	1144	G
6	g	1145	A
6	g	1146	A
6	g	1151	A
6	g	1152	A

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Mol	Chain	Res	Type
6	g	1157	A
6	g	1159	U
6	g	1160	G
6	g	1161	C
6	g	1166	G
6	g	1167	A
6	g	1168	U
6	g	1176	A
6	g	1177	G
6	g	1178	G
6	g	1179	A
6	g	1180	A
6	g	1181	G
6	g	1183	U
6	g	1184	G
6	g	1193	G
6	g	1194	U
6	g	1197	A
6	g	1198	G
6	g	1201	A
6	g	1202	U
6	g	1205	U
6	g	1206	G
6	g	1207	G
6	g	1208	C
6	g	1211	U
6	g	1212	U
6	g	1213	A
6	g	1214	C
6	g	1215	G
6	g	1217	C
6	g	1221	G
6	g	1222	G
6	g	1224	U
6	g	1226	C
6	g	1227	A
6	g	1235	U
6	g	1238	A
6	g	1240	U
6	g	1241	G
6	g	1243	C
6	g	1246	A

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Mol	Chain	Res	Type
6	g	1247	U
6	g	1248	A
6	g	1250	A
6	g	1251	A
6	g	1252	A
6	g	1254	A
6	g	1255	G
6	g	1256	A
6	g	1257	A
6	g	1258	G
6	g	1260	G
6	g	1268	G
6	g	1270	G
6	g	1272	G
6	g	1274	A
6	g	1275	A
6	g	1276	G
6	g	1278	G
6	g	1279	G
6	g	1280	A
6	g	1281	C
6	g	1282	C
6	g	1283	U
6	g	1284	C
6	g	1285	A
6	g	1287	A
6	g	1289	A
6	g	1294	G
6	g	1295	U
6	g	1297	G
6	g	1298	U
6	g	1299	A
6	g	1300	G
6	g	1301	U
6	g	1302	C
6	g	1305	G
6	g	1306	A
6	g	1307	U
6	g	1308	U
6	g	1311	A
6	g	1313	U
6	g	1315	U

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Mol	Chain	Res	Type
6	g	1317	C
6	g	1318	A
6	g	1319	A
6	g	1320	C
6	g	1322	C
6	g	1326	U
6	g	1327	C
6	g	1329	A
6	g	1330	U
6	g	1331	G
6	g	1334	G
6	g	1336	C
6	g	1338	G
6	g	1340	A
6	g	1346	A
6	g	1347	G
6	g	1348	U
6	g	1349	A
6	g	1350	A
6	g	1355	G
6	g	1359	C
6	g	1360	A
6	g	1361	G
6	g	1362	A
6	g	1364	U
6	g	1373	G
6	g	1375	A
6	g	1379	G
6	g	1380	U
6	g	1381	U
6	g	1382	C
6	g	1386	G
6	g	1390	U
6	g	1392	G
6	g	1394	A
6	g	1395	C
6	g	1398	A
6	g	1399	C
6	g	1401	G
6	g	1403	C
6	g	1404	C
6	g	1406	U

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Mol	Chain	Res	Type
6	g	1410	A
6	g	1415	G
6	g	1419	G
6	g	1421	G
6	g	1423	G
6	g	1427	C
6	g	1440	U
6	g	1446	A
6	g	1448	C
6	g	1451	U
6	g	1453	G
6	g	1463	U
6	g	1470	U
6	g	1471	U
6	g	1477	U
6	g	1479	C
6	g	1487	G
6	g	1490	U
6	g	1491	G
6	g	1493	A
6	g	1496	C
6	g	1497	G
6	g	1498	U
6	g	1499	A
6	g	1502	A
6	g	1503	A
6	g	1504	G
6	g	1505	G
6	g	1506	U
6	g	1507	A
6	g	1508	A
6	g	1516	G
6	g	1517	G
6	g	1520	C
6	g	1525	G
6	g	1527	U
6	g	1529	G
6	g	1530	G
6	g	1531	A
6	g	1533	C
6	g	1534	A
6	g	1537	U

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Mol	Chain	Res	Type
6	g	1538	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

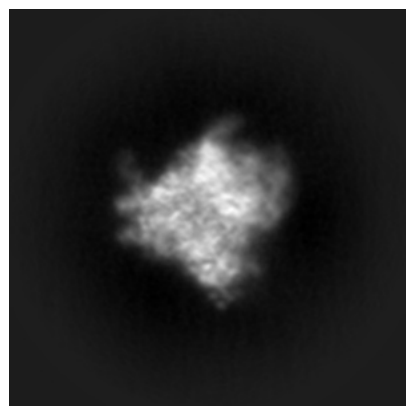
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36619. These allow visual inspection of the internal detail of the map and identification of artifacts.

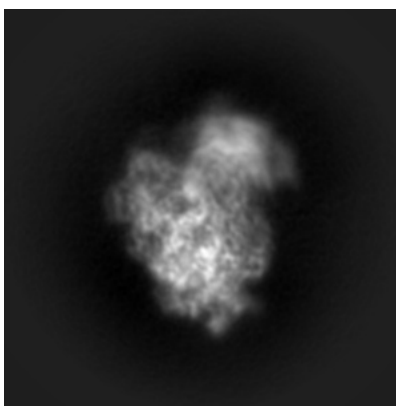
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

