



wwPDB EM Validation Summary Report ⓘ

Jun 19, 2026 – 06:14 am BST

PDB ID : 8QYX / pdb_00008qyx
EMDB ID : EMD-18765
Title : Human 60S ribosomal subunit
Authors : Wiechert, F.; Schacherl, M.; Sprink, T.
Deposited on : 2023-10-26
Resolution : 1.78 Å(reported)
Based on initial model : 6EKO

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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

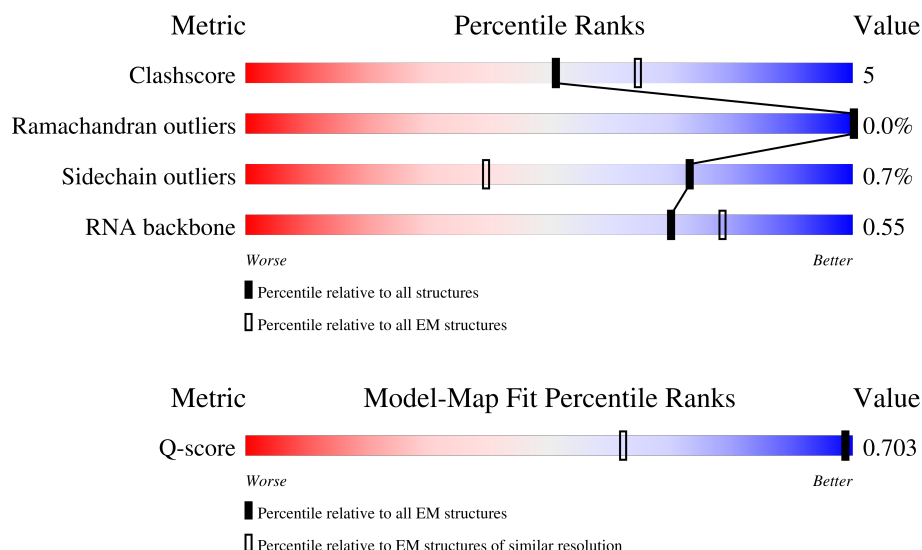
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.78 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.



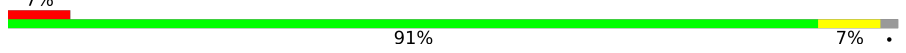
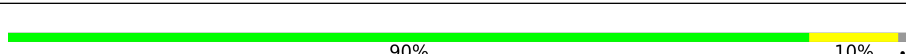
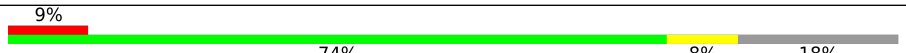
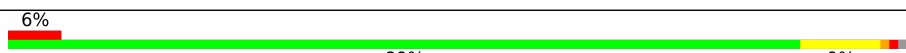
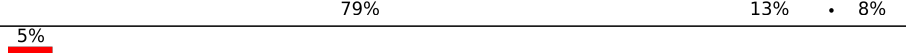
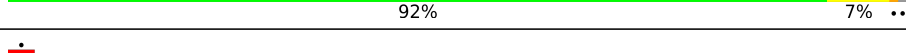
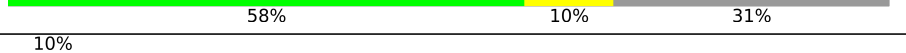
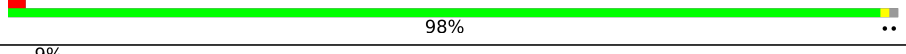
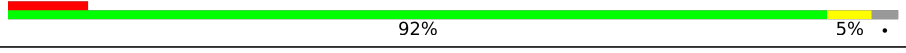
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	707 (1.31 - 2.28)

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	A1	248	
2	B1	266	
3	C1	192	

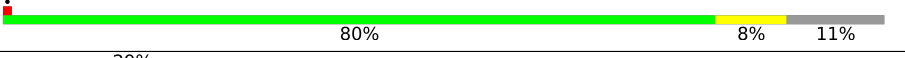
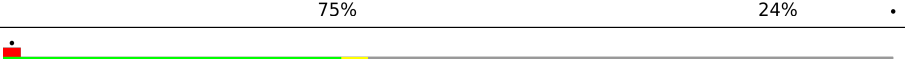
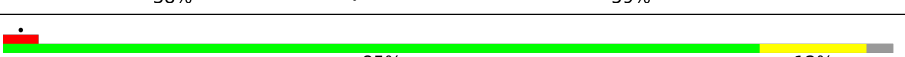
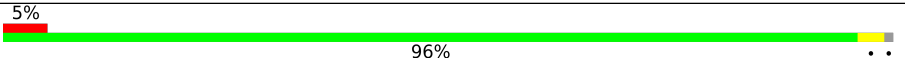
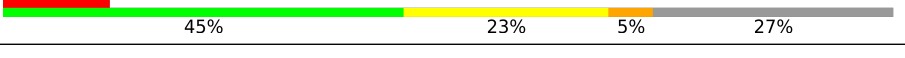
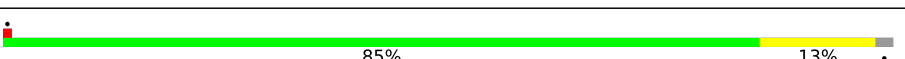
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Mol	Chain	Length	Quality of chain
4	D1	214	
5	E1	178	
6	F1	211	
7	G1	215	
8	H1	204	
9	I1	203	
10	J1	184	
11	K1	188	
12	L1	196	
13	M1	176	
14	N1	160	
15	O1	128	
16	P1	140	
17	Q1	157	
18	R1	156	
19	S1	145	
20	T1	136	
21	U1	148	
22	V1	159	
23	W1	115	
24	X1	125	
25	Y1	135	
26	Z1	110	
27	a1	117	
28	b1	123	

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Mol	Chain	Length	Quality of chain
29	c1	105	
30	d1	97	
31	e1	70	
32	f1	51	
33	g1	128	
34	i1	106	
35	j1	92	
36	k1	137	
37	A2	5069	
38	B2	120	
39	C2	157	
40	D2	257	
41	E2	403	
42	F2	427	
43	G2	297	
44	H2	288	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	PUT	A2	5401	-	-	X	-
46	PUT	A2	5403	-	-	X	-
46	PUT	A2	5404	-	-	X	-
46	PUT	B2	201	-	-	X	-
49	SPD	A2	5407	-	-	X	-
49	SPD	A2	5412	-	-	X	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 149908 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 Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	225	Total	C	N	O	S	2	0
			1887	1213	363	302	9		

- Molecule 2 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	225	Total	C	N	O	S	0	0
			1822	1163	351	304	4		

- Molecule 3 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 4 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	205	Total	C	N	O	S	3	0
			1688	1071	327	277	13		

- Molecule 5 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	171	Total	C	N	O	S	0	0
			1371	867	256	242	6		

- Molecule 6 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	207	Total	C	N	O	S	0	0
			1673	1046	346	277	4		

- Molecule 7 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	136	Total	C	N	O	S	0	0
			1120	719	215	179	7		

- Molecule 8 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	203	Total	C	N	O	S	1	0
			1711	1078	362	267	4		

- Molecule 9 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 10 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	160	Total	C	N	O	S	1	0
			1307	818	252	228	9		

- Molecule 11 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K1	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 12 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L1	161	Total	C	N	O	S	0	0
			1341	834	288	210	9		

- Molecule 13 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M1	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 14 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N1	159	Total	C	N	O	S	1	0
			1304	828	253	217	6		

- Molecule 15 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O1	101	Total	C	N	O	S	1	0
			834	535	146	151	2		

- Molecule 16 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P1	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 17 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q1	62	Total	C	N	O	S	0	0
			519	332	101	83	3		

- Molecule 18 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R1	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 19 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S1	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 20 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T1	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 21 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U1	147	Total	C	N	O	S	0	0
			1163	736	237	187	3		

- Molecule 22 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V1	109	Total	C	N	O	S	0	0
			874	543	190	137	4		

- Molecule 23 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W1	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 24 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X1	109	Total	C	N	O	S	0	0
			901	569	173	157	2		

- Molecule 25 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y1	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 26 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z1	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 27 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a1	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 28 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b1	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 29 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c1	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 30 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d1	86	Total	C	N	O	S	1	0
			716	440	159	112	5		

- Molecule 31 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e1	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 32 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f1	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 33 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g1	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 34 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i1	103	Total	C	N	O	S	1	0
			852	534	175	137	6		

- Molecule 35 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j1	91	Total	C	N	O	S	0	0
			707	445	136	119	7		

- Molecule 36 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k1	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 37 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	A2	3706	Total	C	N	O	P	0	0
			79517	35448	14543	25821	3705		

- Molecule 38 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B2	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 39 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	C2	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 40 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	D2	246	Total	C	N	O	S	0	0
			1888	1183	387	312	6		

- Molecule 41 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	E2	396	Total	C	N	O	S	1	0
			3209	2043	605	547	14		

- Molecule 42 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	F2	359	Total	C	N	O	S	1	0
			2870	1807	573	476	14		

- Molecule 43 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	G2	293	Total	C	N	O	S	0	0
			2386	1510	435	427	14		

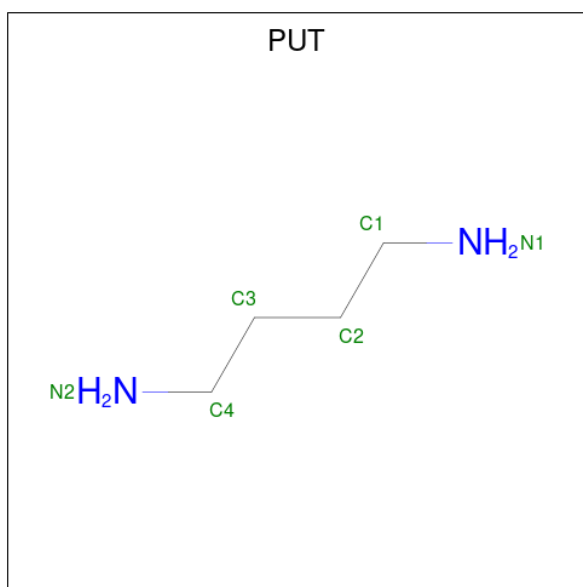
- Molecule 44 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	H2	234	Total	C	N	O	S	1	0
			1903	1222	361	316	4		

- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	D1	1	Total	Mg	0
			1	1	
45	J1	1	Total	Mg	0
			1	1	
45	P1	1	Total	Mg	0
			1	1	
45	Y1	1	Total	Mg	0
			1	1	
45	Z1	1	Total	Mg	0
			1	1	
45	d1	1	Total	Mg	0
			1	1	
45	A2	175	Total	Mg	0
			175	175	
45	B2	2	Total	Mg	0
			2	2	
45	C2	3	Total	Mg	0
			3	3	

- Molecule 46 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
46	H1	1	Total	C	N	1
			12	8	4	
46	A2	1	Total	C	N	0
			6	4	2	
46	A2	1	Total	C	N	0
			6	4	2	
46	A2	1	Total	C	N	0
			6	4	2	
46	A2	1	Total	C	N	0
			6	4	2	
46	B2	1	Total	C	N	0
			6	4	2	

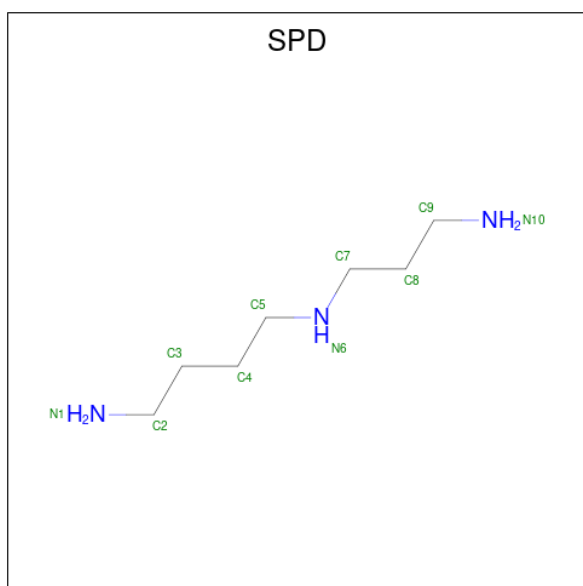
- Molecule 47 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
47	M1	1	Total	K	0
			1	1	
47	N1	1	Total	K	0
			1	1	
47	A2	42	Total	K	0
			42	42	
47	D2	2	Total	K	0
			2	2	

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

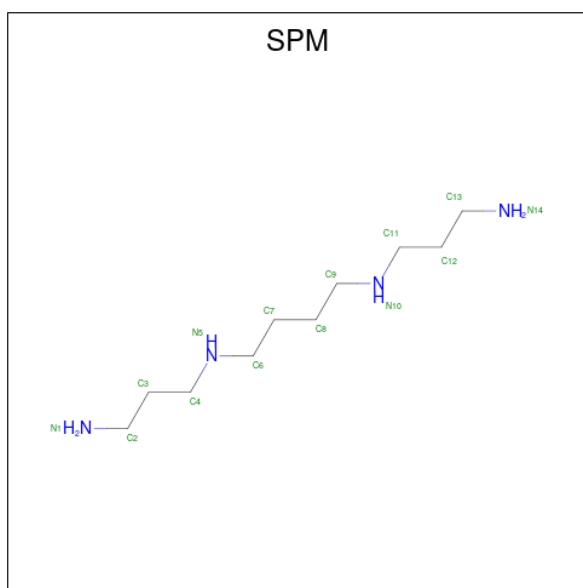
Mol	Chain	Residues	Atoms		AltConf
48	a1	1	Total	Zn	0
			1	1	
48	d1	1	Total	Zn	0
			1	1	
48	g1	1	Total	Zn	0
			1	1	
48	i1	1	Total	Zn	0
			1	1	
48	j1	1	Total	Zn	0
			1	1	

- Molecule 49 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



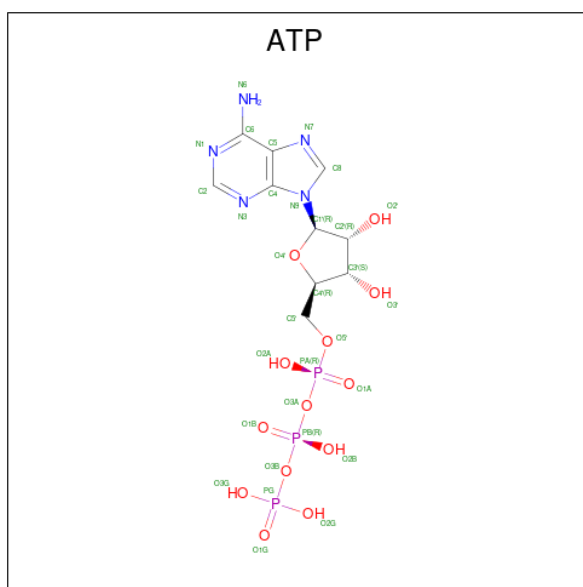
Mol	Chain	Residues	Atoms			AltConf
49	A2	1	Total	C	N	0
			10	7	3	
49	A2	1	Total	C	N	0
			10	7	3	
49	A2	1	Total	C	N	0
			10	7	3	
49	A2	1	Total	C	N	0
			10	7	3	
49	A2	1	Total	C	N	0
			10	7	3	
49	A2	1	Total	C	N	0
			10	7	3	
49	A2	1	Total	C	N	0
			10	7	3	

- Molecule 50 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
50	A2	1	Total	C	N	0
			14	10	4	
50	A2	1	Total	C	N	0
			14	10	4	
50	A2	1	Total	C	N	0
			14	10	4	
50	A2	1	Total	C	N	0
			14	10	4	
50	A2	1	Total	C	N	0
			14	10	4	

- Molecule 51 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
51	A2	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 52 is water.

Mol	Chain	Residues	Atoms	AltConf
52	A1	127	Total O 127 127	0
52	B1	39	Total O 39 39	0
52	C1	24	Total O 24 24	0
52	D1	68	Total O 68 68	0
52	E1	3	Total O 3 3	0
52	F1	90	Total O 90 90	0
52	G1	20	Total O 20 20	0
52	H1	167	Total O 167 167	0
52	I1	94	Total O 94 94	0
52	J1	70	Total O 70 70	0
52	K1	119	Total O 119 119	0

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Mol	Chain	Residues	Atoms		AltConf
52	L1	50	Total 50	O 50	0
52	M1	77	Total 77	O 77	0
52	N1	73	Total 73	O 73	0
52	O1	3	Total 3	O 3	0
52	P1	39	Total 39	O 39	0
52	Q1	15	Total 15	O 15	0
52	R1	38	Total 38	O 38	0
52	S1	45	Total 45	O 45	0
52	T1	9	Total 9	O 9	0
52	U1	89	Total 89	O 89	0
52	V1	46	Total 46	O 46	0
52	W1	5	Total 5	O 5	0
52	X1	32	Total 32	O 32	0
52	Y1	111	Total 111	O 111	0
52	Z1	65	Total 65	O 65	0
52	a1	60	Total 60	O 60	0
52	b1	26	Total 26	O 26	0
52	c1	26	Total 26	O 26	0
52	d1	82	Total 82	O 82	0
52	e1	4	Total 4	O 4	0
52	f1	39	Total 39	O 39	0

Continued on next page...

