



wwPDB EM Validation Summary Report ⓘ

Jun 21, 2026 – 06:20 am BST

PDB ID : 8PPK / pdb_00008ppk
EMDB ID : EMD-17804
Title : Bat-Hp-CoV Nsp1 and eIF1 bound to the human 40S small ribosomal subunit
Authors : Schubert, K.; Karousis, E.D.; Ban, I.; Lapointe, C.P.; Leibundgut, M.; Baeumlin, E.; Kummerant, E.; Scaiola, A.; Schoenhut, T.; Ziegelmueller, J.; Puglisi, J.D.; Muehlemann, O.; Ban, N.
Deposited on : 2023-07-07
Resolution : 2.98 Å (reported)
Based on initial models : 6ZOL, 6ZOK

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:

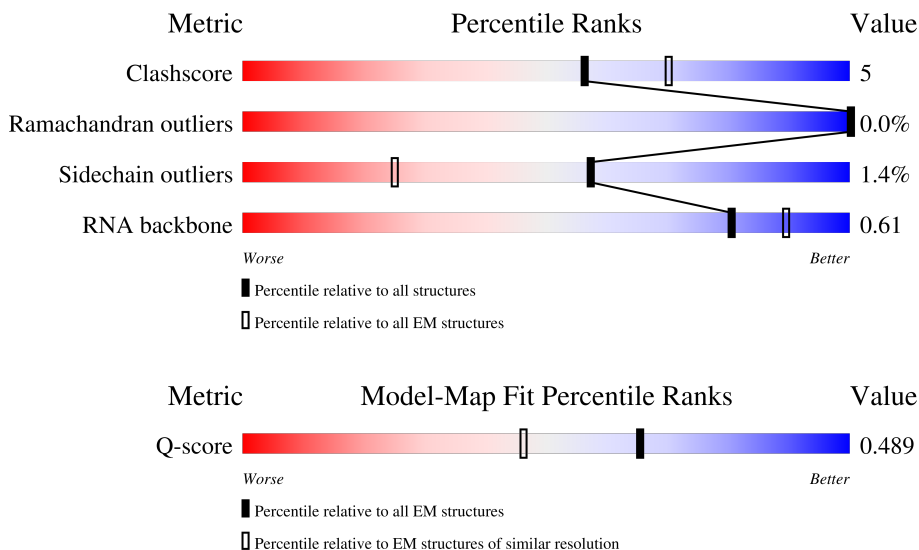
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.98 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13236 (2.48 - 3.48)

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	p	113	
2	2	1869	
3	A	295	


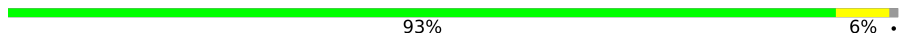







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Mol	Chain	Length	Quality of chain
4	B	264	78% 6% 15%
5	C	293	67% 9% 24%
6	D	243	84% 8% 7%
7	E	263	88% 12%
8	F	204	80% 14% 6%
9	G	249	82% 14%
10	H	194	8% 80% 17%
11	I	208	88% 11%
12	J	194	82% 10% 7%
13	K	165	48% 10% 41%
14	L	158	8% 88% 10%
15	M	132	27% 74% 19% 7%
16	N	151	89% 8%
17	O	151	80% 9% 11%
18	P	145	5% 73% 12% 14%
19	Q	146	84% 14%
20	R	135	84% 15%
21	S	152	73% 22% 5%
22	T	145	92% 7%
23	U	119	76% 8% 15%
24	V	83	89% 10%
25	W	130	88% 12%
26	X	143	90% 9%
27	Y	133	77% 16% 7%
28	Z	125	5% 42% 15% 42%

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Mol	Chain	Length	Quality of chain
29	a	115	
30	b	84	
31	c	69	
32	d	56	
33	e	133	
34	f	156	
35	g	317	
36	h	25	
37	j	188	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 79548 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 Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	p	85	691	438	125	126	2	0	0

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1771	37855	16922	6786	12376	1771	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	216	1708	1085	299	316	8	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	224	1815	1152	328	321	14	0	0

- Molecule 5 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	C	223	1741	1124	300	307	10	1	0

- Molecule 6 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	225	1752	1117	315	313	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 8 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	F	192	1517	948	287	275	7	0	0

- Molecule 9 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	G	240	1945	1212	393	333	7	0	0

- Molecule 10 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	H	189	1523	972	280	270	1	0	0

- Molecule 11 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	I	205	1682	1056	331	290	5	0	0

- Molecule 12 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	J	180	1499	955	300	242	2	0	0

- Molecule 13 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	K	97	816	533	144	133	6	0	0

- Molecule 14 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	155	Total	C	N	O	S	0	0
			1267	807	237	217	6		

- Molecule 15 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 16 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 17 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	138	IAS	ASP	modified residue	UNP P62263

- Molecule 18 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	124	Total	C	N	O	S	0	0
			1016	644	192	173	7		

- Molecule 19 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 20 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	R	134	1082	680	201	197	4	0	0

- Molecule 21 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	S	145	1200	753	242	204	1	0	0

- Molecule 22 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	T	144	1123	704	217	199	3	0	0

- Molecule 23 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	U	101	803	504	153	142	4	0	0

- Molecule 24 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	V	83	639	395	117	122	5	0	0

- Molecule 25 is a protein called 40S ribosomal protein S15a.

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

- Molecule 26 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	X	141	1099	693	219	184	3	0	0

- Molecule 27 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

- Molecule 28 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 29 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 30 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	83	Total	C	N	O	S	0	0
			650	408	121	114	7		

- Molecule 31 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	65	Total	C	N	O	S	0	0
			512	311	103	96	2		

- Molecule 32 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	55	Total	C	N	O	S	0	0
			458	286	94	73	5		

- Molecule 33 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	59	Total	C	N	O	S	0	0
			467	290	102	74	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	f	74	610	385	117	101	7	0	0

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	g	314	2440	1537	425	466	12	0	0

- Molecule 36 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	h	25	239	145	64	27	3	0	0

- Molecule 37 is a protein called Nsp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	j	174	1363	867	239	253	4	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	-13	MET	-	initiating methionine	UNP A0A088DIE1
j	-12	HIS	-	expression tag	UNP A0A088DIE1
j	-11	HIS	-	expression tag	UNP A0A088DIE1
j	-10	HIS	-	expression tag	UNP A0A088DIE1
j	-9	HIS	-	expression tag	UNP A0A088DIE1
j	-8	HIS	-	expression tag	UNP A0A088DIE1
j	-7	HIS	-	expression tag	UNP A0A088DIE1
j	-6	GLU	-	expression tag	UNP A0A088DIE1
j	-5	ASN	-	expression tag	UNP A0A088DIE1
j	-4	LEU	-	expression tag	UNP A0A088DIE1
j	-3	TYR	-	expression tag	UNP A0A088DIE1
j	-2	PHE	-	expression tag	UNP A0A088DIE1
j	-1	GLN	-	expression tag	UNP A0A088DIE1
j	0	SER	-	expression tag	UNP A0A088DIE1

- Molecule 38 is UNKNOWN LIGAND (CCD ID: UNX) (formula: X).

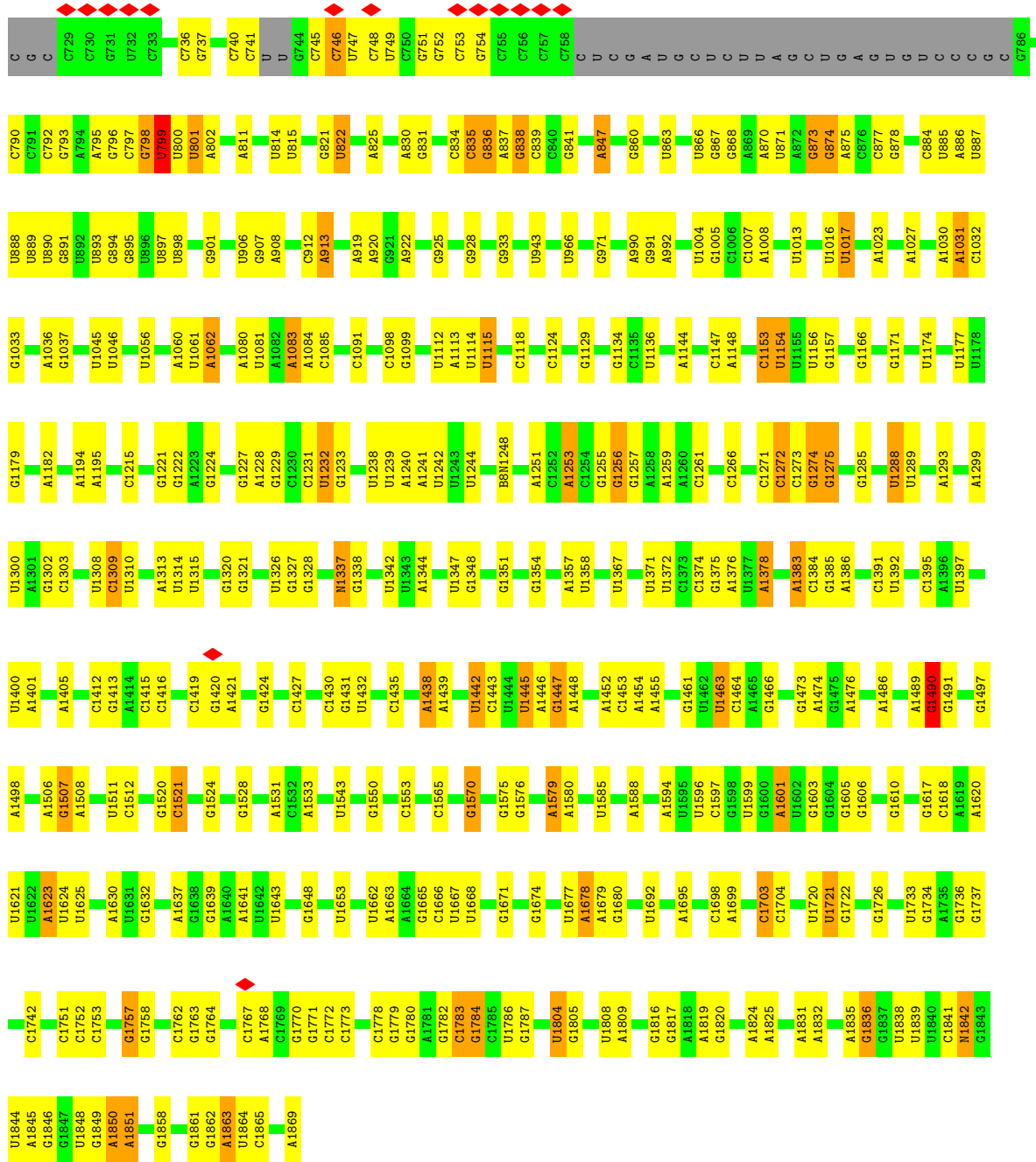
Mol	Chain	Residues	Atoms	AltConf
38	2	108	Total X 108 108	0
38	G	1	Total X 1 1	0
38	H	1	Total X 1 1	0
38	I	1	Total X 1 1	0
38	J	1	Total X 1 1	0
38	L	1	Total X 1 1	0
38	N	1	Total X 1 1	0
38	O	2	Total X 2 2	0
38	X	1	Total X 1 1	0

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

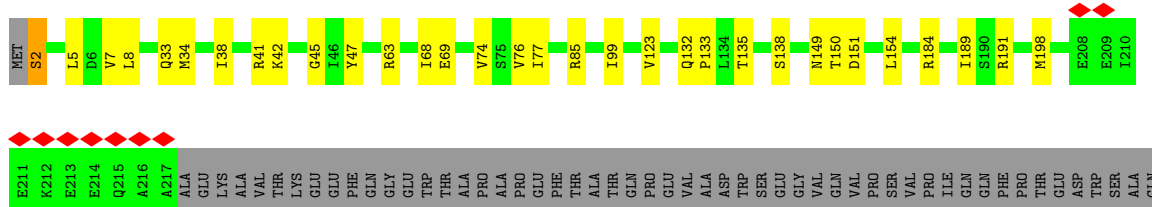
Mol	Chain	Residues	Atoms	AltConf
39	2	110	Total Mg 110 110	0
39	X	1	Total Mg 1 1	0

- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

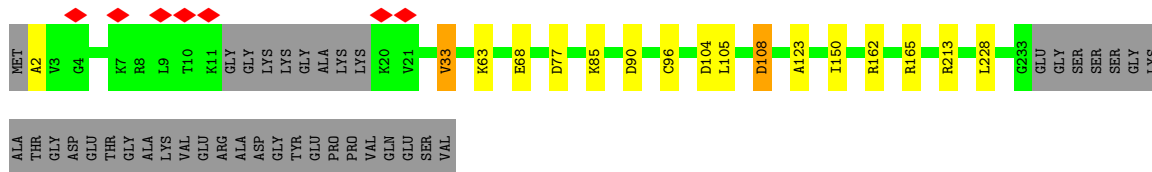
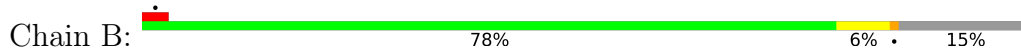


