wwPDB EM Validation Summary Report

Apr 23, 2024 – 12:55 pm BST

PDB ID	:	6ZVH
EMDB ID	:	EMD-11456
Title	:	EDF1-ribosome complex
Authors	:	Best, K.M.; Denk, T.; Cheng, J.; Thoms, M.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2020-07-24
Resolution	:	2.90 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:

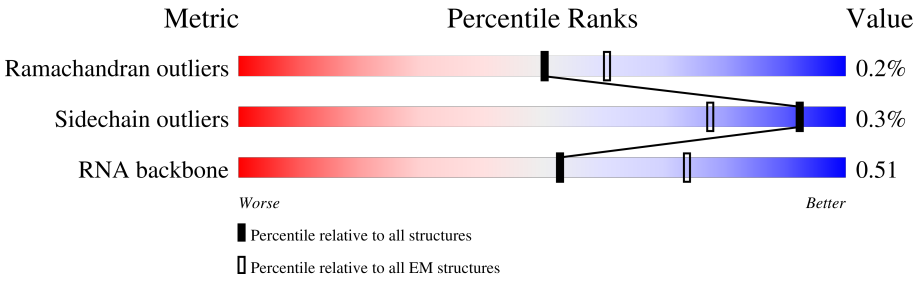
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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)
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	2	1740	9% 76% 23%
2	A	221	10% 99%
3	B	264	81% 19%
4	D	227	11% 99%
5	E	262	100%
6	F	189	96%
7	H	189	33% 97%
8	I	206	12% 99%

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Mol	Chain	Length	Quality of chain
9	K	98	8% 99%
10	L	153	10% 99%
11	P	129	16% 98%
12	Q	144	6% 98%
13	R	135	21% 99%
14	S	145	10% 99%
15	T	143	8% 98%
16	U	104	25% 98%
17	V	83	8% 99%
18	X	141	97%
19	a	102	6% 98%
20	c	64	12% 100%
21	d	55	96%
22	g	313	35% 99%
23	C	222	100%
24	G	237	19% 99%
25	J	185	6% 98%
26	M	122	84% 98%
27	N	150	99%
28	O	140	8% 99%
29	W	129	99%
30	Y	131	15% 98%
31	Z	75	23% 97%
32	b	83	17% 99%
33	e	42	7% 100%

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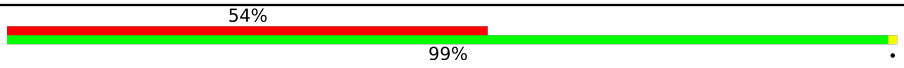
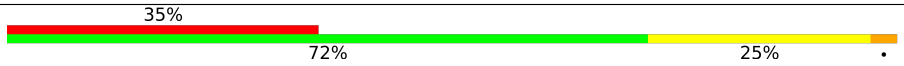
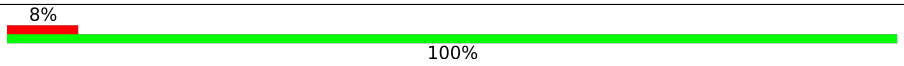
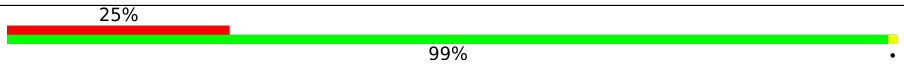
Mol	Chain	Length	Quality of chain
34	f	67	
35	x	75	
36	y	72	
37	i	110	

2 Entry composition (i)

There are 39 unique types of molecules in this entry. The entry contains 79014 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 RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1740	36896	16458	6597	12102	1739	0	0

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	221	1741	1106	305	322	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	214	1738	1103	310	311	14	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	227	1765	1125	317	315	8	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	262	2076	1324	386	358	8	0	0

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	184	1461	914	276	264	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 9 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 11 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	129	Total	C	N	O	S	0	0
			1061	672	202	180	7		

- Molecule 12 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 13 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 14 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 15 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 16 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 17 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	V	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 18 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 19 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 20 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 21 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	d	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 22 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 23 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	C	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 24 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	G	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 25 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	J	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	122	Total	C	N	O	S	0	0
			942	590	165	179	8		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	52	GLN	LEU	conflict	UNP P25398
M	69	LEU	CYS	conflict	UNP P25398
M	99	ASN	LYS	conflict	UNP P25398

- Molecule 27 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 28 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	140	Total	C	N	O	S	0	0
			1049	642	204	197	6		

- Molecule 29 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 32 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 33 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	42	Total	C	N	O	S	0	0
			342	211	78	52	1		

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 35 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	x	75	Total	C	N	O	P	0	0
			1589	710	279	525	75		

- Molecule 36 is a protein called Cell growth-regulating nucleolar protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	y	72	Total	C	N	O	0	0
			603	395	105	103		

- Molecule 37 is a protein called Endothelial differentiation-related factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	i	110	Total	C	N	O	0	0
			865	530	169	166		

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	2	28	Total	Mg	0
			28	28	
38	G	1	Total	Mg	0
			1	1	
38	O	1	Total	Mg	0
			1	1	

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

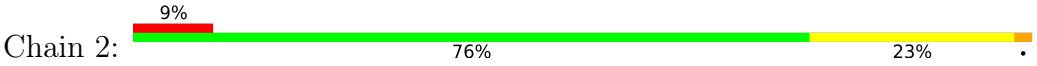
Mol	Chain	Residues	Atoms		AltConf
39	a	1	Total	Zn	0
			1	1	
39	d	1	Total	Zn	0
			1	1	
39	f	1	Total	Zn	0
			1	1	

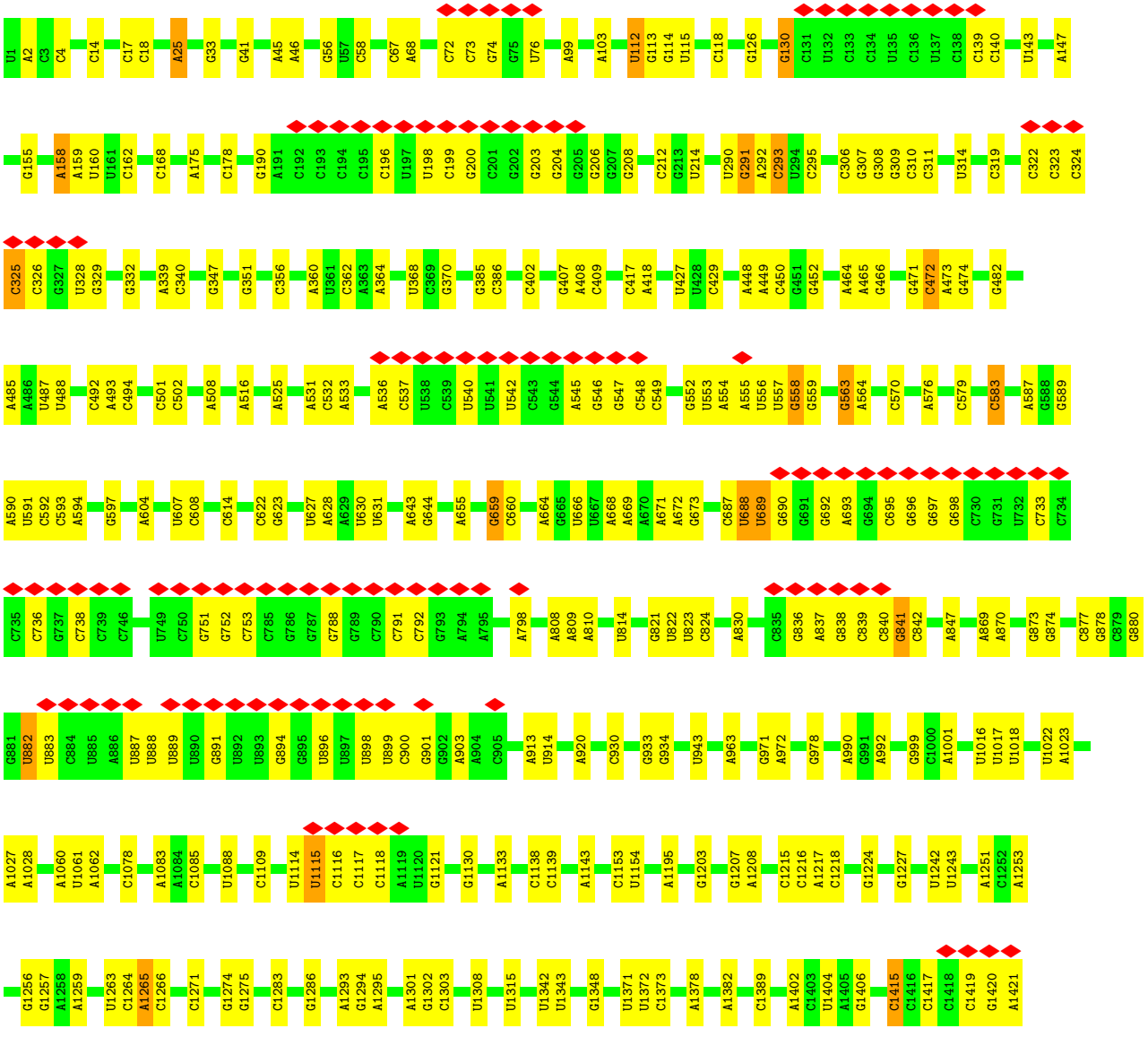
3 Residue-property plots (i)

