Full wwPDB EM Validation Report ⓘ

Jan 1, 2025 – 11:57 PM EST

PDB ID	:	9E6Q
EMDB ID	:	EMD-47578
Title	:	Cryo-EM structure of the Pyrobaculum calidifontis 50S ribosomal subunit in complex with Dri
Authors	:	Nissley, A.J.; Cate, J.H.D.
Deposited on	:	2024-10-30
Resolution	:	1.95 Å(reported)

This is a Full wwPDB EM Validation 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:

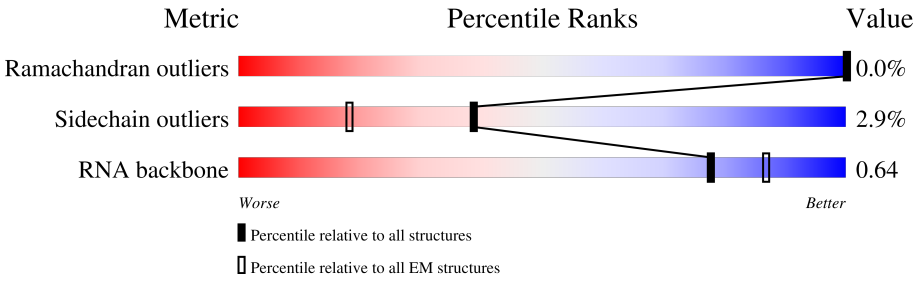
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 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	1	3024	80% 13% 6%
2	2	129	10% 88% 12%
3	3	655	5% 43% 56%
4	AA	244	96%
5	AB	338	99%
6	AC	285	6% 95%
7	AD	178	76% 97%
8	AE	196	17% 96%

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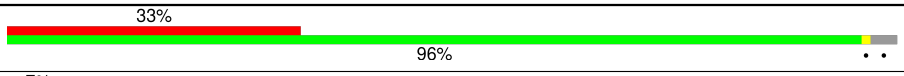
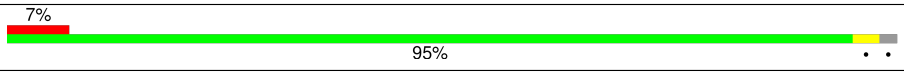
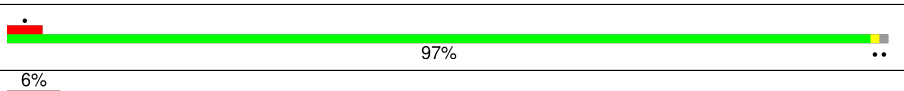
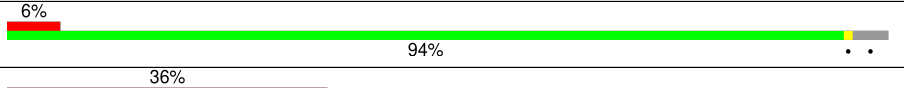
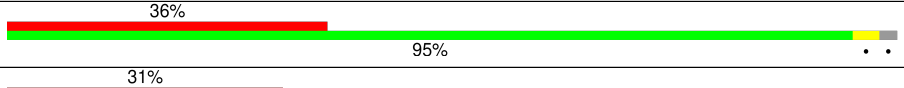
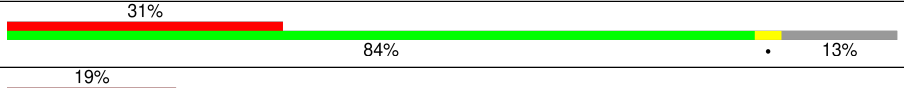
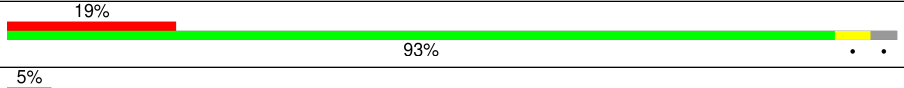
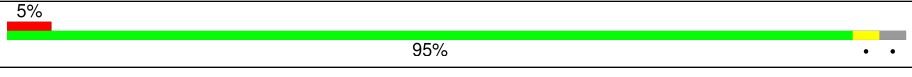
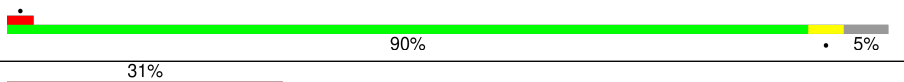
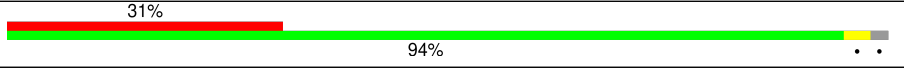
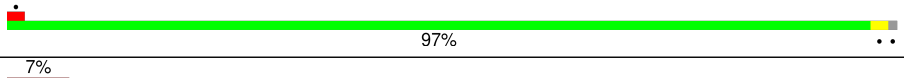
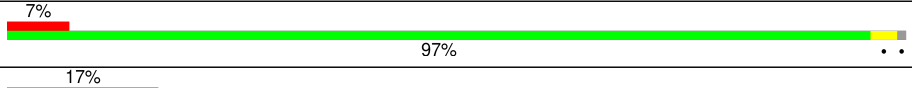
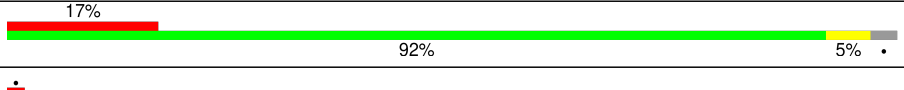
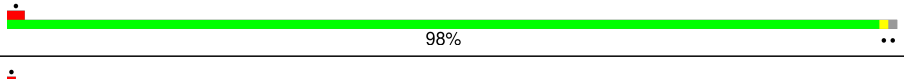
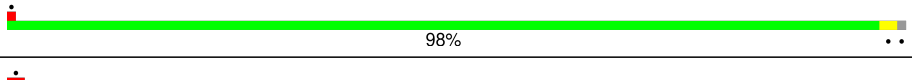
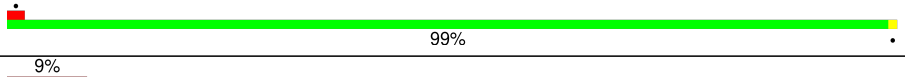
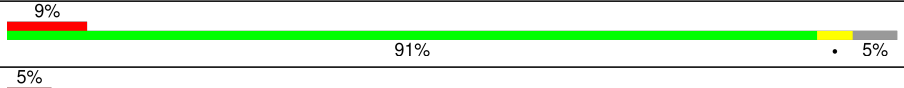
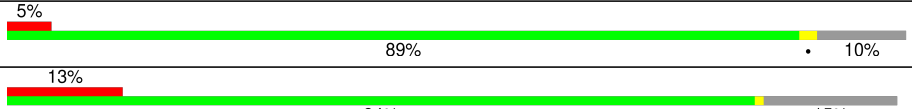
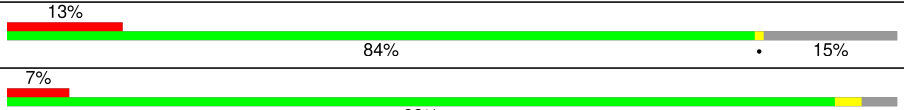
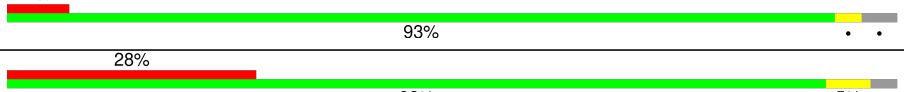
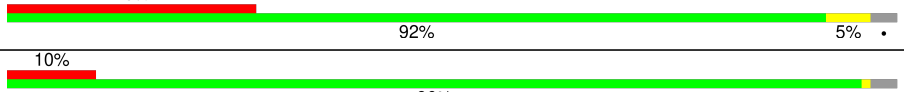
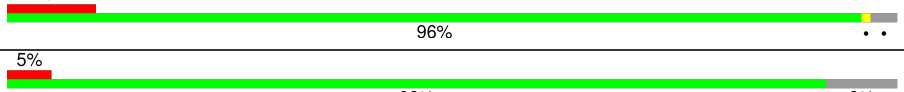
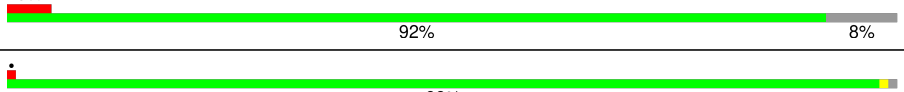
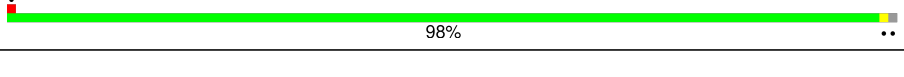
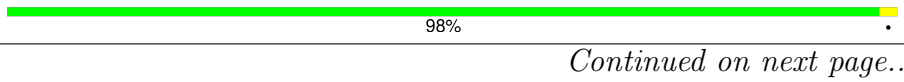
Mol	Chain	Length	Quality of chain
9	AF	149	
10	AG	186	
11	AH	157	
12	AI	144	
13	AJ	103	
13	AK	103	
14	AL	156	
15	AM	189	
16	AN	178	
17	AO	205	
18	AP	122	
19	AQ	147	
20	AR	78	
21	AS	99	
22	AT	184	
23	AU	81	
24	AV	128	
25	AW	62	
26	AX	79	
27	AY	179	
28	AZ	101	
29	Aa	91	
30	Ab	153	
31	Ac	84	
32	Ad	52	

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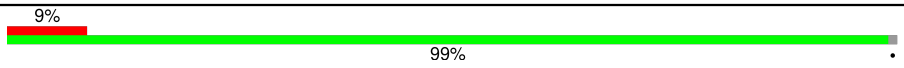
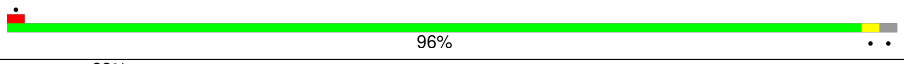
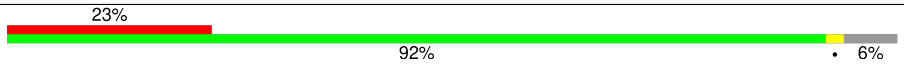
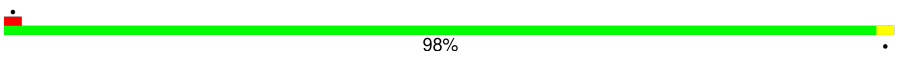
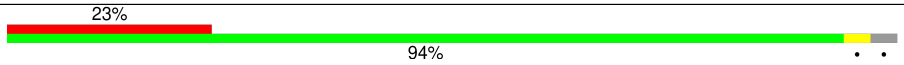
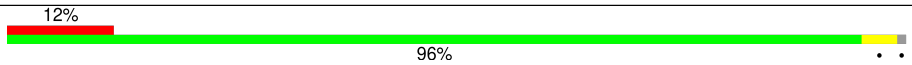
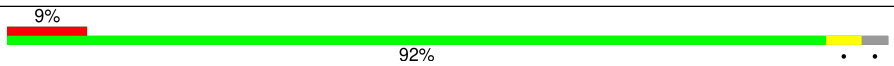
Mol	Chain	Length	Quality of chain
33	Ae	67	
34	Af	51	
35	Ag	53	
36	Ah	91	
37	Ai	102	
38	Aj	184	
39	Ak	93	

2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 114588 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	2842	61237	27268	11426	19701	2842	0	0

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	129	2769	1231	512	897	129	0	0

- Molecule 3 is a protein called Putative signal-transduction protein with CBS domains.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	290	2272	1470	400	399	3	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AA	239	1803	1136	354	308	5	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AB	336	2611	1681	476	450	4	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AC	278	2178	1406	395	371	6	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AD	178	Total	C	N	O	S	0	0
			1412	894	273	238	7		

- Molecule 8 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AE	195	Total	C	N	O	S	0	0
			1520	990	254	272	4		

- Molecule 9 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AF	145	Total	C	N	O	S	0	0
			1095	705	187	202	1		

- Molecule 10 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AG	183	Total	C	N	O	S	0	0
			1510	979	278	246	7		

- Molecule 11 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AH	155	Total	C	N	O	S	0	0
			1244	785	249	209	1		

- Molecule 12 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AI	138	Total	C	N	O	S	0	0
			1068	682	202	181	3		

- Molecule 13 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AJ	101	Total	C	N	O	S	0	0
			788	500	143	144	1		
13	AK	90	Total	C	N	O	S	0	0
			700	441	130	128	1		

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AL	152	Total	C	N	O	S	0	0
			1198	761	232	202	3		

- Molecule 15 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AM	184	Total	C	N	O	S	0	0
			1558	992	315	245	6		

- Molecule 16 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AN	169	Total	C	N	O	S	0	0
			1336	847	254	227	8		

- Molecule 17 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AO	200	Total	C	N	O	S	0	0
			1615	1027	309	278	1		

- Molecule 18 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AP	121	Total	C	N	O	S	0	0
			920	583	181	155	1		

- Molecule 19 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AQ	146	Total	C	N	O	S	0	0
			1214	759	244	208	3		

- Molecule 20 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AR	76	Total	C	N	O	S	0	0
			603	382	109	109	3		

- Molecule 21 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AS	98	Total	C	N	O	S	0	0
			788	503	150	134	1		

- Molecule 22 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AT	183	Total	C	N	O	S	0	0
			1496	978	268	247	3		

- Molecule 23 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AU	81	Total	C	N	O	S	0	0
			651	417	115	117	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AV	121	Total	C	N	O	S	0	0
			976	619	194	161	2		

- Molecule 25 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AW	56	Total	C	N	O	S	0	0
			449	287	86	70	6		

- Molecule 26 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AX	67	Total	C	N	O	S	0	0
			554	343	117	92	2		

- Molecule 27 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AY	172	Total	C	N	O	S	0	0
			1374	888	245	235	6		

- Molecule 28 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AZ	98	Total	C	N	O	S	0	0
			742	481	128	132	1		

- Molecule 29 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Aa	88	Total	C	N	O	0	0
			726	460	146	120		

- Molecule 30 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ab	140	Total	C	N	O	S	0	0
			1183	757	239	186	1		

- Molecule 31 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ac	83	Total	C	N	O	S	0	0
			649	407	138	102	2		

- Molecule 32 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ad	52	Total	C	N	O	S	0	0
			429	265	93	65	6		

- Molecule 33 is a protein called LSU ribosomal protein L38E.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Ae	66	Total	C	N	O	0	0
			552	363	93	96		

- Molecule 34 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Af	50	Total	C	N	O	0	0
			415	260	96	59		

- Molecule 35 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Ag	50	Total	C	N	O	S	0	0
			417	259	88	66	4		

- Molecule 36 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ah	91	Total	C	N	O	S	0	0
			739	467	142	123	7		

- Molecule 37 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ai	99	Total	C	N	O	S	0	0
			769	489	148	127	5		

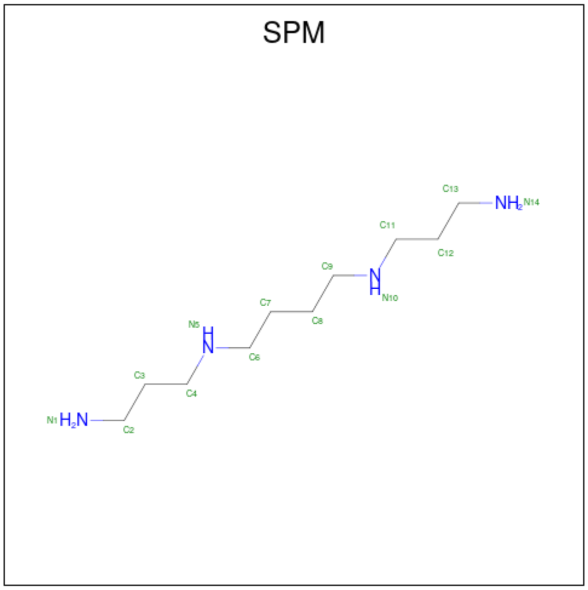
- Molecule 38 is a protein called DJ-1/PfpI domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Aj	183	Total	C	N	O	S	0	0
			1469	954	248	265	2		

- Molecule 39 is a protein called PaREP1 domain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ak	90	Total	C	N	O	S	0	0
			743	478	127	136	2		

- Molecule 40 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	AltConf
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0

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Mol	Chain	Residues	Atoms	AltConf
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0

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Mol	Chain	Residues	Atoms	AltConf
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	1	1	Total C N 14 10 4	0
40	AL	1	Total C N 14 10 4	0
40	AM	1	Total C N 14 10 4	0

- Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
41	1	168	Total Mg 168 168	0
41	AA	1	Total Mg 1 1	0
41	AL	2	Total Mg 2 2	0
41	AN	1	Total Mg 1 1	0
41	AT	1	Total Mg 1 1	0

- Molecule 42 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
42	AW	1	Total Zn 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
42	Ad	1	Total Zn 1 1	0
42	Ag	1	Total Zn 1 1	0
42	Ah	1	Total Zn 1 1	0
42	Ai	1	Total Zn 1 1	0

- Molecule 43 is water.