• Molecule 3: 40S ribosomal protein SA

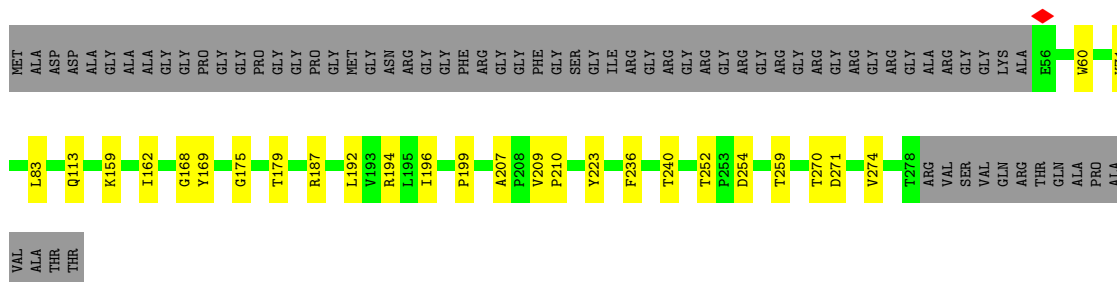
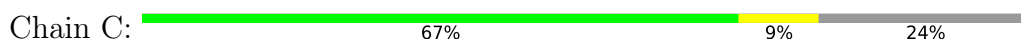


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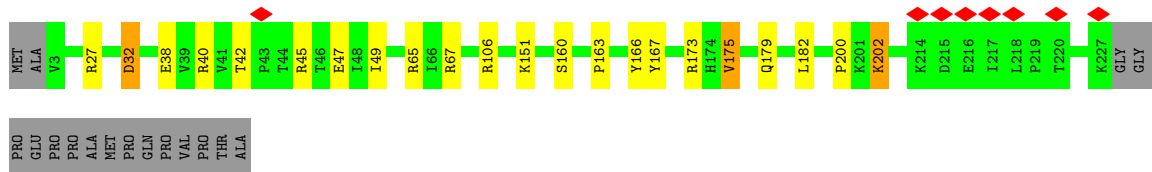
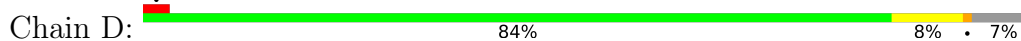
• Molecule 4: 40S ribosomal protein S3a



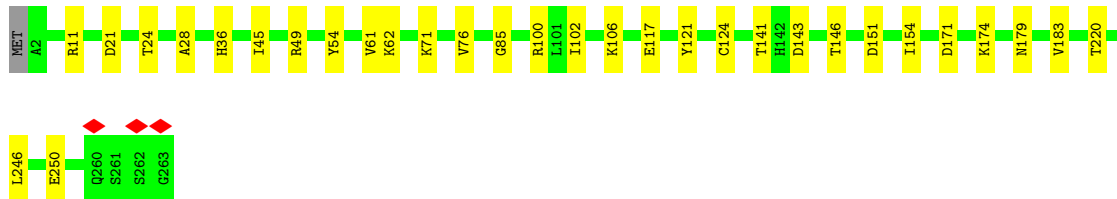
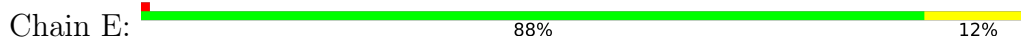
• Molecule 5: 40S ribosomal protein S2



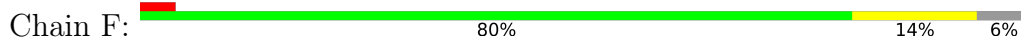
• Molecule 6: 40S ribosomal protein S3

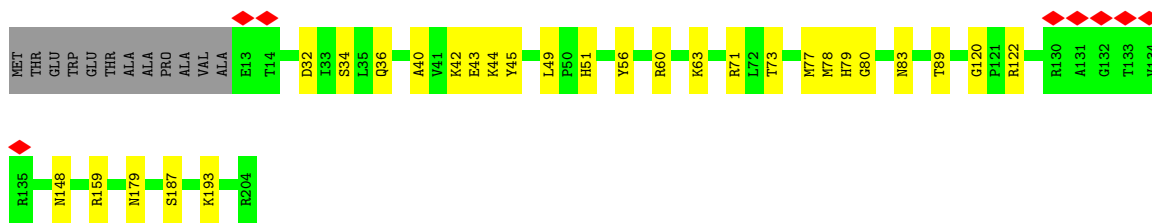


• Molecule 7: 40S ribosomal protein S4, X isoform

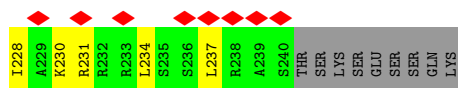
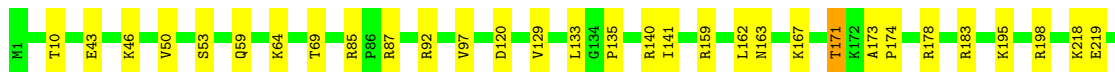
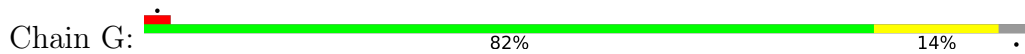


• Molecule 8: 40S ribosomal protein S5

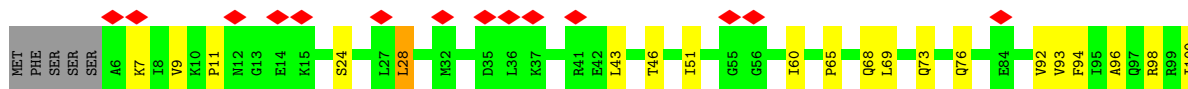
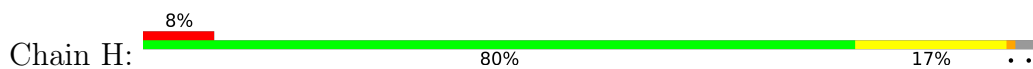




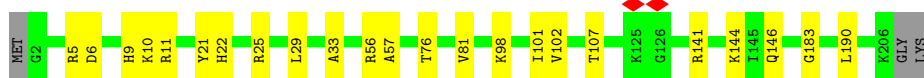
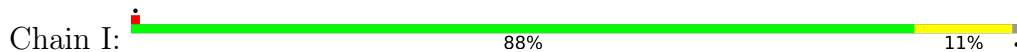
• Molecule 9: 40S ribosomal protein S6



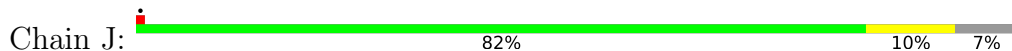
• Molecule 10: 40S ribosomal protein S7



• Molecule 11: 40S ribosomal protein S8

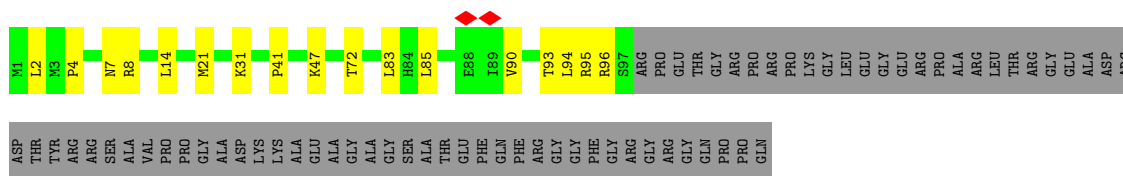


• Molecule 12: 40S ribosomal protein S9

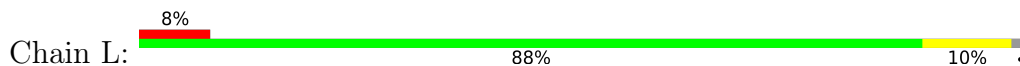


• Molecule 13: 40S ribosomal protein S10

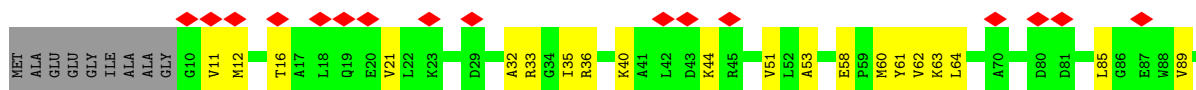
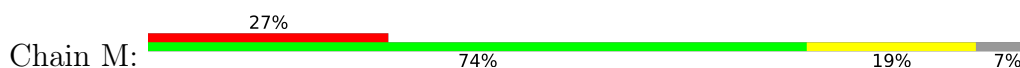




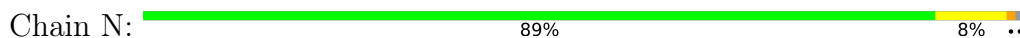
• Molecule 14: 40S ribosomal protein S11



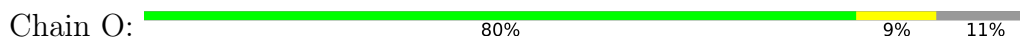
• Molecule 15: 40S ribosomal protein S12



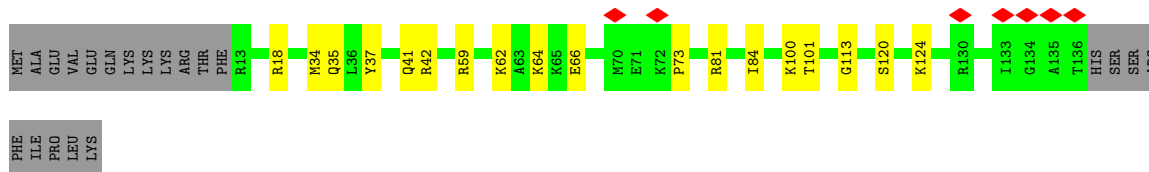
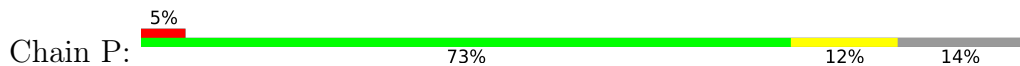
• Molecule 16: 40S ribosomal protein S13



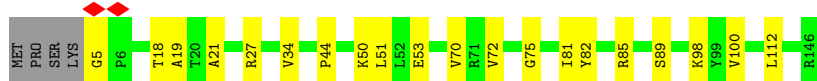
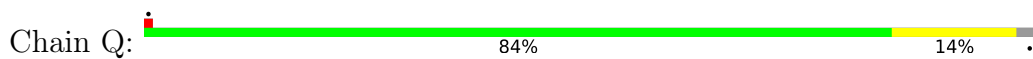
• Molecule 17: 40S ribosomal protein S14



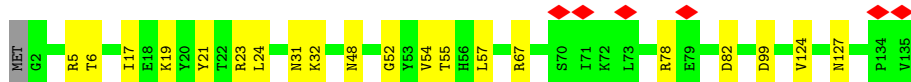
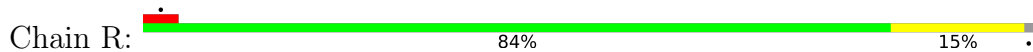
• Molecule 18: 40S ribosomal protein S15



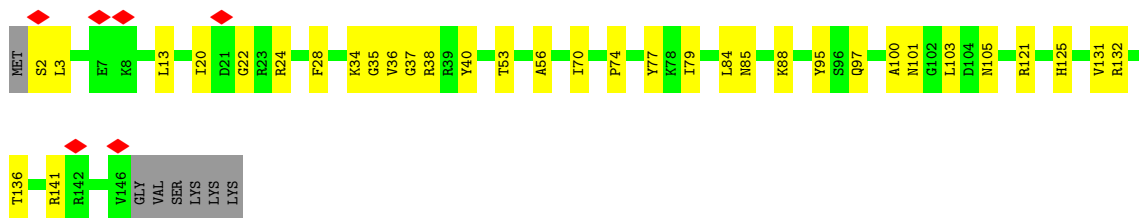
• Molecule 19: 40S ribosomal protein S16



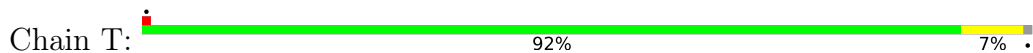
• Molecule 20: 40S ribosomal protein S17



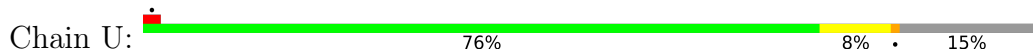
• Molecule 21: Small ribosomal subunit protein uS13