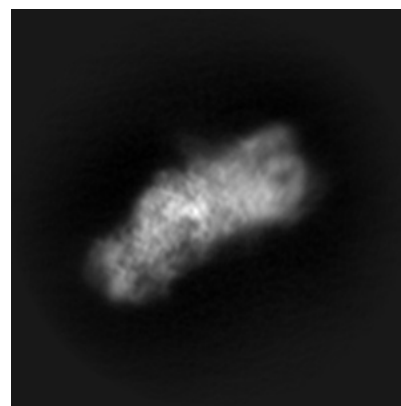
6.1.1 Primary map



X

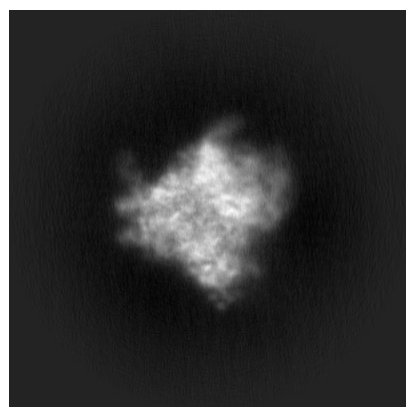


Y

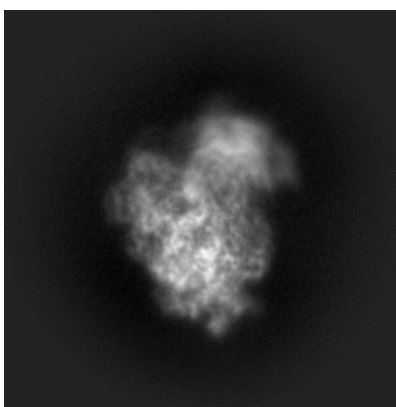


Z

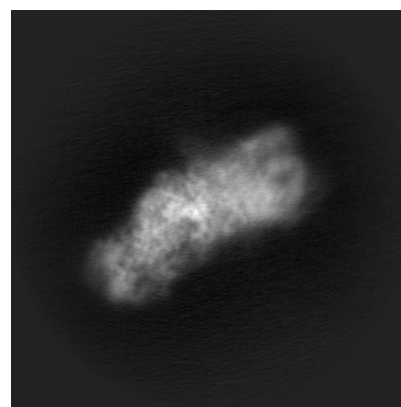
6.1.2 Raw map



X



Y

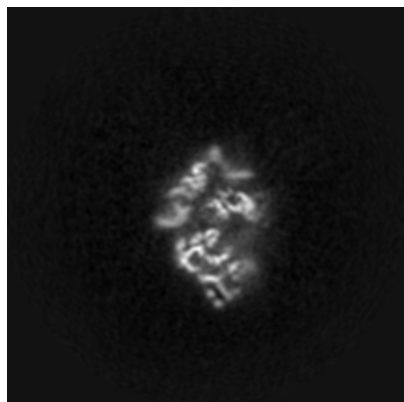


Z

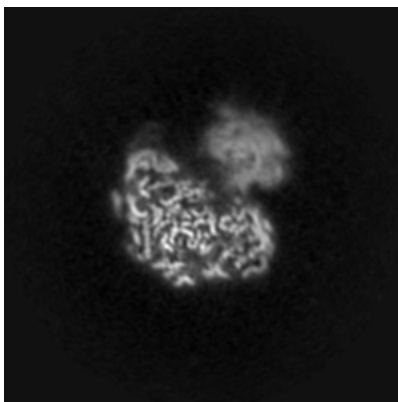
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

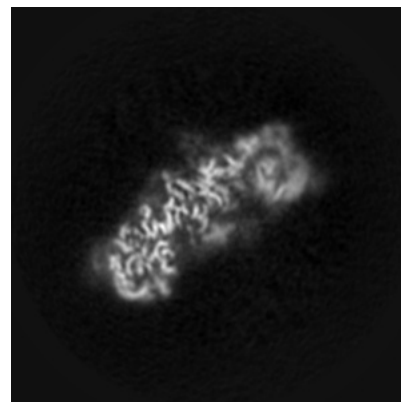
6.2.1 Primary map



X Index: 160



Y Index: 160

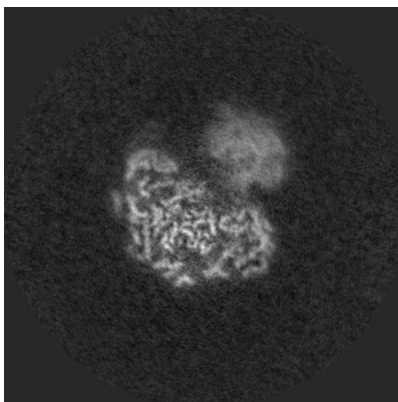


Z Index: 160

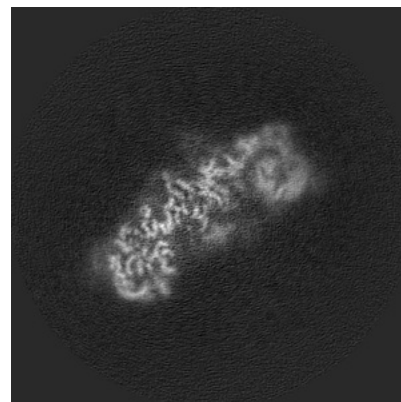
6.2.2 Raw map



X Index: 160



Y Index: 160

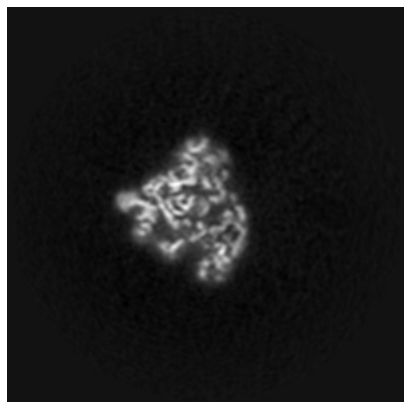


Z Index: 160

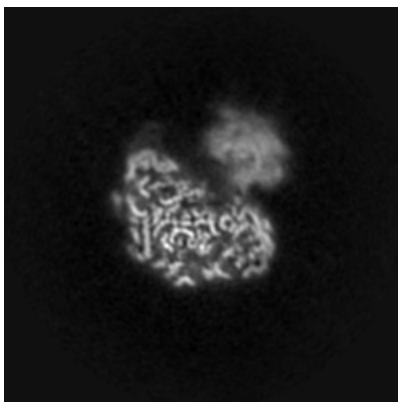
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

