wwPDB EM Validation Summary Report ⓘ

Oct 15, 2024 – 10:28 am BST

PDB ID	:	8S8D
EMDB ID	:	EMD-19801
Title	:	Structure of a yeast 48S-AUC preinitiation complex in closed conformation (model py48S-AUC-2)
Authors	:	Villamayor-Belinchon, L.; Sharma, P.; Llacer, J.L.; Hussain, T.
Deposited on	:	2024-03-06
Resolution	:	3.45 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

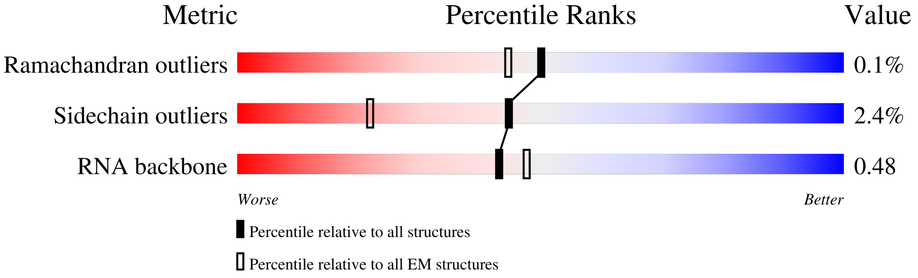
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

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

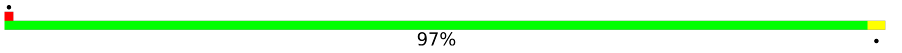
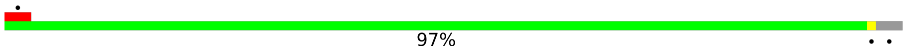
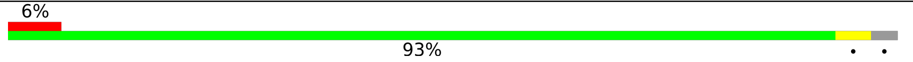
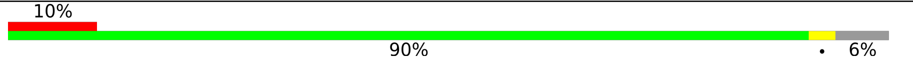
The reported resolution of this entry is 3.45 Å.

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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1798	
2	A	254	
3	B	255	
4	C	259	
5	E	261	
6	G	236	
7	H	190	
8	I	201	

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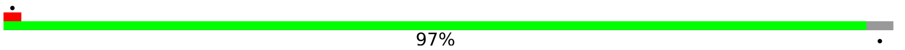
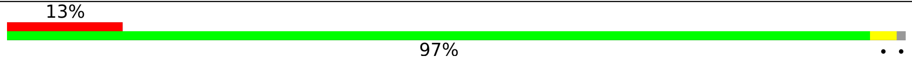
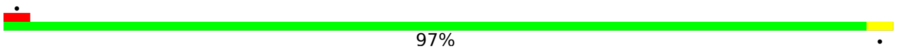
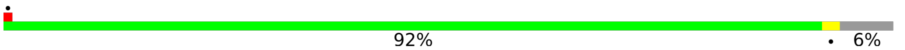
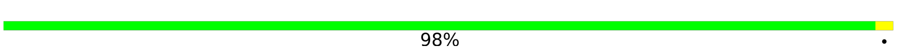
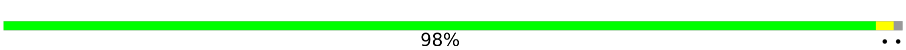
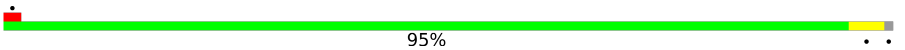
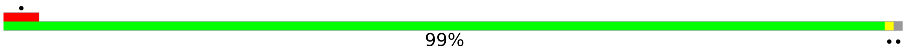
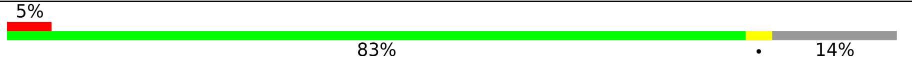
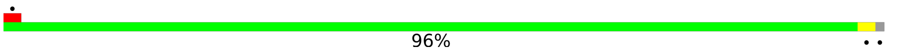
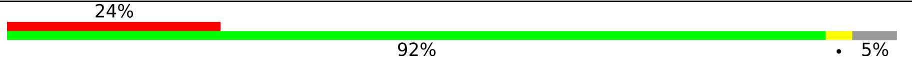
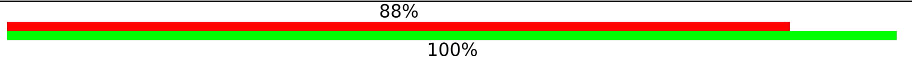
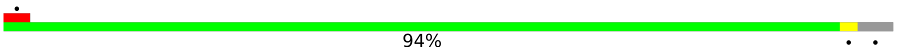
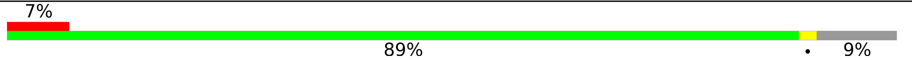
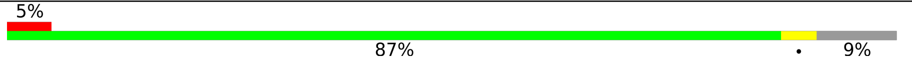
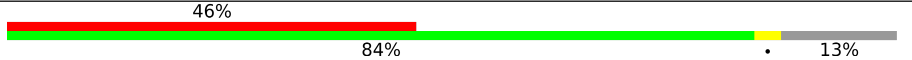
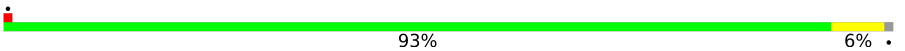
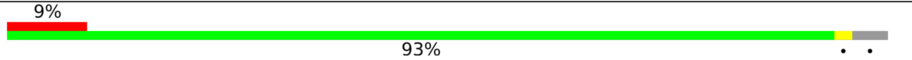
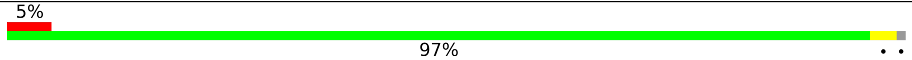
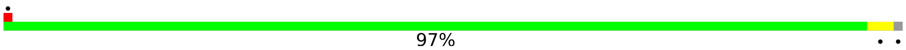
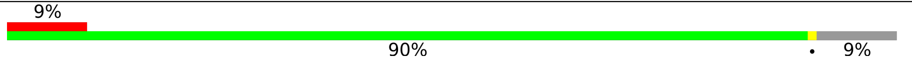
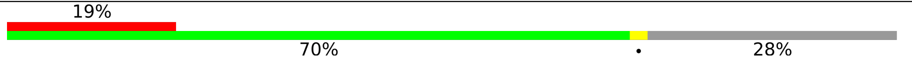
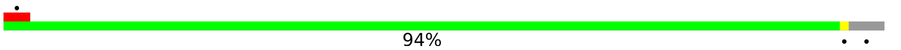
Mol	Chain	Length	Quality of chain
9	J	188	
10	L	156	
11	N	151	
12	O	137	
13	V	87	
14	W	130	
15	X	145	
16	Y	135	
17	a	119	
18	b	82	
19	e	63	
20	h	25	
21	D	237	
22	F	227	
23	K	106	
24	M	134	
25	P	142	
26	Q	143	
27	R	136	
28	S	146	
29	T	144	
30	U	117	
31	Z	108	
32	c	67	
33	d	56	

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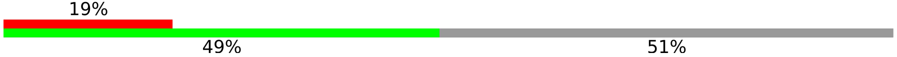
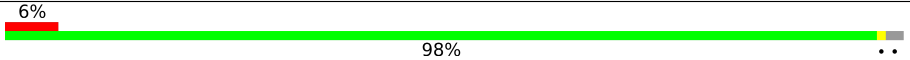
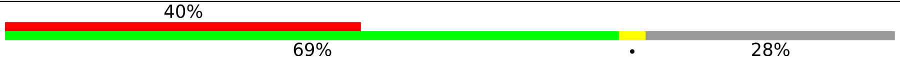
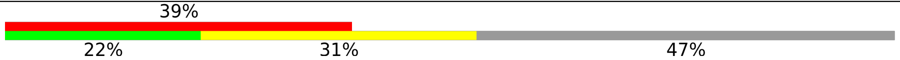
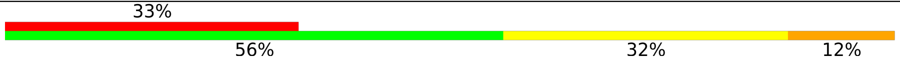
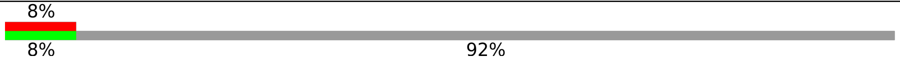
Mol	Chain	Length	Quality of chain
34	f	150	
35	g	326	
36	i	153	
37	3	49	
38	1	75	
39	j	304	
40	k	527	
41	l	285	

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 86108 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1798	Total 38190	C 17073	N 6722	O 12597	P 1798	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	219	Total 1702	C 1085	N 299	O 316	S 2	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	225	Total 1796	C 1135	N 330	O 328	S 3	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	220	Total 1648	C 1053	N 291	O 300	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	260	Total 2078	C 1322	N 393	O 359	S 4	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	230	Total 1832	C 1146	N 352	O 330	S 4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	184	Total 1483	C 950	N 270	O 263	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	188	Total 1489	C 923	N 300	O 265	S 1	0	0

- Molecule 9 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	182	Total 1471	C 929	N 287	O 254	S 1	0	0

- Molecule 10 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	155	Total 1248	C 798	N 237	O 210	S 3	0	0

- Molecule 11 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	151	Total 1195	C 761	N 224	O 207	S 3	0	0

- Molecule 12 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	129	Total 955	C 585	N 191	O 176	S 3	0	0

- Molecule 13 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	87	Total 687	C 424	N 126	O 135	S 2	0	0

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	W	129	1021	651	187	180	3	0	0

- Molecule 15 is a protein called KLLA0B11231p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	X	144	1119	708	218	191	2	0	0

- Molecule 16 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
16	Y	134	1061	665	207	189	0	0

- Molecule 17 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	a	102	797	492	168	132	5	0	0

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	b	81	609	379	112	113	5	0	0

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	e	60	472	295	96	80	1	0	0

- Molecule 20 is a protein called 40S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	h	25	233	142	63	27	1	0	0

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	D	227	1774	1126	320	323	5	0	0

- Molecule 22 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	F	206	1609	1008	298	300	3	0	0

- Molecule 23 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	K	96	809	533	129	146	1	0	0

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	M	117	885	553	161	171	0	0

- Molecule 25 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	P	117	923	592	165	161	5	0	0

- Molecule 26 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	Q	141	1105	709	204	192	0	0

- Molecule 27 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	R	130	1033	643	194	193	3	0	0

- Molecule 28 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	145	Total	C	N	O	S	0	0
			1189	739	239	209	2		

- Molecule 29 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	T	143	Total	C	N	O	0	0
			1110	693	210	207		

- Molecule 30 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	78	Total	C	N	O	S	0	0
			595	376	111	107	1		

- Molecule 32 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	64	Total	C	N	O	S	0	0
			499	308	99	91	1		

- Molecule 33 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	55	Total	C	N	O	S	0	0
			461	289	93	78	1		

- Molecule 34 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	74	Total	C	N	O	S	0	0
			584	374	111	95	4		

- Molecule 35 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	320	Total 2469	C 1561	N 432	O 471	S 5	0	0

- Molecule 36 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	110	Total 870	C 534	N 167	O 164	S 5	0	0

- Molecule 37 is a RNA chain called mRNA (5'-R(P*AP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
37	3	26	Total 536	C 242	N 84	O 184	P 26	0	0

- Molecule 38 is a RNA chain called Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1	75	Total 1639	C 734	N 298	O 531	P 76	0	0

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	267	Total 2139	C 1366	N 355	O 407	S 11	0	0

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	470	Total 3596	C 2279	N 633	O 666	S 18	0	0

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	l	23	Total 190	C 124	N 32	O 34	0	0

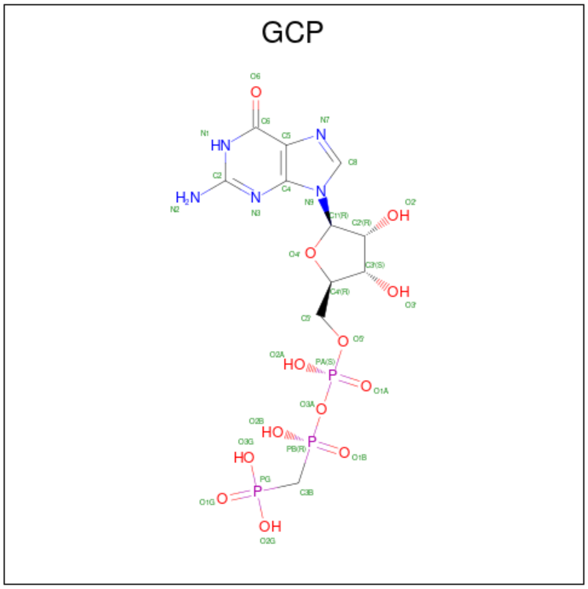
- Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
42	2	112	Total	Mg	0
			112	112	
42	T	1	Total	Mg	0
			1	1	
42	i	1	Total	Mg	0
			1	1	
42	3	1	Total	Mg	0
			1	1	
42	k	1	Total	Mg	0
			1	1	

- Molecule 43 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

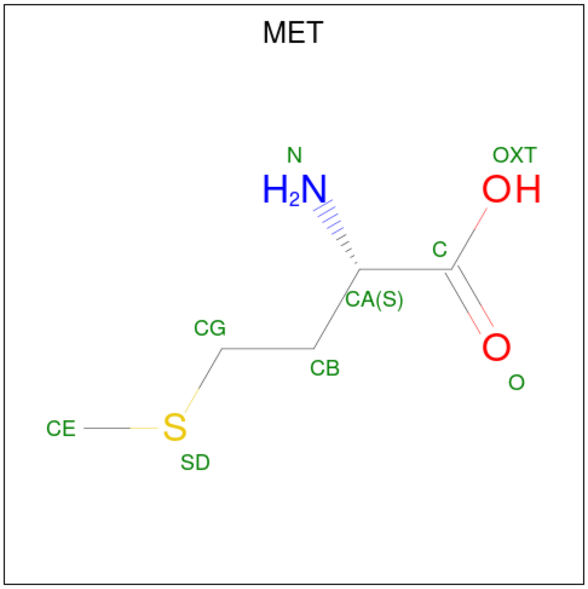
Mol	Chain	Residues	Atoms		AltConf
43	a	1	Total	Zn	0
			1	1	
43	b	1	Total	Zn	0
			1	1	
43	f	1	Total	Zn	0
			1	1	

- Molecule 44 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
44	k	1	Total	C	N	O	P	0
			32	11	5	13	3	

- Molecule 45 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
45	k	1	Total C N O S 8 5 1 1 1	0

