wwPDB EM Validation Summary Report

Nov 2, 2026 – 02:57 PM JST

PDB ID	:	9XJA / pdb_00009xja
EMDB ID	:	EMD-66933
Title	:	In situ portimine A-bound human pre-60S ribosome from intact HEK293T cells
Authors	:	Wang, Y.; Zhang, Y.; Gao, N.
Deposited on	:	2025-11-04
Resolution	:	2.51 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:

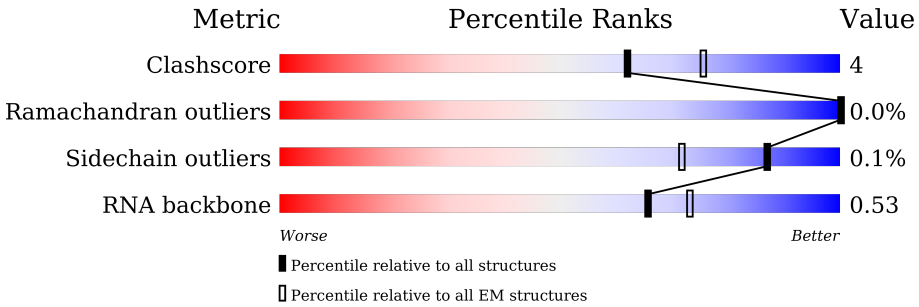
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

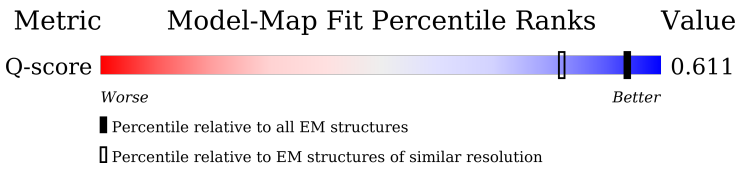
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.51 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	7159 (2.01 - 3.01)

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	LA	252	94% 6%
2	LB	403	92% 7%
3	L8	156	72% 28%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	L5	5069	47% 19% 30%
5	L7	120	84% 15%
6	LC	427	79% 7% 14%
7	LJ	178	5% 76% 20%
8	LH	192	89% 10%
9	LE	288	68% 9% 23%
10	LG	266	10% 77% 13% 9%
11	LO	203	88% 11%
12	LL	211	86% 12%
13	LV	140	91% 5%
14	LM	215	58% 5% 37%
15	La	148	95% 5%
16	LN	204	94% 5%
17	LI	214	86% 9% 5%
18	LD	297	90% 9%
19	LQ	188	92% 7%
20	LR	196	19% 83% 12% 5%
21	LS	176	94% 6%
22	LT	160	94% 5%
23	LP	184	80% 7% 14%
24	LU	128	6% 60% 18% 22%
25	LX	156	73% 24%
26	LY	145	84% 8% 8%
27	LW	157	37% 59%
28	LZ	136	82% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Lr	137	79% 13% 8%
30	Lh	123	90% 9%
31	Lb	159	9% 64% 6% 30%
32	LF	248	84% 7% 9%
33	Lc	115	5% 81% 5% 14%
34	Ld	125	74% 12% 14%
35	Le	135	87% 8% 5%
36	Lf	110	96%
37	Lg	117	91% 6%
38	Li	105	88% 10%
39	Lj	97	87% 11%
40	Lk	70	86% 13%
41	Ll	51	88% 10%
42	Lm	128	40% 59%
43	Ln	25	100% 68% 32%
44	Lo	106	92% 7%
45	Lp	92	95%
46	z	394	76% 63% 26% 10%
47	6	245	41% 67% 24% 9%

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
49	SPD	L5	5227	-	-	X	-

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 140215 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 2 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 3 is a RNA chain called 5.8S rRNA.

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

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L5	3566	76516	34113	13992	24846	3565	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	L7	120	2558	1141	456	842	119	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	LC	366	2914	1832	581	487	14	0	0

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

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

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

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

- Molecule 9 is a protein called Large ribosomal subunit protein eL6.

