wwPDB EM Validation Summary Report

Nov 2, 2026 – 03:15 PM JST

PDB ID	:	9XJH / pdb_00009xjh
EMDB ID	:	EMD-66936
Title	:	In situ 80S ribosome from intact HEK293T cells - consensus map of 60S region
Authors	:	Wang, Y.; Zhang, Y.; Gao, N.
Deposited on	:	2025-11-04
Resolution	:	1.97 Å(reported)

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

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

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

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

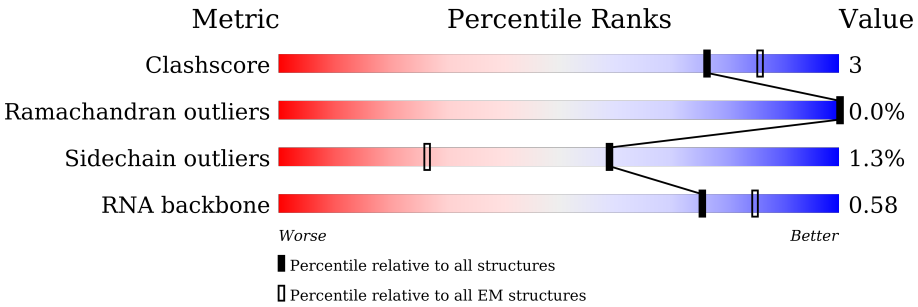
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

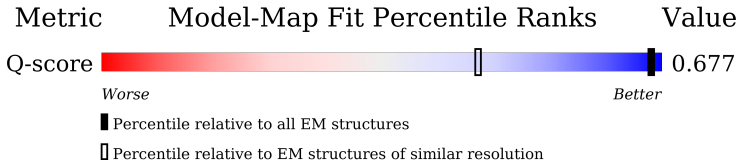
1 Overall quality at a glance

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

The reported resolution of this entry is 1.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	1339 (1.50 - 2.46)

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	A	29	7%, 52%, 34%, 10%, .
2	LA	251	99%, .
3	LB	402	., 93%, 7%

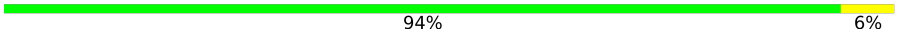
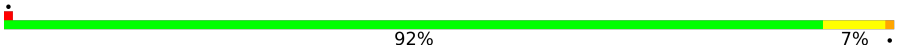
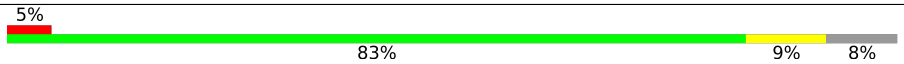
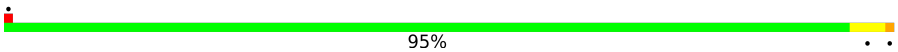
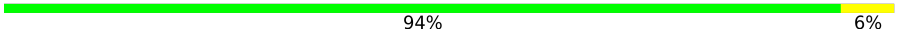
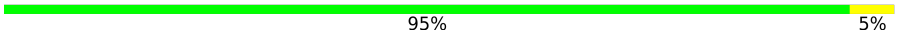
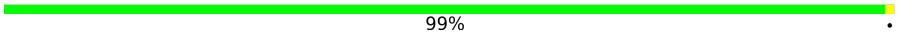
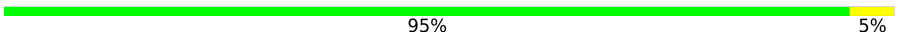
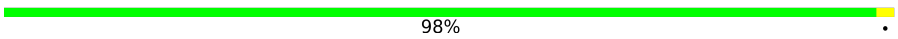
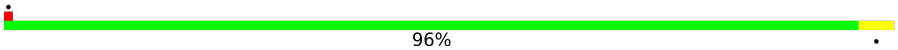
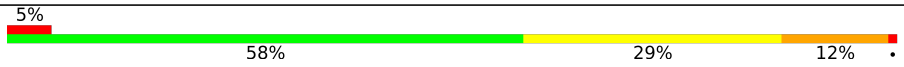
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Mol	Chain	Length	Quality of chain
4	L8	156	76% 22%
5	L5	5069	51% 16% 30%
6	L7	120	89% 9%
7	LC	366	95% 5%
8	LJ	170	88% 12%
9	LH	190	95% 5%
10	LE	288	73% 5% 23%
11	LG	241	94% 6%
12	LO	202	95% 5%
13	LL	206	92% 8%
14	LV	133	95% 5%
15	LM	136	92% 8%
16	La	147	96%
17	LN	203	97%
18	LD	294	91% 9%
19	LQ	187	97%
20	LR	187	6% 90% 10%
21	LS	176	96%
22	LT	159	94% 6%
23	LP	159	93% 7%
24	LU	100	76% 24%
25	LX	118	93% 7%
26	LY	134	96%
27	LW	124	6% 87% 7% 5%
28	LZ	135	90% 10%

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Mol	Chain	Length	Quality of chain
29	Lr	126	
30	Lh	122	
31	Lb	121	
32	LF	225	
33	Lc	99	
34	Ld	107	
35	Le	128	
36	Lf	110	
37	Lg	114	
38	Li	102	
39	Lj	86	
40	Lk	70	
41	Ll	50	
42	Lm	52	
43	Ln	25	
44	Lo	105	
45	Lp	91	
46	mR	3	
47	Pt	77	
48	CB	16	
49	LI	213	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
50	SPD	L5	5113	-	-	X	-

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 137834 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcription factor BTF3.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	29	Total	C	N	O	0	0
			230	142	52	36		

- Molecule 2 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	LA	251	Total	C	N	O	S	1	0
			1930	1209	396	319	6		

- Molecule 3 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	LB	402	Total	C	N	O	S	0	0
			3239	2061	608	556	14		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L8	156	Total	C	N	O	P	0	0
			3316	1482	585	1094	155		

- Molecule 5 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L5	3555	Total	C	N	O	P	1	0
			76304	34019	13953	24777	3555		

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 7 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LC	366	Total	C	N	O	S	0	0
			2914	1832	581	487	14		

- Molecule 8 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 9 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LE	223	Total	C	N	O	S	0	0
			1786	1150	339	293	4		

- Molecule 11 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LG	241	Total	C	N	O	S	0	0
			1926	1228	371	323	4		

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LO	202	Total	C	N	O	S	0	0
			1654	1066	322	261	5		

- Molecule 13 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LL	206	Total	C	N	O	S	1	0
			1672	1046	348	274	4		

- Molecule 14 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LV	133	Total	C	N	O	S	0	0
			988	623	186	174	5		

- Molecule 15 is a protein called Large ribosomal subunit protein eL14.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 17 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LN	203	Total	C	N	O	S	0	0
			1700	1072	359	265	4		

- Molecule 18 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LD	294	Total	C	N	O	S	0	0
			2391	1513	436	428	14		

- Molecule 19 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1512	944	314	249	5		

- Molecule 20 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	187	Total	C	N	O	S	0	0
			1566	971	336	250	9		

- Molecule 21 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	176	Total	C	N	O	S	0	0
			1460	930	284	235	11		

- Molecule 22 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LT	159	Total	C	N	O	S	2	0
			1311	833	256	216	6		

- Molecule 23 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LP	159	Total	C	N	O	S	1	0
			1296	813	251	223	9		

- Molecule 24 is a protein called Large ribosomal subunit protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LU	100	Total	C	N	O	S	0	0
			816	524	142	148	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LX	118	Total	C	N	O	S	0	0
			966	618	181	166	1		

- Molecule 26 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 27 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LW	118	Total	C	N	O	S	0	0
			950	595	192	159	4		

- Molecule 28 is a protein called Large ribosomal subunit protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LZ	135	Total	C	N	O	S	1	0
			1115	719	211	182	3		

- Molecule 29 is a protein called Large ribosomal subunit protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lr	126	Total	C	N	O	S	1	0
			1011	629	208	169	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Lr	1	ACE	-	acetylation	UNP P46779

- Molecule 30 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lh	122	Total	C	N	O	S	0	0
			1014	641	205	167	1		

- Molecule 31 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lb	111	Total	C	N	O	S	0	0
			898	560	195	139	4		

- Molecule 32 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LF	225	Total	C	N	O	S	2	0
			1885	1212	364	300	9		

- Molecule 33 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lc	99	Total	C	N	O	S	0	0
			770	488	136	140	6		

- Molecule 34 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 35 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 36 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lf	110	Total	C	N	O	S	0	0
			883	560	175	144	4		

- Molecule 37 is a protein called Large ribosomal subunit protein eL34.

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

- Molecule 38 is a protein called Large ribosomal subunit protein eL36.

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

- Molecule 39 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lj	86	Total	C	N	O	S	1	0
			712	439	157	111	5		

- Molecule 40 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lk	69	Total	C	N	O	S	0	0
			568	366	103	98	1		

- Molecule 41 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Ll	50	Total	C	N	O	S	0	0
			443	281	98	63	1		

- Molecule 42 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lm	52	Total	C	N	O	S	1	0
			436	272	91	67	6		

- Molecule 43 is a protein called Small ribosomal subunit protein eS32.

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

- Molecule 44 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Lo	105	Total	C	N	O	S	1	0
			870	548	177	139	6		

- Molecule 45 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lp	91	Total	C	N	O	S	1	0
			715	450	139	119	7		

- Molecule 46 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	mR	3	Total	C	N	O	P	0	0
			65	29	12	21	3		

- Molecule 47 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	Pt	77	Total	C	N	O	P	S	0	0
			1646	734	298	536	77	1		

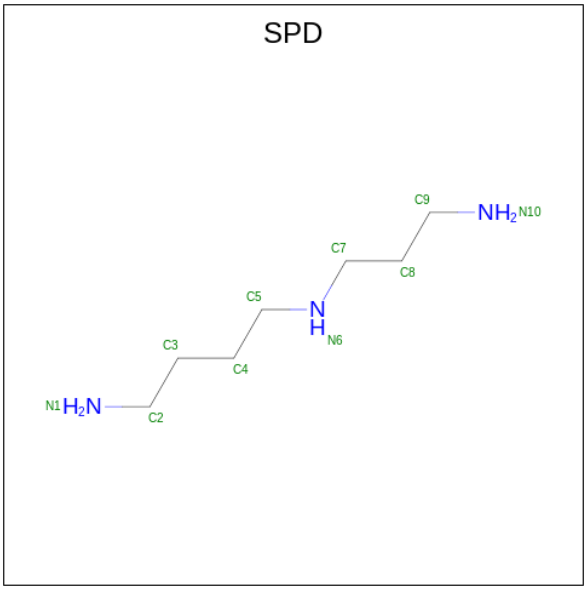
- Molecule 48 is a protein called SERPINE1 mRNA-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	CB	16	Total	C	N	O	S	0	0
			127	80	22	24	1		

- Molecule 49 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	LI	213	Total	C	N	O	S	0	0
			1716	1086	331	285	14		

- Molecule 50 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



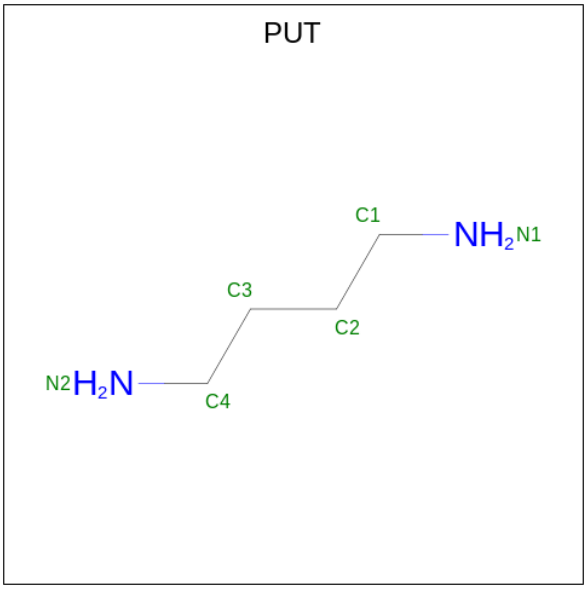
Mol	Chain	Residues	Atoms			AltConf
50	L8	1	Total	C	N	0
			10	7	3	
50	L5	1	Total	C	N	0
			10	7	3	
50	L5	1	Total	C	N	0
			10	7	3	
50	L5	1	Total	C	N	0
			10	7	3	
50	L5	1	Total	C	N	0
			10	7	3	
50	L5	1	Total	C	N	0
			10	7	3	
50	L5	1	Total	C	N	0
			10	7	3	
50	L5	1	Total	C	N	0
			10	7	3	

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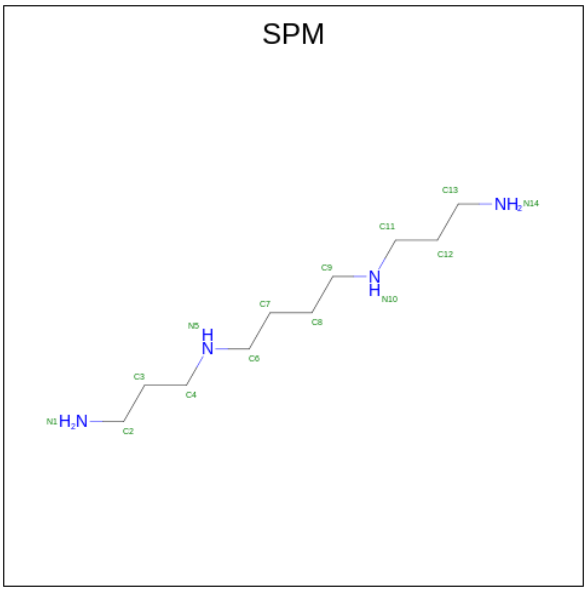
Mol	Chain	Residues	Atoms	AltConf
50	L5	1	Total C N 10 7 3	0
50	L5	1	Total C N 10 7 3	0
50	L5	1	Total C N 10 7 3	0
50	L5	1	Total C N 10 7 3	0
50	LN	1	Total C N 10 7 3	0

- Molecule 51 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



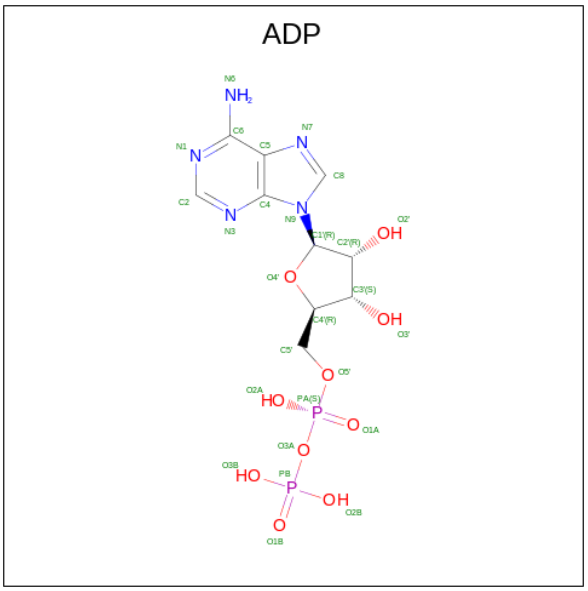
Mol	Chain	Residues	Atoms	AltConf
51	L5	1	Total C N 6 4 2	0

- Molecule 52 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms	AltConf
52	L5	1	Total C N 14 10 4	0
52	L5	1	Total C N 14 10 4	0
52	L5	1	Total C N 14 10 4	0
52	L5	1	Total C N 14 10 4	0
52	L5	1	Total C N 14 10 4	0
52	L5	1	Total C N 14 10 4	0
52	L5	1	Total C N 14 10 4	0
52	L5	1	Total C N 14 10 4	0

- Molecule 53 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
53	L5	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	Lg	1	Total	Zn	0
			1	1	
54	Lj	1	Total	Zn	0
			1	1	
54	Lm	1	Total	Zn	0
			1	1	
54	Lo	1	Total	Zn	0
			1	1	
54	Lp	1	Total	Zn	0
			1	1	

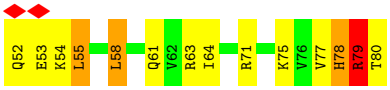
3 Residue-property plots (i)

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

• Molecule 1: Transcription factor BTF3

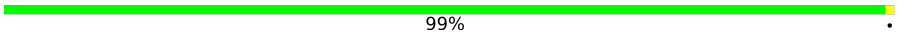
Chain A:





• Molecule 2: Large ribosomal subunit protein uL2

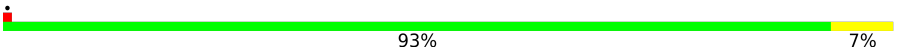
Chain LA:





• Molecule 3: Large ribosomal subunit protein uL3

Chain LB:

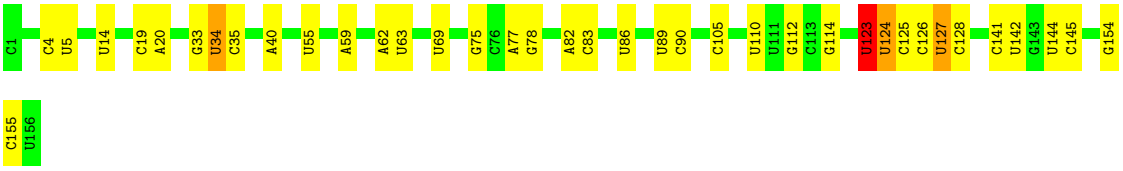




• Molecule 4: 5.8S rRNA

Chain L8:

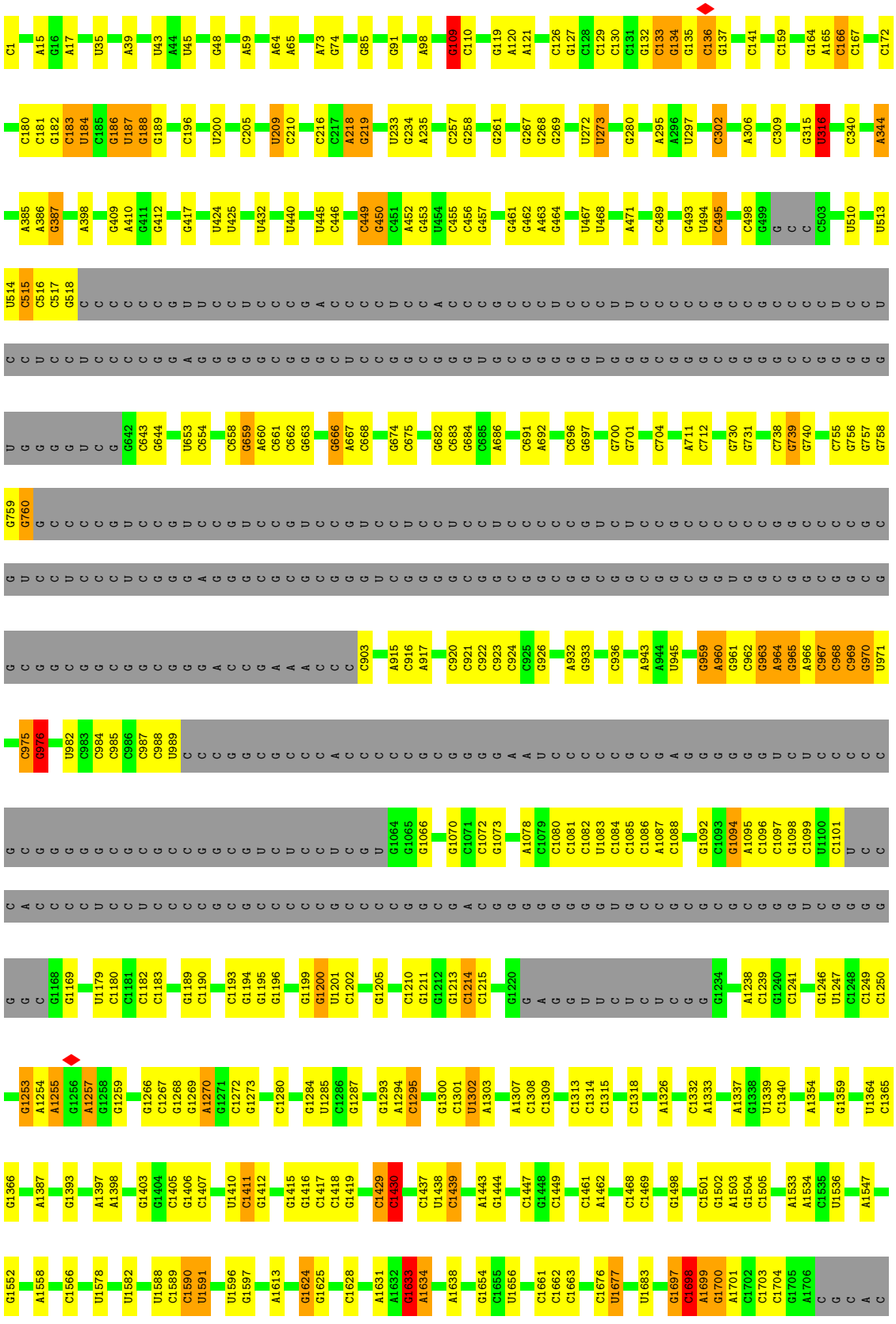


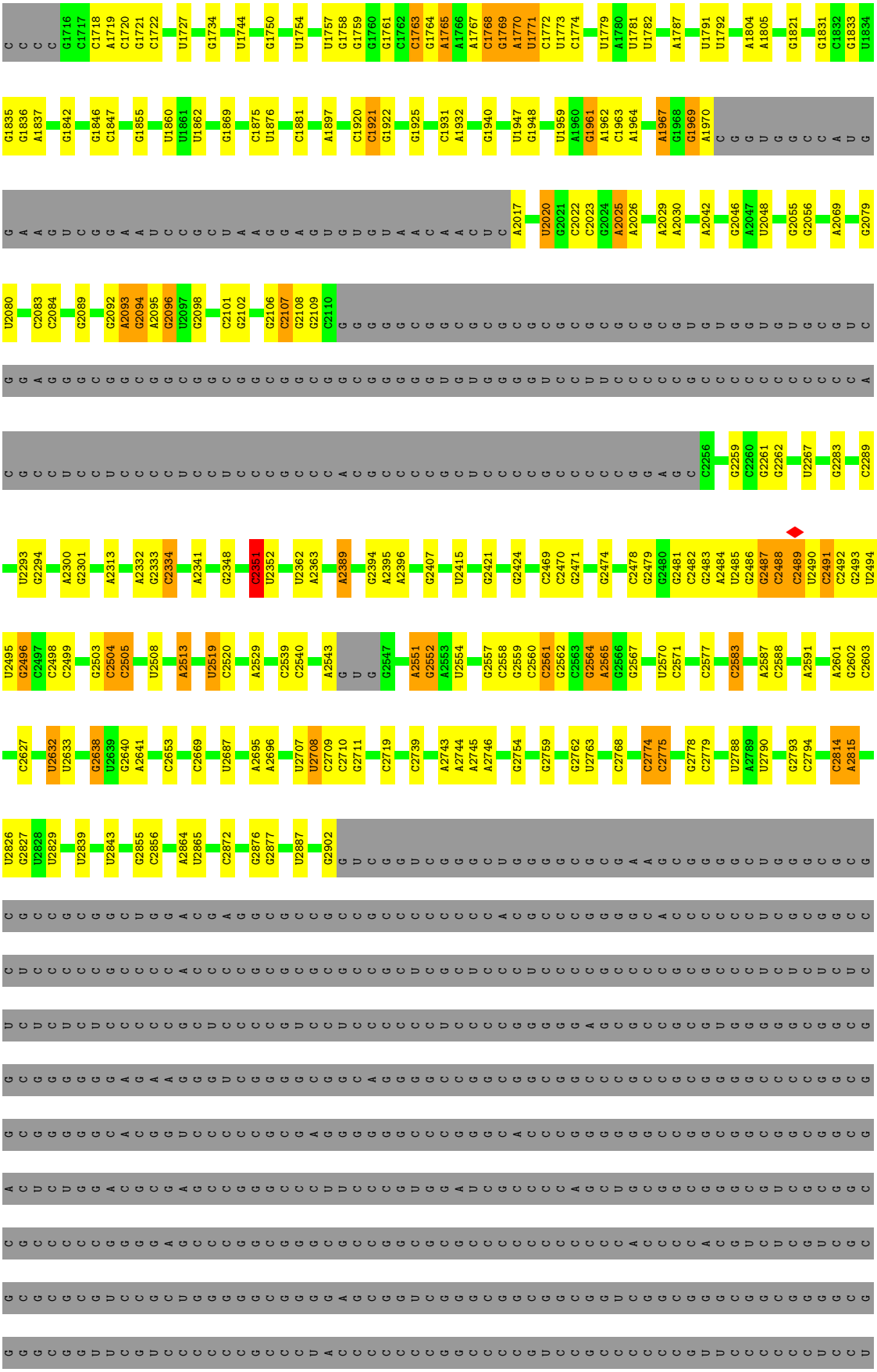


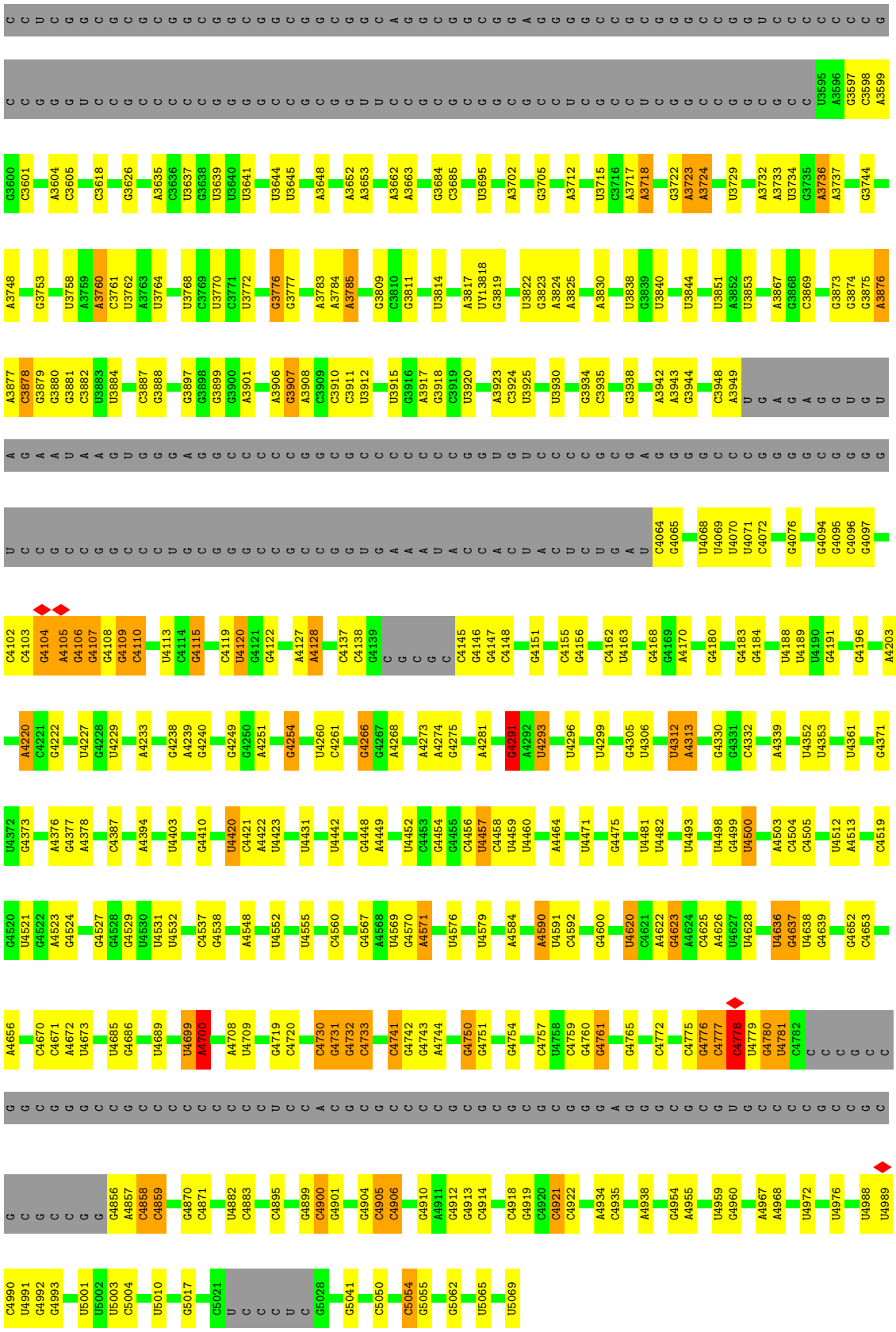
• Molecule 5: 28S rRNA

Chain L5:



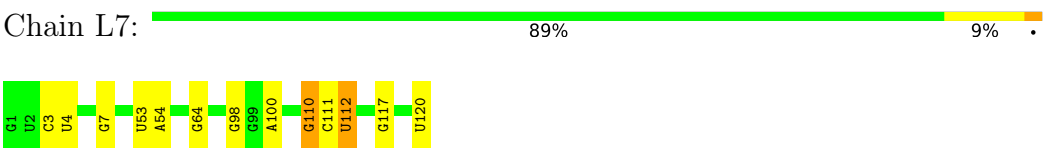






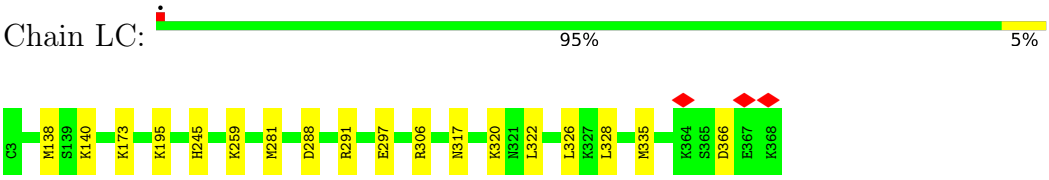
• Molecule 6: 5S rRNA

Chain L7:



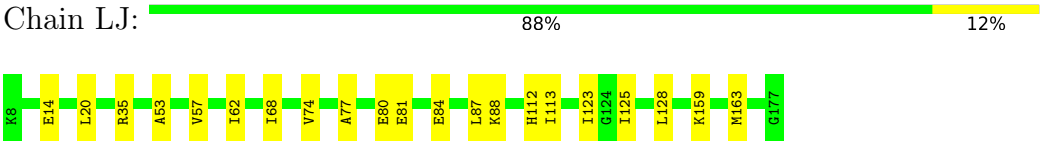
• Molecule 7: Large ribosomal subunit protein uL4

Chain LC:



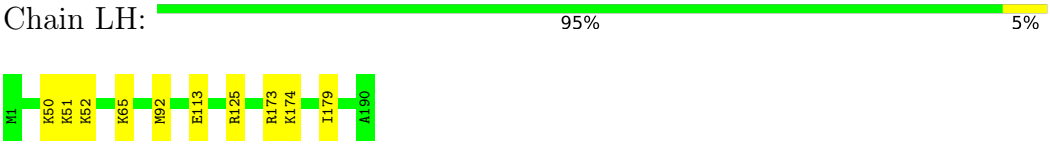
• Molecule 8: Large ribosomal subunit protein uL5

Chain LJ:



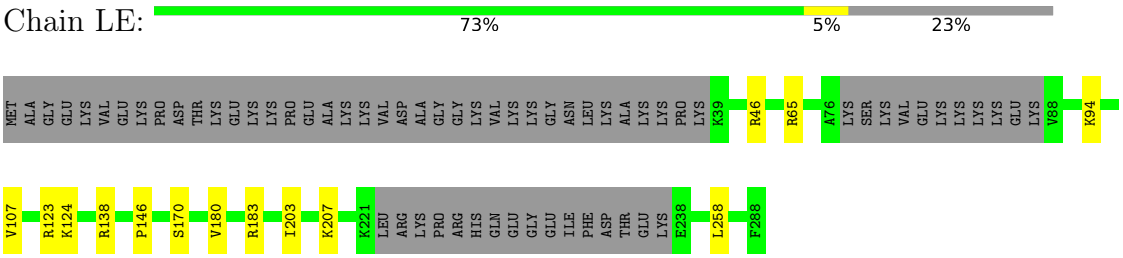
• Molecule 9: Large ribosomal subunit protein uL6

Chain LH:



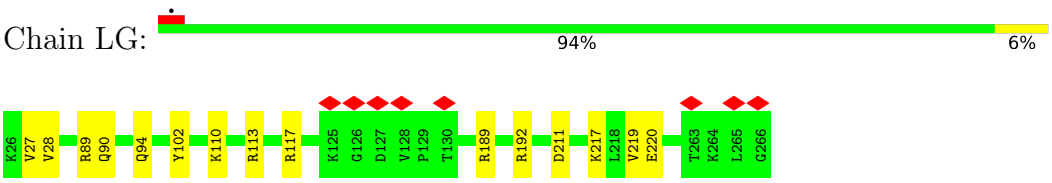
• Molecule 10: Large ribosomal subunit protein eL6

Chain LE:



• Molecule 11: Large ribosomal subunit protein eL8

Chain LG:



• Molecule 12: Large ribosomal subunit protein uL13

Chain LO:

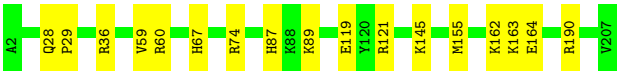




• Molecule 13: Large ribosomal subunit protein eL13

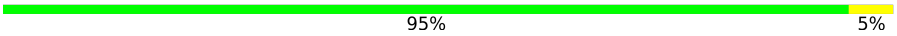
Chain LL:





• Molecule 14: Large ribosomal subunit protein uL14

Chain LV:





• Molecule 15: Large ribosomal subunit protein eL14

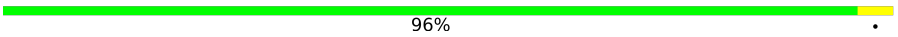
Chain LM:

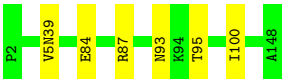




• Molecule 16: Large ribosomal subunit protein uL15

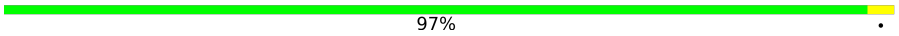
Chain La:

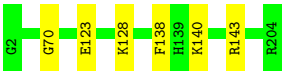




• Molecule 17: Large ribosomal subunit protein eL15

Chain LN:

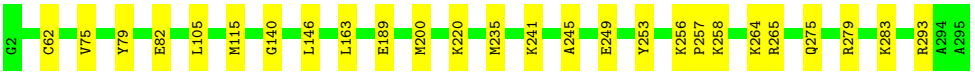




• Molecule 18: Large ribosomal subunit protein uL18

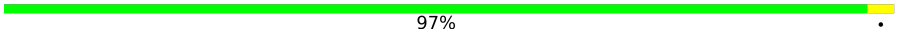
Chain LD:

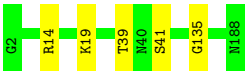




• Molecule 19: Large ribosomal subunit protein eL18

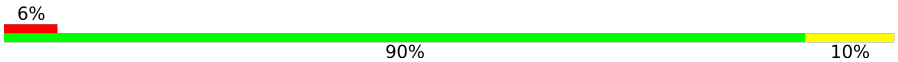
Chain LQ:

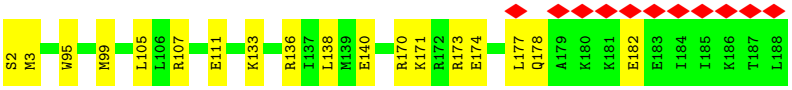




• Molecule 20: Large ribosomal subunit protein eL19

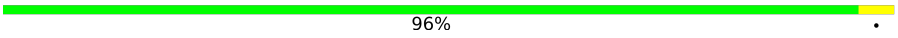
Chain LR:

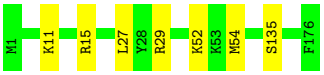




• Molecule 21: Large ribosomal subunit protein eL20

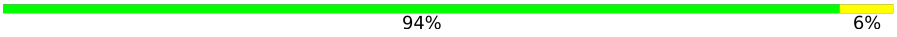
Chain LS:

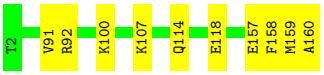




• Molecule 22: Large ribosomal subunit protein eL21

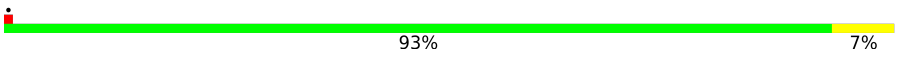
Chain LT:

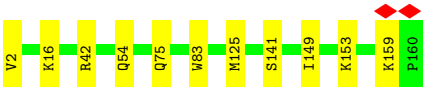




• Molecule 23: Large ribosomal subunit protein uL22

Chain LP:

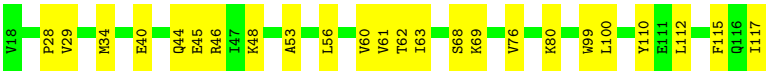




• Molecule 24: Large ribosomal subunit protein eL22

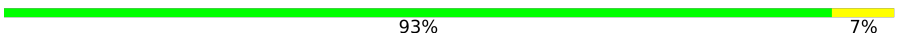
Chain LU:





• Molecule 25: Large ribosomal subunit protein uL23

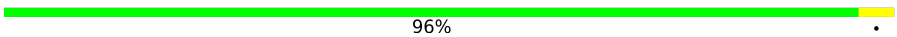
Chain LX:

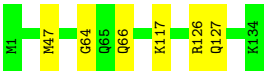




• Molecule 26: Large ribosomal subunit protein uL24

Chain LY:

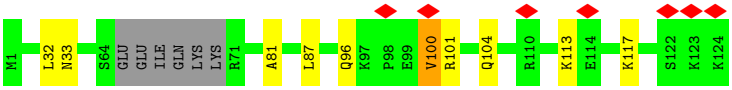




• Molecule 27: Large ribosomal subunit protein eL24

Chain LW:

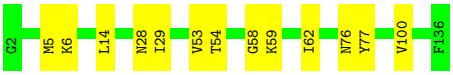




• Molecule 28: Large ribosomal subunit protein eL27

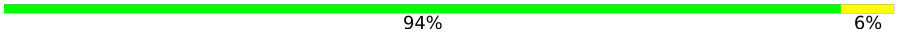
Chain LZ:

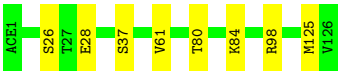




• Molecule 29: Large ribosomal subunit protein eL28

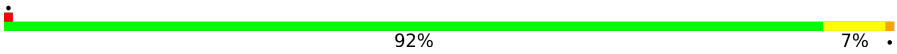
Chain Lr:

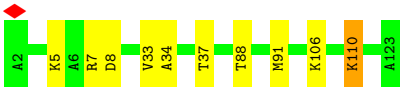




• Molecule 30: Large ribosomal subunit protein uL29

Chain Lh:

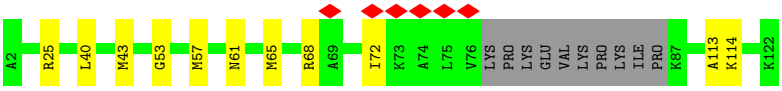




• Molecule 31: Large ribosomal subunit protein eL29

Chain Lb:





• Molecule 32: Large ribosomal subunit protein uL30

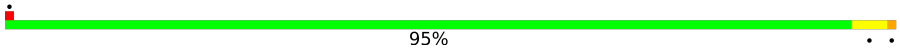
Chain LF:

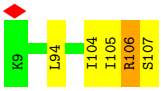




• Molecule 33: Large ribosomal subunit protein eL30

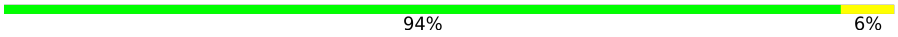
Chain Lc:

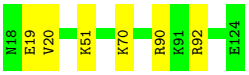




• Molecule 34: Large ribosomal subunit protein eL31

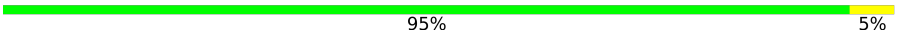
Chain Ld:

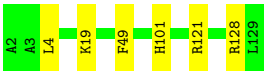




• Molecule 35: Large ribosomal subunit protein eL32

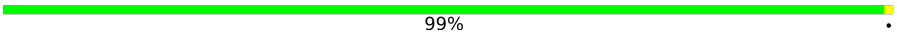
Chain Le:





• Molecule 36: Large ribosomal subunit protein eL33

Chain Lf:

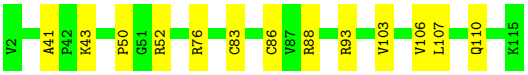




• Molecule 37: Large ribosomal subunit protein eL34

Chain Lg:





• Molecule 38: Large ribosomal subunit protein eL36

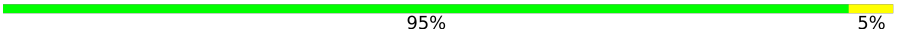
Chain Li:

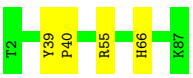




• Molecule 39: Large ribosomal subunit protein eL37

Chain Lj:

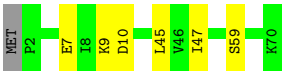




• Molecule 40: Large ribosomal subunit protein eL38

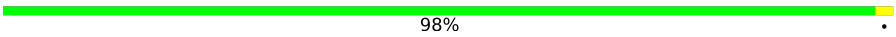
Chain Lk:





• Molecule 41: Large ribosomal subunit protein eL39

Chain Ll:

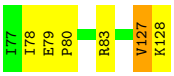




• Molecule 42: Large ribosomal subunit protein eL40

Chain Lm:





• Molecule 43: Small ribosomal subunit protein eS32

Chain Ln:





• Molecule 44: Large ribosomal subunit protein eL42

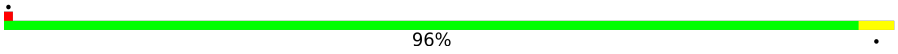
Chain Lo:

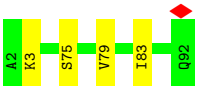




• Molecule 45: Large ribosomal subunit protein eL43

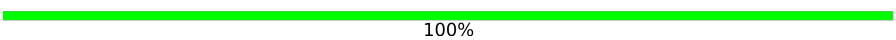
Chain Lp:





• Molecule 46: mRNA

Chain mR:

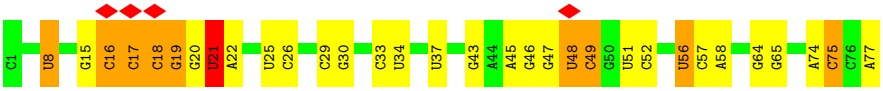


There are no outlier residues recorded for this chain.

• Molecule 47: P-site tRNA

Chain Pt:





• Molecule 48: SERPINE1 mRNA-binding protein 1

Chain CB:



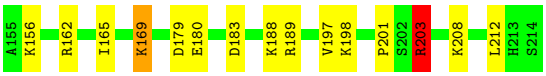


• Molecule 49: Large ribosomal subunit protein uL16

Chain LI:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	676783	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)	300	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	456.0, 456.0, 456.0	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	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: 1MA, PUT, PSU, SPD, A2M, 6MZ, 5MC, ACE, UR3, OMC, M3L, OMG, V5N, ZN, H2U, HIC, UY1, OMU, G7M, ADP, SPM, 4SU, MLZ

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	A	1.03	0/230	1.33	1/301 (0.3%)
2	LA	0.27	0/1958	0.50	0/2623
3	LB	0.24	0/3294	0.45	0/4406
4	L8	0.36	0/3609	0.88	3/5623 (0.1%)
5	L5	0.38	4/82288 (0.0%)	0.92	59/128369 (0.0%)
6	L7	0.32	0/2858	0.81	1/4455 (0.0%)
7	LC	0.22	0/2968	0.42	0/3985
8	LJ	0.18	0/1385	0.42	0/1852
9	LH	0.15	0/1537	0.36	0/2066
10	LE	0.15	0/1820	0.36	0/2442
11	LG	0.21	0/1959	0.40	0/2637
12	LO	0.24	0/1686	0.42	0/2257
13	LL	0.20	0/1706	0.42	0/2284
14	LV	0.20	0/1002	0.45	0/1345
15	LM	0.18	0/1142	0.35	0/1527
16	La	0.25	0/1178	0.45	0/1573
17	LN	0.23	0/1745	0.47	0/2338
18	LD	0.16	0/2437	0.37	0/3263
19	LQ	0.21	0/1536	0.46	0/2052
20	LR	0.19	0/1582	0.40	0/2091
21	LS	0.19	0/1500	0.41	0/2013
22	LT	0.20	0/1345	0.40	0/1795
23	LP	0.25	0/1328	0.43	0/1784
24	LU	0.13	0/830	0.34	0/1114
25	LX	0.19	0/983	0.39	0/1323
26	LY	0.18	0/1132	0.37	0/1504
27	LW	0.18	0/964	0.39	0/1278
28	LZ	0.18	0/1141	0.41	0/1521
29	Lr	0.23	0/1027	0.43	0/1377
30	Lh	0.19	0/1022	0.34	0/1351
31	Lb	0.19	0/900	0.39	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LF	0.27	0/1926	0.44	0/2567
33	Lc	0.29	0/780	0.45	0/1046
34	Ld	0.20	0/903	0.43	0/1216
35	Le	0.22	0/1071	0.45	0/1429
36	Lf	0.21	0/902	0.42	0/1208
37	Lg	0.26	0/916	0.45	0/1220
38	Li	0.16	0/843	0.38	0/1115
39	Lj	0.24	0/731	0.47	0/967
40	Lk	0.14	0/574	0.32	0/761
41	Ll	0.20	0/453	0.37	0/599
42	Lm	0.21	0/433	0.39	0/575
43	Ln	0.20	0/240	0.32	0/305
44	Lo	0.20	0/877	0.43	0/1156
45	Lp	0.21	0/728	0.45	0/967
46	mR	0.28	0/72	0.86	0/110
47	Pt	0.41	0/1722	0.78	0/2682
48	CB	0.93	0/128	1.04	0/171
49	LI	0.93	0/1755	1.18	0/2344
All	All	0.34	4/145146 (0.0%)	0.79	64/214174 (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
1	A	0	2
33	Lc	0	1
48	CB	0	1
49	LI	0	11
All	All	0	15

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L5	4523	A2M	O3'-P	5.36	1.61	1.56
5	L5	3825	A2M	O3'-P	5.26	1.61	1.56
5	L5	3785	A2M	O3'-P	5.22	1.61	1.56
5	L5	3830	A2M	O3'-P	5.20	1.61	1.56

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L5	417	G	O4'-C1'-N9	7.05	113.84	108.20
5	L5	3907	G	O5'-C5'-C4'	6.82	114.85	109.40
5	L5	2469	C	C2-N1-C1'	6.43	125.87	118.80
5	L5	1597	G	O4'-C1'-N9	6.32	112.93	108.50
5	L5	2042	A	O5'-C5'-C4'	6.31	114.44	109.40

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	ARG	Sidechain
1	A	71	ARG	Sidechain
48	CB	16	ARG	Sidechain
49	LI	3	ARG	Sidechain
33	Lc	106	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	230	0	264	14	0
2	LA	1930	0	2028	1	0
3	LB	3239	0	3377	17	0
4	L8	3316	0	1687	19	0
5	L5	76304	0	38651	395	0
6	L7	2558	0	1296	5	0
7	LC	2914	0	3087	13	0
8	LJ	1362	0	1399	12	0
9	LH	1518	0	1601	8	0
10	LE	1786	0	1945	14	0
11	LG	1926	0	2074	8	0
12	LO	1654	0	1799	7	0
13	LL	1672	0	1786	16	0
14	LV	988	0	1047	3	0
15	LM	1120	0	1187	7	0
16	La	1162	0	1206	3	0
17	LN	1700	0	1749	4	0
18	LD	2391	0	2426	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	LQ	1512	0	1628	5	0
20	LR	1566	0	1729	9	0
21	LS	1460	0	1502	3	0
22	LT	1311	0	1392	6	0
23	LP	1296	0	1331	8	0
24	LU	816	0	842	17	0
25	LX	966	0	1040	4	0
26	LY	1115	0	1205	6	0
27	LW	950	0	999	5	0
28	LZ	1115	0	1195	9	0
29	Lr	1011	0	1085	6	0
30	Lh	1014	0	1148	7	0
31	Lb	898	0	983	8	0
32	LF	1885	0	2022	16	0
33	Lc	770	0	809	1	0
34	Ld	888	0	930	4	0
35	Le	1053	0	1147	4	0
36	Lf	883	0	924	1	0
37	Lg	906	0	998	11	0
38	Li	832	0	917	8	0
39	Lj	712	0	744	2	0
40	Lk	568	0	637	3	0
41	Ll	443	0	483	1	0
42	Lm	436	0	477	5	0
43	Ln	239	0	289	2	0
44	Lo	870	0	936	7	0
45	Lp	715	0	769	2	0
46	mR	65	0	33	0	0
47	Pt	1646	0	844	23	0
48	CB	127	0	120	5	0
49	LI	1716	0	1765	10	0
50	L5	110	0	209	14	0
50	L8	10	0	19	0	0
50	LN	10	0	19	1	0
51	L5	6	0	12	1	0
52	L5	112	0	208	6	0
53	L5	27	0	12	0	0
54	Lg	1	0	0	0	0
54	Lj	1	0	0	0	0
54	Lm	1	0	0	0	0
54	Lo	1	0	0	0	0
54	Lp	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	137834	0	100011	698	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 698 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:L5:5113:SPD:C5	50:L5:5113:SPD:N6	1.84	1.41
50:L5:5113:SPD:C9	50:L5:5113:SPD:N10	1.84	1.41
50:L5:5113:SPD:C2	50:L5:5113:SPD:N1	1.83	1.41
50:L5:5113:SPD:C2	50:L5:5113:SPD:C3	2.02	1.38
50:L5:5113:SPD:C9	50:L5:5113:SPD:C8	2.02	1.38