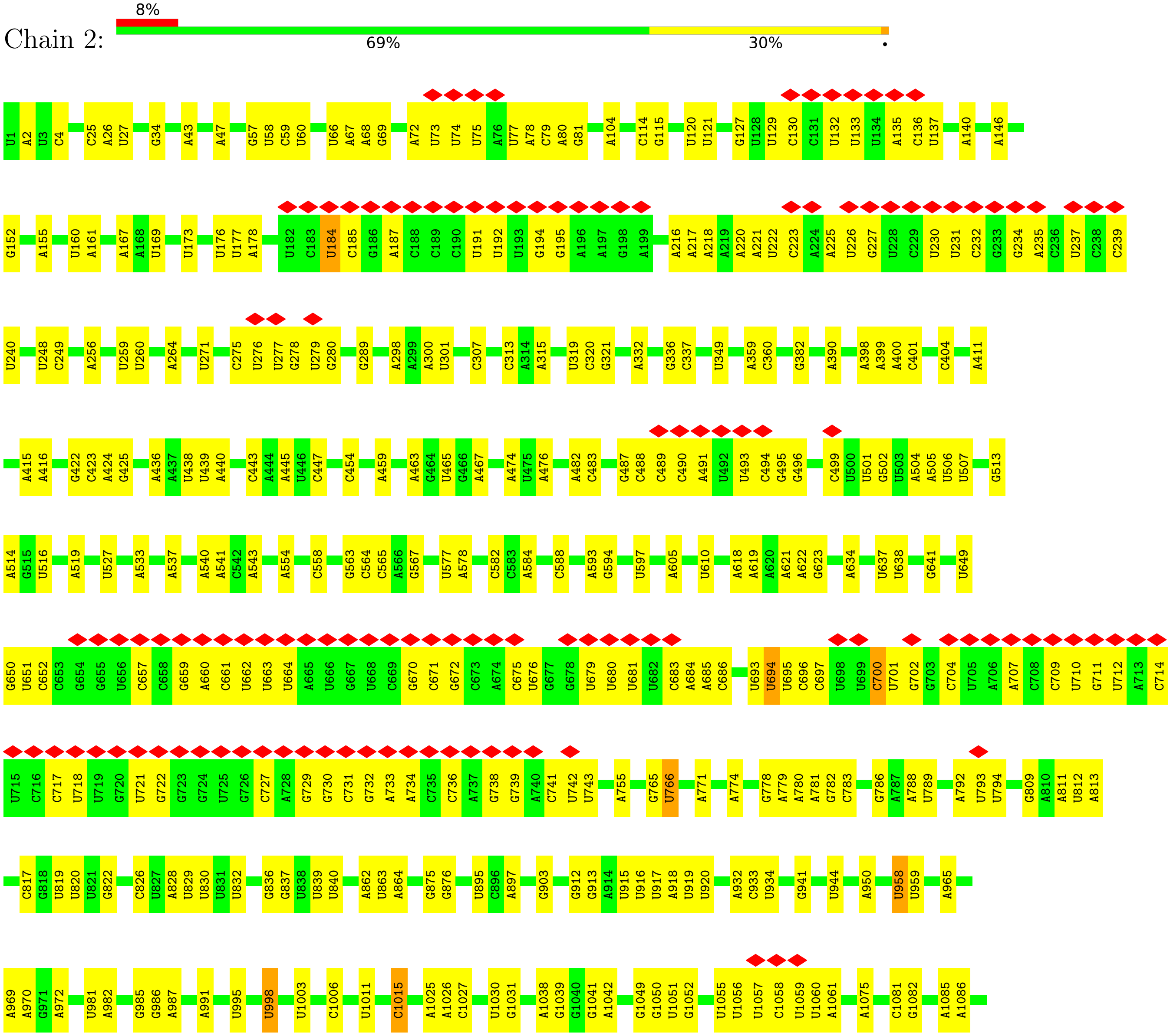
- Molecule 46 is water.

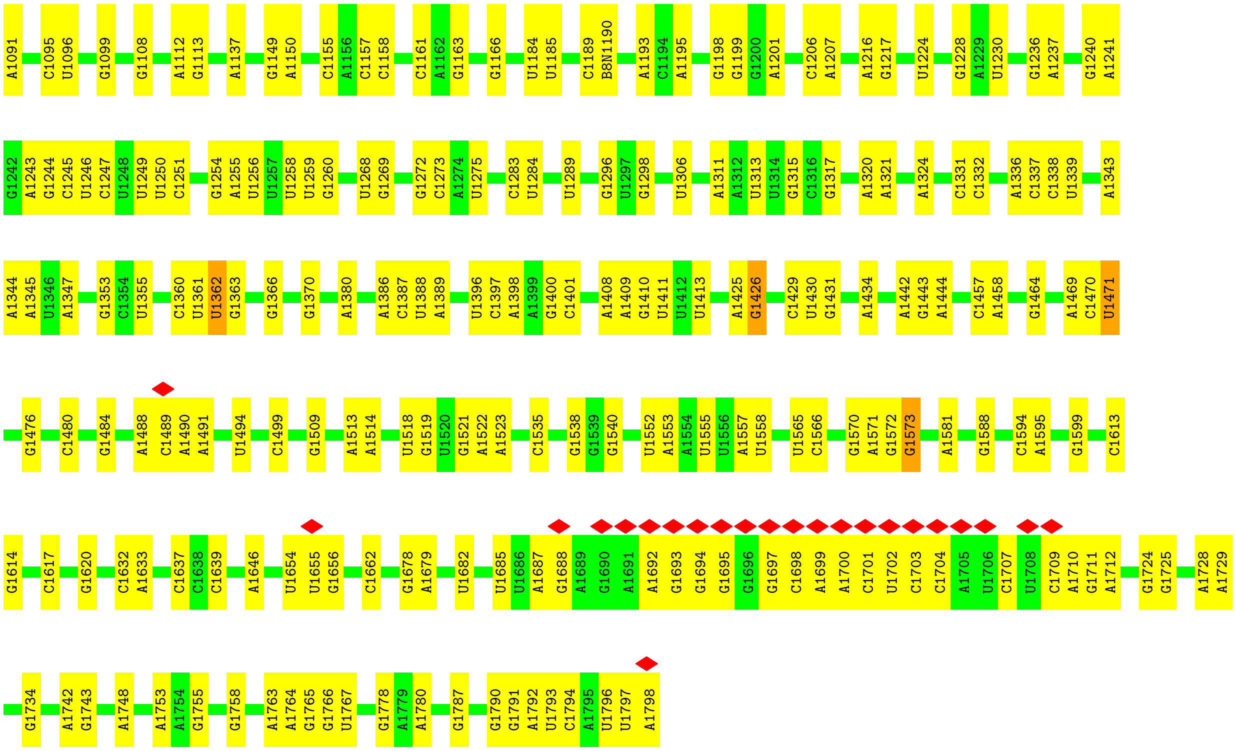
Mol	Chain	Residues	Atoms	AltConf
46	2	3	Total O 3 3	0

3 Residue-property plots ⓘ

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

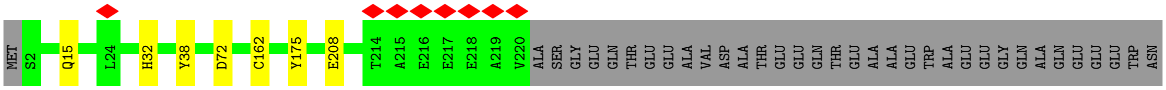
- Molecule 1: 18S ribosomal RNA





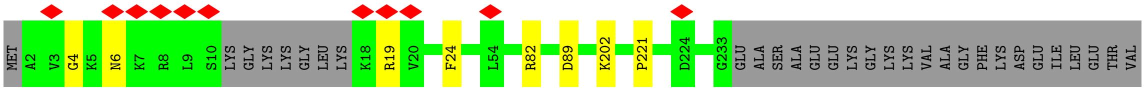
- Molecule 2: Small ribosomal subunit protein uS2

Chain A:



- Molecule 3: Small ribosomal subunit protein eS1

Chain B:

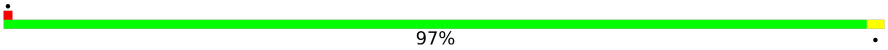


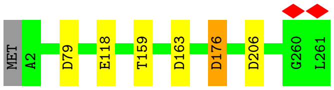
- Molecule 4: Small ribosomal subunit protein uS5

Chain C:

- Molecule 5: 40S ribosomal protein S4

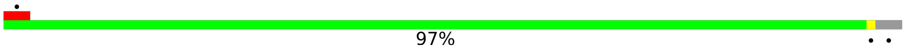
Chain E:

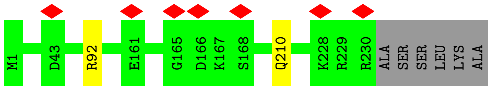




- Molecule 6: Small ribosomal subunit protein eS6

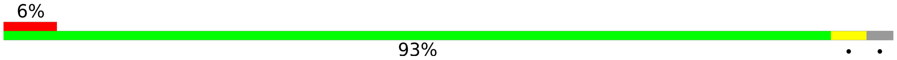
Chain G:

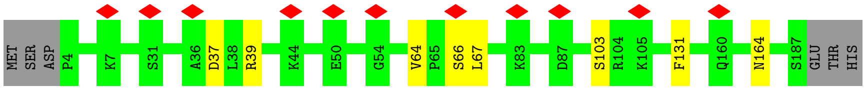




- Molecule 7: 40S ribosomal protein S7

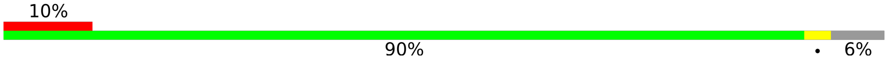
Chain H:

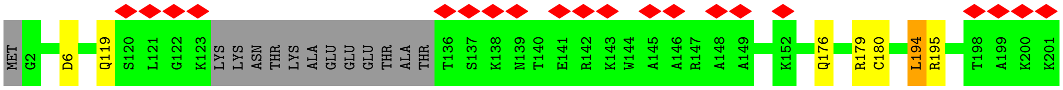




- Molecule 8: 40S ribosomal protein S8

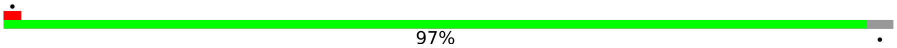
Chain I:

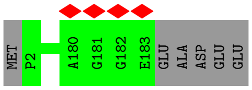




- Molecule 9: KLLA0E23673p

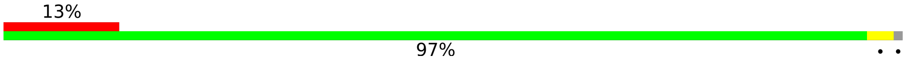
Chain J:

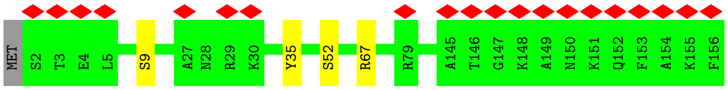




- Molecule 10: KLLA0A10483p

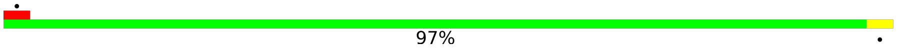
Chain L:

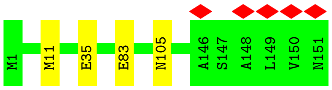




- Molecule 11: KLLA0F18040p

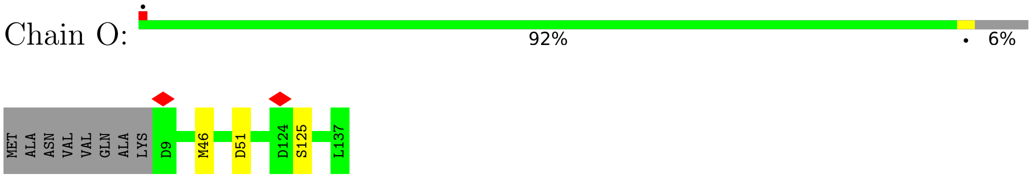
Chain N:





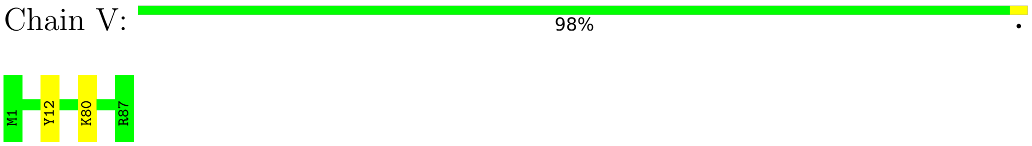
- Molecule 12: Small ribosomal subunit protein uS11

Chain O:



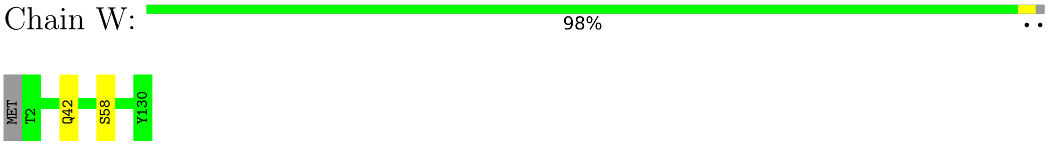
- Molecule 13: 40S ribosomal protein S21

Chain V:



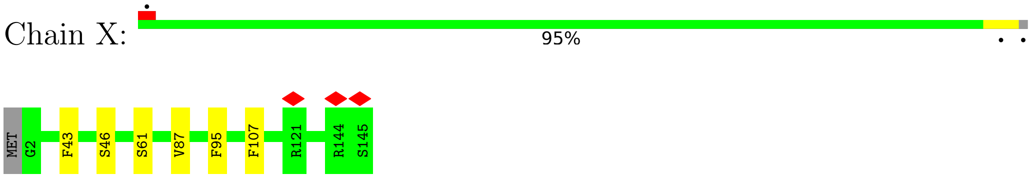
- Molecule 14: Small ribosomal subunit protein uS8

Chain W:



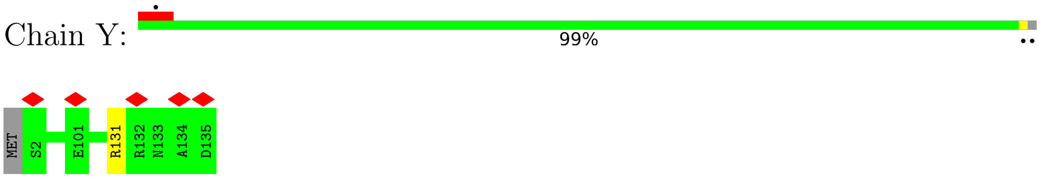
- Molecule 15: KLLA0B11231p

Chain X:



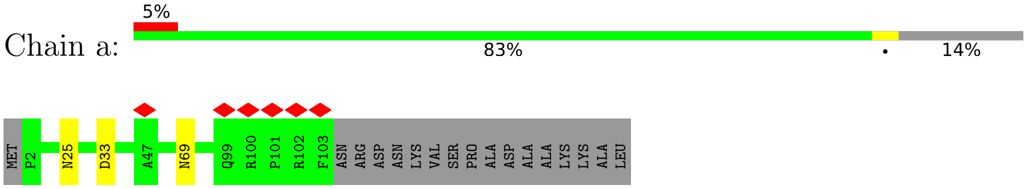
- Molecule 16: 40S ribosomal protein S24

Chain Y:



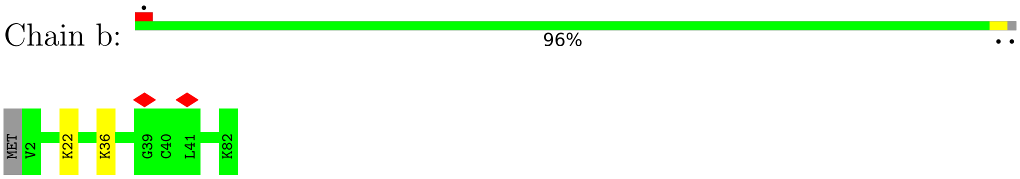
- Molecule 17: 40S ribosomal protein S26

Chain a:

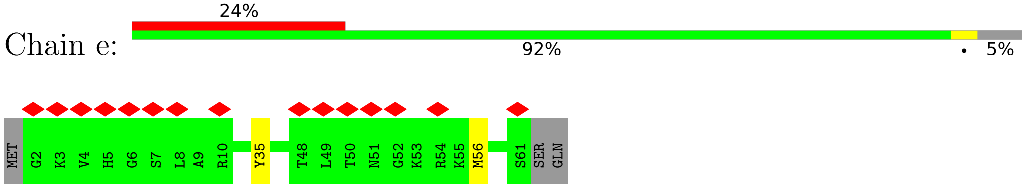


- Molecule 18: 40S ribosomal protein S27

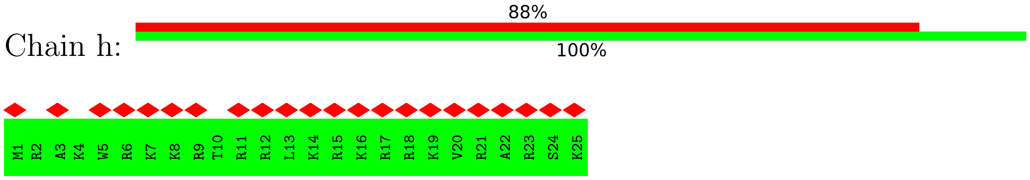
Chain b:



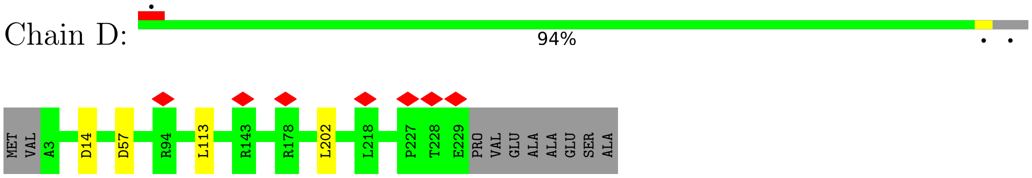
- Molecule 19: 40S ribosomal protein S30



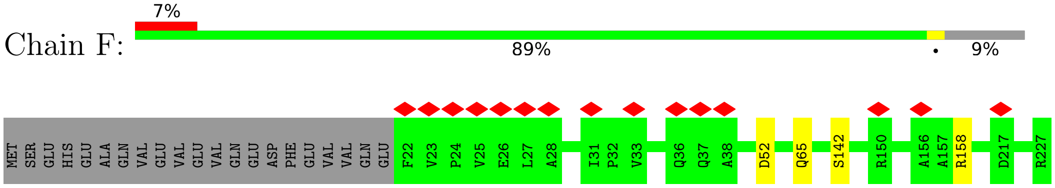
- Molecule 20: 40S ribosomal protein L41-A



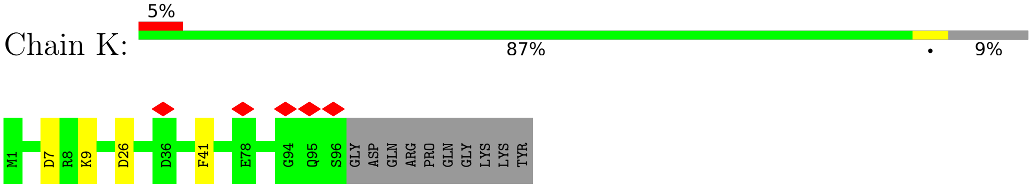
- Molecule 21: 40S ribosomal protein S3



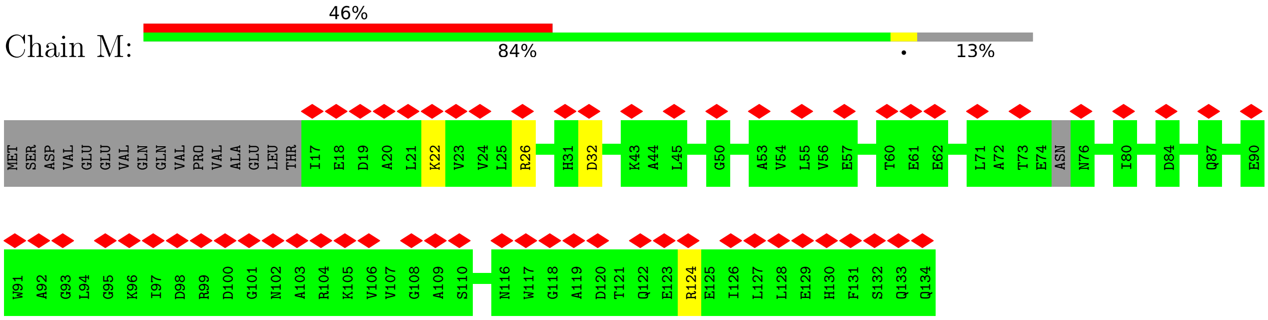
- Molecule 22: KLLA0D10659p



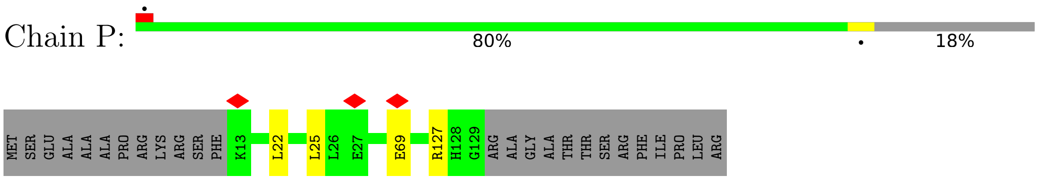
- Molecule 23: KLLA0B08173p



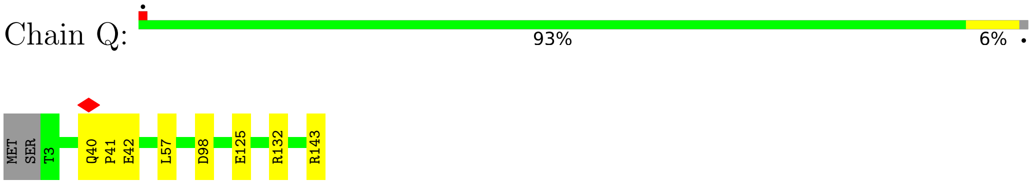
- Molecule 24: 40S ribosomal protein S12



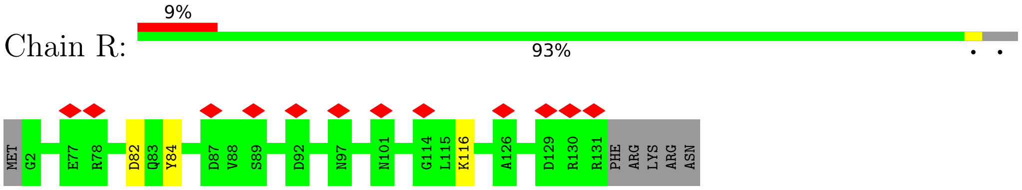
- Molecule 25: KLLA0F07843p



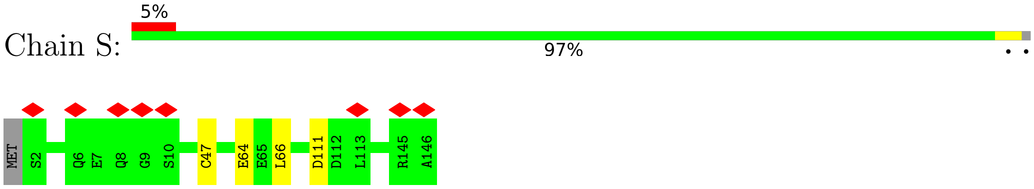
- Molecule 26: Small ribosomal subunit protein uS9



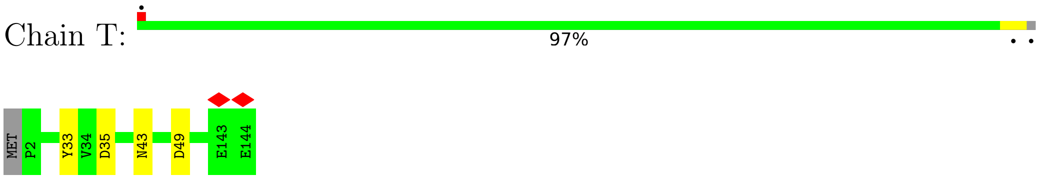
- Molecule 27: KLLA0B01474p



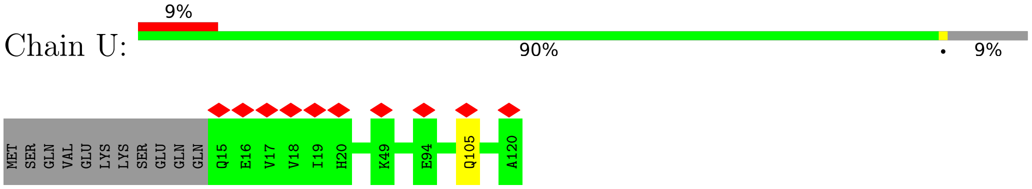
- Molecule 28: KLLA0B01562p



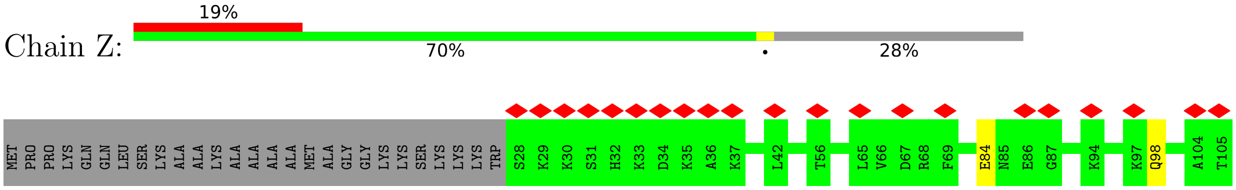
- Molecule 29: KLLA0A07194p



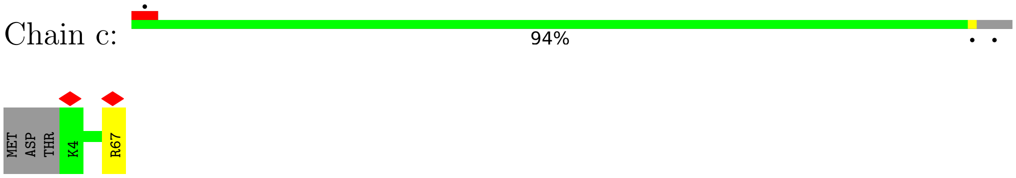
- Molecule 30: Small ribosomal subunit protein uS10



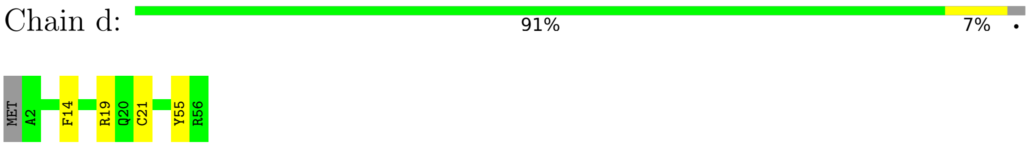
- Molecule 31: 40S ribosomal protein S25



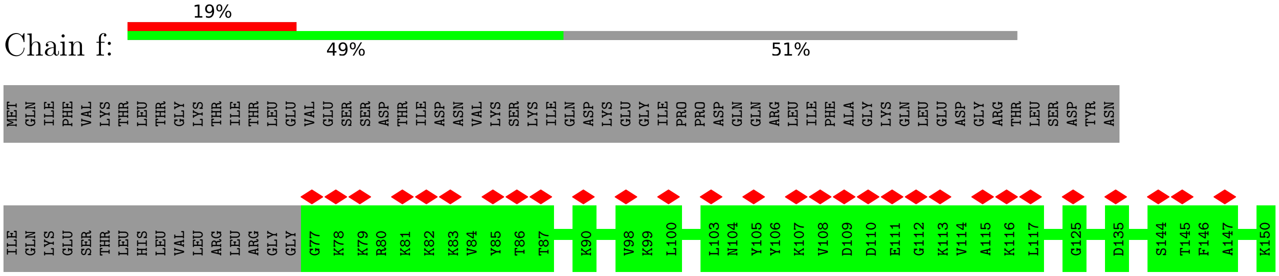
- Molecule 32: Small ribosomal subunit protein eS28



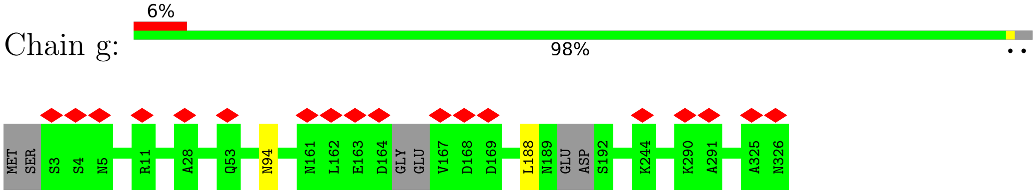
- Molecule 33: Small ribosomal subunit protein uS14



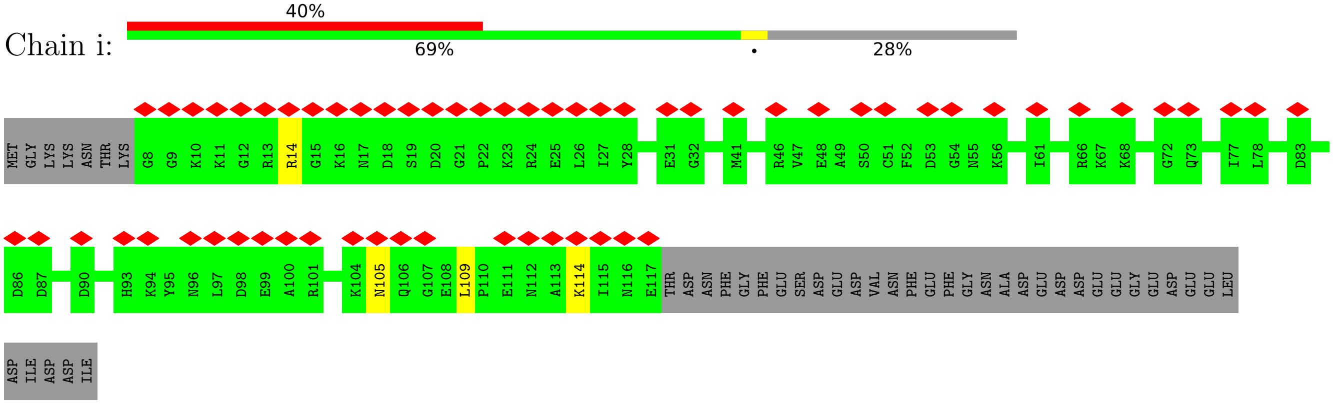
- Molecule 34: Small ribosomal subunit protein eS31