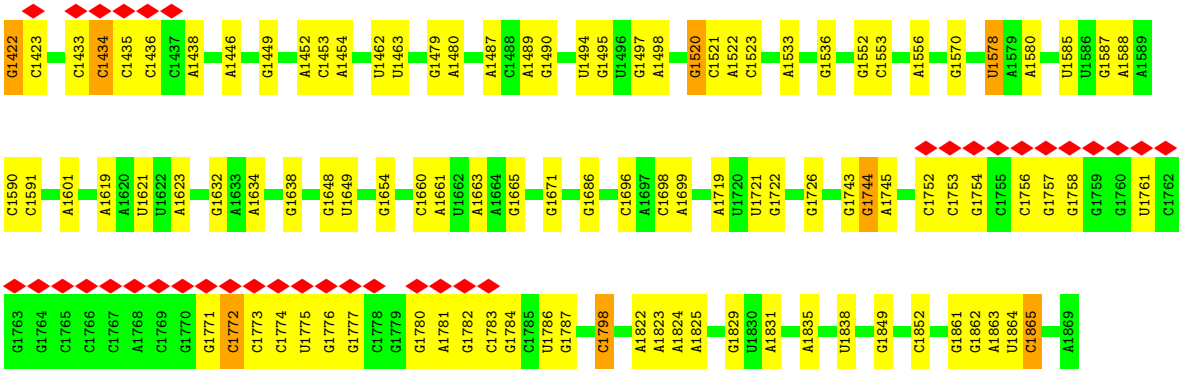
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 18S rRNA

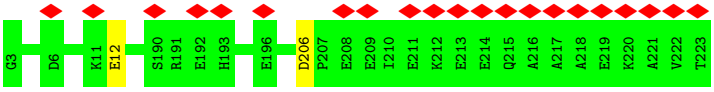
Chain 2:



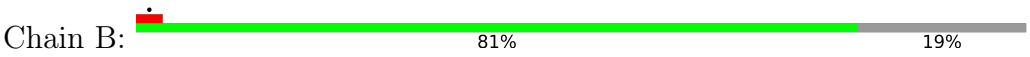


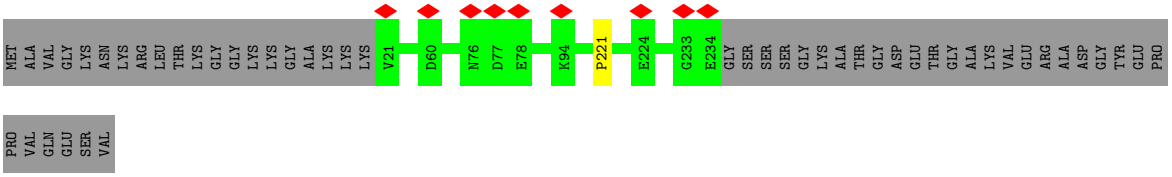


• Molecule 2: 40S ribosomal protein SA

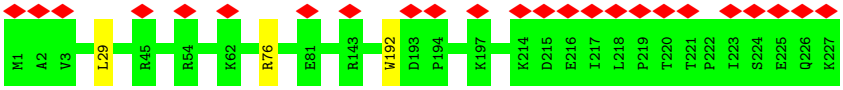


• Molecule 3: 40S ribosomal protein S3a

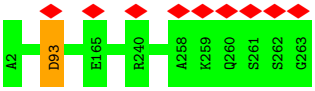




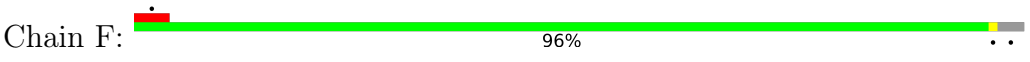
• Molecule 4: 40S ribosomal protein S3

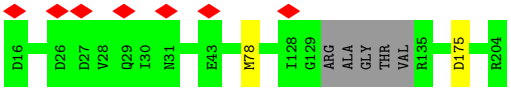


• Molecule 5: 40S ribosomal protein S4, X isoform

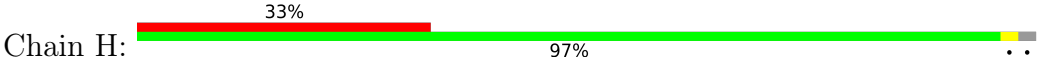


• Molecule 6: 40S ribosomal protein S5

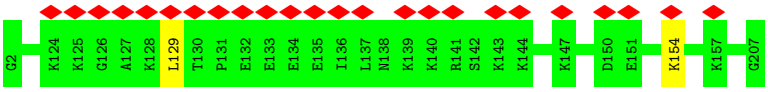




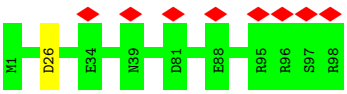
• Molecule 7: 40S ribosomal protein S7



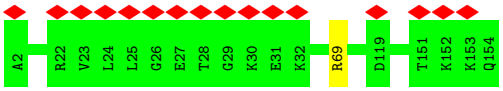
• Molecule 8: 40S ribosomal protein S8



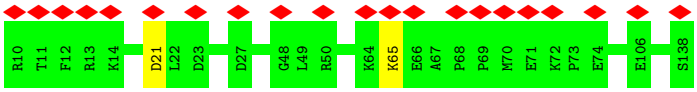
• Molecule 9: 40S ribosomal protein S10



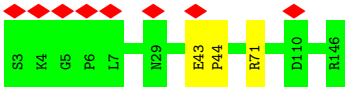
• Molecule 10: 40S ribosomal protein S11



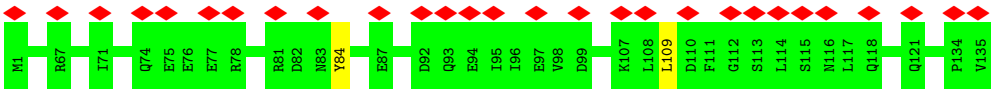
• Molecule 11: 40S ribosomal protein S15



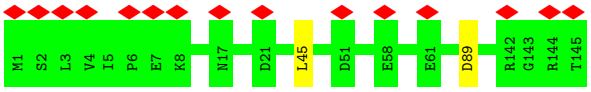
• Molecule 12: 40S ribosomal protein S16



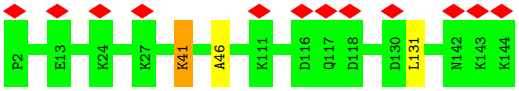
• Molecule 13: 40S ribosomal protein S17



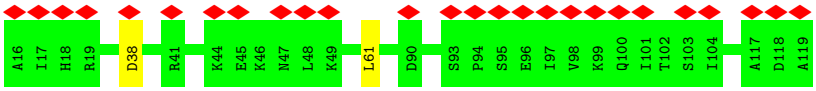
• Molecule 14: 40S ribosomal protein S18



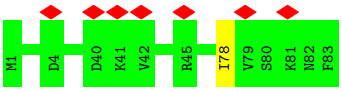
• Molecule 15: 40S ribosomal protein S19



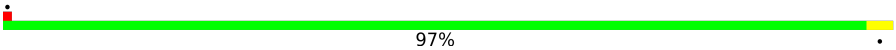
• Molecule 16: 40S ribosomal protein S20



• Molecule 17: 40S ribosomal protein S21

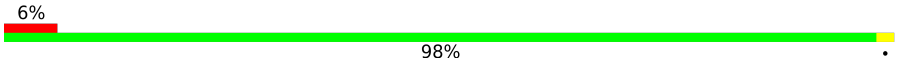


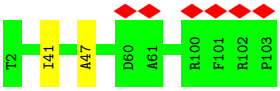
• Molecule 18: 40S ribosomal protein S23



• Molecule 19: 40S ribosomal protein S26

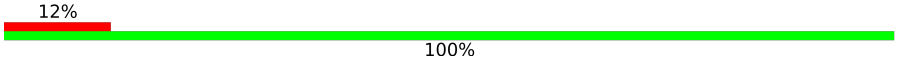
Chain a:

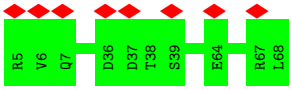




• Molecule 20: 40S ribosomal protein S28

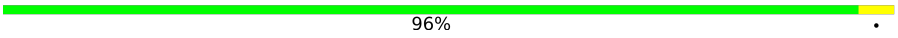
Chain c:





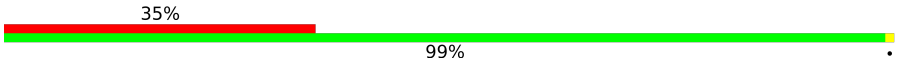
• Molecule 21: 40S ribosomal protein S29

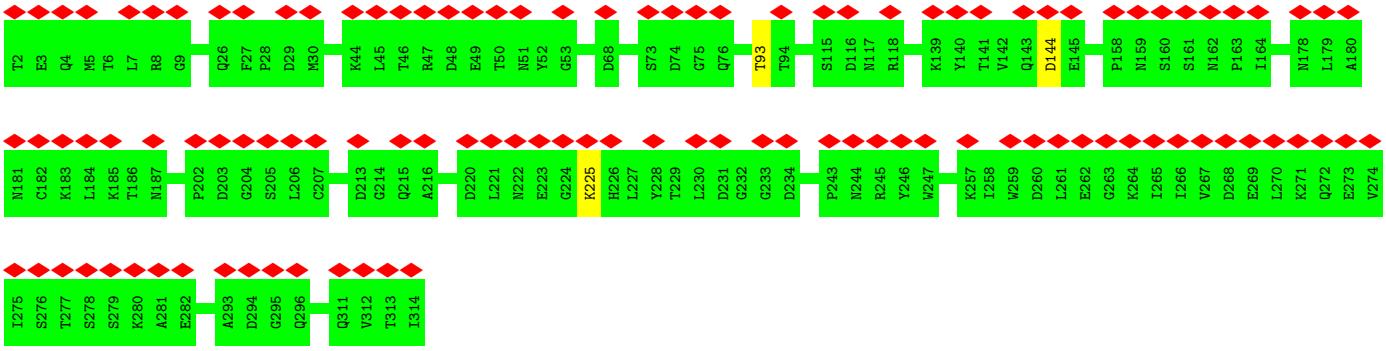
Chain d:



• Molecule 22: Receptor of activated protein C kinase 1

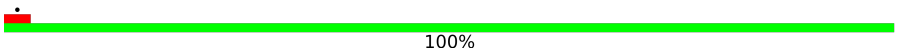
Chain g:

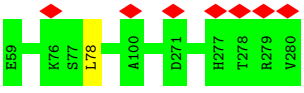




• Molecule 23: 40S ribosomal protein S2

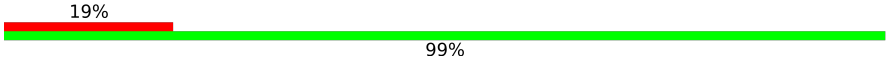
Chain C:

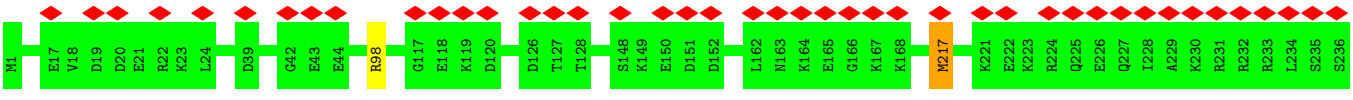




• Molecule 24: 40S ribosomal protein S6

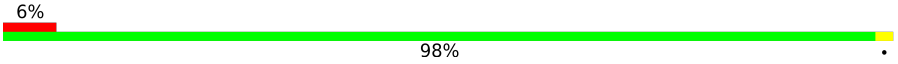
Chain G:

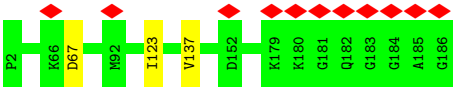




• Molecule 25: 40S ribosomal protein S9

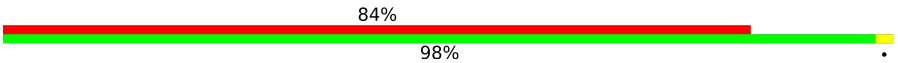
Chain J:

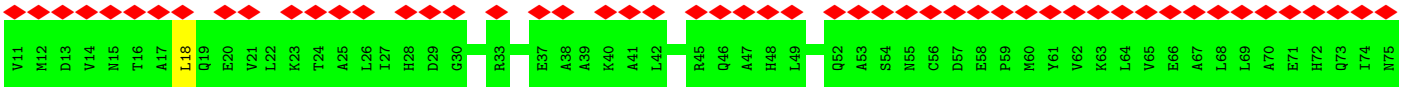


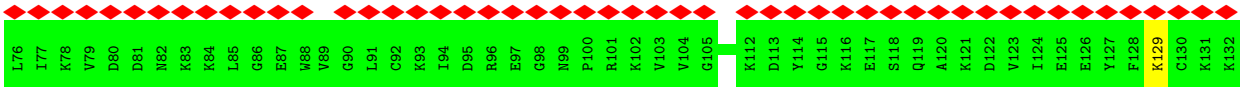


• Molecule 26: 40S ribosomal protein S12

Chain M:

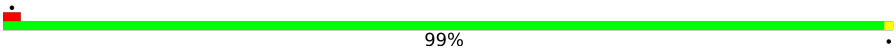


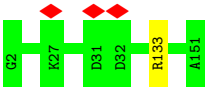




• Molecule 27: 40S ribosomal protein S13

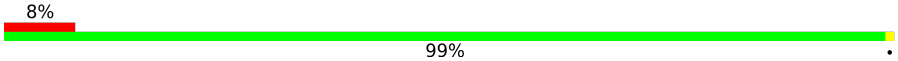
Chain N:

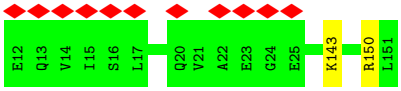




• Molecule 28: 40S ribosomal protein S14

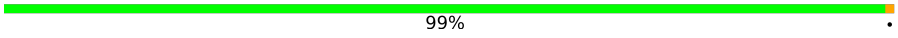
Chain O:





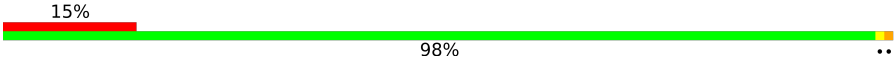
• Molecule 29: 40S ribosomal protein S15a

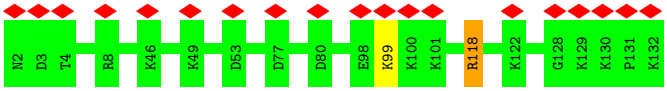
Chain W:



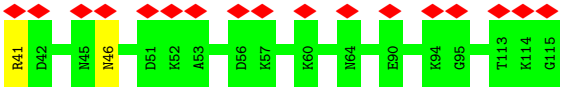
• Molecule 30: 40S ribosomal protein S24

Chain Y:

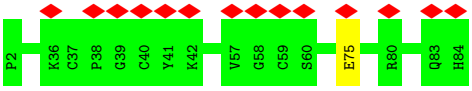




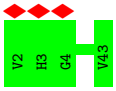
• Molecule 31: 40S ribosomal protein S25



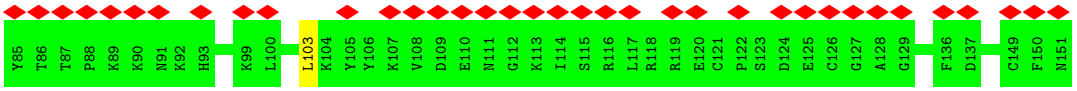
• Molecule 32: 40S ribosomal protein S27



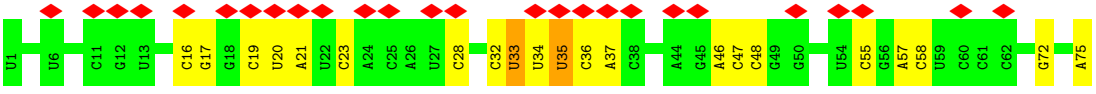
• Molecule 33: 40S ribosomal protein S30



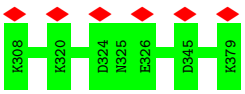
• Molecule 34: Ubiquitin-40S ribosomal protein S27a



• Molecule 35: E-site tRNA

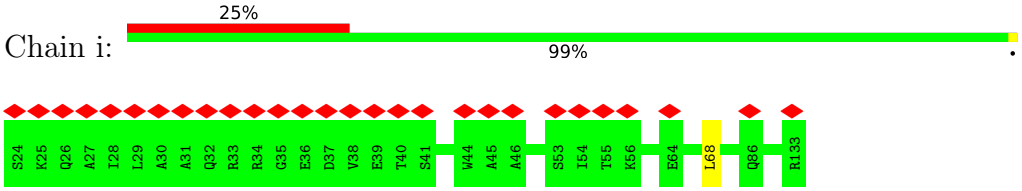


• Molecule 36: Cell growth-regulating nucleolar protein



• Molecule 37: Endothelial differentiation-related factor 1

Chain i:


25%
99%
S24
K25
Q26
A27
I28
L29
A30
A31
Q32
R33
R34
G35
E36
D37
V38
E39
T40
S41
W44
A45
A46
S53
I54
T55
K56
E64
L68
Q86
R133

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81976	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 ($e^-/Å^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.332	Depositor
Minimum map value	-0.064	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	2	0.94	3/41241 (0.0%)	1.04	158/64258 (0.2%)
2	A	0.45	0/1778	0.62	1/2416 (0.0%)
3	B	0.43	0/1765	0.52	0/2362
4	D	0.43	0/1793	0.64	1/2414 (0.0%)
5	E	0.43	0/2118	0.59	1/2849 (0.0%)
6	F	0.43	0/1481	0.62	1/1988 (0.1%)
7	H	0.38	0/1519	0.63	0/2033
8	I	0.44	0/1715	0.59	1/2287 (0.0%)
9	K	0.45	0/851	0.64	1/1147 (0.1%)
10	L	0.50	0/1268	0.60	0/1696
11	P	0.43	0/1082	0.65	1/1446 (0.1%)
12	Q	0.44	0/1160	0.68	0/1553
13	R	0.39	0/1105	0.63	1/1484 (0.1%)
14	S	0.40	0/1216	0.65	2/1628 (0.1%)
15	T	0.42	0/1131	0.64	1/1515 (0.1%)
16	U	0.39	0/831	0.66	1/1115 (0.1%)
17	V	0.45	0/643	0.64	0/860
18	X	0.47	0/1116	0.61	0/1490
19	a	0.46	0/836	0.61	1/1121 (0.1%)
20	c	0.42	0/508	0.70	0/680
21	d	0.50	0/470	0.67	1/623 (0.2%)
22	g	0.37	0/2493	0.63	2/3394 (0.1%)
23	C	0.50	0/1762	0.62	0/2381
24	G	0.37	0/1946	0.58	1/2590 (0.0%)
25	J	0.43	0/1550	0.57	1/2069 (0.0%)
26	M	0.33	0/952	0.69	1/1279 (0.1%)
27	N	0.46	0/1232	0.54	0/1656
28	O	0.42	0/1062	0.63	0/1425
29	W	0.48	0/1051	0.60	1/1406 (0.1%)
30	Y	0.43	0/1083	0.57	0/1438
31	Z	0.34	0/604	0.59	0/810
32	b	0.40	0/665	0.58	0/891

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.39	0/345	0.53	0/451
34	f	0.38	0/560	0.72	1/745 (0.1%)
35	x	0.32	0/1773	0.96	6/2759 (0.2%)
36	y	0.33	0/613	0.52	0/819
37	i	0.32	0/872	0.55	1/1167 (0.1%)
All	All	0.72	3/84190 (0.0%)	0.87	186/122245 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	1
4	D	0	1
6	F	0	1
7	H	0	2
12	Q	0	1
13	R	0	1
15	T	0	1
16	U	0	1
17	V	0	1
18	X	0	3
24	G	0	1
25	J	0	1
28	O	0	1
29	W	0	1
30	Y	0	1
31	Z	0	1
32	b	0	1
All	All	0	20

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1422	G	C6-N1	-6.96	1.34	1.39
1	2	1422	G	C6-O6	-5.24	1.19	1.24
1	2	1417	C	N3-C4	-5.09	1.30	1.33

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1417	C	N3-C4-N4	-29.59	97.29	118.00
1	2	1422	G	N1-C6-O6	-28.04	103.08	119.90
1	2	1417	C	C5-C4-N4	23.82	136.87	120.20
1	2	1422	G	C5-C6-O6	22.55	142.13	128.60
1	2	501	C	N1-C2-O2	14.35	127.51	118.90