Mol	Chain	Residues	Atoms	AltConf
43	1	6534	Total O 6534 6534	0
43	2	147	Total O 147 147	0
43	3	58	Total O 58 58	0
43	AA	83	Total O 83 83	0
43	AB	85	Total O 85 85	0
43	AC	83	Total O 83 83	0
43	AD	16	Total O 16 16	0
43	AE	22	Total O 22 22	0
43	AF	19	Total O 19 19	0
43	AG	50	Total O 50 50	0
43	AH	49	Total O 49 49	0
43	AI	30	Total O 30 30	0
43	AJ	13	Total O 13 13	0
43	AK	15	Total O 15 15	0
43	AL	49	Total O 49 49	0

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Mol	Chain	Residues	Atoms	AltConf
43	AM	66	Total O 66 66	0
43	AN	51	Total O 51 51	0
43	AO	32	Total O 32 32	0
43	AP	28	Total O 28 28	0
43	AQ	45	Total O 45 45	0
43	AR	13	Total O 13 13	0
43	AS	37	Total O 37 37	0
43	AT	46	Total O 46 46	0
43	AU	22	Total O 22 22	0
43	AV	30	Total O 30 30	0
43	AW	13	Total O 13 13	0
43	AX	32	Total O 32 32	0
43	AY	38	Total O 38 38	0
43	AZ	18	Total O 18 18	0
43	Aa	22	Total O 22 22	0
43	Ab	42	Total O 42 42	0
43	Ac	21	Total O 21 21	0
43	Ad	26	Total O 26 26	0
43	Ae	17	Total O 17 17	0
43	Af	18	Total O 18 18	0
43	Ag	11	Total O 11 11	0

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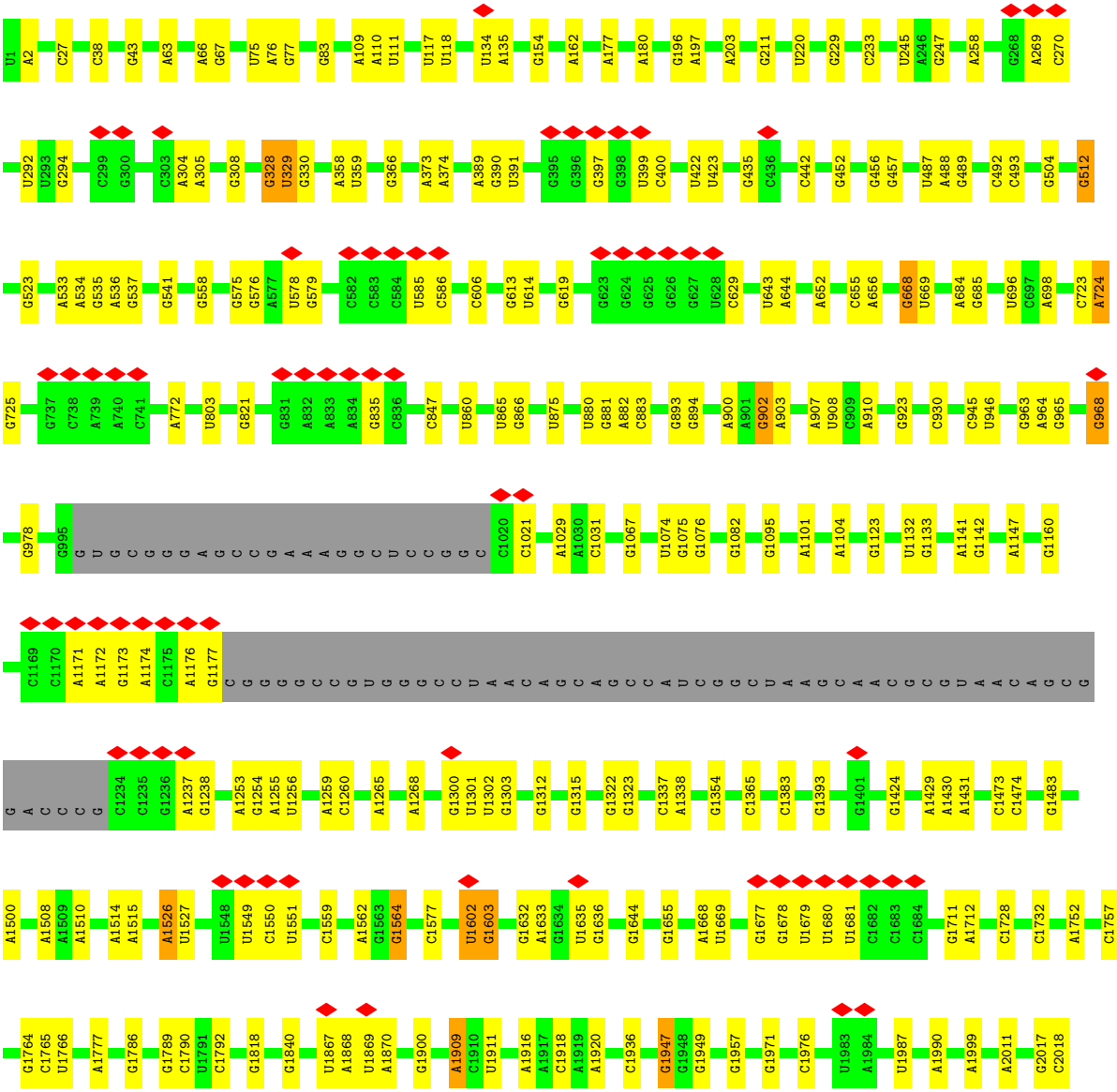
Mol	Chain	Residues	Atoms	AltConf
43	Ah	26	Total O 26 26	0
43	Ai	34	Total O 34 34	0
43	Aj	41	Total O 41 41	0
43	Ak	12	Total O 12 12	0

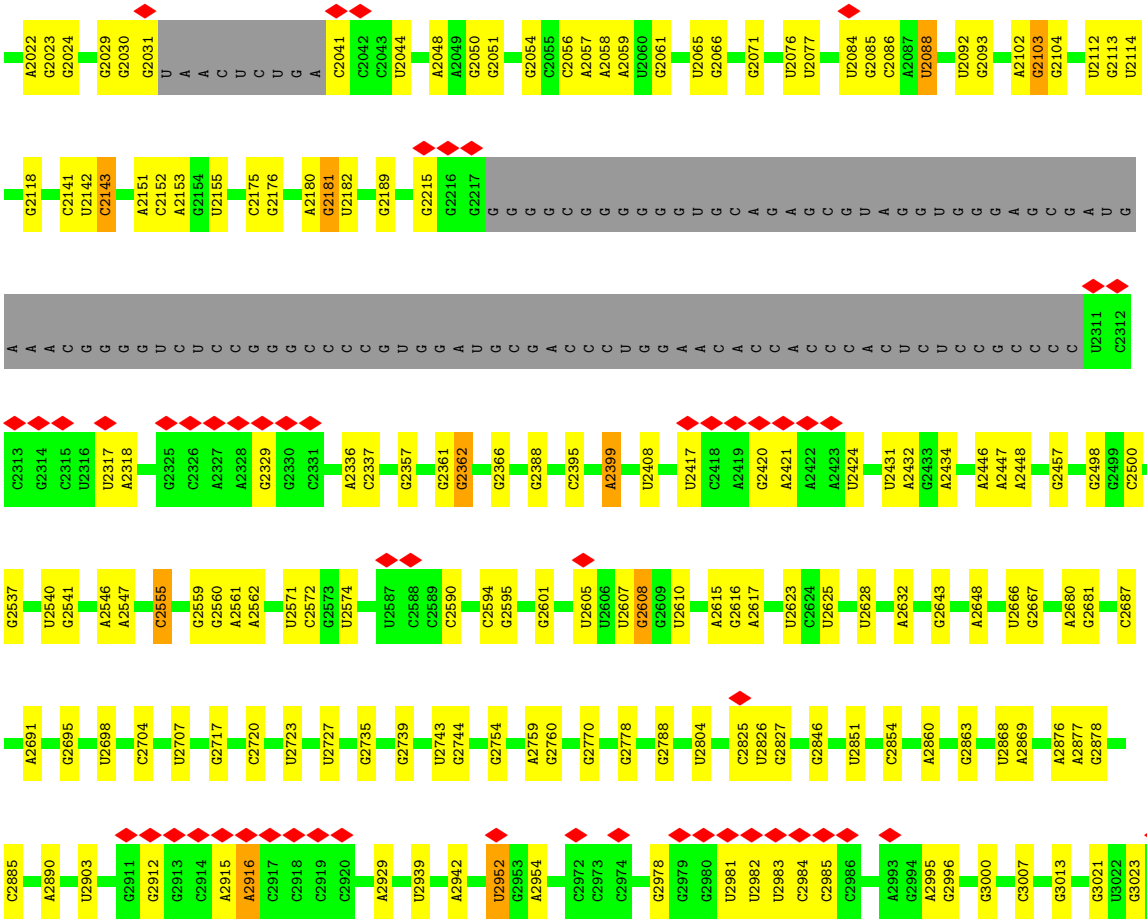
3 Residue-property plots (i)

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

- Molecule 1: 23S rRNA

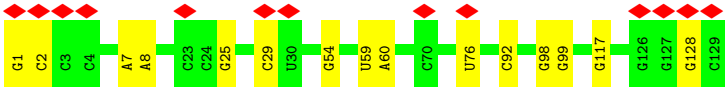
Chain 1:





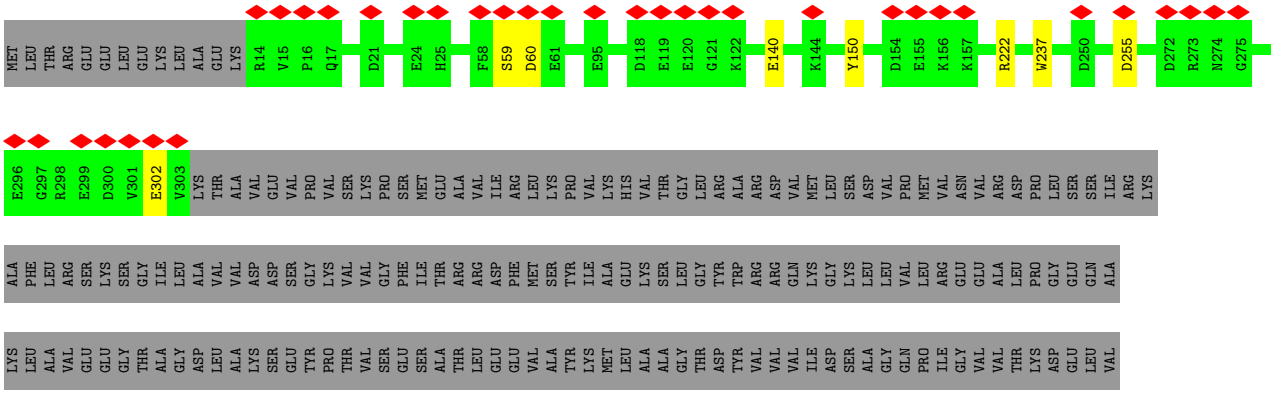
• Molecule 2: 5S rRNA

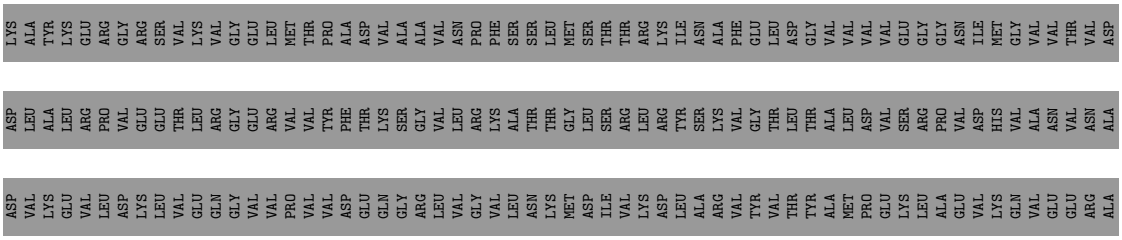
Chain 2:



• Molecule 3: Putative signal-transduction protein with CBS domains

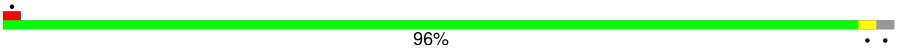
Chain 3:

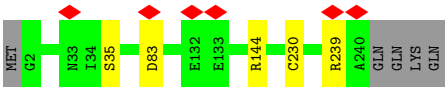




• Molecule 4: Large ribosomal subunit protein uL2

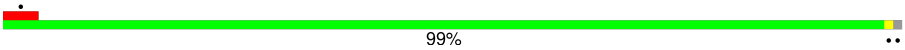
Chain AA:

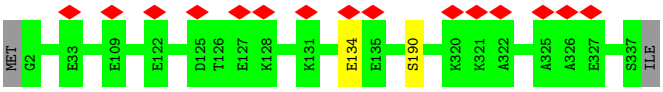




• Molecule 5: Large ribosomal subunit protein uL3

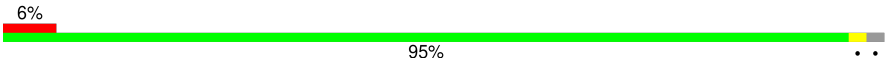
Chain AB:

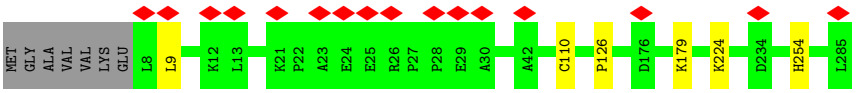




• Molecule 6: Large ribosomal subunit protein uL4

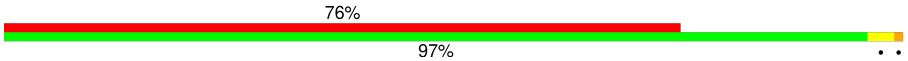
Chain AC:

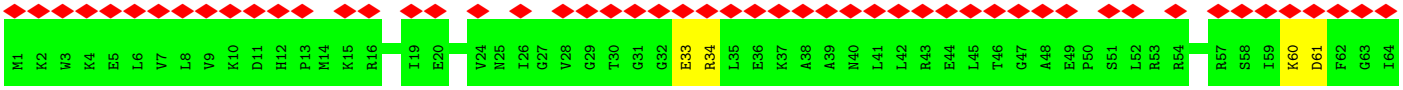


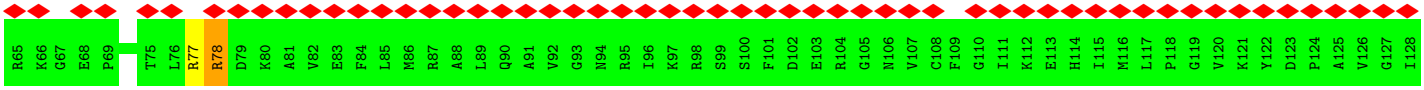


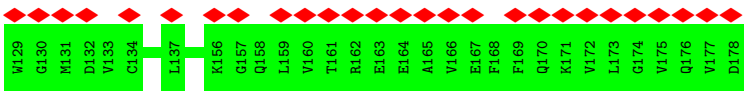
• Molecule 7: Large ribosomal subunit protein uL5

Chain AD:



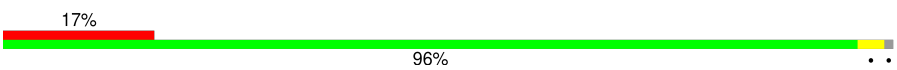


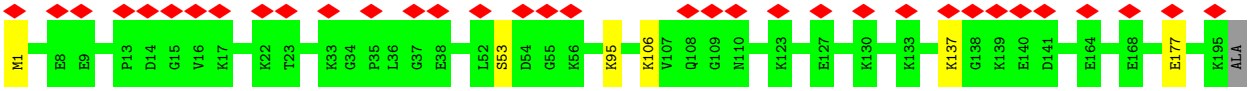




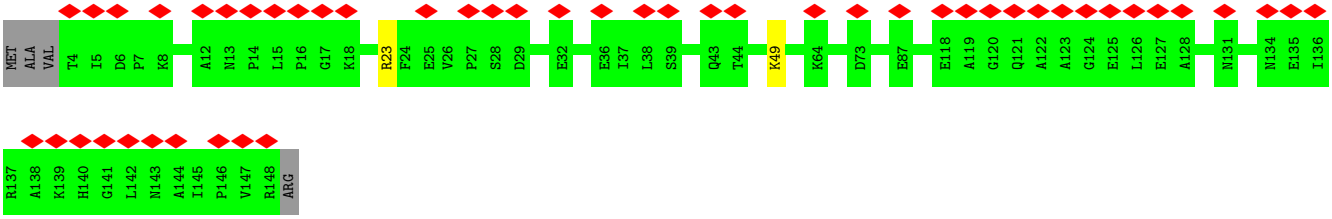
• Molecule 8: Large ribosomal subunit protein uL6

Chain AE:

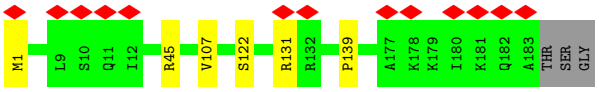




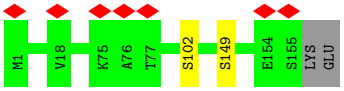
• Molecule 9: Large ribosomal subunit protein eL8



• Molecule 10: Large ribosomal subunit protein uL13

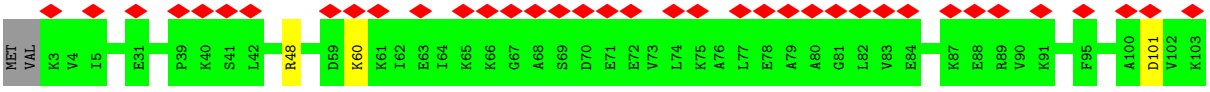


• Molecule 11: Large ribosomal subunit protein eL13

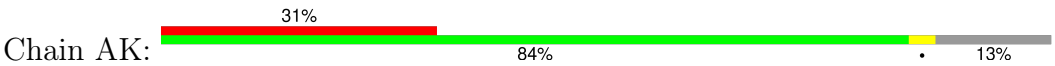


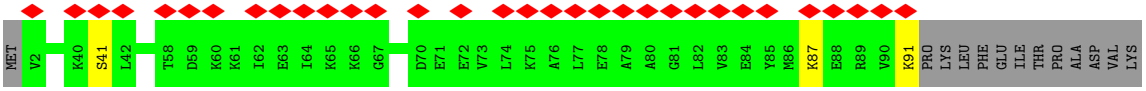
• Molecule 12: Large ribosomal subunit protein uL14

• Molecule 13: eL14



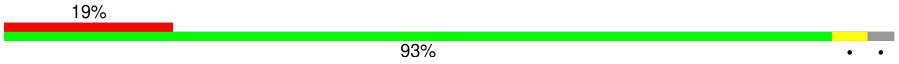
• Molecule 13: eL14

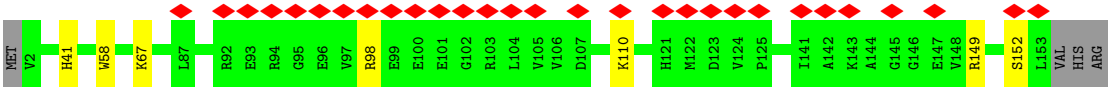




• Molecule 14: Large ribosomal subunit protein uL15

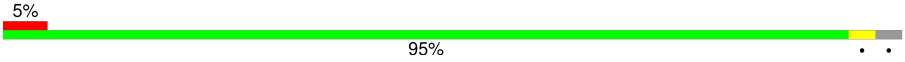
Chain AL:

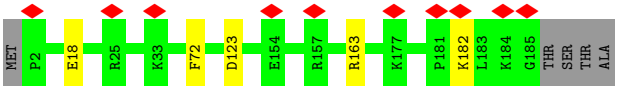




• Molecule 15: 50S ribosomal protein L15e

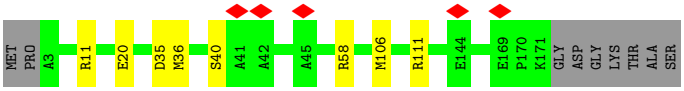
Chain AM:





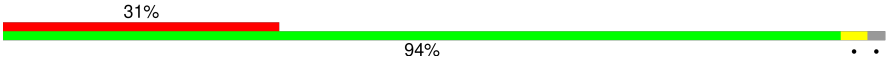
• Molecule 16: Large ribosomal subunit protein uL16

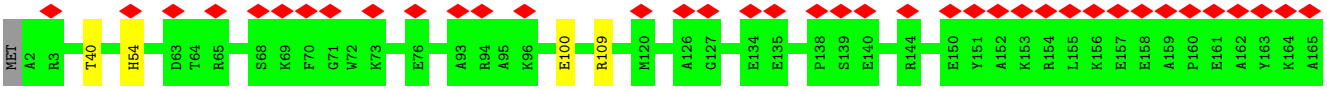
Chain AN:

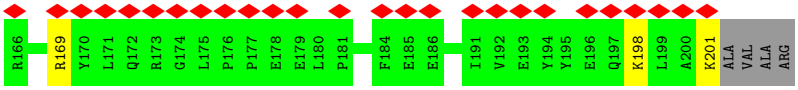


• Molecule 17: Large ribosomal subunit protein uL18

Chain AO:

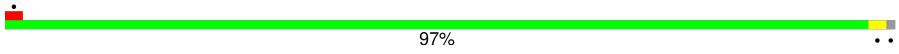


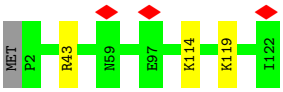




• Molecule 18: Large ribosomal subunit protein eL18

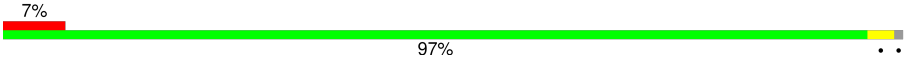
Chain AP:

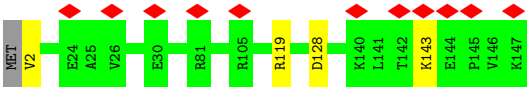




• Molecule 19: Large ribosomal subunit protein eL19

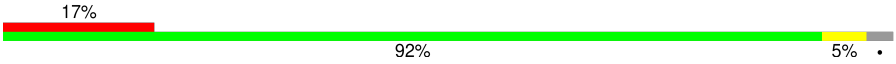
Chain AQ:

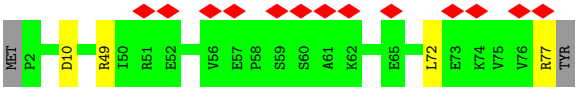




• Molecule 20: Large ribosomal subunit protein eL20

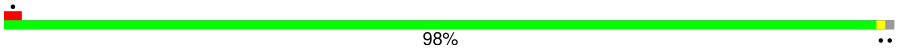
Chain AR:

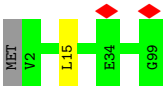




• Molecule 21: Large ribosomal subunit protein eL21

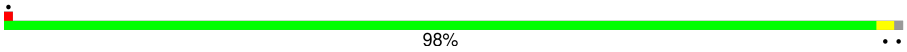
Chain AS:

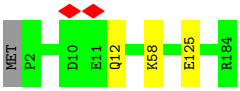




• Molecule 22: Large ribosomal subunit protein uL22

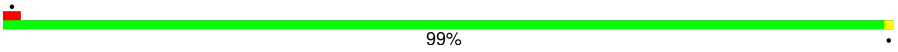
Chain AT:





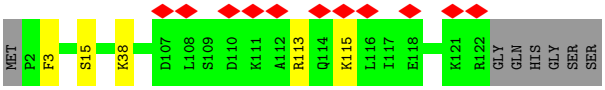
• Molecule 23: Large ribosomal subunit protein uL23

Chain AU:



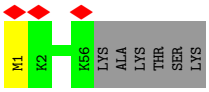
• Molecule 24: Large ribosomal subunit protein uL24

Chain AV:



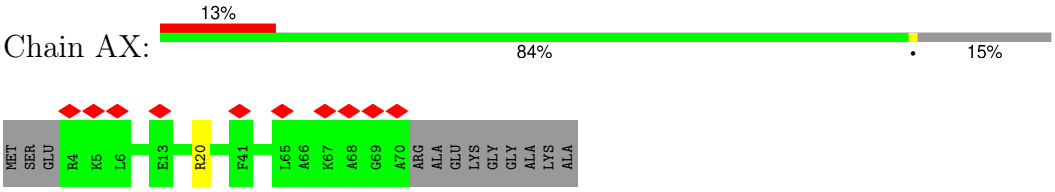
• Molecule 25: Large ribosomal subunit protein eL24

Chain AW:



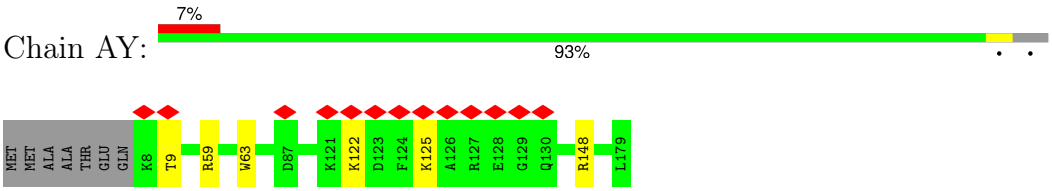
• Molecule 26: Large ribosomal subunit protein uL29

Chain AX:



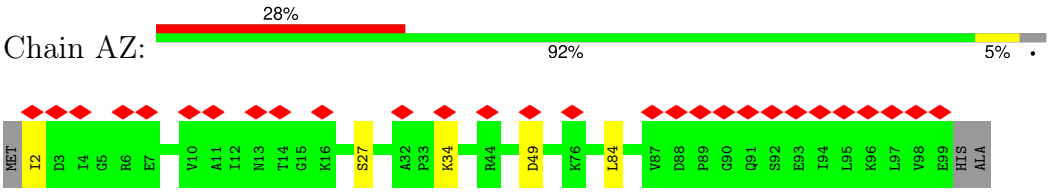
• Molecule 27: Large ribosomal subunit protein uL30

Chain AY:



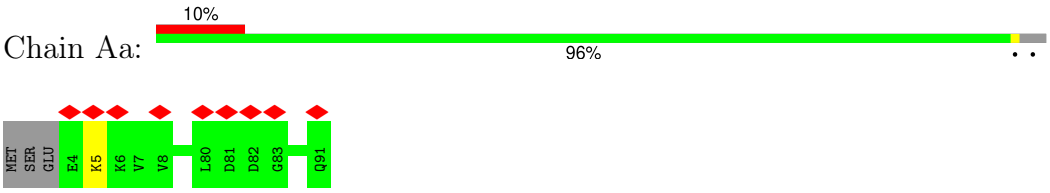
• Molecule 28: Large ribosomal subunit protein eL30

Chain AZ:



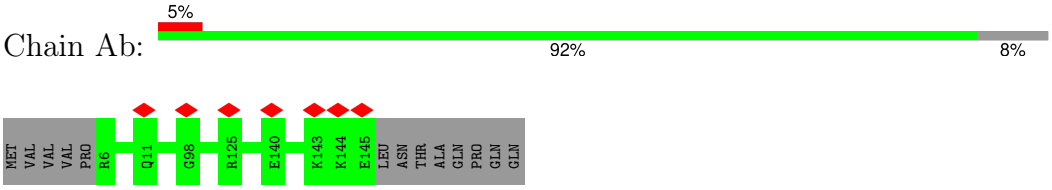
• Molecule 29: Large ribosomal subunit protein eL31

Chain Aa:



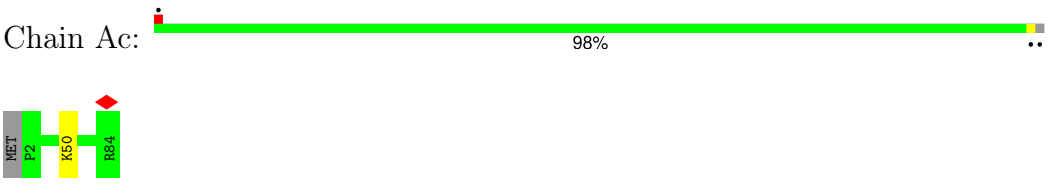
• Molecule 30: Large ribosomal subunit protein eL32

Chain Ab:



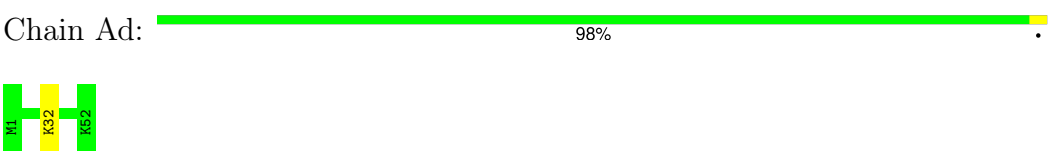
• Molecule 31: Large ribosomal subunit protein eL34

Chain Ac:



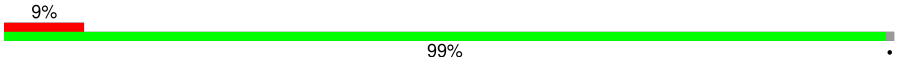
• Molecule 32: Large ribosomal subunit protein eL37

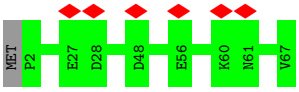
Chain Ad:



• Molecule 33: LSU ribosomal protein L38E

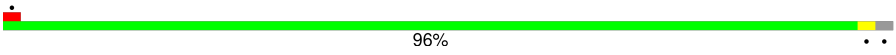
Chain Ae:

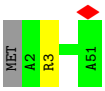




• Molecule 34: Large ribosomal subunit protein eL39

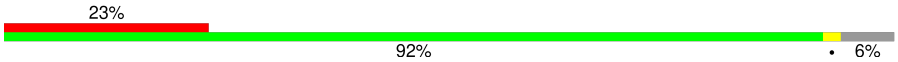
Chain Af:

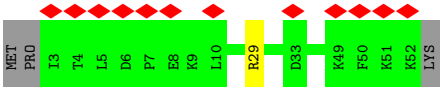




• Molecule 35: Large ribosomal subunit protein eL40

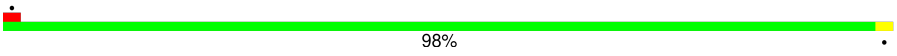
Chain Ag:

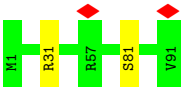




• Molecule 36: eL42

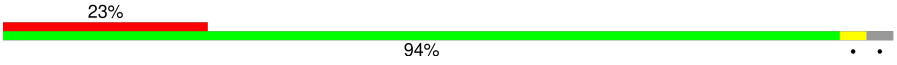
Chain Ah:

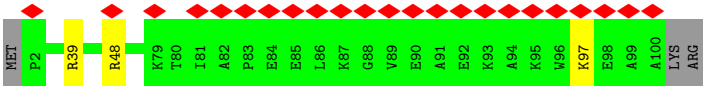




• Molecule 37: Large ribosomal subunit protein eL43

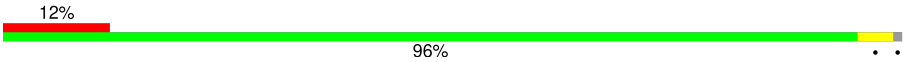
Chain Ai:

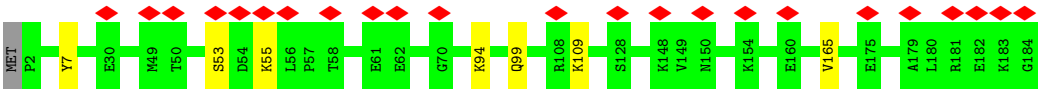




• Molecule 38: DJ-1/PfpI domain-containing protein

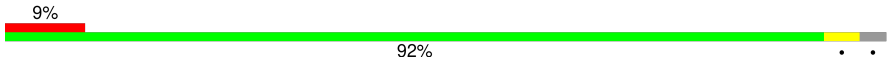
Chain Aj:

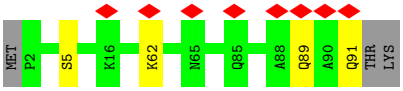




• Molecule 39: PaREP1 domain containing protein

Chain Ak:




MET
P2
S5
K16
K62
N65
Q85
A88
Q89
A90
Q91
THR
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183467	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.352	Depositor
Minimum map value	-0.518	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.152	Depositor
Map size (Å)	504.2144, 504.2144, 504.2144	wwPDB
Map dimensions	608, 608, 608	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8293, 0.8293, 0.8293	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: B8T, MG, 5MC, UR3, OMC, ZN, A2M, OMU, SPM, OMG, 4AC, PSU, G7M

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1	0.87	0/66967	0.86	41/104542 (0.0%)
2	2	0.70	0/3096	0.84	1/4830 (0.0%)
3	3	0.37	0/2323	0.53	0/3153
4	AA	0.42	0/1847	0.61	0/2489
5	AB	0.41	0/2678	0.57	0/3643
6	AC	0.38	0/2234	0.54	0/3024
7	AD	0.33	0/1431	0.58	0/1913
8	AE	0.38	0/1548	0.53	0/2087
9	AF	0.33	0/1114	0.49	0/1513
10	AG	0.38	0/1542	0.54	0/2076
11	AH	0.35	0/1265	0.57	0/1692
12	AI	0.39	0/1093	0.59	0/1487
13	AJ	0.33	0/795	0.54	0/1068
13	AK	0.36	0/704	0.57	0/944
14	AL	0.37	0/1225	0.58	0/1639
15	AM	0.40	0/1594	0.60	0/2138
16	AN	0.38	0/1365	0.57	0/1841
17	AO	0.34	0/1647	0.57	0/2212
18	AP	0.34	0/933	0.55	0/1263
19	AQ	0.34	0/1233	0.57	0/1645
20	AR	0.38	0/610	0.55	0/817
21	AS	0.43	0/805	0.60	0/1081
22	AT	0.37	0/1536	0.51	0/2075
23	AU	0.35	0/655	0.53	0/877
24	AV	0.35	0/990	0.58	0/1325
25	AW	0.40	0/460	0.56	0/613
26	AX	0.31	0/557	0.58	0/738
27	AY	0.38	0/1407	0.55	0/1905
28	AZ	0.31	0/754	0.52	0/1021
29	Aa	0.37	0/735	0.58	0/986
30	Ab	0.37	0/1209	0.59	0/1621
31	Ac	0.41	0/663	0.62	0/889

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Ad	0.43	0/442	0.60	0/587
33	Ae	0.39	0/562	0.46	0/753
34	Af	0.34	0/423	0.62	0/566
35	Ag	0.34	0/424	0.58	0/564
36	Ah	0.40	0/753	0.54	0/1001
37	Ai	0.37	0/788	0.58	0/1057
38	Aj	0.36	0/1497	0.53	0/2029
39	Ak	0.34	0/754	0.45	0/1005
All	All	0.72	0/112658	0.77	42/166709 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	AD	0	2

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2030	G	P-O3'-C3'	-11.54	105.85	119.70
1	1	2041	C	P-O3'-C3'	-10.63	106.94	119.70
1	1	1677	G	P-O3'-C3'	-10.20	107.46	119.70
1	1	2903	U	P-O3'-C3'	-9.81	107.93	119.70
1	1	1678	G	P-O3'-C3'	-8.99	108.91	119.70
1	1	1987	PSU	P-O3'-C3'	-8.94	108.98	119.70
1	1	1603	G	P-O3'-C3'	-8.51	109.49	119.70
1	1	2952	U	P-O3'-C3'	-8.05	110.04	119.70
2	2	1	G	P-O3'-C3'	-7.65	110.53	119.70
1	1	541	G	O4'-C1'-N9	7.12	113.90	108.20
1	1	2399	A	P-O3'-C3'	-6.64	111.73	119.70
1	1	1911	PSU	P-O3'-C3'	-6.45	111.96	119.70
1	1	2050	G	O4'-C1'-N9	6.38	113.30	108.20
1	1	397	G	P-O3'-C3'	-6.33	112.11	119.70
1	1	1564	G	P-O3'-C3'	-6.32	112.12	119.70
1	1	1602	U	P-O3'-C3'	-6.22	112.24	119.70
1	1	2143	OMC	P-O3'-C3'	-6.08	112.41	119.70
1	1	1526	A	C4-N9-C1'	5.96	137.02	126.30
1	1	2695	G	O4'-C1'-N9	5.74	112.79	108.20
1	1	2610	PSU	P-O3'-C3'	-5.67	112.90	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	866	G	O4'-C1'-N9	5.62	112.69	108.20
1	1	1526	A	C8-N9-C4	-5.59	103.56	105.80
1	1	585	U	P-O3'-C3'	-5.51	113.09	119.70
1	1	2029	G	P-O3'-C3'	-5.50	113.10	119.70
1	1	2625	PSU	P-O3'-C3'	-5.46	113.14	119.70
1	1	1679	U	P-O3'-C3'	-5.45	113.17	119.70
1	1	391	U	C2-N1-C1'	5.44	124.23	117.70
1	1	968	G	C4-N9-C1'	-5.42	119.45	126.50
1	1	329	U	OP1-P-OP2	5.40	127.70	119.60
1	1	512	G	O4'-C1'-N9	5.36	112.48	108.20
1	1	821	G	O4'-C1'-N9	5.25	112.40	108.20
1	1	724	A	P-O3'-C3'	5.24	125.99	119.70
1	1	2181	G	O4'-C1'-N9	5.21	112.36	108.20
1	1	2560	G	N1-C6-O6	-5.17	116.80	119.90
1	1	487	U	P-O3'-C3'	-5.15	113.52	119.70
1	1	2572	C	O4'-C1'-N1	5.14	112.31	108.20
1	1	668	G	P-O3'-C3'	5.12	125.85	119.70
1	1	2912	G	N1-C6-O6	-5.12	116.83	119.90
1	1	586	C	P-O3'-C3'	-5.10	113.58	119.70
1	1	1909	A	N9-C1'-C2'	-5.02	106.48	112.00
1	1	328	G	OP1-P-O3'	-5.02	94.16	105.20
1	1	2916	A	P-O3'-C3'	-5.01	113.68	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	AD	77	ARG	Sidechain
7	AD	78	ARG	Sidechain

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	
3	3	288/655 (44%)	282 (98%)	6 (2%)	0	100	100
4	AA	237/244 (97%)	229 (97%)	8 (3%)	0	100	100
5	AB	334/338 (99%)	327 (98%)	7 (2%)	0	100	100
6	AC	276/285 (97%)	267 (97%)	9 (3%)	0	100	100
7	AD	176/178 (99%)	168 (96%)	8 (4%)	0	100	100
8	AE	193/196 (98%)	190 (98%)	3 (2%)	0	100	100
9	AF	143/149 (96%)	141 (99%)	2 (1%)	0	100	100
10	AG	181/186 (97%)	180 (99%)	1 (1%)	0	100	100
11	AH	153/157 (98%)	152 (99%)	1 (1%)	0	100	100
12	AI	136/144 (94%)	134 (98%)	2 (2%)	0	100	100
13	AJ	99/103 (96%)	97 (98%)	2 (2%)	0	100	100
13	AK	88/103 (85%)	84 (96%)	3 (3%)	1 (1%)	12	4
14	AL	150/156 (96%)	144 (96%)	6 (4%)	0	100	100
15	AM	182/189 (96%)	179 (98%)	3 (2%)	0	100	100
16	AN	167/178 (94%)	165 (99%)	2 (1%)	0	100	100
17	AO	198/205 (97%)	197 (100%)	1 (0%)	0	100	100
18	AP	119/122 (98%)	118 (99%)	1 (1%)	0	100	100
19	AQ	144/147 (98%)	144 (100%)	0	0	100	100
20	AR	74/78 (95%)	73 (99%)	1 (1%)	0	100	100
21	AS	96/99 (97%)	91 (95%)	5 (5%)	0	100	100
22	AT	181/184 (98%)	176 (97%)	5 (3%)	0	100	100
23	AU	79/81 (98%)	75 (95%)	4 (5%)	0	100	100
24	AV	119/128 (93%)	117 (98%)	1 (1%)	1 (1%)	16	8
25	AW	54/62 (87%)	54 (100%)	0	0	100	100
26	AX	65/79 (82%)	65 (100%)	0	0	100	100
27	AY	170/179 (95%)	165 (97%)	5 (3%)	0	100	100
28	AZ	96/101 (95%)	92 (96%)	4 (4%)	0	100	100
29	Aa	86/91 (94%)	85 (99%)	1 (1%)	0	100	100
30	Ab	138/153 (90%)	137 (99%)	1 (1%)	0	100	100
31	Ac	81/84 (96%)	78 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	Ad	50/52 (96%)	48 (96%)	2 (4%)	0	100	100
33	Ae	64/67 (96%)	64 (100%)	0	0	100	100
34	Af	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
35	Ag	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
36	Ah	89/91 (98%)	89 (100%)	0	0	100	100
37	Ai	97/102 (95%)	91 (94%)	6 (6%)	0	100	100
38	Aj	181/184 (98%)	172 (95%)	9 (5%)	0	100	100
39	Ak	88/93 (95%)	88 (100%)	0	0	100	100
All	All	5168/5747 (90%)	5051 (98%)	115 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	AK	41	SER
24	AV	3	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	243/552 (44%)	235 (97%)	8 (3%)	33	23
4	AA	181/186 (97%)	176 (97%)	5 (3%)	38	29
5	AB	280/282 (99%)	278 (99%)	2 (1%)	81	81
6	AC	226/231 (98%)	220 (97%)	6 (3%)	40	31
7	AD	149/149 (100%)	144 (97%)	5 (3%)	32	22
8	AE	165/165 (100%)	159 (96%)	6 (4%)	30	20
9	AF	115/118 (98%)	113 (98%)	2 (2%)	56	52
10	AG	163/165 (99%)	157 (96%)	6 (4%)	29	19
11	AH	133/135 (98%)	131 (98%)	2 (2%)	60	57
12	AI	115/118 (98%)	113 (98%)	2 (2%)	56	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AJ	87/89 (98%)	84 (97%)	3 (3%)	32	22
13	AK	77/89 (86%)	75 (97%)	2 (3%)	41	33
14	AL	121/125 (97%)	114 (94%)	7 (6%)	17	7
15	AM	161/165 (98%)	156 (97%)	5 (3%)	35	25
16	AN	134/140 (96%)	126 (94%)	8 (6%)	16	6
17	AO	166/169 (98%)	159 (96%)	7 (4%)	25	15
18	AP	99/100 (99%)	96 (97%)	3 (3%)	36	27
19	AQ	127/128 (99%)	123 (97%)	4 (3%)	35	25
20	AR	69/71 (97%)	65 (94%)	4 (6%)	17	7
21	AS	84/85 (99%)	83 (99%)	1 (1%)	67	65
22	AT	157/158 (99%)	154 (98%)	3 (2%)	52	47
23	AU	71/71 (100%)	70 (99%)	1 (1%)	62	59
24	AV	107/112 (96%)	103 (96%)	4 (4%)	29	19
25	AW	48/53 (91%)	47 (98%)	1 (2%)	48	43
26	AX	58/65 (89%)	57 (98%)	1 (2%)	56	52
27	AY	147/152 (97%)	141 (96%)	6 (4%)	26	15
28	AZ	77/79 (98%)	72 (94%)	5 (6%)	14	5
29	Aa	78/81 (96%)	77 (99%)	1 (1%)	65	62
30	Ab	125/137 (91%)	125 (100%)	0	100	100
31	Ac	67/68 (98%)	66 (98%)	1 (2%)	60	57
32	Ad	44/44 (100%)	43 (98%)	1 (2%)	45	39
33	Ae	60/61 (98%)	60 (100%)	0	100	100
34	Af	42/43 (98%)	41 (98%)	1 (2%)	44	37
35	Ag	46/49 (94%)	45 (98%)	1 (2%)	47	41
36	Ah	82/82 (100%)	80 (98%)	2 (2%)	44	37
37	Ai	77/80 (96%)	74 (96%)	3 (4%)	27	17
38	Aj	161/162 (99%)	154 (96%)	7 (4%)	25	14
39	Ak	79/82 (96%)	75 (95%)	4 (5%)	20	9
All	All	4421/4841 (91%)	4291 (97%)	130 (3%)	39	28