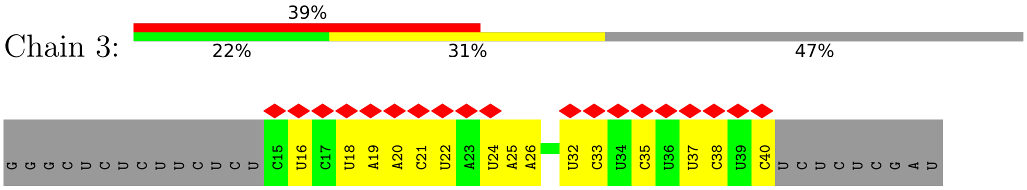
- Molecule 35: KLLA0E12277p



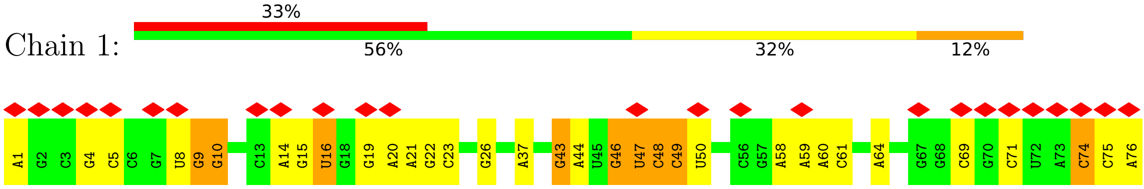
- Molecule 36: Eukaryotic translation initiation factor 1A



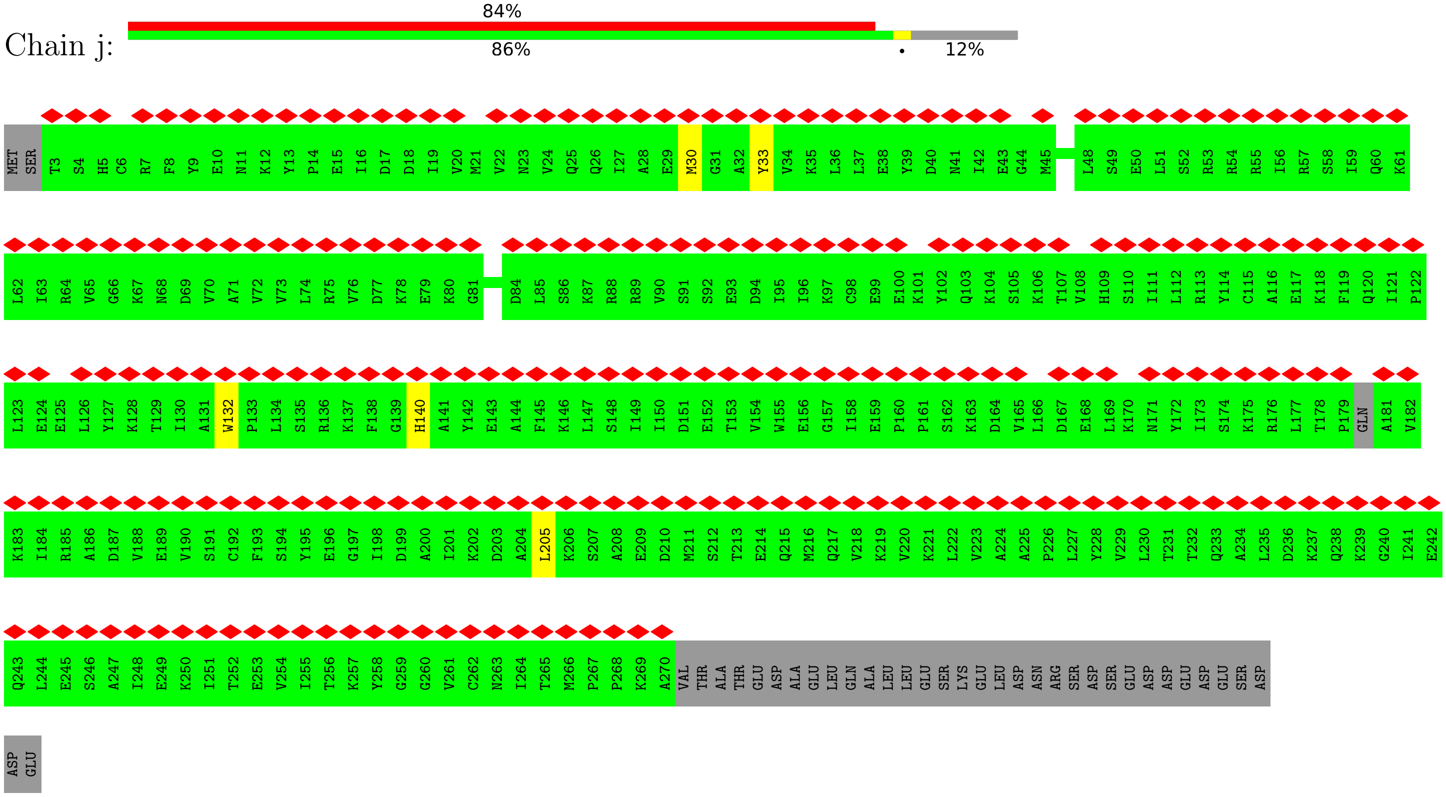
- Molecule 37: mRNA (5'-R(P*AP*AP*U)-3')



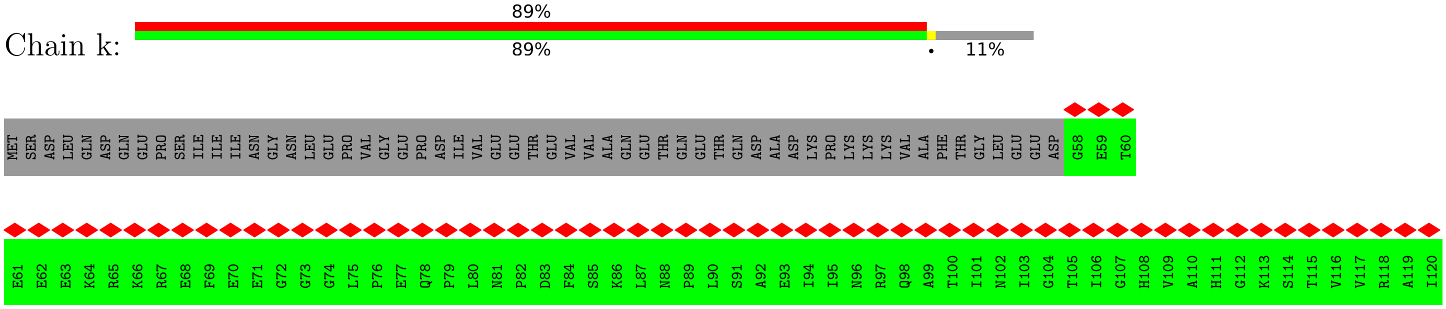
- Molecule 38: Met-tRNAi

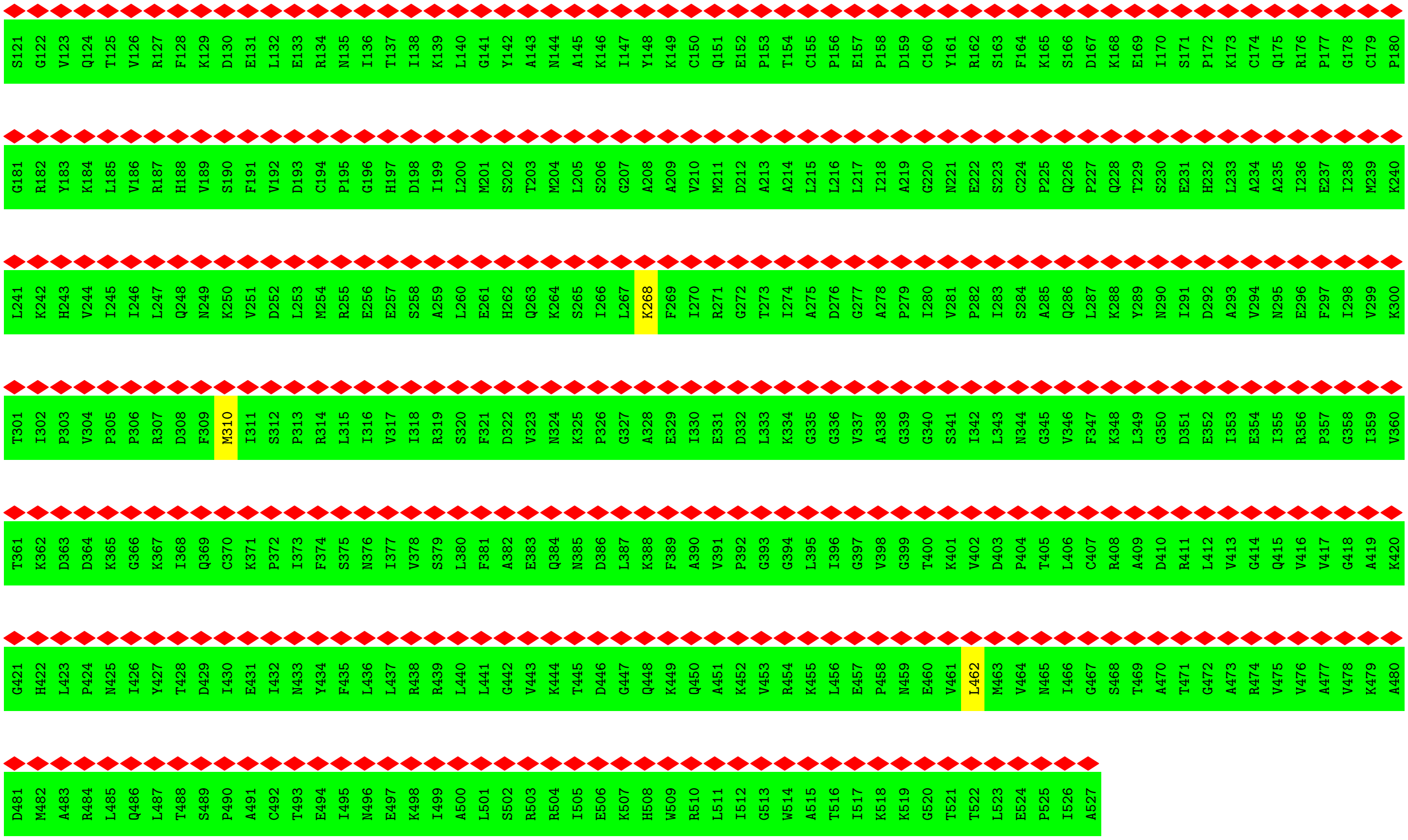


- Molecule 39: Eukaryotic translation initiation factor 2 subunit alpha

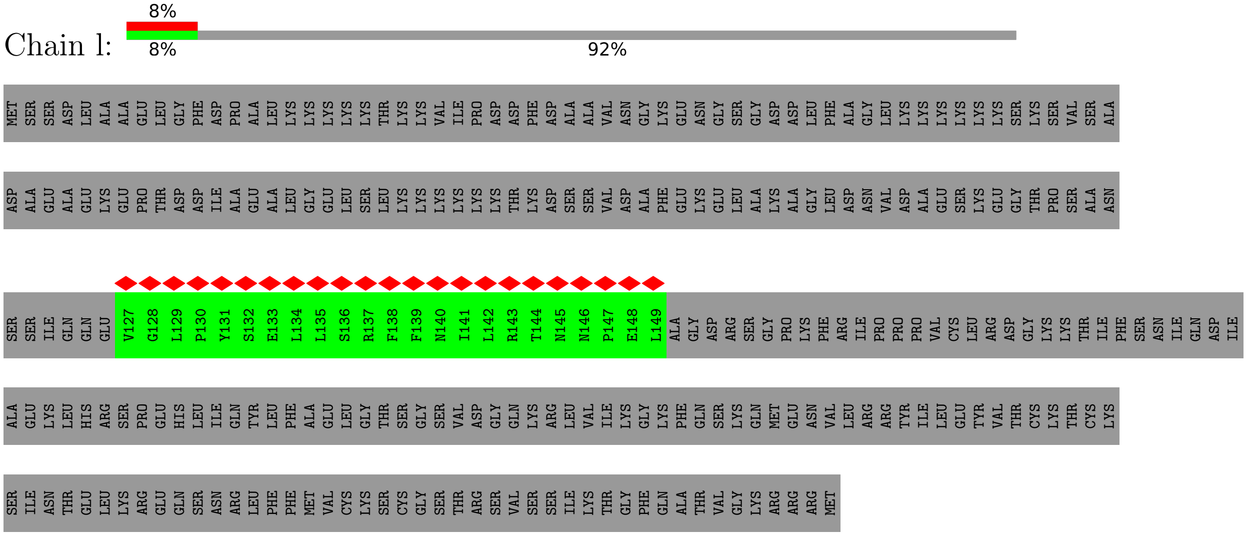


- Molecule 40: Eukaryotic translation initiation factor 2 subunit gamma





- Molecule 41: Eukaryotic translation initiation factor 2 subunit beta



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141338	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 ($e^-/\text{Å}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.670	Depositor
Minimum map value	-0.330	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, M2G, MG, RIA, 2MG, 7MG, B8N, GCP, 1MG, 1MA, H2U, MA6, PSU, T6A, 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	0.22	0/42410	0.84	31/66079 (0.0%)
2	A	0.27	0/1742	0.54	0/2383
3	B	0.28	0/1820	0.60	0/2448
4	C	0.26	0/1678	0.51	0/2277
5	E	0.26	0/2122	0.58	1/2861 (0.0%)
6	G	0.24	0/1855	0.53	0/2479
7	H	0.30	0/1507	0.58	0/2028
8	I	0.27	0/1515	0.64	1/2029 (0.0%)
9	J	0.27	0/1495	0.59	0/2001
10	L	0.26	0/1276	0.56	0/1718
11	N	0.26	0/1218	0.55	0/1638
12	O	0.28	0/966	0.68	1/1297 (0.1%)
13	V	0.29	0/696	0.61	0/938
14	W	0.26	0/1039	0.53	0/1399
15	X	0.28	0/1137	0.57	0/1516
16	Y	0.27	0/1075	0.58	0/1433
17	a	0.26	0/810	0.62	0/1087
18	b	0.25	0/619	0.54	0/837
19	e	0.27	0/480	0.59	0/640
20	h	0.25	0/234	0.70	0/300
21	D	0.27	0/1800	0.61	3/2421 (0.1%)
22	F	0.26	0/1628	0.60	1/2198 (0.0%)
23	K	0.31	0/831	0.60	0/1123
24	M	0.25	0/891	0.64	1/1201 (0.1%)
25	P	0.29	0/942	0.64	1/1269 (0.1%)
26	Q	0.30	0/1125	0.60	0/1510
27	R	0.25	0/1044	0.55	0/1402
28	S	0.26	0/1208	0.65	1/1624 (0.1%)
29	T	0.28	0/1129	0.60	1/1520 (0.1%)
30	U	0.26	0/857	0.58	0/1158
31	Z	0.32	0/604	0.66	0/815
32	c	0.25	0/501	0.67	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
33	d	0.25	0/473	0.55	0/629
34	f	0.25	0/597	0.53	0/795
35	g	0.26	0/2523	0.55	0/3434
36	i	0.27	0/880	0.61	0/1170
37	3	0.14	0/595	0.69	0/920
38	1	0.37	1/1529 (0.1%)	0.86	3/2376 (0.1%)
39	j	0.26	0/2171	0.51	1/2924 (0.0%)
40	k	0.26	0/3657	0.50	0/4946
41	l	0.25	0/194	0.48	0/263
All	All	0.25	1/90873 (0.0%)	0.73	46/131759 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	1	A	OP3-P	-10.56	1.48	1.61

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	T	35	ASP	CB-CG-OD1	8.28	125.75	118.30
22	F	52	ASP	CB-CG-OD1	7.92	125.42	118.30
8	I	194	LEU	CA-CB-CG	7.19	131.84	115.30
1	2	700	C	C2-N1-C1'	7.04	126.55	118.80
1	2	1471	U	C2-N1-C1'	7.03	126.14	117.70

There are no chirality outliers.