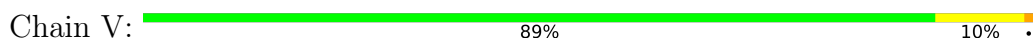
• Molecule 22: Small ribosomal subunit protein eS19



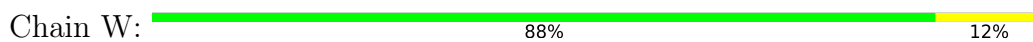
• Molecule 23: 40S ribosomal protein S20



• Molecule 24: 40S ribosomal protein S21

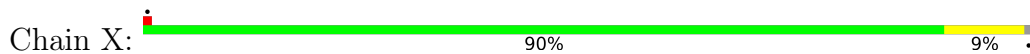


• Molecule 25: 40S ribosomal protein S15a

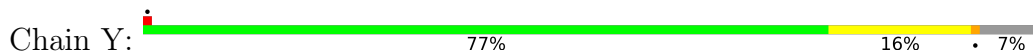




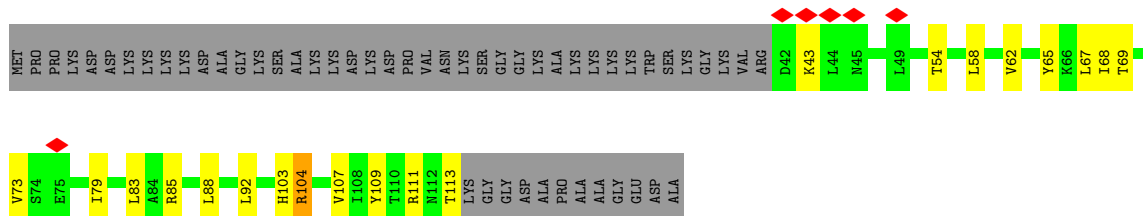
• Molecule 26: 40S ribosomal protein S23



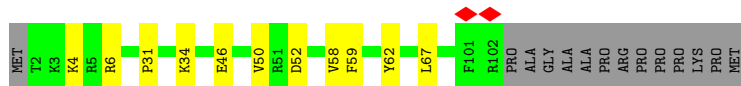
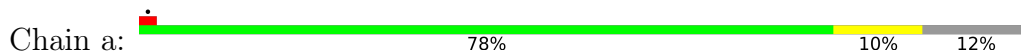
• Molecule 27: 40S ribosomal protein S24



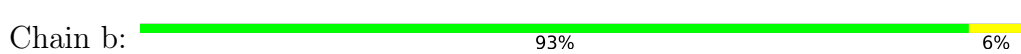
• Molecule 28: 40S ribosomal protein S25



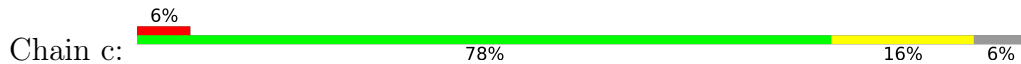
• Molecule 29: 40S ribosomal protein S26



• Molecule 30: 40S ribosomal protein S27

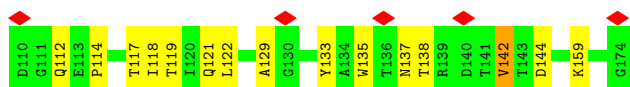


• Molecule 31: 40S ribosomal protein S28





- Molecule 37: Nsp1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98750	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.378	Depositor
Minimum map value	-0.548	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.16	Depositor
Map size (\AA)	596.4, 596.4, 596.4	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.065, 1.065, 1.065	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: ZN, IAS, A2M, AME, MG, MA6, OMG, B8N, OMU, G7M, 4AC, SAC, HY3, PSU, UNX, OMC, 6MZ, NMM

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	p	0.07	0/701	0.16	0/936
2	2	0.16	2/40280 (0.0%)	0.17	0/62782
3	A	0.10	0/1736	0.20	0/2359
4	B	0.10	0/1841	0.20	0/2459
5	C	0.11	0/1781	0.21	0/2405
6	D	0.09	0/1780	0.20	0/2397
7	E	0.12	0/2118	0.22	0/2849
8	F	0.08	0/1539	0.24	0/2071
9	G	0.09	0/1968	0.19	0/2619
10	H	0.09	0/1546	0.23	0/2071
11	I	0.10	0/1711	0.20	0/2282
12	J	0.11	0/1524	0.19	0/2035
13	K	0.08	0/840	0.22	0/1133
14	L	0.11	0/1289	0.19	0/1724
15	M	0.07	0/963	0.24	0/1291
16	N	0.10	0/1226	0.21	0/1649
17	O	0.10	0/1014	0.21	0/1358
18	P	0.06	0/1035	0.17	0/1383
19	Q	0.09	0/1146	0.21	0/1534
20	R	0.08	0/1097	0.20	0/1474
21	S	0.07	0/1209	0.20	0/1620
22	T	0.07	0/1130	0.17	0/1513
23	U	0.08	0/813	0.21	0/1092
24	V	0.10	0/635	0.19	0/850
25	W	0.13	0/1051	0.23	0/1406
26	X	0.11	0/1107	0.22	0/1475
27	Y	0.10	0/1031	0.19	0/1370
28	Z	0.09	0/580	0.24	0/780
29	a	0.11	0/828	0.21	0/1109
30	b	0.10	0/664	0.21	0/891
31	c	0.09	0/514	0.21	0/688

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	0.09	0/469	0.20	0/623
33	e	0.12	0/473	0.26	0/623
34	f	0.34	0/622	0.40	0/822
35	g	0.09	0/2497	0.24	0/3399
36	h	0.08	0/240	0.15	0/305
37	j	0.11	0/1399	0.27	0/1903
All	All	0.14	2/82397 (0.0%)	0.19	0/119280

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	627	OMU	O3'-P	5.17	1.61	1.56
2	2	1639	G7M	O3'-P	5.02	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	p	691	0	706	5	0
2	2	37855	0	19186	304	0
3	A	1708	0	1710	20	0
4	B	1815	0	1908	11	0
5	C	1741	0	1827	20	0
6	D	1752	0	1848	15	0
7	E	2076	0	2177	21	0
8	F	1517	0	1569	20	0
9	G	1945	0	2112	26	0
10	H	1523	0	1622	27	0
11	I	1682	0	1769	17	0
12	J	1499	0	1618	12	0
13	K	816	0	841	9	0
14	L	1267	0	1340	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	M	953	0	990	18	0
16	N	1202	0	1289	9	0
17	O	1010	0	1033	8	0
18	P	1016	0	1066	13	0
19	Q	1128	0	1195	11	0
20	R	1082	0	1137	15	0
21	S	1200	0	1262	22	0
22	T	1123	0	1152	7	0
23	U	803	0	873	5	0
24	V	639	0	638	9	0
25	W	1034	0	1080	12	0
26	X	1099	0	1162	7	0
27	Y	1014	0	1082	15	0
28	Z	574	0	627	12	0
29	a	814	0	863	7	0
30	b	650	0	672	3	0
31	c	512	0	541	7	0
32	d	458	0	448	3	0
33	e	467	0	516	2	0
34	f	610	0	634	19	0
35	g	2440	0	2396	32	0
36	h	239	0	289	3	0
37	j	1363	0	1342	20	0
38	2	108	0	0	0	0
38	G	1	0	0	0	0
38	H	1	0	0	0	0
38	I	1	0	0	0	0
38	J	1	0	0	0	0
38	L	1	0	0	0	0
38	N	1	0	0	0	0
38	O	2	0	0	0	0
38	X	1	0	0	0	0
39	2	110	0	0	0	0
39	X	1	0	0	0	0
40	a	1	0	0	0	0
40	d	1	0	0	0	0
40	f	1	0	0	0	0
All	All	79548	0	62520	641	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 5.

The worst 5 of 641 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)
2:2:1091:C:HO2'	25:W:2:VAL:N	1.71	0.88
2:2:229:A:H62	2:2:887:U:H3	1.29	0.77
35:g:191:HIS:HE2	35:g:209:SER:HG	1.33	0.74
9:G:64:LYS:HB2	9:G:97:VAL:HG11	1.68	0.73
31:c:7:GLN:HE22	31:c:61:SER:H	1.37	0.72

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	p	83/113 (74%)	82 (99%)	1 (1%)	0	100	100
3	A	214/295 (72%)	211 (99%)	3 (1%)	0	100	100
4	B	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
5	C	222/293 (76%)	218 (98%)	4 (2%)	0	100	100
6	D	223/243 (92%)	221 (99%)	2 (1%)	0	100	100
7	E	260/263 (99%)	255 (98%)	5 (2%)	0	100	100
8	F	190/204 (93%)	182 (96%)	8 (4%)	0	100	100
9	G	238/249 (96%)	236 (99%)	2 (1%)	0	100	100
10	H	187/194 (96%)	183 (98%)	4 (2%)	0	100	100
11	I	203/208 (98%)	201 (99%)	2 (1%)	0	100	100
12	J	178/194 (92%)	175 (98%)	3 (2%)	0	100	100
13	K	95/165 (58%)	93 (98%)	2 (2%)	0	100	100
14	L	153/158 (97%)	149 (97%)	4 (3%)	0	100	100
15	M	121/132 (92%)	117 (97%)	4 (3%)	0	100	100
16	N	147/151 (97%)	142 (97%)	5 (3%)	0	100	100
17	O	131/151 (87%)	128 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	P	122/145 (84%)	122 (100%)	0	0	100	100
19	Q	140/146 (96%)	138 (99%)	2 (1%)	0	100	100
20	R	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
21	S	143/152 (94%)	141 (99%)	2 (1%)	0	100	100
22	T	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
23	U	99/119 (83%)	96 (97%)	3 (3%)	0	100	100
24	V	81/83 (98%)	81 (100%)	0	0	100	100
25	W	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
26	X	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
27	Y	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
28	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
29	a	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
30	b	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
31	c	63/69 (91%)	62 (98%)	1 (2%)	0	100	100
32	d	53/56 (95%)	53 (100%)	0	0	100	100
33	e	57/133 (43%)	54 (95%)	3 (5%)	0	100	100
34	f	72/156 (46%)	63 (88%)	8 (11%)	1 (1%)	9	34
35	g	312/317 (98%)	297 (95%)	15 (5%)	0	100	100
36	h	23/25 (92%)	23 (100%)	0	0	100	100
37	j	172/188 (92%)	165 (96%)	6 (4%)	1 (1%)	21	53
All	All	5112/5876 (87%)	4994 (98%)	116 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	j	129	ALA
34	f	84	SER

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	p	74/96 (77%)	72 (97%)	2 (3%)	39	70
3	A	179/242 (74%)	178 (99%)	1 (1%)	78	88
4	B	203/231 (88%)	200 (98%)	3 (2%)	57	79
5	C	190/225 (84%)	190 (100%)	0	100	100
6	D	189/202 (94%)	186 (98%)	3 (2%)	55	78
7	E	224/225 (100%)	224 (100%)	0	100	100
8	F	162/170 (95%)	162 (100%)	0	100	100
9	G	209/218 (96%)	206 (99%)	3 (1%)	59	80
10	H	169/174 (97%)	168 (99%)	1 (1%)	78	88
11	I	178/180 (99%)	175 (98%)	3 (2%)	53	77
12	J	160/168 (95%)	159 (99%)	1 (1%)	78	88
13	K	88/136 (65%)	85 (97%)	3 (3%)	32	64
14	L	139/142 (98%)	138 (99%)	1 (1%)	76	87
15	M	104/108 (96%)	102 (98%)	2 (2%)	50	75
16	N	130/131 (99%)	127 (98%)	3 (2%)	44	72
17	O	104/118 (88%)	103 (99%)	1 (1%)	68	83
18	P	110/130 (85%)	110 (100%)	0	100	100
19	Q	117/121 (97%)	114 (97%)	3 (3%)	40	70
20	R	121/122 (99%)	117 (97%)	4 (3%)	33	65
21	S	125/131 (95%)	124 (99%)	1 (1%)	73	86
22	T	113/114 (99%)	113 (100%)	0	100	100
23	U	93/107 (87%)	90 (97%)	3 (3%)	34	65
24	V	66/66 (100%)	65 (98%)	1 (2%)	57	79
25	W	112/113 (99%)	111 (99%)	1 (1%)	70	85
26	X	112/114 (98%)	111 (99%)	1 (1%)	70	85
27	Y	108/115 (94%)	107 (99%)	1 (1%)	70	85
28	Z	64/103 (62%)	61 (95%)	3 (5%)	23	56
29	a	88/98 (90%)	87 (99%)	1 (1%)	65	82
30	b	75/76 (99%)	74 (99%)	1 (1%)	61	81
31	c	58/62 (94%)	58 (100%)	0	100	100
32	d	48/49 (98%)	47 (98%)	1 (2%)	47	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	e	48/104 (46%)	46 (96%)	2 (4%)	26	59
34	f	67/140 (48%)	65 (97%)	2 (3%)	36	67
35	g	272/275 (99%)	267 (98%)	5 (2%)	51	76
36	h	24/24 (100%)	24 (100%)	0	100	100
37	j	144/158 (91%)	138 (96%)	6 (4%)	26	59
All	All	4467/4988 (90%)	4404 (99%)	63 (1%)	57	80