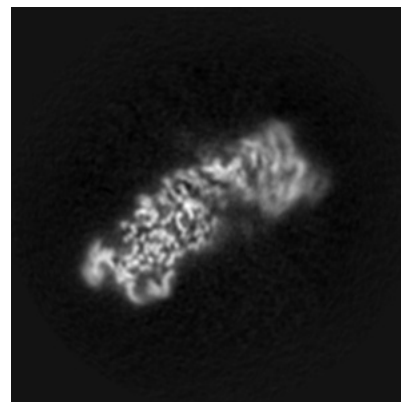
6.3.1 Primary map



X Index: 122

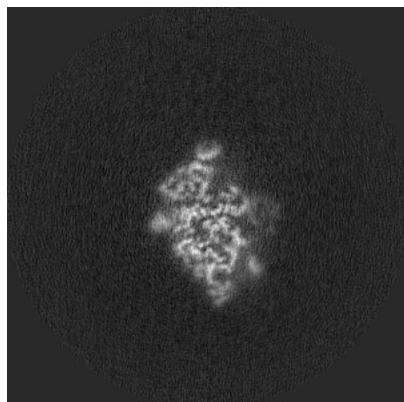


Y Index: 159

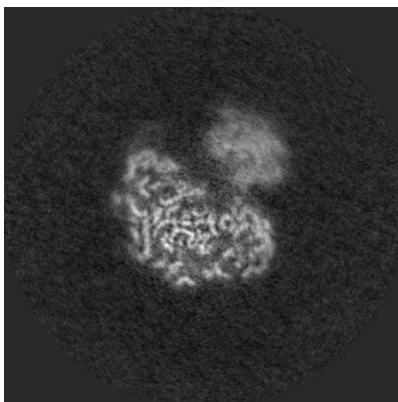


Z Index: 167

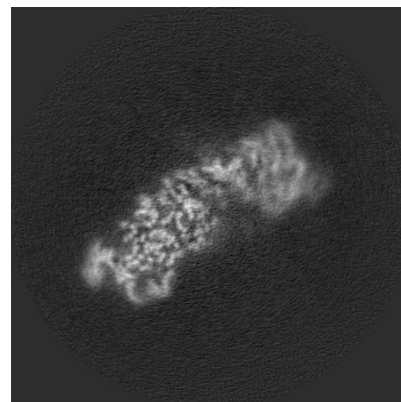
6.3.2 Raw map



X Index: 152



Y Index: 159

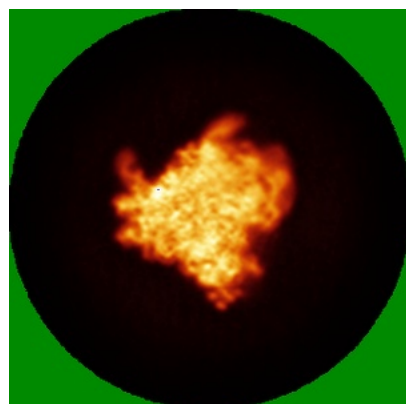


Z Index: 167

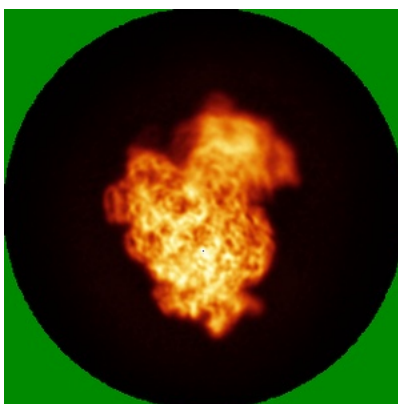
The images above show the largest variance slices of the map in three orthogonal directions.

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

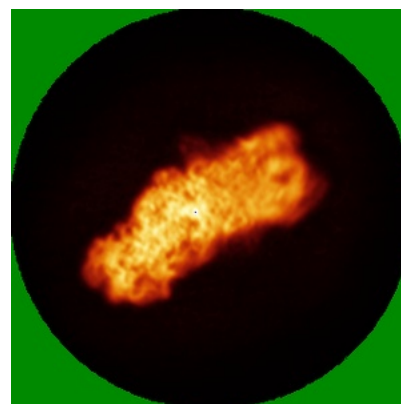
6.4.1 Primary map



X

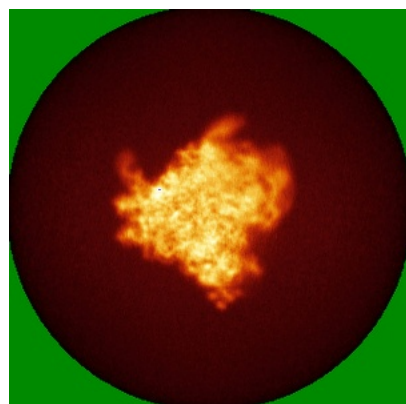


Y

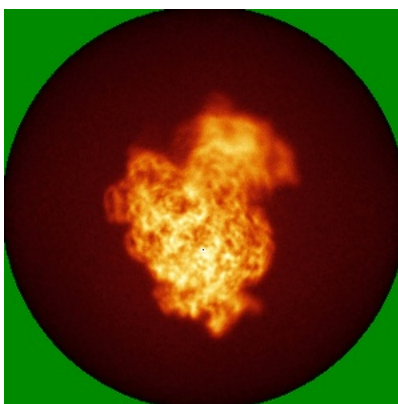


Z

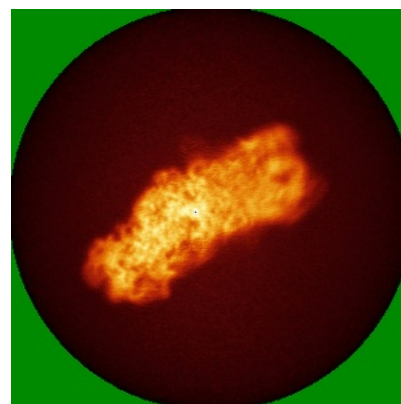
6.4.2 Raw map



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](#)

