



wwPDB EM Validation Summary 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 wwPDB EM Validation Summary 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

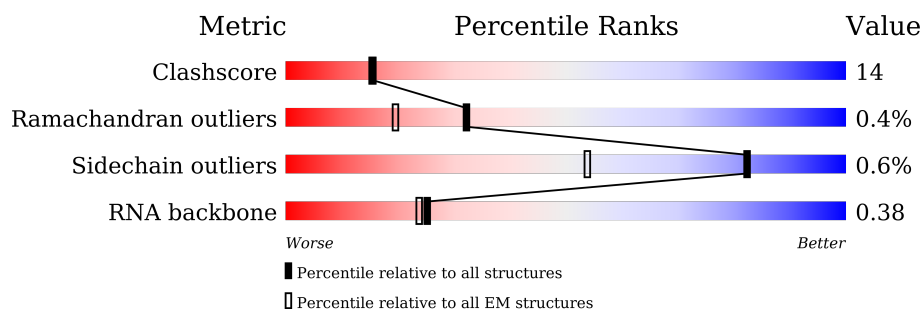
1 Overall quality at a glance

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.

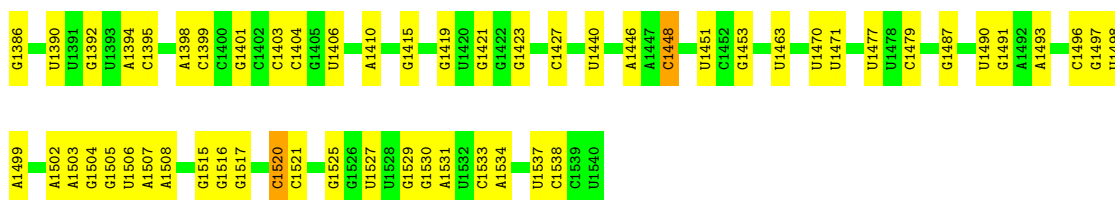
Mol	Chain	Residues	Atoms					AltConf	Trace
22	j	218	Total 1705	C 1081	N 305	O 312	S 7	0	0

THR	ASP	K3	V11	V12	S13	D14	K15	M16	E17	K18	S19	R26	F27	K38	H46	D47	E48	I60	C63	R64	K68	T69	K70	V78	E79	K80	A81	V82
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• Molecule 6: 16S ribosomal RNA

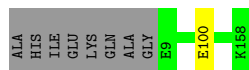
Chain g:  63% 37%

A	A2	A3	A4	U5	G6	A7	A8	G9	U14	G15	A16	G22	A26	U30	G31	A32	A33	C47	C48	U49	A50	A51	A55	U56	A72	C73	A74	A77	A78	A80	A81	C82	C83	U84	U85	G86	U93	G94	G108	A109	C110	A116	U121	G122	A129						
A130	A131	G134	U140	G141	G142	A143	G144	C153	G163	A182	C183	G184	C188	A189	A32	A190	A195	A196	C322	U439	G198	A51	A55	U56	C210	U219	C222	A223	U224	C225	G226	G227	A228	U229	G240	U244	U245	A246	G247	G251	G254	G257	G258	G259	G260	U261					
A262	G399	G265	G266	C267	U268	G281	A288	G289	G293	G299	A303	A306	A315	G319	A320	A321	C322	C328	A329	G332	U340	A344	C345	G351	C352	A353	G354	C355	U367	U478	U479	U480	G481	A482	U486	A487	A493	C494	A495	U390	G391	A498	A393	G122	A129						
U398	G399	C400	C401	G406	U407	A411	A412	C413	A414	C418	C419	G423	G424	G425	U429	A435	C436	U437	U438	U439	C440	G450	G454	C462	A466	U467	A468	C469	U476	C477	A478	U479	U480	G481	A482	U486	A487	A493	C494	A495	G497	A498	A499	A502							
G505	U508	C511	C518	C519	A520	A521	G521	C525	C526	G527	G530	U531	G538	A547	G550	A559	A560	U561	U562	C564	A563	U565	G566	G570	A571	A572	A573	A574	G575	C576	G577	C578	A579	A596	G606	A609	U610	A621	A622	G623	G628	A629	U632								
U644	G650	U653	G654	A655	A665	G671	A675	U678	G685	U686	A687	G688	C689	G690	G691	U692	G693	A694	A695	G698	A702	G703	A704	G710	G714	U717	A718	C719	G720	G721	G722	U723	G724	A728	A729	G730	G731	C732	G734	C735	G741	A747	G748								
A749	A753	G754	G755	C758	A759	G760	G761	A767	G773	A777	G778	C779	A780	A781	A782	U788	U789	A792	U793	A794	C795	G796	U801	A807	C808	G809	U813	A814	C817	G818	U828	G829	G832	U835	C839	C840	C841	U842	U843	A845	G846	C849									
U850	G851	U855	A864	U870	U871	A872	A873	C879	C880	C883	U884	A889	G890	U891	C896	A907	A913	A914	G917	A918	A919	U921	G922	A923	C924	G925	G926	U927	G928	G929	G933	C934	A935	A938	G941	G942	G945	G951	U952	G953	U954	U957									
U960	U961	C962	G963	A964	U965	G966	C967	A968	A969	C970	G971	C972	A974	A975	G976	A977	A978	C979	C980	U981	U982	A983	C990	A1000	C1001	U1002	G1003	A1004	A1005	G1006	U1007	U1008	U1009	U1010	C1011	G1015	A1016	U1017	G1018	U1023	G945	G951	G952	G953	G954	U957					
G1032	G1033	G1034	A1035	A1036	C1037	A1042	G1043	A1044	C1045	U1046	G1047	G1048	U1049	C1054	A1055	U1056	G1057	G1058	C1059	U1060	G1064	U1065	C1066	U1070	U1078	G1079	A1080	U1081	A1082	U1083	G1084	U1091	G1094	U1095	C1096	C1100	A1101	U1123	U1124	U1125	U1126	G1127	C1128	G1129	A1130	G1131	G1132	G1133	G1134		
U1135	G1136	C1137	G1138	A1139	G1142	G1143	A1144	A1145	A1146	A1151	A1152	A1157	C1158	U1159	G1160	C1161	G1166	A1167	U1168	A1176	G1177	U1178	A1179	A1180	G1181	U1182	G1183	A1184	G1193	U1194	A1197	G1198	A1201	U1202	U1205	G1206	C1207	A1208	U1211	U1212	A1213	C1214	G1215	A1216	C1217	G1221	G1222	C1223			
U1224	A1225	A1226	A1227	U1235	A1238	A1239	U1240	G1241	G1242	C1243	A1246	U1247	A1248	G1249	A1250	A1251	A1252	G1253	A1254	G1255	A1256	A1257	G1268	A1269	G1270	A1271	G1272	G1273	A1274	A1275	G1276	G1277	G1278	G1279	A1280	C1281	C1282	U1283	G1284	A1285	U1286	A1287	A1288	U1289	G1294	U1295	C1296	G1297	U1298	A1299	C1300
U1301	C1302	G1305	A1306	U1307	U1308	A1311	G1312	U1313	G1314	U1315	G1316	C1317	A1318	A1319	C1320	U1321	C1322	U1326	C1327	G1328	A1329	U1330	G1331	G1334	U1335	C1336	G1337	G1338	A1339	A1340	A1346	G1347	U1348	A1349	A1350	G1355	C1359	A1360	G1361	A1362	A1363	U1364	G1373	A1374	A1375	G1379	U1380	U1381	C1382		