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	Q	51	LEU
35	g	294	ASP
23	U	25	THR
35	g	266	ILE
37	j	133	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
35	g	305	ASN
37	j	10	GLN
37	j	137	ASN
14	L	18	GLN
14	L	11	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	2	1765/1869 (94%)	213 (12%)	1 (0%)

5 of 213 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	2	4	C
2	2	17	C
2	2	33	G
2	2	41	G
2	2	46	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	873	G

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

92 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	2	1703	2	19,22,23	0.83	0	26,31,34	0.89	1 (3%)
2	PSU	2	109	2	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
2	MA6	2	1850	2	23,26,27	2.26	5 (21%)	34,38,41	3.70	13 (38%)
2	PSU	2	119	2	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
2	PSU	2	1238	2	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
2	A2M	2	512	2	22,25,26	1.45	4 (18%)	31,36,39	2.15	9 (29%)
2	PSU	2	651	2	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
2	A2M	2	1031	2	22,25,26	1.44	4 (18%)	31,36,39	2.12	10 (32%)
2	OMU	2	354	2	19,22,23	1.22	3 (15%)	26,31,34	1.72	5 (19%)
2	A2M	2	27	39,2	22,25,26	1.50	4 (18%)	31,36,39	2.14	10 (32%)
2	OMG	2	601	2	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
2	PSU	2	814	2	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
2	OMU	2	116	2	19,22,23	1.21	3 (15%)	26,31,34	1.70	4 (15%)
2	A2M	2	99	39,2	22,25,26	1.51	4 (18%)	31,36,39	2.14	10 (32%)
2	PSU	2	1174	2	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
2	6MZ	2	1832	39,2	22,25,26	1.42	4 (18%)	30,36,39	2.16	8 (26%)
2	PSU	2	1244	2	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
2	PSU	2	609	2	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
2	PSU	2	1367	2	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
2	A2M	2	1678	2	22,25,26	1.45	4 (18%)	31,36,39	2.16	9 (29%)
2	OMG	2	644	2	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMC	2	462	2	19,22,23	0.81	0	26,31,34	0.81	0
2	PSU	2	1643	39,2	18,21,22	1.37	2 (11%)	22,30,33	1.87	3 (13%)
2	PSU	2	1347	2	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
2	A2M	2	668	39,2	22,25,26	1.44	4 (18%)	31,36,39	2.11	9 (29%)
2	OMU	2	1326	39,2	19,22,23	1.19	2 (10%)	26,31,34	1.72	5 (19%)
2	PSU	2	1177	2	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
2	G7M	2	1639	2	23,26,27	3.11	8 (34%)	35,39,42	3.31	13 (37%)
2	OMU	2	1804	2	19,22,23	1.21	3 (15%)	26,31,34	1.71	4 (15%)
2	PSU	2	686	2	18,21,22	1.33	2 (11%)	22,30,33	1.93	4 (18%)
2	PSU	2	1081	2	18,21,22	1.38	3 (16%)	22,30,33	1.88	3 (13%)
2	OMU	2	121	2	19,22,23	1.21	3 (15%)	26,31,34	1.69	5 (19%)
2	PSU	2	966	2	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
2	OMU	2	1442	39,2	19,22,23	1.23	2 (10%)	26,31,34	1.70	4 (15%)
2	PSU	2	1232	2	18,21,22	1.34	2 (11%)	22,30,33	1.92	4 (18%)
2	OMG	2	1447	2	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
2	OMU	2	428	2	19,22,23	1.19	3 (15%)	26,31,34	1.71	5 (19%)
2	PSU	2	34	2	18,21,22	1.37	2 (11%)	22,30,33	1.95	3 (13%)
2	A2M	2	159	2	22,25,26	1.51	4 (18%)	31,36,39	2.13	10 (32%)
2	A2M	2	166	2	22,25,26	1.45	4 (18%)	31,36,39	2.16	10 (32%)
2	OMU	2	172	2	19,22,23	1.21	2 (10%)	26,31,34	1.73	5 (19%)
2	PSU	2	681	2	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
2	OMG	2	509	39,2	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
2	PSU	2	801	2	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
2	OMC	2	1272	2	19,22,23	0.83	0	26,31,34	0.89	1 (3%)
2	PSU	2	1136	2	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
2	PSU	2	1004	2	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
2	OMG	2	1490	39,2	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
2	OMC	2	517	2	19,22,23	0.82	0	26,31,34	0.82	0
2	OMC	2	1391	2	19,22,23	0.81	0	26,31,34	0.83	0
2	PSU	2	1692	2	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
2	A2M	2	1383	2	22,25,26	1.46	4 (18%)	31,36,39	2.16	10 (32%)
2	PSU	2	1625	2	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
2	PSU	2	1046	2	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
26	HY3	X	62	26	6,8,9	2.16	1 (16%)	5,10,12	1.16	1 (20%)
2	PSU	2	210	2	18,21,22	1.35	2 (11%)	22,30,33	1.87	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	2	218	2	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
2	PSU	2	296	2	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
2	PSU	2	863	2	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
2	OMG	2	683	2	23,26,27	1.20	3 (13%)	33,38,41	1.93	6 (18%)
2	OMC	2	174	39,2	19,22,23	0.82	0	26,31,34	0.79	0
2	OMC	2	797	2	19,22,23	0.82	0	26,31,34	0.87	1 (3%)
2	PSU	2	1445	2	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
2	PSU	2	105	2	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
2	PSU	2	406	2	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
17	IAS	O	138	17	6,7,8	0.97	0	6,8,10	1.32	1 (16%)
2	4AC	2	1337	2	21,24,25	1.10	2 (9%)	29,34,37	1.02	2 (6%)
2	PSU	2	866	2	18,21,22	1.34	2 (11%)	22,30,33	1.93	4 (18%)
22	NMM	T	67	22	9,11,12	0.59	0	6,12,14	0.55	0
2	B8N	2	1248	2	24,29,30	1.29	3 (12%)	29,42,45	1.26	3 (10%)
2	PSU	2	822	2	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
2	PSU	2	1056	2	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
2	PSU	2	93	2	18,21,22	1.38	2 (11%)	22,30,33	1.95	3 (13%)
2	OMG	2	436	2	23,26,27	1.20	3 (13%)	33,38,41	1.96	6 (18%)
2	OMU	2	799	2	19,22,23	1.21	3 (15%)	26,31,34	1.72	5 (19%)
2	MA6	2	1851	2	23,26,27	2.27	5 (21%)	34,38,41	3.64	12 (35%)
3	SAC	A	2	3	7,8,9	0.52	0	8,9,11	0.86	1 (12%)
2	PSU	2	572	2	18,21,22	1.36	2 (11%)	22,30,33	1.93	3 (13%)
2	PSU	2	815	2	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
2	OMU	2	627	2	19,22,23	1.20	2 (10%)	26,31,34	1.67	5 (19%)
2	A2M	2	468	2	22,25,26	1.45	4 (18%)	31,36,39	2.13	10 (32%)
2	A2M	2	590	2	22,25,26	1.46	4 (18%)	31,36,39	2.19	7 (22%)
2	OMU	2	1288	2	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
2	4AC	2	1842	2	21,24,25	1.11	2 (9%)	29,34,37	1.23	3 (10%)
2	PSU	2	36	2	18,21,22	1.37	2 (11%)	22,30,33	1.95	3 (13%)
2	A2M	2	484	2	22,25,26	1.45	4 (18%)	31,36,39	2.11	9 (29%)
21	SAC	S	2	21	7,8,9	0.53	0	8,9,11	0.91	1 (12%)
2	A2M	2	576	2	22,25,26	1.45	4 (18%)	31,36,39	2.13	10 (32%)
24	AME	V	1	24	9,10,11	0.47	0	9,11,13	0.88	1 (11%)
2	PSU	2	649	2	18,21,22	1.34	2 (11%)	22,30,33	1.90	4 (18%)
2	OMG	2	1328	2	23,26,27	1.20	3 (13%)	33,38,41	1.94	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	2	1045	2	18,21,22	1.33	2 (11%)	22,30,33	1.89	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	2	1703	2	-	1/9/27/28	0/2/2/2
2	PSU	2	109	2	-	0/7/25/26	0/2/2/2
2	MA6	2	1850	2	-	0/11/29/30	0/3/3/3
2	PSU	2	119	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1238	2	-	0/7/25/26	0/2/2/2
2	A2M	2	512	2	-	3/9/27/28	0/3/3/3
2	PSU	2	651	2	-	0/7/25/26	0/2/2/2
2	A2M	2	1031	2	-	0/9/27/28	0/3/3/3
2	OMU	2	354	2	-	1/9/27/28	0/2/2/2
2	A2M	2	27	39,2	-	0/9/27/28	0/3/3/3
2	OMG	2	601	2	-	0/9/27/28	0/3/3/3
2	PSU	2	814	2	-	0/7/25/26	0/2/2/2
2	OMU	2	116	2	-	1/9/27/28	0/2/2/2
2	A2M	2	99	39,2	-	2/9/27/28	0/3/3/3
2	PSU	2	1174	2	-	0/7/25/26	0/2/2/2
2	6MZ	2	1832	39,2	-	0/9/27/28	0/3/3/3
2	PSU	2	1244	2	-	0/7/25/26	0/2/2/2
2	PSU	2	609	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1367	2	-	0/7/25/26	0/2/2/2
2	A2M	2	1678	2	-	0/9/27/28	0/3/3/3
2	OMG	2	644	2	-	3/9/27/28	0/3/3/3
2	OMC	2	462	2	-	0/9/27/28	0/2/2/2
2	PSU	2	1643	39,2	-	0/7/25/26	0/2/2/2
2	PSU	2	1347	2	-	0/7/25/26	0/2/2/2
2	A2M	2	668	39,2	-	4/9/27/28	0/3/3/3
2	OMU	2	1326	39,2	-	0/9/27/28	0/2/2/2
2	PSU	2	1177	2	-	0/7/25/26	0/2/2/2
2	G7M	2	1639	2	-	0/7/25/26	0/3/3/3
2	OMU	2	1804	2	-	0/9/27/28	0/2/2/2
2	PSU	2	686	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1081	2	-	1/7/25/26	0/2/2/2
2	OMU	2	121	2	-	0/9/27/28	0/2/2/2
2	PSU	2	966	2	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	2	1442	39,2	-	0/9/27/28	0/2/2/2
2	PSU	2	1232	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1447	2	-	2/9/27/28	0/3/3/3
2	OMU	2	428	2	-	4/9/27/28	0/2/2/2
2	PSU	2	34	2	-	0/7/25/26	0/2/2/2
2	A2M	2	159	2	-	0/9/27/28	0/3/3/3
2	A2M	2	166	2	-	0/9/27/28	0/3/3/3
2	OMU	2	172	2	-	0/9/27/28	0/2/2/2
2	PSU	2	681	2	-	0/7/25/26	0/2/2/2
2	OMG	2	509	39,2	-	3/9/27/28	0/3/3/3
2	PSU	2	801	2	-	1/7/25/26	0/2/2/2
2	OMC	2	1272	2	-	1/9/27/28	0/2/2/2
2	PSU	2	1136	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1004	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1490	39,2	-	0/9/27/28	0/3/3/3
2	OMC	2	517	2	-	0/9/27/28	0/2/2/2
2	OMC	2	1391	2	-	1/9/27/28	0/2/2/2
2	PSU	2	1692	2	-	0/7/25/26	0/2/2/2
2	A2M	2	1383	2	-	0/9/27/28	0/3/3/3
2	PSU	2	1625	2	-	0/7/25/26	0/2/2/2
2	PSU	2	1046	2	-	0/7/25/26	0/2/2/2
26	HY3	X	62	26	-	1/1/12/14	0/1/1/1
2	PSU	2	210	2	-	0/7/25/26	0/2/2/2
2	PSU	2	218	2	-	0/7/25/26	0/2/2/2
2	PSU	2	296	2	-	0/7/25/26	0/2/2/2
2	PSU	2	863	2	-	0/7/25/26	0/2/2/2
2	OMG	2	683	2	-	1/9/27/28	0/3/3/3
2	OMC	2	174	39,2	-	0/9/27/28	0/2/2/2
2	OMC	2	797	2	-	1/9/27/28	0/2/2/2
2	PSU	2	1445	2	-	0/7/25/26	0/2/2/2
2	PSU	2	105	2	-	0/7/25/26	0/2/2/2
2	PSU	2	406	2	-	0/7/25/26	0/2/2/2
17	IAS	O	138	17	-	1/7/7/8	-
2	4AC	2	1337	2	-	2/11/29/30	0/2/2/2
2	PSU	2	866	2	-	0/7/25/26	0/2/2/2
22	NMM	T	67	22	-	0/9/11/13	-
2	B8N	2	1248	2	-	4/16/34/35	0/2/2/2
2	PSU	2	822	2	-	2/7/25/26	0/2/2/2
2	PSU	2	1056	2	-	0/7/25/26	0/2/2/2
2	PSU	2	93	2	-	0/7/25/26	0/2/2/2
2	OMG	2	436	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMU	2	799	2	-	2/9/27/28	0/2/2/2
2	MA6	2	1851	2	-	1/11/29/30	0/3/3/3
3	SAC	A	2	3	-	1/7/8/10	-
2	PSU	2	572	2	-	0/7/25/26	0/2/2/2
2	PSU	2	815	2	-	0/7/25/26	0/2/2/2
2	OMU	2	627	2	-	1/9/27/28	0/2/2/2
2	A2M	2	468	2	-	0/9/27/28	0/3/3/3
2	A2M	2	590	2	-	3/9/27/28	0/3/3/3
2	OMU	2	1288	2	-	0/9/27/28	0/2/2/2
2	4AC	2	1842	2	-	2/11/29/30	0/2/2/2
2	PSU	2	36	2	-	0/7/25/26	0/2/2/2
2	A2M	2	484	2	-	2/9/27/28	0/3/3/3
21	SAC	S	2	21	-	0/7/8/10	-
2	A2M	2	576	2	-	3/9/27/28	0/3/3/3
24	AME	V	1	24	-	2/9/10/12	-
2	PSU	2	649	2	-	0/7/25/26	0/2/2/2
2	OMG	2	1328	2	-	0/9/27/28	0/3/3/3
2	PSU	2	1045	2	-	0/7/25/26	0/2/2/2