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	221	PRO	Peptide
4	D	192	TRP	Peptide
6	F	78	MET	Peptide
7	H	15	LYS	Peptide
7	H	29	GLU	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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
2	A	219/221 (99%)	206 (94%)	12 (6%)	1 (0%)	29 61
3	B	212/264 (80%)	205 (97%)	7 (3%)	0	100 100
4	D	225/227 (99%)	209 (93%)	16 (7%)	0	100 100
5	E	260/262 (99%)	252 (97%)	7 (3%)	1 (0%)	34 66
6	F	180/189 (95%)	171 (95%)	9 (5%)	0	100 100
7	H	182/189 (96%)	171 (94%)	11 (6%)	0	100 100
8	I	204/206 (99%)	199 (98%)	5 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	K	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
10	L	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
11	P	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
12	Q	142/144 (99%)	129 (91%)	12 (8%)	1 (1%)	22	54
13	R	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
14	S	143/145 (99%)	137 (96%)	6 (4%)	0	100	100
15	T	141/143 (99%)	135 (96%)	5 (4%)	1 (1%)	22	54
16	U	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
17	V	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
18	X	139/141 (99%)	131 (94%)	7 (5%)	1 (1%)	22	54
19	a	100/102 (98%)	94 (94%)	5 (5%)	1 (1%)	15	45
20	c	62/64 (97%)	54 (87%)	8 (13%)	0	100	100
21	d	53/55 (96%)	51 (96%)	1 (2%)	1 (2%)	8	28
22	g	311/313 (99%)	292 (94%)	19 (6%)	0	100	100
23	C	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	29	61
24	G	235/237 (99%)	227 (97%)	8 (3%)	0	100	100
25	J	183/185 (99%)	176 (96%)	6 (3%)	1 (0%)	29	61
26	M	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
27	N	148/150 (99%)	148 (100%)	0	0	100	100
28	O	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
29	W	127/129 (98%)	122 (96%)	5 (4%)	0	100	100
30	Y	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
31	Z	73/75 (97%)	64 (88%)	9 (12%)	0	100	100
32	b	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
33	e	40/42 (95%)	40 (100%)	0	0	100	100
34	f	65/67 (97%)	58 (89%)	7 (11%)	0	100	100
36	y	70/72 (97%)	68 (97%)	2 (3%)	0	100	100
37	i	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
All	All	5000/5132 (97%)	4747 (95%)	244 (5%)	9 (0%)	50	78

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	X	127	ASN
23	C	78	LEU
15	T	41	LYS
25	J	123	ILE
2	A	12	GLU

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
2	A	183/183 (100%)	183 (100%)	0	100 100
3	B	195/231 (84%)	195 (100%)	0	100 100
4	D	190/190 (100%)	189 (100%)	1 (0%)	88 96
5	E	224/224 (100%)	224 (100%)	0	100 100
6	F	156/159 (98%)	156 (100%)	0	100 100
7	H	166/169 (98%)	165 (99%)	1 (1%)	86 96
8	I	178/178 (100%)	177 (99%)	1 (1%)	86 96
9	K	89/89 (100%)	89 (100%)	0	100 100
10	L	137/137 (100%)	136 (99%)	1 (1%)	84 95
11	P	115/115 (100%)	114 (99%)	1 (1%)	78 93
12	Q	119/119 (100%)	118 (99%)	1 (1%)	81 94
13	R	122/122 (100%)	122 (100%)	0	100 100
14	S	126/126 (100%)	126 (100%)	0	100 100
15	T	113/113 (100%)	112 (99%)	1 (1%)	78 93
16	U	94/94 (100%)	94 (100%)	0	100 100
17	V	67/67 (100%)	67 (100%)	0	100 100
18	X	113/113 (100%)	113 (100%)	0	100 100
19	a	89/89 (100%)	89 (100%)	0	100 100
20	c	57/57 (100%)	57 (100%)	0	100 100
21	d	48/48 (100%)	48 (100%)	0	100 100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
22	g	272/272 (100%)	271 (100%)	1 (0%)	91 97
23	C	188/188 (100%)	188 (100%)	0	100 100
24	G	207/207 (100%)	206 (100%)	1 (0%)	88 96
25	J	161/161 (100%)	161 (100%)	0	100 100
26	M	102/104 (98%)	101 (99%)	1 (1%)	76 92
27	N	130/130 (100%)	129 (99%)	1 (1%)	81 94
28	O	110/110 (100%)	109 (99%)	1 (1%)	78 93
29	W	112/112 (100%)	112 (100%)	0	100 100
30	Y	113/113 (100%)	111 (98%)	2 (2%)	59 85
31	Z	66/66 (100%)	65 (98%)	1 (2%)	65 87
32	b	75/75 (100%)	75 (100%)	0	100 100
33	e	34/34 (100%)	34 (100%)	0	100 100
34	f	60/60 (100%)	60 (100%)	0	100 100
36	y	68/68 (100%)	68 (100%)	0	100 100
37	i	92/92 (100%)	92 (100%)	0	100 100
All	All	4371/4415 (99%)	4356 (100%)	15 (0%)	92 98

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	g	225	LYS
30	Y	118	ARG
24	G	98	ARG
31	Z	41	ARG
28	O	150	ARG

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

Mol	Chain	Res	Type
9	K	7	ASN
12	Q	97	GLN
16	U	100	GLN
26	M	52	GLN
36	y	321	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1717/1740 (98%)	377 (21%)	11 (0%)
35	x	74/75 (98%)	20 (27%)	0
All	All	1791/1815 (98%)	397 (22%)	11 (0%)

5 of 397 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	17	C
1	2	25	A
1	2	33	G
1	2	41	G

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	688	U
1	2	1265	A
1	2	1520	G
1	2	1434	C
1	2	552	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 33 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	753:C	O3'	785:C	P	30.20
1	2	698:G	O3'	730:C	P	15.36
1	2	739:C	O3'	746:C	P	12.19
1	2	225:G	O3'	287:U	P	7.08

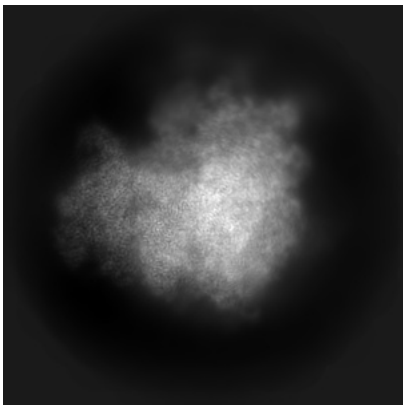
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11456. These allow visual inspection of the internal detail of the map and identification of artifacts.

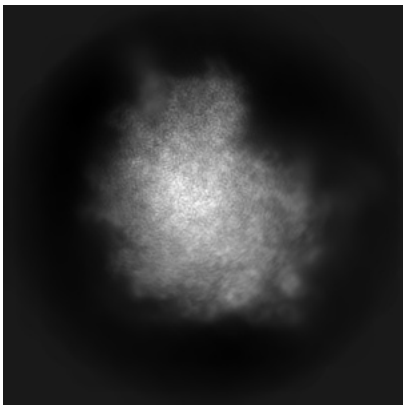
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

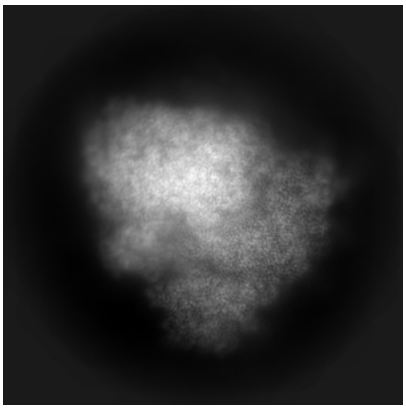
6.1.1 Primary map



X

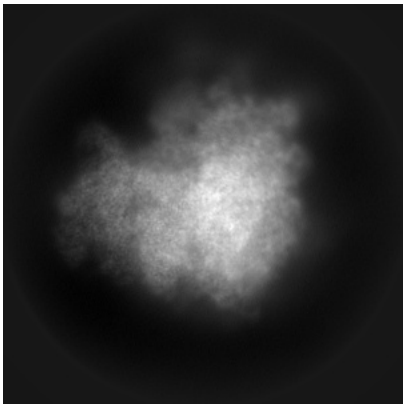


Y

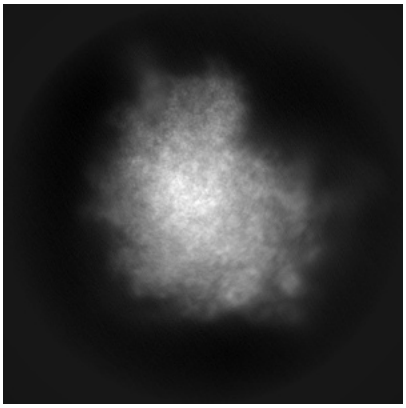


Z

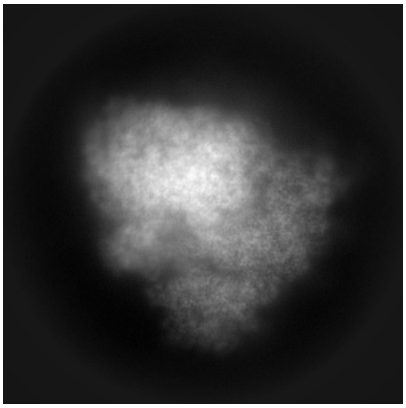
6.1.2 Raw map



X



Y

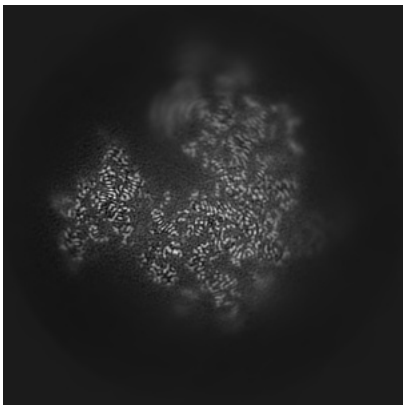


Z

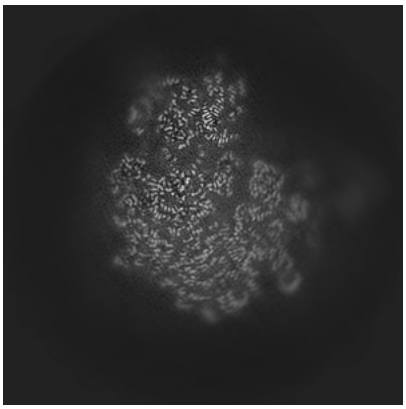
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