There are no planarity outliers.

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	217/254 (85%)	194 (89%)	23 (11%)	0	100	100
3	B	221/255 (87%)	202 (91%)	17 (8%)	2 (1%)	14	48
4	C	218/259 (84%)	208 (95%)	10 (5%)	0	100	100
5	E	258/261 (99%)	240 (93%)	18 (7%)	0	100	100
6	G	228/236 (97%)	220 (96%)	8 (4%)	0	100	100
7	H	182/190 (96%)	168 (92%)	13 (7%)	1 (0%)	25	59
8	I	184/201 (92%)	164 (89%)	20 (11%)	0	100	100
9	J	180/188 (96%)	173 (96%)	7 (4%)	0	100	100
10	L	153/156 (98%)	141 (92%)	12 (8%)	0	100	100
11	N	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
12	O	127/137 (93%)	115 (91%)	12 (9%)	0	100	100
13	V	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
14	W	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
15	X	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
16	Y	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
17	a	100/119 (84%)	81 (81%)	19 (19%)	0	100	100
18	b	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
19	e	58/63 (92%)	52 (90%)	6 (10%)	0	100	100
20	h	23/25 (92%)	23 (100%)	0	0	100	100
21	D	225/237 (95%)	216 (96%)	9 (4%)	0	100	100
22	F	204/227 (90%)	184 (90%)	20 (10%)	0	100	100
23	K	94/106 (89%)	86 (92%)	8 (8%)	0	100	100
24	M	113/134 (84%)	99 (88%)	14 (12%)	0	100	100
25	P	115/142 (81%)	104 (90%)	11 (10%)	0	100	100
26	Q	139/143 (97%)	122 (88%)	15 (11%)	2 (1%)	9	40
27	R	128/136 (94%)	117 (91%)	11 (9%)	0	100	100
28	S	143/146 (98%)	130 (91%)	13 (9%)	0	100	100
29	T	141/144 (98%)	131 (93%)	10 (7%)	0	100	100
30	U	104/117 (89%)	92 (88%)	12 (12%)	0	100	100
31	Z	76/108 (70%)	69 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	c	62/67 (92%)	57 (92%)	5 (8%)	0	100	100
33	d	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
34	f	72/150 (48%)	58 (81%)	14 (19%)	0	100	100
35	g	314/326 (96%)	291 (93%)	23 (7%)	0	100	100
36	i	108/153 (71%)	99 (92%)	9 (8%)	0	100	100
39	j	263/304 (86%)	244 (93%)	19 (7%)	0	100	100
40	k	468/527 (89%)	438 (94%)	30 (6%)	0	100	100
41	l	21/285 (7%)	21 (100%)	0	0	100	100
All	All	5706/6582 (87%)	5266 (92%)	435 (8%)	5 (0%)	50	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	64	VAL
26	Q	41	PRO
26	Q	42	GLU
3	B	221	PRO
3	B	4	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	180/211 (85%)	173 (96%)	7 (4%)	27	58
3	B	202/228 (89%)	196 (97%)	6 (3%)	36	65
4	C	177/203 (87%)	175 (99%)	2 (1%)	70	83
5	E	223/224 (100%)	217 (97%)	6 (3%)	40	67
6	G	192/200 (96%)	190 (99%)	2 (1%)	73	84
7	H	164/170 (96%)	157 (96%)	7 (4%)	25	54
8	I	147/159 (92%)	140 (95%)	7 (5%)	21	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	J	153/158 (97%)	153 (100%)	0	100	100
10	L	136/137 (99%)	132 (97%)	4 (3%)	37	65
11	N	128/128 (100%)	124 (97%)	4 (3%)	35	64
12	O	97/104 (93%)	95 (98%)	2 (2%)	48	72
13	V	73/73 (100%)	71 (97%)	2 (3%)	40	67
14	W	110/111 (99%)	108 (98%)	2 (2%)	54	75
15	X	119/120 (99%)	113 (95%)	6 (5%)	20	50
16	Y	108/109 (99%)	107 (99%)	1 (1%)	75	86
17	a	83/100 (83%)	80 (96%)	3 (4%)	30	60
18	b	71/72 (99%)	69 (97%)	2 (3%)	38	66
19	e	51/55 (93%)	49 (96%)	2 (4%)	27	58
20	h	23/23 (100%)	23 (100%)	0	100	100
21	D	188/196 (96%)	187 (100%)	1 (0%)	86	92
22	F	174/194 (90%)	171 (98%)	3 (2%)	56	75
23	K	88/96 (92%)	84 (96%)	4 (4%)	23	54
24	M	93/109 (85%)	90 (97%)	3 (3%)	34	63
25	P	99/119 (83%)	96 (97%)	3 (3%)	36	65
26	Q	117/119 (98%)	111 (95%)	6 (5%)	20	49
27	R	116/124 (94%)	113 (97%)	3 (3%)	41	68
28	S	127/129 (98%)	124 (98%)	3 (2%)	44	70
29	T	117/118 (99%)	114 (97%)	3 (3%)	41	68
30	U	96/107 (90%)	95 (99%)	1 (1%)	73	84
31	Z	60/88 (68%)	58 (97%)	2 (3%)	33	62
32	c	55/59 (93%)	54 (98%)	1 (2%)	54	75
33	d	47/48 (98%)	43 (92%)	4 (8%)	8	33
34	f	60/133 (45%)	60 (100%)	0	100	100
35	g	264/272 (97%)	262 (99%)	2 (1%)	79	87
36	i	90/130 (69%)	86 (96%)	4 (4%)	24	54
39	j	239/274 (87%)	235 (98%)	4 (2%)	56	75
40	k	393/449 (88%)	390 (99%)	3 (1%)	79	87
41	l	22/246 (9%)	22 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	4882/5595 (87%)	4767 (98%)	115 (2%)	45	70

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	Y	131	ARG
39	j	132	TRP
23	K	26	ASP
39	j	33	TYR
33	d	19	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
40	k	263	GLN
40	k	465	ASN
19	e	46	ASN
22	F	65	GLN
22	F	226	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1795/1798 (99%)	520 (28%)	30 (1%)
37	3	25/49 (51%)	15 (60%)	0
38	1	71/75 (94%)	28 (39%)	2 (2%)
All	All	1891/1922 (98%)	563 (29%)	32 (1%)

5 of 563 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	25	C
1	2	26	A
1	2	27	U

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1613	C
1	2	1765	G
1	2	649	U
1	2	637	U
38	1	43	G

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

23 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	$\#\|Z\| > 2$
1	PSU	2	998	1	18,21,22	4.29	7 (38%)	22,30,33	1.88	6 (27%)
38	2MG	1	10	38	18,26,27	2.54	7 (38%)	16,38,41	1.37	3 (18%)
1	PSU	2	766	1	18,21,22	4.32	8 (44%)	22,30,33	1.85	6 (27%)
38	1MA	1	58	38	16,25,26	4.38	4 (25%)	18,37,40	1.77	3 (16%)
38	7MG	1	46	38	22,26,27	3.91	10 (45%)	29,39,42	2.07	9 (31%)
1	PSU	2	465	1	18,21,22	4.29	7 (38%)	22,30,33	1.82	5 (22%)
38	5MC	1	48	38	18,22,23	3.59	7 (38%)	26,32,35	1.09	2 (7%)
38	T6A	1	37	38	27,34,35	2.17	7 (25%)	29,49,52	2.20	6 (20%)
1	5MC	2	1006	1	18,22,23	3.55	7 (38%)	26,32,35	1.13	2 (7%)
1	MA6	2	1780	1	18,26,27	1.02	2 (11%)	19,38,41	3.60	2 (10%)
38	1MG	1	9	38	18,26,27	3.01	5 (27%)	19,39,42	1.50	4 (21%)
1	PSU	2	1289	1	18,21,22	4.33	7 (38%)	22,30,33	1.73	5 (22%)
38	H2U	1	16	38	18,21,22	3.07	4 (22%)	21,30,33	2.03	5 (23%)
38	M2G	1	26	38	20,27,28	3.89	8 (40%)	22,40,43	1.46	5 (22%)
1	B8N	2	1190	1	24,29,30	3.00	5 (20%)	29,42,45	1.70	6 (20%)
38	RIA	1	64	38	31,38,39	0.57	0	39,57,60	0.74	1 (2%)
1	PSU	2	120	1	18,21,22	4.32	7 (38%)	22,30,33	1.82	5 (22%)
1	5MC	2	1637	1	18,22,23	3.60	7 (38%)	26,32,35	0.98	1 (3%)
38	5MC	1	49	38	18,22,23	3.64	7 (38%)	26,32,35	1.16	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	7MG	2	1573	38,1	22,26,27	3.90	10 (45%)	29,39,42	2.07	9 (31%)
1	2MG	2	1570	1	18,26,27	2.55	7 (38%)	16,38,41	1.36	3 (18%)
1	2MG	2	1426	42,1	18,26,27	2.53	7 (38%)	16,38,41	1.35	4 (25%)
38	H2U	1	47	38	18,21,22	3.12	4 (22%)	21,30,33	1.93	4 (19%)

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
1	PSU	2	998	1	-	3/7/25/26	0/2/2/2
38	2MG	1	10	38	-	1/5/27/28	0/3/3/3
1	PSU	2	766	1	-	1/7/25/26	0/2/2/2
38	1MA	1	58	38	-	0/3/25/26	0/3/3/3
38	7MG	1	46	38	-	1/7/37/38	0/3/3/3
1	PSU	2	465	1	-	0/7/25/26	0/2/2/2
38	5MC	1	48	38	-	3/7/25/26	0/2/2/2
38	T6A	1	37	38	-	1/19/41/42	0/3/3/3
1	5MC	2	1006	1	-	0/7/25/26	0/2/2/2
1	MA6	2	1780	1	-	3/7/29/30	0/3/3/3
38	1MG	1	9	38	-	2/3/25/26	0/3/3/3
1	PSU	2	1289	1	-	0/7/25/26	0/2/2/2
38	H2U	1	16	38	-	5/7/38/39	0/2/2/2
38	M2G	1	26	38	-	0/7/29/30	0/3/3/3
1	B8N	2	1190	1	-	5/16/34/35	0/2/2/2
38	RIA	1	64	38	-	4/13/51/52	0/4/4/4
1	PSU	2	120	1	-	0/7/25/26	0/2/2/2
1	5MC	2	1637	1	-	0/7/25/26	0/2/2/2
38	5MC	1	49	38	-	4/7/25/26	0/2/2/2
1	7MG	2	1573	38,1	-	2/7/37/38	0/3/3/3
1	2MG	2	1570	1	-	0/5/27/28	0/3/3/3
1	2MG	2	1426	42,1	-	0/5/27/28	0/3/3/3
38	H2U	1	47	38	-	5/7/38/39	0/2/2/2

The worst 5 of 144 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	58	1MA	C2-N3	15.80	1.48	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1	26	M2G	C2-N3	13.49	1.47	1.30
1	2	1289	PSU	C6-C5	11.31	1.48	1.35
1	2	120	PSU	C6-C5	11.26	1.48	1.35
1	2	766	PSU	C6-C5	11.24	1.48	1.35

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1780	MA6	N1-C6-N6	-14.48	101.82	117.06
38	1	16	H2U	C4-N3-C2	-6.90	120.07	125.79
38	1	47	H2U	C4-N3-C2	-6.55	120.36	125.79
38	1	37	T6A	N3-C2-N1	-5.59	119.94	128.68
1	2	1780	MA6	N3-C2-N1	-5.55	120.00	128.68

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	998	PSU	O4'-C4'-C5'-O5'
1	2	1780	MA6	O4'-C4'-C5'-O5'
38	1	9	1MG	O4'-C4'-C5'-O5'
38	1	9	1MG	C3'-C4'-C5'-O5'
38	1	16	H2U	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 121 ligands modelled in this entry, 119 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
45	MET	k	603	-	6,7,8	0.47	0	2,7,9	0.22	0
44	GCP	k	601	-	27,34,34	4.76	10 (37%)	34,54,54	1.70	7 (20%)

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
45	MET	k	603	-	-	0/5/6/8	-
44	GCP	k	601	-	-	2/15/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	k	601	GCP	O4'-C1'	15.11	1.62	1.41
44	k	601	GCP	C2'-C1'	-14.88	1.31	1.53
44	k	601	GCP	O4'-C4'	-6.30	1.30	1.45
44	k	601	GCP	PB-O3A	6.24	1.65	1.58
44	k	601	GCP	C2-N2	5.82	1.45	1.33

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	k	601	GCP	N3-C2-N1	-5.29	120.16	127.22
44	k	601	GCP	C2-N3-C4	4.12	120.06	115.36
44	k	601	GCP	C3'-C2'-C1'	2.97	105.45	100.98
44	k	601	GCP	PB-O3A-PA	-2.71	123.97	132.56
44	k	601	GCP	N2-C2-N3	2.57	121.98	117.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

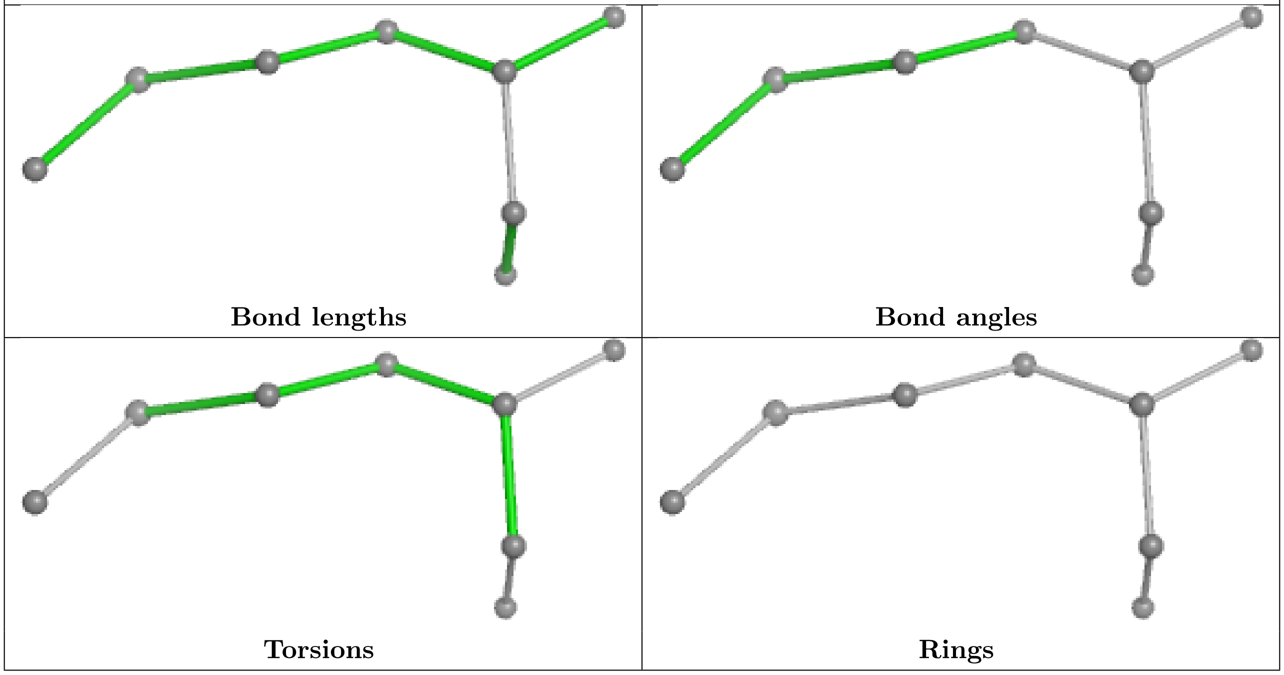
Mol	Chain	Res	Type	Atoms
44	k	601	GCP	O4'-C4'-C5'-O5'
44	k	601	GCP	C3'-C4'-C5'-O5'

There are no ring outliers.