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	59	SER
3	3	60	ASP
3	3	140	GLU
3	3	150	TYR
3	3	222	ARG
3	3	237	TRP
3	3	255	ASP
3	3	302	GLU
4	AA	35	SER
4	AA	83	ASP
4	AA	144	ARG
4	AA	230	CYS
4	AA	239	ARG
5	AB	134	GLU
5	AB	190	SER
6	AC	9	LEU
6	AC	110	CYS
6	AC	126	PRO
6	AC	179	LYS
6	AC	224	LYS
6	AC	254	HIS
7	AD	33	GLU
7	AD	34	ARG
7	AD	60	LYS
7	AD	61	ASP
7	AD	78	ARG
8	AE	1	MET
8	AE	53	SER
8	AE	95	LYS
8	AE	106	LYS
8	AE	137	LYS
8	AE	177	GLU
9	AF	23	ARG
9	AF	49	LYS
10	AG	1	MET
10	AG	45	ARG
10	AG	107	VAL
10	AG	122	SER
10	AG	131	ARG
10	AG	139	PRO
11	AH	102	SER
11	AH	149	SER
12	AI	37	LYS

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Mol	Chain	Res	Type
12	AI	90	ARG
13	AJ	48	ARG
13	AJ	60	LYS
13	AJ	101	ASP
13	AK	87	LYS
13	AK	91	LYS
14	AL	41	HIS
14	AL	58	TRP
14	AL	67	LYS
14	AL	98	ARG
14	AL	110	LYS
14	AL	149	ARG
14	AL	152	SER
15	AM	18	GLU
15	AM	72	PHE
15	AM	123	ASP
15	AM	163	ARG
15	AM	182	LYS
16	AN	11	ARG
16	AN	20	GLU
16	AN	35	ASP
16	AN	36	MET
16	AN	40	SER
16	AN	58	ARG
16	AN	106	MET
16	AN	111	ARG
17	AO	40	THR
17	AO	54	HIS
17	AO	100	GLU
17	AO	109	ARG
17	AO	169	ARG
17	AO	198	LYS
17	AO	201	LYS
18	AP	43	ARG
18	AP	114	LYS
18	AP	119	LYS
19	AQ	2	VAL
19	AQ	119	ARG
19	AQ	128	ASP
19	AQ	143	LYS
20	AR	10	ASP
20	AR	49	ARG

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Mol	Chain	Res	Type
20	AR	72	LEU
20	AR	77	ARG
21	AS	15	LEU
22	AT	12	GLN
22	AT	58	LYS
22	AT	125	GLU
23	AU	13	ARG
24	AV	15	SER
24	AV	38	LYS
24	AV	113	ARG
24	AV	115	LYS
25	AW	1	MET
26	AX	20	ARG
27	AY	9	THR
27	AY	59	ARG
27	AY	63	TRP
27	AY	122	LYS
27	AY	125	LYS
27	AY	148	ARG
28	AZ	2	ILE
28	AZ	27	SER
28	AZ	34	LYS
28	AZ	49	ASP
28	AZ	84	LEU
29	Aa	5	LYS
31	Ac	50	LYS
32	Ad	32	LYS
34	Af	3	ARG
35	Ag	29	ARG
36	Ah	31	ARG
36	Ah	81	SER
37	Ai	39	ARG
37	Ai	48	ARG
37	Ai	97	LYS
38	Aj	7	TYR
38	Aj	53	SER
38	Aj	55	LYS
38	Aj	94	LYS
38	Aj	99	GLN
38	Aj	109	LYS
38	Aj	165	VAL
39	Ak	5	SER

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Mol	Chain	Res	Type
39	Ak	62	LYS
39	Ak	89	GLN
39	Ak	91	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2834/3024 (93%)	342 (12%)	32 (1%)
2	2	128/129 (99%)	13 (10%)	1 (0%)
All	All	2962/3153 (93%)	355 (11%)	33 (1%)

All (355) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	A
1	1	27	C
1	1	43	G
1	1	63	A
1	1	66	A
1	1	67	G
1	1	75	U
1	1	76	A
1	1	77	G
1	1	83	G
1	1	109	A
1	1	110	A
1	1	111	U
1	1	118	U
1	1	134	U
1	1	135	A
1	1	154	G
1	1	162	A
1	1	177	A
1	1	196	G
1	1	197	A
1	1	203	A
1	1	211	G
1	1	220	U

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Mol	Chain	Res	Type
1	1	229	G
1	1	233	C
1	1	245	U
1	1	247	G
1	1	258	A
1	1	269	A
1	1	270	C
1	1	292	U
1	1	294	G
1	1	304	A
1	1	305	A
1	1	308	G
1	1	328	G
1	1	329	U
1	1	330	G
1	1	358	A
1	1	359	U
1	1	366	G
1	1	373	A
1	1	374	A
1	1	389	A
1	1	390	G
1	1	399	U
1	1	400	C
1	1	422	U
1	1	423	U
1	1	435	G
1	1	442	C
1	1	452	G
1	1	457	G
1	1	488	A
1	1	489	G
1	1	504	G
1	1	512	G
1	1	523	G
1	1	534	A
1	1	535	G
1	1	536	A
1	1	537	G
1	1	558	G
1	1	575	G
1	1	576	G

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Mol	Chain	Res	Type
1	1	578	U
1	1	579	G
1	1	606	C
1	1	613	G
1	1	614	U
1	1	619	G
1	1	629	C
1	1	643	U
1	1	644	A
1	1	652	A
1	1	655	C
1	1	656	A
1	1	668	G
1	1	669	U
1	1	684	A
1	1	685	G
1	1	696	U
1	1	698	A
1	1	723	C
1	1	724	A
1	1	725	G
1	1	772	A
1	1	803	U
1	1	835	G
1	1	847	C
1	1	860	U
1	1	865	U
1	1	881	G
1	1	882	A
1	1	883	C
1	1	893	G
1	1	894	G
1	1	900	A
1	1	902	OMG
1	1	903	A
1	1	907	A
1	1	910	A
1	1	923	G
1	1	930	C
1	1	945	C
1	1	946	U
1	1	964	A

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Mol	Chain	Res	Type
1	1	965	G
1	1	968	G
1	1	978	G
1	1	1021	C
1	1	1029	A
1	1	1031	C
1	1	1067	G
1	1	1074	U
1	1	1075	G
1	1	1076	G
1	1	1082	G
1	1	1095	G
1	1	1101	A
1	1	1104	A
1	1	1123	G
1	1	1132	U
1	1	1133	G
1	1	1141	A
1	1	1142	G
1	1	1147	A
1	1	1160	G
1	1	1171	A
1	1	1172	A
1	1	1173	G
1	1	1174	A
1	1	1176	A
1	1	1177	G
1	1	1237	A
1	1	1238	G
1	1	1254	G
1	1	1255	A
1	1	1256	U
1	1	1259	A
1	1	1260	C
1	1	1265	A
1	1	1268	A
1	1	1300	G
1	1	1301	U
1	1	1302	U
1	1	1303	G
1	1	1312	G
1	1	1315	G

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Mol	Chain	Res	Type
1	1	1322	G
1	1	1323	G
1	1	1338	A
1	1	1354	G
1	1	1365	C
1	1	1383	C
1	1	1393	G
1	1	1424	G
1	1	1429	A
1	1	1430	A
1	1	1431	A
1	1	1474	C
1	1	1483	G
1	1	1500	A
1	1	1508	A
1	1	1510	A
1	1	1514	A
1	1	1515	A
1	1	1526	A
1	1	1527	U
1	1	1549	U
1	1	1550	C
1	1	1551	U
1	1	1559	C
1	1	1562	A
1	1	1564	G
1	1	1577	C
1	1	1602	U
1	1	1603	G
1	1	1632	G
1	1	1633	A
1	1	1635	U
1	1	1636	G
1	1	1644	G
1	1	1655	G
1	1	1668	A
1	1	1669	U
1	1	1680	U
1	1	1681	U
1	1	1711	G
1	1	1712	A
1	1	1728	C

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Mol	Chain	Res	Type
1	1	1732	C
1	1	1752	A
1	1	1757	C
1	1	1764	G
1	1	1765	C
1	1	1766	U
1	1	1777	A
1	1	1786	G
1	1	1789	G
1	1	1790	C
1	1	1792	C
1	1	1818	G
1	1	1840	G
1	1	1867	U
1	1	1868	A
1	1	1869	U
1	1	1870	A
1	1	1900	G
1	1	1909	A
1	1	1916	A
1	1	1918	C
1	1	1920	A
1	1	1936	C
1	1	1947	OMG
1	1	1999	A
1	1	2022	A
1	1	2023	G
1	1	2024	G
1	1	2031	G
1	1	2048	A
1	1	2051	G
1	1	2054	G
1	1	2057	A
1	1	2058	A
1	1	2061	G
1	1	2065	U
1	1	2076	U
1	1	2084	U
1	1	2085	G
1	1	2086	C
1	1	2088	OMU
1	1	2092	U

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Mol	Chain	Res	Type
1	1	2093	G
1	1	2103	OMG
1	1	2112	U
1	1	2113	G
1	1	2114	U
1	1	2118	G
1	1	2141	C
1	1	2142	U
1	1	2143	OMC
1	1	2151	A
1	1	2152	C
1	1	2153	A
1	1	2175	C
1	1	2180	A
1	1	2181	G
1	1	2182	U
1	1	2189	G
1	1	2215	G
1	1	2317	U
1	1	2318	A
1	1	2329	G
1	1	2336	A
1	1	2337	C
1	1	2357	G
1	1	2361	G
1	1	2362	OMG
1	1	2395	C
1	1	2399	A
1	1	2417	U
1	1	2420	G
1	1	2421	A
1	1	2424	U
1	1	2432	A
1	1	2434	A
1	1	2446	A
1	1	2447	A
1	1	2448	A
1	1	2457	G
1	1	2498	G
1	1	2500	C
1	1	2518	C
1	1	2540	U

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Mol	Chain	Res	Type
1	1	2541	G
1	1	2546	A
1	1	2547	A
1	1	2555	OMC
1	1	2559	G
1	1	2561	A
1	1	2562	A
1	1	2590	C
1	1	2594	C
1	1	2595	G
1	1	2605	U
1	1	2608	OMG
1	1	2615	A
1	1	2616	G
1	1	2617	A
1	1	2632	A
1	1	2643	G
1	1	2648	A
1	1	2680	A
1	1	2681	G
1	1	2687	C
1	1	2717	G
1	1	2723	U
1	1	2727	U
1	1	2735	G
1	1	2739	G
1	1	2743	U
1	1	2744	G
1	1	2754	G
1	1	2759	A
1	1	2760	G
1	1	2770	G
1	1	2778	G
1	1	2788	G
1	1	2804	U
1	1	2825	C
1	1	2826	U
1	1	2827	G
1	1	2846	G
1	1	2854	C
1	1	2860	A
1	1	2863	G

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Mol	Chain	Res	Type
1	1	2869	A
1	1	2876	A
1	1	2877	A
1	1	2878	G
1	1	2890	A
1	1	2915	A
1	1	2916	A
1	1	2929	A
1	1	2939	U
1	1	2942	A
1	1	2952	U
1	1	2954	A
1	1	2978	G
1	1	2981	U
1	1	2982	U
1	1	2983	U
1	1	2984	C
1	1	2985	C
1	1	2995	A
1	1	2996	G
1	1	3000	G
1	1	3007	C
1	1	3013	G
1	1	3021	G
2	2	2	C
2	2	8	A
2	2	25	G
2	2	29	C
2	2	54	G
2	2	59	U
2	2	60	A
2	2	76	U
2	2	92	C
2	2	98	G
2	2	99	G
2	2	117	G
2	2	128	G

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	117	U

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Mol	Chain	Res	Type
1	1	134	U
1	1	180	A
1	1	456	G
1	1	533	A
1	1	536	A
1	1	575	G
1	1	613	G
1	1	668	G
1	1	724	A
1	1	880	U
1	1	882	A
1	1	902	OMG
1	1	963	G
1	1	1075	G
1	1	1253	A
1	1	1337	C
1	1	1473	C
1	1	1514	A
1	1	1526	A
1	1	1868	A
1	1	2022	A
1	1	2065	U
1	1	2102	A
1	1	2336	A
1	1	2361	G
1	1	2420	G
1	1	2431	U
1	1	2615	A
1	1	2868	U
1	1	2984	C
1	1	2995	A
2	2	7	A