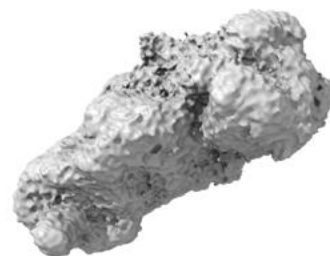
6.5.1 Primary map



X



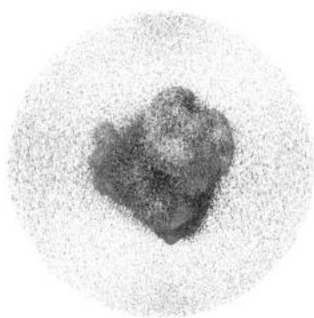
Y



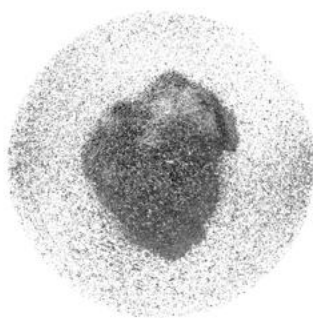
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00126. 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.

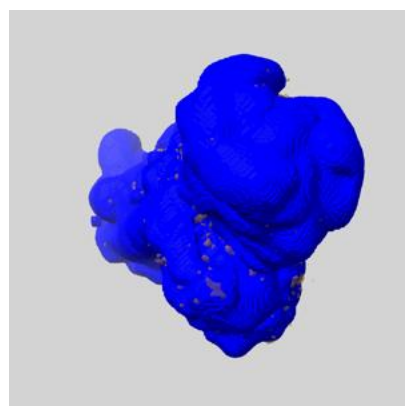
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

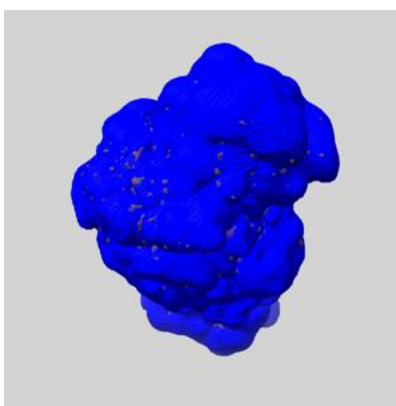
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

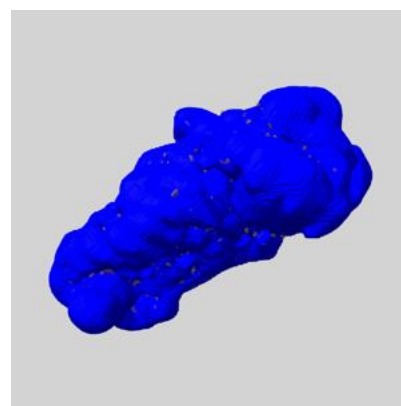
6.6.1 emd_36619_msk_1.map [i](#)