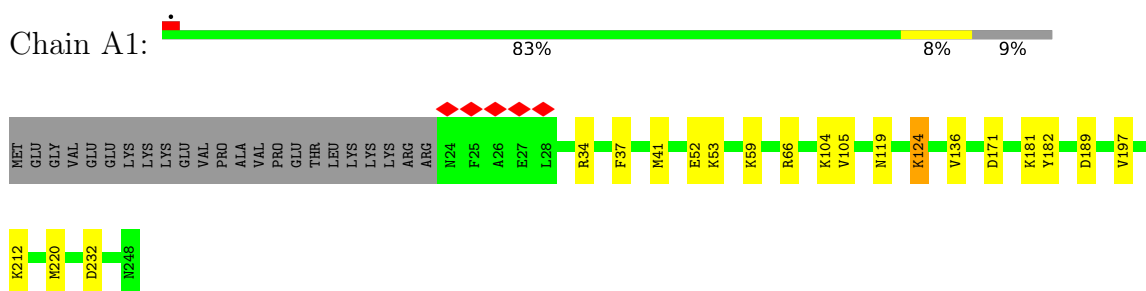
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
52	g1	22	Total 22	O 22	0
52	i1	49	Total 49	O 49	0
52	j1	27	Total 27	O 27	0
52	k1	59	Total 59	O 59	0
52	A2	8755	Total 8755	O 8755	0
52	B2	213	Total 213	O 213	0
52	C2	379	Total 379	O 379	0
52	D2	119	Total 119	O 119	0
52	E2	161	Total 161	O 161	0
52	F2	201	Total 201	O 201	0
52	G2	42	Total 42	O 42	0
52	H2	35	Total 35	O 35	0

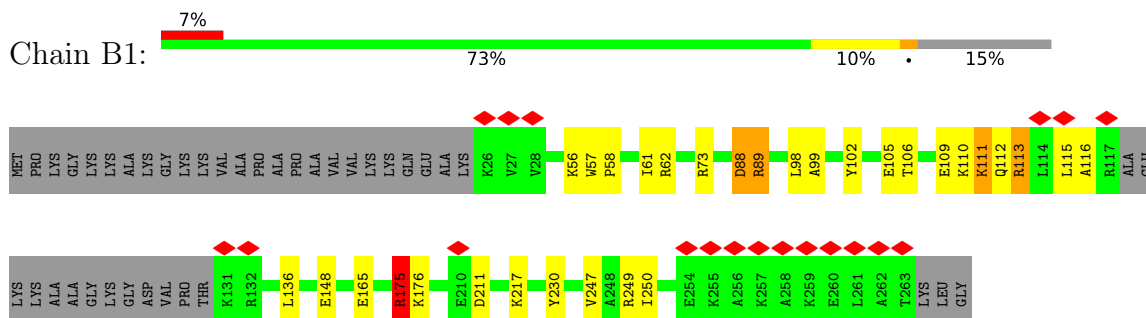
3 Residue-property plots

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.

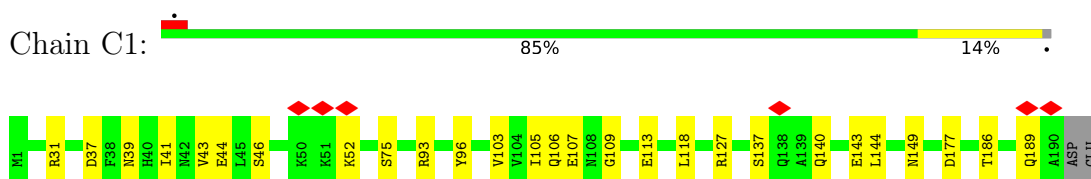
- Molecule 1: Large ribosomal subunit protein uL30



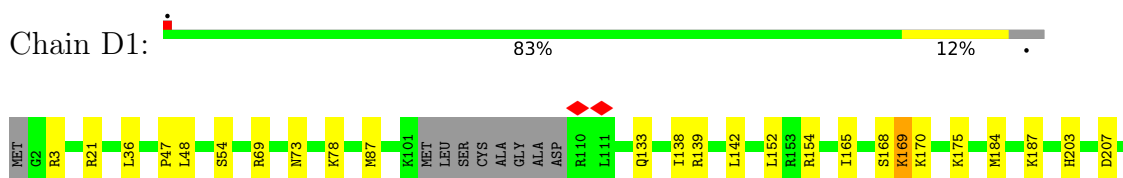
- Molecule 2: 60S ribosomal protein L7a



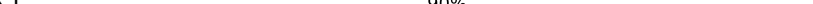
- Molecule 3: 60S ribosomal protein L9



- Molecule 4: Ribosomal protein uL16-like

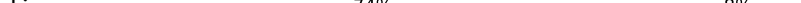


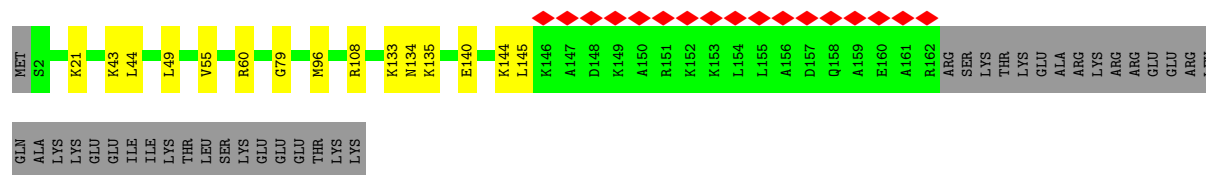
- Molecule 11: 60S ribosomal protein L18

Chain K1:  90% 10%



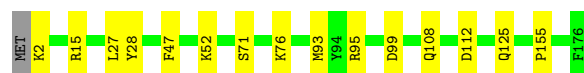
- Molecule 12: 60S ribosomal protein L19

Chain L1: 



- Molecule 13: 60S ribosomal protein L18a

Chain M1: 91% 9%

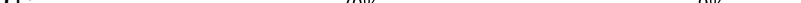


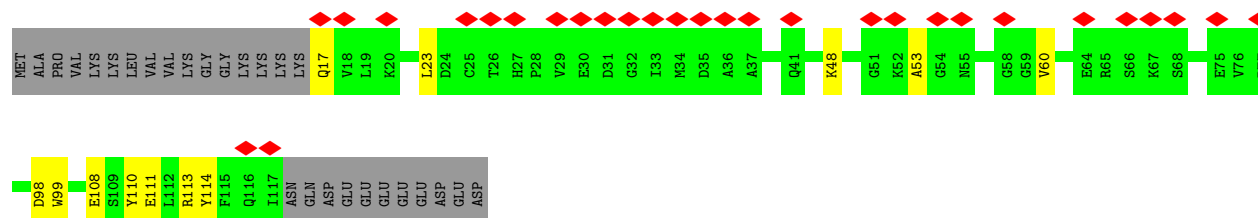
- Molecule 14: 60S ribosomal protein L21

Chain N1: 6% 89% 9% ...



- Molecule 15: 60S ribosomal protein L22

Chain O1: 



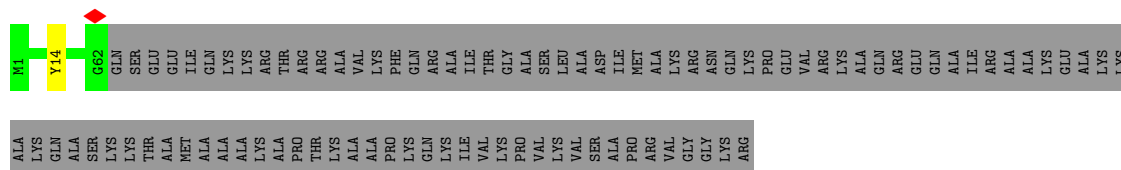
- Molecule 16: 60S ribosomal protein L23

Chain P1:  82% 11% 6%



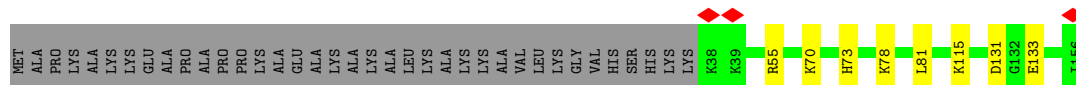
- Molecule 17: 60S ribosomal protein L24

Chain Q1:  39% 61%



- Molecule 18: 60S ribosomal protein L23a

Chain R1:  71% 5% 24%

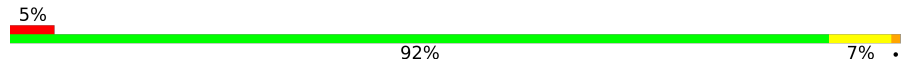


- Molecule 19: 60S ribosomal protein L26

Chain S1:  79% 13% 8%



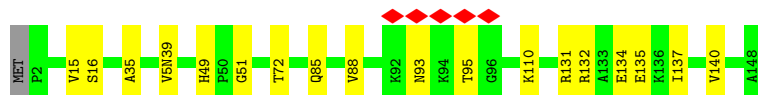
- Molecule 20: 60S ribosomal protein L27

Chain T1:  5% 92% 7% ..



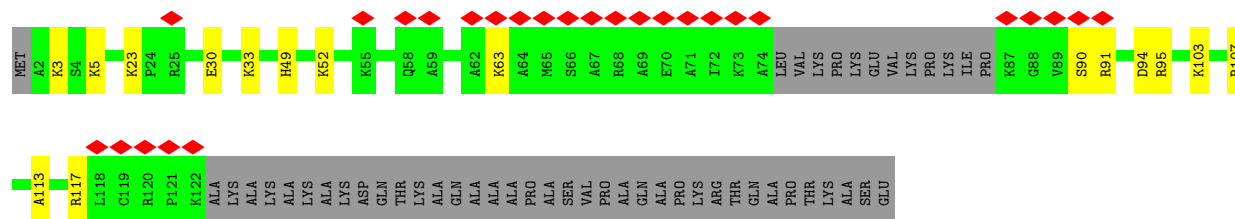
- Molecule 21: Large ribosomal subunit protein uL15

Chain U1:  87% 12%

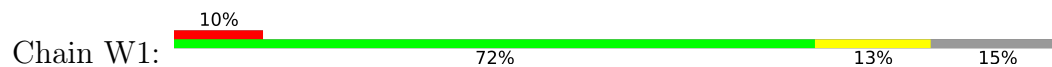


- Molecule 22: 60S ribosomal protein L29

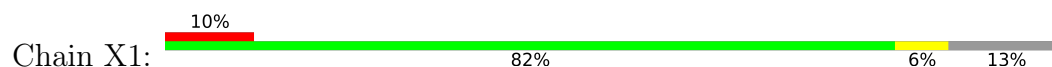
Chain V1:  17% 58% 10% 31%



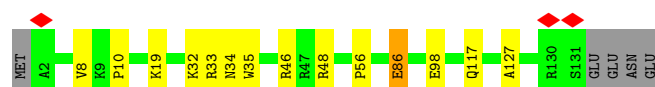
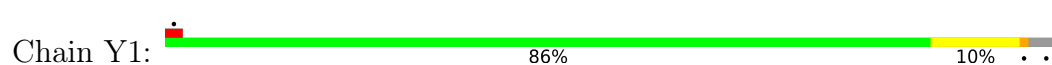
- Molecule 23: 60S ribosomal protein L30



- Molecule 24: 60S ribosomal protein L31



- Molecule 25: 60S ribosomal protein L32



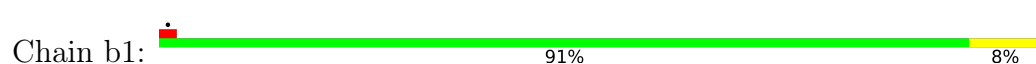
- Molecule 26: 60S ribosomal protein L35a



- Molecule 27: 60S ribosomal protein L34

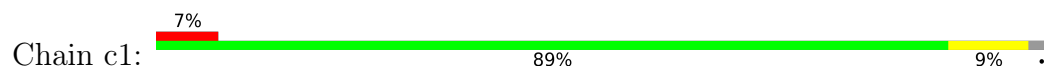


- Molecule 28: 60S ribosomal protein L35

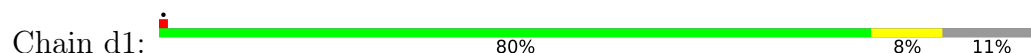




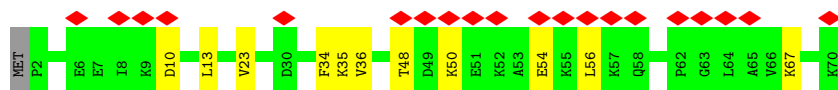
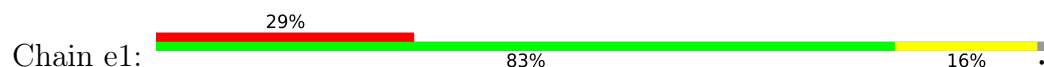
- Molecule 29: 60S ribosomal protein L36



- Molecule 30: 60S ribosomal protein L37



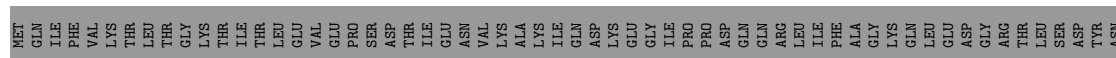
- Molecule 31: 60S ribosomal protein L38



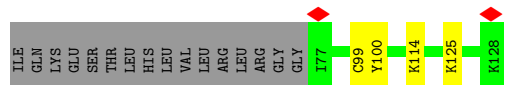
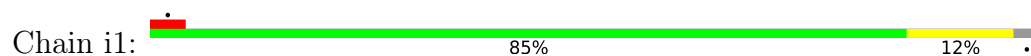
- Molecule 32: 60S ribosomal protein L39



- Molecule 33: Large ribosomal subunit protein eL40



- Molecule 34: 60S ribosomal protein L36a

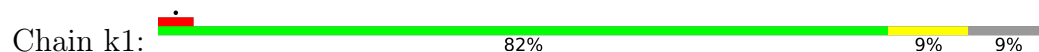




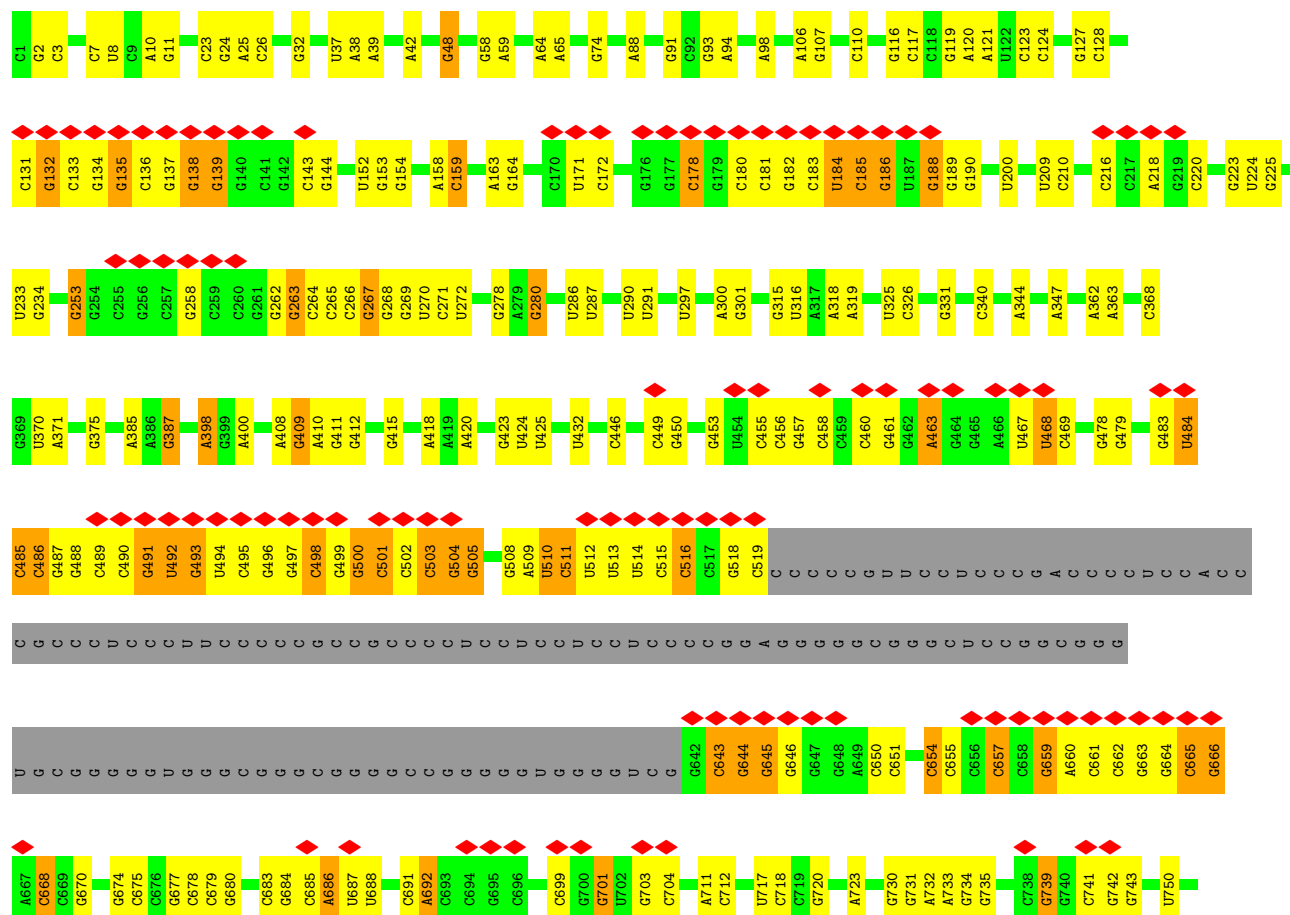
- Molecule 35: 60S ribosomal protein L37a