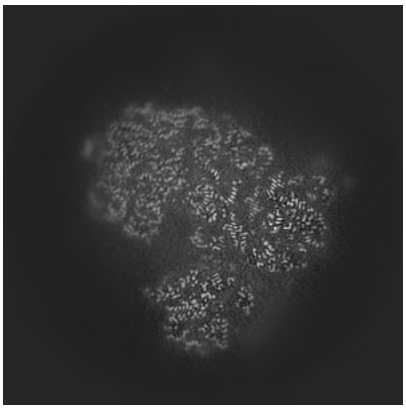
6.2.1 Primary map



X Index: 200

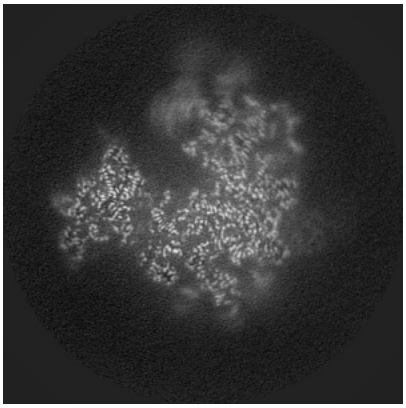


Y Index: 200

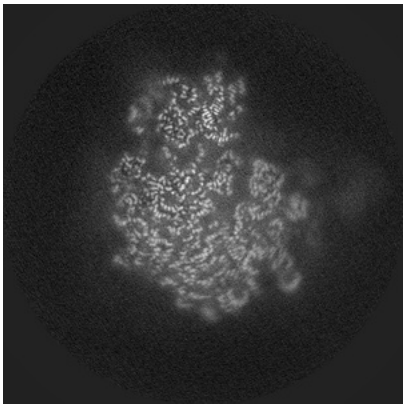


Z Index: 200

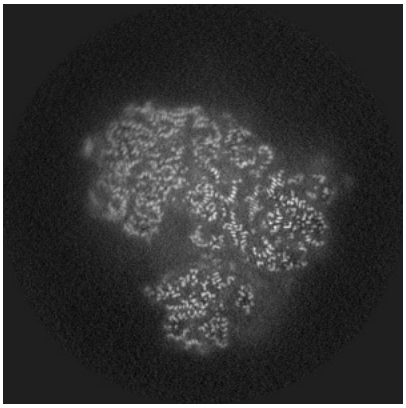
6.2.2 Raw map



X Index: 200



Y Index: 200

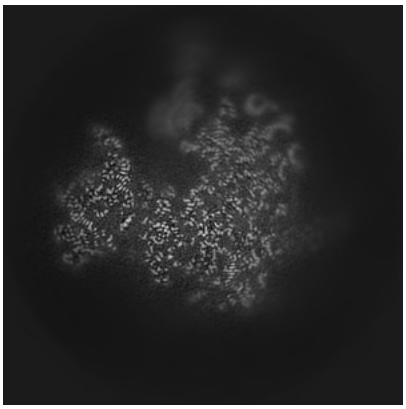


Z Index: 200

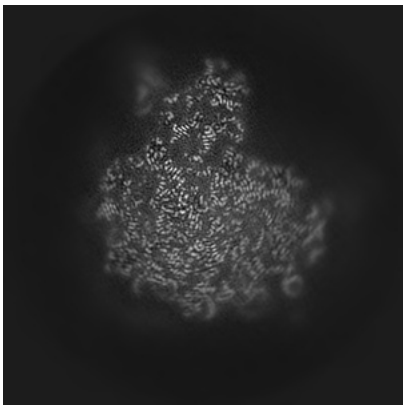
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

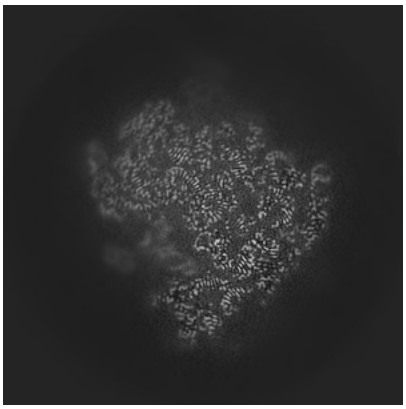
6.3.1 Primary map



X Index: 211

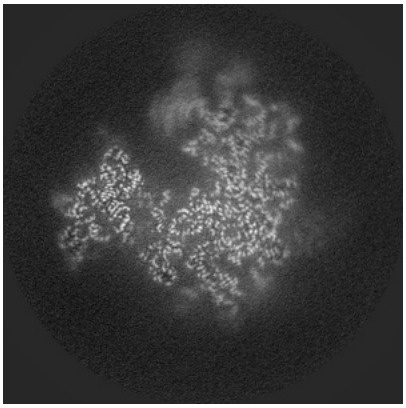


Y Index: 214

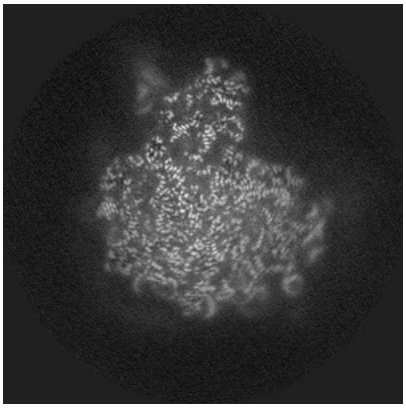


Z Index: 182

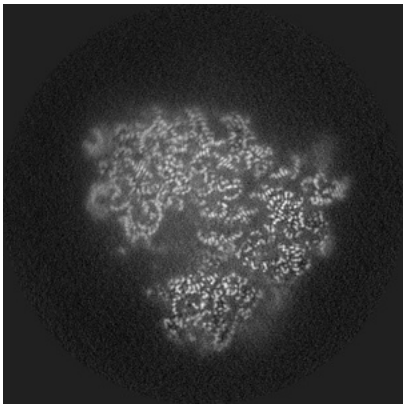
6.3.2 Raw map



X Index: 201



Y Index: 214

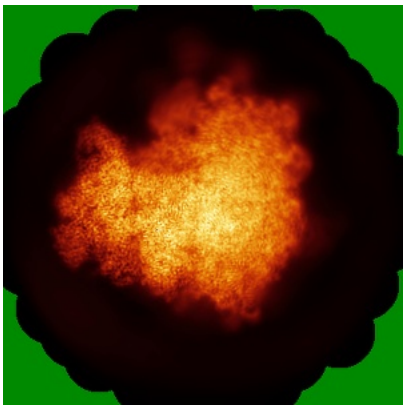


Z Index: 208

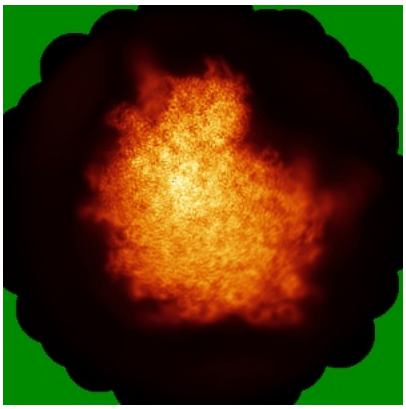
The images above show the largest variance slices of the map in three orthogonal directions.

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

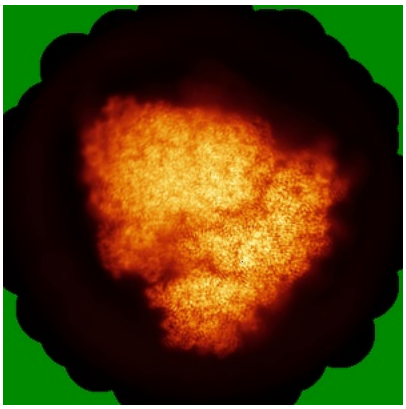
6.4.1 Primary map



X

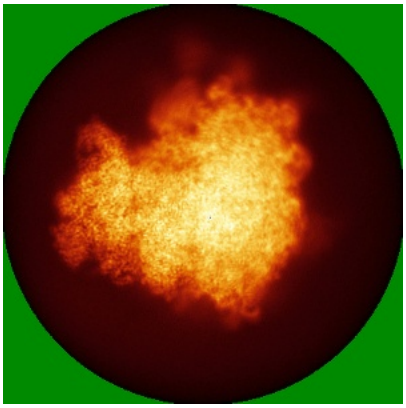


Y

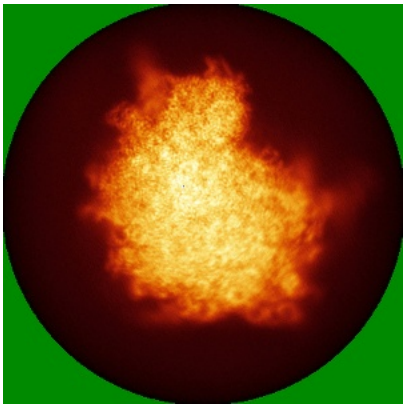


Z

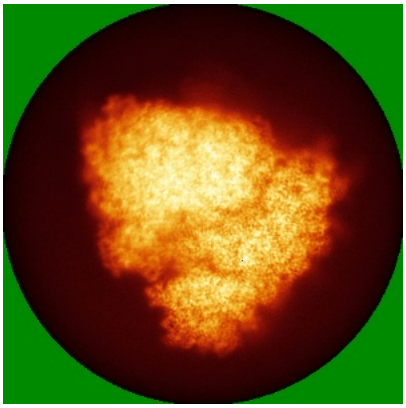
6.4.2 Raw map



X



Y

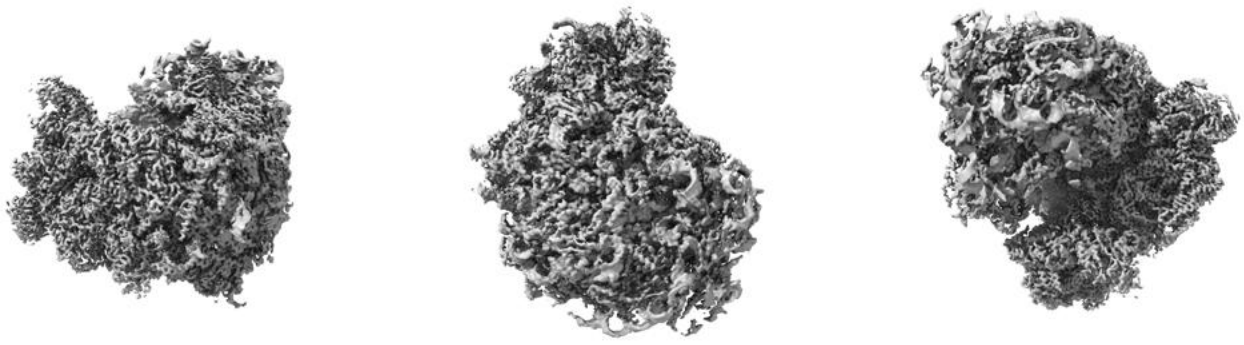


Z

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)