X



Y

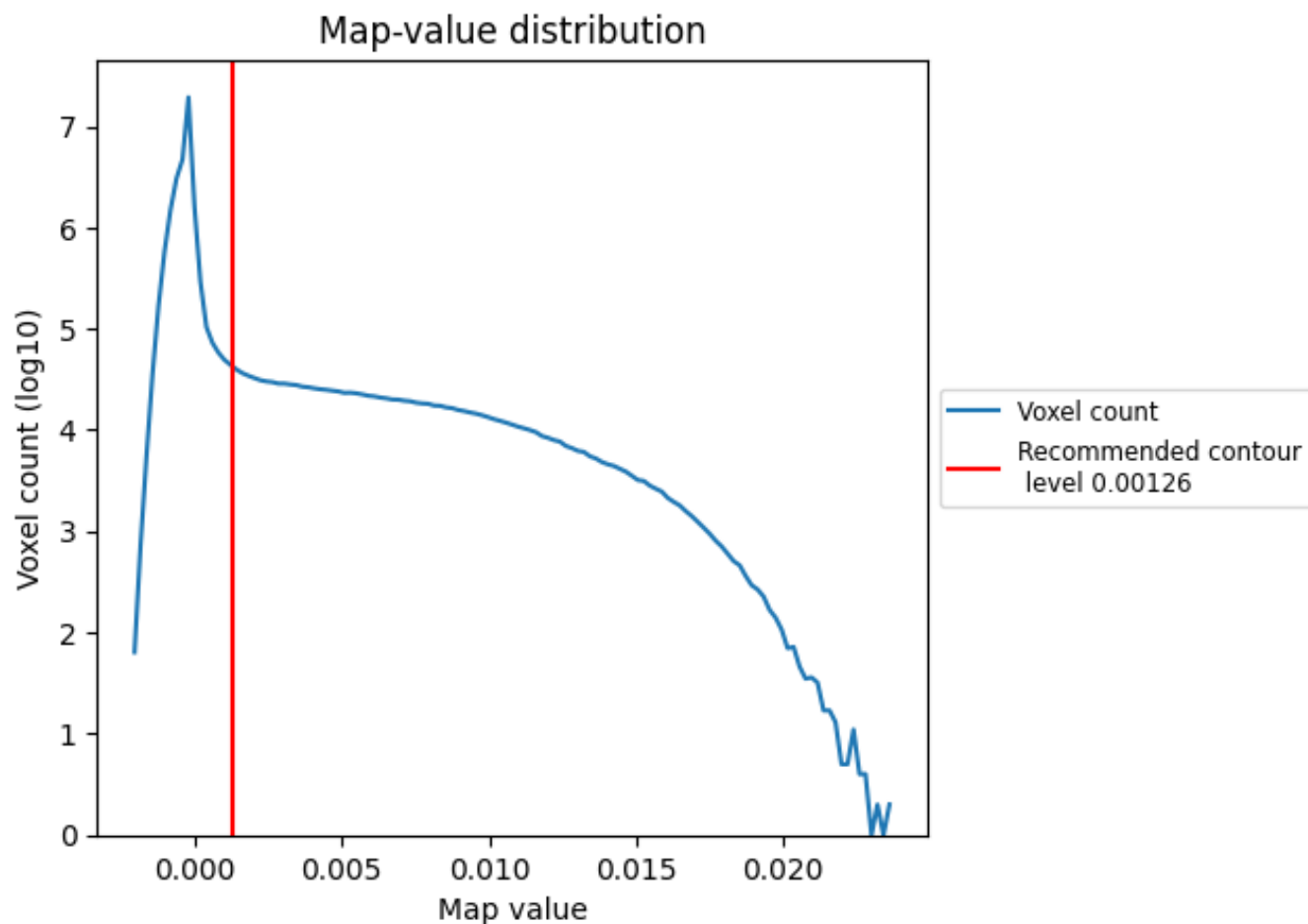


Z

7 Map analysis [i](#)

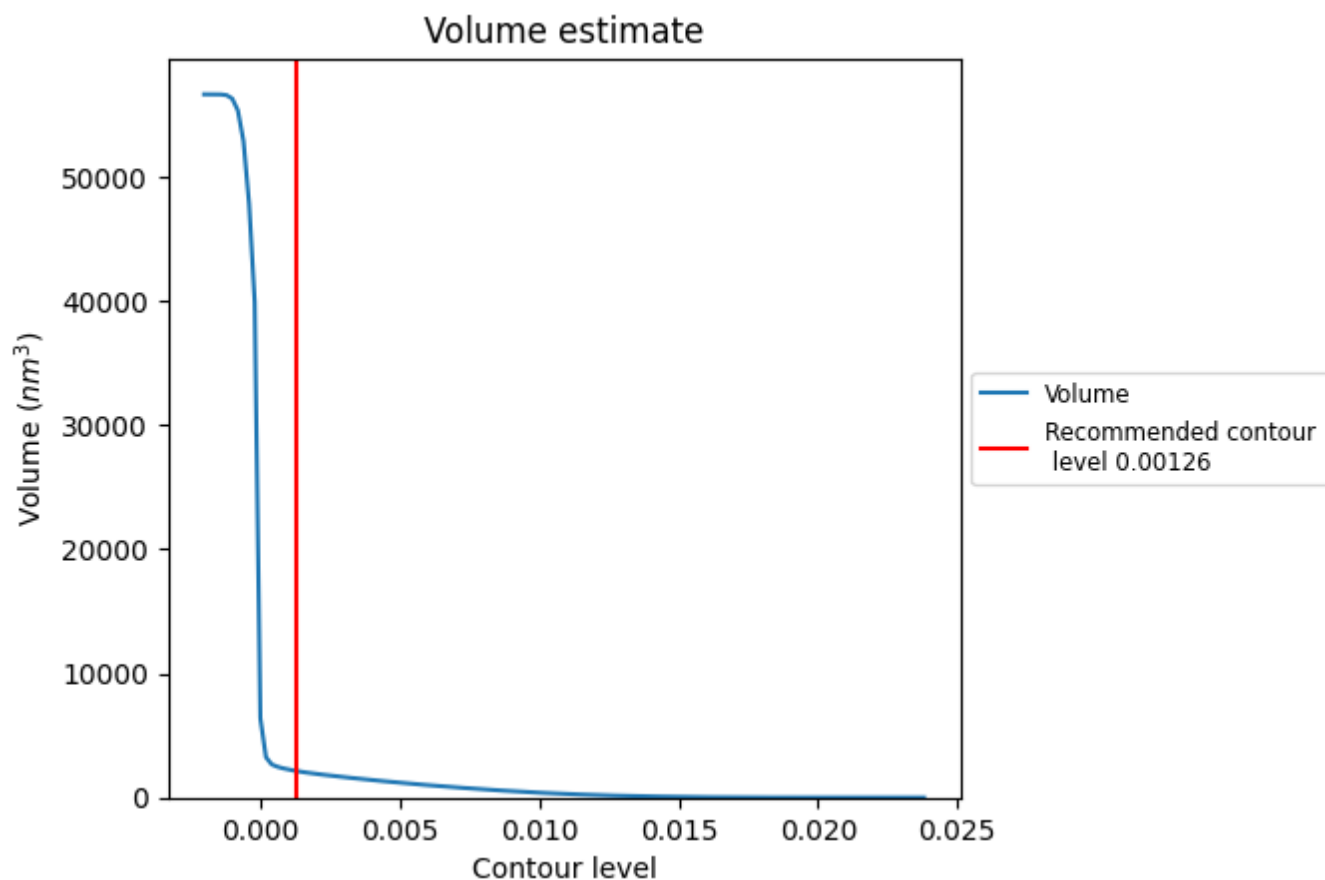
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