- Molecule 36: 60S ribosomal protein L28



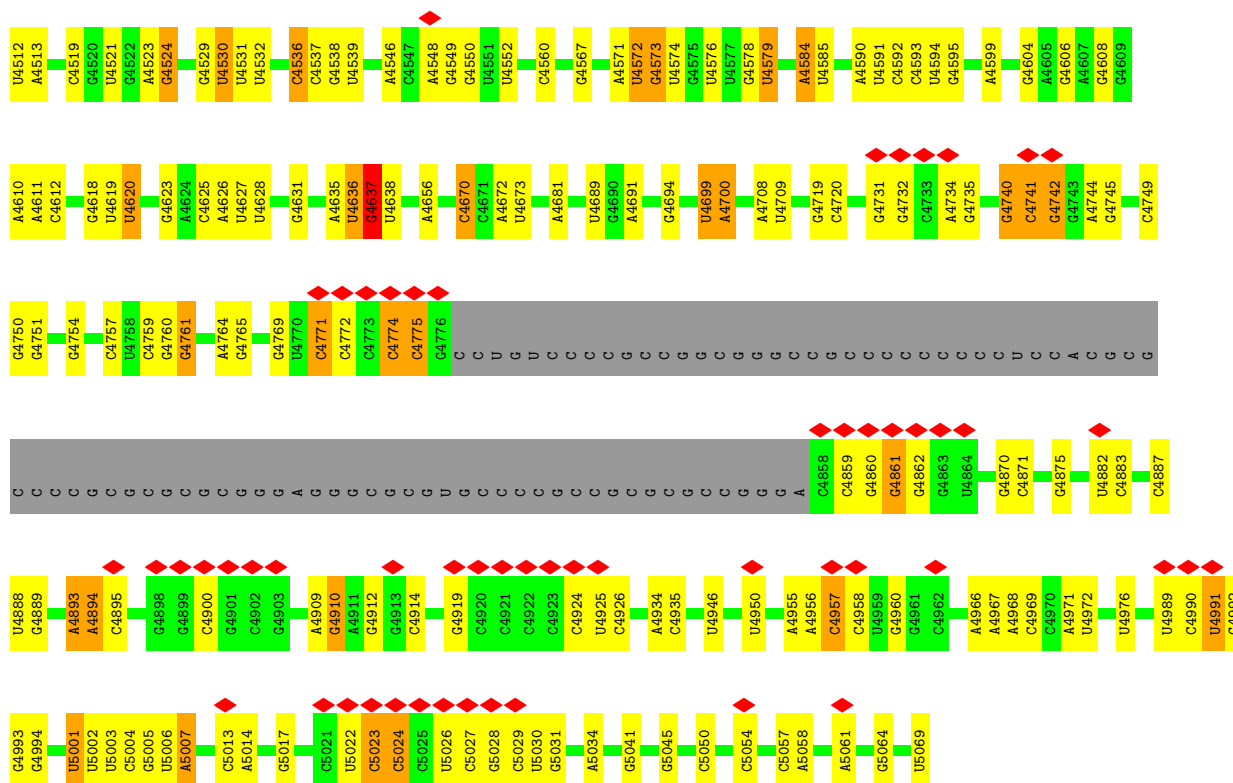
- Molecule 37: 28S rRNA



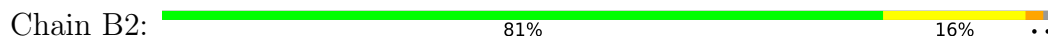




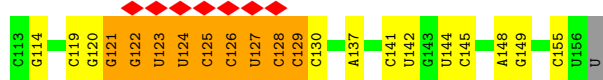
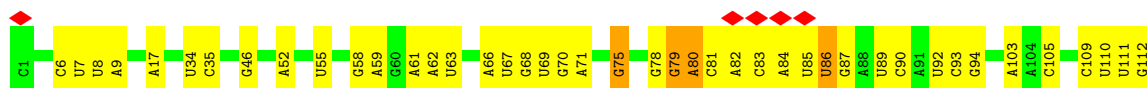




• Molecule 38: 5S rRNA

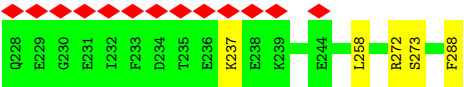


• Molecule 39: 5.8S rRNA



• Molecule 40: Large ribosomal subunit protein uL2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	880876	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 ($e^-/\text{\AA}^2$)	49	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	48.268	Depositor
Minimum map value	-17.531	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.86	Depositor
Map size ($\text{\AA}$)	394.24, 394.24, 394.24	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.616, 0.616, 0.616	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UY1, SPM, V5N, UR3, OMG, MG, PUT, 5MC, ZN, ATP, 1MA, OMU, MLZ, 6MZ, PSU, B8T, OMC, SPD, K, A2M, HIC

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	A1	0.30	0/1925	0.37	0/2564
2	B1	0.58	3/1853 (0.2%)	0.49	1/2495 (0.0%)
3	C1	0.40	0/1537	0.44	0/2066
4	D1	0.36	0/1727	0.43	2/2303 (0.1%)
5	E1	0.45	1/1394 (0.1%)	0.58	3/1863 (0.2%)
6	F1	0.21	0/1704	0.35	0/2282
7	G1	0.17	0/1142	0.29	0/1527
8	H1	0.21	0/1757	0.35	0/2353
9	I1	0.26	0/1682	0.37	0/2250
10	J1	0.36	0/1335	0.45	1/1793 (0.1%)
11	K1	0.21	0/1537	0.35	0/2052
12	L1	0.17	0/1357	0.27	0/1797
13	M1	0.21	0/1493	0.29	0/2003
14	N1	0.32	0/1335	0.42	1/1781 (0.1%)
15	O1	0.18	0/848	0.38	0/1137
16	P1	0.19	0/993	0.36	0/1332
17	Q1	0.17	0/532	0.29	0/708
18	R1	0.16	0/993	0.26	0/1334
19	S1	0.41	2/1132 (0.2%)	0.49	3/1504 (0.2%)
20	T1	0.20	0/1130	0.35	0/1507
21	U1	0.41	1/1179 (0.1%)	0.37	0/1573
22	V1	0.44	0/887	0.51	0/1170
23	W1	0.17	0/774	0.29	0/1038
24	X1	0.18	0/916	0.32	0/1234
25	Y1	0.20	0/1088	0.35	0/1451
26	Z1	0.21	0/895	0.31	0/1198
27	a1	0.18	0/916	0.31	0/1220
28	b1	0.17	0/1023	0.30	0/1351
29	c1	0.15	0/843	0.28	0/1115
30	d1	0.22	0/731	0.36	0/966
31	e1	0.18	0/575	0.37	0/761

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	f1	0.20	0/454	0.36	0/599
33	g1	0.23	0/425	0.32	0/561
34	i1	0.46	1/866 (0.1%)	0.45	0/1143
35	j1	0.18	0/717	0.31	0/953
36	k1	0.19	0/1017	0.31	0/1364
37	A2	0.24	1/86206 (0.0%)	0.30	0/134491
38	B2	0.22	0/2836	0.26	0/4421
39	C2	0.25	0/3631	0.30	0/5657
40	D2	0.29	0/1913	0.41	0/2563
41	E2	0.39	3/3264 (0.1%)	0.50	5/4366 (0.1%)
42	F2	0.26	0/2924	0.36	0/3927
43	G2	0.18	0/2432	0.32	0/3256
44	H2	0.23	0/1941	0.36	0/2603
All	All	0.26	12/145859 (0.0%)	0.33	16/215632 (0.0%)

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B1	175	ARG	C-O	-15.08	1.06	1.24
2	B1	175	ARG	CA-CB	-11.01	1.36	1.53
41	E2	300	LYS	CA-C	-10.80	1.38	1.52
34	i1	37	GLY	C-N	-9.67	1.20	1.33
19	S1	2	LYS	C-N	9.05	1.47	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	E2	301	ASN	N-CA-C	-10.46	88.52	110.80
41	E2	302	ASN	N-CA-C	-9.56	90.43	110.80
19	S1	2	LYS	CA-C-N	-9.55	107.25	122.24
19	S1	2	LYS	C-N-CA	-9.55	107.25	122.24
5	E1	118	LYS	N-CA-C	7.41	119.89	110.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	1887	0	2021	16	0
2	B1	1822	0	1962	24	0
3	C1	1518	0	1601	17	0
4	D1	1688	0	1737	20	0
5	E1	1371	0	1412	27	0
6	F1	1673	0	1779	15	0
7	G1	1120	0	1187	6	0
8	H1	1711	0	1755	25	0
9	I1	1650	0	1794	18	0
10	J1	1307	0	1337	13	0
11	K1	1513	0	1628	14	0
12	L1	1341	0	1475	16	0
13	M1	1453	0	1490	11	0
14	N1	1304	0	1379	18	0
15	O1	834	0	862	7	0
16	P1	979	0	1039	10	0
17	Q1	519	0	533	1	0
18	R1	976	0	1053	7	0
19	S1	1115	0	1205	16	0
20	T1	1107	0	1182	8	0
21	U1	1163	0	1206	11	0
22	V1	874	0	944	13	0
23	W1	764	0	804	9	0
24	X1	901	0	946	4	0
25	Y1	1070	0	1165	11	0
26	Z1	876	0	912	1	0
27	a1	906	0	998	5	0
28	b1	1015	0	1148	10	0
29	c1	832	0	917	6	0
30	d1	716	0	748	8	0
31	e1	569	0	637	12	0
32	f1	444	0	483	13	0
33	g1	430	0	466	3	0
34	i1	852	0	918	10	0
35	j1	707	0	756	3	0
36	k1	1002	0	1068	9	0
37	A2	79517	0	40246	762	0
38	B2	2538	0	1286	19	0
39	C2	3315	0	1685	52	0
40	D2	1888	0	1976	18	0
41	E2	3209	0	3351	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	F2	2870	0	3044	26	0
43	G2	2386	0	2421	19	0
44	H2	1903	0	2057	19	0
45	A2	175	0	0	0	0
45	B2	2	0	0	0	0
45	C2	3	0	0	0	0
45	D1	1	0	0	0	0
45	J1	1	0	0	0	0
45	P1	1	0	0	0	0
45	Y1	1	0	0	0	0
45	Z1	1	0	0	0	0
45	d1	1	0	0	0	0
46	A2	30	0	60	20	0
46	B2	6	0	12	5	0
46	H1	12	0	24	4	0
47	A2	42	0	0	0	0
47	D2	2	0	0	0	0
47	M1	1	0	0	0	0
47	N1	1	0	0	0	0
48	a1	1	0	0	0	0
48	d1	1	0	0	0	0
48	g1	1	0	0	0	0
48	i1	1	0	0	0	0
48	j1	1	0	0	0	0
49	A2	70	0	132	29	0
50	A2	70	0	130	4	0
51	A2	31	0	12	8	0
52	A1	127	0	0	3	0
52	A2	8755	0	0	74	0
52	B1	39	0	0	0	0
52	B2	213	0	0	2	0
52	C1	24	0	0	0	0
52	C2	379	0	0	3	0
52	D1	68	0	0	1	0
52	D2	119	0	0	4	0
52	E1	3	0	0	0	0
52	E2	161	0	0	3	0
52	F1	90	0	0	2	0
52	F2	201	0	0	8	0
52	G1	20	0	0	0	0
52	G2	42	0	0	1	0
52	H1	167	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	H2	35	0	0	1	0
52	I1	94	0	0	1	0
52	J1	70	0	0	1	0
52	K1	119	0	0	4	0
52	L1	50	0	0	0	0
52	M1	77	0	0	1	0
52	N1	73	0	0	3	0
52	O1	3	0	0	0	0
52	P1	39	0	0	0	0
52	Q1	15	0	0	0	0
52	R1	38	0	0	2	0
52	S1	45	0	0	0	0
52	T1	9	0	0	1	0
52	U1	89	0	0	0	0
52	V1	46	0	0	1	0
52	W1	5	0	0	0	0
52	X1	32	0	0	0	0
52	Y1	111	0	0	4	0
52	Z1	65	0	0	0	0
52	a1	60	0	0	1	0
52	b1	26	0	0	1	0
52	c1	26	0	0	1	0
52	d1	82	0	0	3	0
52	e1	4	0	0	0	0
52	f1	39	0	0	4	0
52	g1	22	0	0	0	0
52	i1	49	0	0	2	0
52	j1	27	0	0	0	0
52	k1	59	0	0	1	0
All	All	149908	0	98983	1259	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 1259 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)
5:E1:57:VAL:O	5:E1:58:ARG:HG2	1.24	1.38
5:E1:89:VAL:HG13	5:E1:114:ASP:OD2	1.37	1.21
31:e1:34:PHE:CE2	31:e1:56:LEU:HD22	1.90	1.06
5:E1:57:VAL:O	5:E1:58:ARG:CG	2.03	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E1:95:ARG:HD3	5:E1:178:LYS:O	1.56	1.04

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	A1	225/248 (91%)	221 (98%)	4 (2%)	0	100	100
2	B1	221/266 (83%)	217 (98%)	4 (2%)	0	100	100
3	C1	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
4	D1	204/214 (95%)	203 (100%)	1 (0%)	0	100	100
5	E1	169/178 (95%)	162 (96%)	7 (4%)	0	100	100
6	F1	205/211 (97%)	197 (96%)	8 (4%)	0	100	100
7	G1	134/215 (62%)	130 (97%)	4 (3%)	0	100	100
8	H1	202/204 (99%)	200 (99%)	2 (1%)	0	100	100
9	I1	199/203 (98%)	198 (100%)	1 (0%)	0	100	100
10	J1	159/184 (86%)	152 (96%)	7 (4%)	0	100	100
11	K1	185/188 (98%)	183 (99%)	2 (1%)	0	100	100
12	L1	159/196 (81%)	159 (100%)	0	0	100	100
13	M1	173/176 (98%)	172 (99%)	1 (1%)	0	100	100
14	N1	158/160 (99%)	155 (98%)	3 (2%)	0	100	100
15	O1	100/128 (78%)	93 (93%)	7 (7%)	0	100	100
16	P1	129/140 (92%)	127 (98%)	2 (2%)	0	100	100
17	Q1	60/157 (38%)	60 (100%)	0	0	100	100
18	R1	117/156 (75%)	114 (97%)	3 (3%)	0	100	100
19	S1	132/145 (91%)	131 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T1	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
21	U1	144/148 (97%)	140 (97%)	3 (2%)	1 (1%)	18	8
22	V1	105/159 (66%)	100 (95%)	5 (5%)	0	100	100
23	W1	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
24	X1	107/125 (86%)	101 (94%)	6 (6%)	0	100	100
25	Y1	128/135 (95%)	128 (100%)	0	0	100	100
26	Z1	107/110 (97%)	107 (100%)	0	0	100	100
27	a1	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
28	b1	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
29	c1	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
30	d1	85/97 (88%)	85 (100%)	0	0	100	100
31	e1	67/70 (96%)	67 (100%)	0	0	100	100
32	f1	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
33	g1	49/128 (38%)	49 (100%)	0	0	100	100
34	i1	102/106 (96%)	97 (95%)	5 (5%)	0	100	100
35	j1	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
36	k1	123/137 (90%)	123 (100%)	0	0	100	100
40	D2	243/257 (95%)	236 (97%)	7 (3%)	0	100	100
41	E2	394/403 (98%)	382 (97%)	11 (3%)	1 (0%)	36	22
42	F2	358/427 (84%)	355 (99%)	3 (1%)	0	100	100
43	G2	291/297 (98%)	285 (98%)	6 (2%)	0	100	100
44	H2	231/288 (80%)	223 (96%)	8 (4%)	0	100	100
All	All	6351/7187 (88%)	6213 (98%)	136 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
41	E2	300	LYS
21	U1	15	VAL