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

- Molecule 10 is a protein called Large ribosomal subunit protein eL8.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 12 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 14 is a protein called Large ribosomal subunit protein eL14.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 16 is a protein called Large ribosomal subunit protein eL15.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LI	203	Total	C	N	O	S	0	0
			1645	1045	317	270	13		

- 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	64	Total	C	N	O	S	0	0
			534	340	104	87	3		

- 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	2	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	1	0
			1061	672	219	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 Ubiquitin-ribosomal protein eL40 fusion protein.

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 protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	z	354	Total	C	N	O	S	13	0
			2837	1792	483	543	19		

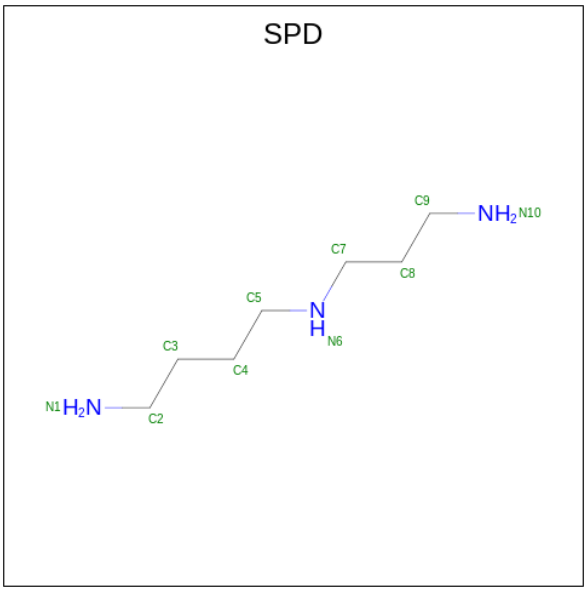
- Molecule 47 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	6	224	Total	C	N	O	S	0	0
			1704	1060	294	339	11		

- Molecule 48 is POTASSIUM ION (CCD ID: K) (formula: K).

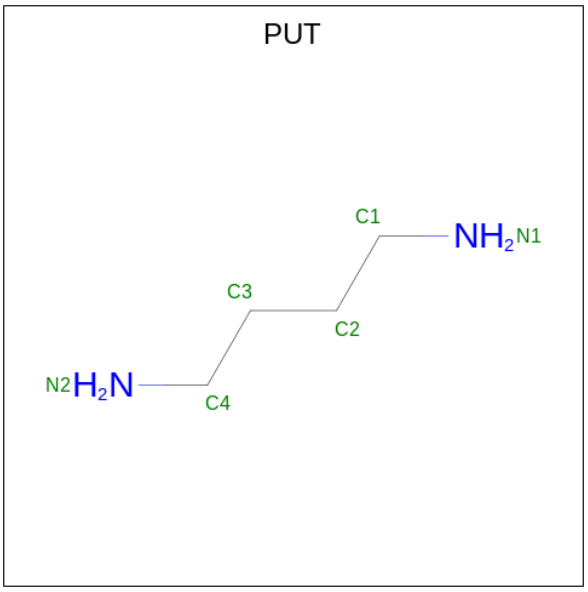
Mol	Chain	Residues	Atoms	AltConf
48	LA	3	Total K 3 3	0
48	LB	1	Total K 1 1	0
48	L8	2	Total K 2 2	0
48	L5	111	Total K 111 111	0
48	L7	4	Total K 4 4	0
48	LH	1	Total K 1 1	0
48	LN	2	Total K 2 2	0
48	LI	1	Total K 1 1	0
48	LQ	1	Total K 1 1	0
48	Lb	1	Total K 1 1	0
48	Le	1	Total K 1 1	0
48	Lf	2	Total K 2 2	0
48	Lg	1	Total K 1 1	0
48	Ll	1	Total K 1 1	0