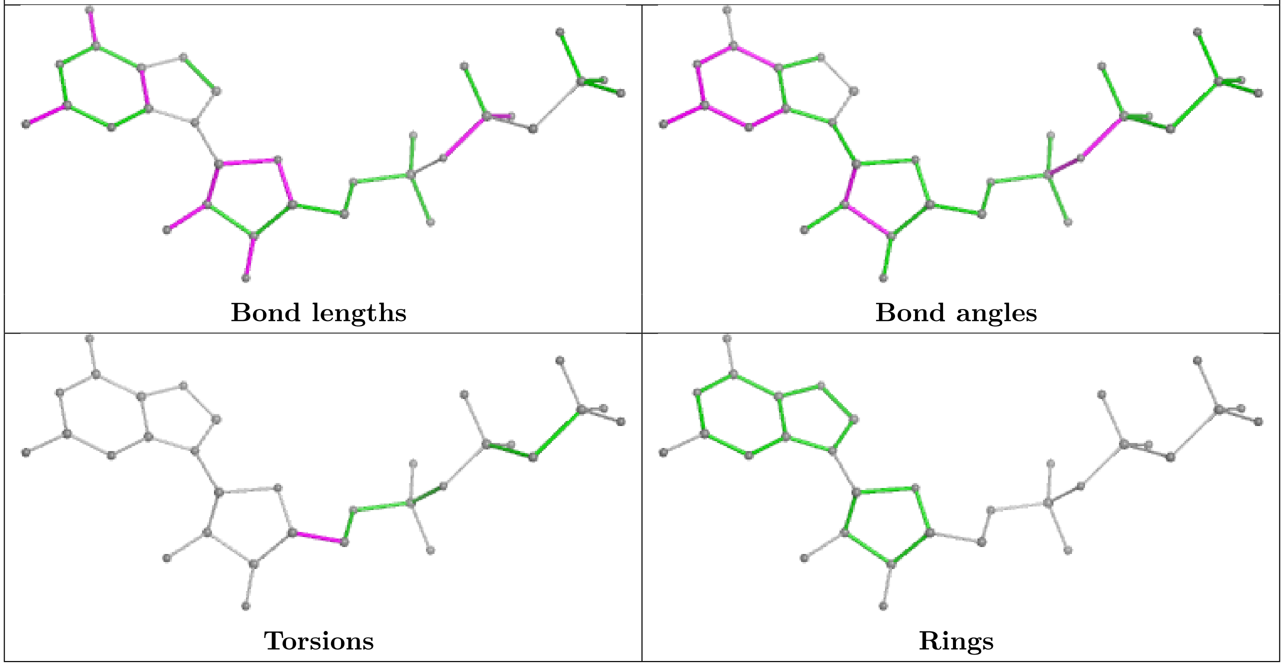
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand MET k 603



Ligand GCP k 601



Bond lengths

Bond angles

Torsions

Rings

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
38	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	64:RIA	O3’	65:G	P	9.21
1	1	16:H2U	O3’	18:G	P	3.56
1	1	63:G	O3’	64:RIA	P	3.47

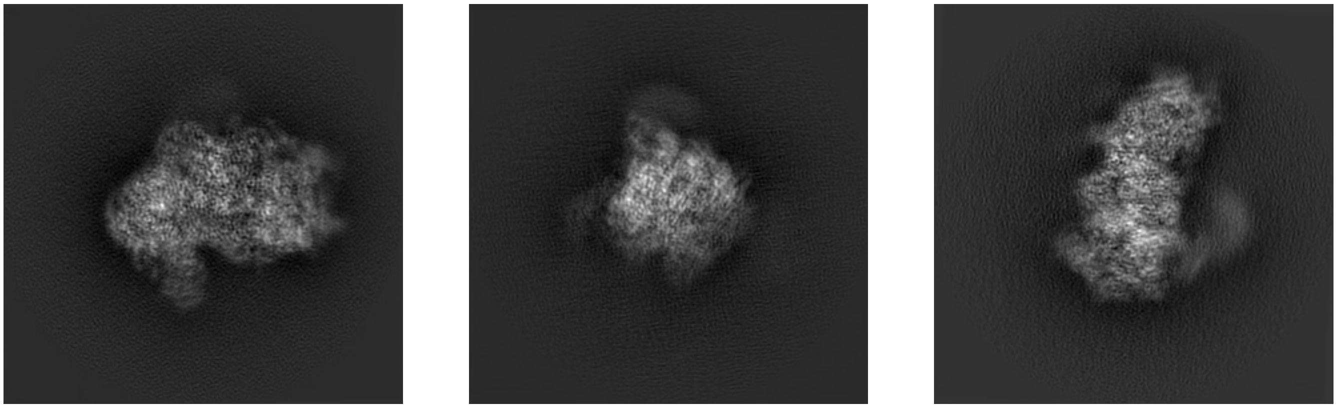
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-19801. 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.

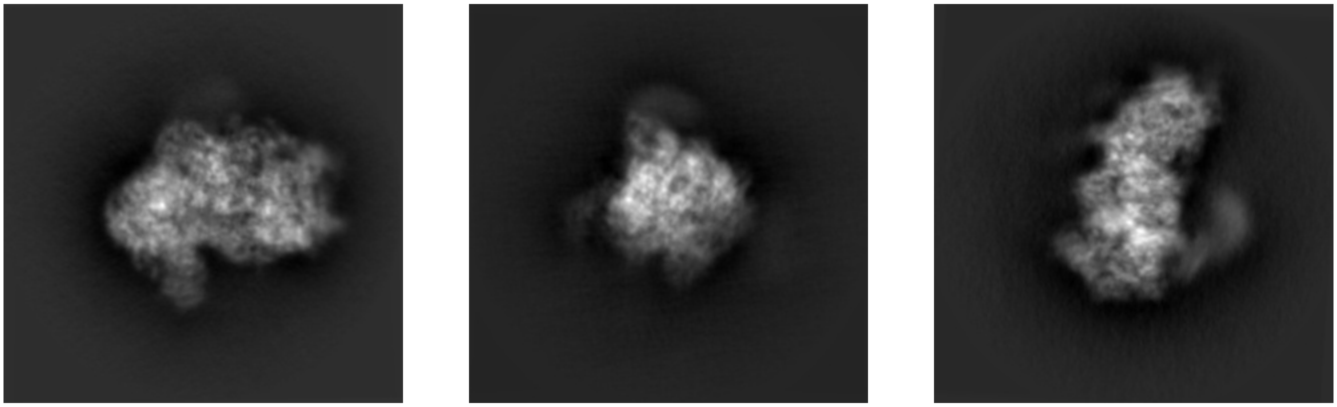
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

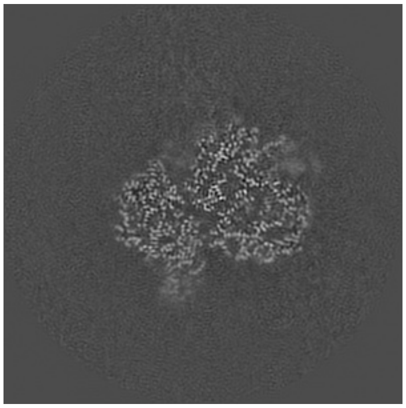


X Y Z

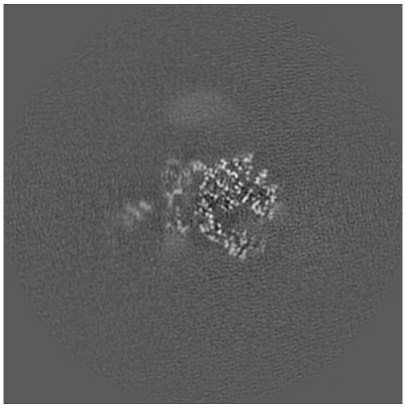
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

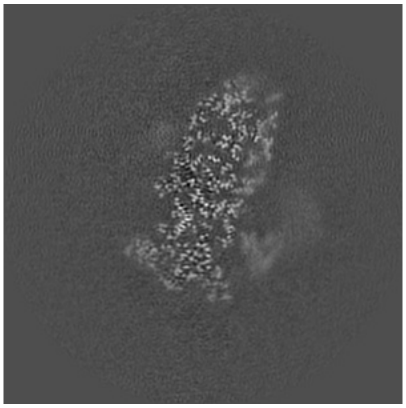
6.2.1 Primary map



X Index: 150

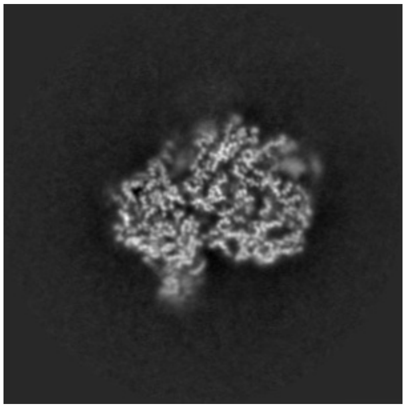


Y Index: 150

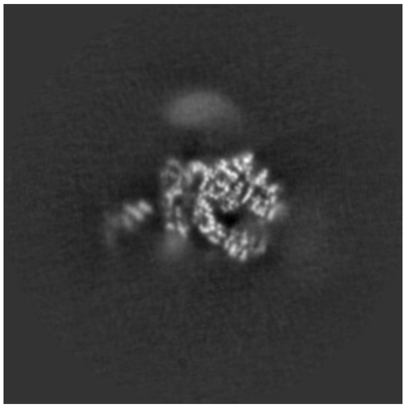


Z Index: 150

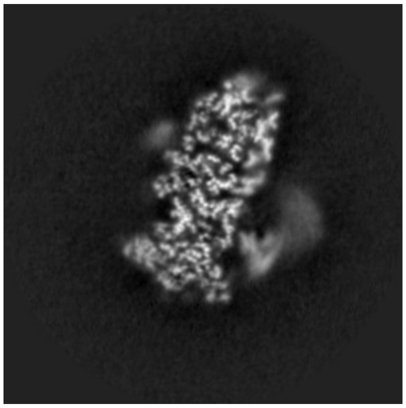
6.2.2 Raw map



X Index: 150



Y Index: 150

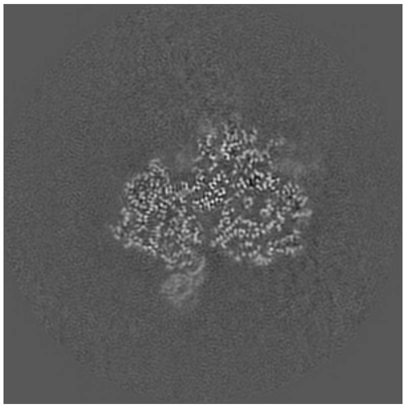


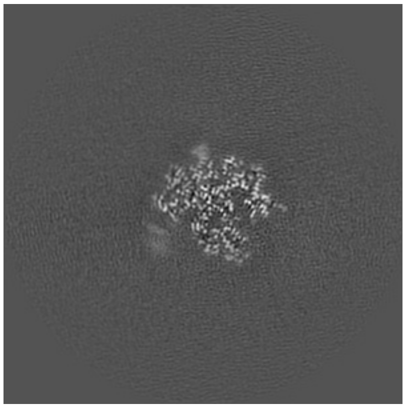
Z Index: 150

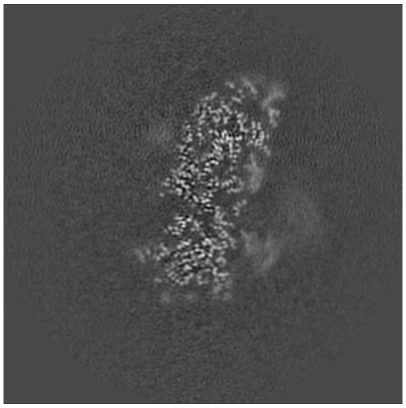
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

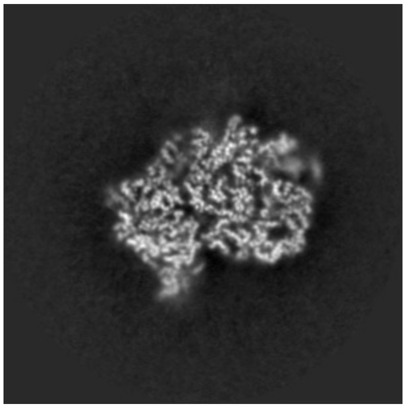
6.3.1 Primary map

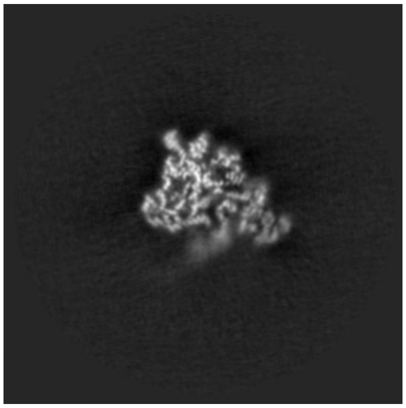

X Index: 148

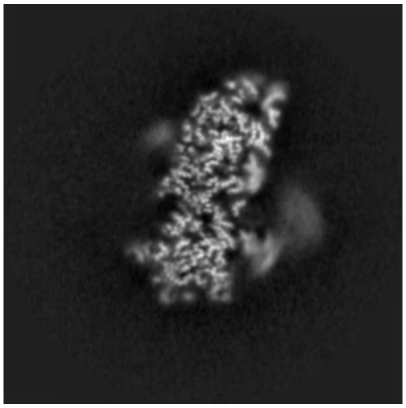

Y Index: 166


Z Index: 146

6.3.2 Raw map


X Index: 152

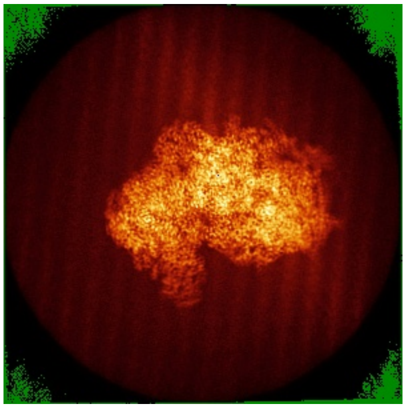

Y Index: 198

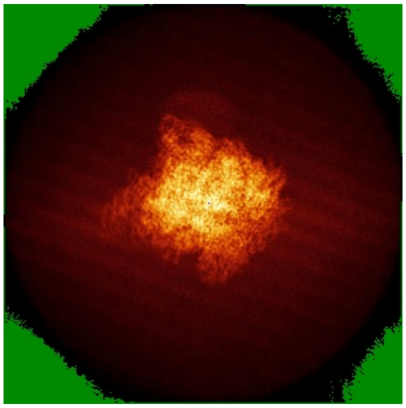

Z Index: 146

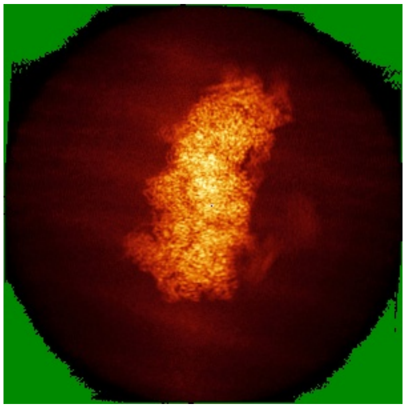
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