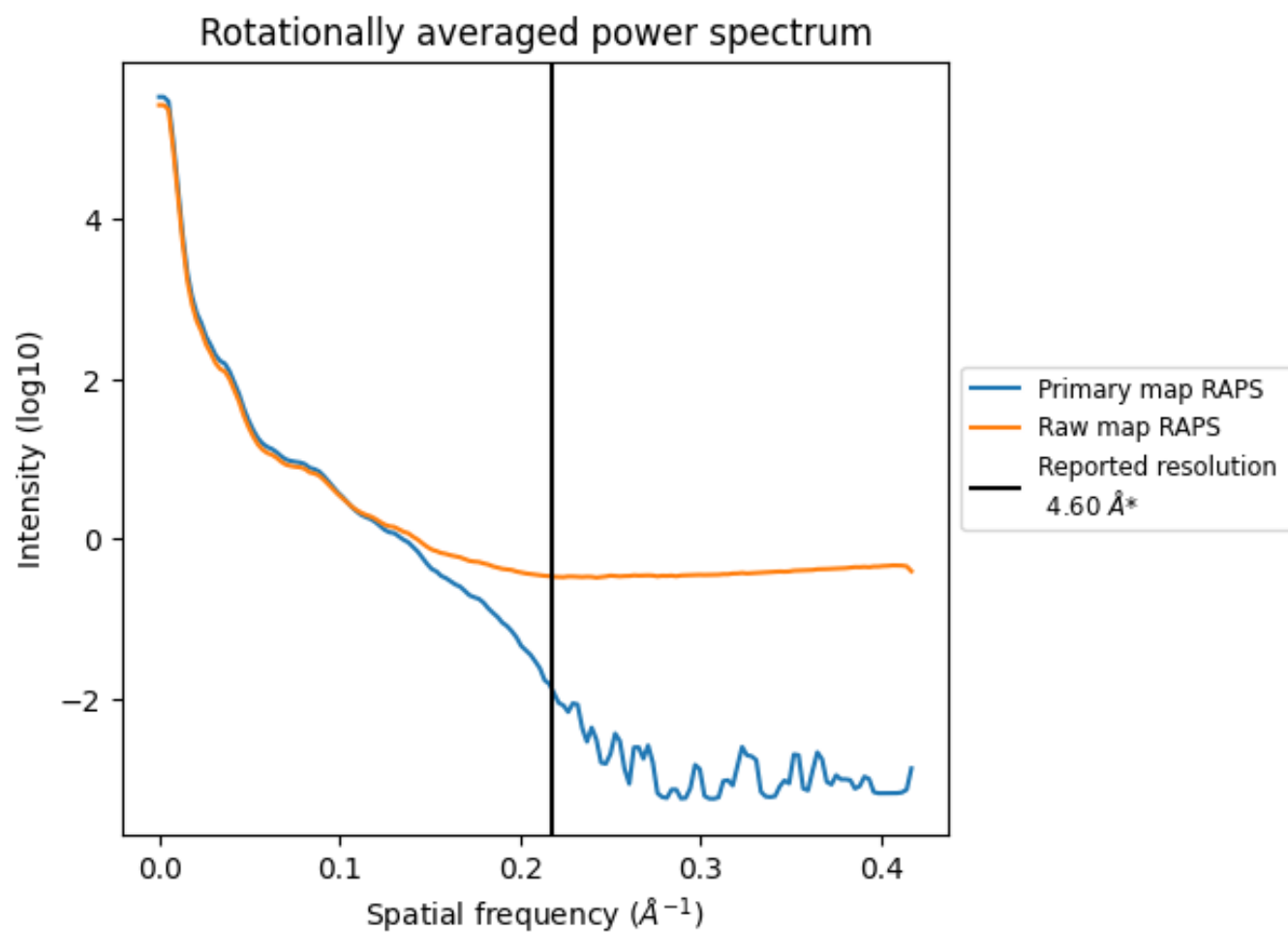
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2144 nm³; this corresponds to an approximate mass of 1937 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](#)