- 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%



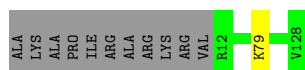
- Molecule 10: Small ribosomal subunit protein uS8

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%



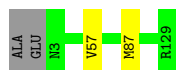
- Molecule 16: Small ribosomal subunit protein uS7

Chain m: 99%



- Molecule 17: Small ribosomal subunit protein uS9

Chain o: 97%



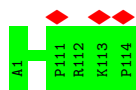
- Molecule 18: Small ribosomal subunit protein uS10

Chain r: 93%



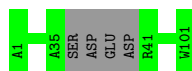
- Molecule 19: Small ribosomal subunit protein uS13

Chain s: 100%



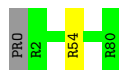
- Molecule 20: Small ribosomal subunit protein uS14

Chain w: 96%



- Molecule 21: Small ribosomal subunit protein uS19

Chain z: 98% ..



- Molecule 22: Small ribosomal subunit protein uS2

Chain j: 96% ..



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.

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
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

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.

The worst 5 of 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	n	38	ARG
11	q	79	LYS
22	j	104	LYS
16	m	130	LYS
21	z	54	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
21	z	56	HIS
21	z	51	HIS
11	q	37	GLN
9	n	63	ASN
11	q	39	ASN

5.3.3 RNA ⓘ

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

5 of 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

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.

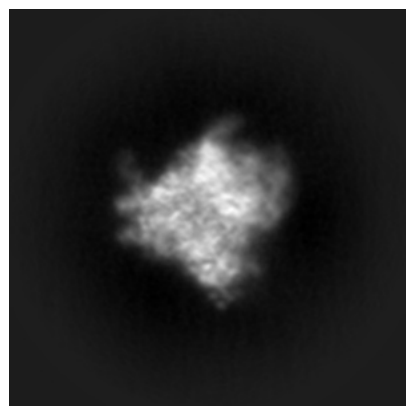
6 Map visualisation [i](#)

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.

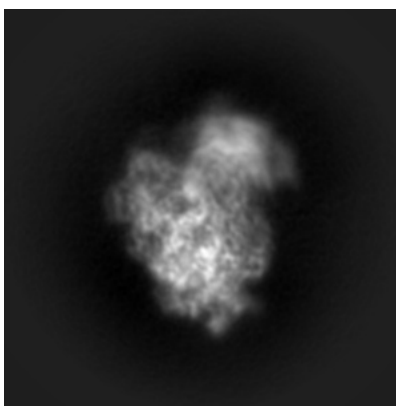
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

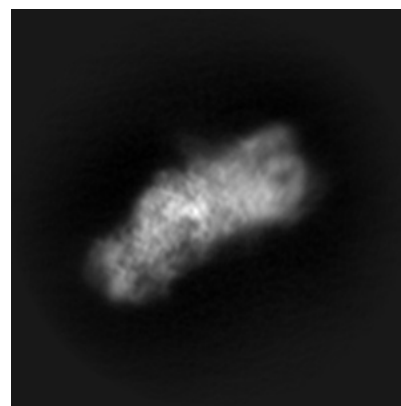
6.1.1 Primary map



X

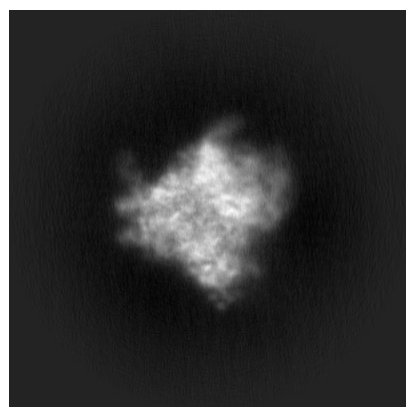


Y

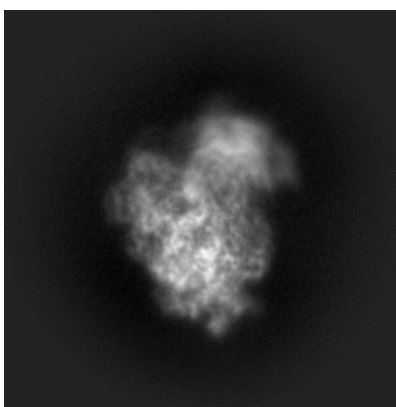


Z

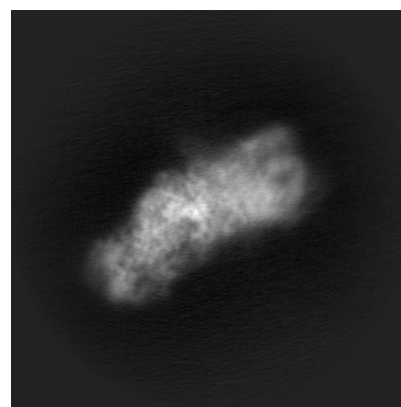
6.1.2 Raw map



X



Y

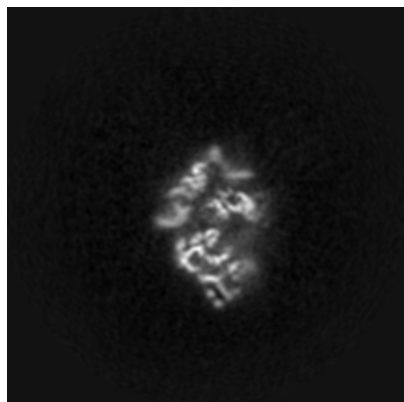


Z

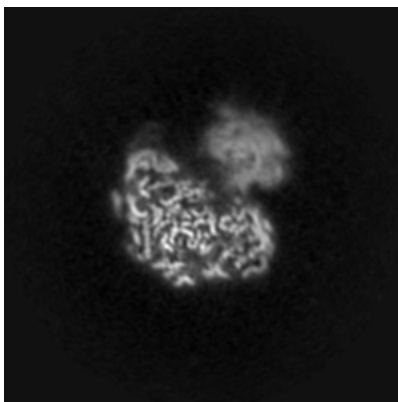
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