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



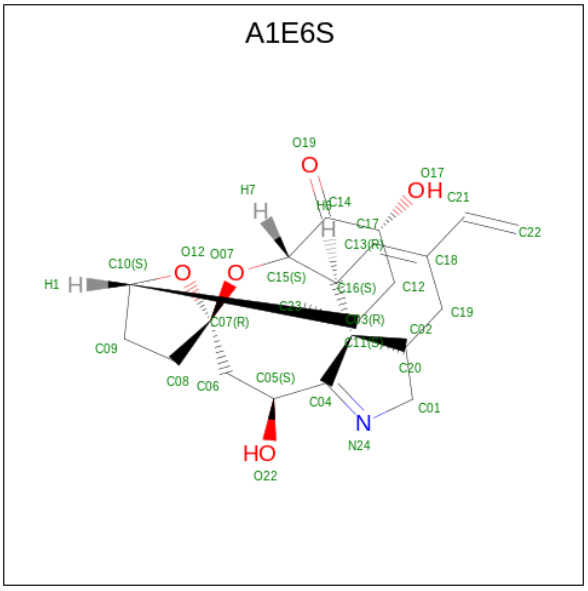
Mol	Chain	Residues	Atoms	AltConf
49	L5	1	Total C N 10 7 3	0
49	L5	1	Total C N 10 7 3	0
49	L5	1	Total C N 10 7 3	0
49	L5	1	Total C N 10 7 3	0
49	L5	1	Total C N 10 7 3	0
49	L5	1	Total C N 10 7 3	0
49	L5	1	Total C N 10 7 3	0
49	L5	1	Total C N 10 7 3	0
49	L5	1	Total C N 10 7 3	0
49	L5	1	Total C N 10 7 3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

- Molecule 50 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



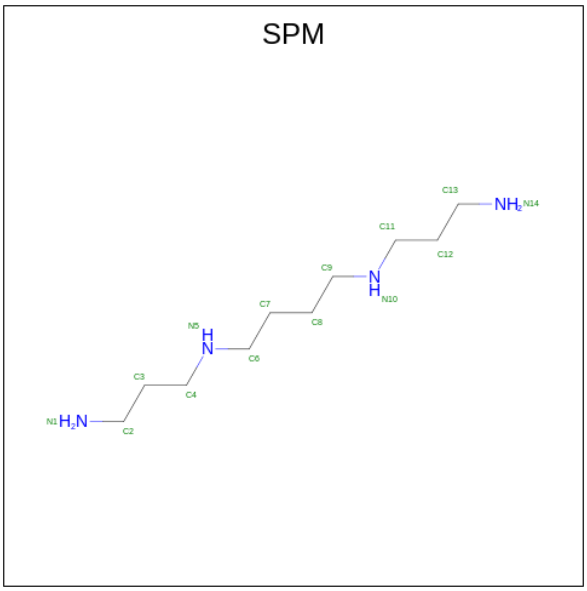
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
50	L5	1	6	4	2	0

- Molecule 51 is (1R,3S,8R,13S,14S,16R,18S,19S)-11-ethenyl-3,16-dihydroxy-18-methyl-22,23-dioxa-5-azapentacyclo[12.7.1.11,19.04,8.08,13]tricosa-4,11-dien-15-one (CCD ID: A1E6S) (formula: $C_{23}H_{31}NO_5$) (labeled as "Ligand of Interest" by depositor).