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

65 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	1	1987	1	18,21,22	0.92	1 (5%)	21,30,33	0.72	0
1	OMG	1	2071	1	19,26,27	0.96	1 (5%)	21,38,41	1.09	2 (9%)
1	PSU	1	2571	1	18,21,22	0.93	1 (5%)	21,30,33	0.68	0
1	PSU	1	2625	1	18,21,22	0.92	1 (5%)	21,30,33	0.78	0
1	OMC	1	493	1	19,22,23	0.82	1 (5%)	25,31,34	0.79	0
1	OMU	1	2574	1	19,22,23	1.34	3 (15%)	25,31,34	1.81	4 (16%)
1	OMC	1	2116	1	19,22,23	0.79	0	25,31,34	0.74	0
1	OMU	1	2623	1	19,22,23	1.34	4 (21%)	25,31,34	1.94	4 (16%)
1	OMG	1	2066	1	19,26,27	0.93	1 (5%)	21,38,41	1.07	2 (9%)
1	A2M	1	2059	1,41	18,25,26	0.69	0	20,36,39	0.92	1 (5%)
1	OMU	1	2666	1	19,22,23	1.29	3 (15%)	25,31,34	1.99	5 (20%)
1	OMG	1	2366	1	19,26,27	0.93	1 (5%)	21,38,41	1.08	2 (9%)
1	OMG	1	2667	1	19,26,27	0.92	1 (5%)	21,38,41	1.08	2 (9%)
1	OMC	1	2624	1	19,22,23	0.29	0	25,31,34	0.31	0
1	A2M	1	2691	1,41	18,25,26	0.67	0	20,36,39	0.76	1 (5%)
1	OMG	1	2608	1	19,26,27	1.06	3 (15%)	21,38,41	0.72	1 (4%)
1	OMG	1	902	1,41	19,26,27	0.93	1 (5%)	21,38,41	1.19	2 (9%)
1	PSU	1	1911	1	18,21,22	0.93	1 (5%)	21,30,33	0.77	0
1	OMC	1	2143	1	19,22,23	0.29	0	25,31,34	0.38	0
1	OMG	1	1949	1	19,26,27	0.96	1 (5%)	21,38,41	1.11	2 (9%)
1	OMC	1	872	1	19,22,23	0.79	0	25,31,34	0.80	0
1	OMU	1	908	1,41	19,22,23	1.35	4 (21%)	25,31,34	2.02	8 (32%)
1	OMC	1	2720	1	19,22,23	0.78	0	25,31,34	0.94	1 (4%)
1	B8T	1	79	1	19,22,23	0.43	0	25,31,34	0.35	0
1	OMC	1	2555	1	19,22,23	0.79	0	25,31,34	0.88	1 (4%)
1	G7M	1	3023	1	20,26,27	2.37	3 (15%)	16,39,42	0.38	0
1	OMU	1	875	1	19,22,23	1.28	3 (15%)	25,31,34	1.87	5 (20%)
1	4AC	1	2016	1	21,24,25	0.37	0	28,34,37	0.40	0
1	PSU	1	2610	1	18,21,22	0.91	1 (5%)	21,30,33	0.83	1 (4%)
1	OMG	1	2388	1	19,26,27	0.91	1 (5%)	21,38,41	1.20	2 (9%)
1	OMU	1	2851	1	19,22,23	1.33	3 (15%)	25,31,34	1.81	4 (16%)
1	OMU	1	2408	1	19,22,23	1.31	4 (21%)	25,31,34	1.91	5 (20%)
1	OMC	1	2018	1	19,22,23	0.80	1 (5%)	25,31,34	0.81	0
1	OMC	1	673	1	19,22,23	0.80	0	25,31,34	0.87	0
1	UR3	1	2698	1	19,22,23	0.94	1 (5%)	26,32,35	1.77	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMC	1	2704	1	19,22,23	0.82	1 (5%)	25,31,34	0.85	0
1	OMG	1	1947	1	19,26,27	0.90	1 (5%)	21,38,41	1.21	2 (9%)
1	OMU	1	2088	1	19,22,23	1.37	3 (15%)	25,31,34	1.84	5 (20%)
1	OMG	1	2537	1	19,26,27	0.92	1 (5%)	21,38,41	1.08	2 (9%)
1	OMU	1	2155	1	19,22,23	1.39	3 (15%)	25,31,34	2.03	5 (20%)
1	PSU	1	2044	1	18,21,22	0.88	1 (5%)	21,30,33	0.68	0
1	OMG	1	2017	1	19,26,27	0.87	1 (5%)	21,38,41	1.11	3 (14%)
1	5MC	1	38	1	19,22,23	1.42	3 (15%)	26,32,35	1.31	3 (11%)
1	OMC	1	2538	1	19,22,23	0.78	0	25,31,34	0.75	0
1	OMU	1	2077	1	19,22,23	1.34	3 (15%)	25,31,34	1.86	4 (16%)
1	OMG	1	1957	1	19,26,27	0.95	1 (5%)	21,38,41	1.07	2 (9%)
1	OMC	1	1976	1	19,22,23	0.82	1 (5%)	25,31,34	0.98	1 (4%)
1	A2M	1	2011	1	18,25,26	0.67	0	20,36,39	0.73	1 (5%)
1	5MC	1	2056	1,41	19,22,23	1.41	3 (15%)	26,32,35	1.13	3 (11%)
1	OMG	1	2104	1	19,26,27	0.96	1 (5%)	21,38,41	1.22	2 (9%)
1	PSU	1	2607	1	18,21,22	0.95	1 (5%)	21,30,33	0.72	0
1	OMC	1	492	1	19,22,23	0.80	1 (5%)	25,31,34	0.88	1 (4%)
1	OMG	1	2176	1,41	19,26,27	0.89	1 (5%)	21,38,41	1.12	3 (14%)
1	OMC	1	2884	1	19,22,23	0.80	0	25,31,34	0.77	0
1	OMU	1	2707	1	19,22,23	1.36	4 (21%)	25,31,34	1.84	5 (20%)
1	OMC	1	1816	1	19,22,23	0.76	0	25,31,34	0.77	0
1	OMG	1	2362	1	19,26,27	0.98	1 (5%)	21,38,41	1.10	2 (9%)
1	OMC	1	2115	1	19,22,23	0.81	0	25,31,34	0.76	0
1	OMG	1	2103	1	19,26,27	0.89	1 (5%)	21,38,41	1.14	2 (9%)
1	OMG	1	2601	1,41	19,26,27	0.91	1 (5%)	21,38,41	1.09	3 (14%)
1	OMC	1	2885	1	19,22,23	0.80	0	25,31,34	0.78	1 (4%)
1	A2M	1	1990	1	18,25,26	0.69	0	20,36,39	0.83	1 (5%)
1	OMU	1	2628	1	19,22,23	1.36	3 (15%)	25,31,34	1.89	5 (20%)
1	OMG	1	1971	1	19,26,27	0.93	1 (5%)	21,38,41	0.99	2 (9%)
1	B8T	1	2937	1	19,22,23	0.42	0	25,31,34	0.33	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
1	PSU	1	1987	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2071	1	-	0/5/27/28	0/3/3/3
1	PSU	1	2571	1	-	0/7/25/26	0/2/2/2
1	PSU	1	2625	1	-	0/7/25/26	0/2/2/2
1	OMC	1	493	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2574	1	-	0/9/27/28	0/2/2/2
1	OMC	1	2116	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2623	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2066	1	-	0/5/27/28	0/3/3/3
1	A2M	1	2059	1,41	-	1/5/27/28	0/3/3/3
1	OMU	1	2666	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2366	1	-	0/5/27/28	0/3/3/3
1	OMG	1	2667	1	-	0/5/27/28	0/3/3/3
1	OMC	1	2624	1	-	0/9/27/28	0/2/2/2
1	A2M	1	2691	1,41	-	0/5/27/28	0/3/3/3
1	OMG	1	2608	1	-	2/5/27/28	0/3/3/3
1	OMG	1	902	1,41	-	0/5/27/28	0/3/3/3
1	PSU	1	1911	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2143	1	-	2/9/27/28	0/2/2/2
1	OMG	1	1949	1	-	0/5/27/28	0/3/3/3
1	OMC	1	872	1	-	0/9/27/28	0/2/2/2
1	OMU	1	908	1,41	-	5/9/27/28	0/2/2/2
1	OMC	1	2720	1	-	0/9/27/28	0/2/2/2
1	B8T	1	79	1	-	0/7/27/28	0/2/2/2
1	OMC	1	2555	1	-	1/9/27/28	0/2/2/2
1	G7M	1	3023	1	-	0/3/25/26	0/3/3/3
1	OMU	1	875	1	-	0/9/27/28	0/2/2/2
1	4AC	1	2016	1	-	0/11/29/30	0/2/2/2
1	PSU	1	2610	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2388	1	-	1/5/27/28	0/3/3/3
1	OMU	1	2851	1	-	1/9/27/28	0/2/2/2
1	OMU	1	2408	1	-	0/9/27/28	0/2/2/2
1	OMC	1	2018	1	-	0/9/27/28	0/2/2/2
1	OMC	1	673	1	-	0/9/27/28	0/2/2/2
1	UR3	1	2698	1	-	0/7/25/26	0/2/2/2
1	OMC	1	2704	1	-	0/9/27/28	0/2/2/2
1	OMG	1	1947	1	-	2/5/27/28	0/3/3/3
1	OMU	1	2088	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2537	1	-	1/5/27/28	0/3/3/3
1	OMU	1	2155	1	-	3/9/27/28	0/2/2/2
1	PSU	1	2044	1	-	0/7/25/26	0/2/2/2
1	OMG	1	2017	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1	38	1	-	1/7/25/26	0/2/2/2
1	OMC	1	2538	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2077	1	-	0/9/27/28	0/2/2/2
1	OMG	1	1957	1	-	0/5/27/28	0/3/3/3
1	OMC	1	1976	1	-	0/9/27/28	0/2/2/2
1	A2M	1	2011	1	-	0/5/27/28	0/3/3/3
1	5MC	1	2056	1,41	-	0/7/25/26	0/2/2/2
1	OMG	1	2104	1	-	0/5/27/28	0/3/3/3
1	PSU	1	2607	1	-	0/7/25/26	0/2/2/2
1	OMC	1	492	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2176	1,41	-	0/5/27/28	0/3/3/3
1	OMC	1	2884	1	-	0/9/27/28	0/2/2/2
1	OMU	1	2707	1	-	0/9/27/28	0/2/2/2
1	OMC	1	1816	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2362	1	-	0/5/27/28	0/3/3/3
1	OMC	1	2115	1	-	0/9/27/28	0/2/2/2
1	OMG	1	2103	1	-	0/5/27/28	0/3/3/3
1	OMG	1	2601	1,41	-	1/5/27/28	0/3/3/3
1	OMC	1	2885	1	-	0/9/27/28	0/2/2/2
1	A2M	1	1990	1	-	1/5/27/28	0/3/3/3
1	OMU	1	2628	1	-	0/9/27/28	0/2/2/2
1	OMG	1	1971	1	-	1/5/27/28	0/3/3/3
1	B8T	1	2937	1	-	2/7/27/28	0/2/2/2

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	3023	G7M	C8-N9	7.30	1.46	1.33
1	1	3023	G7M	C8-N7	7.02	1.45	1.33
1	1	2056	5MC	C5-C4	4.75	1.47	1.44
1	1	38	5MC	C5-C4	4.75	1.47	1.44
1	1	2571	PSU	C6-C5	3.61	1.39	1.35
1	1	2607	PSU	C6-C5	3.59	1.39	1.35
1	1	2610	PSU	C6-C5	3.59	1.39	1.35
1	1	2625	PSU	C6-C5	3.57	1.39	1.35
1	1	1911	PSU	C6-C5	3.56	1.39	1.35
1	1	2088	OMU	C4-N3	-3.46	1.32	1.38
1	1	1987	PSU	C6-C5	3.46	1.39	1.35
1	1	2707	OMU	C4-N3	-3.42	1.32	1.38
1	1	2628	OMU	C4-N3	-3.41	1.32	1.38
1	1	2155	OMU	C4-N3	-3.41	1.32	1.38
1	1	2044	PSU	C6-C5	3.39	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2574	OMU	C4-N3	-3.30	1.33	1.38
1	1	2623	OMU	C4-N3	-3.26	1.33	1.38
1	1	2851	OMU	C4-N3	-3.23	1.33	1.38
1	1	2408	OMU	C4-N3	-3.20	1.33	1.38
1	1	2666	OMU	C4-N3	-3.20	1.33	1.38
1	1	2077	OMU	C4-N3	-3.14	1.33	1.38
1	1	2362	OMG	C6-N1	-3.14	1.33	1.37
1	1	875	OMU	C4-N3	-3.12	1.33	1.38
1	1	2071	OMG	C6-N1	-3.08	1.33	1.37
1	1	908	OMU	C4-N3	-3.06	1.33	1.38
1	1	2155	OMU	C2-N3	-3.01	1.32	1.38
1	1	2104	OMG	C6-N1	-3.01	1.33	1.37
1	1	1949	OMG	C6-N1	-3.01	1.33	1.37
1	1	2366	OMG	C6-N1	-2.98	1.33	1.37
1	1	1971	OMG	C6-N1	-2.98	1.33	1.37
1	1	902	OMG	C6-N1	-2.96	1.33	1.37
1	1	38	5MC	C6-N1	-2.95	1.33	1.38
1	1	2066	OMG	C6-N1	-2.94	1.33	1.37
1	1	2707	OMU	C2-N3	-2.93	1.32	1.38
1	1	1957	OMG	C6-N1	-2.93	1.33	1.37
1	1	2537	OMG	C6-N1	-2.85	1.33	1.37
1	1	2077	OMU	C2-N3	-2.85	1.33	1.38
1	1	2623	OMU	C2-N3	-2.85	1.33	1.38
1	1	2088	OMU	C2-N3	-2.84	1.33	1.38
1	1	2601	OMG	C6-N1	-2.83	1.33	1.37
1	1	1947	OMG	C6-N1	-2.80	1.33	1.37
1	1	2103	OMG	C6-N1	-2.80	1.33	1.37
1	1	2408	OMU	C2-N3	-2.80	1.33	1.38
1	1	2667	OMG	C6-N1	-2.79	1.33	1.37
1	1	2574	OMU	C2-N3	-2.76	1.33	1.38
1	1	2628	OMU	C2-N3	-2.75	1.33	1.38
1	1	2176	OMG	C6-N1	-2.75	1.33	1.37
1	1	2388	OMG	C6-N1	-2.74	1.33	1.37
1	1	2666	OMU	C2-N3	-2.73	1.33	1.38
1	1	2851	OMU	C2-N3	-2.72	1.33	1.38
1	1	2608	OMG	C5-C6	-2.67	1.42	1.47
1	1	875	OMU	C2-N3	-2.67	1.33	1.38
1	1	908	OMU	C2-N3	-2.66	1.33	1.38
1	1	2017	OMG	C6-N1	-2.65	1.33	1.37
1	1	2056	5MC	C6-N1	-2.58	1.33	1.38
1	1	2707	OMU	C5-C4	-2.44	1.38	1.43
1	1	908	OMU	C5-C4	-2.41	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2628	OMU	C5-C4	-2.40	1.38	1.43
1	1	875	OMU	C5-C4	-2.38	1.38	1.43
1	1	2077	OMU	C5-C4	-2.37	1.38	1.43
1	1	2088	OMU	C5-C4	-2.36	1.38	1.43
1	1	2574	OMU	C5-C4	-2.36	1.38	1.43
1	1	2056	5MC	C6-C5	2.34	1.38	1.34
1	1	2623	OMU	C5-C4	-2.34	1.38	1.43
1	1	2851	OMU	C5-C4	-2.31	1.38	1.43
1	1	2408	OMU	C5-C4	-2.28	1.38	1.43
1	1	2155	OMU	C5-C4	-2.28	1.38	1.43
1	1	2666	OMU	C5-C4	-2.22	1.38	1.43
1	1	2608	OMG	C8-N7	-2.17	1.31	1.34
1	1	2698	UR3	C5-C4	-2.16	1.38	1.43
1	1	38	5MC	C6-C5	2.14	1.38	1.34
1	1	908	OMU	C2-N1	2.13	1.41	1.38
1	1	1976	OMC	C6-N1	-2.12	1.33	1.38
1	1	3023	G7M	C5-C6	-2.11	1.40	1.45
1	1	2018	OMC	C6-N1	-2.06	1.33	1.38
1	1	2608	OMG	C5-C4	-2.04	1.38	1.43
1	1	493	OMC	C6-N1	-2.04	1.33	1.38
1	1	2704	OMC	C6-N1	-2.03	1.33	1.38
1	1	2408	OMU	C6-N1	-2.03	1.33	1.38
1	1	2623	OMU	C6-N1	-2.02	1.33	1.38
1	1	2707	OMU	C6-N1	-2.02	1.33	1.38
1	1	492	OMC	C6-N1	-2.01	1.33	1.38

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2698	UR3	C4-N3-C2	-6.86	119.06	124.58
1	1	2666	OMU	C4-N3-C2	-5.44	119.85	126.61
1	1	2155	OMU	C4-N3-C2	-5.41	119.90	126.61
1	1	2408	OMU	C4-N3-C2	-5.18	120.18	126.61
1	1	2623	OMU	C4-N3-C2	-5.17	120.19	126.61
1	1	2707	OMU	C4-N3-C2	-4.95	120.47	126.61
1	1	875	OMU	C4-N3-C2	-4.91	120.52	126.61
1	1	2077	OMU	C4-N3-C2	-4.84	120.60	126.61
1	1	2851	OMU	C4-N3-C2	-4.83	120.61	126.61
1	1	908	OMU	C1'-N1-C2	4.83	126.27	117.59
1	1	2628	OMU	C4-N3-C2	-4.83	120.62	126.61
1	1	2574	OMU	C4-N3-C2	-4.80	120.65	126.61
1	1	2088	OMU	C4-N3-C2	-4.72	120.75	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2155	OMU	N3-C2-N1	4.70	121.01	114.89
1	1	2628	OMU	N3-C2-N1	4.65	120.94	114.89
1	1	2666	OMU	N3-C2-N1	4.61	120.89	114.89
1	1	2623	OMU	N3-C2-N1	4.52	120.77	114.89
1	1	2408	OMU	N3-C2-N1	4.46	120.70	114.89
1	1	2666	OMU	C5-C4-N3	4.35	120.90	114.80
1	1	2574	OMU	N3-C2-N1	4.35	120.55	114.89
1	1	875	OMU	N3-C2-N1	4.35	120.55	114.89
1	1	2707	OMU	N3-C2-N1	4.34	120.55	114.89
1	1	2155	OMU	C5-C4-N3	4.29	120.80	114.80
1	1	2088	OMU	N3-C2-N1	4.26	120.44	114.89
1	1	2077	OMU	N3-C2-N1	4.25	120.42	114.89
1	1	908	OMU	C4-N3-C2	-4.23	121.37	126.61
1	1	2623	OMU	C5-C4-N3	4.20	120.69	114.80
1	1	2851	OMU	C5-C4-N3	4.12	120.57	114.80
1	1	2077	OMU	C5-C4-N3	4.11	120.55	114.80
1	1	2408	OMU	C5-C4-N3	4.09	120.53	114.80
1	1	2707	OMU	C5-C4-N3	4.09	120.53	114.80
1	1	2088	OMU	C5-C4-N3	4.08	120.51	114.80
1	1	2574	OMU	C5-C4-N3	4.07	120.50	114.80
1	1	875	OMU	C5-C4-N3	4.03	120.45	114.80
1	1	908	OMU	N3-C2-N1	3.98	120.08	114.89
1	1	2851	OMU	N3-C2-N1	3.98	120.08	114.89
1	1	2628	OMU	C5-C4-N3	3.97	120.36	114.80
1	1	908	OMU	C5-C4-N3	3.86	120.21	114.80
1	1	38	5MC	C5-C6-N1	-3.52	119.49	123.31
1	1	2698	UR3	C5-C4-N3	3.47	119.61	115.04
1	1	2623	OMU	O4-C4-C5	-3.27	119.53	125.16
1	1	875	OMU	O4-C4-C5	-3.23	119.60	125.16
1	1	2056	5MC	C5-C6-N1	-3.22	119.81	123.31
1	1	2666	OMU	O4-C4-C5	-3.14	119.75	125.16
1	1	38	5MC	C5-C4-N3	-3.12	118.56	121.75
1	1	2103	OMG	C8-N7-C5	3.09	107.81	102.55
1	1	2388	OMG	C8-N7-C5	3.09	107.81	102.55
1	1	902	OMG	C8-N7-C5	3.07	107.78	102.55
1	1	2851	OMU	O4-C4-C5	-3.07	119.88	125.16
1	1	2077	OMU	O4-C4-C5	-3.05	119.89	125.16
1	1	2408	OMU	O4-C4-C5	-3.05	119.90	125.16
1	1	2104	OMG	C8-N7-C5	3.02	107.69	102.55
1	1	2362	OMG	C8-N7-C5	3.02	107.69	102.55
1	1	2155	OMU	O4-C4-C5	-2.99	120.00	125.16
1	1	2537	OMG	C8-N7-C5	2.99	107.64	102.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	908	OMU	O4-C4-C5	-2.99	120.01	125.16
1	1	1949	OMG	C8-N7-C5	2.98	107.62	102.55
1	1	2707	OMU	O4-C4-C5	-2.97	120.04	125.16
1	1	2088	OMU	O4-C4-C5	-2.95	120.07	125.16
1	1	2366	OMG	C8-N7-C5	2.89	107.47	102.55
1	1	875	OMU	O2-C2-N1	-2.86	119.08	122.80
1	1	1957	OMG	C8-N7-C5	2.85	107.40	102.55
1	1	2017	OMG	C8-N7-C5	2.85	107.40	102.55
1	1	2628	OMU	O4-C4-C5	-2.84	120.26	125.16
1	1	2667	OMG	C8-N7-C5	2.84	107.38	102.55
1	1	2056	5MC	C5-C4-N3	-2.83	118.85	121.75
1	1	1976	OMC	O2-C2-N3	-2.83	117.87	122.33
1	1	1947	OMG	C8-N7-C5	2.82	107.36	102.55
1	1	2574	OMU	O4-C4-C5	-2.76	120.40	125.16
1	1	2071	OMG	C8-N7-C5	2.74	107.22	102.55
1	1	1971	OMG	C8-N7-C5	2.74	107.22	102.55
1	1	2666	OMU	O2-C2-N1	-2.72	119.25	122.80
1	1	2601	OMG	C8-N7-C5	2.72	107.18	102.55
1	1	2066	OMG	C8-N7-C5	2.69	107.13	102.55
1	1	38	5MC	O2-C2-N3	-2.68	118.10	122.33
1	1	2176	OMG	C8-N7-C5	2.68	107.11	102.55
1	1	2155	OMU	O2'-C2'-C1'	2.67	114.05	108.99
1	1	908	OMU	C1'-N1-C6	-2.62	115.18	120.78
1	1	2408	OMU	O2-C2-N1	-2.56	119.47	122.80
1	1	902	OMG	C5-C6-N1	2.44	118.73	114.07
1	1	2388	OMG	C5-C6-N1	2.42	118.69	114.07
1	1	2610	PSU	C3'-C2'-C1'	2.42	104.54	101.69
1	1	2691	A2M	C5-C6-N6	2.40	123.97	120.31
1	1	2555	OMC	O2-C2-N3	-2.37	118.59	122.33
1	1	2628	OMU	C1'-N1-C2	2.36	121.83	117.59
1	1	2088	OMU	C1'-N1-C2	2.34	121.79	117.59
1	1	2176	OMG	C5-C6-N1	2.32	118.49	114.07
1	1	2056	5MC	O2-C2-N3	-2.31	118.68	122.33
1	1	2698	UR3	C3U-N3-C4	2.31	121.07	117.87
1	1	2362	OMG	C5-C6-N1	2.29	118.44	114.07
1	1	1949	OMG	C5-C6-N1	2.29	118.44	114.07
1	1	492	OMC	O2-C2-N3	-2.23	118.81	122.33
1	1	1990	A2M	C5-C6-N6	2.21	123.69	120.31
1	1	2011	A2M	C5-C6-N6	2.21	123.67	120.31
1	1	2366	OMG	C5-C6-N1	2.18	118.22	114.07
1	1	1947	OMG	C5-C6-N1	2.17	118.22	114.07
1	1	2601	OMG	C5-C6-N1	2.17	118.21	114.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	2537	OMG	C5-C6-N1	2.16	118.19	114.07
1	1	2707	OMU	O2-C2-N1	-2.15	119.99	122.80
1	1	908	OMU	O2-C2-N3	-2.13	117.56	121.49
1	1	2066	OMG	C5-C6-N1	2.12	118.12	114.07
1	1	2071	OMG	C5-C6-N1	2.12	118.12	114.07
1	1	2720	OMC	O2-C2-N3	-2.11	119.00	122.33
1	1	2667	OMG	C5-C6-N1	2.11	118.10	114.07
1	1	2104	OMG	C5-C6-N1	2.11	118.09	114.07
1	1	2059	A2M	C5-C6-N6	2.09	123.50	120.31
1	1	2017	OMG	C5-C6-N1	2.09	118.06	114.07
1	1	2601	OMG	O6-C6-C5	-2.08	120.19	124.32
1	1	1957	OMG	C5-C6-N1	2.08	118.03	114.07
1	1	2176	OMG	O6-C6-C5	-2.07	120.21	124.32
1	1	2103	OMG	C5-C6-N1	2.04	117.96	114.07
1	1	2017	OMG	O6-C6-C5	-2.04	120.28	124.32
1	1	2885	OMC	O2-C2-N3	-2.04	119.12	122.33
1	1	908	OMU	C6-N1-C2	-2.03	118.53	121.00
1	1	2698	UR3	C6-N1-C2	-2.03	120.14	121.80
1	1	1971	OMG	C5-C6-N1	2.01	117.90	114.07
1	1	2608	OMG	O6-C6-C5	2.00	128.29	124.32