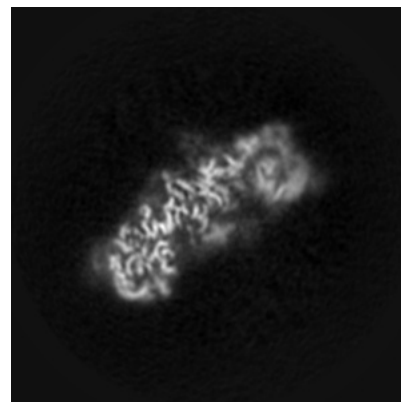
6.2.1 Primary map



X Index: 160



Y Index: 160

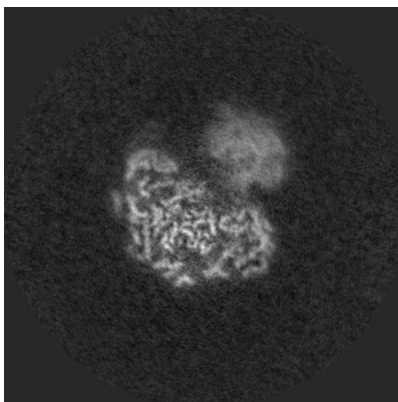


Z Index: 160

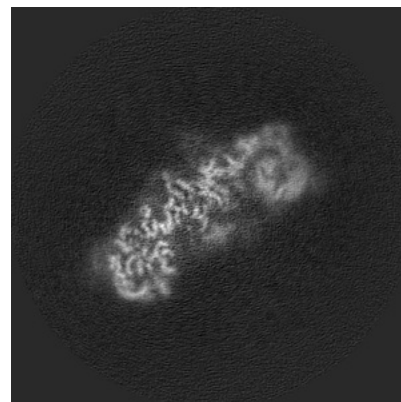
6.2.2 Raw map



X Index: 160



Y Index: 160

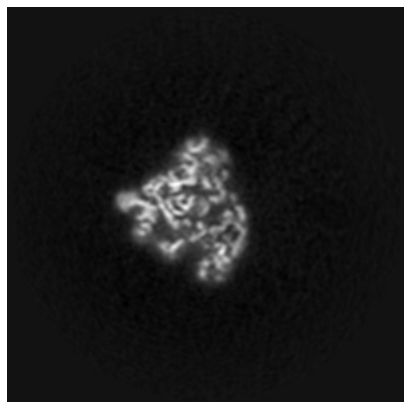


Z Index: 160

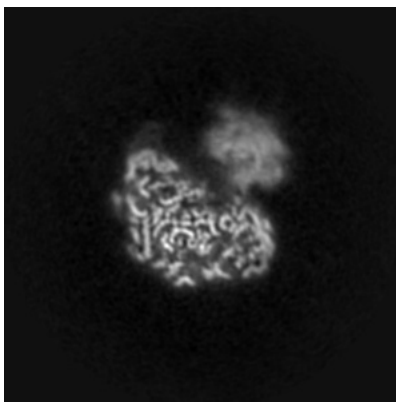
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