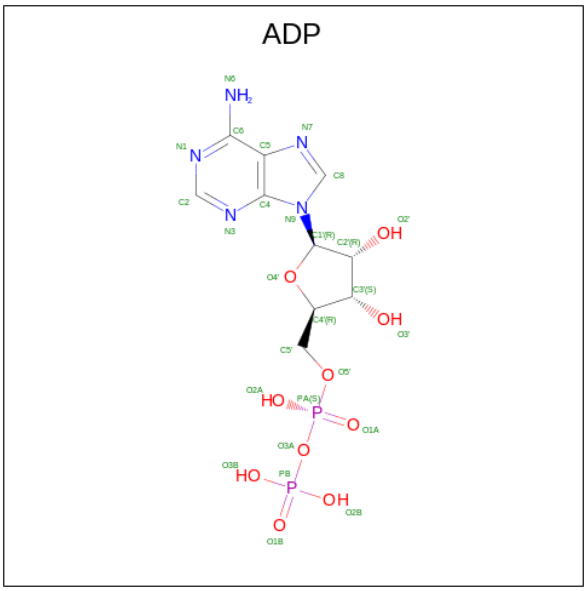
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
51	L5	1	29	23	1	5	0

- 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
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).

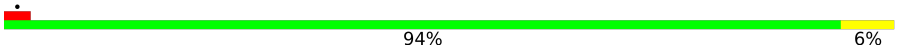
Mol	Chain	Residues	Atoms		AltConf
54	Lg	1	Total	Zn	0
			1	1	
54	Lj	1	Total	Zn	0
			1	1	
54	Lm	1	Total	Zn	0
			1	1	
54	Lo	1	Total	Zn	0
			1	1	
54	Lp	1	Total	Zn	0
			1	1	

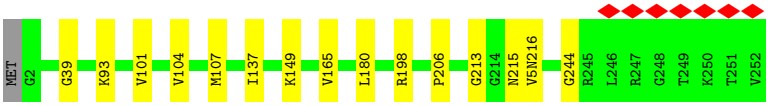
3 Residue-property plots (i)

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: Large ribosomal subunit protein uL2

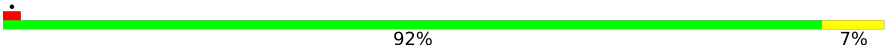
Chain LA:

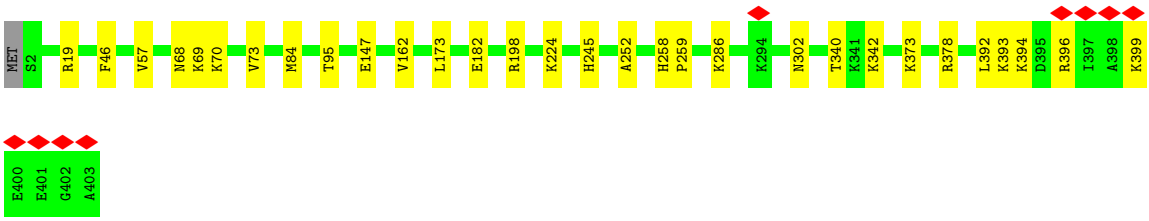




• Molecule 2: Large ribosomal subunit protein uL3

Chain LB:

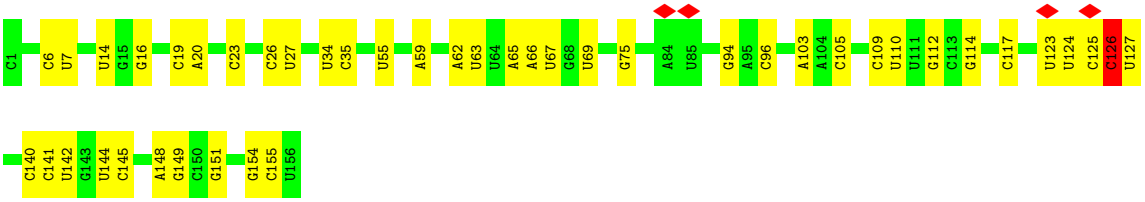




• Molecule 3: 5.8S rRNA

Chain L8:

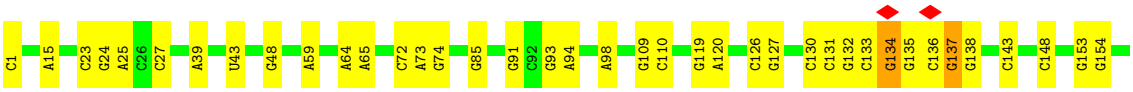


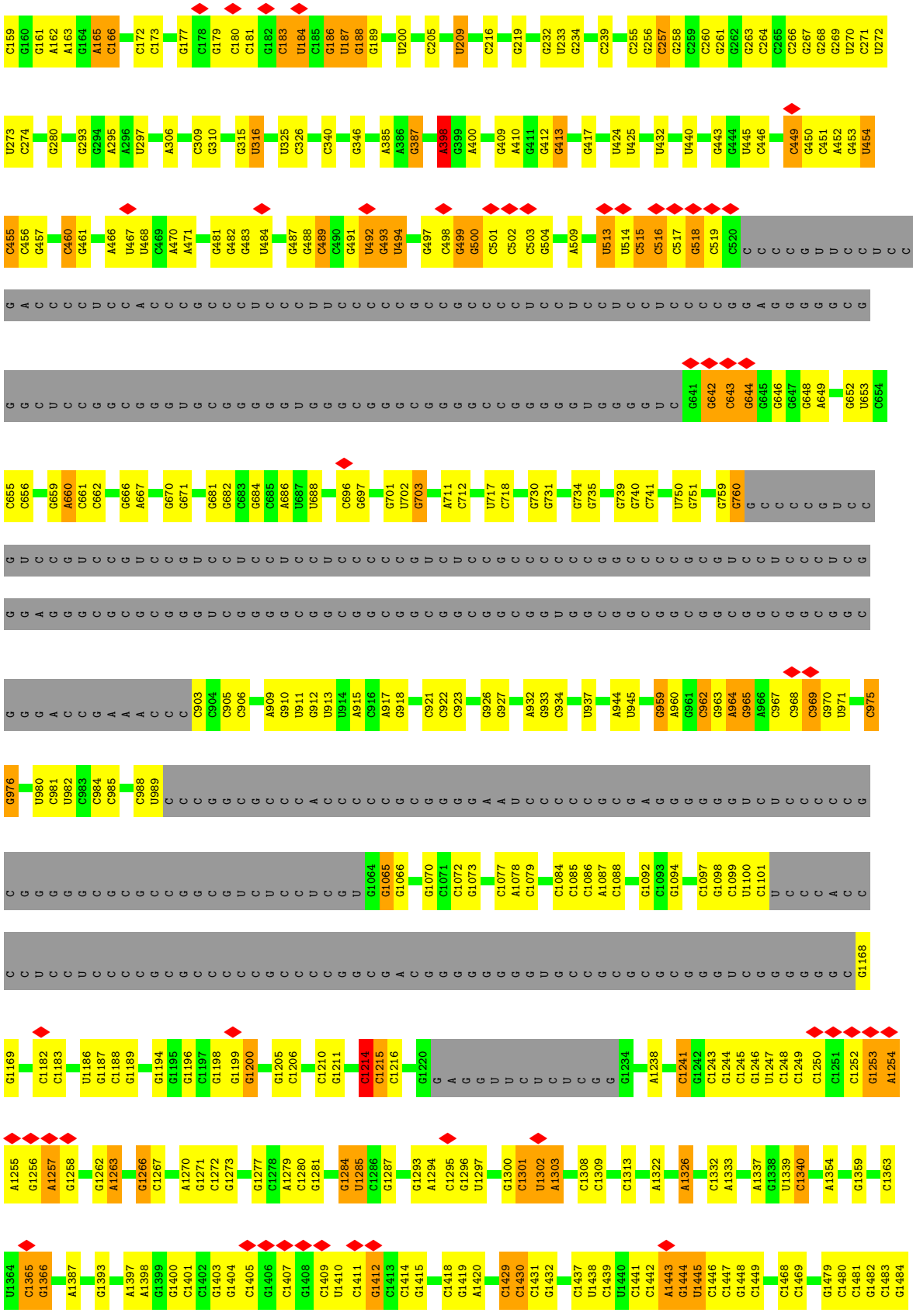