The worst 5 of 216 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1639	G7M	C4-N9	7.91	1.58	1.38
2	2	1639	G7M	O6-C6	7.52	1.37	1.23
2	2	1850	MA6	C5-N7	6.82	1.51	1.39
2	2	1851	MA6	C5-N7	6.81	1.51	1.39
2	2	1639	G7M	C5-C4	6.17	1.53	1.38

The worst 5 of 410 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	1850	MA6	C4-N9-C8	14.46	121.39	105.73
2	2	1851	MA6	C4-N9-C8	14.39	121.32	105.73
2	2	1639	G7M	C8-N7-C5	11.31	121.92	107.78
2	2	1850	MA6	N3-C4-N9	6.98	138.59	127.08
2	2	590	A2M	C5-C4-N3	-6.97	117.66	126.75

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	428	OMU	C2'-C1'-N1-C2
2	2	428	OMU	C2'-C1'-N1-C6
2	2	644	OMG	O4'-C4'-C5'-O5'
2	2	644	OMG	C3'-C4'-C5'-O5'
2	2	668	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

38 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	1703	OMC	1	0
2	2	1850	MA6	1	0
2	2	512	A2M	1	0
2	2	1031	A2M	2	0
2	2	354	OMU	1	0
2	2	27	A2M	1	0
2	2	601	OMG	1	0
2	2	116	OMU	1	0
2	2	1678	A2M	1	0
2	2	462	OMC	1	0
2	2	668	A2M	1	0
2	2	1804	OMU	1	0
2	2	121	OMU	1	0
2	2	1442	OMU	1	0
2	2	1232	PSU	1	0
2	2	1447	OMG	2	0
2	2	428	OMU	1	0
2	2	166	A2M	2	0
2	2	681	PSU	1	0
2	2	509	OMG	2	0
2	2	801	PSU	1	0
2	2	1272	OMC	2	0
2	2	1490	OMG	1	0
2	2	517	OMC	1	0
2	2	1391	OMC	1	0
2	2	1383	A2M	1	0
2	2	1445	PSU	1	0
2	2	1337	4AC	2	0
2	2	436	OMG	2	0
2	2	799	OMU	4	0
3	A	2	SAC	1	0
2	2	468	A2M	1	0
2	2	1288	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	1842	4AC	2	0
2	2	36	PSU	1	0
2	2	484	A2M	1	0
2	2	576	A2M	1	0
24	V	1	AME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 117 are unknown and 114 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

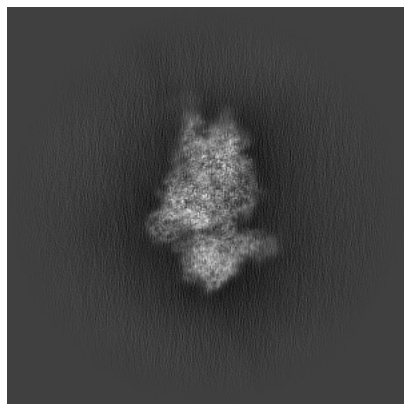
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17804. These allow visual inspection of the internal detail of the map and identification of artifacts.

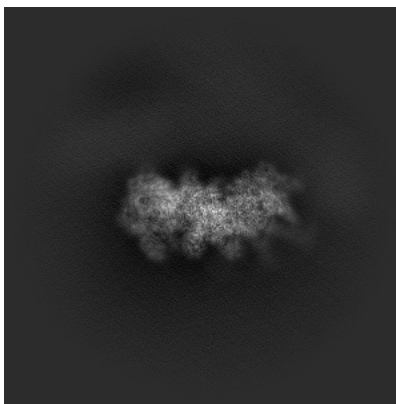
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

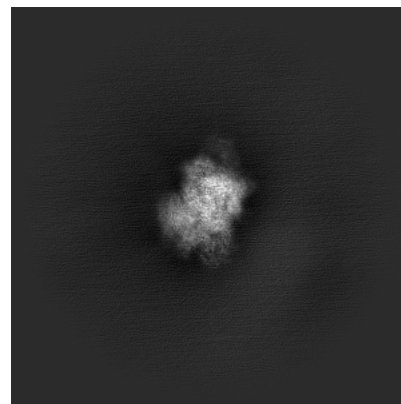
6.1.1 Primary map



X

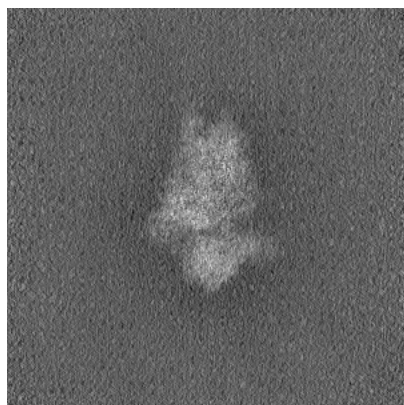


Y

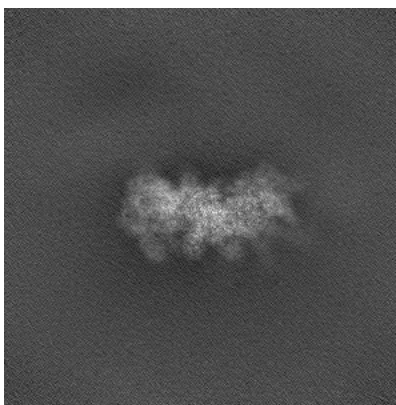


Z

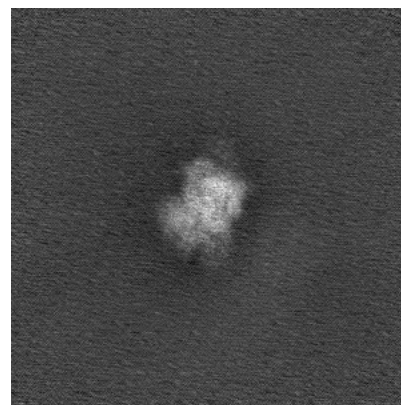
6.1.2 Raw map



X



Y

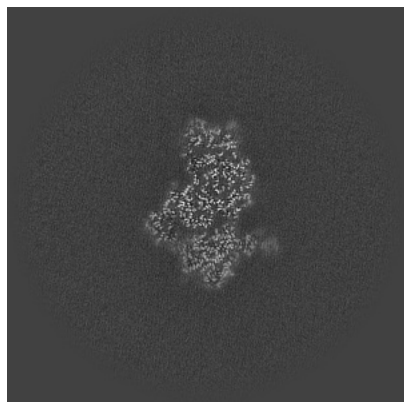


Z

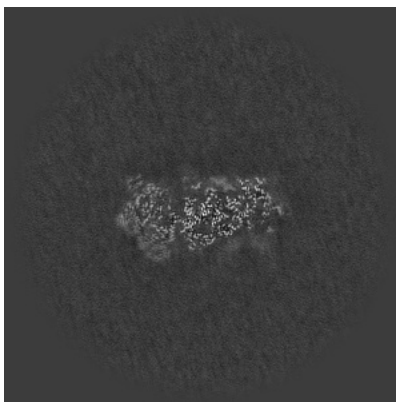
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

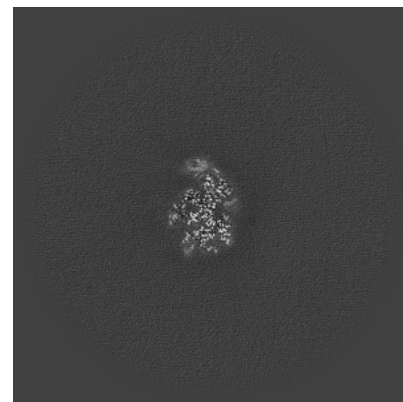
6.2.1 Primary map



X Index: 280

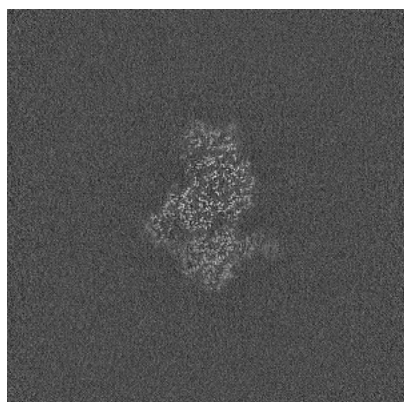


Y Index: 280

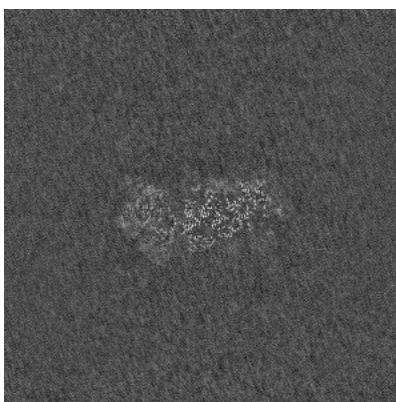


Z Index: 280

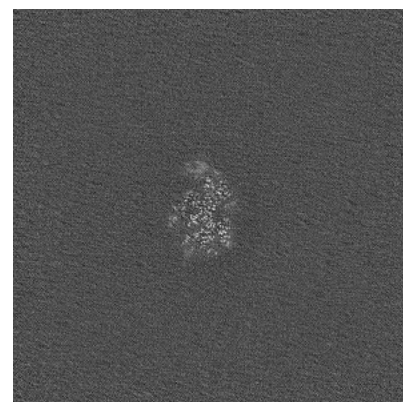
6.2.2 Raw map



X Index: 280



Y Index: 280

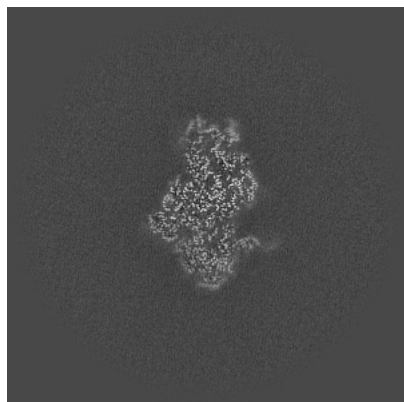


Z Index: 280

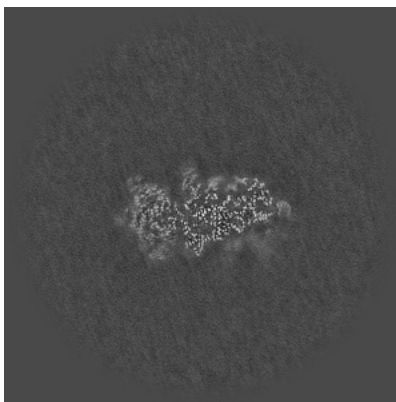
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