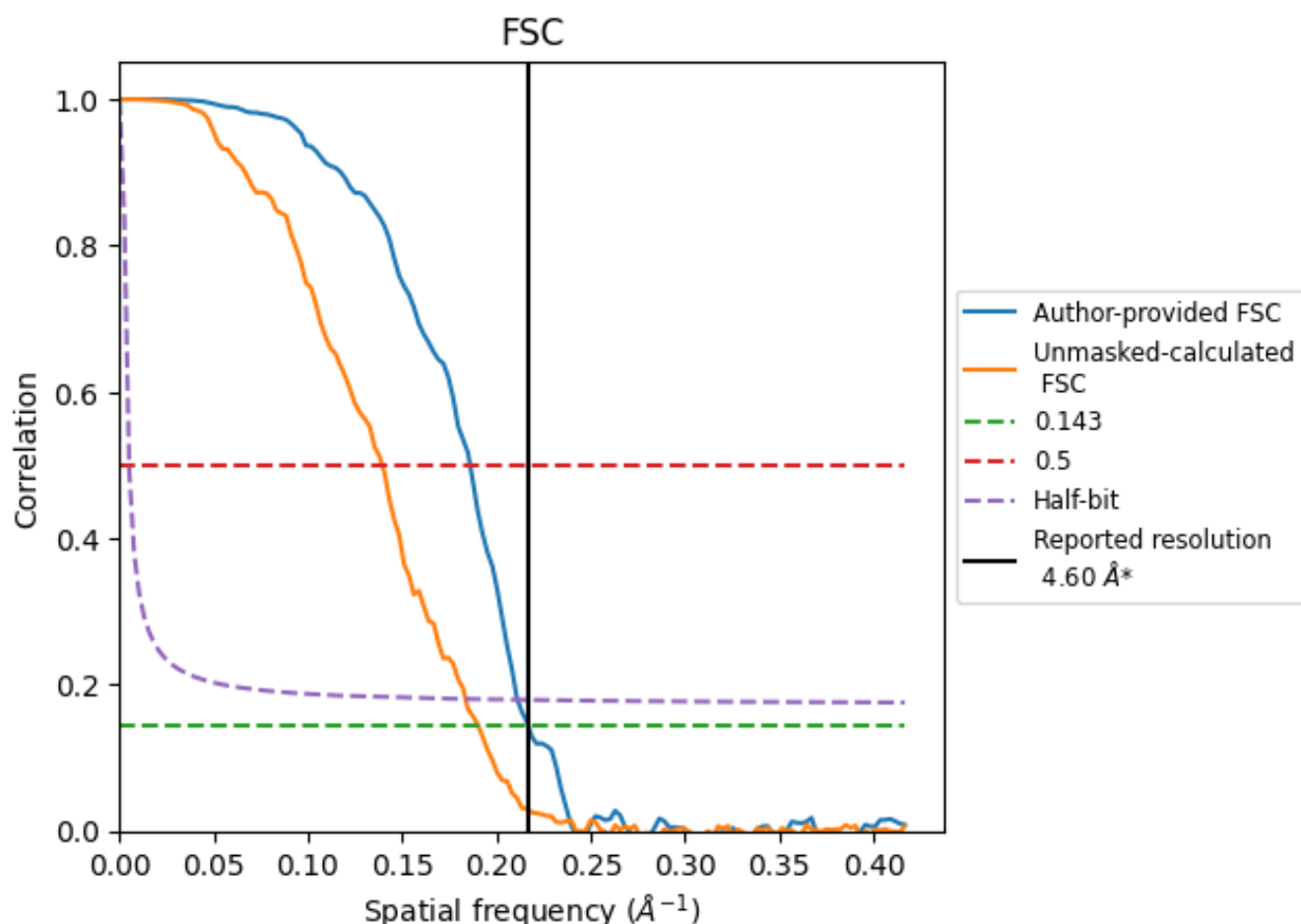


*Reported resolution corresponds to spatial frequency of 0.217 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

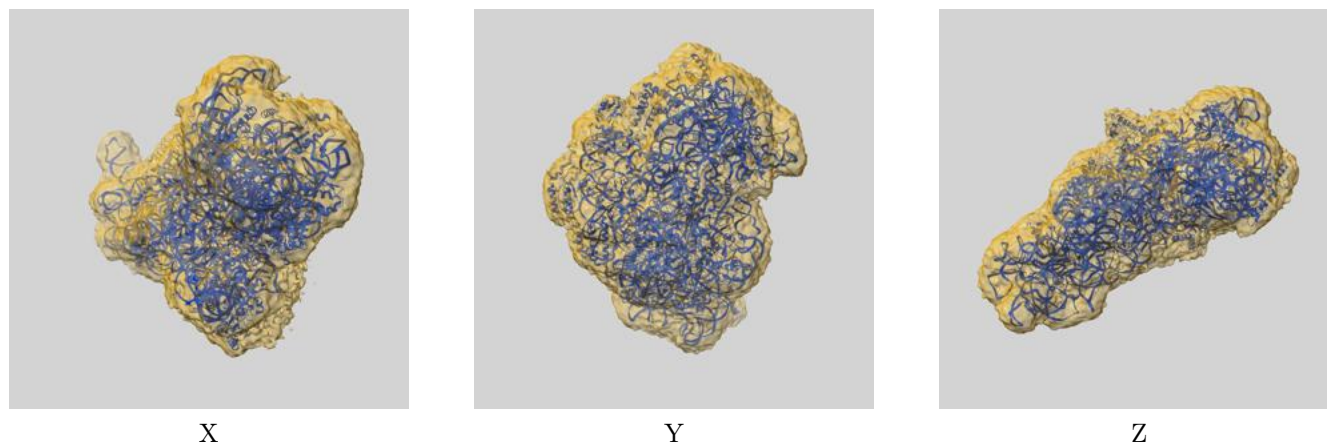
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.61	5.38	4.73
Unmasked-calculated*	5.25	7.17	5.44

*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 5.25 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

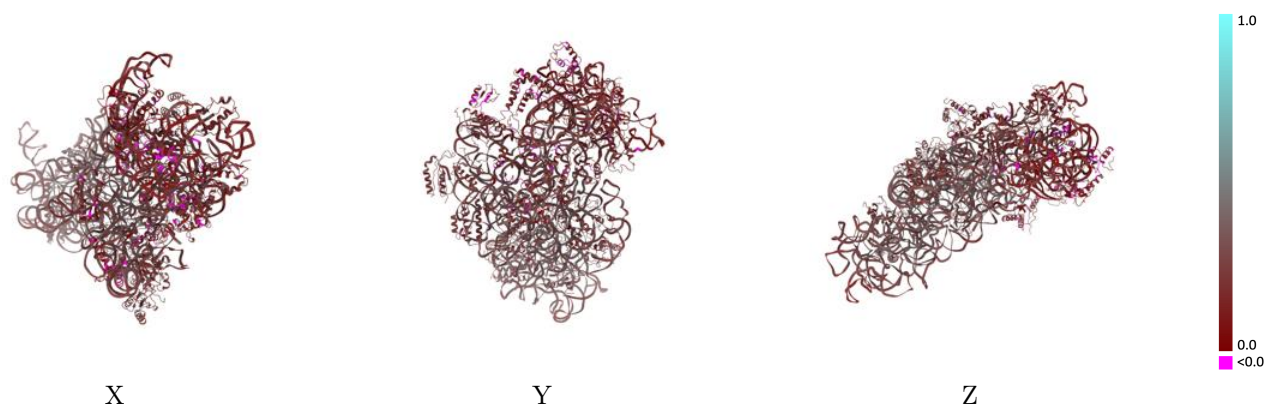
This section contains information regarding the fit between EMDB map EMD-36619 and PDB model 8JSG. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