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	27/29 (93%)	22 (82%)	3 (11%)	2 (7%)	1 0
2	LA	249/251 (99%)	242 (97%)	7 (3%)	0	100 100
3	LB	399/402 (99%)	394 (99%)	5 (1%)	0	100 100
7	LC	364/366 (100%)	363 (100%)	1 (0%)	0	100 100
8	LJ	168/170 (99%)	168 (100%)	0	0	100 100
9	LH	188/190 (99%)	186 (99%)	2 (1%)	0	100 100
10	LE	217/288 (75%)	209 (96%)	8 (4%)	0	100 100
11	LG	239/241 (99%)	235 (98%)	4 (2%)	0	100 100
12	LO	200/202 (99%)	196 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	LL	205/206 (100%)	201 (98%)	4 (2%)	0	100	100
14	LV	131/133 (98%)	130 (99%)	1 (1%)	0	100	100
15	LM	134/136 (98%)	133 (99%)	1 (1%)	0	100	100
16	La	144/147 (98%)	138 (96%)	6 (4%)	0	100	100
17	LN	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
18	LD	292/294 (99%)	288 (99%)	4 (1%)	0	100	100
19	LQ	185/187 (99%)	182 (98%)	3 (2%)	0	100	100
20	LR	185/187 (99%)	184 (100%)	1 (0%)	0	100	100
21	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
22	LT	159/159 (100%)	157 (99%)	2 (1%)	0	100	100
23	LP	158/159 (99%)	154 (98%)	4 (2%)	0	100	100
24	LU	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
25	LX	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
26	LY	132/134 (98%)	131 (99%)	1 (1%)	0	100	100
27	LW	114/124 (92%)	109 (96%)	5 (4%)	0	100	100
28	LZ	134/135 (99%)	133 (99%)	1 (1%)	0	100	100
29	Lr	125/126 (99%)	124 (99%)	1 (1%)	0	100	100
30	Lh	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
31	Lb	106/121 (88%)	104 (98%)	2 (2%)	0	100	100
32	LF	225/225 (100%)	219 (97%)	6 (3%)	0	100	100
33	Lc	97/99 (98%)	96 (99%)	0	1 (1%)	12	5
34	Ld	105/107 (98%)	105 (100%)	0	0	100	100
35	Le	126/128 (98%)	126 (100%)	0	0	100	100
36	Lf	108/110 (98%)	108 (100%)	0	0	100	100
37	Lg	112/114 (98%)	111 (99%)	1 (1%)	0	100	100
38	Li	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
39	Lj	85/86 (99%)	84 (99%)	1 (1%)	0	100	100
40	Lk	67/70 (96%)	67 (100%)	0	0	100	100
41	Ll	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
42	Lm	50/52 (96%)	50 (100%)	0	0	100	100
43	Ln	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	Lo	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
45	Lp	90/91 (99%)	85 (94%)	5 (6%)	0	100	100
48	CB	14/16 (88%)	14 (100%)	0	0	100	100
49	LI	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
All	All	6528/6699 (97%)	6420 (98%)	105 (2%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
33	Lc	106	ARG
1	A	78	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	23/23 (100%)	19 (83%)	4 (17%)	2	0
2	LA	193/192 (100%)	193 (100%)	0	100	100
3	LB	347/347 (100%)	346 (100%)	1 (0%)	86	86
7	LC	305/305 (100%)	303 (99%)	2 (1%)	76	73
8	LJ	143/143 (100%)	141 (99%)	2 (1%)	59	54
9	LH	169/169 (100%)	168 (99%)	1 (1%)	78	76
10	LE	196/252 (78%)	196 (100%)	0	100	100
11	LG	203/205 (99%)	200 (98%)	3 (2%)	57	52
12	LO	173/173 (100%)	173 (100%)	0	100	100
13	LL	173/172 (101%)	173 (100%)	0	100	100
14	LV	102/102 (100%)	100 (98%)	2 (2%)	48	42
15	LM	116/116 (100%)	115 (99%)	1 (1%)	70	67
16	La	119/119 (100%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	LN	171/171 (100%)	171 (100%)	0	100 100
18	LD	247/247 (100%)	244 (99%)	3 (1%)	63 58
19	LQ	164/164 (100%)	164 (100%)	0	100 100
20	LR	166/166 (100%)	164 (99%)	2 (1%)	63 58
21	LS	157/157 (100%)	156 (99%)	1 (1%)	78 76
22	LT	141/139 (101%)	141 (100%)	0	100 100
23	LP	141/140 (101%)	140 (99%)	1 (1%)	76 73
24	LU	90/90 (100%)	88 (98%)	2 (2%)	45 38
25	LX	106/106 (100%)	106 (100%)	0	100 100
26	LY	124/124 (100%)	124 (100%)	0	100 100
27	LW	95/103 (92%)	94 (99%)	1 (1%)	65 61
28	LZ	118/117 (101%)	117 (99%)	1 (1%)	73 71
29	Lr	110/109 (101%)	110 (100%)	0	100 100
30	Lh	109/109 (100%)	108 (99%)	1 (1%)	70 67
31	Lb	90/100 (90%)	90 (100%)	0	100 100
32	LF	196/194 (101%)	195 (100%)	1 (0%)	81 79
33	Lc	84/84 (100%)	82 (98%)	2 (2%)	43 35
34	Ld	98/98 (100%)	98 (100%)	0	100 100
35	Le	114/114 (100%)	114 (100%)	0	100 100
36	Lf	89/89 (100%)	89 (100%)	0	100 100
37	Lg	98/98 (100%)	98 (100%)	0	100 100
38	Li	86/86 (100%)	84 (98%)	2 (2%)	44 37
39	Lj	74/73 (101%)	73 (99%)	1 (1%)	59 54
40	Lk	64/65 (98%)	63 (98%)	1 (2%)	55 50
41	Ll	47/47 (100%)	47 (100%)	0	100 100
42	Lm	48/47 (102%)	47 (98%)	1 (2%)	47 40
43	Ln	24/24 (100%)	24 (100%)	0	100 100
44	Lo	93/92 (101%)	92 (99%)	1 (1%)	65 61
45	Lp	75/74 (101%)	74 (99%)	1 (1%)	61 57
48	CB	14/14 (100%)	14 (100%)	0	100 100
49	LI	180/180 (100%)	147 (82%)	33 (18%)	2 0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5675/5739 (99%)	5604 (99%)	71 (1%)	59 57

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	LI	148	VAL
49	LI	156	LYS
49	LI	189	ARG
24	LU	76	VAL
24	LU	62	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
18	LD	202	GLN
49	LI	130	HIS
24	LU	55	ASN
49	LI	112	GLN
39	Lj	13	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	L8	155/156 (99%)	13 (8%)	0
46	mR	2/3 (66%)	0	0
47	Pt	76/77 (98%)	11 (14%)	0
5	L5	3538/5069 (69%)	479 (13%)	21 (0%)
6	L7	119/120 (99%)	8 (6%)	0
All	All	3890/5425 (71%)	511 (13%)	21 (0%)

5 of 511 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	L8	34	U
4	L8	35	C
4	L8	59	A
4	L8	62	A
4	L8	63	U

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L5	2774	C
5	L5	4779	U
5	L5	4905	C
5	L5	4780	G
5	L5	4699	U

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

144 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	$\#\|Z\| > 2$
5	PSU	L5	4420	5	18,21,22	1.10	2 (11%)	22,30,33	1.75	5 (22%)
5	PSU	L5	3637	5	18,21,22	1.07	1 (5%)	22,30,33	1.84	3 (13%)
5	A2M	L5	1326	5	22,25,26	0.20	0	31,36,39	0.31	0
5	OMG	L5	4618	5	23,26,27	0.47	0	33,38,41	0.63	0
5	PSU	L5	4493	5	18,21,22	1.07	1 (5%)	22,30,33	1.71	4 (18%)
5	PSU	L5	4576	5	18,21,22	1.02	1 (5%)	22,30,33	1.71	4 (18%)
47	G7M	Pt	47	47	23,26,27	0.71	1 (4%)	35,39,42	0.59	0
5	PSU	L5	4972	5	18,21,22	1.10	1 (5%)	22,30,33	1.67	4 (18%)
5	OMG	L5	3792	5	23,26,27	0.48	0	33,38,41	0.56	0
5	A2M	L5	2815	5	22,25,26	0.19	0	31,36,39	0.35	0
5	A2M	L5	3867	5	22,25,26	3.17	9 (40%)	31,36,39	2.87	10 (32%)
5	OMG	L5	4637	5	23,26,27	0.49	0	33,38,41	0.54	0
5	PSU	L5	3639	5	18,21,22	1.08	1 (5%)	22,30,33	1.59	3 (13%)
5	OMG	L5	2364	5	23,26,27	0.28	0	33,38,41	0.34	0
5	A2M	L5	3723	5	22,25,26	3.17	9 (40%)	31,36,39	2.94	10 (32%)
5	PSU	L5	3920	5	18,21,22	1.06	1 (5%)	22,30,33	1.64	2 (9%)
5	OMU	L5	4306	5	19,22,23	3.09	8 (42%)	26,31,34	1.72	5 (19%)
5	PSU	L5	4353	5	18,21,22	1.07	1 (5%)	22,30,33	1.62	2 (9%)
5	PSU	L5	4361	5	18,21,22	0.99	1 (5%)	22,30,33	1.81	3 (13%)
5	A2M	L5	2401	5	22,25,26	0.19	0	31,36,39	0.42	0
5	PSU	L5	1744	5	18,21,22	0.84	1 (5%)	22,30,33	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PSU	L5	1677	5	18,21,22	0.84	1 (5%)	22,30,33	0.87	1 (4%)
5	PSU	L5	3758	5	18,21,22	1.07	1 (5%)	22,30,33	1.79	4 (18%)
5	PSU	L5	4689	5	18,21,22	1.05	1 (5%)	22,30,33	1.78	4 (18%)
5	PSU	L5	4312	5	18,21,22	1.00	1 (5%)	22,30,33	1.79	4 (18%)
5	PSU	L5	1582	5	18,21,22	1.07	1 (5%)	22,30,33	1.65	4 (18%)
5	A2M	L5	3830	5	22,25,26	3.15	9 (40%)	31,36,39	2.87	12 (38%)
5	OMG	L5	4228	5	23,26,27	0.45	0	33,38,41	0.63	0
5	OMG	L5	4392	5	23,26,27	0.47	0	33,38,41	0.49	0
3	HIC	LB	245	3	10,11,12	0.44	0	8,14,16	0.60	0
5	PSU	L5	3884	5	18,21,22	1.06	1 (5%)	22,30,33	1.64	4 (18%)
5	PSU	L5	3715	5	18,21,22	1.06	1 (5%)	22,30,33	1.79	5 (22%)
5	PSU	L5	1782	5	18,21,22	0.85	1 (5%)	22,30,33	0.66	0
5	A2M	L5	3825	5	22,25,26	3.12	9 (40%)	31,36,39	2.86	11 (35%)
5	OMG	L5	4494	5	23,26,27	0.49	0	33,38,41	0.54	0
5	A2M	L5	3724	5	22,25,26	3.15	9 (40%)	31,36,39	2.91	10 (32%)
5	OMG	L5	1316	5	23,26,27	0.51	0	33,38,41	0.67	0
5	OMU	L5	3925	5	19,22,23	3.01	8 (42%)	26,31,34	1.71	4 (15%)
5	PSU	L5	4500	5	18,21,22	1.06	1 (5%)	22,30,33	1.67	5 (22%)
5	OMG	L5	2876	5	23,26,27	0.51	0	33,38,41	0.56	0
5	PSU	L5	1792	5	18,21,22	0.86	1 (5%)	22,30,33	0.70	0
5	A2M	L5	2787	5	22,25,26	0.19	0	31,36,39	0.49	0
5	OMC	L5	3841	5	19,22,23	0.59	0	26,31,34	0.71	0
5	UR3	L5	4530	5	19,22,23	0.30	0	26,32,35	0.69	0
5	OMG	L5	3944	5	23,26,27	0.49	0	33,38,41	0.54	0
5	PSU	L5	1683	5	18,21,22	0.85	1 (5%)	22,30,33	0.72	0
5	OMC	L5	3887	5	19,22,23	0.58	0	26,31,34	0.64	0
4	OMG	L8	75	4	23,26,27	0.47	0	33,38,41	0.50	0
5	OMC	L5	2422	5	19,22,23	0.57	0	26,31,34	0.75	0
5	OMC	L5	2861	5	19,22,23	0.29	0	26,31,34	0.29	0
5	PSU	L5	4457	5	18,21,22	1.03	1 (5%)	22,30,33	1.67	4 (18%)
5	PSU	L5	4531	5	18,21,22	0.89	1 (5%)	22,30,33	0.63	0
5	A2M	L5	4523	5	22,25,26	3.15	9 (40%)	31,36,39	2.88	10 (32%)
42	M3L	Lm	98	42	10,11,12	0.55	0	9,14,16	0.46	0
5	PSU	L5	3764	5	18,21,22	1.07	1 (5%)	22,30,33	1.74	5 (22%)
5	OMU	L5	2837	5	19,22,23	0.22	0	26,31,34	0.71	0
5	PSU	L5	4673	5	18,21,22	1.09	1 (5%)	22,30,33	1.65	3 (13%)
5	PSU	L5	3844	5	18,21,22	0.97	1 (5%)	22,30,33	1.61	3 (13%)
5	PSU	L5	3729	5	18,21,22	1.02	1 (5%)	22,30,33	1.73	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PSU	L5	4442	5	18,21,22	1.03	1 (5%)	22,30,33	1.77	5 (22%)
5	PSU	L5	4628	5	18,21,22	1.01	1 (5%)	22,30,33	1.61	4 (18%)
5	OMC	L5	3701	5	19,22,23	0.62	0	26,31,34	0.71	0
5	OMG	L5	1625	5	23,26,27	0.56	0	33,38,41	0.48	0
5	6MZ	L5	4220	5	22,25,26	1.39	4 (18%)	30,36,39	2.15	9 (30%)
5	PSU	L5	4403	5	18,21,22	1.04	1 (5%)	22,30,33	1.99	6 (27%)
5	PSU	L5	3768	5	18,21,22	1.09	1 (5%)	22,30,33	1.67	3 (13%)
5	PSU	L5	4569	5	18,21,22	1.09	1 (5%)	22,30,33	1.81	3 (13%)
5	PSU	L5	4579	5	18,21,22	1.05	1 (5%)	22,30,33	1.70	4 (18%)
5	PSU	L5	4293	5	18,21,22	1.06	1 (5%)	22,30,33	1.56	3 (13%)
5	OMG	L5	3744	5	23,26,27	0.48	0	33,38,41	0.53	0
5	OMC	L5	4456	5	19,22,23	0.58	0	26,31,34	0.56	0
47	PSU	Pt	56	47	18,21,22	0.88	1 (5%)	22,30,33	0.59	0
5	A2M	L5	400	5	22,25,26	0.16	0	31,36,39	0.37	0
5	A2M	L5	1871	5	22,25,26	0.19	0	31,36,39	0.64	0
5	OMC	L5	2824	5	19,22,23	0.55	0	26,31,34	0.70	0
5	PSU	L5	1862	5	18,21,22	0.87	1 (5%)	22,30,33	0.69	0
5	PSU	L5	4296	5	18,21,22	1.02	1 (5%)	22,30,33	1.70	4 (18%)
4	OMU	L8	14	5,4	19,22,23	0.26	0	26,31,34	0.29	0
5	A2M	L5	4571	5	22,25,26	3.23	9 (40%)	31,36,39	2.94	12 (38%)
5	A2M	L5	3760	5	22,25,26	3.21	9 (40%)	31,36,39	2.97	10 (32%)
5	OMU	L5	2415	5	19,22,23	0.24	0	26,31,34	0.37	0
5	OMG	L5	4196	47,5	23,26,27	0.49	0	33,38,41	0.55	0
5	OMU	L5	4498	5	19,22,23	3.05	8 (42%)	26,31,34	1.77	4 (15%)
5	PSU	L5	4521	5	18,21,22	1.02	1 (5%)	22,30,33	1.81	4 (18%)
5	OMU	L5	4620	5	19,22,23	2.99	8 (42%)	26,31,34	1.44	4 (15%)
5	UY1	L5	3818	5	19,22,23	1.39	3 (15%)	22,31,34	2.05	4 (18%)
5	PSU	L5	4431	5	18,21,22	1.01	1 (5%)	22,30,33	1.70	3 (13%)
5	PSU	L5	1860	5	18,21,22	0.85	1 (5%)	22,30,33	0.74	0
47	OMC	Pt	33	47	19,22,23	0.29	0	26,31,34	0.30	0
5	OMC	L5	1881	5	19,22,23	0.56	0	26,31,34	0.75	0
5	PSU	L5	5010	5	18,21,22	1.09	1 (5%)	22,30,33	1.73	4 (18%)
5	PSU	L5	4636	5	18,21,22	1.07	1 (5%)	22,30,33	1.77	5 (22%)
5	PSU	L5	3851	5	18,21,22	1.14	1 (5%)	22,30,33	1.68	4 (18%)
4	PSU	L8	55	4	18,21,22	0.86	1 (5%)	22,30,33	0.68	0
2	V5N	LA	216	2	9,11,12	0.49	0	9,14,16	1.10	1 (11%)
5	PSU	L5	1536	5	18,21,22	1.18	1 (5%)	22,30,33	1.57	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PSU	L5	3695	5	18,21,22	1.05	1 (5%)	22,30,33	1.82	6 (27%)
5	OMC	L5	2804	5	19,22,23	0.54	0	26,31,34	0.68	0
47	H2U	Pt	21	47	18,21,22	0.43	0	21,30,33	1.09	1 (4%)
5	PSU	L5	4552	5	18,21,22	0.98	1 (5%)	22,30,33	1.79	3 (13%)
5	PSU	L5	3853	5	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
5	PSU	L5	4471	5	18,21,22	1.04	1 (5%)	22,30,33	1.75	3 (13%)
5	1MA	L5	1322	5	21,25,26	0.48	0	31,37,40	0.76	0
5	OMG	L5	2424	5	23,26,27	0.51	0	33,38,41	0.47	0
5	OMG	L5	3899	5	23,26,27	0.53	0	33,38,41	0.70	0
5	OMG	L5	4623	5	23,26,27	0.67	0	33,38,41	0.67	0
5	OMC	L5	2351	5	19,22,23	0.56	0	26,31,34	1.06	2 (7%)
5	OMG	L5	3627	5	23,26,27	0.53	0	33,38,41	0.61	0
5	A2M	L5	1534	5	22,25,26	0.18	0	31,36,39	0.44	0
5	PSU	L5	1781	5	18,21,22	0.87	1 (5%)	22,30,33	0.65	0
5	5MC	L5	4447	5	18,22,23	0.73	0	26,32,35	0.61	0
31	MLZ	Lb	5	31	8,9,10	0.72	0	4,9,11	0.67	0
16	V5N	La	39	16	9,11,12	0.47	0	9,14,16	0.97	1 (11%)
5	OMG	L5	1522	5	23,26,27	0.49	0	33,38,41	0.61	0
5	PSU	L5	2632	5	18,21,22	1.08	1 (5%)	22,30,33	1.64	5 (22%)
5	OMC	L5	3808	5	19,22,23	0.57	0	26,31,34	0.59	0
5	A2M	L5	2363	5	22,25,26	0.20	0	31,36,39	0.37	0
5	PSU	L5	4299	5	18,21,22	1.01	1 (5%)	22,30,33	1.65	3 (13%)
5	OMU	L5	4227	5	19,22,23	3.06	8 (42%)	26,31,34	1.69	4 (15%)
5	PSU	L5	2839	5	18,21,22	0.89	1 (5%)	22,30,33	0.66	0
5	OMC	L5	3869	5	19,22,23	0.57	0	26,31,34	0.71	0
5	PSU	L5	4423	5	18,21,22	1.02	1 (5%)	22,30,33	1.77	3 (13%)
5	OMC	L5	2365	5	19,22,23	0.29	0	26,31,34	0.50	0
5	PSU	L5	3770	5	18,21,22	1.04	1 (5%)	22,30,33	1.75	4 (18%)
5	PSU	L5	4532	5	18,21,22	0.90	1 (5%)	22,30,33	0.66	0
5	A2M	L5	3718	5	22,25,26	3.19	10 (45%)	31,36,39	2.85	11 (35%)
5	PSU	L5	5001	5	18,21,22	1.08	1 (5%)	22,30,33	1.82	5 (22%)
5	A2M	L5	398	5	22,25,26	0.16	0	31,36,39	0.40	0
5	OMG	L5	4370	5	23,26,27	0.47	0	33,38,41	0.56	0
5	A2M	L5	4590	5	22,25,26	3.15	9 (40%)	31,36,39	2.97	13 (41%)
5	PSU	L5	2508	5	18,21,22	1.01	1 (5%)	22,30,33	1.73	4 (18%)
47	4SU	Pt	8	47	18,21,22	0.36	0	26,30,33	1.21	3 (11%)
5	A2M	L5	1524	5	22,25,26	0.23	0	31,36,39	0.54	0
44	MLZ	Lo	53	44	8,9,10	0.74	0	4,9,11	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	OMG	L5	4499	5	23,26,27	0.49	0	33,38,41	0.56	0
5	PSU	L5	3762	5	18,21,22	1.11	1 (5%)	22,30,33	1.74	4 (18%)
5	5MC	L5	3782	5	18,22,23	0.57	0	26,32,35	0.56	0
5	A2M	L5	3785	5	22,25,26	3.18	10 (45%)	31,36,39	3.09	14 (45%)
5	OMC	L5	4536	5	19,22,23	0.58	0	26,31,34	0.67	0
5	PSU	L5	3734	5	18,21,22	0.98	1 (5%)	22,30,33	1.71	4 (18%)
5	OMC	L5	1340	5	19,22,23	0.56	0	26,31,34	0.77	0
4	PSU	L8	69	4	18,21,22	0.87	1 (5%)	22,30,33	0.78	1 (4%)
5	PSU	L5	1779	5	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
5	PSU	L5	2843	5	18,21,22	0.89	1 (5%)	22,30,33	0.82	1 (4%)