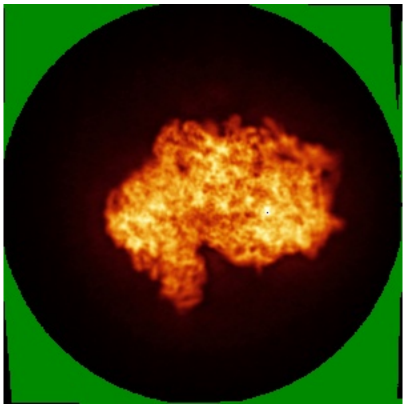
6.4.1 Primary map

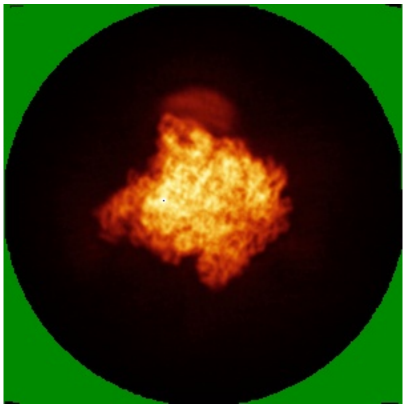

X

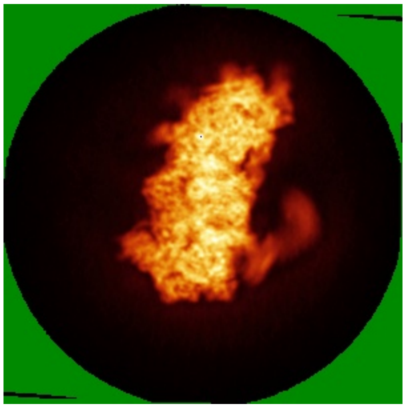

Y


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

6.5.1 Primary map

X

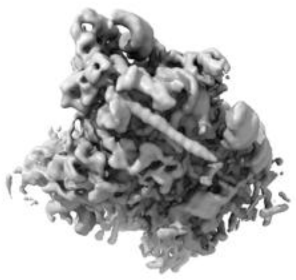
Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. 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.

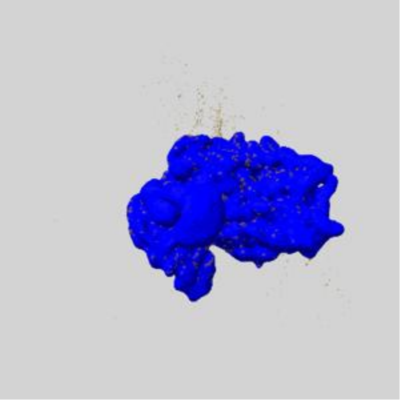
6.6 Mask visualisation

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

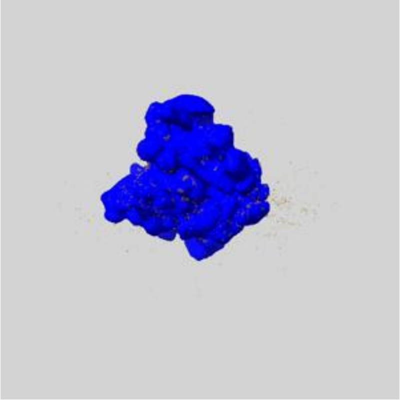
A mask typically either:

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

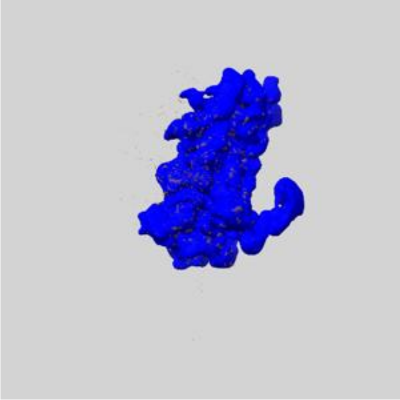
6.6.1 emd_19801_msk_1.map



X



Y

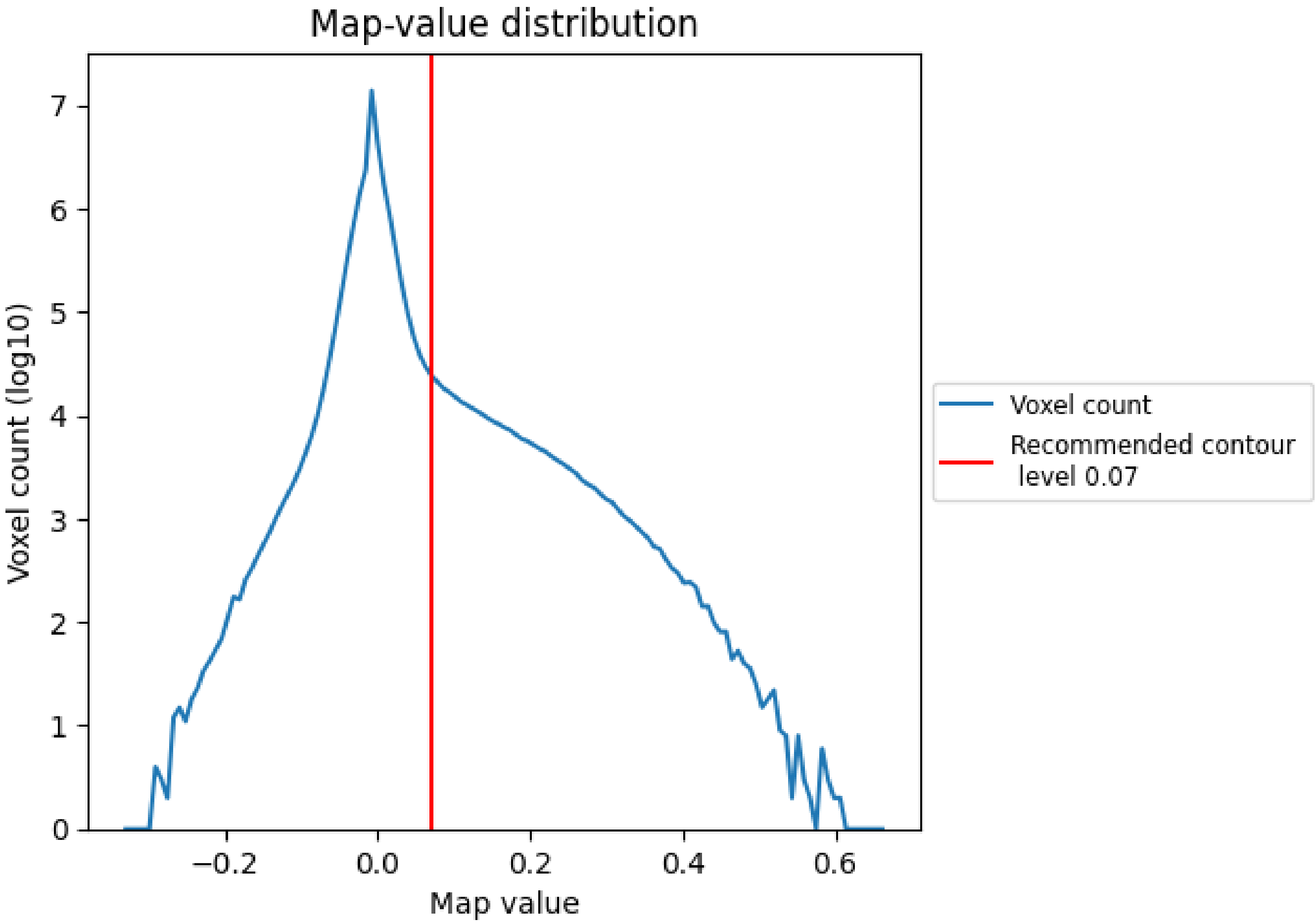


Z

7 Map analysis ⓘ

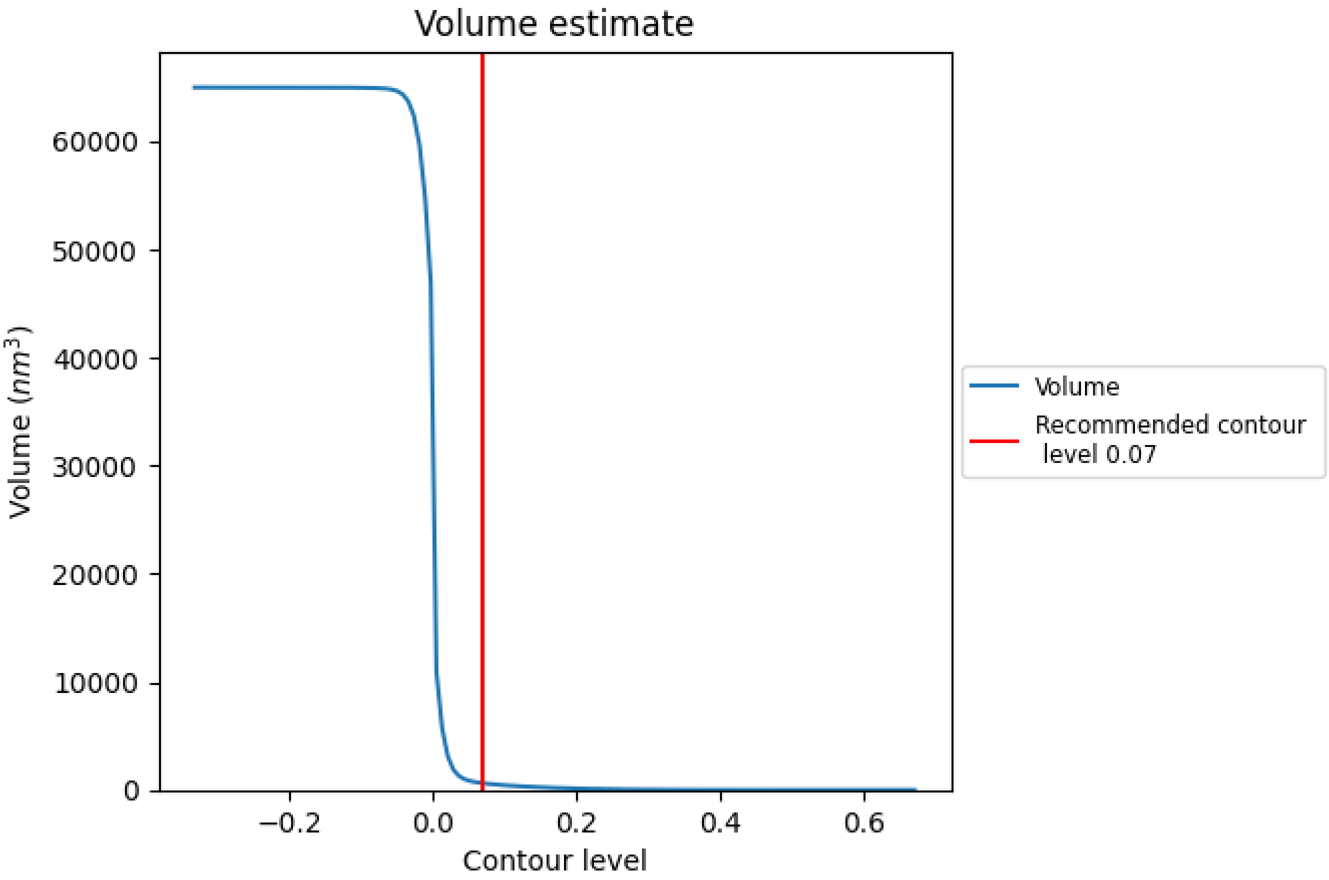
This section contains the results of statistical analysis of the map.

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.

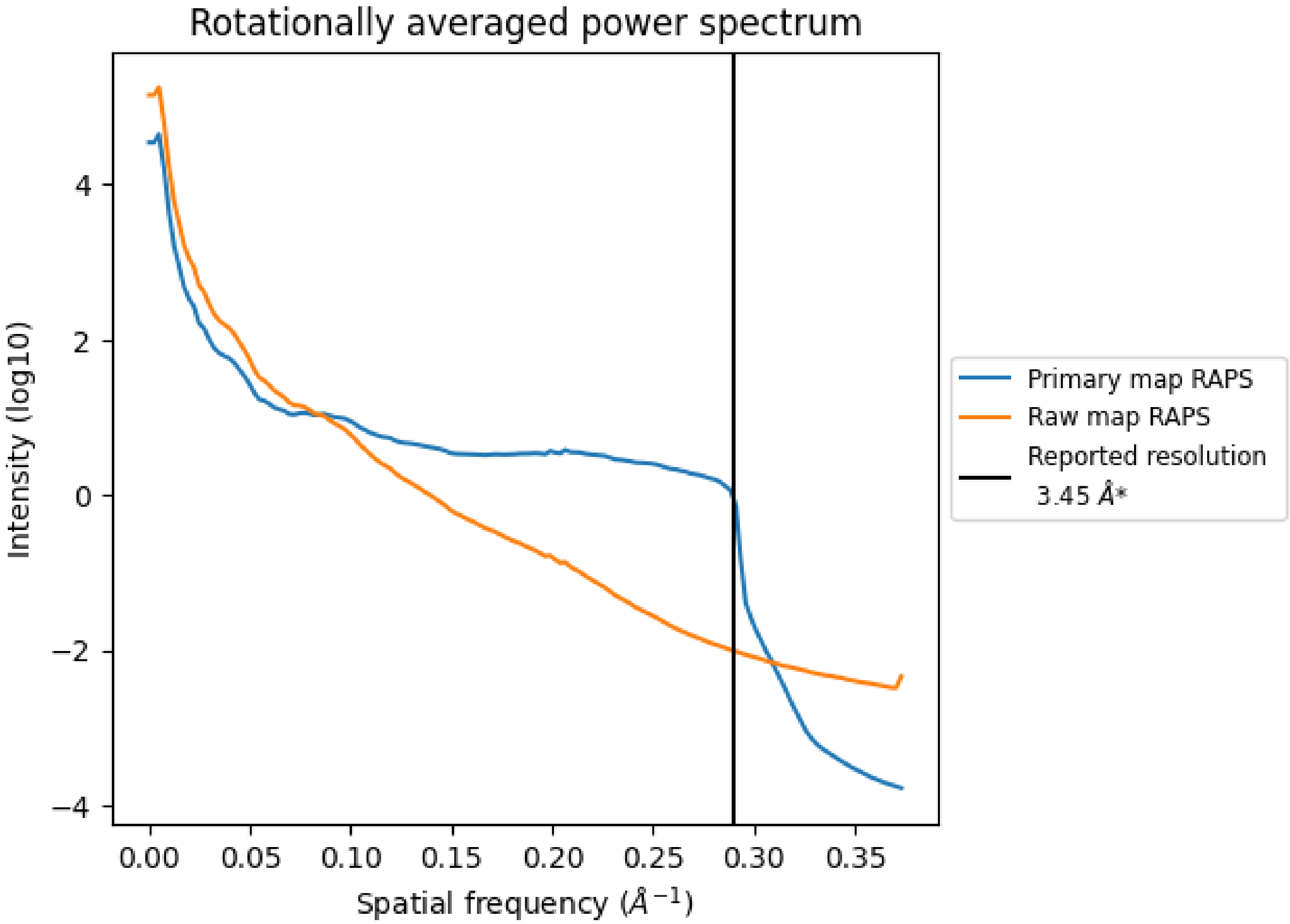
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 623 nm^3; this corresponds to an approximate mass of 563 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 ⓘ