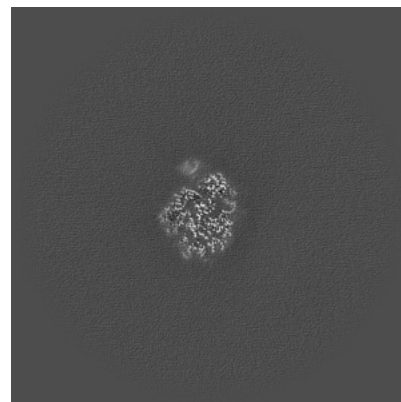
6.3.1 Primary map



X Index: 274

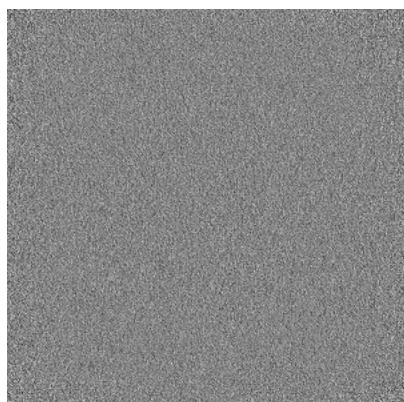


Y Index: 275

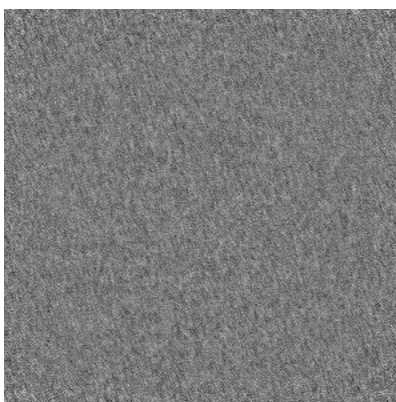


Z Index: 274

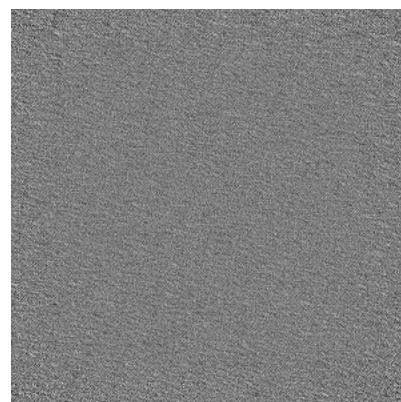
6.3.2 Raw map



X Index: 0



Y Index: 0

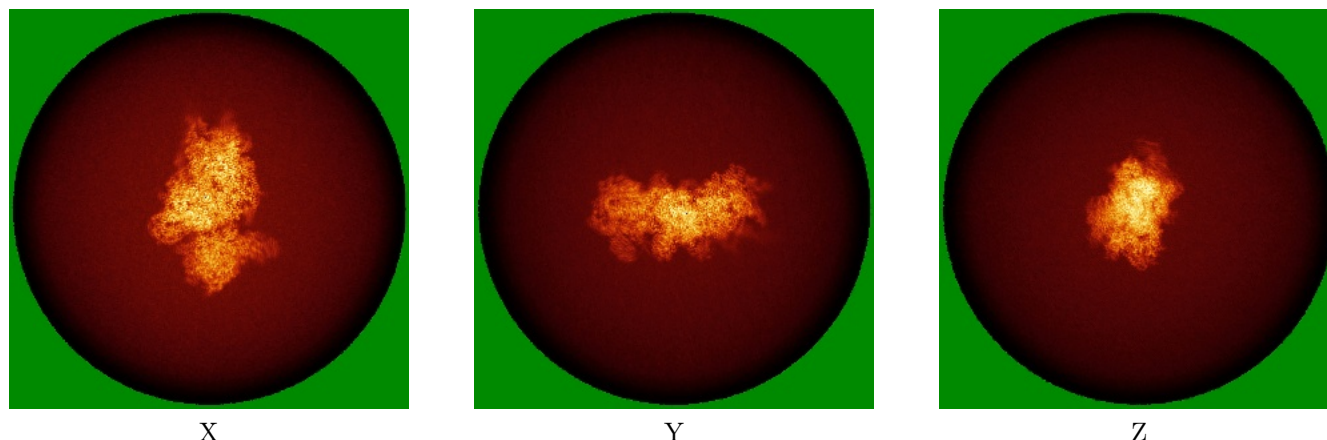


Z Index: 0

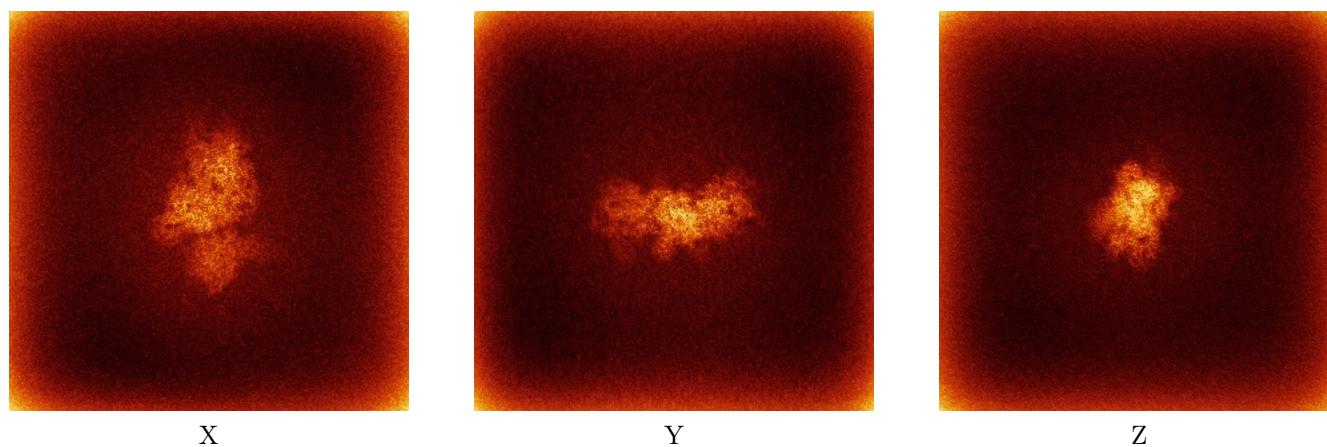
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



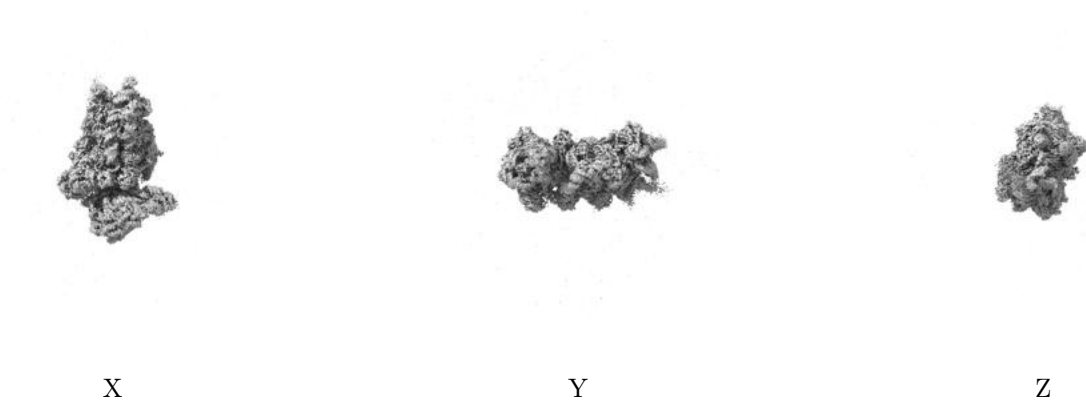
6.4.2 Raw map



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.

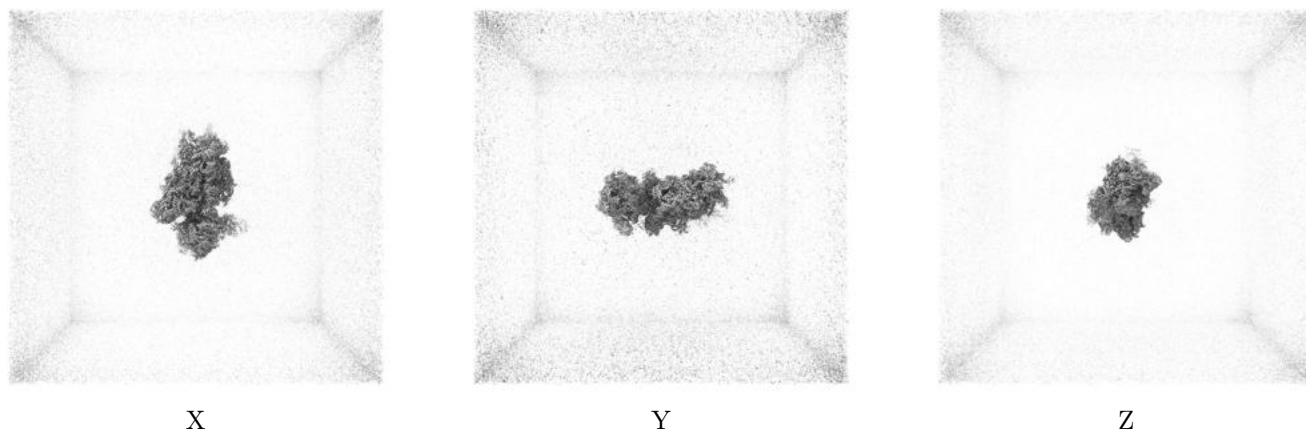
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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



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

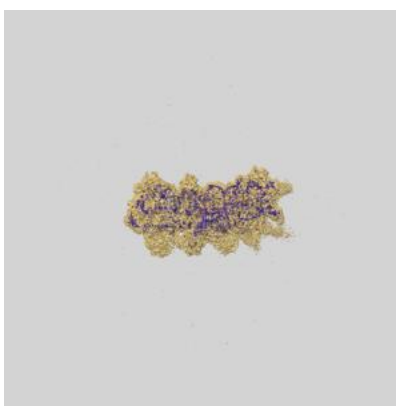
A mask typically either:

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

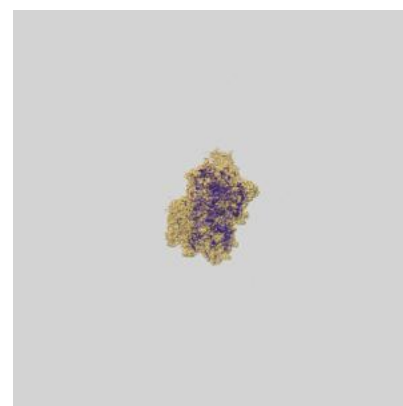
6.6.1 emd_17804_msk_1.map [i](#)



X

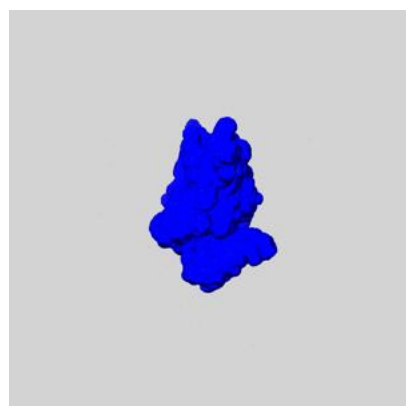


Y

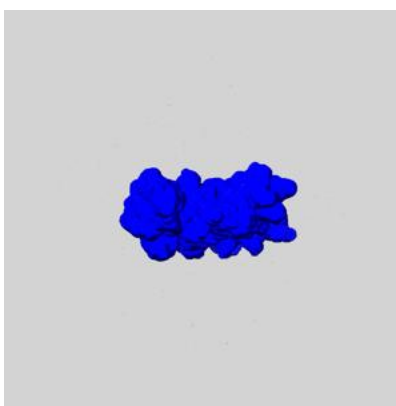


Z

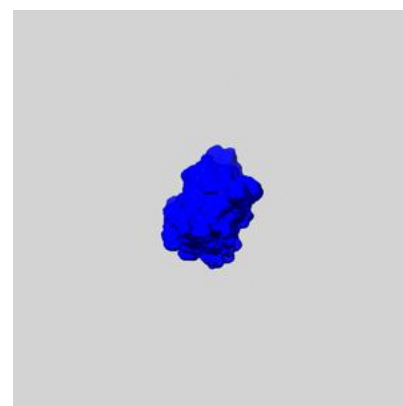
6.6.2 emd_17804_msk_2.map [i](#)