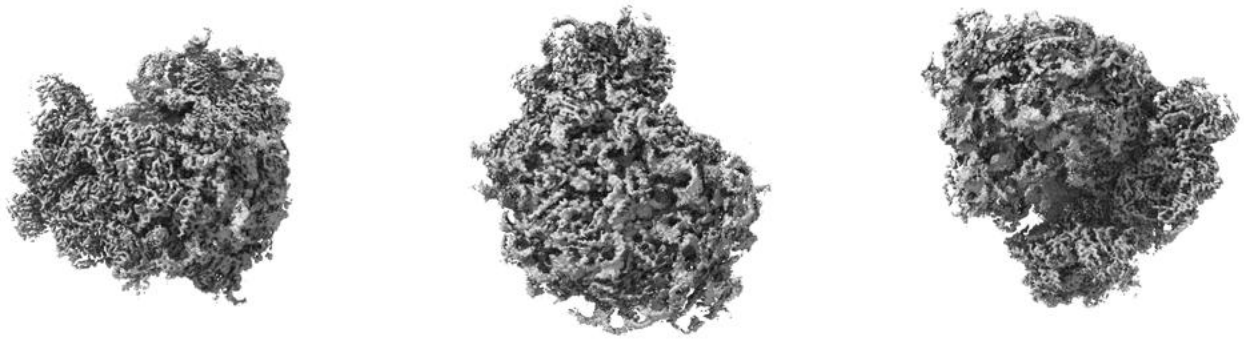
6.5.1 Primary map



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.

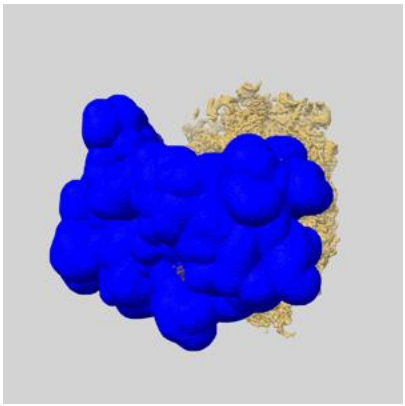
6.6 Mask visualisation (i)

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

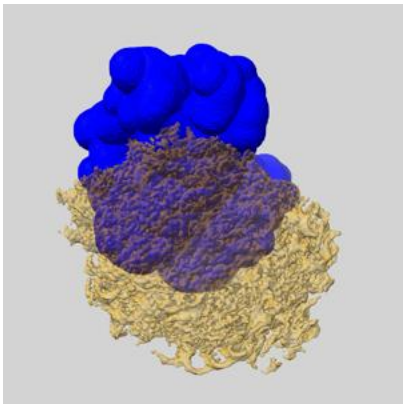
A mask typically either:

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

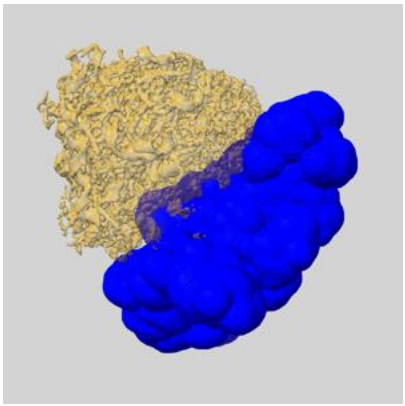
6.6.1 emd_11456_msk_1.map (i)