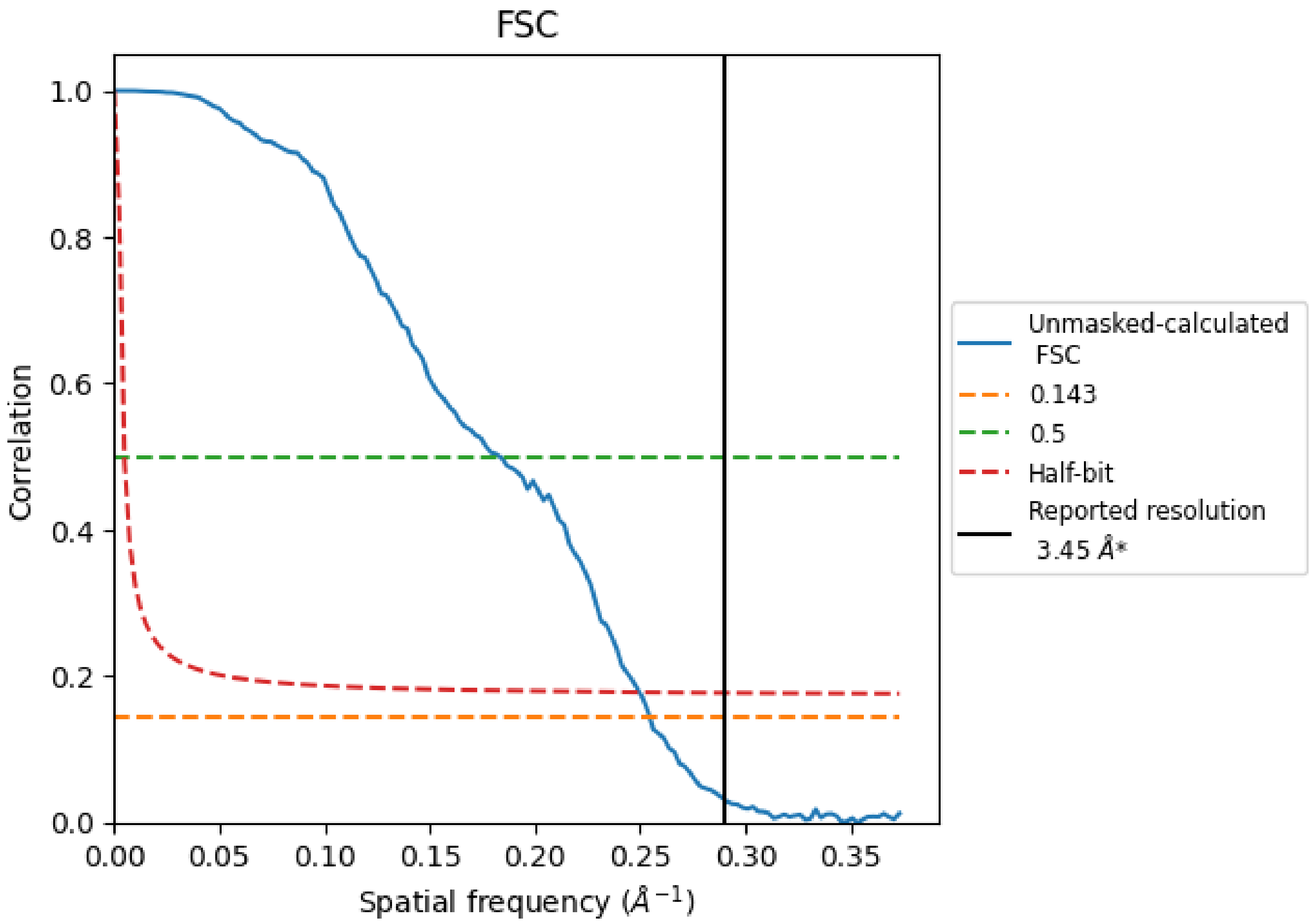


*Reported resolution corresponds to spatial frequency of 0.290 $Å^{-1}$

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 0.290 Å^{-1}

8.2 Resolution estimates ⓘ

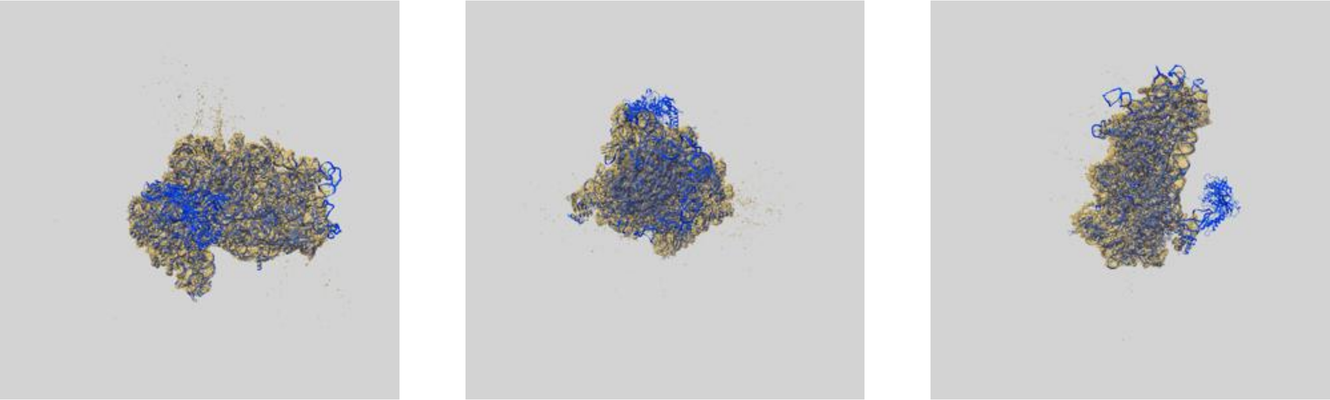
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.93	5.46	4.01

*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 3.93 differs from the reported value 3.45 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-19801 and PDB model 8S8D. Per-residue inclusion information can be found in section 3 on page 13.

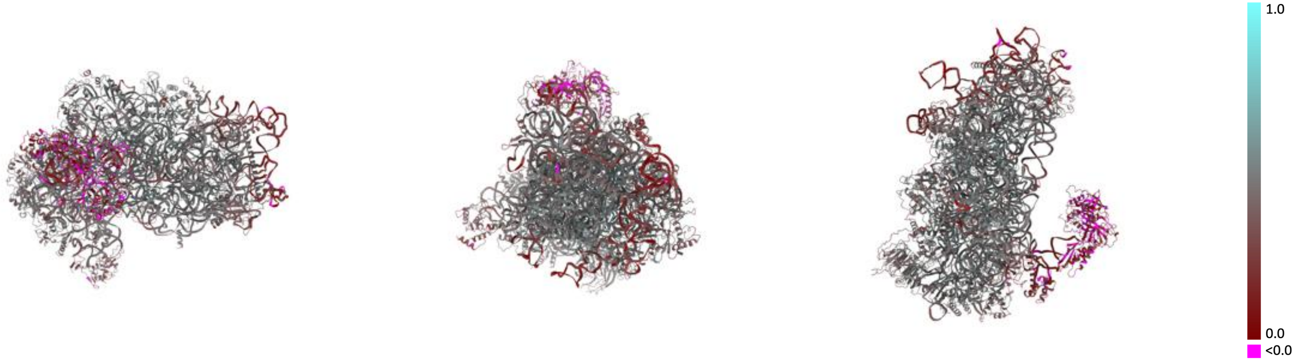
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

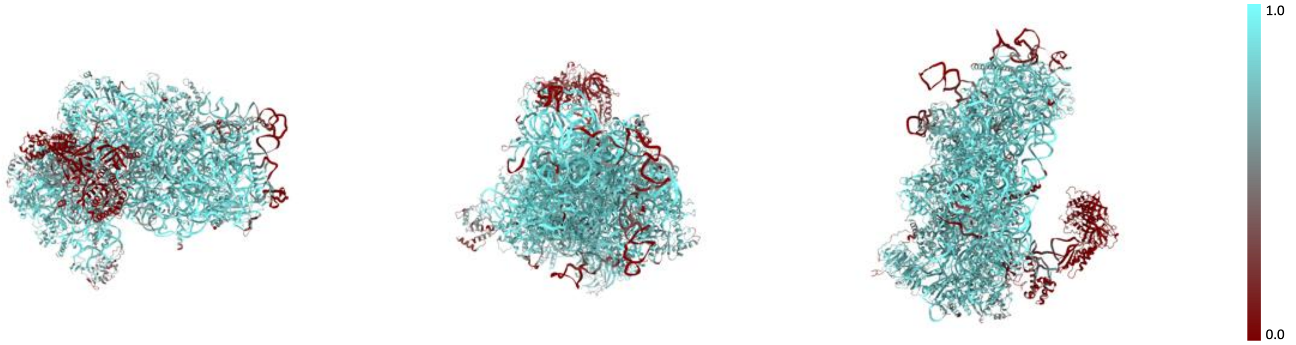
9.2 Q-score mapped to coordinate model



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.

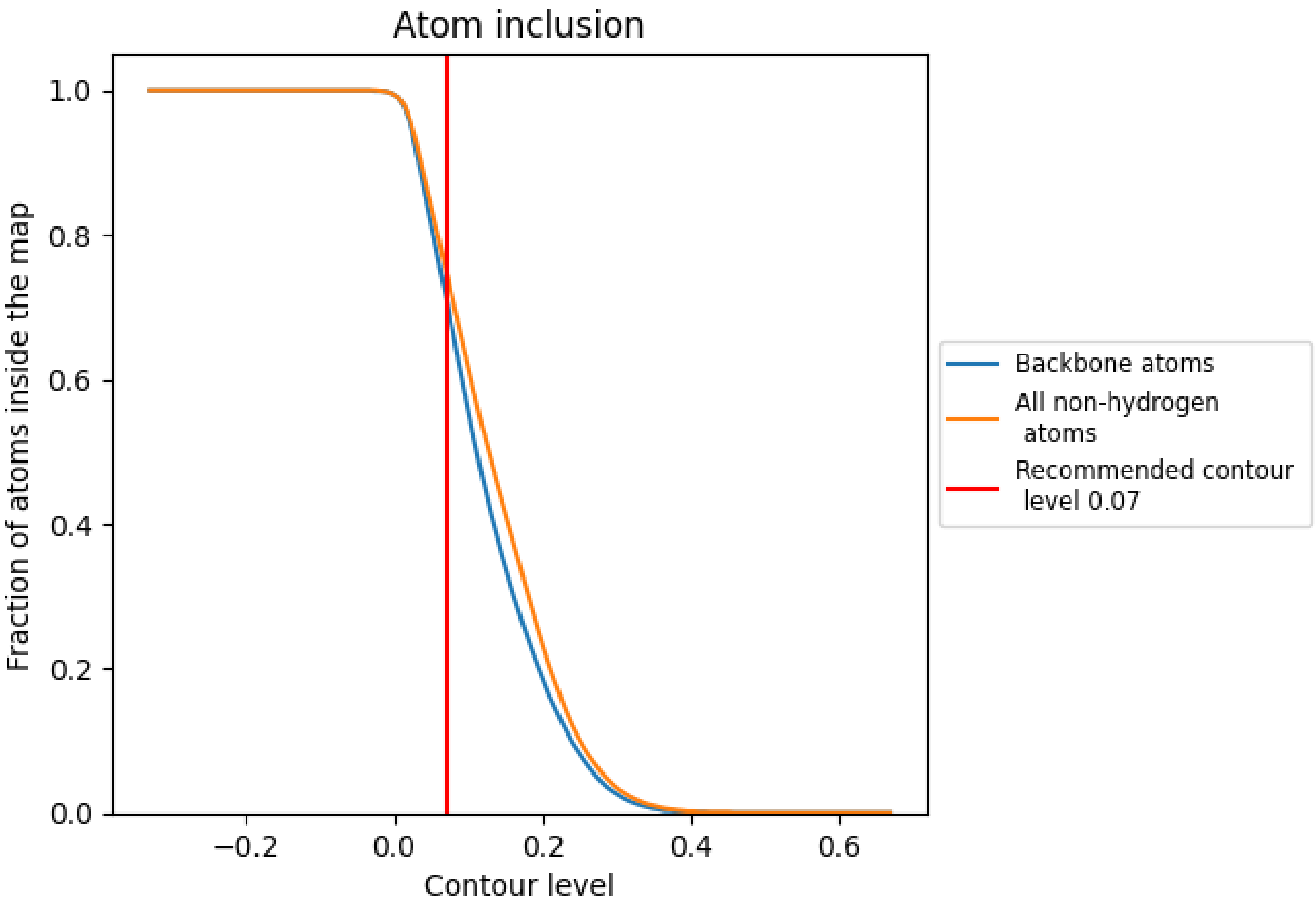
9.3 Atom inclusion mapped to coordinate model



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 (0.07).

9.4 Atom inclusion ⓘ



At the recommended contour level, 71% of all backbone atoms, 75% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7500	0.4150
1	0.5430	0.2450
2	0.8700	0.4250
3	0.3020	0.3440
A	0.8340	0.4730
B	0.7880	0.4590
C	0.8600	0.5090
D	0.7720	0.4600
E	0.8590	0.4940
F	0.7730	0.4670
G	0.7690	0.4110
H	0.6970	0.4230
I	0.7660	0.4360
J	0.8470	0.4890
K	0.7640	0.4310
L	0.7570	0.4730
M	0.3670	0.2750
N	0.8450	0.4840
O	0.8270	0.4680
P	0.8070	0.4460
Q	0.8550	0.4730
R	0.7290	0.4400
S	0.7880	0.4350
T	0.8590	0.4700
U	0.6980	0.4350
V	0.8790	0.4880
W	0.8560	0.5080
X	0.8090	0.5000
Y	0.8400	0.4710
Z	0.5660	0.3660
a	0.8400	0.5000
b	0.8240	0.4840
c	0.7520	0.4890
d	0.8690	0.5090
e	0.6860	0.4520

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Chain	Atom inclusion	Q-score
f	0.5010	0.3390
g	0.7650	0.4310
h	0.1790	0.4090
i	0.3800	0.4070
j	0.0630	0.1960
k	0.0010	0.1080
l	0.0050	0.0760