X



Y

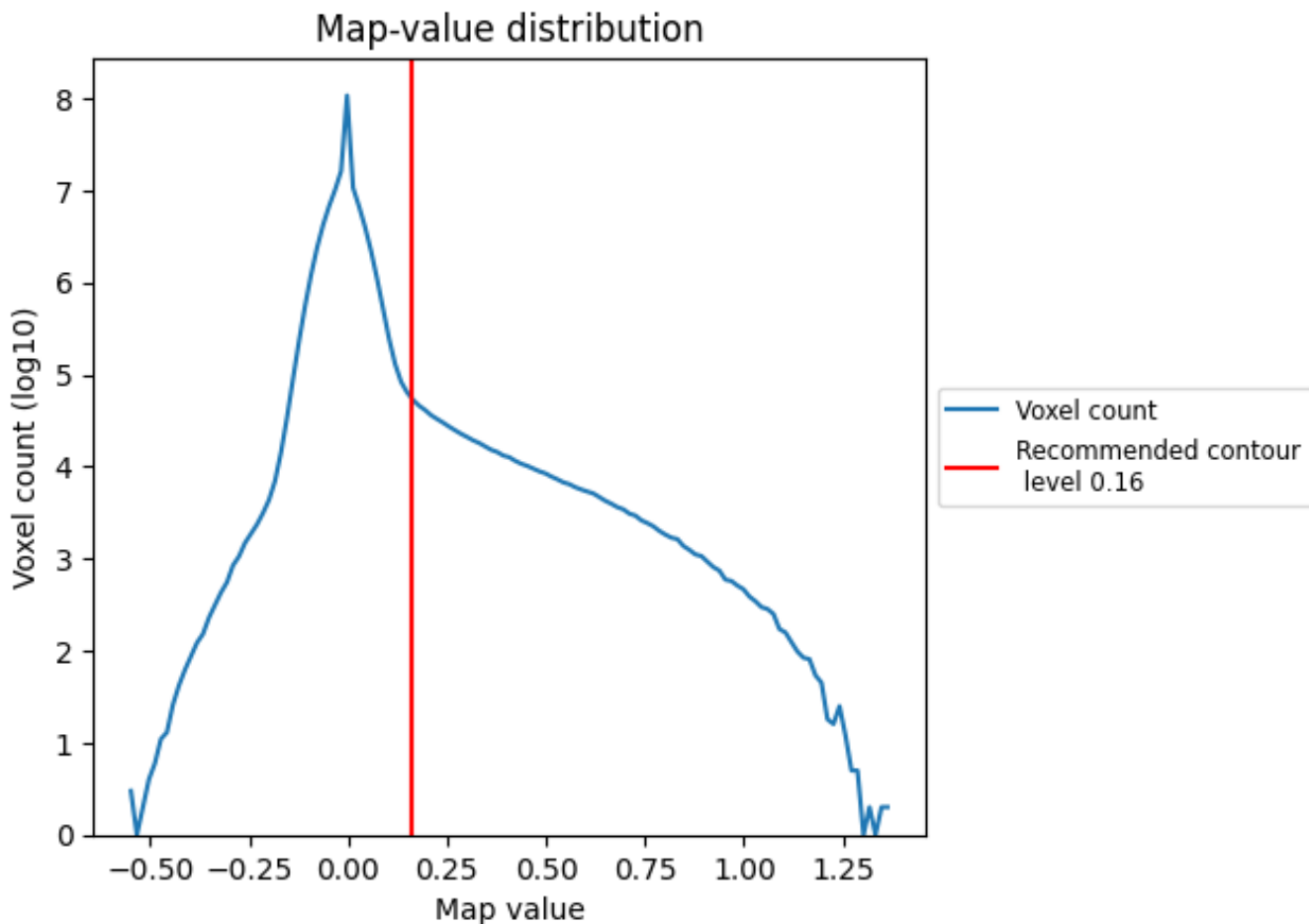


Z

7 Map analysis [i](#)

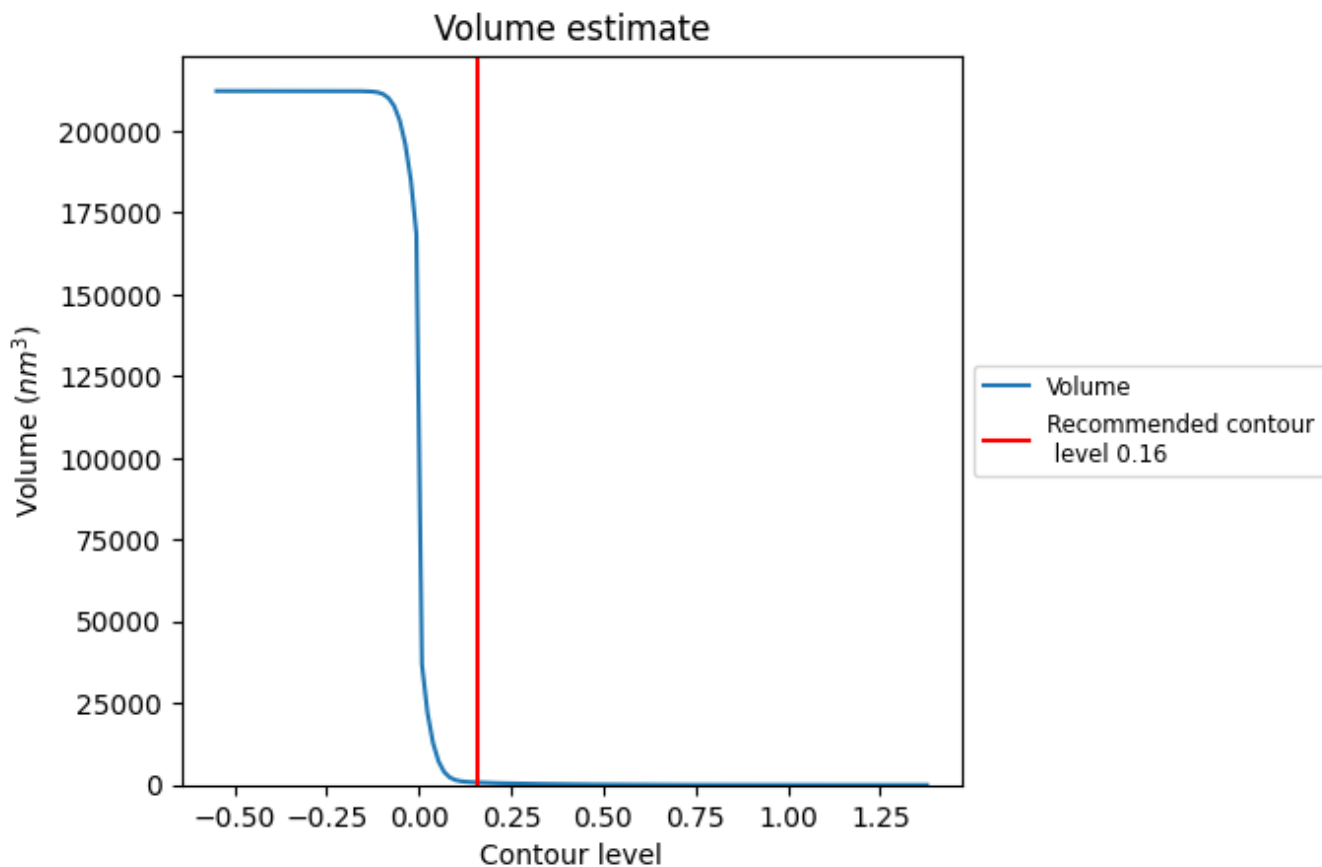
This section contains the results of statistical analysis of the map.

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.

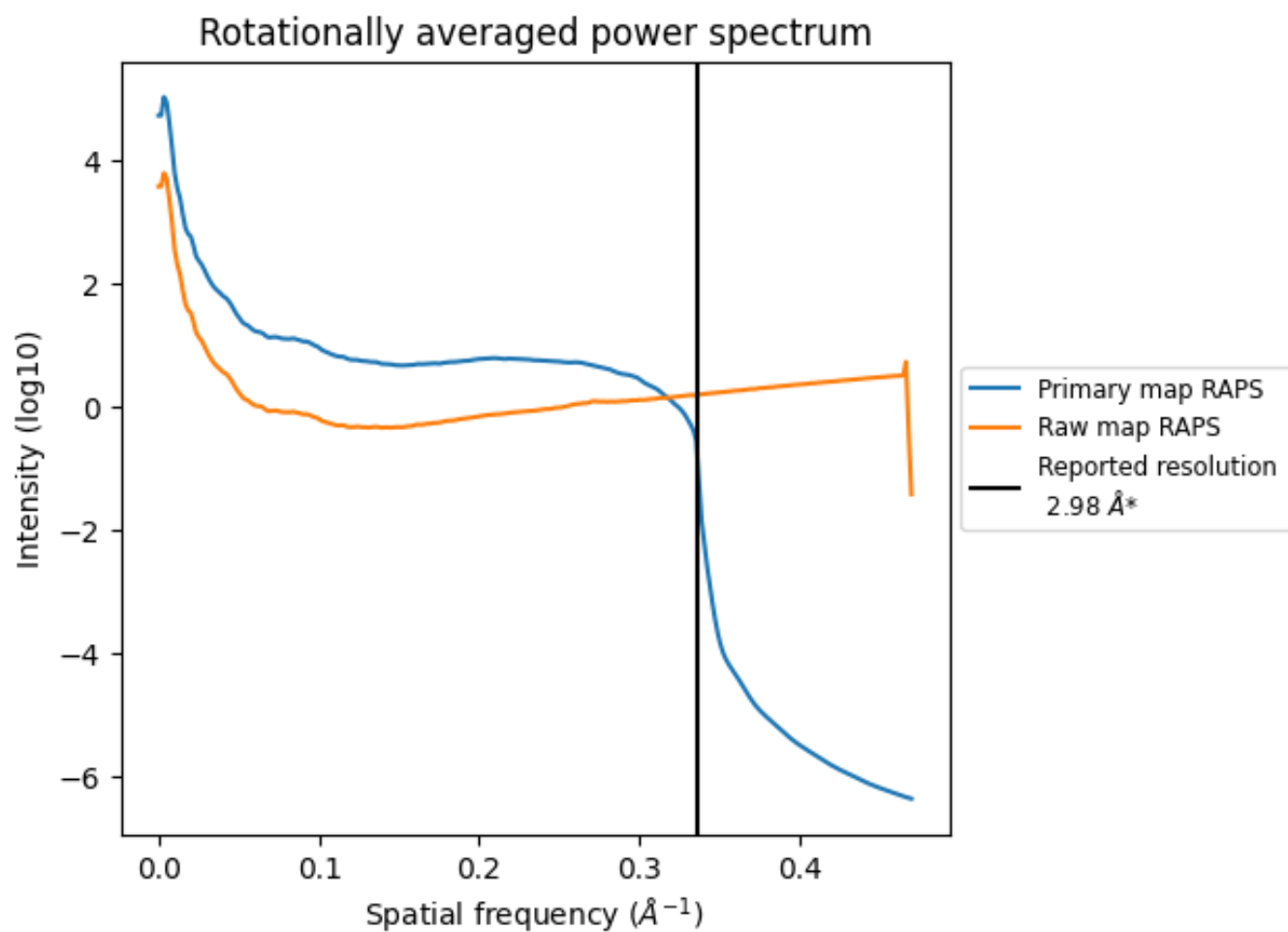
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 753 nm³; this corresponds to an approximate mass of 680 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