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
5	PSU	L5	4420	5	-	4/7/25/26	0/2/2/2
5	PSU	L5	3637	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	1326	5	-	2/9/27/28	0/3/3/3
5	OMG	L5	4618	5	-	0/9/27/28	0/3/3/3
5	PSU	L5	4493	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4576	5	-	0/7/25/26	0/2/2/2
47	G7M	Pt	47	47	-	0/7/25/26	0/3/3/3
5	PSU	L5	4972	5	-	0/7/25/26	0/2/2/2
5	OMG	L5	3792	5	-	0/9/27/28	0/3/3/3
5	A2M	L5	2815	5	-	2/9/27/28	0/3/3/3
5	A2M	L5	3867	5	-	1/9/27/28	0/3/3/3
5	OMG	L5	4637	5	-	1/9/27/28	0/3/3/3
5	PSU	L5	3639	5	-	0/7/25/26	0/2/2/2
5	OMG	L5	2364	5	-	2/9/27/28	0/3/3/3
5	A2M	L5	3723	5	-	1/9/27/28	0/3/3/3
5	PSU	L5	3920	5	-	0/7/25/26	0/2/2/2
5	OMU	L5	4306	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	4353	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4361	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	2401	5	-	0/9/27/28	0/3/3/3
5	PSU	L5	1744	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	1677	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	3758	5	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	L5	4689	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4312	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	1582	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	3830	5	-	0/9/27/28	0/3/3/3
5	OMG	L5	4228	5	-	0/9/27/28	0/3/3/3
5	OMG	L5	4392	5	-	0/9/27/28	0/3/3/3
3	HIC	LB	245	3	-	0/5/6/8	0/1/1/1
5	PSU	L5	3884	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	3715	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	1782	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	3825	5	-	0/9/27/28	0/3/3/3
5	OMG	L5	4494	5	-	1/9/27/28	0/3/3/3
5	A2M	L5	3724	5	-	1/9/27/28	0/3/3/3
5	OMG	L5	1316	5	-	0/9/27/28	0/3/3/3
5	OMU	L5	3925	5	-	1/9/27/28	0/2/2/2
5	PSU	L5	4500	5	-	1/7/25/26	0/2/2/2
5	OMG	L5	2876	5	-	0/9/27/28	0/3/3/3
5	PSU	L5	1792	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	2787	5	-	3/9/27/28	0/3/3/3
5	OMC	L5	3841	5	-	0/9/27/28	0/2/2/2
5	UR3	L5	4530	5	-	0/7/25/26	0/2/2/2
5	OMG	L5	3944	5	-	1/9/27/28	0/3/3/3
5	PSU	L5	1683	5	-	0/7/25/26	0/2/2/2
5	OMC	L5	3887	5	-	0/9/27/28	0/2/2/2
4	OMG	L8	75	4	-	1/9/27/28	0/3/3/3
5	OMC	L5	2422	5	-	2/9/27/28	0/2/2/2
5	OMC	L5	2861	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	4457	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4531	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	4523	5	-	0/9/27/28	0/3/3/3
42	M3L	Lm	98	42	-	0/9/10/12	-
5	PSU	L5	3764	5	-	1/7/25/26	0/2/2/2
5	OMU	L5	2837	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	4673	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	3844	5	-	1/7/25/26	0/2/2/2
5	PSU	L5	3729	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4442	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4628	5	-	0/7/25/26	0/2/2/2
5	OMC	L5	3701	5	-	4/9/27/28	0/2/2/2
5	OMG	L5	1625	5	-	1/9/27/28	0/3/3/3
5	6MZ	L5	4220	5	-	0/9/27/28	0/3/3/3
5	PSU	L5	4403	5	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	L5	3768	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4569	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4579	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4293	5	-	1/7/25/26	0/2/2/2
5	OMG	L5	3744	5	-	0/9/27/28	0/3/3/3
5	OMC	L5	4456	5	-	0/9/27/28	0/2/2/2
47	PSU	Pt	56	47	-	0/7/25/26	0/2/2/2
5	A2M	L5	400	5	-	0/9/27/28	0/3/3/3
5	A2M	L5	1871	5	-	0/9/27/28	0/3/3/3
5	OMC	L5	2824	5	-	1/9/27/28	0/2/2/2
5	PSU	L5	1862	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4296	5	-	0/7/25/26	0/2/2/2
4	OMU	L8	14	5,4	-	1/9/27/28	0/2/2/2
5	A2M	L5	4571	5	-	0/9/27/28	0/3/3/3
5	A2M	L5	3760	5	-	3/9/27/28	0/3/3/3
5	OMU	L5	2415	5	-	1/9/27/28	0/2/2/2
5	OMG	L5	4196	47,5	-	1/9/27/28	0/3/3/3
5	OMU	L5	4498	5	-	1/9/27/28	0/2/2/2
5	PSU	L5	4521	5	-	1/7/25/26	0/2/2/2
5	OMU	L5	4620	5	-	1/9/27/28	0/2/2/2
5	UY1	L5	3818	5	-	2/9/27/28	0/2/2/2
5	PSU	L5	4431	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	1860	5	-	0/7/25/26	0/2/2/2
47	OMC	Pt	33	47	-	1/9/27/28	0/2/2/2
5	OMC	L5	1881	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	5010	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4636	5	-	2/7/25/26	0/2/2/2
5	PSU	L5	3851	5	-	1/7/25/26	0/2/2/2
4	PSU	L8	55	4	-	0/7/25/26	0/2/2/2
2	V5N	LA	216	2	-	1/9/10/12	0/1/1/1
5	PSU	L5	1536	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	3695	5	-	0/7/25/26	0/2/2/2
5	OMC	L5	2804	5	-	0/9/27/28	0/2/2/2
47	H2U	Pt	21	47	-	3/7/38/39	0/2/2/2
5	PSU	L5	4552	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	3853	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4471	5	-	0/7/25/26	0/2/2/2
5	1MA	L5	1322	5	-	0/7/25/26	0/3/3/3
5	OMG	L5	2424	5	-	0/9/27/28	0/3/3/3
5	OMG	L5	3899	5	-	0/9/27/28	0/3/3/3
5	OMG	L5	4623	5	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OMC	L5	2351	5	-	3/9/27/28	0/2/2/2
5	OMG	L5	3627	5	-	0/9/27/28	0/3/3/3
5	A2M	L5	1534	5	-	2/9/27/28	0/3/3/3
5	PSU	L5	1781	5	-	0/7/25/26	0/2/2/2
5	5MC	L5	4447	5	-	4/7/25/26	0/2/2/2
31	MLZ	Lb	5	31	-	2/7/8/10	-
16	V5N	La	39	16	-	1/9/10/12	0/1/1/1
5	OMG	L5	1522	5	-	0/9/27/28	0/3/3/3
5	PSU	L5	2632	5	-	0/7/25/26	0/2/2/2
5	OMC	L5	3808	5	-	0/9/27/28	0/2/2/2
5	A2M	L5	2363	5	-	0/9/27/28	0/3/3/3
5	PSU	L5	4299	5	-	0/7/25/26	0/2/2/2
5	OMU	L5	4227	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	2839	5	-	0/7/25/26	0/2/2/2
5	OMC	L5	3869	5	-	2/9/27/28	0/2/2/2
5	PSU	L5	4423	5	-	0/7/25/26	0/2/2/2
5	OMC	L5	2365	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	3770	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	4532	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	3718	5	-	0/9/27/28	0/3/3/3
5	PSU	L5	5001	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	398	5	-	1/9/27/28	0/3/3/3
5	OMG	L5	4370	5	-	0/9/27/28	0/3/3/3
5	A2M	L5	4590	5	-	2/9/27/28	0/3/3/3
5	PSU	L5	2508	5	-	0/7/25/26	0/2/2/2
47	4SU	Pt	8	47	-	0/7/25/26	0/2/2/2
5	A2M	L5	1524	5	-	1/9/27/28	0/3/3/3
44	MLZ	Lo	53	44	-	2/7/8/10	-
5	OMG	L5	4499	5	-	1/9/27/28	0/3/3/3
5	PSU	L5	3762	5	-	0/7/25/26	0/2/2/2
5	5MC	L5	3782	5	-	0/7/25/26	0/2/2/2
5	A2M	L5	3785	5	-	3/9/27/28	0/3/3/3
5	OMC	L5	4536	5	-	0/9/27/28	0/2/2/2
5	PSU	L5	3734	5	-	0/7/25/26	0/2/2/2
5	OMC	L5	1340	5	-	0/9/27/28	0/2/2/2
4	PSU	L8	69	4	-	0/7/25/26	0/2/2/2
5	PSU	L5	1779	5	-	0/7/25/26	0/2/2/2
5	PSU	L5	2843	5	-	0/7/25/26	0/2/2/2

The worst 5 of 213 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L5	3760	A2M	C3'-C4'	-8.78	1.30	1.53
5	L5	3723	A2M	C3'-C4'	-8.70	1.30	1.53
5	L5	4571	A2M	C3'-C4'	-8.68	1.30	1.53
5	L5	3867	A2M	C3'-C4'	-8.60	1.31	1.53
5	L5	3718	A2M	C3'-C4'	-8.55	1.31	1.53

The worst 5 of 349 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L5	3760	A2M	N6-C6-N1	-6.89	103.25	118.35
5	L5	3718	A2M	N6-C6-N1	-6.89	103.25	118.35
5	L5	4590	A2M	N6-C6-N1	-6.70	103.68	118.35
5	L5	3724	A2M	N6-C6-N1	-6.68	103.73	118.35
5	L5	4571	A2M	N6-C6-N1	-6.57	103.97	118.35

There are no chirality outliers.