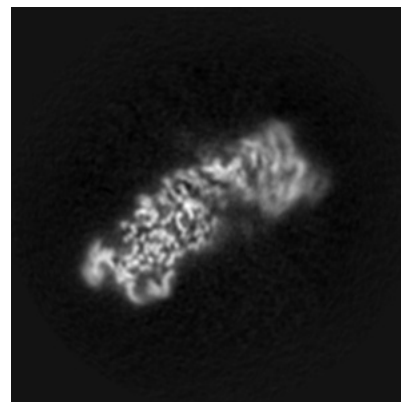
6.3.1 Primary map



X Index: 122

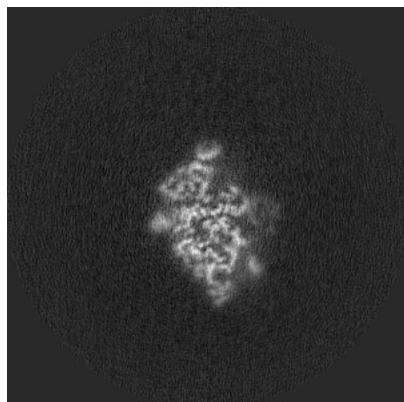


Y Index: 159

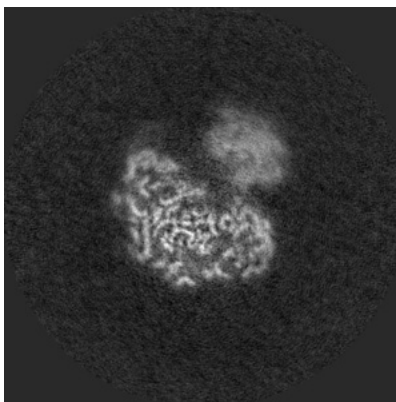


Z Index: 167

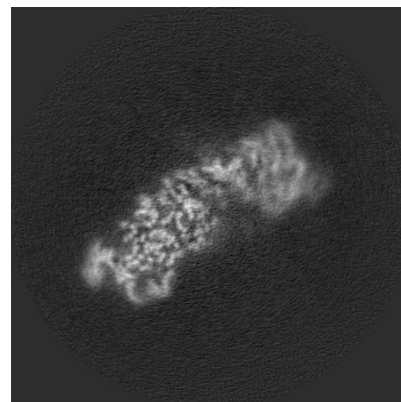
6.3.2 Raw map



X Index: 152



Y Index: 159

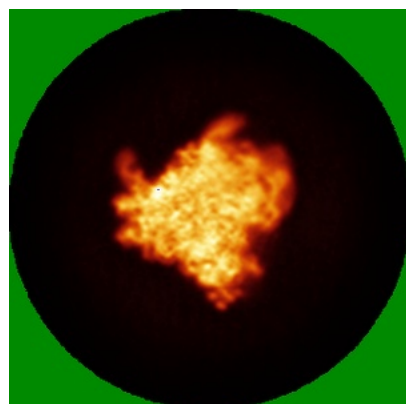


Z Index: 167

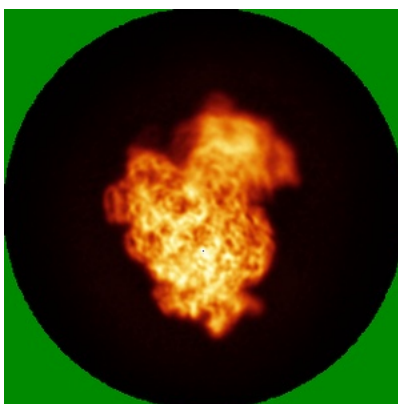
The images above show the largest variance slices of the map in three orthogonal directions.

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

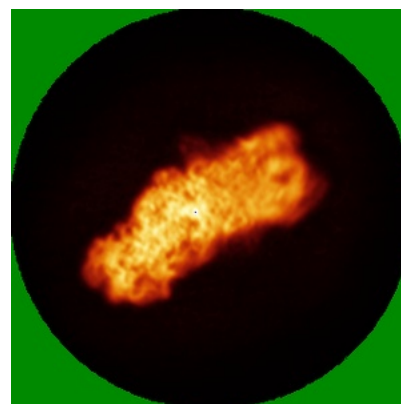
6.4.1 Primary map



X

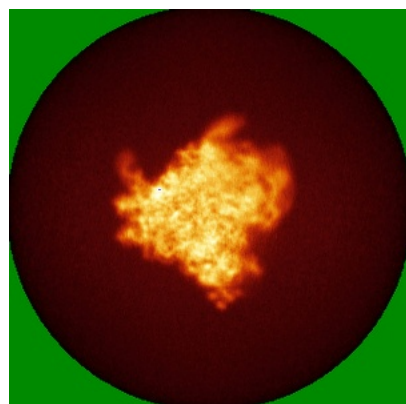


Y

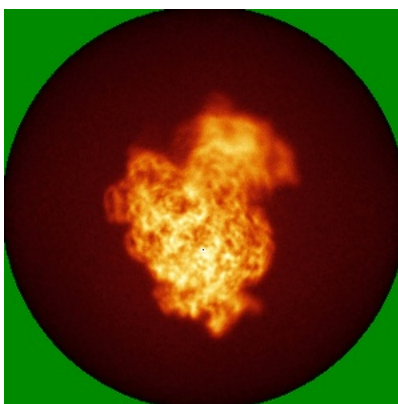


Z

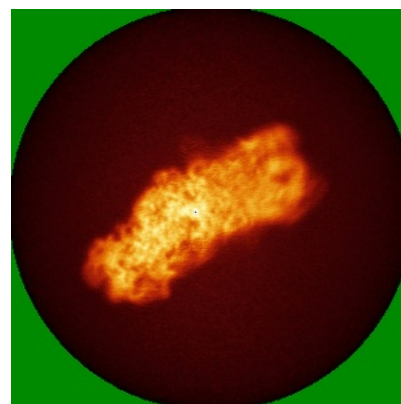
6.4.2 Raw map



X



Y



Z

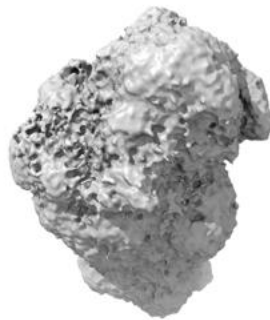
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



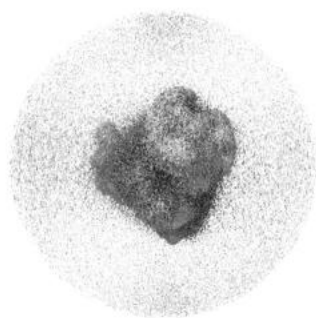
Y



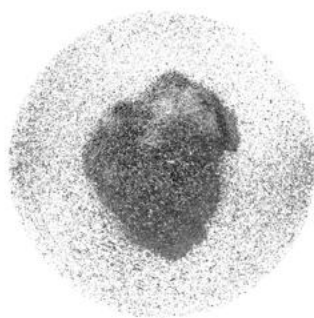
Z

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.

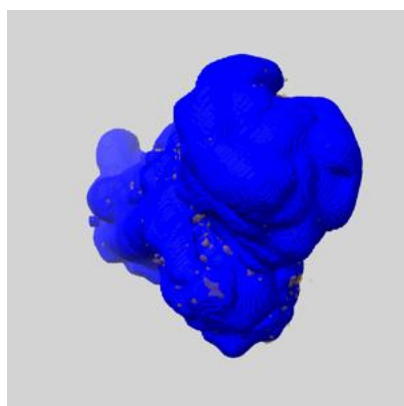
6.6 Mask visualisation [i](#)

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

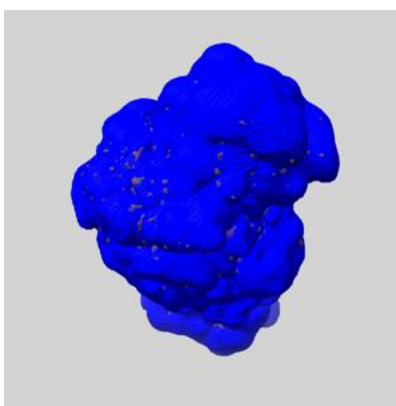
A mask typically either:

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

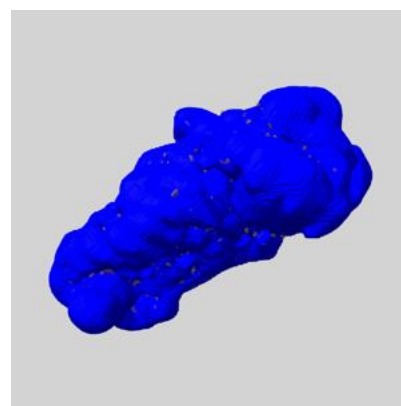
6.6.1 emd_36619_msk_1.map [i](#)