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	196/215 (91%)	194 (99%)	2 (1%)	68	55
2	B1	195/223 (87%)	188 (96%)	7 (4%)	31	10
3	C1	169/171 (99%)	168 (99%)	1 (1%)	78	70
4	D1	178/181 (98%)	176 (99%)	2 (1%)	65	51
5	E1	144/149 (97%)	142 (99%)	2 (1%)	59	44
6	F1	173/177 (98%)	173 (100%)	0	100	100
7	G1	116/161 (72%)	116 (100%)	0	100	100
8	H1	172/172 (100%)	172 (100%)	0	100	100
9	I1	173/174 (99%)	172 (99%)	1 (1%)	78	70
10	J1	142/163 (87%)	139 (98%)	3 (2%)	47	27
11	K1	164/165 (99%)	164 (100%)	0	100	100
12	L1	142/175 (81%)	141 (99%)	1 (1%)	76	66
13	M1	156/157 (99%)	156 (100%)	0	100	100
14	N1	140/140 (100%)	138 (99%)	2 (1%)	59	44
15	O1	92/115 (80%)	91 (99%)	1 (1%)	65	51
16	P1	101/107 (94%)	101 (100%)	0	100	100
17	Q1	54/126 (43%)	54 (100%)	0	100	100
18	R1	107/133 (80%)	107 (100%)	0	100	100
19	S1	124/135 (92%)	123 (99%)	1 (1%)	73	63
20	T1	117/118 (99%)	116 (99%)	1 (1%)	70	59
21	U1	119/120 (99%)	119 (100%)	0	100	100
22	V1	87/126 (69%)	85 (98%)	2 (2%)	44	25
23	W1	83/97 (86%)	83 (100%)	0	100	100
24	X1	99/110 (90%)	99 (100%)	0	100	100
25	Y1	116/121 (96%)	114 (98%)	2 (2%)	53	36
26	Z1	88/89 (99%)	88 (100%)	0	100	100
27	a1	98/100 (98%)	98 (100%)	0	100	100
28	b1	109/110 (99%)	109 (100%)	0	100	100
29	c1	86/89 (97%)	86 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	d1	74/80 (92%)	74 (100%)	0	100	100
31	e1	64/65 (98%)	64 (100%)	0	100	100
32	f1	47/48 (98%)	47 (100%)	0	100	100
33	g1	47/115 (41%)	47 (100%)	0	100	100
34	i1	92/94 (98%)	91 (99%)	1 (1%)	65	51
35	j1	74/75 (99%)	74 (100%)	0	100	100
36	k1	109/121 (90%)	108 (99%)	1 (1%)	70	59
40	D2	188/198 (95%)	186 (99%)	2 (1%)	65	51
41	E2	345/348 (99%)	343 (99%)	2 (1%)	78	70
42	F2	300/348 (86%)	297 (99%)	3 (1%)	68	55
43	G2	247/250 (99%)	247 (100%)	0	100	100
44	H2	210/252 (83%)	209 (100%)	1 (0%)	81	73
All	All	5537/6113 (91%)	5499 (99%)	38 (1%)	73	66

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	i1	59	LYS
42	F2	291	ARG
36	k1	5	LEU
41	E2	300	LYS
44	H2	207	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
26	Z1	99	HIS
41	E2	145	GLN
27	a1	114	GLN
34	i1	102	GLN
41	E2	289	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
37	A2	3695/5069 (72%)	657 (17%)	21 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
38	B2	118/120 (98%)	9 (7%)	0
39	C2	155/157 (98%)	28 (18%)	1 (0%)
All	All	3968/5346 (74%)	694 (17%)	22 (0%)

5 of 694 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
37	A2	39	A
37	A2	42	A
37	A2	48	G
37	A2	58	G
37	A2	59	A

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
37	A2	3876	A
37	A2	4142	C
37	A2	4106	G
37	A2	4378	A
37	A2	1625	OMG

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

122 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	$\# Z > 2$
37	OMC	A2	2351	45,37	19,22,23	2.89	8 (42%)	26,31,34	0.76	0
37	OMC	A2	1881	45,37	19,22,23	2.88	8 (42%)	26,31,34	0.76	0
37	A2M	A2	1326	37	22,25,26	3.07	8 (36%)	31,36,39	3.75	12 (38%)
37	OMC	A2	2804	37	19,22,23	2.89	8 (42%)	26,31,34	0.64	0
37	PSU	A2	2839	37	18,21,22	4.18	7 (38%)	22,30,33	1.87	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	A2M	A2	398	37	22,25,26	3.09	7 (31%)	31,36,39	3.81	12 (38%)
37	PSU	A2	4299	37	18,21,22	4.16	7 (38%)	22,30,33	1.87	5 (22%)
37	OMG	A2	3669	37	23,26,27	2.41	8 (34%)	33,38,41	2.34	11 (33%)
37	OMG	A2	4228	37	23,26,27	2.39	8 (34%)	33,38,41	2.34	10 (30%)
37	OMC	A2	2365	37	19,22,23	2.89	8 (42%)	26,31,34	0.68	0
40	V5N	D2	216	40	9,11,12	2.72	2 (22%)	9,14,16	1.25	1 (11%)
37	PSU	A2	4442	37	18,21,22	4.18	7 (38%)	22,30,33	1.93	6 (27%)
37	A2M	A2	4523	45,37	22,25,26	3.06	7 (31%)	31,36,39	3.87	13 (41%)
37	PSU	A2	1792	37	18,21,22	4.16	8 (44%)	22,30,33	1.83	5 (22%)
37	OMC	A2	3701	47,37	19,22,23	2.92	8 (42%)	26,31,34	0.77	0
37	PSU	A2	4972	37	18,21,22	4.18	7 (38%)	22,30,33	1.86	5 (22%)
37	A2M	A2	2787	37	22,25,26	3.09	9 (40%)	31,36,39	3.80	13 (41%)
37	PSU	A2	4521	45,37	18,21,22	4.15	7 (38%)	22,30,33	1.97	6 (27%)
37	OMC	A2	3841	37	19,22,23	2.89	8 (42%)	26,31,34	0.70	0
37	PSU	A2	4296	37	18,21,22	4.21	7 (38%)	22,30,33	1.92	5 (22%)
37	OMG	A2	2876	37	23,26,27	2.44	8 (34%)	33,38,41	2.26	10 (30%)
37	A2M	A2	1524	37	22,25,26	3.04	9 (40%)	31,36,39	3.75	13 (41%)
37	PSU	A2	1782	37	18,21,22	4.19	7 (38%)	22,30,33	1.92	5 (22%)
37	OMU	A2	4306	37	19,22,23	3.00	8 (42%)	26,31,34	1.68	4 (15%)
37	OMC	A2	4536	37	19,22,23	2.90	8 (42%)	26,31,34	0.75	0
37	PSU	A2	3884	37	18,21,22	4.17	7 (38%)	22,30,33	1.91	5 (22%)
37	OMC	A2	2824	37	19,22,23	2.93	8 (42%)	26,31,34	0.70	0
37	A2M	A2	3825	37	22,25,26	3.08	7 (31%)	31,36,39	3.81	12 (38%)
37	OMG	A2	3627	37	23,26,27	2.39	8 (34%)	33,38,41	2.35	10 (30%)
37	PSU	A2	1677	37	18,21,22	4.26	8 (44%)	22,30,33	1.94	5 (22%)
37	5MC	A2	4447	47,37	18,22,23	3.42	7 (38%)	26,32,35	1.08	1 (3%)
37	UR3	A2	4530	37	19,22,23	2.78	6 (31%)	26,32,35	1.57	5 (19%)
37	PSU	A2	4576	37	18,21,22	4.18	7 (38%)	22,30,33	1.83	5 (22%)
37	A2M	A2	1323	37	22,25,26	3.07	8 (36%)	31,36,39	3.72	12 (38%)
37	A2M	A2	3718	37	22,25,26	3.09	8 (36%)	31,36,39	3.83	12 (38%)
37	OMG	A2	4196	37	23,26,27	2.41	8 (34%)	33,38,41	2.23	10 (30%)
37	PSU	A2	4403	37	18,21,22	4.15	7 (38%)	22,30,33	1.98	6 (27%)
37	OMG	A2	1625	37	23,26,27	2.42	7 (30%)	33,38,41	2.19	9 (27%)
37	PSU	A2	1860	37	18,21,22	4.17	7 (38%)	22,30,33	1.91	5 (22%)
37	PSU	A2	4673	45,37	18,21,22	4.14	7 (38%)	22,30,33	1.90	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PSU	A2	4532	37	18,21,22	4.21	7 (38%)	22,30,33	1.81	5 (22%)
37	5MC	A2	3782	45,37	18,22,23	3.43	7 (38%)	26,32,35	1.01	2 (7%)
37	OMG	A2	2424	37	23,26,27	2.41	8 (34%)	33,38,41	2.24	9 (27%)
37	PSU	A2	4457	37	18,21,22	4.14	7 (38%)	22,30,33	1.86	6 (27%)
39	OMG	C2	75	39	23,26,27	2.39	8 (34%)	33,38,41	2.26	10 (30%)
37	A2M	A2	3830	37	22,25,26	3.07	8 (36%)	31,36,39	3.85	12 (38%)
37	PSU	A2	224	37	18,21,22	4.21	7 (38%)	22,30,33	1.93	5 (22%)
37	OMG	A2	3899	37	23,26,27	2.39	7 (30%)	33,38,41	2.28	10 (30%)
41	HIC	E2	245	41	10,11,12	1.44	1 (10%)	8,14,16	1.00	0
37	PSU	A2	4431	37	18,21,22	4.15	7 (38%)	22,30,33	1.86	5 (22%)
37	A2M	A2	1871	45,37	22,25,26	3.07	7 (31%)	31,36,39	3.75	12 (38%)
37	PSU	A2	1781	37	18,21,22	4.21	7 (38%)	22,30,33	1.84	5 (22%)
37	A2M	A2	2363	45,37	22,25,26	3.07	8 (36%)	31,36,39	3.80	12 (38%)
37	OMG	A2	4623	37	23,26,27	2.41	8 (34%)	33,38,41	2.29	10 (30%)
37	PSU	A2	4500	37	18,21,22	4.19	7 (38%)	22,30,33	1.93	6 (27%)
37	OMG	A2	4499	37	23,26,27	2.42	8 (34%)	33,38,41	2.27	10 (30%)
37	OMU	A2	3925	37	19,22,23	3.01	8 (42%)	26,31,34	1.74	5 (19%)
37	PSU	A2	1536	37	18,21,22	4.10	7 (38%)	22,30,33	1.91	5 (22%)
37	OMC	A2	2861	37	19,22,23	2.94	8 (42%)	26,31,34	0.71	0
37	PSU	A2	4353	37	18,21,22	4.16	7 (38%)	22,30,33	1.98	5 (22%)
37	1MA	A2	1322	45,37	21,25,26	2.95	7 (33%)	31,37,40	1.94	8 (25%)
37	OMG	A2	1522	37	23,26,27	2.41	8 (34%)	33,38,41	2.34	10 (30%)
37	A2M	A2	3785	37	22,25,26	3.07	7 (31%)	31,36,39	4.08	14 (45%)
37	OMG	A2	4637	37	23,26,27	2.39	7 (30%)	33,38,41	2.25	10 (30%)
37	OMG	A2	1316	37	23,26,27	2.40	7 (30%)	33,38,41	2.26	10 (30%)
37	PSU	A2	4552	37	18,21,22	4.14	7 (38%)	22,30,33	1.81	5 (22%)
37	PSU	A2	4312	37	18,21,22	4.16	7 (38%)	22,30,33	1.85	5 (22%)
37	PSU	A2	2632	37	18,21,22	4.25	8 (44%)	22,30,33	1.76	5 (22%)
37	6MZ	A2	4220	37	22,25,26	2.90	6 (27%)	30,36,39	2.49	9 (30%)
37	OMU	A2	4227	37	19,22,23	3.04	8 (42%)	26,31,34	1.73	5 (19%)
37	PSU	A2	4471	37	18,21,22	4.16	7 (38%)	22,30,33	1.83	5 (22%)
37	PSU	A2	5001	37	18,21,22	4.19	7 (38%)	22,30,33	1.89	5 (22%)
37	PSU	A2	4423	37	18,21,22	4.21	7 (38%)	22,30,33	1.88	5 (22%)
37	PSU	A2	1744	37	18,21,22	4.16	7 (38%)	22,30,33	1.87	5 (22%)
37	B8T	A2	1859	37	19,22,23	3.15	8 (42%)	26,31,34	0.83	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	OMC	A2	2422	45,37	19,22,23	2.92	8 (42%)	26,31,34	0.70	0
37	OMC	A2	3869	37	19,22,23	2.91	8 (42%)	26,31,34	0.71	0
37	A2M	A2	400	37	22,25,26	3.08	8 (36%)	31,36,39	3.81	11 (35%)
37	OMG	A2	4392	37	23,26,27	2.40	7 (30%)	33,38,41	2.26	10 (30%)
37	OMG	A2	3744	37	23,26,27	2.41	8 (34%)	33,38,41	2.26	10 (30%)
37	OMC	A2	3808	37	19,22,23	2.94	8 (42%)	26,31,34	0.83	0
37	OMG	A2	3792	37	23,26,27	2.39	7 (30%)	33,38,41	2.17	9 (27%)
37	PSU	A2	3637	47,37	18,21,22	4.14	7 (38%)	22,30,33	1.96	5 (22%)
37	OMG	A2	4618	37	23,26,27	2.40	8 (34%)	33,38,41	2.29	10 (30%)
33	MLZ	g1	98	33	8,9,10	0.76	0	4,9,11	0.61	0
37	OMU	A2	4498	45,37	19,22,23	3.01	8 (42%)	26,31,34	1.75	5 (19%)
37	OMC	A2	4456	37	19,22,23	2.88	8 (42%)	26,31,34	0.73	0
37	OMG	A2	2364	37	23,26,27	2.39	7 (30%)	33,38,41	2.19	9 (27%)
37	PSU	A2	4293	37	18,21,22	4.12	7 (38%)	22,30,33	1.75	5 (22%)
37	PSU	A2	3639	37	18,21,22	4.13	7 (38%)	22,30,33	1.91	5 (22%)
37	PSU	A2	4689	37	18,21,22	4.13	7 (38%)	22,30,33	1.95	5 (22%)
37	A2M	A2	4571	37	22,25,26	3.09	8 (36%)	31,36,39	4.00	12 (38%)
37	OMG	A2	4494	37	23,26,27	2.42	8 (34%)	33,38,41	2.25	10 (30%)
37	PSU	A2	1779	37	18,21,22	4.21	7 (38%)	22,30,33	1.88	5 (22%)
37	A2M	A2	2401	37	22,25,26	3.08	7 (31%)	31,36,39	3.80	12 (38%)
37	PSU	A2	4361	37	18,21,22	4.14	7 (38%)	22,30,33	1.82	5 (22%)
39	PSU	C2	55	39	18,21,22	4.19	7 (38%)	22,30,33	1.88	5 (22%)
37	OMU	A2	4620	37	19,22,23	2.99	8 (42%)	26,31,34	1.71	5 (19%)
37	A2M	A2	3867	37	22,25,26	3.08	8 (36%)	31,36,39	3.83	12 (38%)
37	PSU	A2	1862	37	18,21,22	4.13	7 (38%)	22,30,33	1.91	5 (22%)
21	V5N	U1	39	21	9,11,12	2.73	2 (22%)	9,14,16	1.25	1 (11%)
37	PSU	A2	4493	47,37	18,21,22	4.18	7 (38%)	22,30,33	1.80	5 (22%)
37	PSU	A2	1683	47,37	18,21,22	4.12	7 (38%)	22,30,33	1.91	5 (22%)
37	OMU	A2	2837	37	19,22,23	3.00	8 (42%)	26,31,34	1.77	5 (19%)
37	PSU	A2	3822	37	18,21,22	4.18	7 (38%)	22,30,33	1.97	5 (22%)
37	PSU	A2	4628	37	18,21,22	4.12	7 (38%)	22,30,33	2.02	5 (22%)
37	OMC	A2	1340	37	19,22,23	2.89	8 (42%)	26,31,34	0.66	0
37	PSU	A2	3844	37	18,21,22	4.16	7 (38%)	22,30,33	1.85	5 (22%)
37	PSU	A2	4420	37	18,21,22	4.34	8 (44%)	22,30,33	1.75	5 (22%)
37	PSU	A2	3851	37	18,21,22	4.17	7 (38%)	22,30,33	1.91	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PSU	A2	3920	45,37	18,21,22	4.15	7 (38%)	22,30,33	1.87	6 (27%)
37	PSU	A2	4579	37	18,21,22	4.16	7 (38%)	22,30,33	1.88	5 (22%)
37	PSU	A2	2508	37	18,21,22	4.17	7 (38%)	22,30,33	1.86	5 (22%)
37	A2M	A2	2815	45,37	22,25,26	3.07	7 (31%)	31,36,39	3.75	12 (38%)
39	PSU	C2	69	39	18,21,22	4.19	7 (38%)	22,30,33	1.93	6 (27%)
37	OMG	A2	4370	37	23,26,27	2.41	8 (34%)	33,38,41	2.30	10 (30%)
37	OMU	A2	2415	37	19,22,23	3.04	8 (42%)	26,31,34	1.72	5 (19%)
37	PSU	A2	3715	37	18,21,22	4.22	7 (38%)	22,30,33	1.94	6 (27%)
37	UY1	A2	3818	47,37	19,22,23	4.11	9 (47%)	22,31,34	2.07	5 (22%)
37	A2M	A2	1534	45,37	22,25,26	3.10	8 (36%)	31,36,39	3.81	12 (38%)
37	PSU	A2	3695	37	18,21,22	4.21	8 (44%)	22,30,33	1.83	6 (27%)
37	OMC	A2	3887	37	19,22,23	2.91	8 (42%)	26,31,34	0.71	0