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1947	OMG	O4'-C4'-C5'-O5'
1	1	1990	A2M	C1'-C2'-O2'-CM'
1	1	2155	OMU	C1'-C2'-O2'-CM2
1	1	2608	OMG	O4'-C4'-C5'-O5'
1	1	1947	OMG	C3'-C4'-C5'-O5'
1	1	2143	OMC	C3'-C4'-C5'-O5'
1	1	2143	OMC	O4'-C4'-C5'-O5'
1	1	2937	B8T	C3'-C4'-C5'-O5'
1	1	38	5MC	C4'-C5'-O5'-P
1	1	2608	OMG	C3'-C4'-C5'-O5'
1	1	2937	B8T	O4'-C4'-C5'-O5'
1	1	2388	OMG	C4'-C5'-O5'-P
1	1	2555	OMC	C4'-C5'-O5'-P
1	1	2851	OMU	C3'-C4'-C5'-O5'
1	1	908	OMU	C2'-C1'-N1-C6
1	1	2155	OMU	C2'-C1'-N1-C6
1	1	908	OMU	C2'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
1	1	2537	OMG	O4'-C4'-C5'-O5'
1	1	908	OMU	O4'-C1'-N1-C6
1	1	908	OMU	O4'-C1'-N1-C2
1	1	2059	A2M	O4'-C4'-C5'-O5'
1	1	908	OMU	C3'-C2'-O2'-CM2
1	1	2155	OMU	O4'-C1'-N1-C6
1	1	2601	OMG	C3'-C4'-C5'-O5'
1	1	1971	OMG	C3'-C2'-O2'-CM2

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 224 ligands modelled in this entry, 178 are monoatomic - leaving 46 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	$\#\|Z\| > 2$
40	SPM	1	3120	-	13,13,13	0.17	0	12,12,12	0.23	0
40	SPM	1	3110	-	13,13,13	0.14	0	12,12,12	0.16	0
40	SPM	1	3138	-	13,13,13	0.16	0	12,12,12	0.18	0
40	SPM	AL	201	-	13,13,13	0.16	0	12,12,12	0.20	0
40	SPM	1	3143	-	13,13,13	0.19	0	12,12,12	0.44	0
40	SPM	1	3127	-	13,13,13	0.16	0	12,12,12	0.22	0
40	SPM	1	3102	-	13,13,13	0.17	0	12,12,12	0.43	0
40	SPM	1	3131	-	13,13,13	0.15	0	12,12,12	0.25	0
40	SPM	1	3137	-	13,13,13	0.17	0	12,12,12	0.27	0
40	SPM	1	3144	-	13,13,13	0.19	0	12,12,12	0.24	0
40	SPM	AM	201	-	13,13,13	0.18	0	12,12,12	0.28	0
40	SPM	1	3116	-	13,13,13	0.21	0	12,12,12	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	SPM	1	3124	-	13,13,13	0.16	0	12,12,12	0.34	0
40	SPM	1	3133	-	13,13,13	0.16	0	12,12,12	0.29	0
40	SPM	1	3142	-	13,13,13	0.17	0	12,12,12	0.37	0
40	SPM	1	3111	-	13,13,13	0.14	0	12,12,12	0.19	0
40	SPM	1	3109	-	13,13,13	0.17	0	12,12,12	0.26	0
40	SPM	1	3134	-	13,13,13	0.17	0	12,12,12	0.29	0
40	SPM	1	3139	-	13,13,13	0.18	0	12,12,12	0.14	0
40	SPM	1	3119	-	13,13,13	0.20	0	12,12,12	0.21	0
40	SPM	1	3135	-	13,13,13	0.15	0	12,12,12	0.33	0
40	SPM	1	3105	-	13,13,13	0.17	0	12,12,12	0.18	0
40	SPM	1	3104	-	13,13,13	0.16	0	12,12,12	0.40	0
40	SPM	1	3114	-	13,13,13	0.20	0	12,12,12	0.31	0
40	SPM	1	3122	-	13,13,13	0.17	0	12,12,12	0.20	0
40	SPM	1	3129	-	13,13,13	0.18	0	12,12,12	0.31	0
40	SPM	1	3125	-	13,13,13	0.14	0	12,12,12	0.28	0
40	SPM	1	3123	-	13,13,13	0.18	0	12,12,12	0.33	0
40	SPM	1	3113	-	13,13,13	0.16	0	12,12,12	0.21	0
40	SPM	1	3121	-	13,13,13	0.24	0	12,12,12	0.24	0
40	SPM	1	3108	-	13,13,13	0.18	0	12,12,12	0.35	0
40	SPM	1	3106	-	13,13,13	0.20	0	12,12,12	0.24	0
40	SPM	1	3112	-	13,13,13	0.19	0	12,12,12	0.40	0
40	SPM	1	3132	-	13,13,13	0.17	0	12,12,12	0.19	0
40	SPM	1	3115	-	13,13,13	0.18	0	12,12,12	0.26	0
40	SPM	1	3126	-	13,13,13	0.14	0	12,12,12	0.42	0
40	SPM	1	3117	-	13,13,13	0.20	0	12,12,12	0.32	0
40	SPM	1	3140	-	13,13,13	0.15	0	12,12,12	0.26	0
40	SPM	1	3103	-	13,13,13	0.16	0	12,12,12	0.34	0
40	SPM	1	3130	-	13,13,13	0.15	0	12,12,12	0.22	0
40	SPM	1	3136	-	13,13,13	0.18	0	12,12,12	0.37	0
40	SPM	1	3118	-	13,13,13	0.16	0	12,12,12	0.26	0
40	SPM	1	3141	-	13,13,13	0.16	0	12,12,12	0.17	0
40	SPM	1	3107	-	13,13,13	0.16	0	12,12,12	0.18	0
40	SPM	1	3128	-	13,13,13	0.19	0	12,12,12	0.32	0
40	SPM	1	3101	-	13,13,13	0.18	0	12,12,12	0.27	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
40	SPM	1	3120	-	-	1/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	SPM	1	3110	-	-	4/11/11/11	-
40	SPM	1	3138	-	-	8/11/11/11	-
40	SPM	AL	201	-	-	3/11/11/11	-
40	SPM	1	3143	-	-	4/11/11/11	-
40	SPM	1	3127	-	-	0/11/11/11	-
40	SPM	1	3102	-	-	1/11/11/11	-
40	SPM	1	3131	-	-	1/11/11/11	-
40	SPM	1	3137	-	-	2/11/11/11	-
40	SPM	1	3144	-	-	2/11/11/11	-
40	SPM	AM	201	-	-	0/11/11/11	-
40	SPM	1	3116	-	-	3/11/11/11	-
40	SPM	1	3124	-	-	0/11/11/11	-
40	SPM	1	3133	-	-	2/11/11/11	-
40	SPM	1	3142	-	-	1/11/11/11	-
40	SPM	1	3111	-	-	8/11/11/11	-
40	SPM	1	3109	-	-	1/11/11/11	-
40	SPM	1	3134	-	-	1/11/11/11	-
40	SPM	1	3139	-	-	2/11/11/11	-
40	SPM	1	3119	-	-	2/11/11/11	-
40	SPM	1	3135	-	-	1/11/11/11	-
40	SPM	1	3105	-	-	1/11/11/11	-
40	SPM	1	3104	-	-	2/11/11/11	-
40	SPM	1	3114	-	-	3/11/11/11	-
40	SPM	1	3122	-	-	9/11/11/11	-
40	SPM	1	3129	-	-	2/11/11/11	-
40	SPM	1	3125	-	-	1/11/11/11	-
40	SPM	1	3123	-	-	3/11/11/11	-
40	SPM	1	3113	-	-	9/11/11/11	-
40	SPM	1	3121	-	-	1/11/11/11	-
40	SPM	1	3108	-	-	4/11/11/11	-
40	SPM	1	3106	-	-	7/11/11/11	-
40	SPM	1	3112	-	-	1/11/11/11	-
40	SPM	1	3132	-	-	9/11/11/11	-
40	SPM	1	3115	-	-	1/11/11/11	-
40	SPM	1	3126	-	-	1/11/11/11	-
40	SPM	1	3117	-	-	1/11/11/11	-
40	SPM	1	3140	-	-	1/11/11/11	-
40	SPM	1	3103	-	-	0/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	SPM	1	3130	-	-	0/11/11/11	-
40	SPM	1	3136	-	-	0/11/11/11	-
40	SPM	1	3118	-	-	0/11/11/11	-
40	SPM	1	3141	-	-	7/11/11/11	-
40	SPM	1	3107	-	-	3/11/11/11	-
40	SPM	1	3128	-	-	1/11/11/11	-
40	SPM	1	3101	-	-	4/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	1	3106	SPM	C12-C11-N10-C9
40	1	3113	SPM	C12-C11-N10-C9
40	1	3122	SPM	C12-C11-N10-C9
40	1	3138	SPM	C3-C4-N5-C6
40	1	3134	SPM	N5-C6-C7-C8
40	1	3122	SPM	N10-C11-C12-C13
40	1	3132	SPM	C7-C8-C9-N10
40	1	3106	SPM	C7-C8-C9-N10
40	1	3122	SPM	C7-C8-C9-N10
40	1	3141	SPM	N5-C6-C7-C8
40	1	3106	SPM	C2-C3-C4-N5
40	1	3106	SPM	N10-C11-C12-C13
40	1	3113	SPM	C2-C3-C4-N5
40	1	3101	SPM	C7-C8-C9-N10
40	1	3102	SPM	C3-C4-N5-C6
40	1	3110	SPM	C2-C3-C4-N5
40	1	3113	SPM	N10-C11-C12-C13
40	1	3141	SPM	C2-C3-C4-N5
40	1	3138	SPM	C7-C8-C9-N10
40	1	3106	SPM	C8-C9-N10-C11
40	1	3122	SPM	C8-C9-N10-C11
40	1	3132	SPM	C3-C4-N5-C6
40	1	3137	SPM	C7-C8-C9-N10
40	1	3113	SPM	C8-C9-N10-C11
40	1	3132	SPM	C7-C6-N5-C4
40	1	3138	SPM	C2-C3-C4-N5

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Mol	Chain	Res	Type	Atoms
40	1	3143	SPM	C2-C3-C4-N5
40	1	3142	SPM	N5-C6-C7-C8
40	1	3101	SPM	C12-C11-N10-C9
40	1	3119	SPM	C8-C9-N10-C11
40	1	3132	SPM	C11-C12-C13-N14
40	1	3138	SPM	C8-C9-N10-C11
40	1	3141	SPM	N1-C2-C3-C4
40	1	3132	SPM	C6-C7-C8-C9
40	1	3144	SPM	C6-C7-C8-C9
40	1	3132	SPM	C2-C3-C4-N5
40	1	3108	SPM	C7-C8-C9-N10
40	1	3117	SPM	C8-C9-N10-C11
40	1	3129	SPM	C8-C9-N10-C11
40	1	3114	SPM	C6-C7-C8-C9
40	1	3123	SPM	C6-C7-C8-C9
40	1	3111	SPM	N10-C11-C12-C13
40	1	3113	SPM	C6-C7-C8-C9
40	1	3101	SPM	C8-C9-N10-C11
40	1	3110	SPM	C3-C4-N5-C6
40	1	3113	SPM	C11-C12-C13-N14
40	1	3114	SPM	C11-C12-C13-N14
40	1	3138	SPM	C11-C12-C13-N14
40	1	3139	SPM	C8-C9-N10-C11
40	1	3141	SPM	C11-C12-C13-N14
40	1	3143	SPM	C3-C4-N5-C6
40	1	3111	SPM	C6-C7-C8-C9
40	1	3114	SPM	C2-C3-C4-N5
40	1	3132	SPM	N5-C6-C7-C8
40	1	3111	SPM	C3-C4-N5-C6
40	1	3113	SPM	C7-C6-N5-C4
40	1	3141	SPM	C7-C6-N5-C4
40	1	3128	SPM	C6-C7-C8-C9
40	1	3108	SPM	N5-C6-C7-C8
40	1	3133	SPM	C6-C7-C8-C9
40	1	3113	SPM	C3-C4-N5-C6
40	1	3105	SPM	C6-C7-C8-C9
40	1	3125	SPM	C6-C7-C8-C9
40	1	3116	SPM	N5-C6-C7-C8
40	1	3107	SPM	C6-C7-C8-C9
40	1	3138	SPM	C7-C6-N5-C4
40	1	3107	SPM	C2-C3-C4-N5
40	1	3112	SPM	C7-C8-C9-N10

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Mol	Chain	Res	Type	Atoms
40	1	3111	SPM	N1-C2-C3-C4
40	1	3122	SPM	N1-C2-C3-C4
40	1	3122	SPM	C11-C12-C13-N14
40	1	3132	SPM	N1-C2-C3-C4
40	1	3132	SPM	C8-C9-N10-C11
40	1	3138	SPM	N1-C2-C3-C4
40	1	3140	SPM	C3-C4-N5-C6
40	1	3143	SPM	C6-C7-C8-C9
40	1	3101	SPM	C7-C6-N5-C4
40	1	3104	SPM	C8-C9-N10-C11
40	1	3126	SPM	C7-C6-N5-C4
40	1	3113	SPM	C7-C8-C9-N10
40	1	3115	SPM	C12-C11-N10-C9
40	1	3123	SPM	C8-C9-N10-C11
40	1	3122	SPM	N5-C6-C7-C8
40	1	3110	SPM	N10-C11-C12-C13
40	1	3111	SPM	N5-C6-C7-C8
40	1	3121	SPM	C7-C6-N5-C4
40	1	3120	SPM	C7-C6-N5-C4
40	1	3129	SPM	C12-C11-N10-C9
40	1	3144	SPM	C7-C6-N5-C4
40	1	3133	SPM	N5-C6-C7-C8
40	1	3143	SPM	C7-C8-C9-N10
40	1	3111	SPM	C2-C3-C4-N5
40	1	3116	SPM	C12-C11-N10-C9
40	AL	201	SPM	C7-C6-N5-C4
40	1	3104	SPM	C2-C3-C4-N5
40	1	3111	SPM	C12-C11-N10-C9
40	1	3122	SPM	C3-C4-N5-C6
40	1	3141	SPM	C12-C11-N10-C9
40	1	3135	SPM	N10-C11-C12-C13
40	1	3108	SPM	C8-C9-N10-C11
40	1	3110	SPM	N5-C6-C7-C8
40	1	3139	SPM	C6-C7-C8-C9
40	1	3122	SPM	C6-C7-C8-C9
40	1	3138	SPM	C6-C7-C8-C9
40	1	3106	SPM	C7-C6-N5-C4
40	1	3111	SPM	C8-C9-N10-C11
40	1	3137	SPM	C12-C11-N10-C9
40	1	3141	SPM	C3-C4-N5-C6
40	1	3116	SPM	C6-C7-C8-C9
40	1	3108	SPM	C7-C6-N5-C4

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Mol	Chain	Res	Type	Atoms
40	1	3123	SPM	C3-C4-N5-C6
40	AL	201	SPM	C6-C7-C8-C9
40	1	3131	SPM	C6-C7-C8-C9
40	1	3109	SPM	C12-C11-N10-C9
40	1	3107	SPM	C7-C8-C9-N10
40	1	3106	SPM	C3-C4-N5-C6
40	1	3119	SPM	C7-C6-N5-C4
40	AL	201	SPM	C12-C11-N10-C9

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

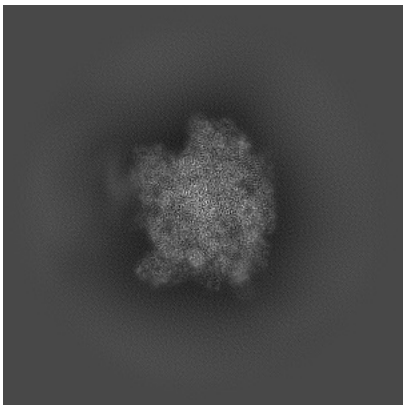
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-47578. These allow visual inspection of the internal detail of the map and identification of artifacts.