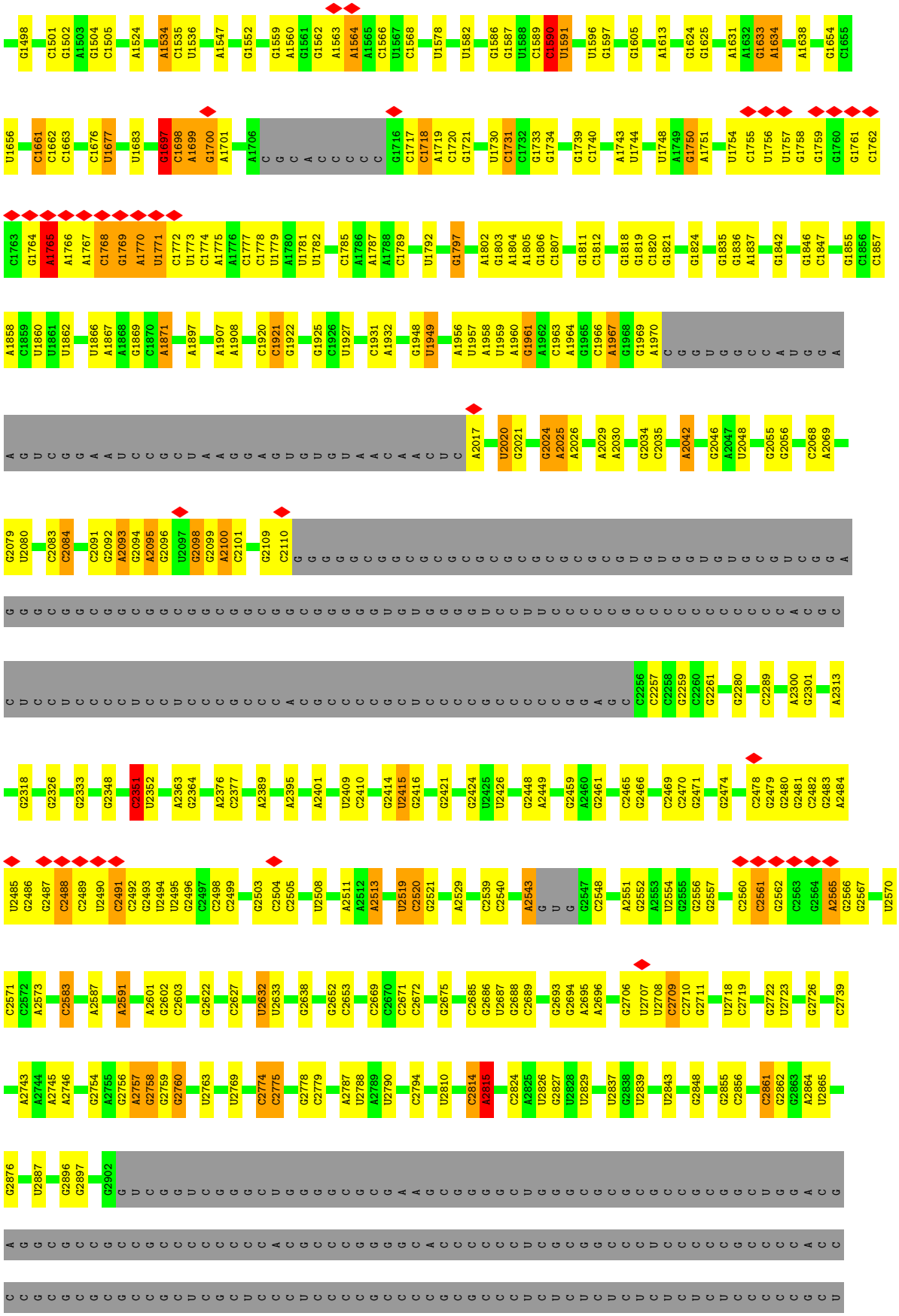