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
37	OMC	A2	2351	45,37	-	1/9/27/28	0/2/2/2
37	OMC	A2	1881	45,37	-	0/9/27/28	0/2/2/2
37	A2M	A2	1326	37	-	0/9/27/28	0/3/3/3
37	OMC	A2	2804	37	-	0/9/27/28	0/2/2/2
37	PSU	A2	2839	37	-	0/7/25/26	0/2/2/2
37	A2M	A2	398	37	-	1/9/27/28	0/3/3/3
37	PSU	A2	4299	37	-	0/7/25/26	0/2/2/2
37	OMG	A2	3669	37	-	2/9/27/28	0/3/3/3
37	OMG	A2	4228	37	-	0/9/27/28	0/3/3/3
37	OMC	A2	2365	37	-	0/9/27/28	0/2/2/2
40	V5N	D2	216	40	-	1/9/10/12	0/1/1/1
37	PSU	A2	4442	37	-	0/7/25/26	0/2/2/2
37	A2M	A2	4523	45,37	-	0/9/27/28	0/3/3/3
37	PSU	A2	1792	37	-	0/7/25/26	0/2/2/2
37	OMC	A2	3701	47,37	-	4/9/27/28	0/2/2/2
37	PSU	A2	4972	37	-	0/7/25/26	0/2/2/2
37	A2M	A2	2787	37	-	4/9/27/28	0/3/3/3
37	PSU	A2	4521	45,37	-	0/7/25/26	0/2/2/2
37	OMC	A2	3841	37	-	0/9/27/28	0/2/2/2
37	PSU	A2	4296	37	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	OMG	A2	2876	37	-	1/9/27/28	0/3/3/3
37	A2M	A2	1524	37	-	1/9/27/28	0/3/3/3
37	PSU	A2	1782	37	-	0/7/25/26	0/2/2/2
37	OMU	A2	4306	37	-	0/9/27/28	0/2/2/2
37	OMC	A2	4536	37	-	0/9/27/28	0/2/2/2
37	PSU	A2	3884	37	-	0/7/25/26	0/2/2/2
37	OMC	A2	2824	37	-	1/9/27/28	0/2/2/2
37	A2M	A2	3825	37	-	0/9/27/28	0/3/3/3
37	OMG	A2	3627	37	-	0/9/27/28	0/3/3/3
37	PSU	A2	1677	37	-	0/7/25/26	0/2/2/2
37	5MC	A2	4447	47,37	-	4/7/25/26	0/2/2/2
37	UR3	A2	4530	37	-	2/7/25/26	0/2/2/2
37	PSU	A2	4576	37	-	0/7/25/26	0/2/2/2
37	A2M	A2	1323	37	-	1/9/27/28	0/3/3/3
37	A2M	A2	3718	37	-	1/9/27/28	0/3/3/3
37	OMG	A2	4196	37	-	3/9/27/28	0/3/3/3
37	PSU	A2	4403	37	-	0/7/25/26	0/2/2/2
37	OMG	A2	1625	37	-	1/9/27/28	0/3/3/3
37	PSU	A2	1860	37	-	0/7/25/26	0/2/2/2
37	PSU	A2	4673	45,37	-	0/7/25/26	0/2/2/2
37	PSU	A2	4532	37	-	0/7/25/26	0/2/2/2
37	5MC	A2	3782	45,37	-	0/7/25/26	0/2/2/2
37	OMG	A2	2424	37	-	1/9/27/28	0/3/3/3
37	PSU	A2	4457	37	-	0/7/25/26	0/2/2/2
39	OMG	C2	75	39	-	0/9/27/28	0/3/3/3
37	A2M	A2	3830	37	-	1/9/27/28	0/3/3/3
37	PSU	A2	224	37	-	2/7/25/26	0/2/2/2
37	OMG	A2	3899	37	-	0/9/27/28	0/3/3/3
41	HIC	E2	245	41	-	1/5/6/8	0/1/1/1
37	PSU	A2	4431	37	-	0/7/25/26	0/2/2/2
37	A2M	A2	1871	45,37	-	0/9/27/28	0/3/3/3
37	PSU	A2	1781	37	-	1/7/25/26	0/2/2/2
37	A2M	A2	2363	45,37	-	0/9/27/28	0/3/3/3
37	OMG	A2	4623	37	-	0/9/27/28	0/3/3/3
37	PSU	A2	4500	37	-	3/7/25/26	0/2/2/2
37	OMG	A2	4499	37	-	0/9/27/28	0/3/3/3
37	OMU	A2	3925	37	-	0/9/27/28	0/2/2/2
37	PSU	A2	1536	37	-	0/7/25/26	0/2/2/2
37	OMC	A2	2861	37	-	0/9/27/28	0/2/2/2
37	PSU	A2	4353	37	-	0/7/25/26	0/2/2/2
37	1MA	A2	1322	45,37	-	1/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	OMG	A2	1522	37	-	0/9/27/28	0/3/3/3
37	A2M	A2	3785	37	-	2/9/27/28	0/3/3/3
37	OMG	A2	4637	37	-	1/9/27/28	0/3/3/3
37	OMG	A2	1316	37	-	0/9/27/28	0/3/3/3
37	PSU	A2	4552	37	-	0/7/25/26	0/2/2/2
37	PSU	A2	4312	37	-	0/7/25/26	0/2/2/2
37	PSU	A2	2632	37	-	0/7/25/26	0/2/2/2
37	6MZ	A2	4220	37	-	0/9/27/28	0/3/3/3
37	OMU	A2	4227	37	-	0/9/27/28	0/2/2/2
37	PSU	A2	4471	37	-	0/7/25/26	0/2/2/2
37	PSU	A2	5001	37	-	0/7/25/26	0/2/2/2
37	PSU	A2	4423	37	-	0/7/25/26	0/2/2/2
37	PSU	A2	1744	37	-	0/7/25/26	0/2/2/2
37	B8T	A2	1859	37	-	0/7/27/28	0/2/2/2
37	OMC	A2	2422	45,37	-	2/9/27/28	0/2/2/2
37	OMC	A2	3869	37	-	0/9/27/28	0/2/2/2
37	A2M	A2	400	37	-	0/9/27/28	0/3/3/3
37	OMG	A2	4392	37	-	0/9/27/28	0/3/3/3
37	OMG	A2	3744	37	-	1/9/27/28	0/3/3/3
37	OMC	A2	3808	37	-	0/9/27/28	0/2/2/2
37	OMG	A2	3792	37	-	2/9/27/28	0/3/3/3
37	PSU	A2	3637	47,37	-	0/7/25/26	0/2/2/2
37	OMG	A2	4618	37	-	0/9/27/28	0/3/3/3
33	MLZ	g1	98	33	-	1/7/8/10	-
37	OMU	A2	4498	45,37	-	1/9/27/28	0/2/2/2
37	OMC	A2	4456	37	-	0/9/27/28	0/2/2/2
37	OMG	A2	2364	37	-	0/9/27/28	0/3/3/3
37	PSU	A2	4293	37	-	0/7/25/26	0/2/2/2
37	PSU	A2	3639	37	-	0/7/25/26	0/2/2/2
37	PSU	A2	4689	37	-	0/7/25/26	0/2/2/2
37	A2M	A2	4571	37	-	1/9/27/28	0/3/3/3
37	OMG	A2	4494	37	-	1/9/27/28	0/3/3/3
37	PSU	A2	1779	37	-	0/7/25/26	0/2/2/2
37	A2M	A2	2401	37	-	1/9/27/28	0/3/3/3
37	PSU	A2	4361	37	-	0/7/25/26	0/2/2/2
39	PSU	C2	55	39	-	0/7/25/26	0/2/2/2
37	OMU	A2	4620	37	-	0/9/27/28	0/2/2/2
37	A2M	A2	3867	37	-	2/9/27/28	0/3/3/3
37	PSU	A2	1862	37	-	0/7/25/26	0/2/2/2
21	V5N	U1	39	21	-	1/9/10/12	0/1/1/1
37	PSU	A2	4493	47,37	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	PSU	A2	1683	47,37	-	0/7/25/26	0/2/2/2
37	OMU	A2	2837	37	-	0/9/27/28	0/2/2/2
37	PSU	A2	3822	37	-	0/7/25/26	0/2/2/2
37	PSU	A2	4628	37	-	0/7/25/26	0/2/2/2
37	OMC	A2	1340	37	-	0/9/27/28	0/2/2/2
37	PSU	A2	3844	37	-	1/7/25/26	0/2/2/2
37	PSU	A2	4420	37	-	4/7/25/26	0/2/2/2
37	PSU	A2	3851	37	-	1/7/25/26	0/2/2/2
37	PSU	A2	3920	45,37	-	0/7/25/26	0/2/2/2
37	PSU	A2	4579	37	-	0/7/25/26	0/2/2/2
37	PSU	A2	2508	37	-	0/7/25/26	0/2/2/2
37	A2M	A2	2815	45,37	-	3/9/27/28	0/3/3/3
39	PSU	C2	69	39	-	0/7/25/26	0/2/2/2
37	OMG	A2	4370	37	-	1/9/27/28	0/3/3/3
37	OMU	A2	2415	37	-	0/9/27/28	0/2/2/2
37	PSU	A2	3715	37	-	0/7/25/26	0/2/2/2
37	UY1	A2	3818	47,37	-	1/9/27/28	0/2/2/2
37	A2M	A2	1534	45,37	-	2/9/27/28	0/3/3/3
37	PSU	A2	3695	37	-	0/7/25/26	0/2/2/2
37	OMC	A2	3887	37	-	0/9/27/28	0/2/2/2

The worst 5 of 886 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	A2	4420	PSU	C6-C5	11.20	1.48	1.35
37	A2	2632	PSU	C6-C5	11.06	1.48	1.35
37	A2	4296	PSU	C6-C5	10.94	1.48	1.35
37	A2	4532	PSU	C6-C5	10.94	1.48	1.35
37	A2	1781	PSU	C6-C5	10.94	1.48	1.35

The worst 5 of 754 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	A2	3785	A2M	N6-C6-N1	-10.12	96.18	118.35
37	A2	4571	A2M	N6-C6-N1	-9.96	96.54	118.35
37	A2	3718	A2M	N6-C6-N1	-9.95	96.55	118.35
37	A2	3830	A2M	N6-C6-N1	-9.94	96.57	118.35
37	A2	3867	A2M	N6-C6-N1	-9.92	96.63	118.35

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	D2	216	V5N	O-C-CA-CB
41	E2	245	HIC	O-C-CA-CB
37	A2	224	PSU	C2'-C1'-C5-C4
37	A2	398	A2M	C1'-C2'-O2'-CM'
37	A2	1323	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

41 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	A2	2351	OMC	1	0
37	A2	1326	A2M	1	0
37	A2	2804	OMC	1	0
37	A2	398	A2M	1	0
37	A2	3701	OMC	1	0
37	A2	4296	PSU	1	0
37	A2	2876	OMG	1	0
37	A2	1524	A2M	2	0
37	A2	4536	OMC	1	0
37	A2	3884	PSU	1	0
37	A2	2824	OMC	1	0
37	A2	4447	5MC	1	0
37	A2	4530	UR3	1	0
37	A2	3718	A2M	3	0
37	A2	4196	OMG	1	0
37	A2	2424	OMG	1	0
37	A2	4457	PSU	1	0
39	C2	75	OMG	2	0
37	A2	4431	PSU	1	0
37	A2	1871	A2M	2	0
37	A2	1781	PSU	1	0
37	A2	2363	A2M	2	0
37	A2	4499	OMG	2	0
37	A2	2861	OMC	1	0
37	A2	4637	OMG	2	0
37	A2	2632	PSU	1	0
37	A2	5001	PSU	1	0
37	A2	3744	OMG	1	0
37	A2	3792	OMG	1	0
37	A2	3637	PSU	1	0
37	A2	4498	OMU	1	0
37	A2	4456	OMC	1	0
37	A2	2364	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	A2	4620	OMU	2	0
37	A2	3867	A2M	2	0
37	A2	1340	OMC	1	0
37	A2	4579	PSU	2	0
37	A2	2815	A2M	1	0
37	A2	4370	OMG	1	0
37	A2	2415	OMU	1	0
37	A2	1534	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 258 ligands modelled in this entry, 237 are monoatomic - leaving 21 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	$\# Z > 2$
49	SPD	A2	5410	-	9,9,9	0.35	0	8,8,8	0.65	0
49	SPD	A2	5408	-	9,9,9	0.31	0	8,8,8	0.98	0
51	ATP	A2	5418	-	29,33,33	1.23	2 (6%)	44,52,52	2.29	15 (34%)
50	SPM	A2	5414	-	13,13,13	0.36	0	12,12,12	0.94	0
49	SPD	A2	5411	-	9,9,9	0.30	0	8,8,8	0.70	0
50	SPM	A2	5415	-	13,13,13	0.26	0	12,12,12	0.96	0
50	SPM	A2	5416	-	13,13,13	0.26	0	12,12,12	1.21	1 (8%)
49	SPD	A2	5407	-	9,9,9	0.32	0	8,8,8	0.85	0
46	PUT	A2	5402	-	5,5,5	0.19	0	4,4,4	0.23	0
49	SPD	A2	5406	-	9,9,9	0.34	0	8,8,8	0.76	0
49	SPD	A2	5409	-	9,9,9	0.32	0	8,8,8	0.92	1 (12%)
50	SPM	A2	5417	-	13,13,13	0.26	0	12,12,12	1.48	1 (8%)
46	PUT	H1	301[A]	-	5,5,5	0.22	0	4,4,4	0.51	0
46	PUT	B2	201	-	5,5,5	0.18	0	4,4,4	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	SPM	A2	5413	-	13,13,13	0.35	0	12,12,12	0.94	0
46	PUT	A2	5404	-	5,5,5	0.17	0	4,4,4	0.53	0
46	PUT	H1	301[B]	-	5,5,5	0.15	0	4,4,4	0.48	0
49	SPD	A2	5412	-	9,9,9	0.46	0	8,8,8	1.00	0
46	PUT	A2	5401	-	5,5,5	0.28	0	4,4,4	0.70	0
46	PUT	A2	5405	-	5,5,5	0.11	0	4,4,4	0.53	0
46	PUT	A2	5403	-	5,5,5	0.32	0	4,4,4	0.70	0

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
49	SPD	A2	5410	-	-	6/7/7/7	-
49	SPD	A2	5408	-	-	0/7/7/7	-
51	ATP	A2	5418	-	-	7/22/38/38	0/3/3/3
50	SPM	A2	5414	-	-	0/11/11/11	-
49	SPD	A2	5411	-	-	3/7/7/7	-
50	SPM	A2	5415	-	-	3/11/11/11	-
50	SPM	A2	5416	-	-	4/11/11/11	-
49	SPD	A2	5407	-	-	4/7/7/7	-
46	PUT	A2	5402	-	-	1/3/3/3	-
49	SPD	A2	5406	-	-	3/7/7/7	-
49	SPD	A2	5409	-	-	3/7/7/7	-
50	SPM	A2	5417	-	-	8/11/11/11	-
46	PUT	H1	301[A]	-	-	1/3/3/3	-
46	PUT	B2	201	-	-	1/3/3/3	-
50	SPM	A2	5413	-	-	0/11/11/11	-
46	PUT	A2	5404	-	-	0/3/3/3	-
46	PUT	H1	301[B]	-	-	1/3/3/3	-
49	SPD	A2	5412	-	-	6/7/7/7	-
46	PUT	A2	5401	-	-	1/3/3/3	-
46	PUT	A2	5405	-	-	1/3/3/3	-
46	PUT	A2	5403	-	-	1/3/3/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A2	5418	ATP	C5-C4	3.60	1.45	1.39

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	A2	5418	ATP	C5-N7	-2.55	1.34	1.39