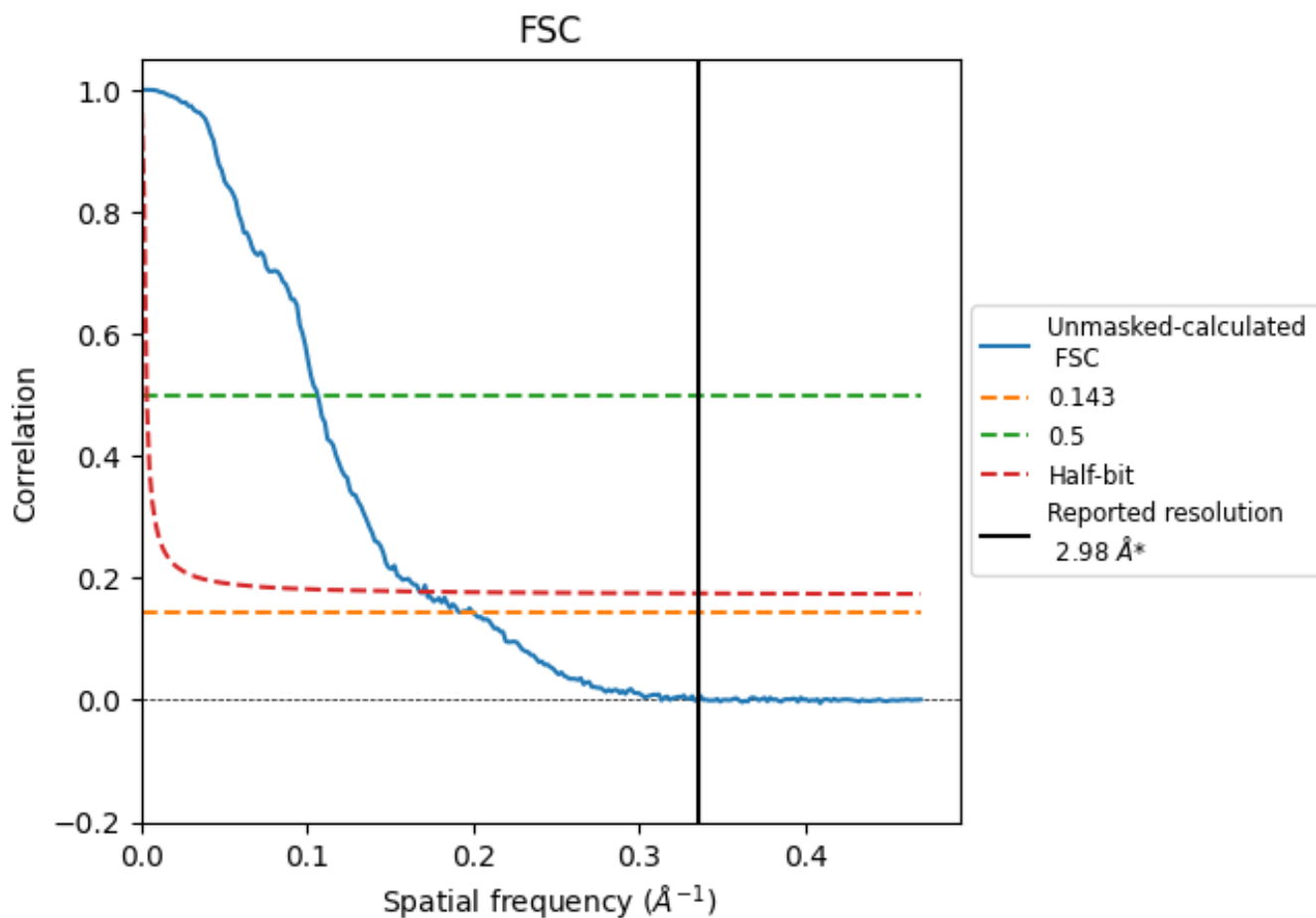


*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

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 0.336 Å⁻¹

8.2 Resolution estimates [i](#)

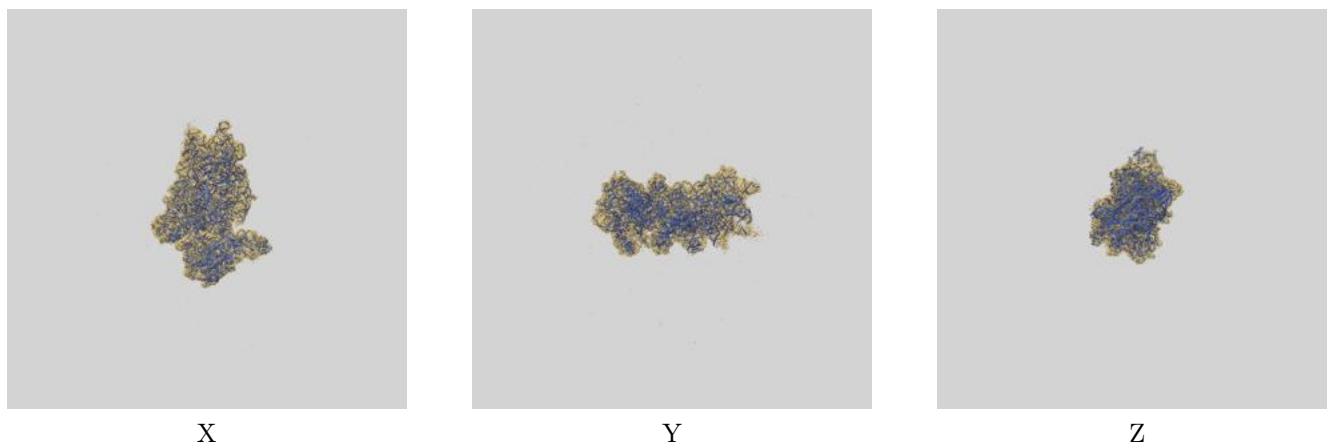
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.00	9.42	5.97

*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 5.00 differs from the reported value 2.98 by more than 10 %

9 Map-model fit [i](#)

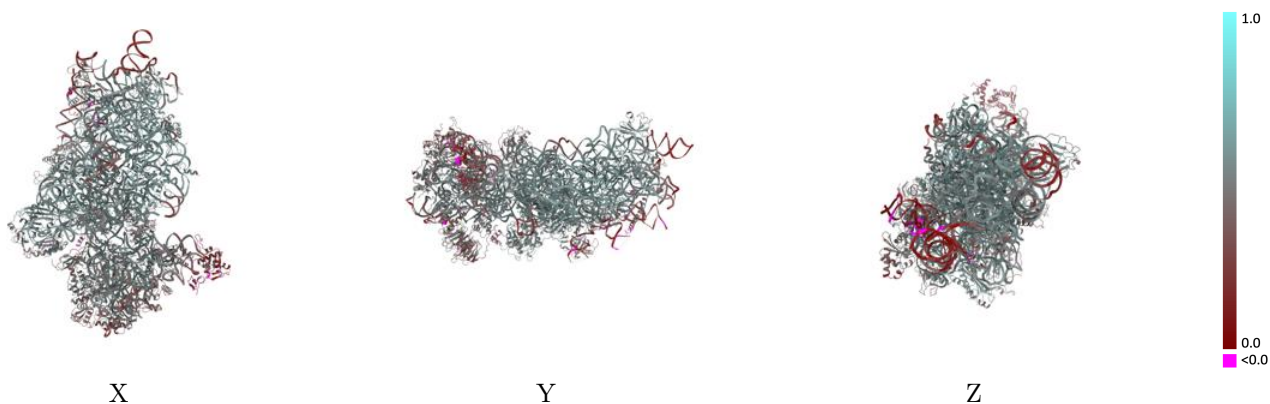
This section contains information regarding the fit between EMDB map EMD-17804 and PDB model 8PPK. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



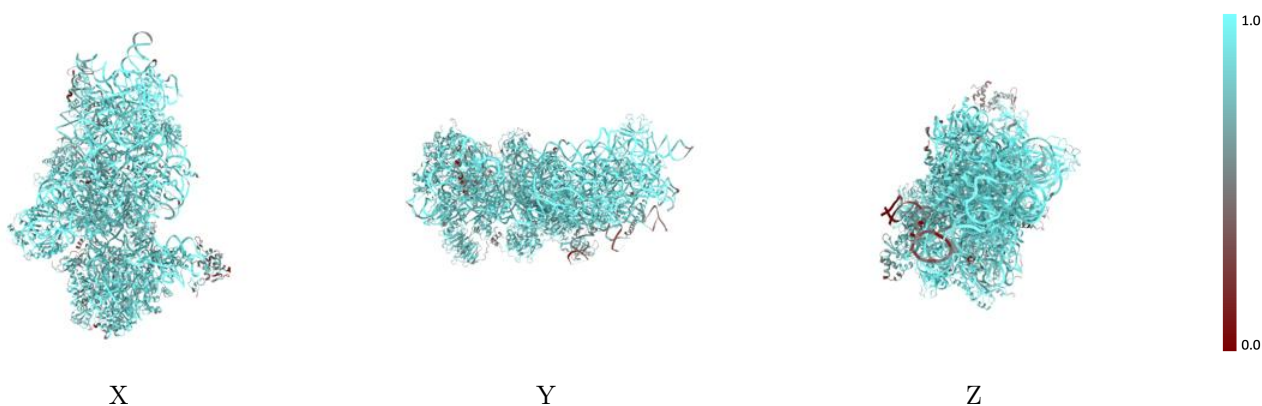
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



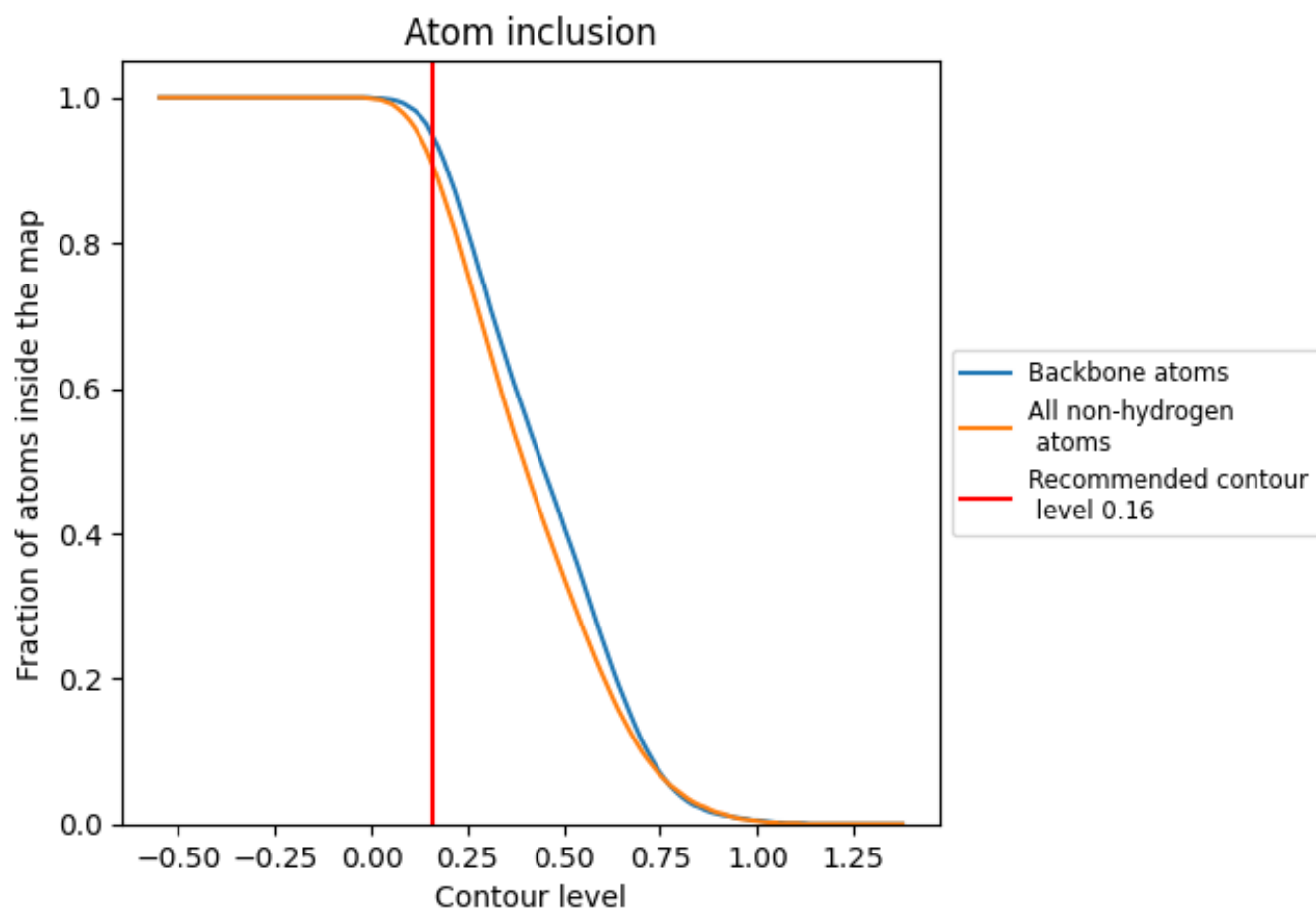
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 91% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9070	 0.4890
2	 0.9540	 0.4970
A	 0.9080	 0.5210
B	 0.9050	 0.5110
C	 0.9470	 0.5610
D	 0.8700	 0.4880
E	 0.9470	 0.5620
F	 0.8420	 0.4650
G	 0.8870	 0.4820
H	 0.7610	 0.4380
I	 0.9050	 0.5210
J	 0.9490	 0.5590
K	 0.8740	 0.4470
L	 0.8670	 0.5160
M	 0.5190	 0.2090
N	 0.9400	 0.5330
O	 0.9210	 0.5210
P	 0.8050	 0.4120
Q	 0.9010	 0.5030
R	 0.8180	 0.4470
S	 0.7800	 0.3990
T	 0.8730	 0.4730
U	 0.8440	 0.4530
V	 0.9390	 0.5570
W	 0.9590	 0.5730
X	 0.9510	 0.5700
Y	 0.9540	 0.5550
Z	 0.7380	 0.3720
a	 0.9250	 0.5380
b	 0.9070	 0.5000
c	 0.7700	 0.4200
d	 0.9500	 0.5380
e	 0.8500	 0.5220
f	 0.5080	 0.2000
g	 0.8130	 0.3880



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Chain	Atom inclusion	Q-score
h	 0.7710	 0.4760
j	 0.7960	 0.4640
p	 0.7730	 0.4460