5 of 78 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	Lb	5	MLZ	N-CA-CB-CG
31	Lb	5	MLZ	C-CA-CB-CG
4	L8	14	OMU	C1'-C2'-O2'-CM2
4	L8	75	OMG	C1'-C2'-O2'-CM2
5	L5	398	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

36 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L5	2815	A2M	1	0
5	L5	4637	OMG	1	0
5	L5	3723	A2M	3	0
5	L5	4312	PSU	1	0
5	L5	3724	A2M	1	0
5	L5	2876	OMG	1	0
5	L5	3944	OMG	1	0
5	L5	3887	OMC	1	0
4	L8	75	OMG	1	0
5	L5	4457	PSU	1	0
5	L5	4220	6MZ	1	0
5	L5	4293	PSU	1	0
5	L5	3744	OMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L5	4456	OMC	1	0
47	Pt	56	PSU	1	0
4	L8	14	OMU	1	0
5	L5	4571	A2M	1	0
5	L5	2415	OMU	1	0
5	L5	4196	OMG	1	0
5	L5	4620	OMU	1	0
47	Pt	33	OMC	1	0
5	L5	1881	OMC	1	0
47	Pt	21	H2U	1	0
5	L5	2424	OMG	1	0
5	L5	3899	OMG	1	0
5	L5	4623	OMG	3	0
5	L5	2351	OMC	1	0
5	L5	2632	PSU	1	0
5	L5	2363	A2M	1	0
5	L5	3869	OMC	2	0
5	L5	3718	A2M	4	0
5	L5	398	A2M	1	0
47	Pt	8	4SU	1	0
5	L5	4499	OMG	1	0
5	L5	3785	A2M	1	0
5	L5	1340	OMC	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 5 are monoatomic - leaving 23 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	$\#\|Z\|>2$

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	SPD	L5	5106	-	9,9,9	0.32	0	8,8,8	0.92	0
50	SPD	L5	5101	-	9,9,9	0.32	0	8,8,8	0.78	0
52	SPM	L5	5118	-	13,13,13	0.38	0	12,12,12	0.90	0
52	SPM	L5	5116	-	13,13,13	0.34	0	12,12,12	1.09	0
53	ADP	L5	5121	-	27,29,29	1.37	4 (14%)	42,45,45	1.91	10 (23%)
50	SPD	L5	5107	-	9,9,9	0.35	0	8,8,8	0.74	0
50	SPD	L5	5109	-	9,9,9	0.32	0	8,8,8	0.42	0
52	SPM	L5	5111	-	13,13,13	0.36	0	12,12,12	0.86	0
52	SPM	L5	5120	-	13,13,13	0.36	0	12,12,12	0.88	0
50	SPD	L5	5113	-	9,9,9	8.37	7 (77%)	8,8,8	0.67	0
50	SPD	L5	5102	-	9,9,9	0.37	0	8,8,8	0.76	0
50	SPD	L5	5112	-	9,9,9	0.34	0	8,8,8	0.81	0
52	SPM	L5	5119	-	13,13,13	0.37	0	12,12,12	0.78	0
51	PUT	L5	5110	-	5,5,5	0.12	0	4,4,4	0.20	0
52	SPM	L5	5117	-	13,13,13	0.35	0	12,12,12	0.83	0
50	SPD	L5	5103	-	9,9,9	0.32	0	8,8,8	0.81	0
50	SPD	L5	5104	-	9,9,9	0.33	0	8,8,8	0.82	0
50	SPD	L5	5105	-	9,9,9	0.33	0	8,8,8	0.75	0
52	SPM	L5	5114	-	13,13,13	0.37	0	12,12,12	0.84	0
52	SPM	L5	5115	-	13,13,13	0.35	0	12,12,12	0.80	0
50	SPD	L8	201	-	9,9,9	0.32	0	8,8,8	0.81	0
50	SPD	LN	301	-	9,9,9	0.30	0	8,8,8	0.75	0
50	SPD	L5	5108	-	9,9,9	0.32	0	8,8,8	0.79	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
50	SPD	L5	5106	-	-	4/7/7/7	-
50	SPD	L5	5101	-	-	0/7/7/7	-
52	SPM	L5	5118	-	-	3/11/11/11	-
52	SPM	L5	5116	-	-	6/11/11/11	-
53	ADP	L5	5121	-	-	5/16/32/32	0/3/3/3
50	SPD	L5	5107	-	-	4/7/7/7	-
50	SPD	L5	5109	-	-	3/7/7/7	-
52	SPM	L5	5111	-	-	3/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	SPM	L5	5120	-	-	3/11/11/11	-
50	SPD	L5	5113	-	-	2/7/7/7	-
50	SPD	L5	5102	-	-	2/7/7/7	-
50	SPD	L5	5112	-	-	1/7/7/7	-
52	SPM	L5	5119	-	-	4/11/11/11	-
51	PUT	L5	5110	-	-	0/3/3/3	-
52	SPM	L5	5117	-	-	2/11/11/11	-
50	SPD	L5	5103	-	-	1/7/7/7	-
50	SPD	L5	5104	-	-	1/7/7/7	-
50	SPD	L5	5105	-	-	2/7/7/7	-
52	SPM	L5	5114	-	-	2/11/11/11	-
52	SPM	L5	5115	-	-	3/11/11/11	-
50	SPD	L8	201	-	-	1/7/7/7	-
50	SPD	LN	301	-	-	1/7/7/7	-
50	SPD	L5	5108	-	-	1/7/7/7	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	L5	5113	SPD	C4-C5	12.55	2.02	1.51
50	L5	5113	SPD	C5-N6	11.16	1.84	1.46
50	L5	5113	SPD	C3-C2	10.54	2.02	1.51
50	L5	5113	SPD	C8-C9	10.47	2.02	1.51
50	L5	5113	SPD	C4-C3	9.08	2.02	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	L5	5121	ADP	C5-C4-N3	-6.35	118.47	126.75
53	L5	5121	ADP	N3-C4-N9	4.82	135.03	127.08
53	L5	5121	ADP	C2-N3-C4	3.88	120.91	111.75
53	L5	5121	ADP	C4-C5-N7	-3.50	106.36	110.62
53	L5	5121	ADP	N3-C2-N1	-2.96	123.97	128.60

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	L5	5121	ADP	C5'-O5'-PA-O1A
50	L5	5113	SPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
50	L5	5108	SPD	C3-C4-C5-N6
52	L5	5116	SPM	N5-C6-C7-C8
52	L5	5119	SPM	C7-C8-C9-N10

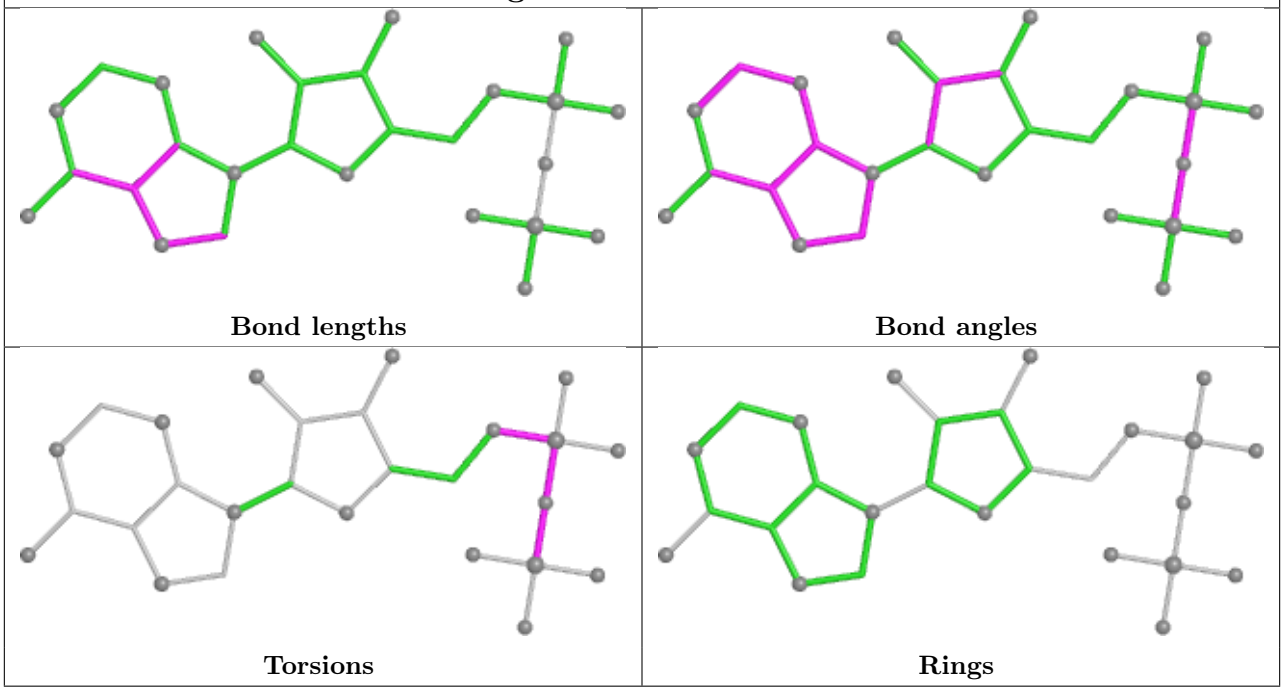
There are no ring outliers.

10 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	L5	5118	SPM	2	0
50	L5	5109	SPD	4	0
52	L5	5111	SPM	1	0
52	L5	5120	SPM	1	0
50	L5	5113	SPD	9	0
51	L5	5110	PUT	1	0
52	L5	5117	SPM	1	0
50	L5	5105	SPD	1	0
52	L5	5115	SPM	1	0
50	LN	301	SPD	1	0

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

Ligand ADP L5 5121



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.

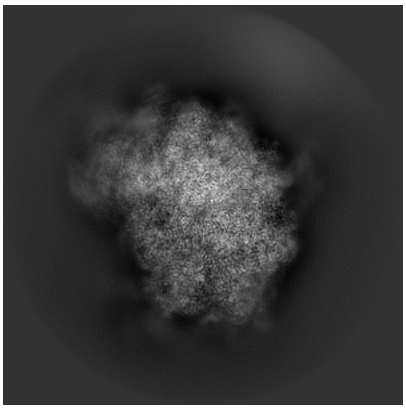
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66936. These allow visual inspection of the internal detail of the map and identification of artifacts.

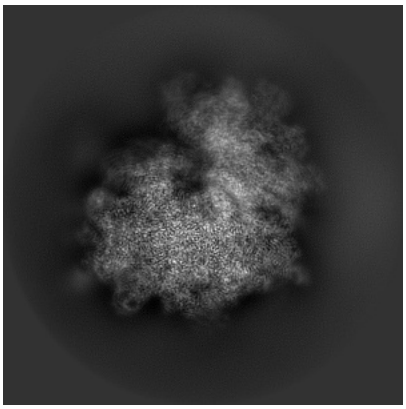
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

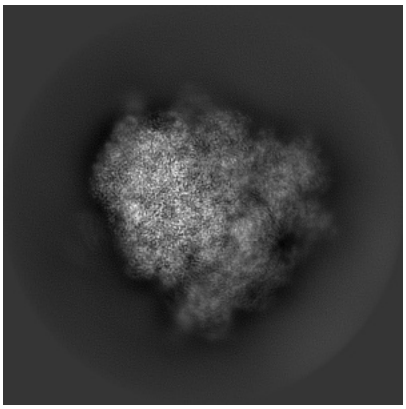
6.1.1 Primary map



X

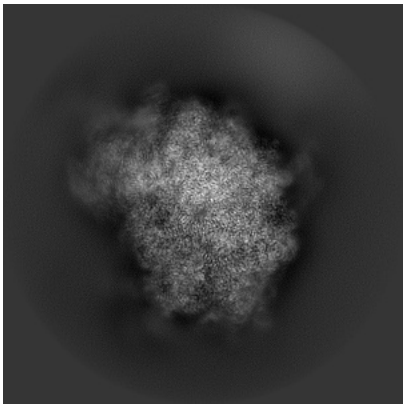


Y

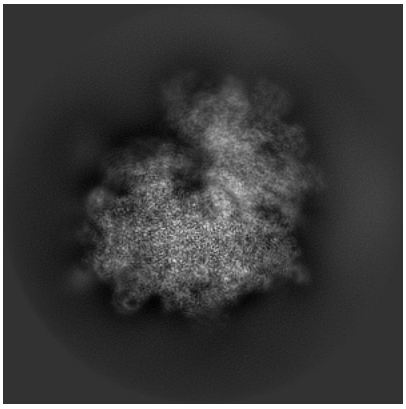


Z

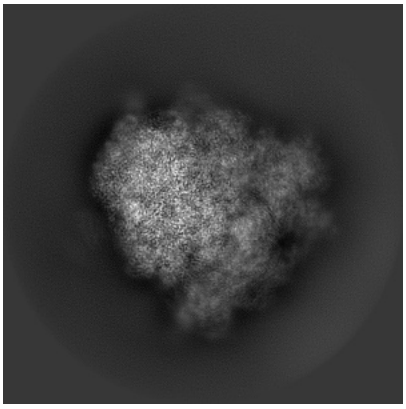
6.1.2 Raw map



X



Y

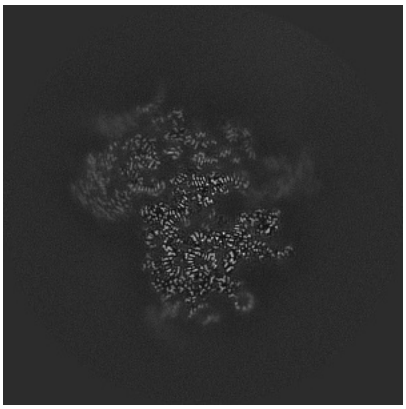


Z

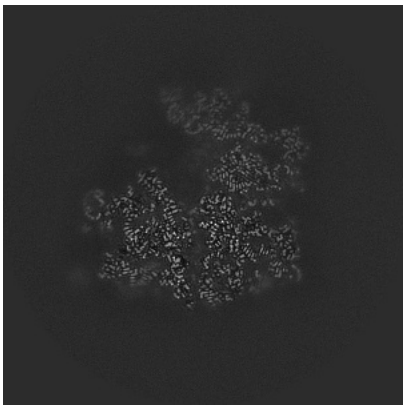
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

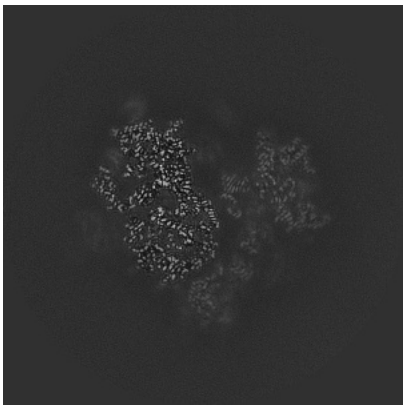
6.2.1 Primary map



X Index: 240

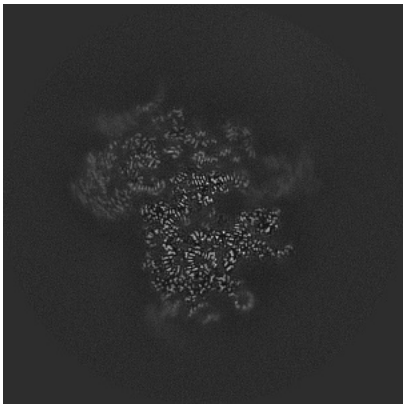


Y Index: 240

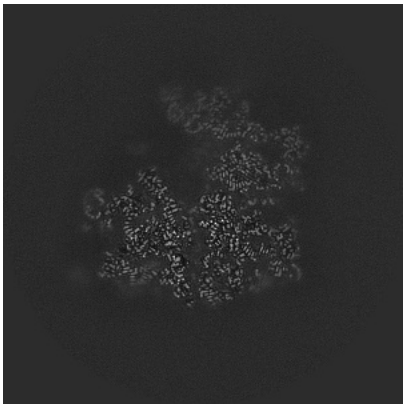


Z Index: 240

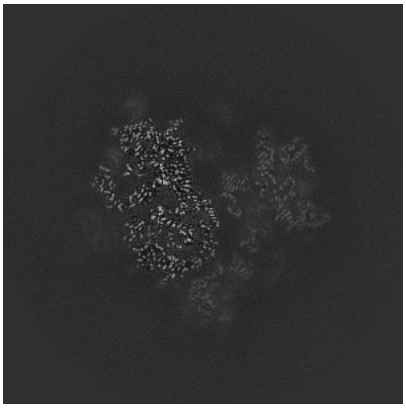
6.2.2 Raw map



X Index: 240



Y Index: 240

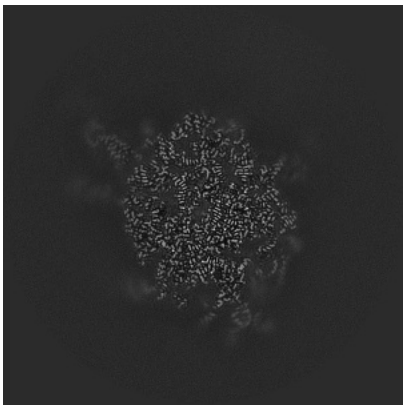


Z Index: 240

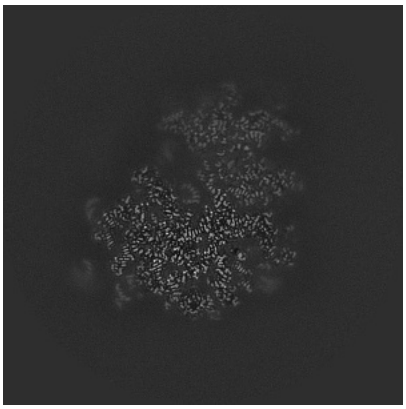
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