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	A2	5418	ATP	C5-C4-N3	-6.57	118.17	126.75
51	A2	5418	ATP	N3-C4-N9	5.81	136.65	127.08
51	A2	5418	ATP	PB-O3B-PG	-4.50	117.37	132.83
51	A2	5418	ATP	C2-N3-C4	4.45	122.27	111.75
51	A2	5418	ATP	N3-C2-N1	-3.95	122.42	128.60

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	A2	5407	SPD	C8-C7-N6-C5
49	A2	5412	SPD	C4-C5-N6-C7
51	A2	5418	ATP	PB-O3A-PA-O5'
51	A2	5418	ATP	C5'-O5'-PA-O2A
51	A2	5418	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

17 monomers are involved in 70 short contacts:

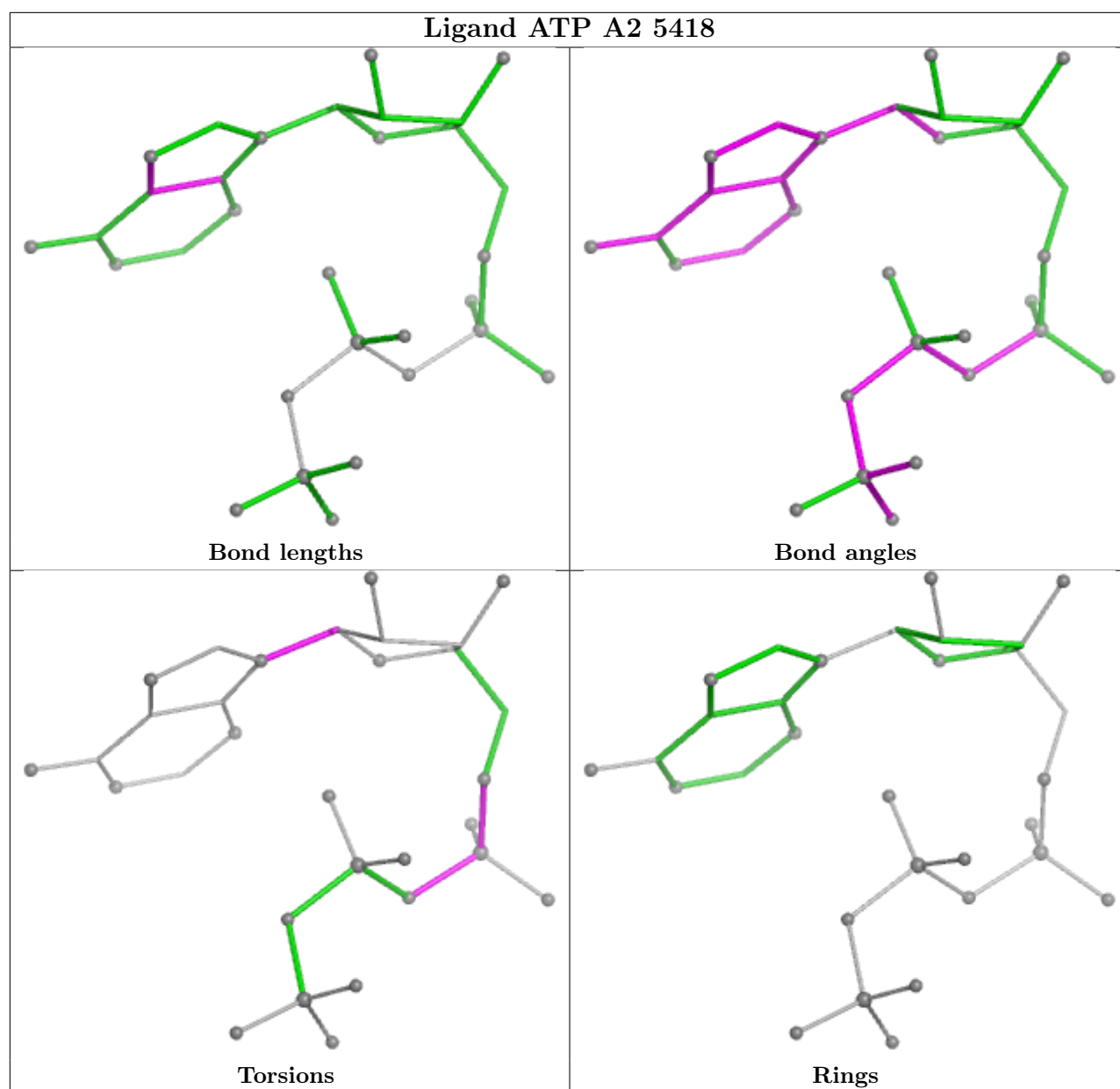
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	A2	5410	SPD	4	0
51	A2	5418	ATP	8	0
50	A2	5416	SPM	1	0
49	A2	5407	SPD	12	0
46	A2	5402	PUT	3	0
49	A2	5406	SPD	1	0
49	A2	5409	SPD	1	0
50	A2	5417	SPM	1	0
46	H1	301[A]	PUT	2	0
46	B2	201	PUT	5	0
50	A2	5413	SPM	2	0
46	A2	5404	PUT	4	0
46	H1	301[B]	PUT	2	0
49	A2	5412	SPD	11	0
46	A2	5401	PUT	6	0
46	A2	5405	PUT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A2	5403	PUT	6	0

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 than 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.



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.

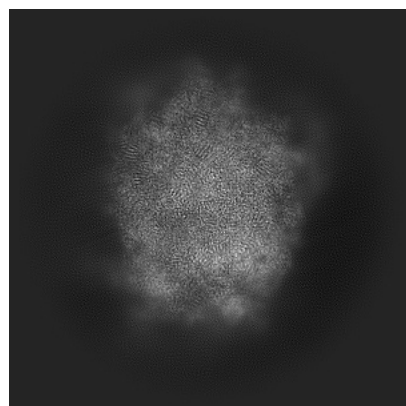
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18765. These allow visual inspection of the internal detail of the map and identification of artifacts.

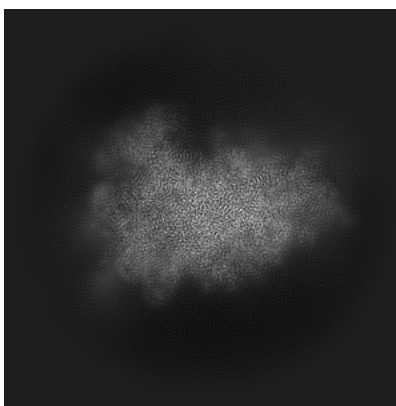
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

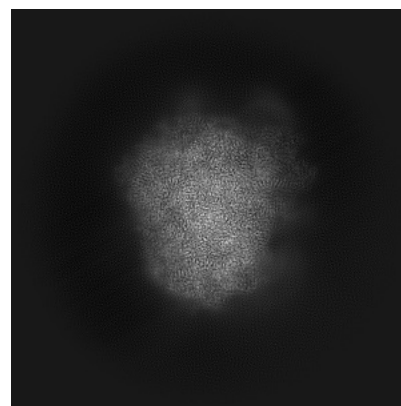
6.1.1 Primary map



X

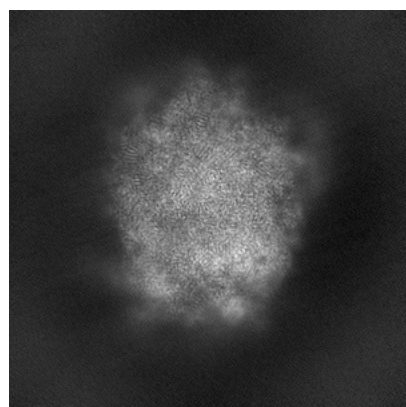


Y

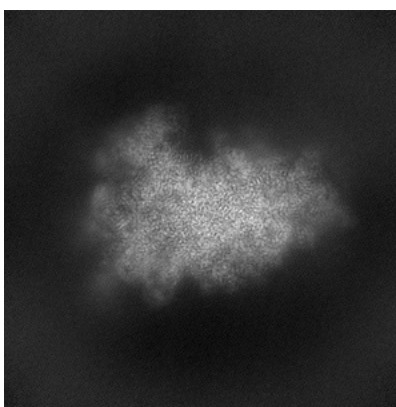


Z

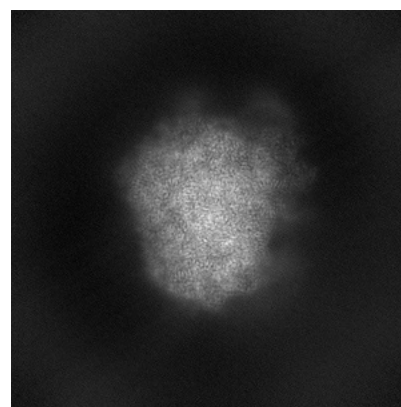
6.1.2 Raw map



X



Y

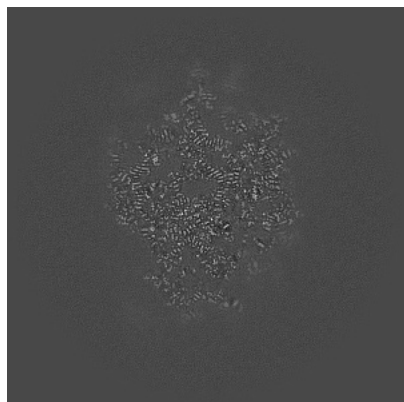


Z

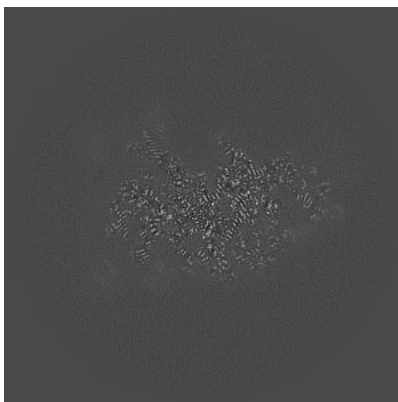
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

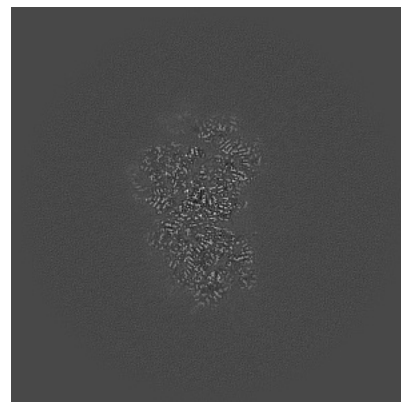
6.2.1 Primary map



X Index: 320

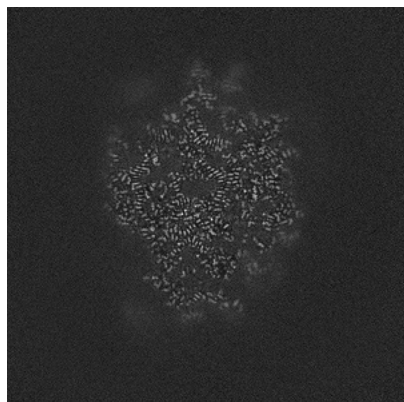


Y Index: 320

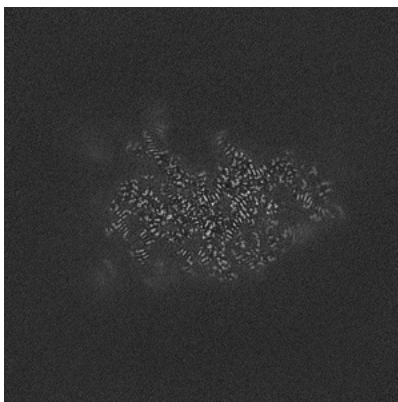


Z Index: 320

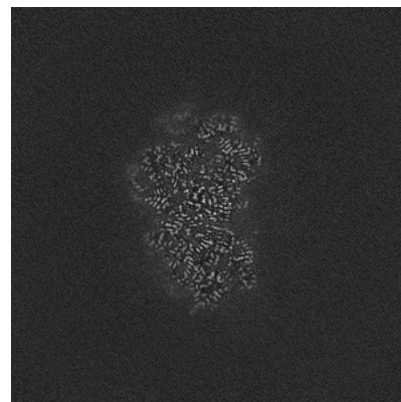
6.2.2 Raw map



X Index: 320



Y Index: 320

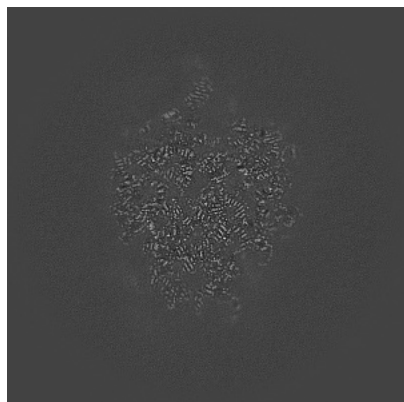


Z Index: 320

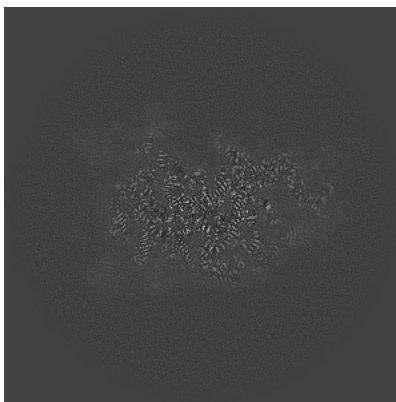
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

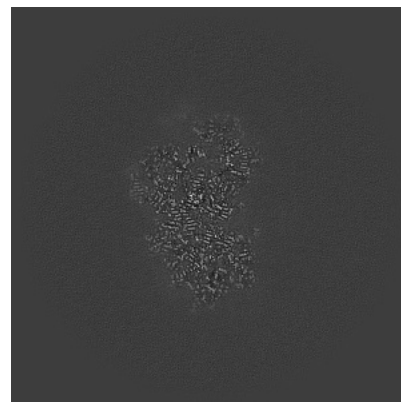
6.3.1 Primary map



X Index: 305

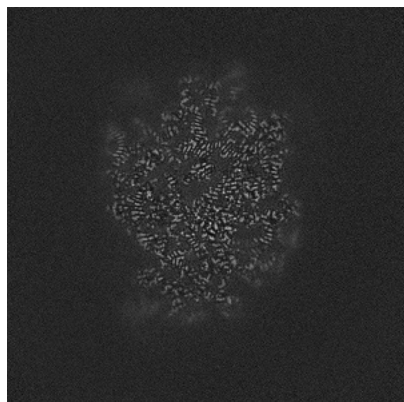


Y Index: 325

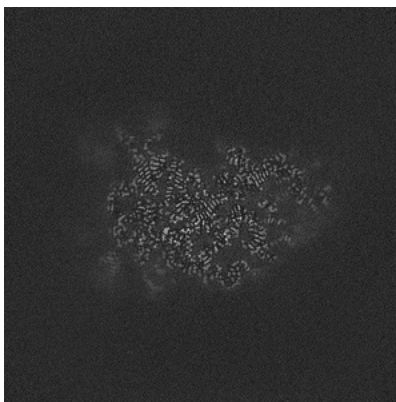


Z Index: 323

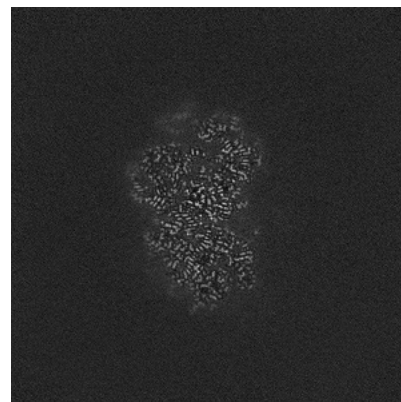
6.3.2 Raw map



X Index: 328



Y Index: 333

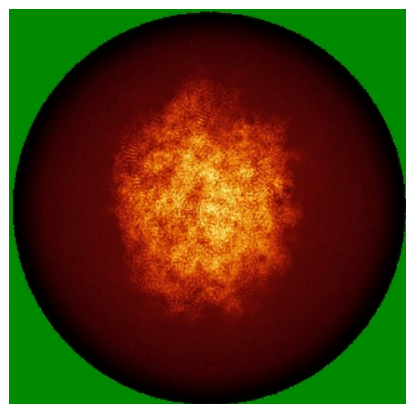


Z Index: 321

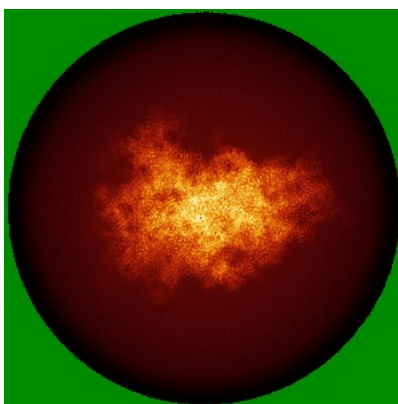
The images above show the largest variance slices of the map in three orthogonal directions.