X



Y

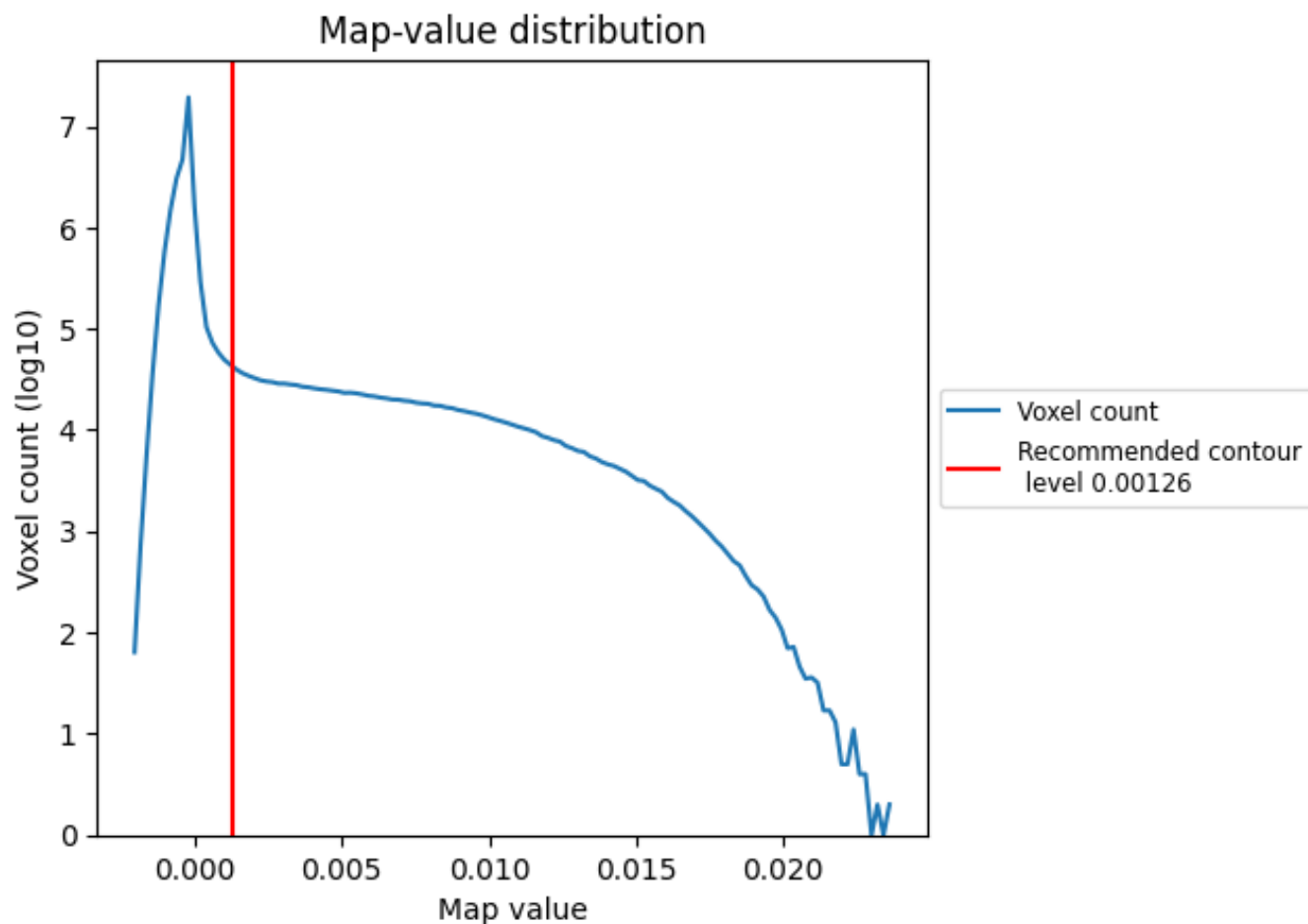


Z

7 Map analysis [i](#)

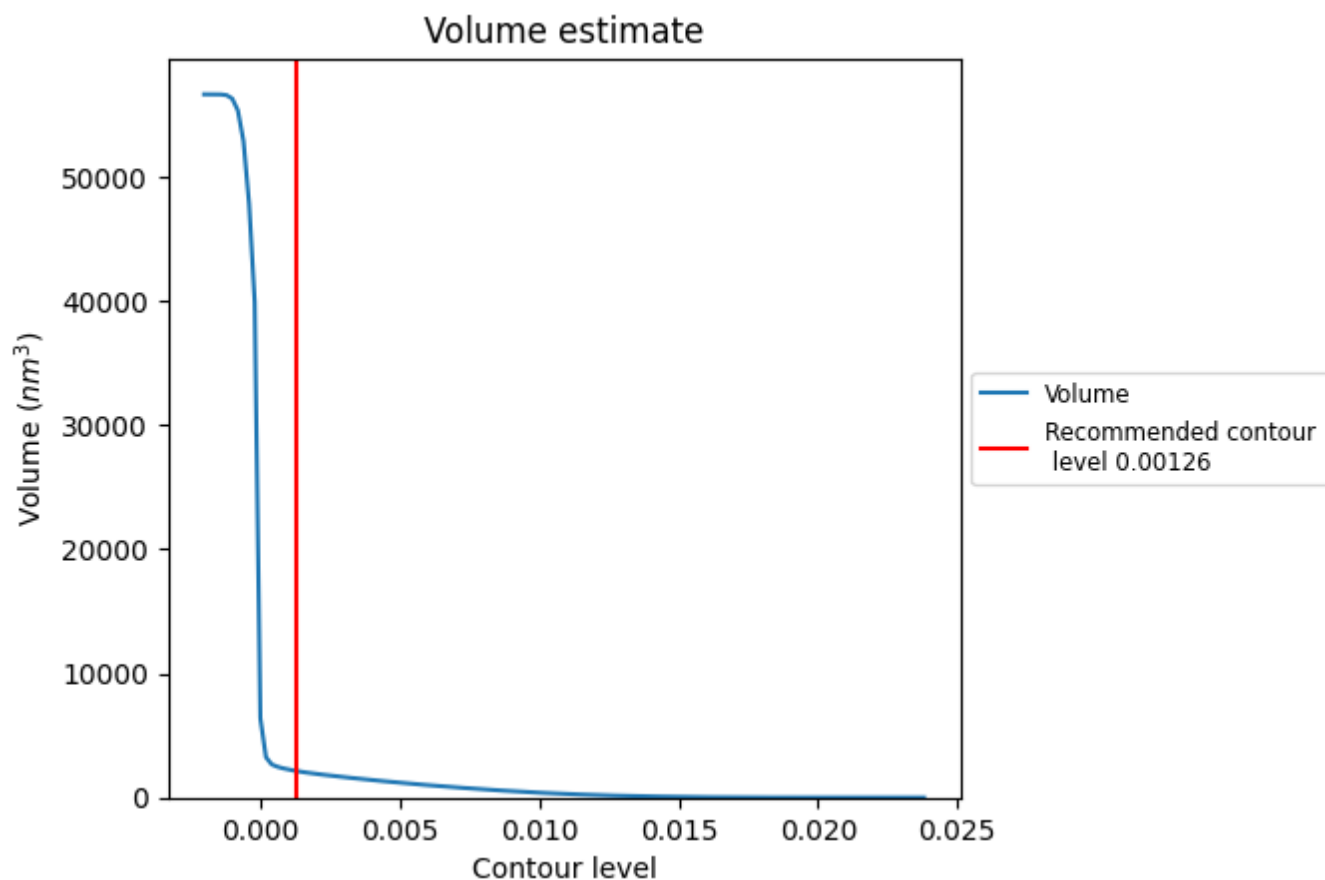
This section contains the results of statistical analysis of the map.