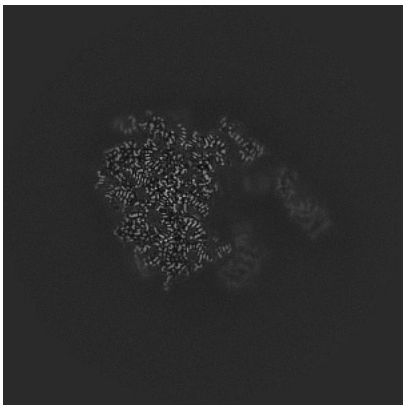
6.3.1 Primary map



X Index: 207

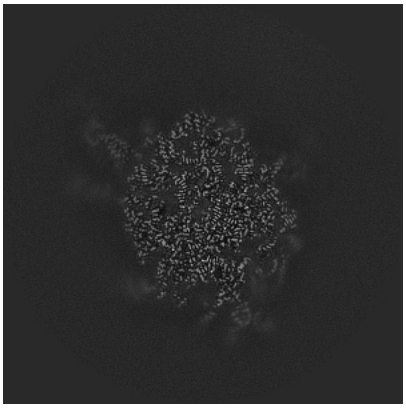


Y Index: 255

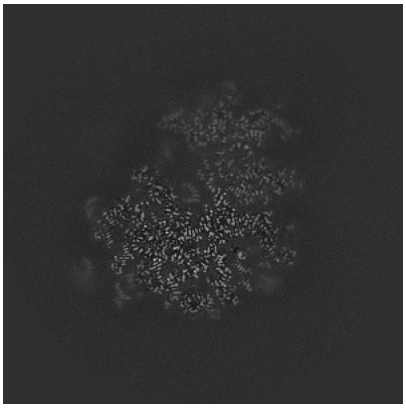


Z Index: 204

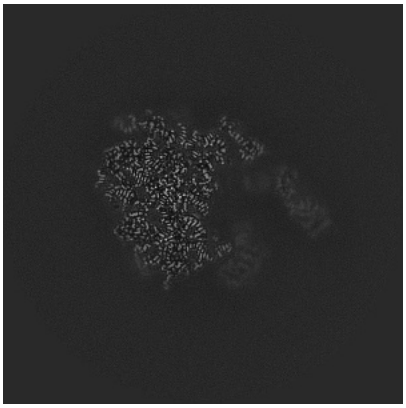
6.3.2 Raw map



X Index: 207



Y Index: 255

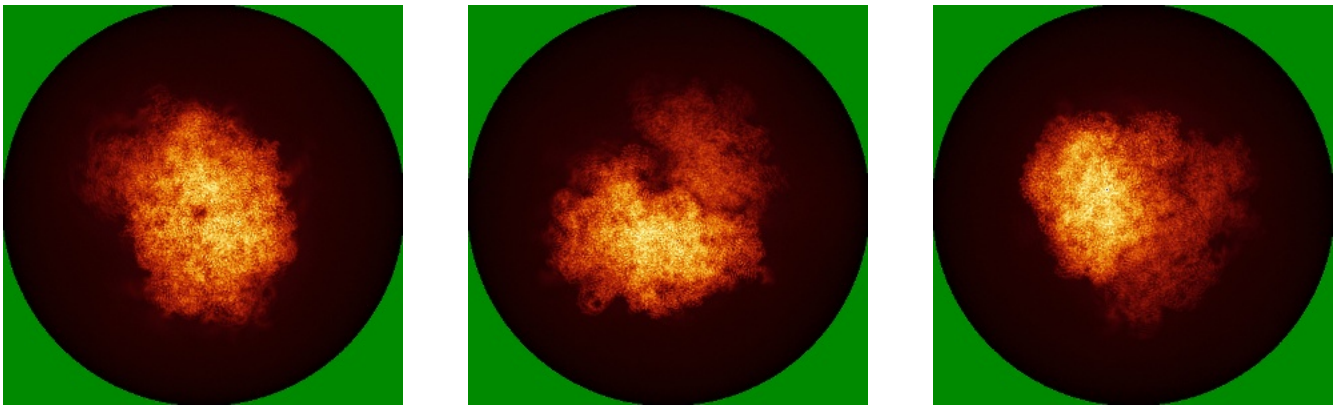


Z Index: 204

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

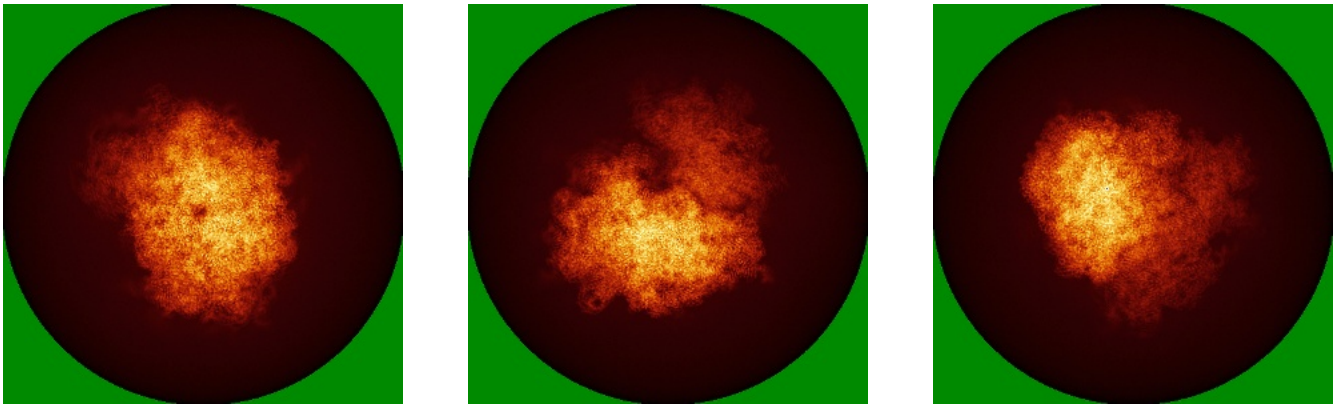
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

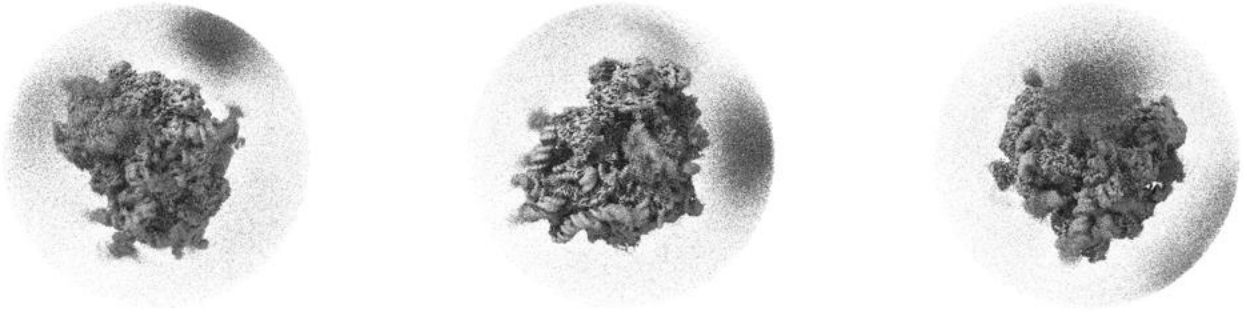


X Y Z

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)

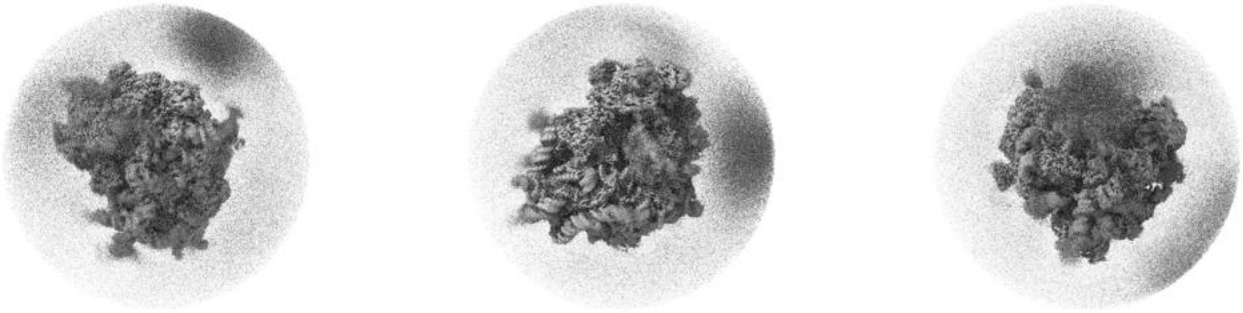
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.003. 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.

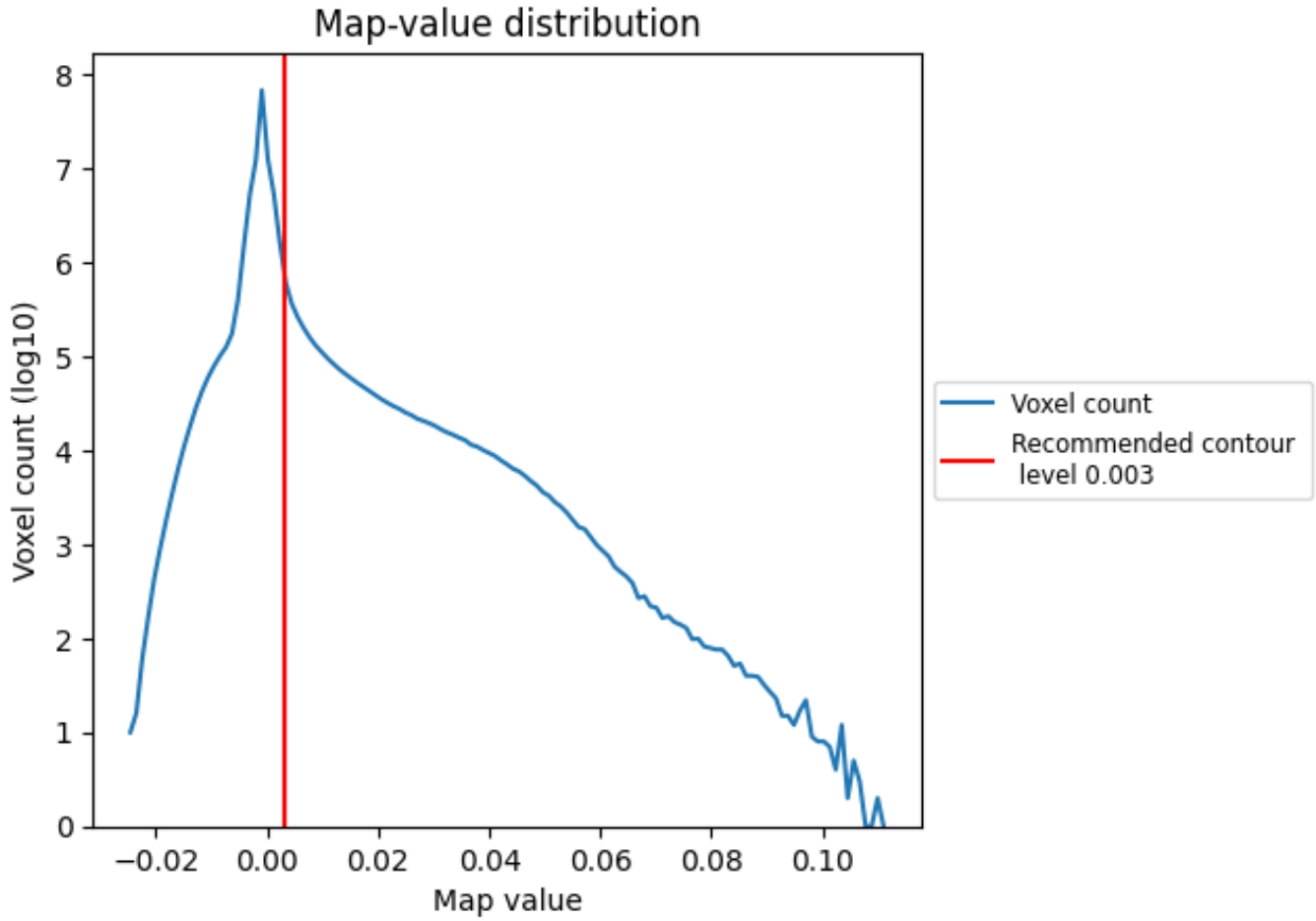
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

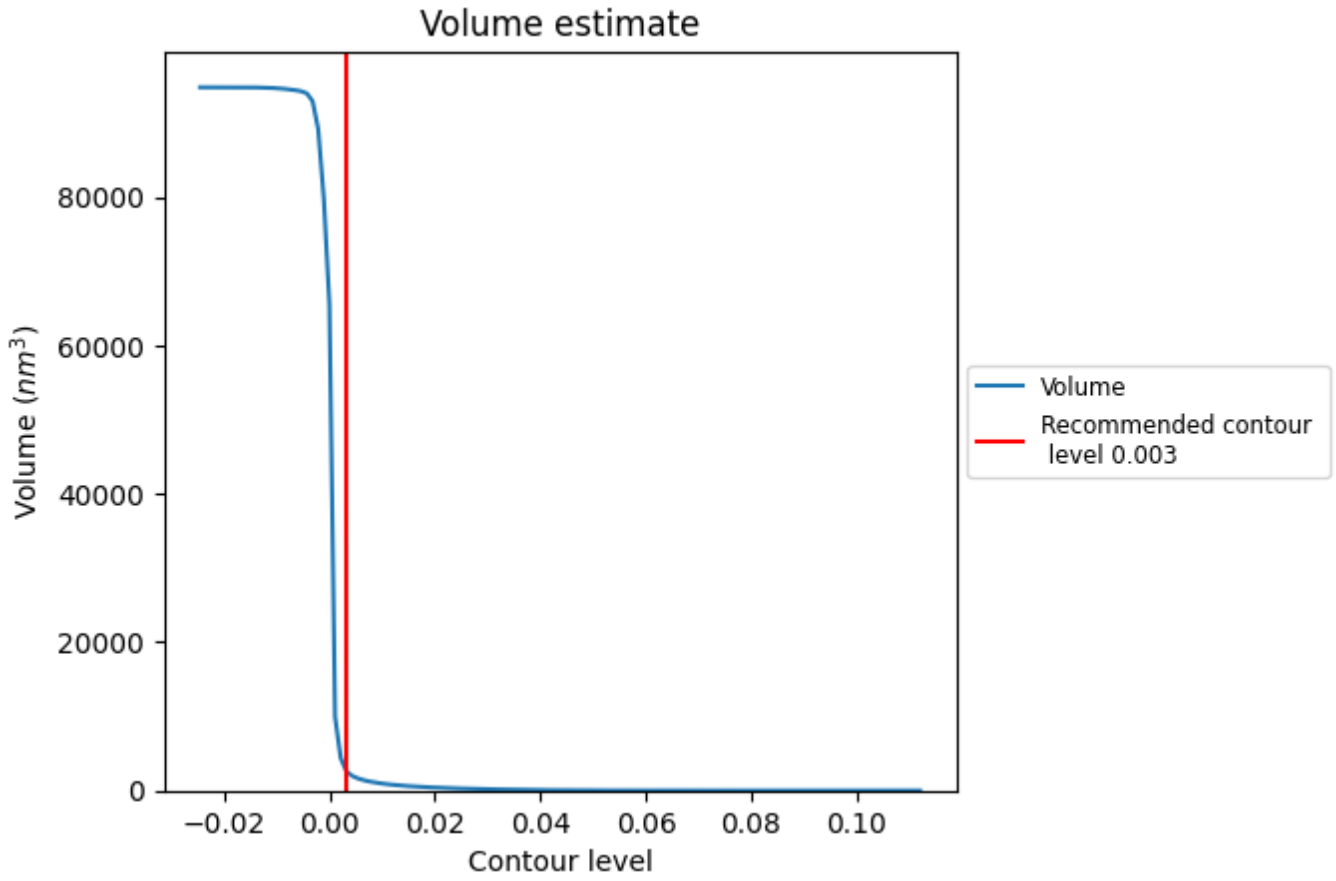
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