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

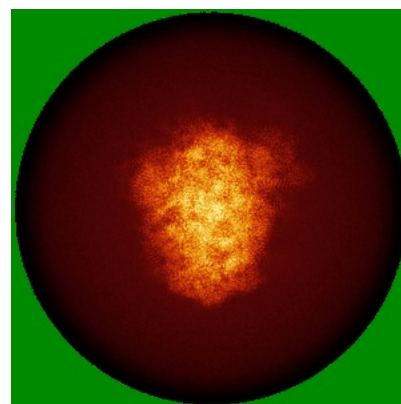
6.4.1 Primary map



X

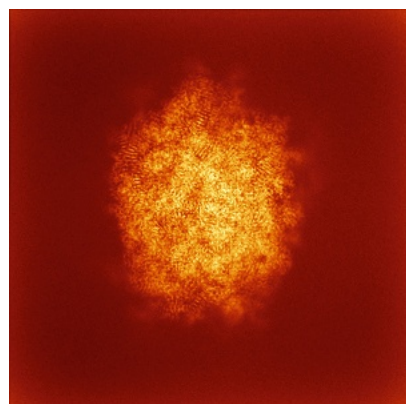


Y

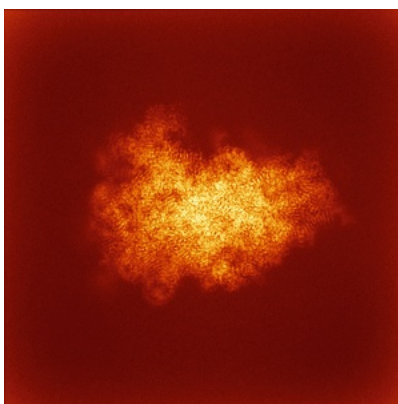


Z

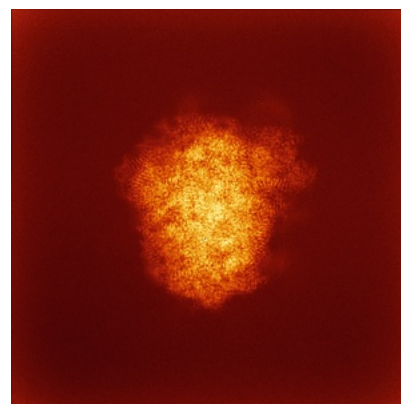
6.4.2 Raw map



X



Y

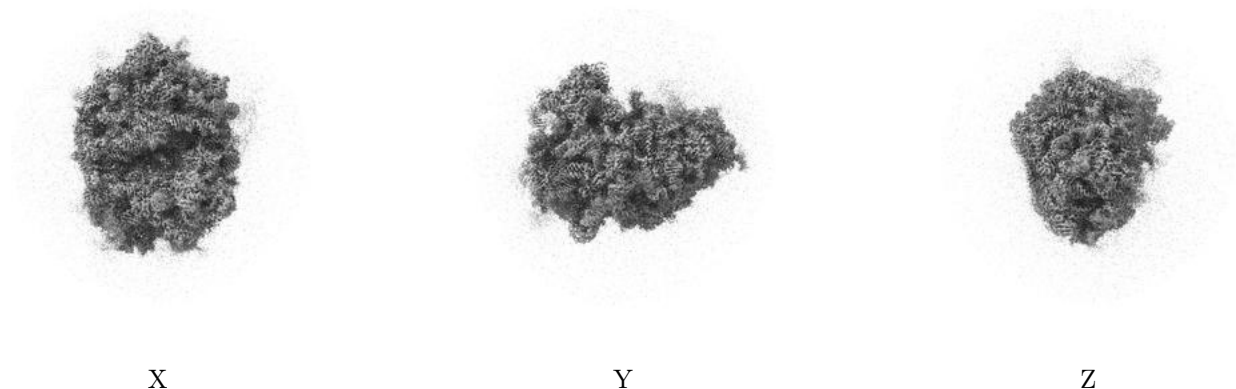


Z

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

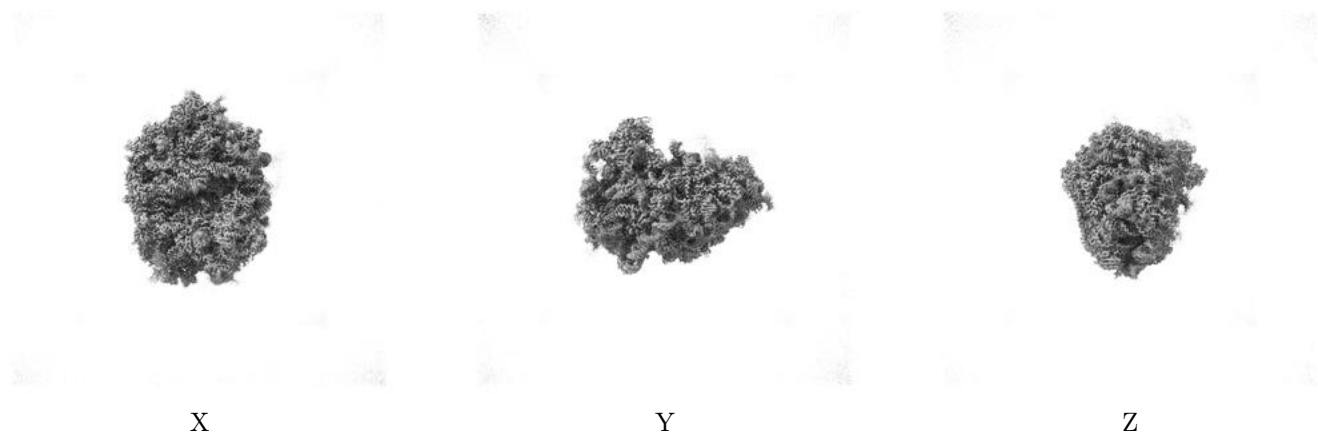
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.86. 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.

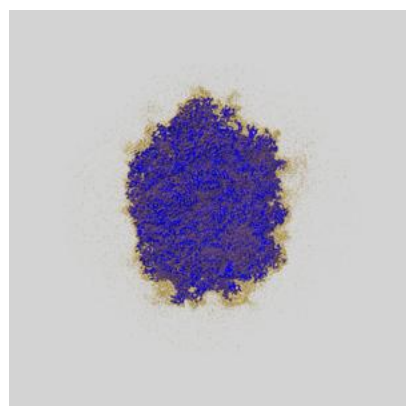
6.6 Mask visualisation [i](#)

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

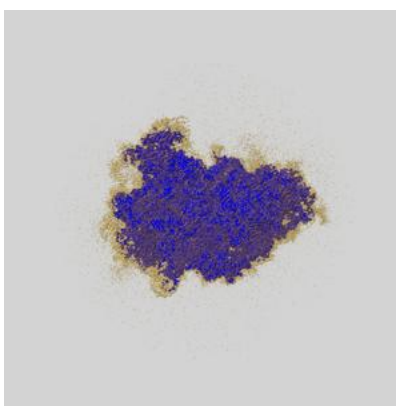
A mask typically either:

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

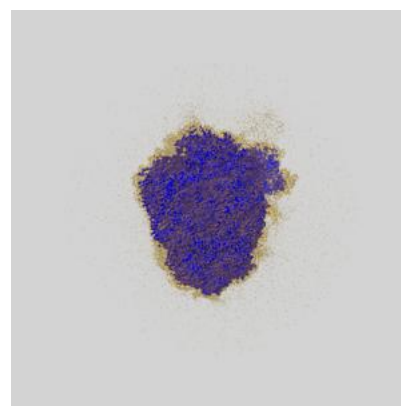
6.6.1 emd_18765_msk_1.map [i](#)



X



Y

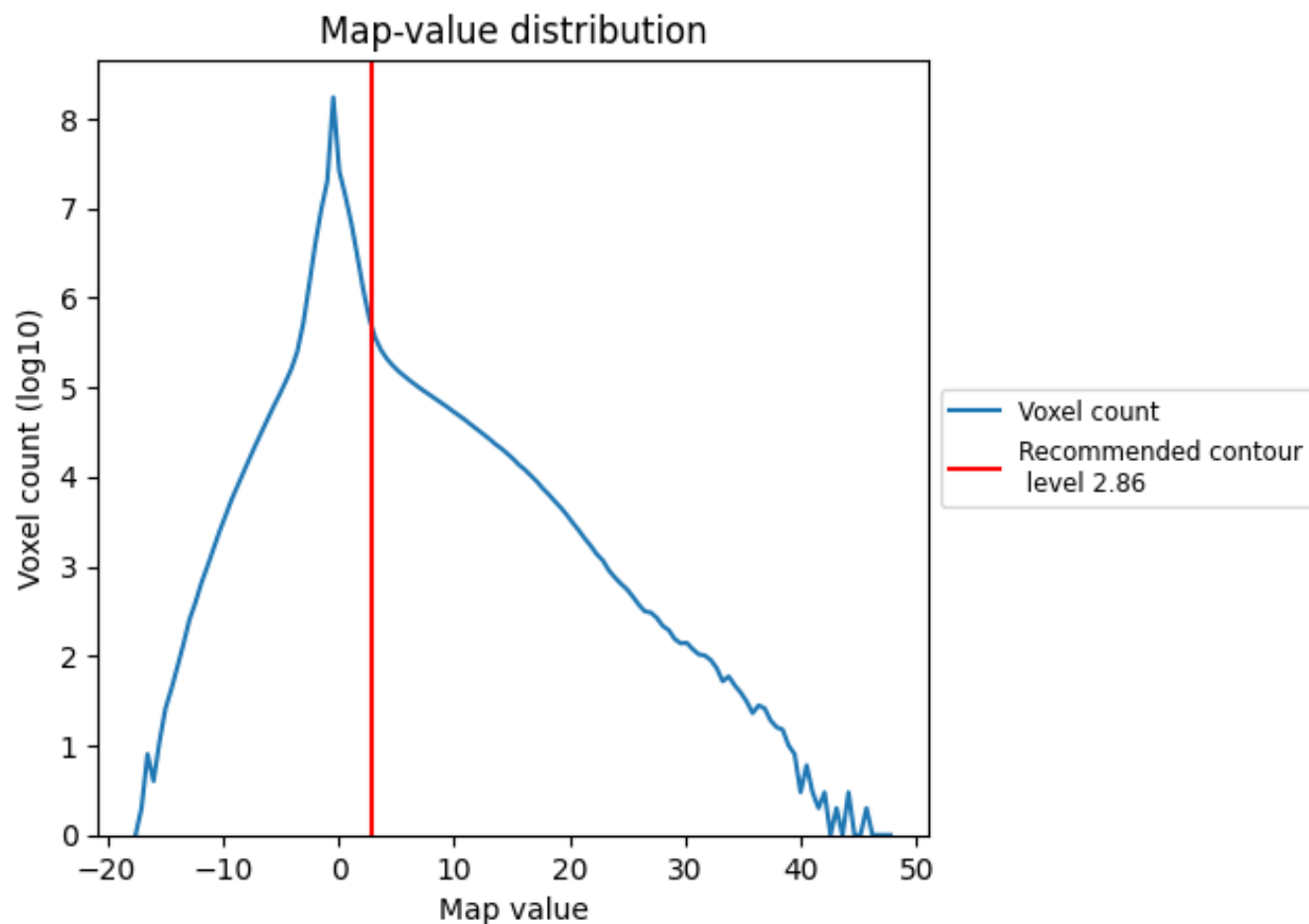


Z

7 Map analysis [i](#)

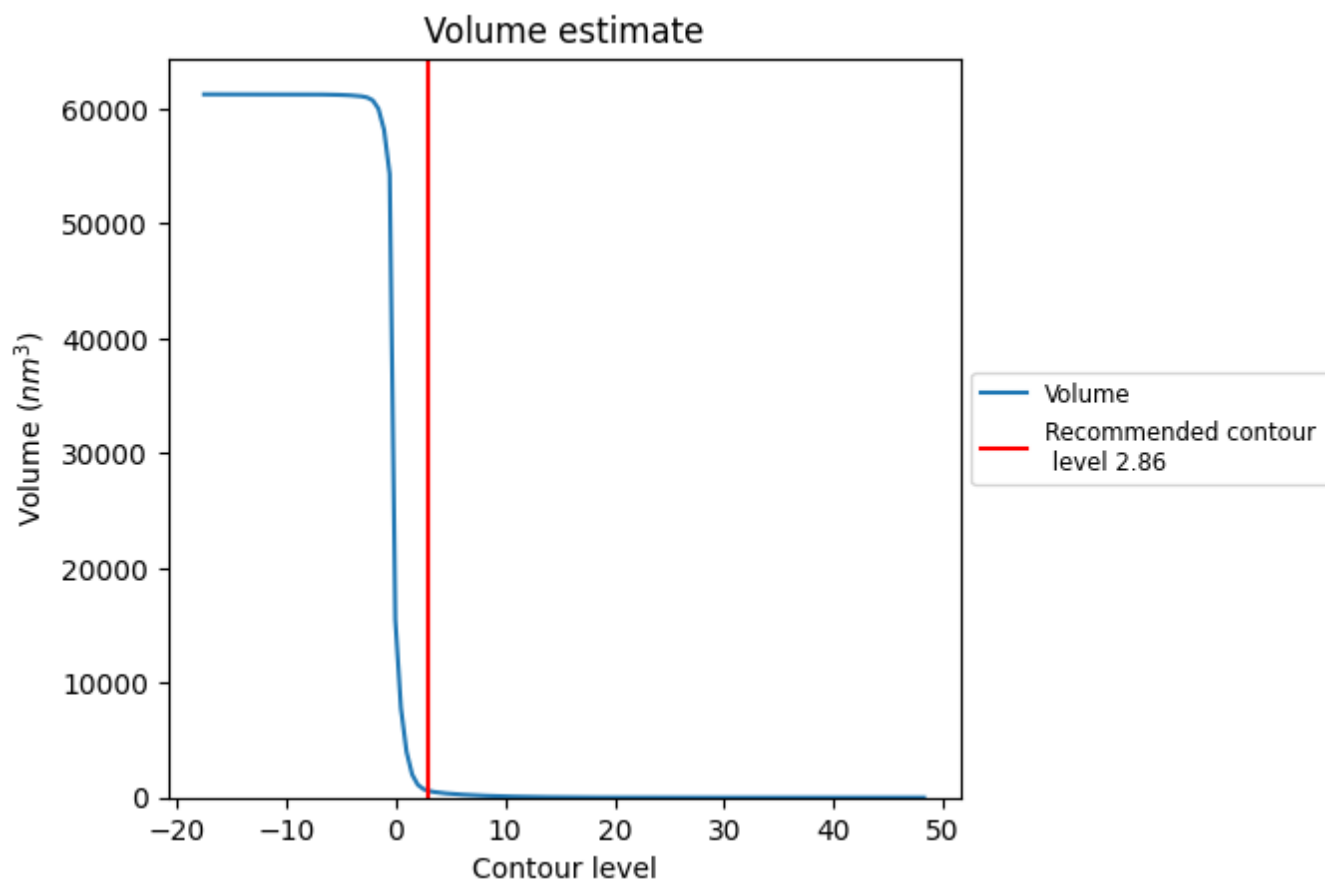
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