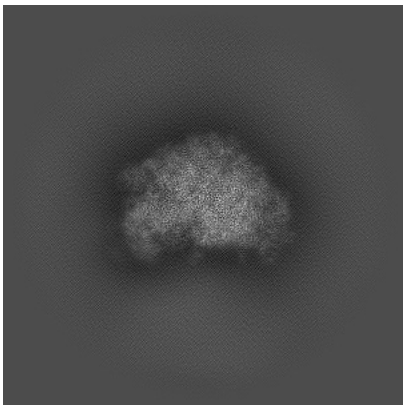
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

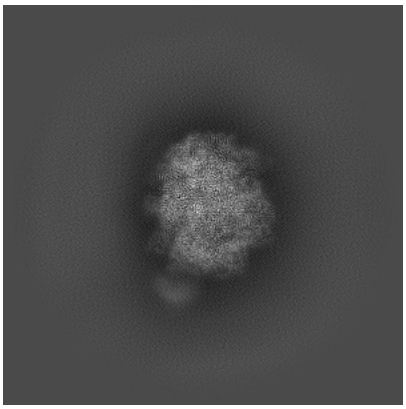
6.1.1 Primary map



X

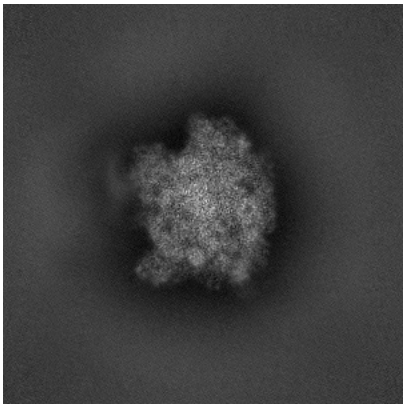


Y

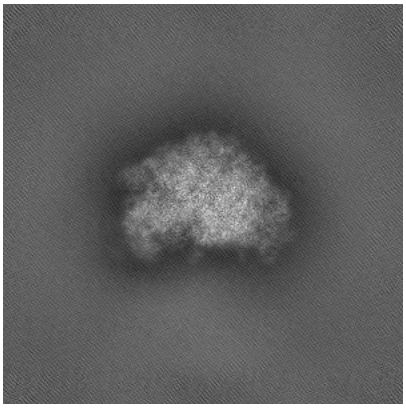


Z

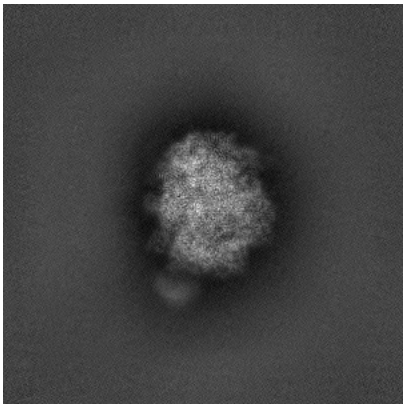
6.1.2 Raw map



X



Y

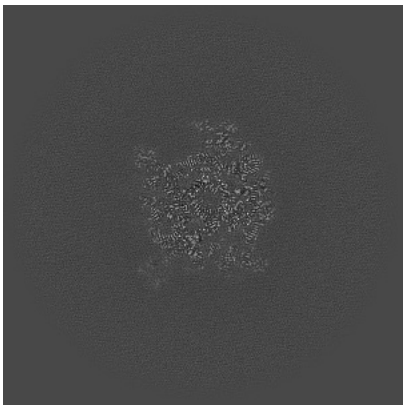


Z

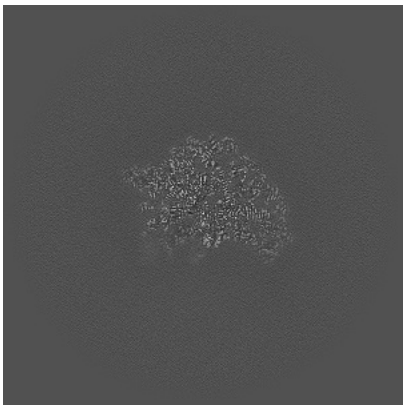
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

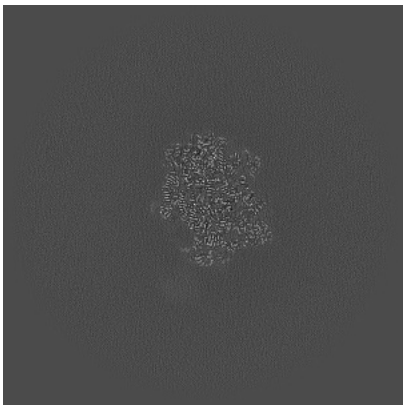
6.2.1 Primary map



X Index: 304

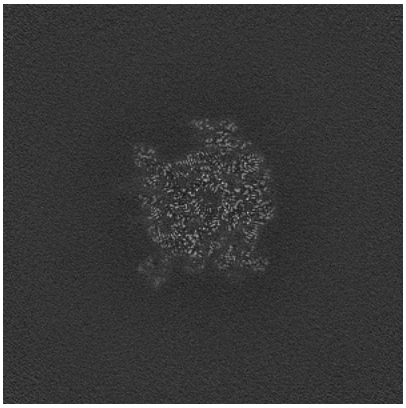


Y Index: 304

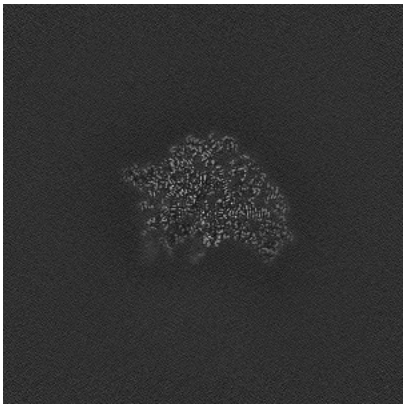


Z Index: 304

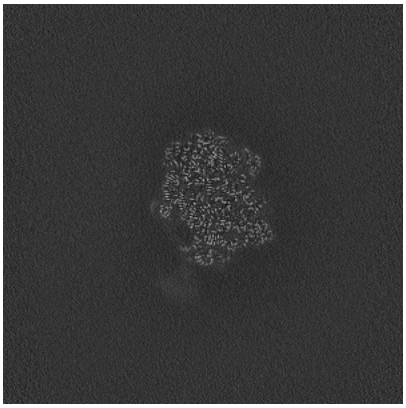
6.2.2 Raw map



X Index: 304



Y Index: 304

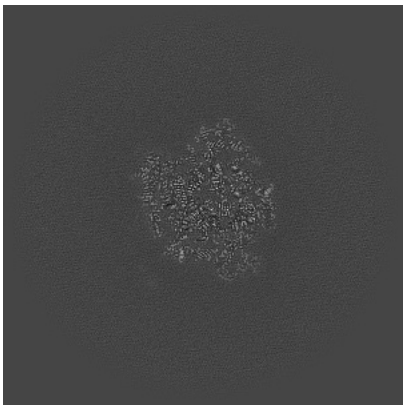


Z Index: 304

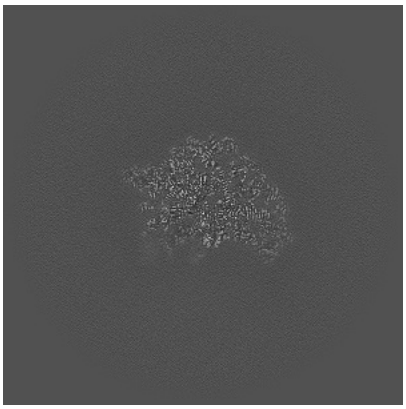
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

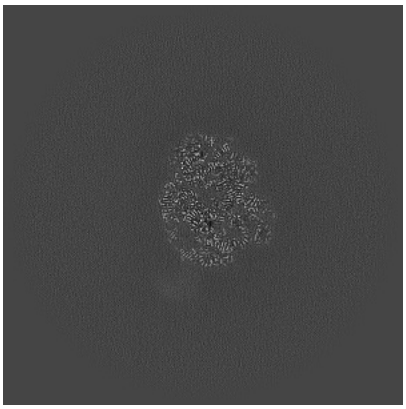
6.3.1 Primary map



X Index: 316

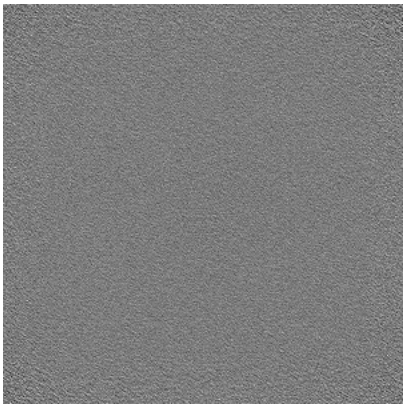


Y Index: 304

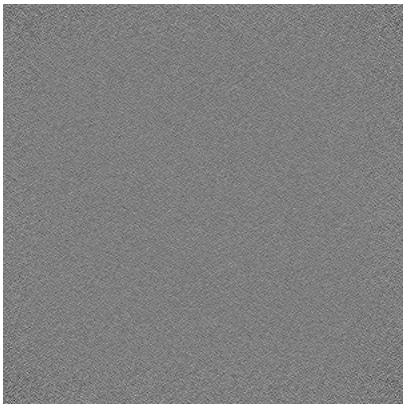


Z Index: 311

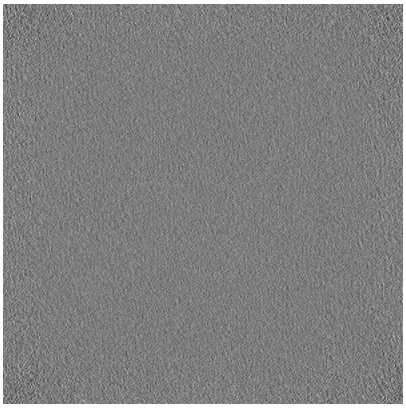
6.3.2 Raw map



X Index: 0



Y Index: 0

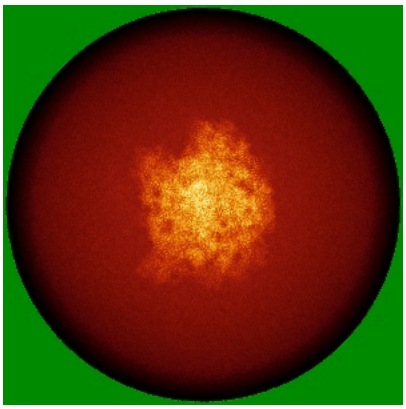


Z Index: 0

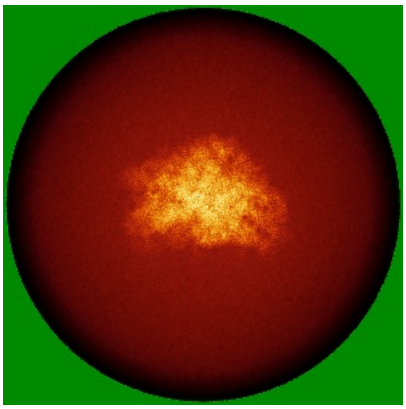
The images above show the largest variance slices of the map in three orthogonal directions.

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

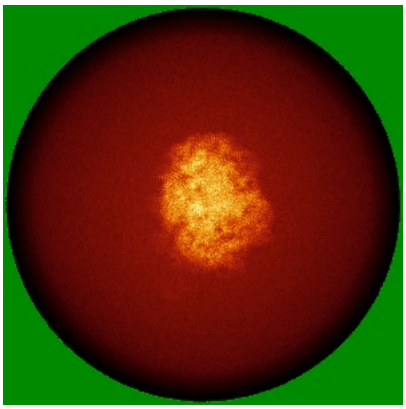
6.4.1 Primary map



X

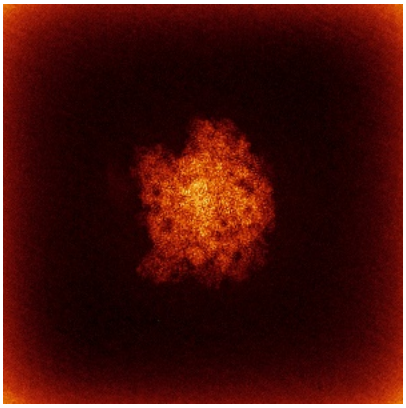


Y

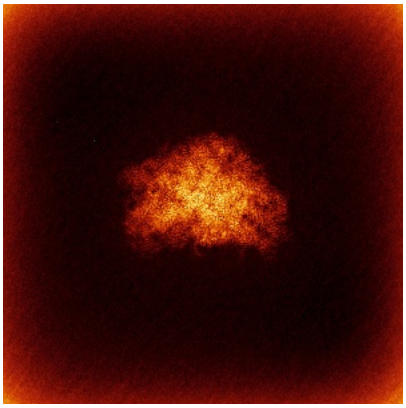


Z

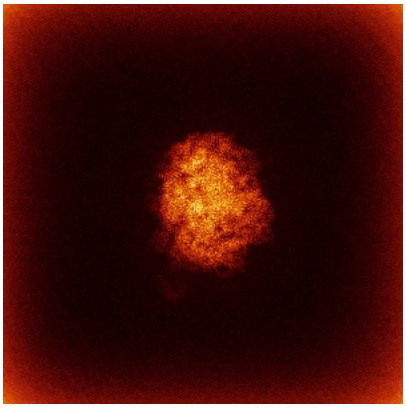
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.152. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X

Y

Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

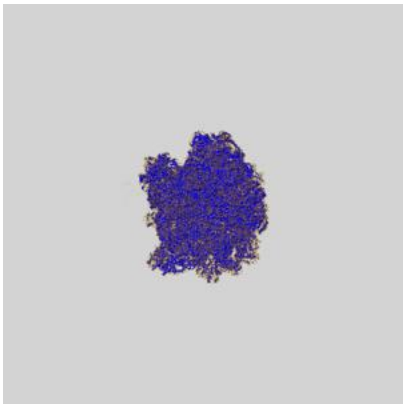
6.6 Mask visualisation (i)

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

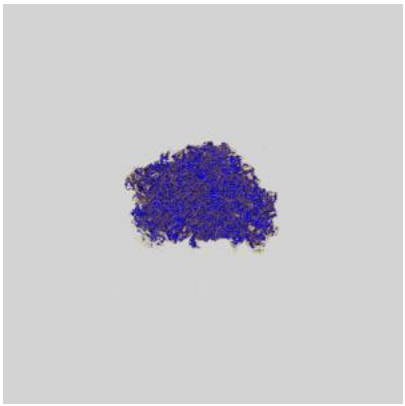
A mask typically either:

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

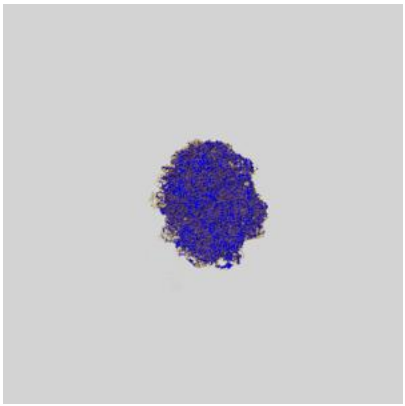
6.6.1 emd_47578_msk_1.map (i)



X



Y

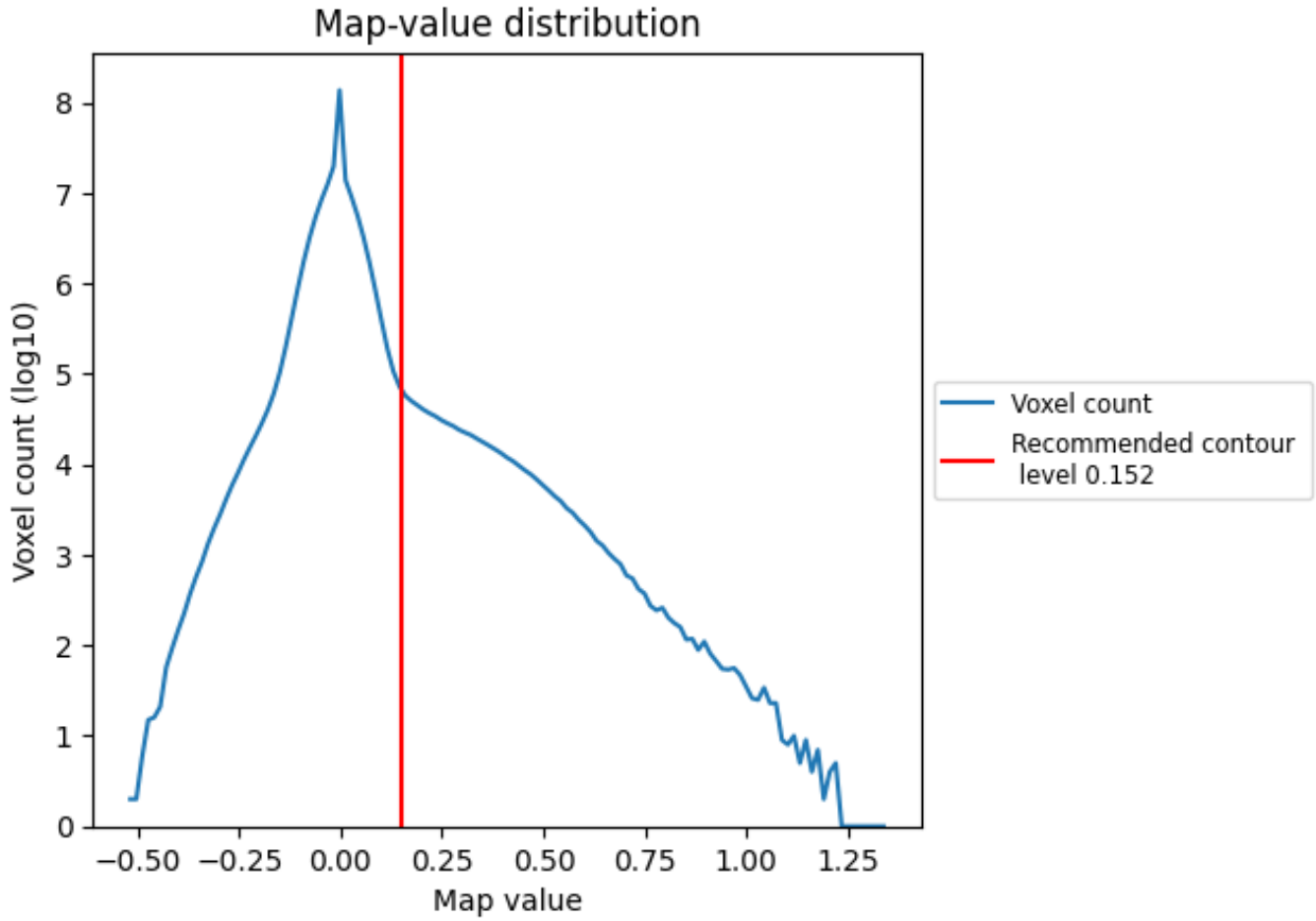


Z

7 Map analysis

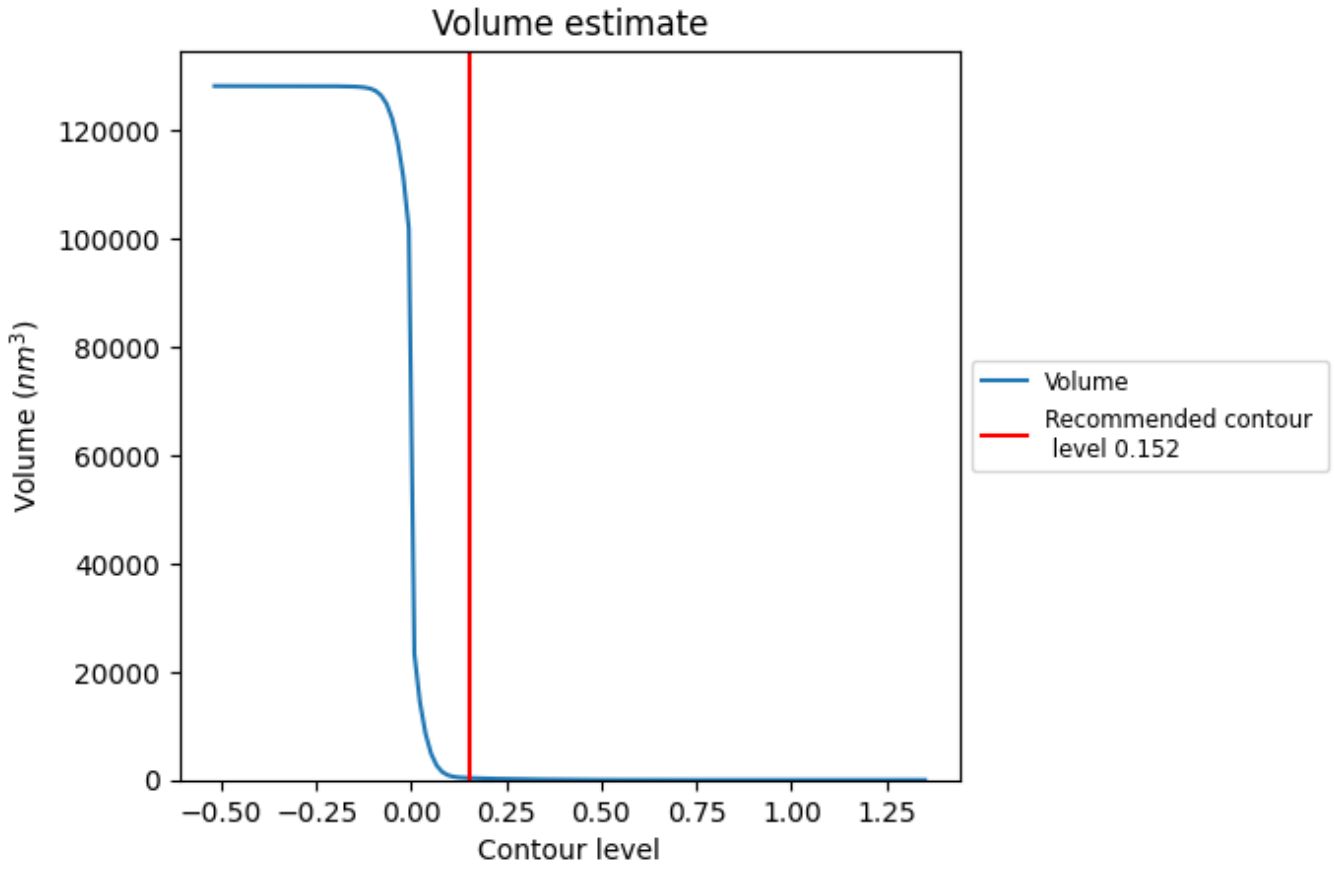
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