X



Y

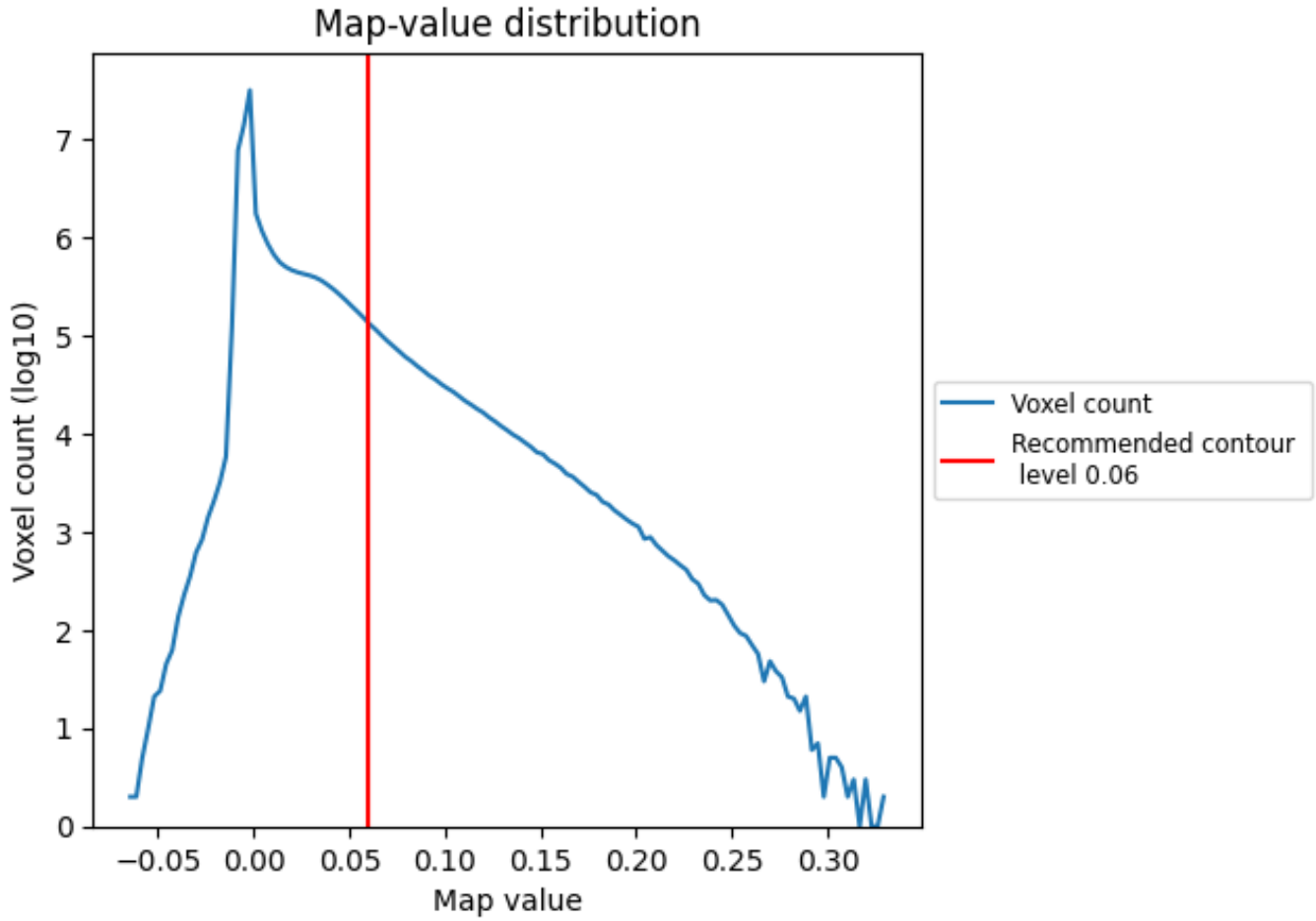


Z

7 Map analysis

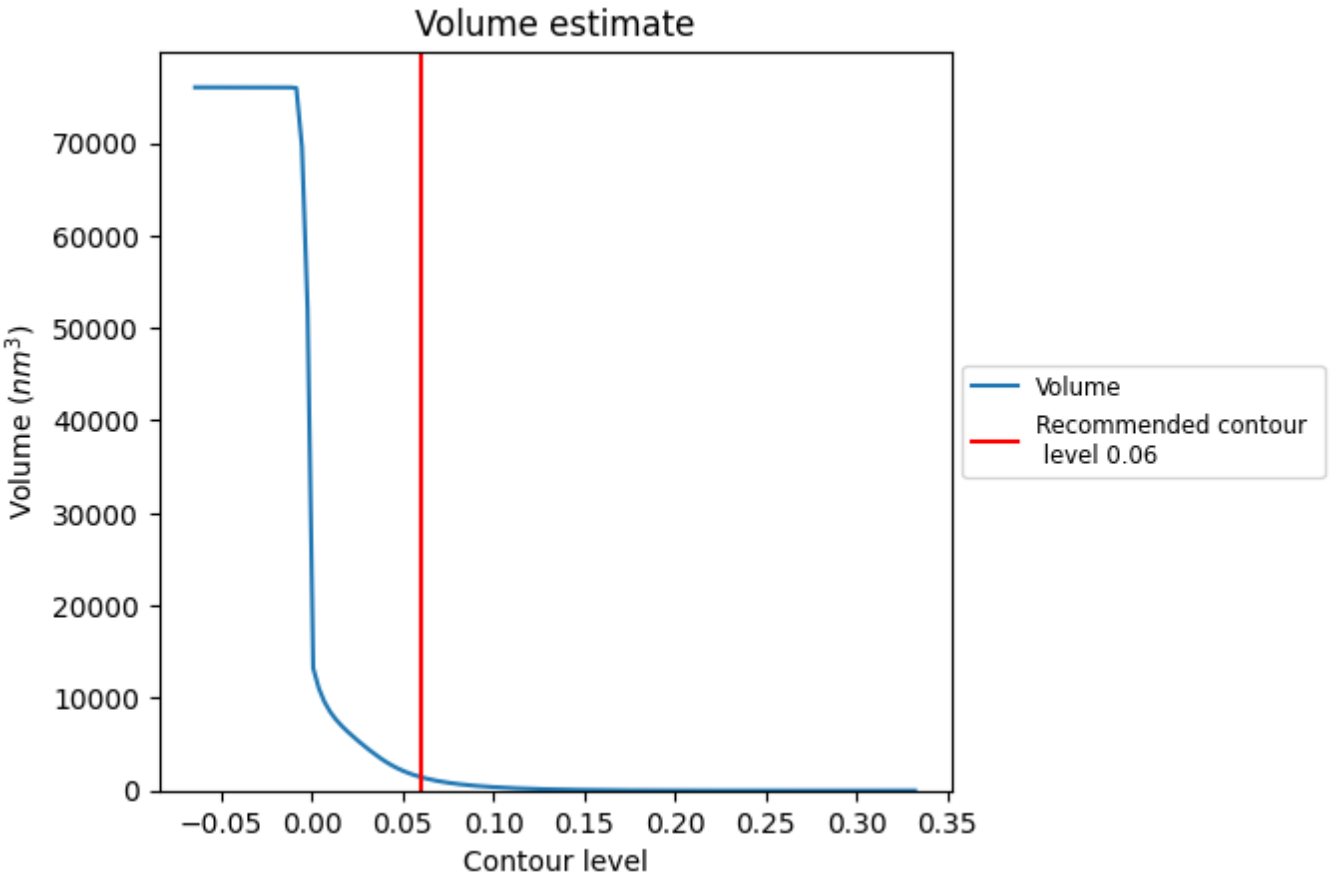
This section contains the results of statistical analysis of the map.

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.

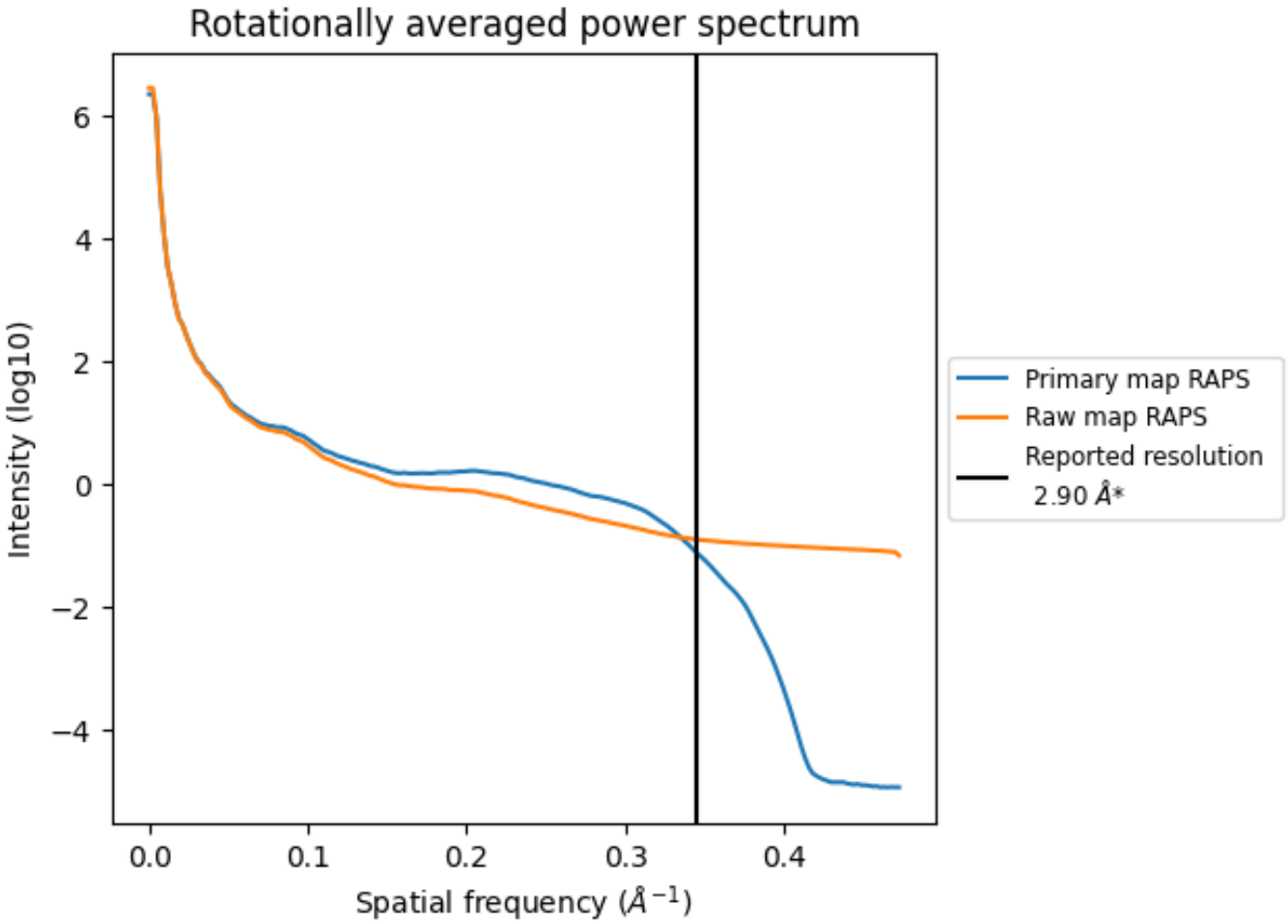
7.2 Volume estimate (i)



The volume at the recommended contour level is 1454 nm^3; this corresponds to an approximate mass of 1313 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)

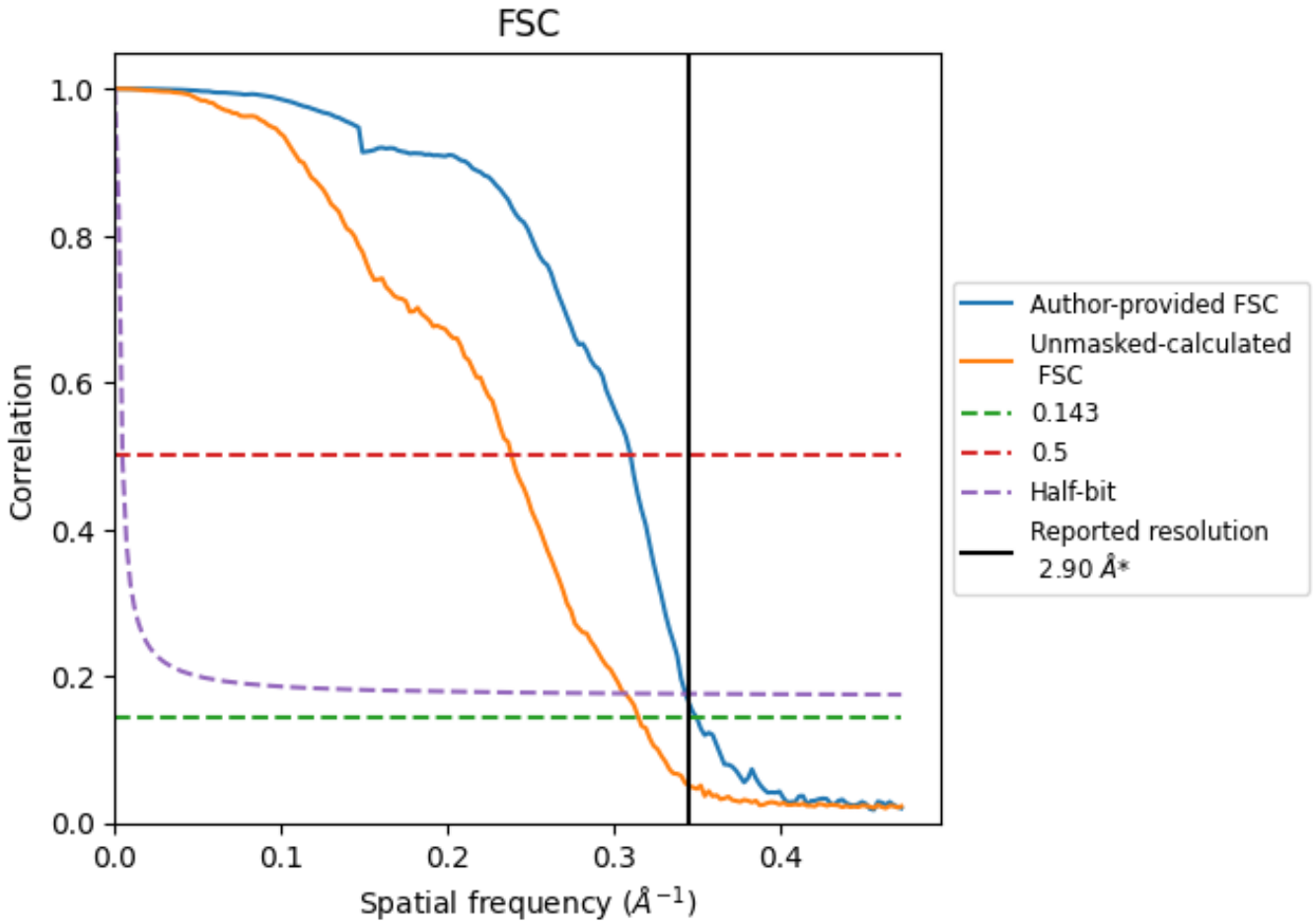


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

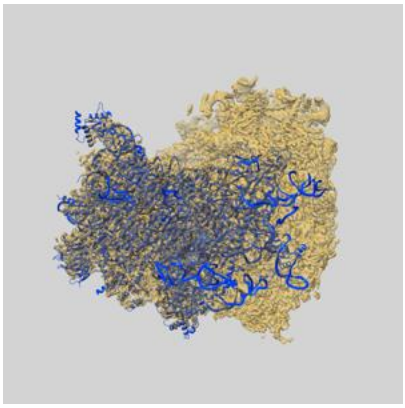
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.86	3.23	2.92
Unmasked-calculated*	3.18	4.20	3.27

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

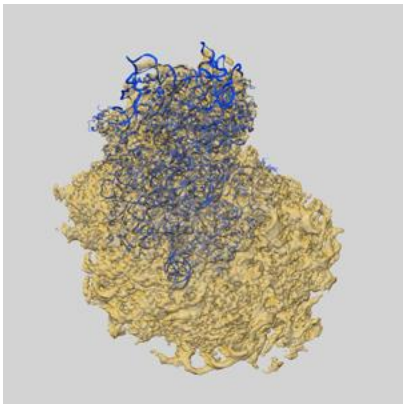
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11456 and PDB model 6ZVH. Per-residue inclusion information can be found in section 3 on page 11.