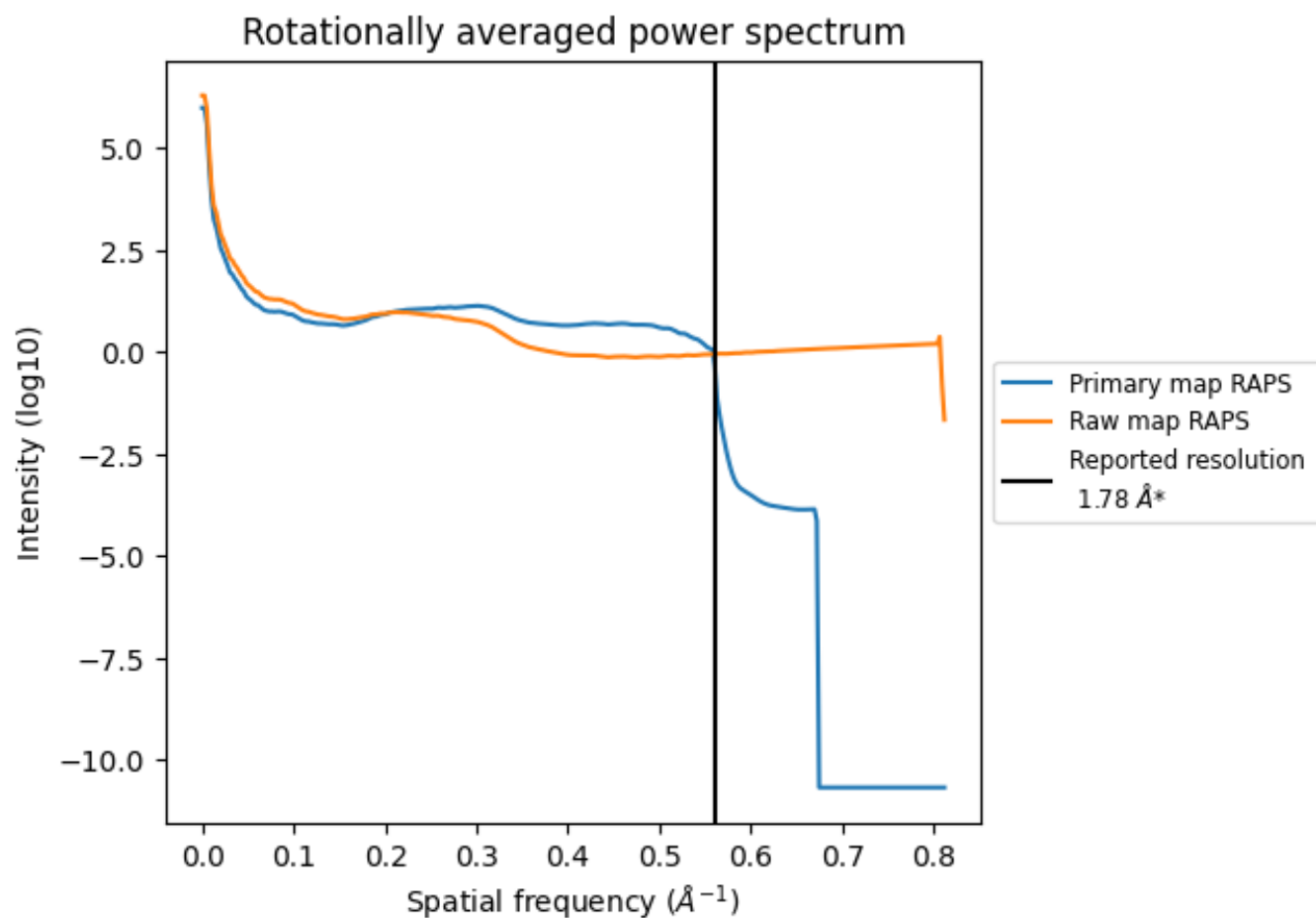
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 629 nm^3 ; this corresponds to an approximate mass of 568 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 ⓘ

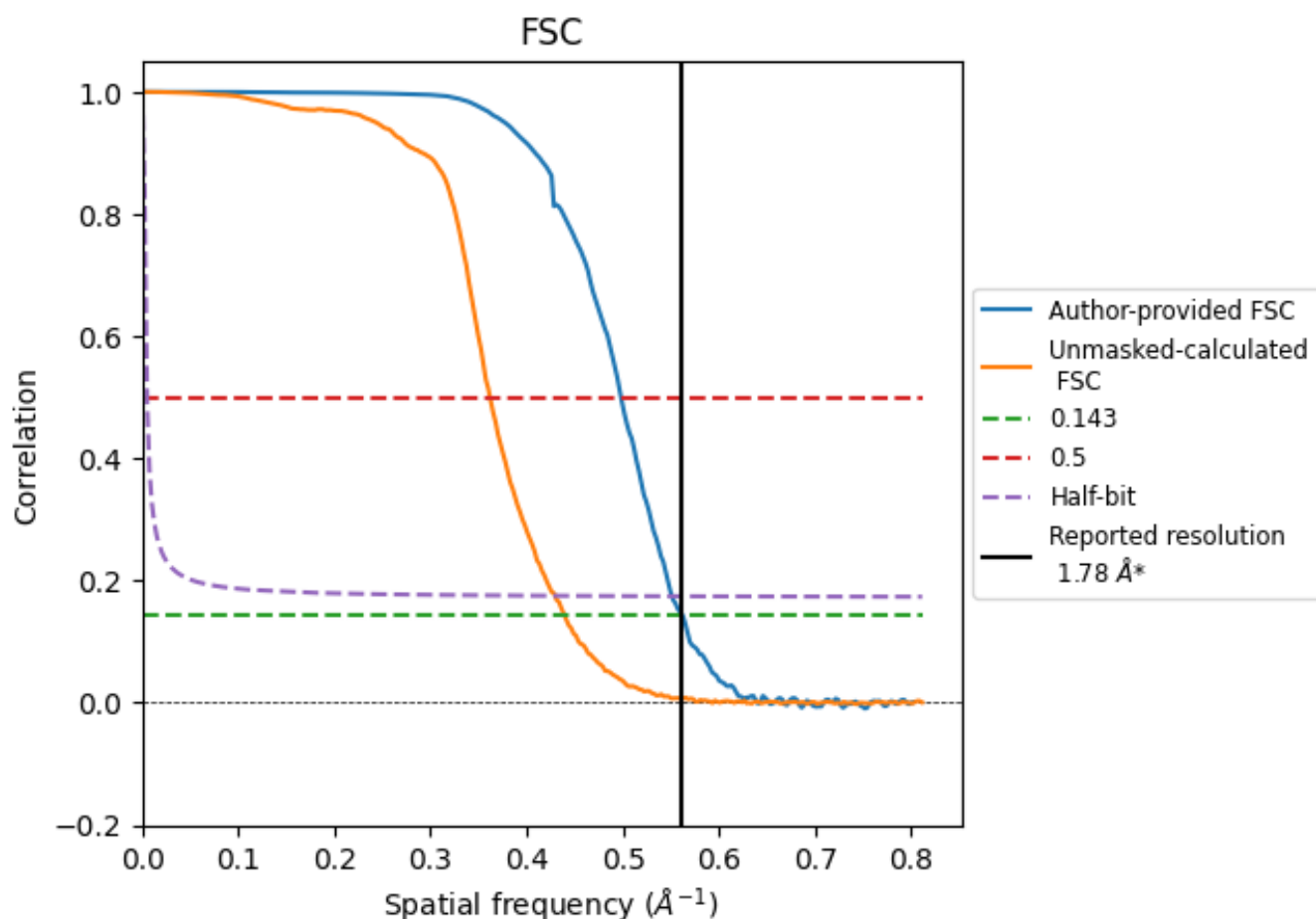


*Reported resolution corresponds to spatial frequency of 0.562 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.562 Å⁻¹

8.2 Resolution estimates [i](#)

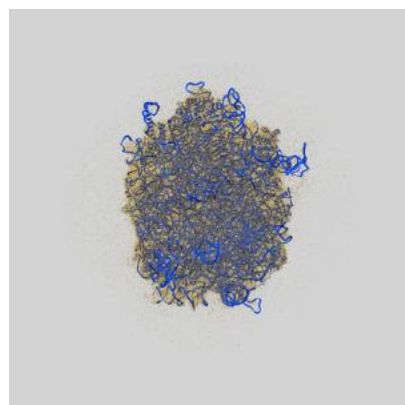
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.78	-	-
Author-provided FSC curve	1.78	2.01	1.81
Unmasked-calculated*	2.28	2.76	2.33

*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 2.28 differs from the reported value 1.78 by more than 10 %

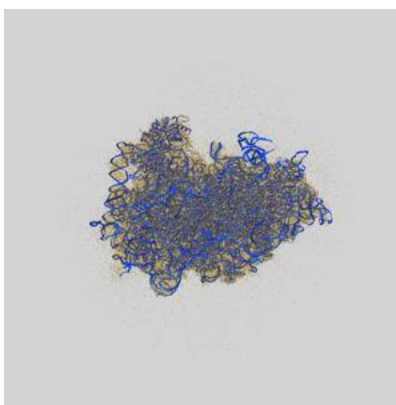
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18765 and PDB model 8QYX. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

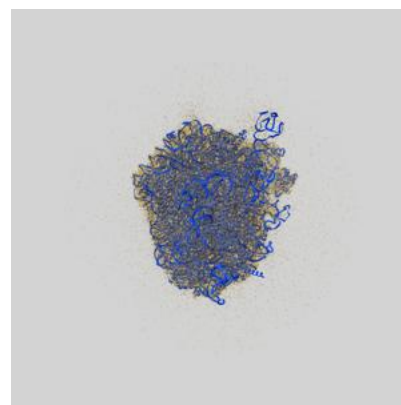
9.1 Map-model overlay [i](#)



X



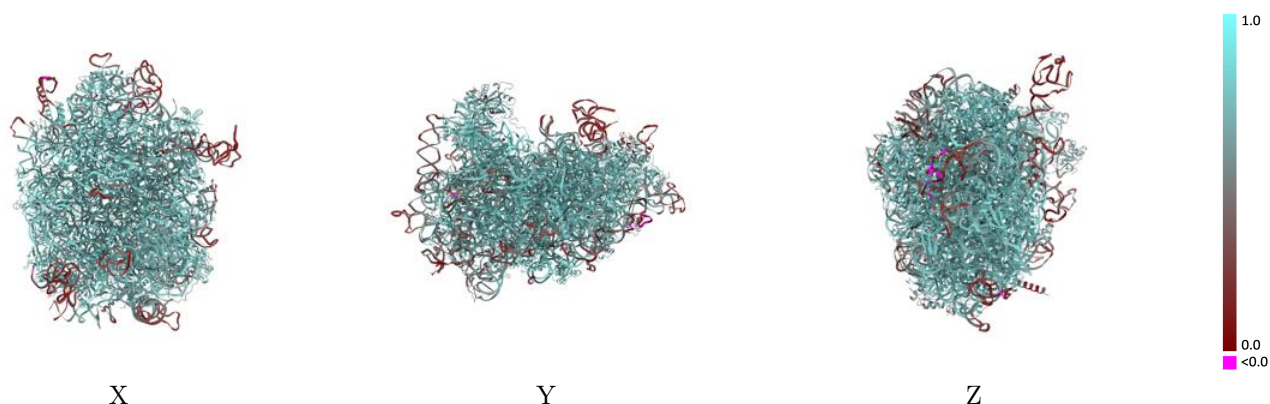
Y



Z

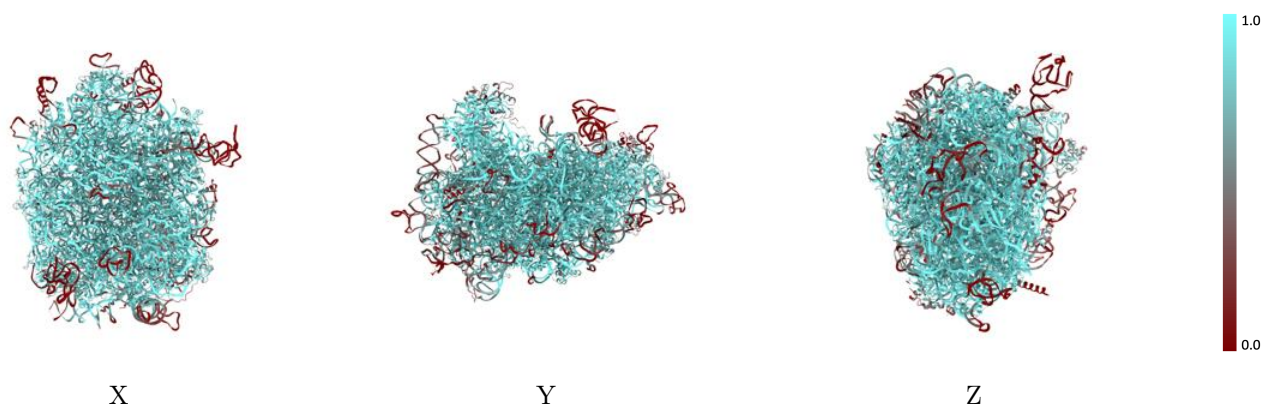
The images above show the 3D surface view of the map at the recommended contour level 2.86 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



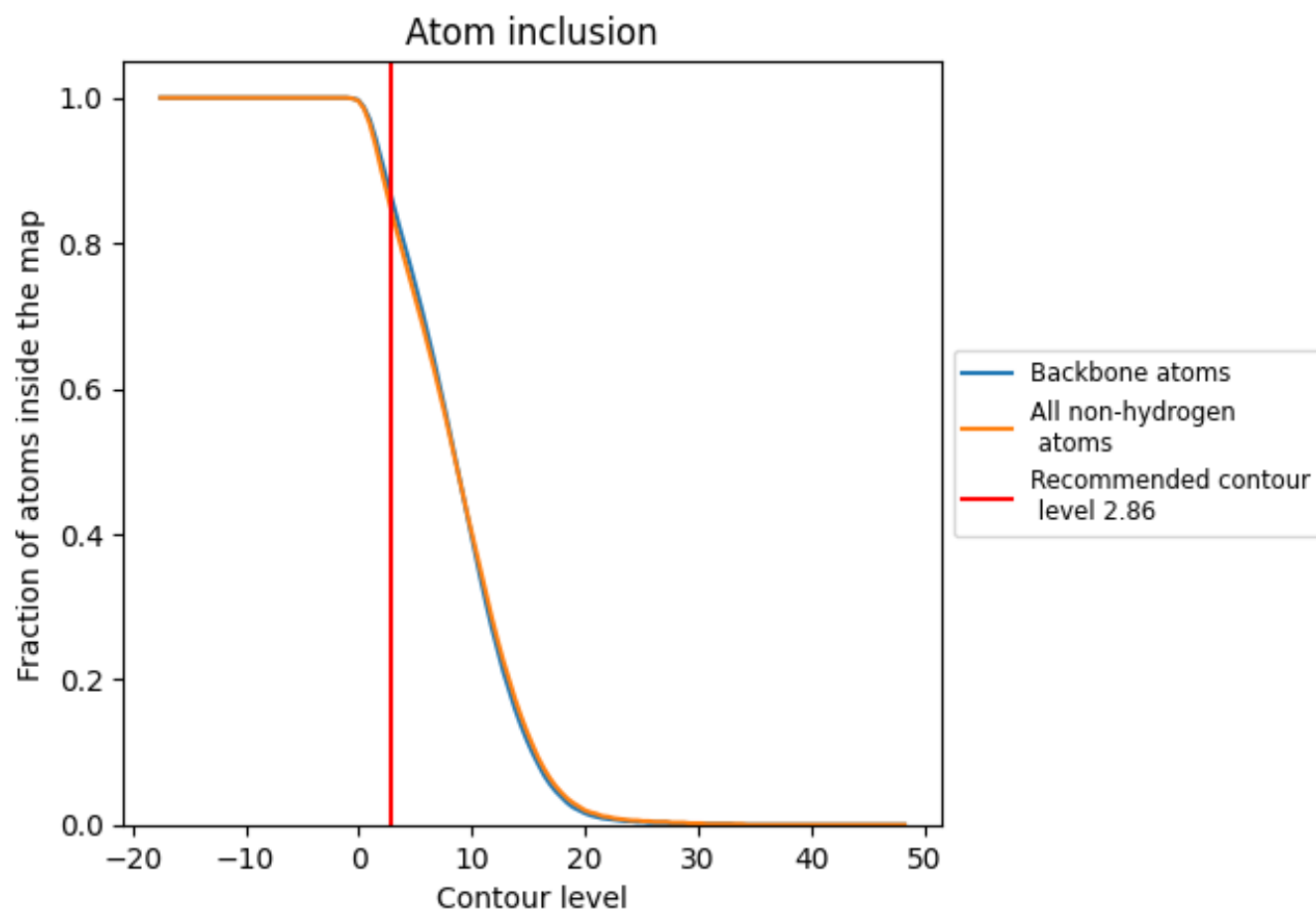
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.86).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (2.86) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8450	 0.7030
A1	 0.9360	 0.7940
A2	 0.8100	 0.6690
B1	 0.8340	 0.7110
B2	 0.9800	 0.7530
C1	 0.8940	 0.7480
C2	 0.9050	 0.7120
D1	 0.9100	 0.7540
D2	 0.9720	 0.8020
E1	 0.6970	 0.6340
E2	 0.9240	 0.7770
F1	 0.8730	 0.7430
F2	 0.9460	 0.7890
G1	 0.9150	 0.7600
G2	 0.8430	 0.7120
H1	 0.9900	 0.8120
H2	 0.7930	 0.6770
I1	 0.9410	 0.7840
J1	 0.8890	 0.7490
K1	 0.9700	 0.8050
L1	 0.8540	 0.7190
M1	 0.9690	 0.7940
N1	 0.8770	 0.7380
O1	 0.6220	 0.6020
P1	 0.9350	 0.7820
Q1	 0.9100	 0.7640
R1	 0.9020	 0.7460
S1	 0.8940	 0.7550
T1	 0.8560	 0.7220
U1	 0.9480	 0.7970
V1	 0.7360	 0.6750
W1	 0.8030	 0.7030
X1	 0.8520	 0.7290
Y1	 0.9530	 0.7990
Z1	 0.9640	 0.8050



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Chain	Atom inclusion	Q-score
a1	 0.8720	 0.7410
b1	 0.8870	 0.7500
c1	 0.8370	 0.7280
d1	 0.9820	 0.8030
e1	 0.6700	 0.6320
f1	 0.9390	 0.7600
g1	 0.9040	 0.7570
i1	 0.8890	 0.7570
j1	 0.8950	 0.7620
k1	 0.9440	 0.7840