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.

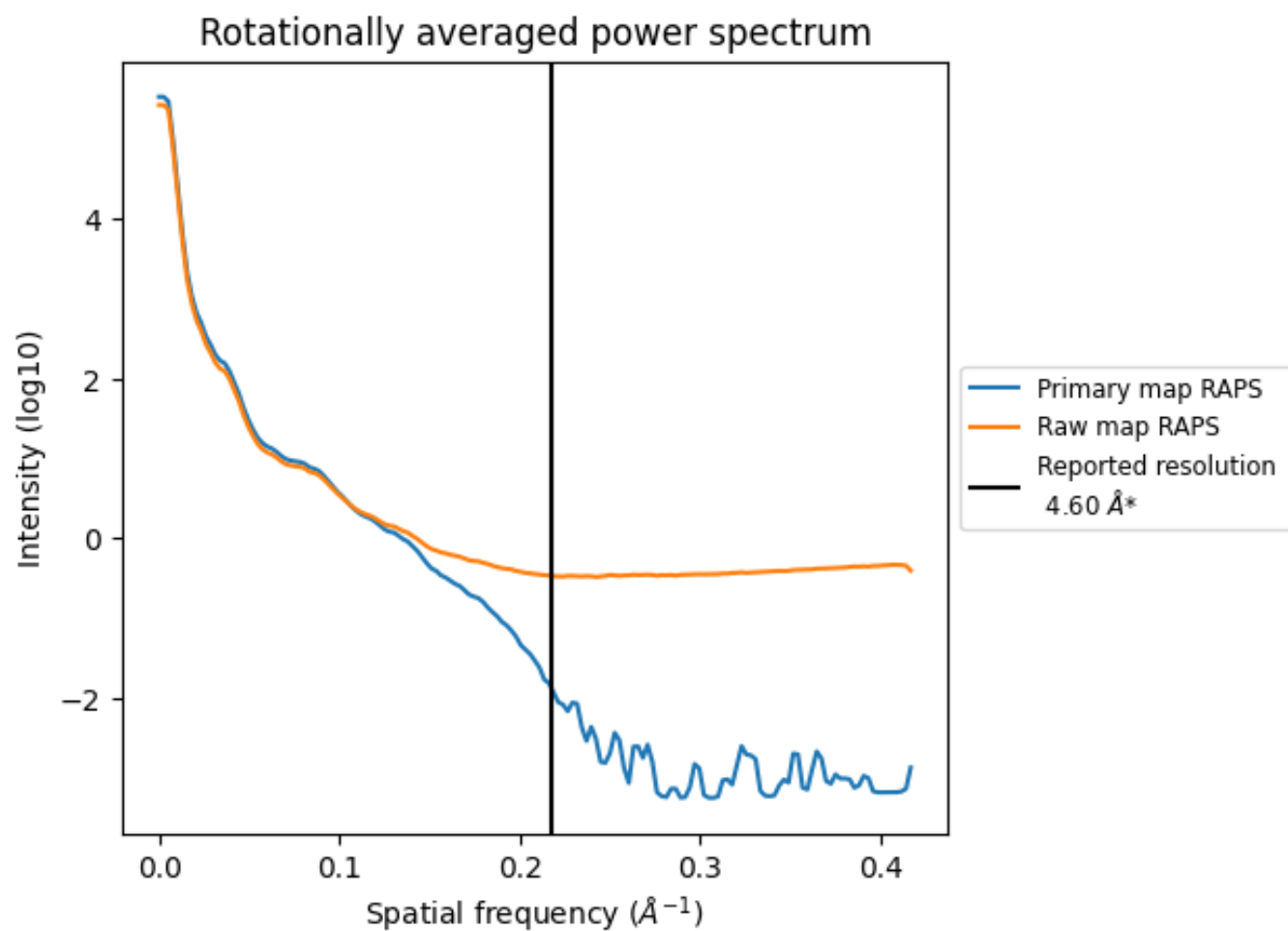
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2144 nm^3 ; 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](#)