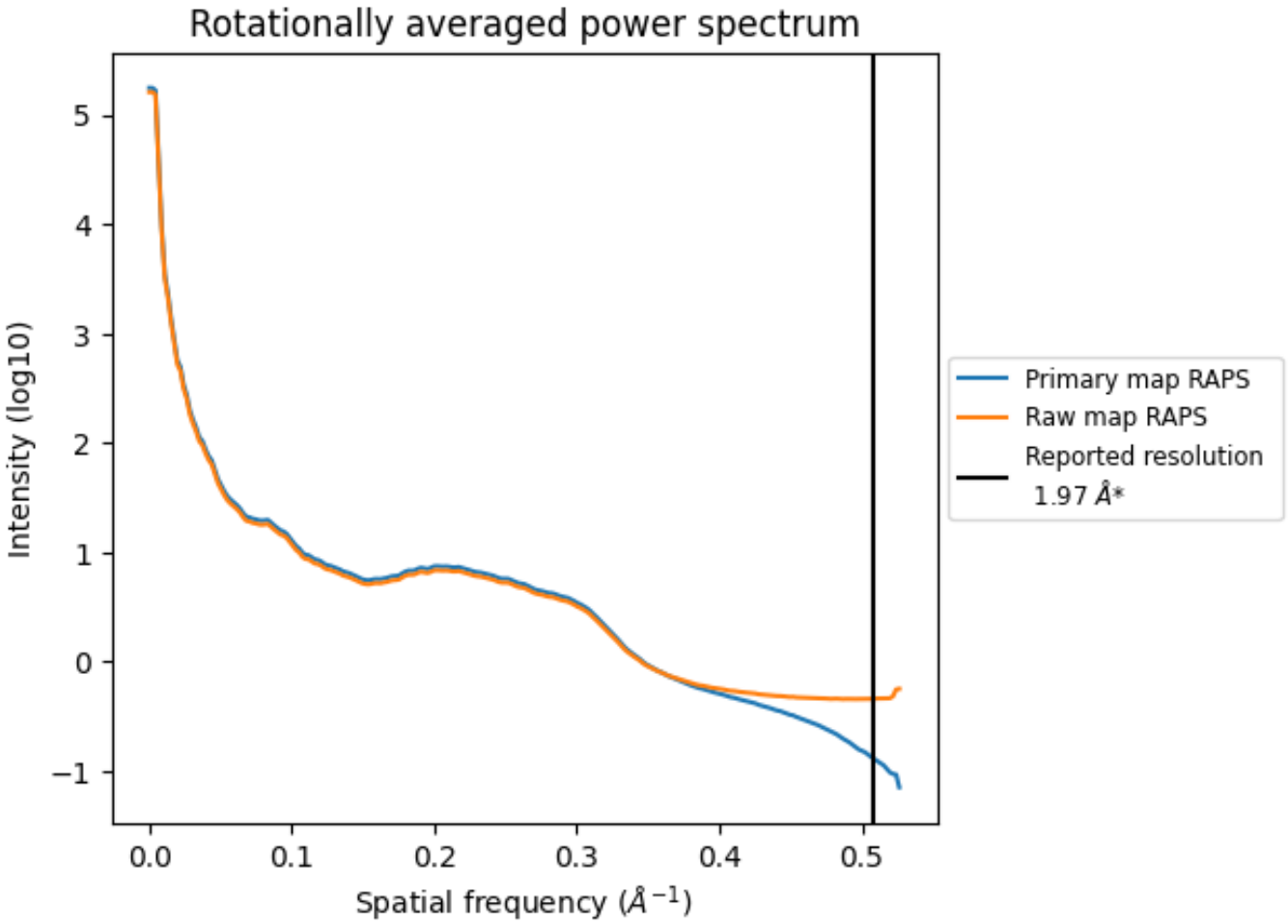
7.2 Volume estimate (i)



The volume at the recommended contour level is 2886 nm^3; this corresponds to an approximate mass of 2607 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)

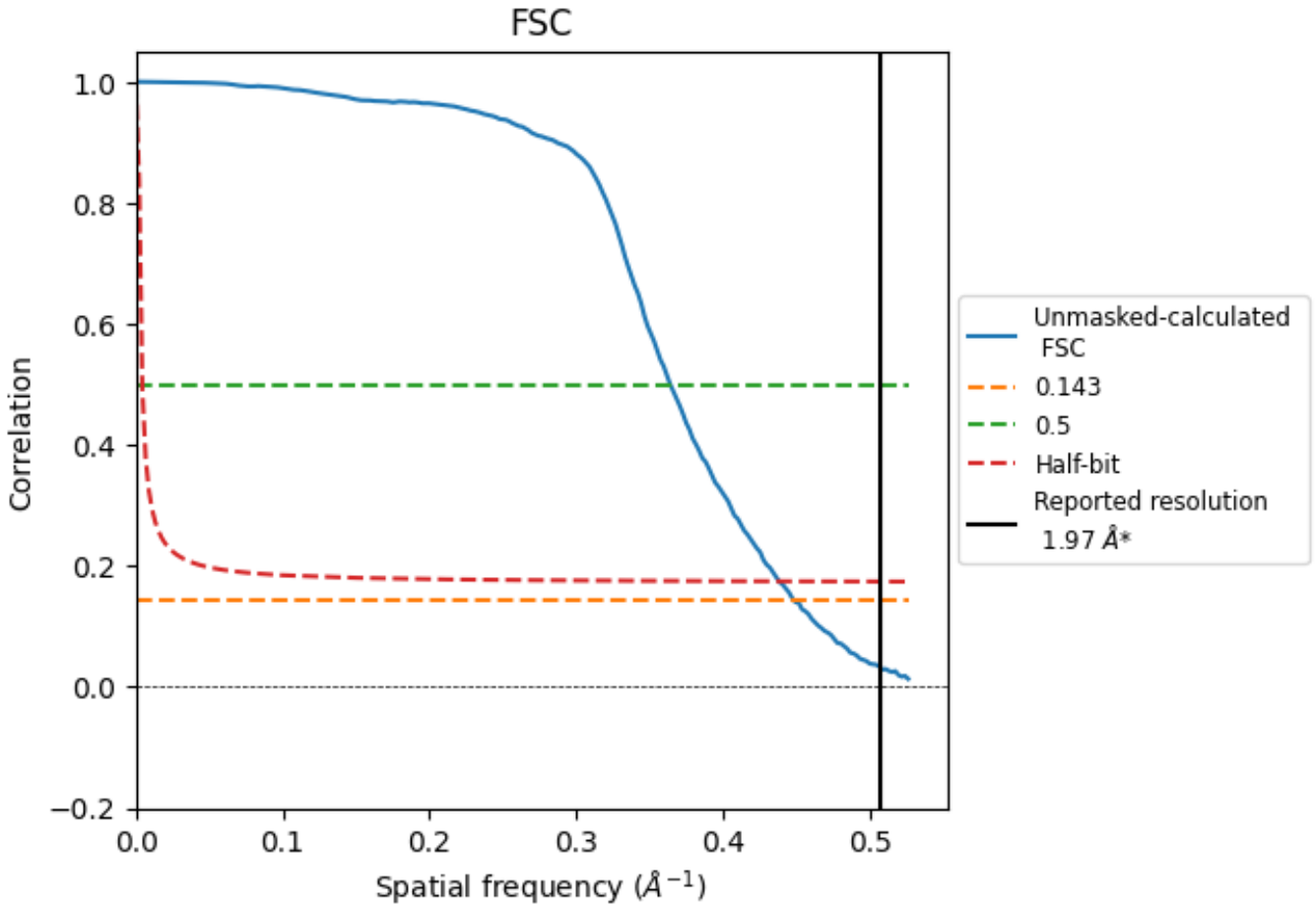


*Reported resolution corresponds to spatial frequency of 0.508 Å^{-1}

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 0.508 Å^{-1}

8.2 Resolution estimates (i)

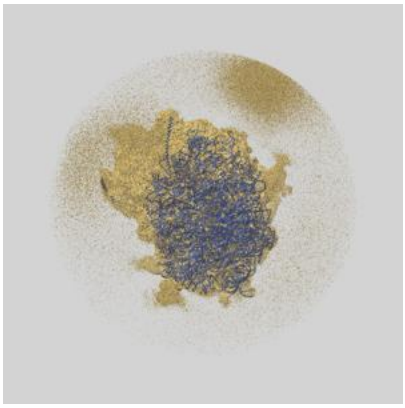
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.97	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.23	2.75	2.28

*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 2.23 differs from the reported value 1.97 by more than 10 %

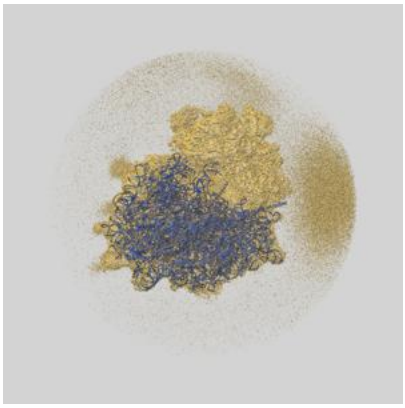
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66936 and PDB model 9XJH. Per-residue inclusion information can be found in section 3 on page 16.

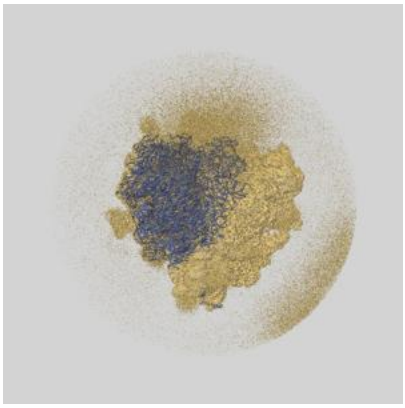
9.1 Map-model overlay



X



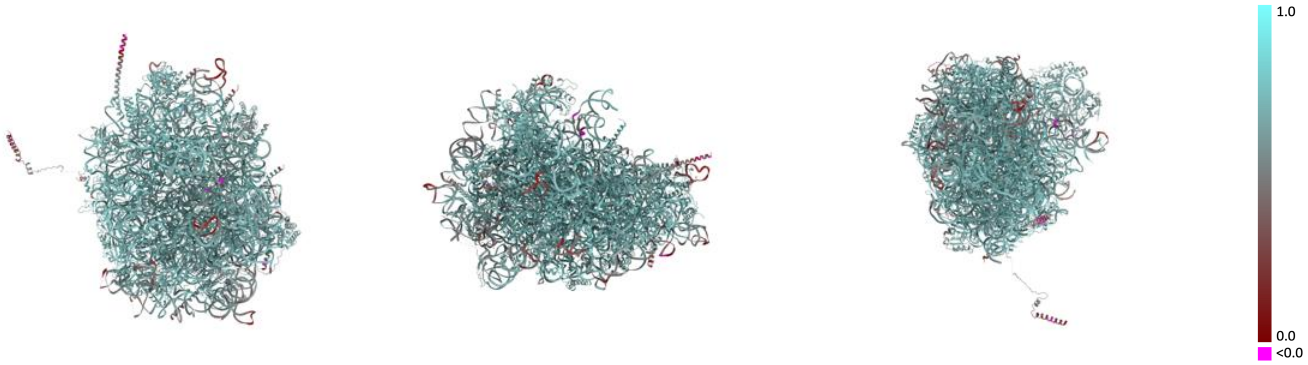
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003 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.

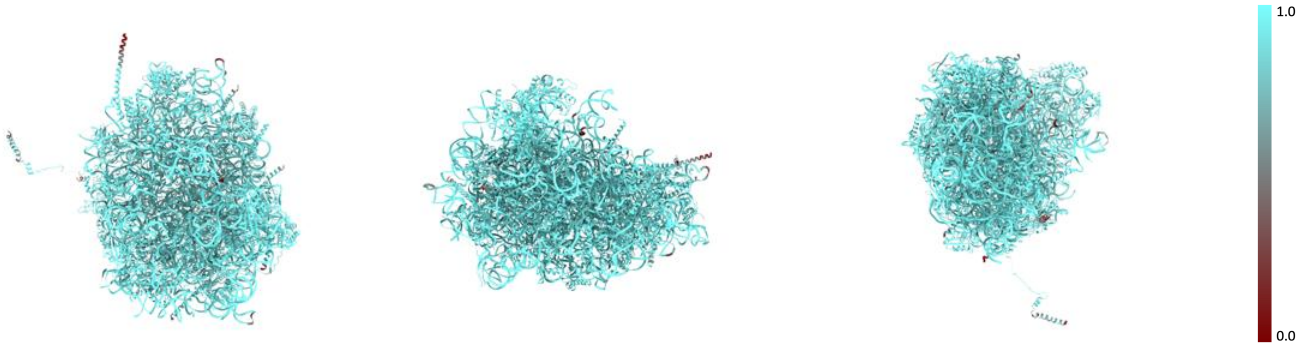
9.2 Q-score mapped to coordinate model (i)



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.

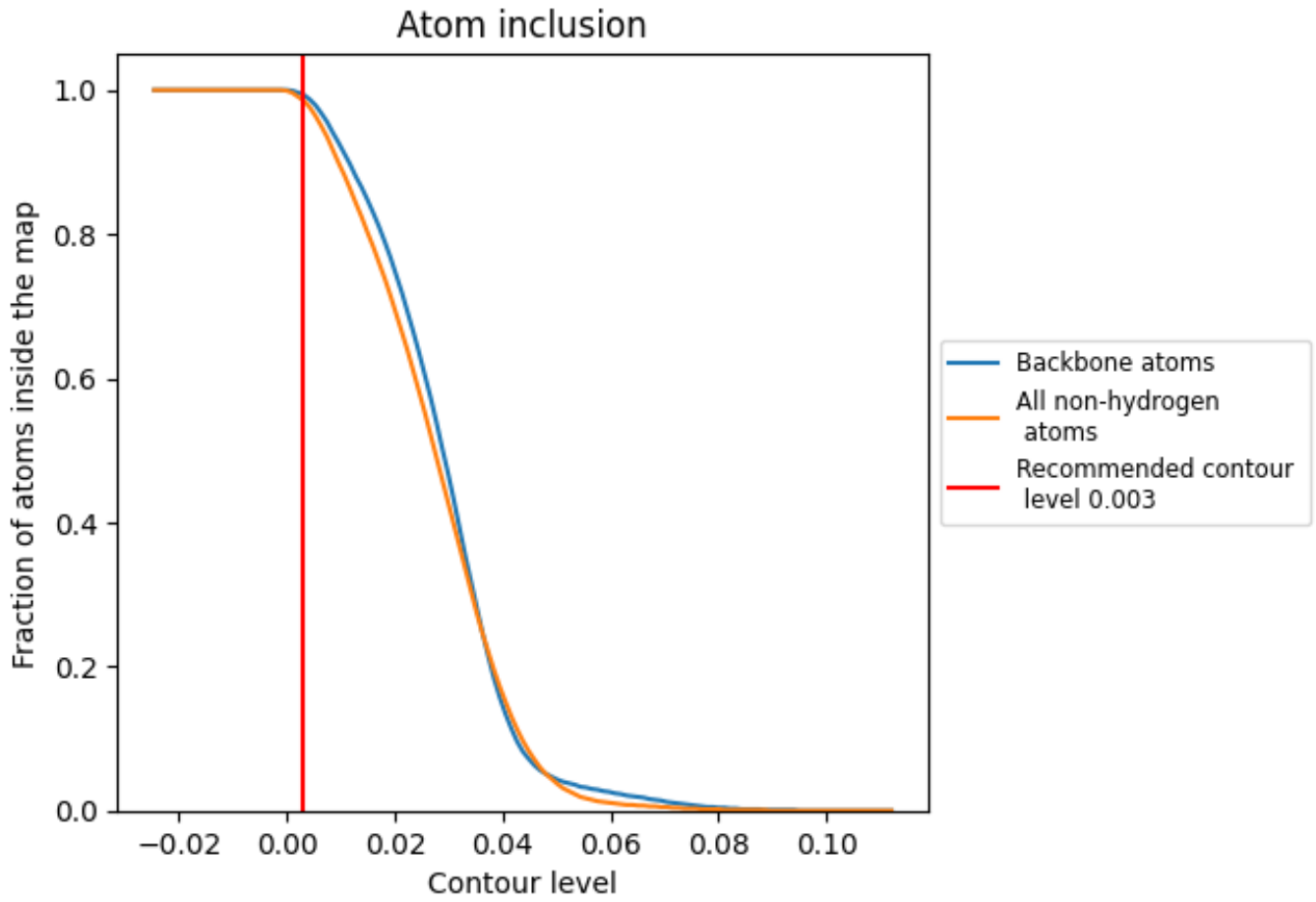
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.003).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9860	0.6770
A	0.8150	0.5350
CB	0.9600	0.6660
L5	0.9920	0.6650
L7	0.9970	0.6870
L8	0.9970	0.6890
LA	0.9940	0.7410
LB	0.9820	0.7170
LC	0.9830	0.7190
LD	0.9760	0.6630
LE	0.9880	0.6770
LF	0.9930	0.7160
LG	0.9440	0.6500
LH	0.9860	0.6900
LI	0.9810	0.6960
LJ	0.9720	0.6290
LL	0.9790	0.7000
LM	0.9910	0.6960
LN	0.9990	0.7470
LO	0.9930	0.7210
LP	0.9720	0.7200
LQ	0.9970	0.7370
LR	0.9090	0.6320
LS	0.9970	0.7200
LT	0.9740	0.6960
LU	0.9550	0.5940
LV	0.9950	0.7270
LW	0.8720	0.5230
LX	0.9850	0.7070
LY	0.9850	0.7000
LZ	0.9860	0.6880
La	0.9940	0.7380
Lb	0.9440	0.6380
Lc	0.9750	0.6880
Ld	0.9760	0.6890



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Chain	Atom inclusion	Q-score
Le	0.9930	0.7350
Lf	0.9910	0.7350
Lg	0.9760	0.7040
Lh	0.9840	0.6970
Li	0.9760	0.6850
Lj	0.9990	0.7420
Lk	0.9500	0.6330
Ll	0.9950	0.7200
Lm	0.9880	0.7050
Ln	0.9860	0.6920
Lo	0.9910	0.7120
Lp	0.9800	0.7140
Lr	0.9940	0.7170
Pt	0.9480	0.5630
mR	1.0000	0.6720