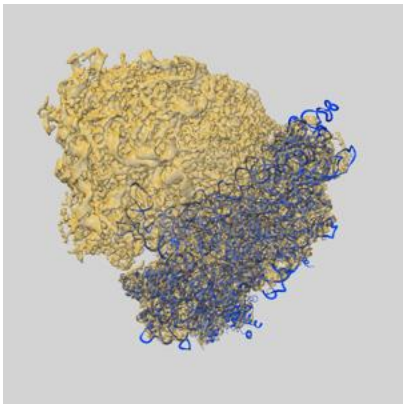
9.1 Map-model overlay



X



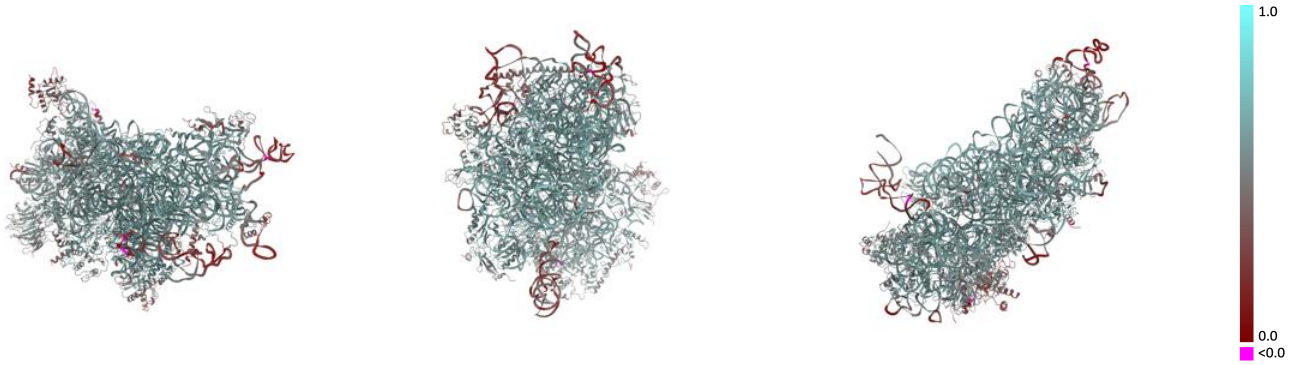
Y



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.

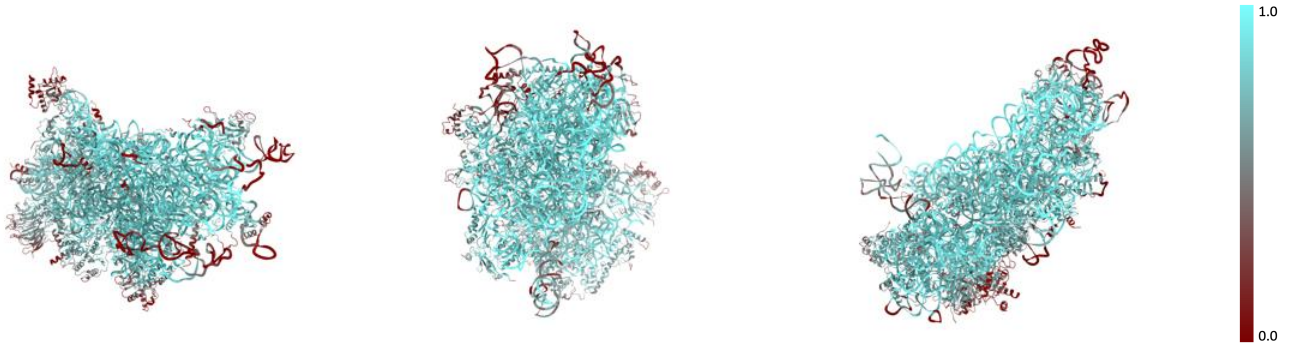
9.2 Q-score mapped to coordinate model (i)



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.

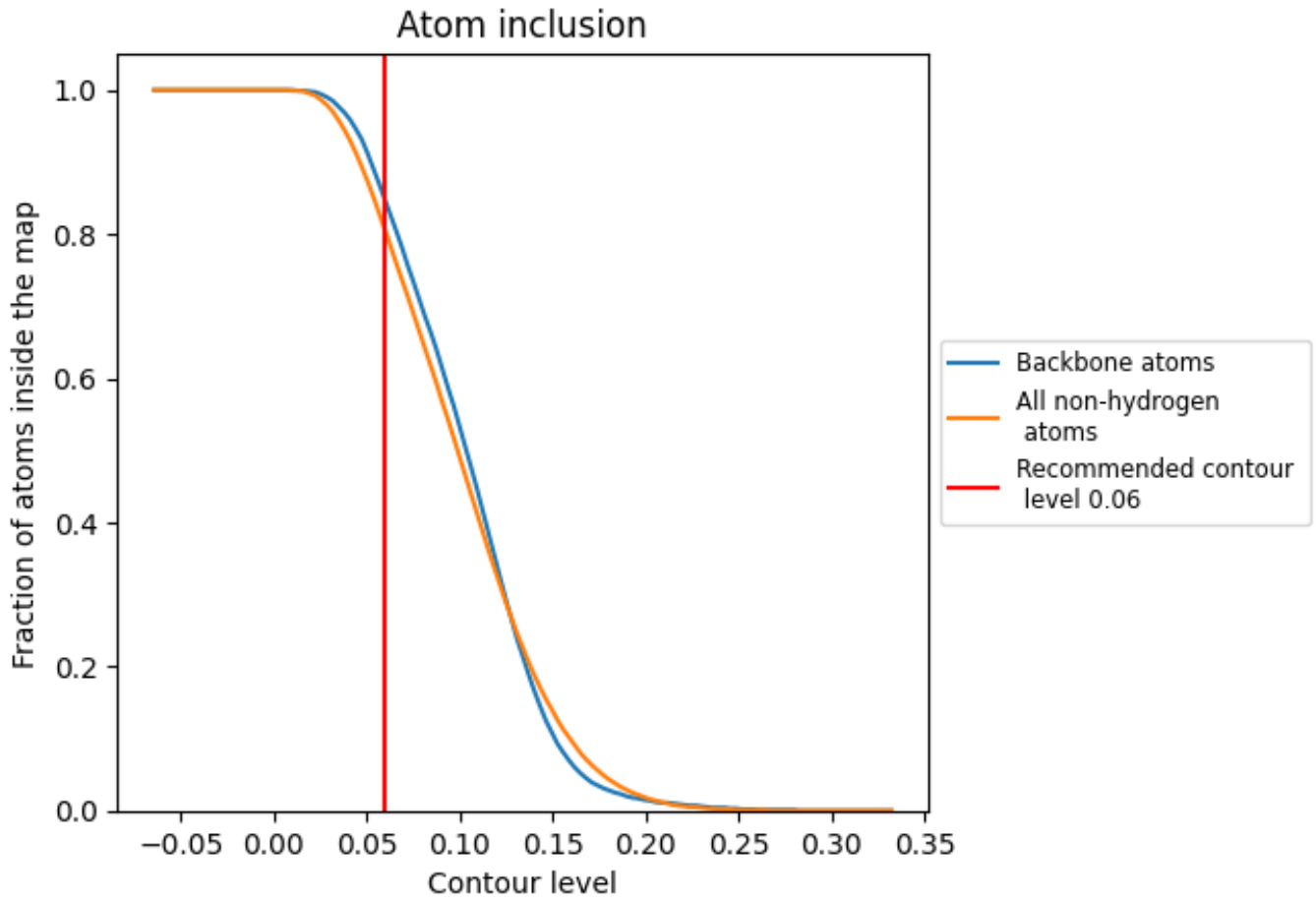
9.3 Atom inclusion mapped to coordinate model (i)



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, 85% of all backbone atoms, 80% 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	0.8040	0.5570
2	0.8950	0.5830
A	0.7610	0.5670
B	0.8160	0.5780
C	0.8520	0.5930
D	0.7360	0.5340
E	0.8420	0.5890
F	0.8050	0.5540
G	0.6620	0.5190
H	0.5430	0.4920
I	0.8040	0.5590
J	0.8310	0.5740
K	0.7470	0.5410
L	0.8430	0.5890
M	0.1840	0.3390
N	0.8820	0.6000
O	0.8470	0.5700
P	0.6870	0.5240
Q	0.7870	0.5680
R	0.6600	0.5180
S	0.7230	0.5280
T	0.7380	0.5470
U	0.6550	0.5060
V	0.7600	0.5680
W	0.9250	0.6180
X	0.9250	0.6110
Y	0.7180	0.5360
Z	0.5820	0.4910
a	0.8720	0.5860
b	0.7110	0.5550
c	0.6960	0.5220
d	0.9390	0.6100
e	0.8140	0.5780
f	0.3410	0.4070
g	0.4880	0.4870

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Chain	Atom inclusion	Q-score
i	0.5750	0.5310
x	0.4910	0.2680
y	0.7420	0.5410