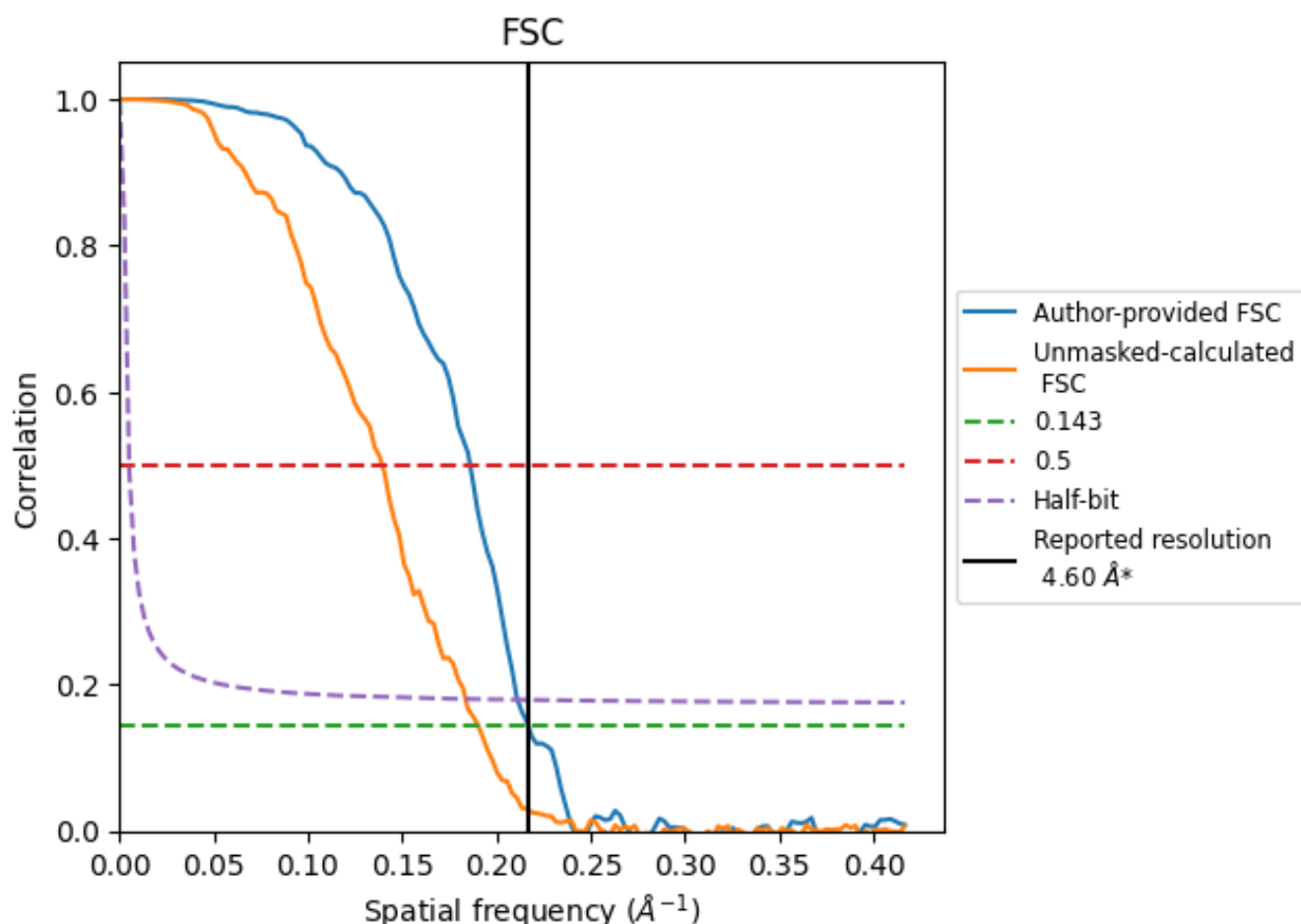


*Reported resolution corresponds to spatial frequency of 0.217 \AA^{-1}

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 \AA^{-1}

8.2 Resolution estimates [i](#)

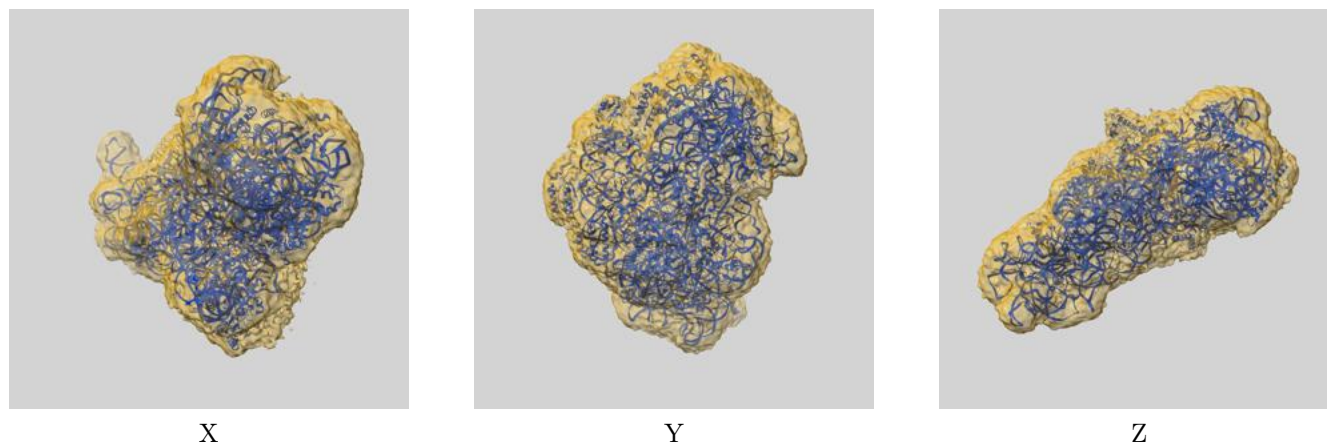
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.61	5.38	4.73
Unmasked-calculated*	5.25	7.17	5.44

*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](#)

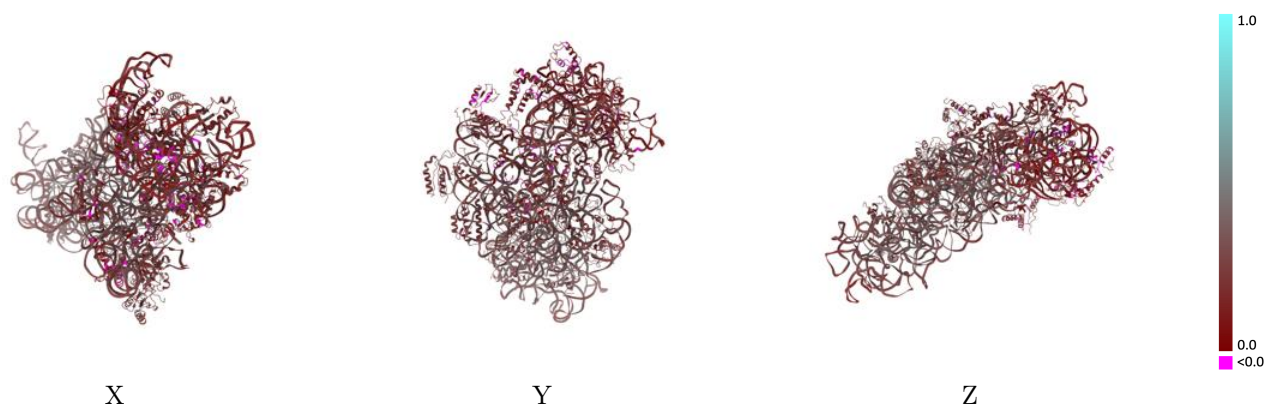
This section contains information regarding the fit between EMDB map EMD-36619 and PDB model 8JSG. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