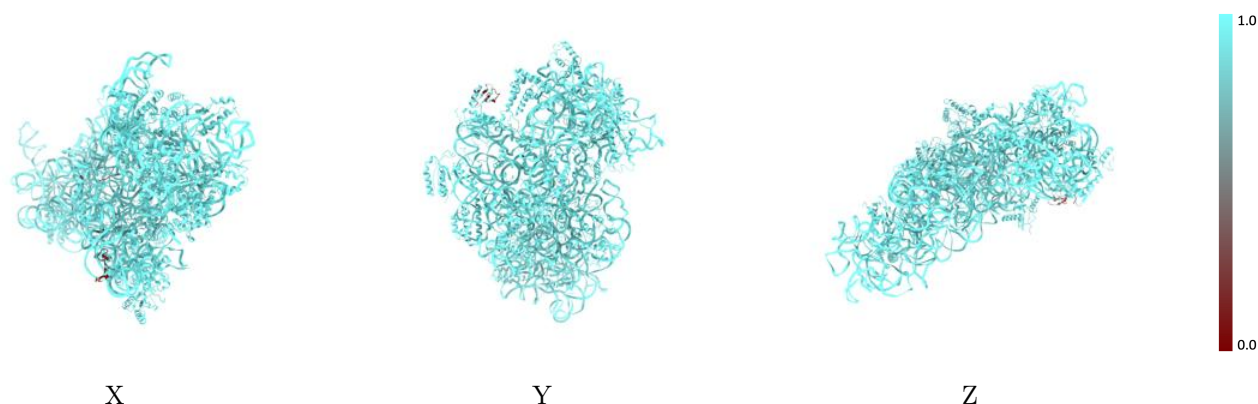
The images above show the 3D surface view of the map at the recommended contour level 0.00126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



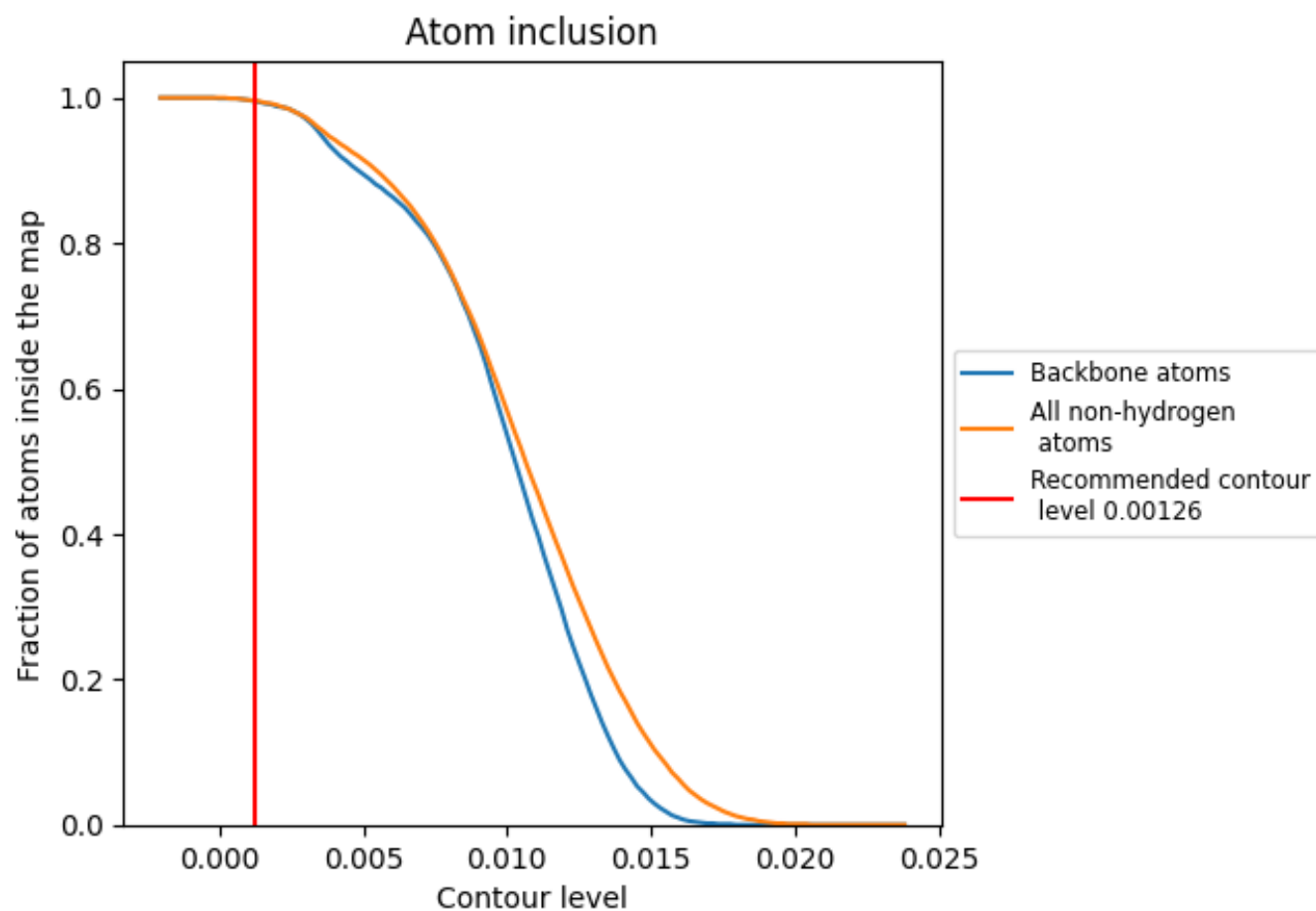
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00126).















































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.00126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9960	 0.2650
1	 1.0000	 0.2820
2	 1.0000	 0.0730
3	 1.0000	 0.2600
A	 0.8590	 0.1680
P	 1.0000	 0.3160
g	 1.0000	 0.2870
h	 1.0000	 0.2420
j	 0.9970	 0.2110
k	 1.0000	 0.3070
l	 1.0000	 0.2700
m	 1.0000	 0.1540
n	 1.0000	 0.2640
o	 1.0000	 0.1680
p	 1.0000	 0.2920
q	 1.0000	 0.2560
r	 1.0000	 0.2070
s	 0.9640	 0.1120
t	 1.0000	 0.3230
u	 1.0000	 0.2580
w	 1.0000	 0.1770
y	 1.0000	 0.3020
z	 1.0000	 0.1170