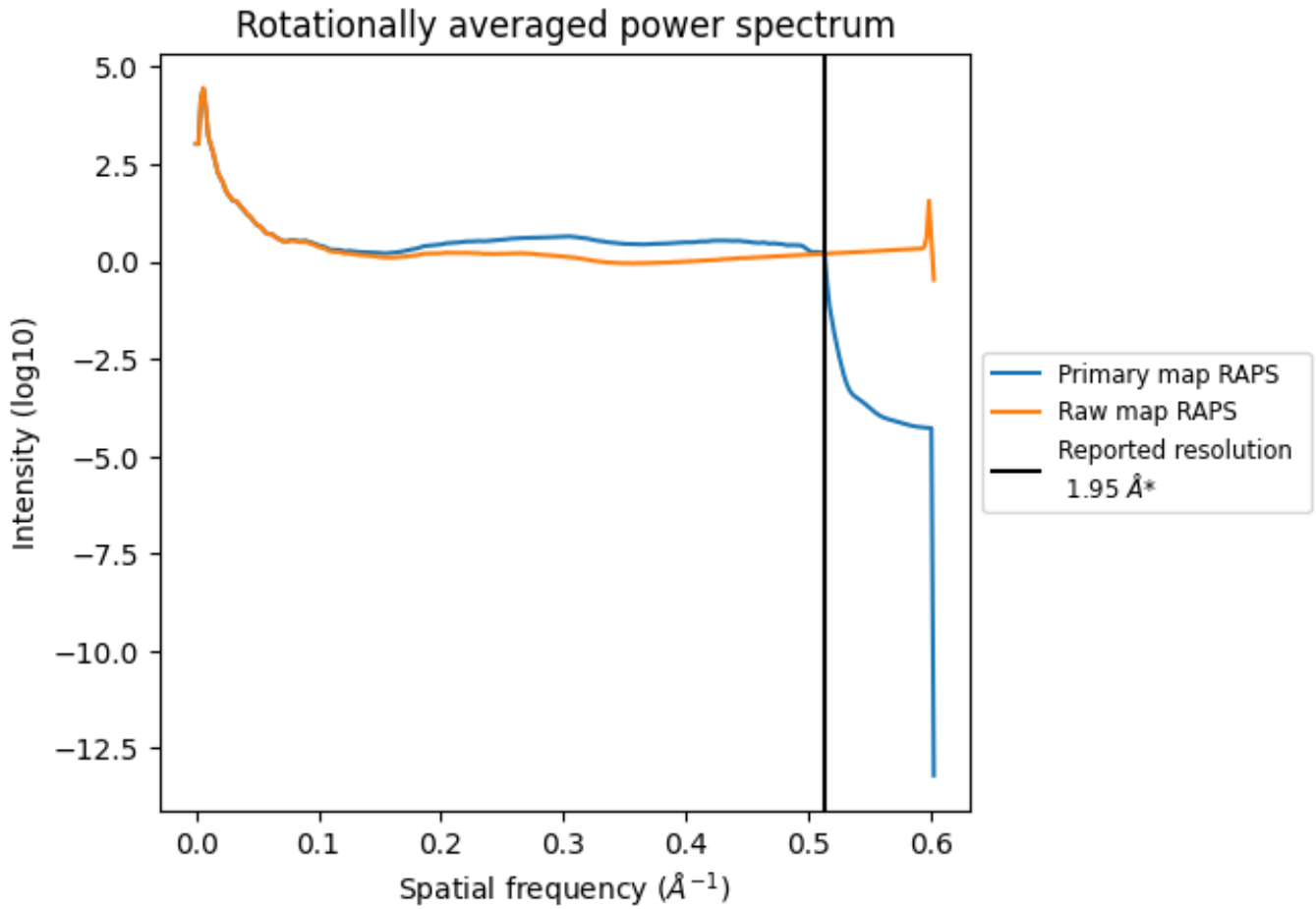
7.2 Volume estimate



The volume at the recommended contour level is 360 nm^3; this corresponds to an approximate mass of 325 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

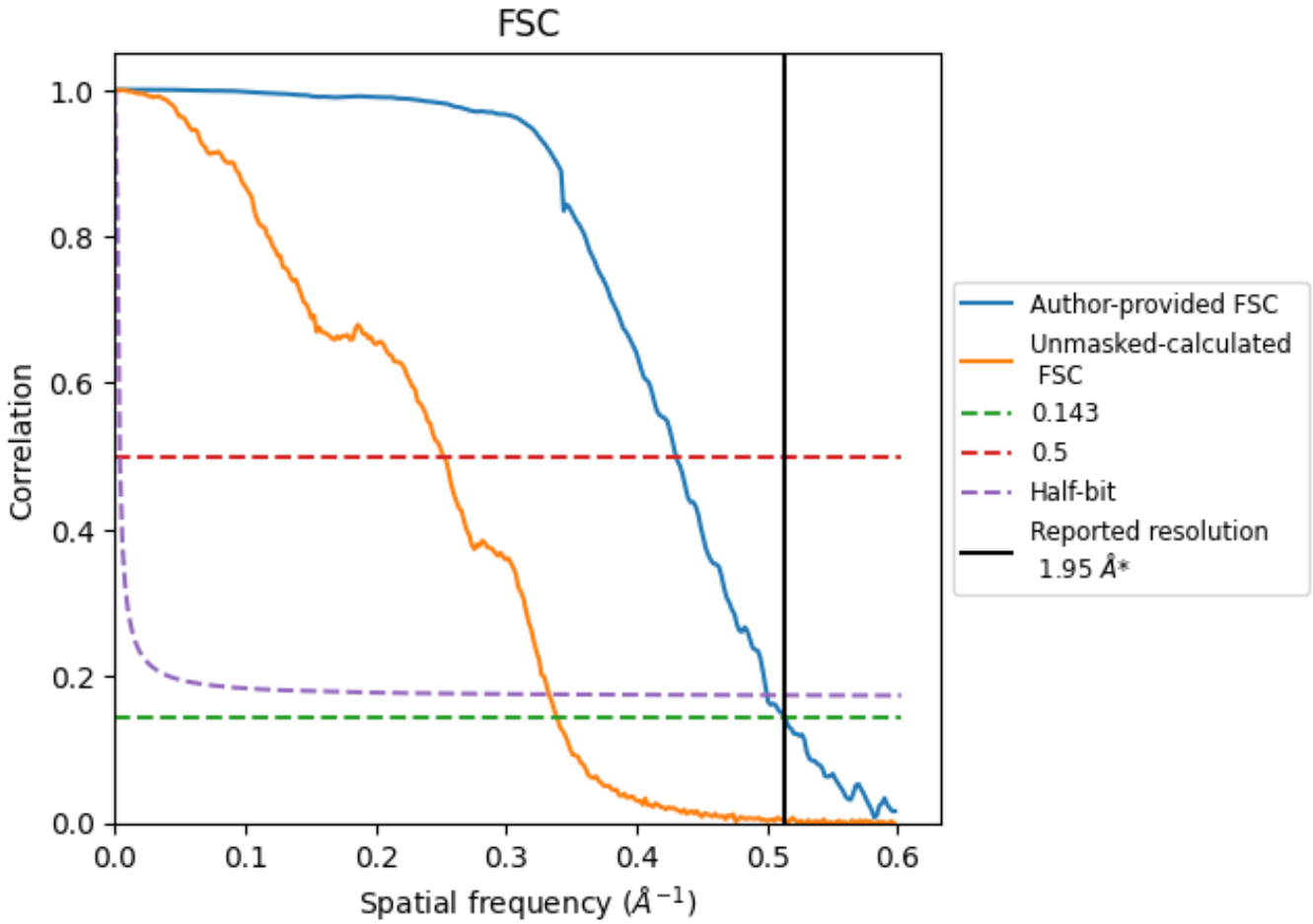


*Reported resolution corresponds to spatial frequency of 0.513 $Å^{-1}$

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 0.513 Å^{-1}

8.2 Resolution estimates (i)

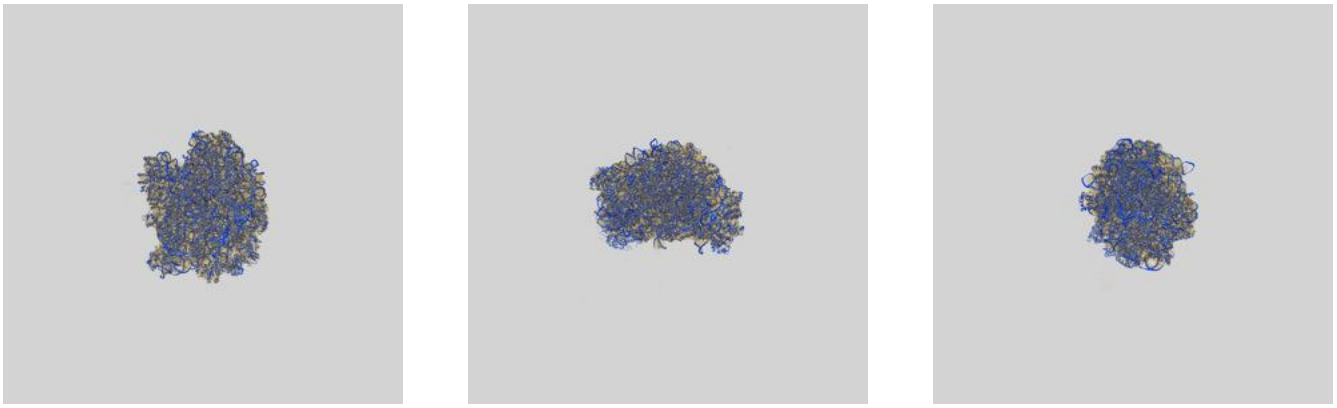
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.95	-	-
Author-provided FSC curve	1.95	2.32	2.00
Unmasked-calculated*	2.95	3.97	3.00

*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 2.95 differs from the reported value 1.95 by more than 10 %

9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-47578 and PDB model 9E6Q. Per-residue inclusion information can be found in section 3 on page 17.

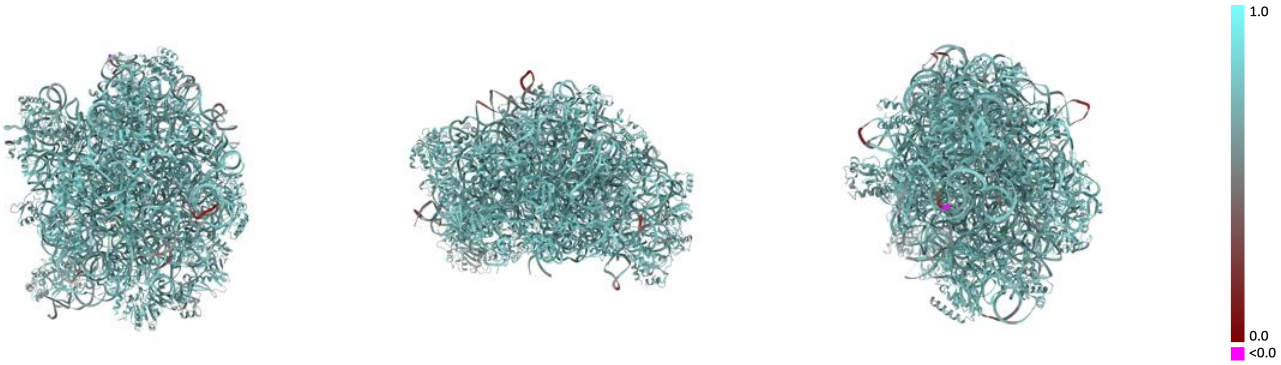
9.1 Map-model overlay



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.152 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

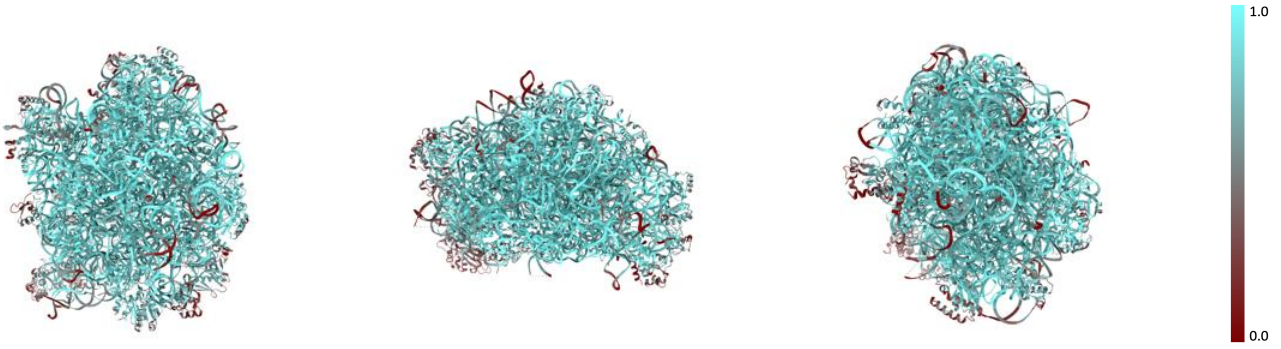
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

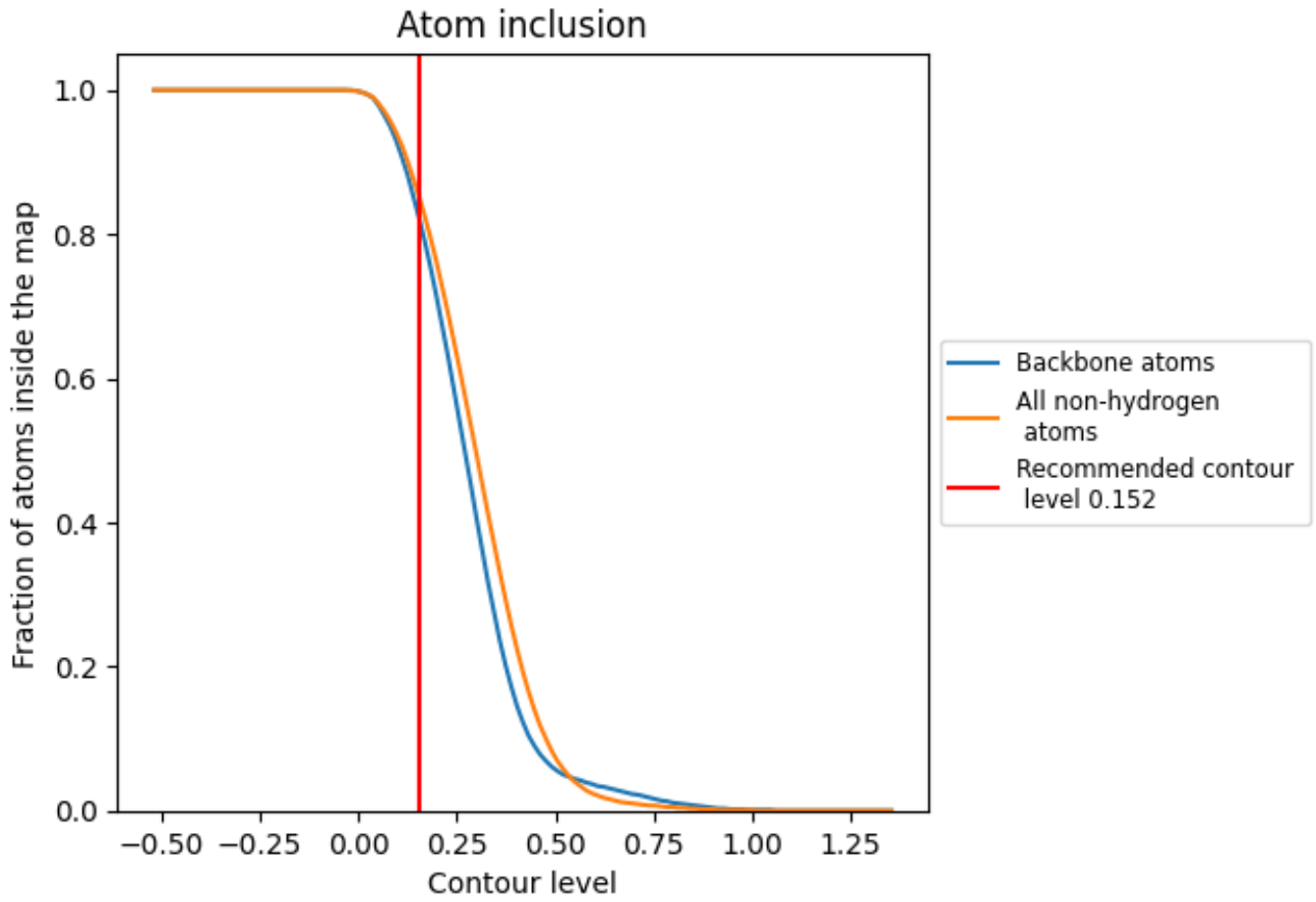
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.152).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 86% 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 (0.152) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8560	0.7260
1	0.9130	0.7290
2	0.7540	0.6710
3	0.7710	0.7220
AA	0.9030	0.7590
AB	0.8970	0.7600
AC	0.8650	0.7470
AD	0.2720	0.5760
AE	0.6660	0.6980
AF	0.6050	0.6730
AG	0.8300	0.7460
AH	0.8600	0.7470
AI	0.8620	0.7510
AJ	0.5470	0.6460
AK	0.6000	0.6720
AL	0.7260	0.7070
AM	0.8720	0.7510
AN	0.8770	0.7540
AO	0.5930	0.6730
AP	0.8620	0.7470
AQ	0.8160	0.7380
AR	0.6980	0.7080
AS	0.9020	0.7540
AT	0.8960	0.7620
AU	0.8540	0.7510
AV	0.8030	0.7280
AW	0.8430	0.7430
AX	0.7160	0.7100
AY	0.8510	0.7400
AZ	0.5860	0.6720
Aa	0.8210	0.7410
Ab	0.8490	0.7490
Ac	0.9060	0.7420
Ad	0.9830	0.7900
Ae	0.7940	0.7310

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Chain	Atom inclusion	Q-score
Af	0.9240	0.7650
Ag	0.6930	0.6920
Ah	0.8760	0.7430
Ai	0.7120	0.7150
Aj	0.7260	0.7120
Ak	0.7250	0.7020