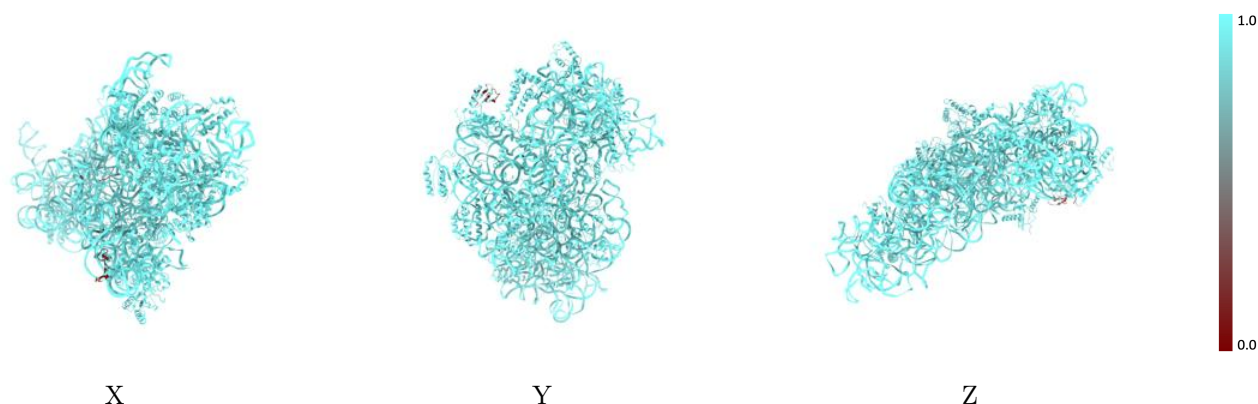
The images above show the 3D surface view of the map at the recommended contour level 0.00126 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



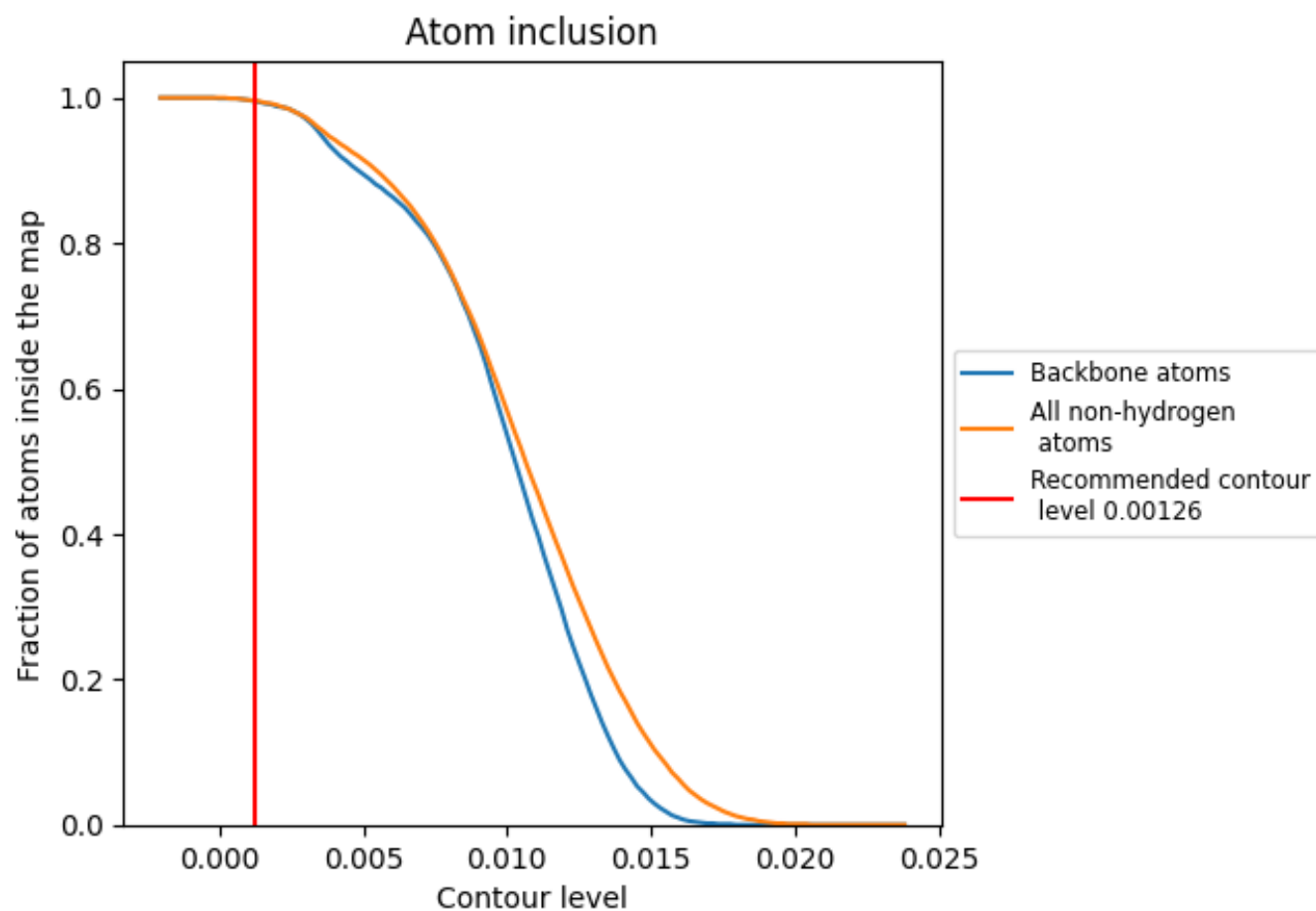
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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















































9.4 Atom inclusion ⓘ



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