• Molecule 4: 28S rRNA

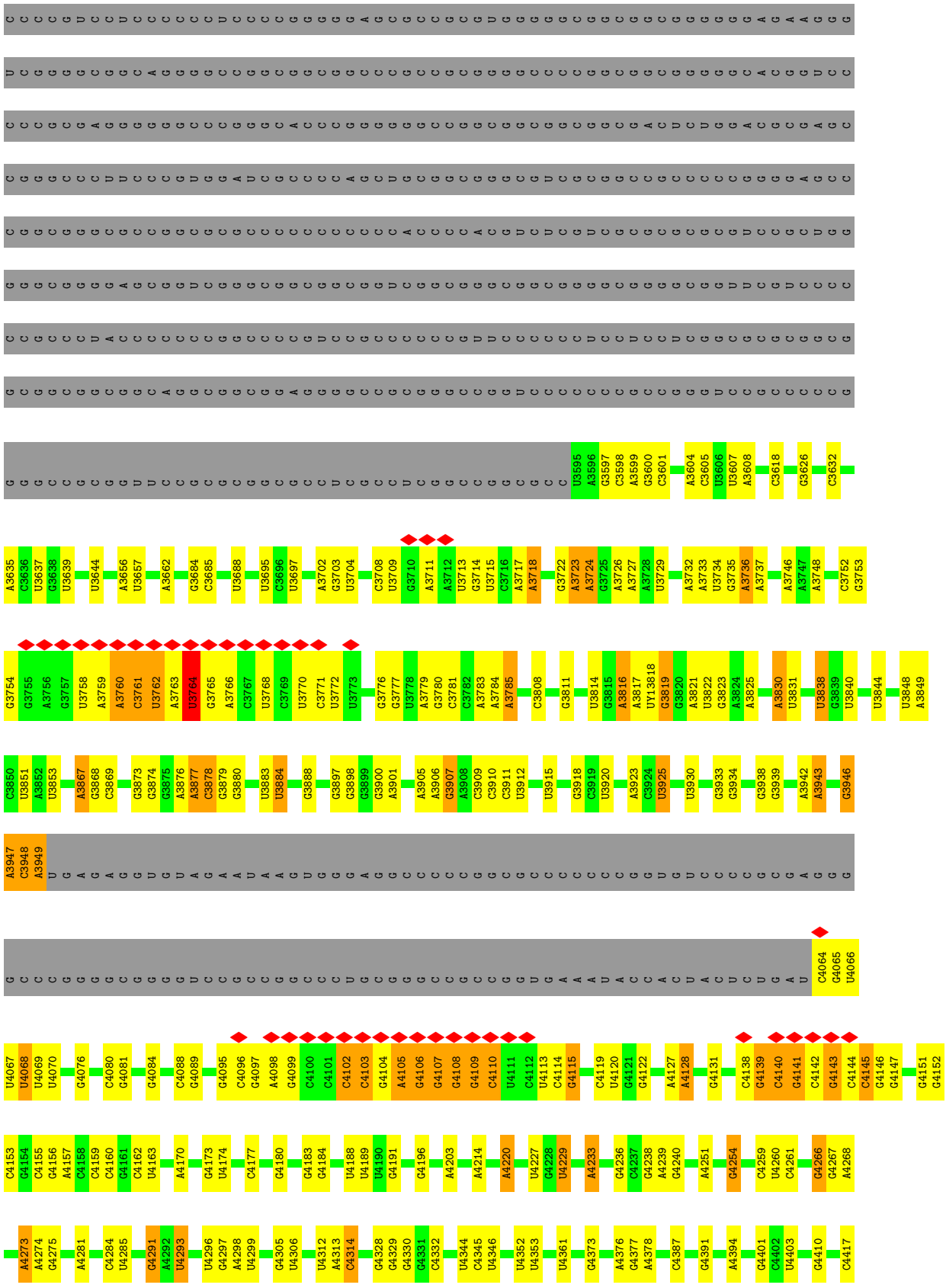
Chain L5:

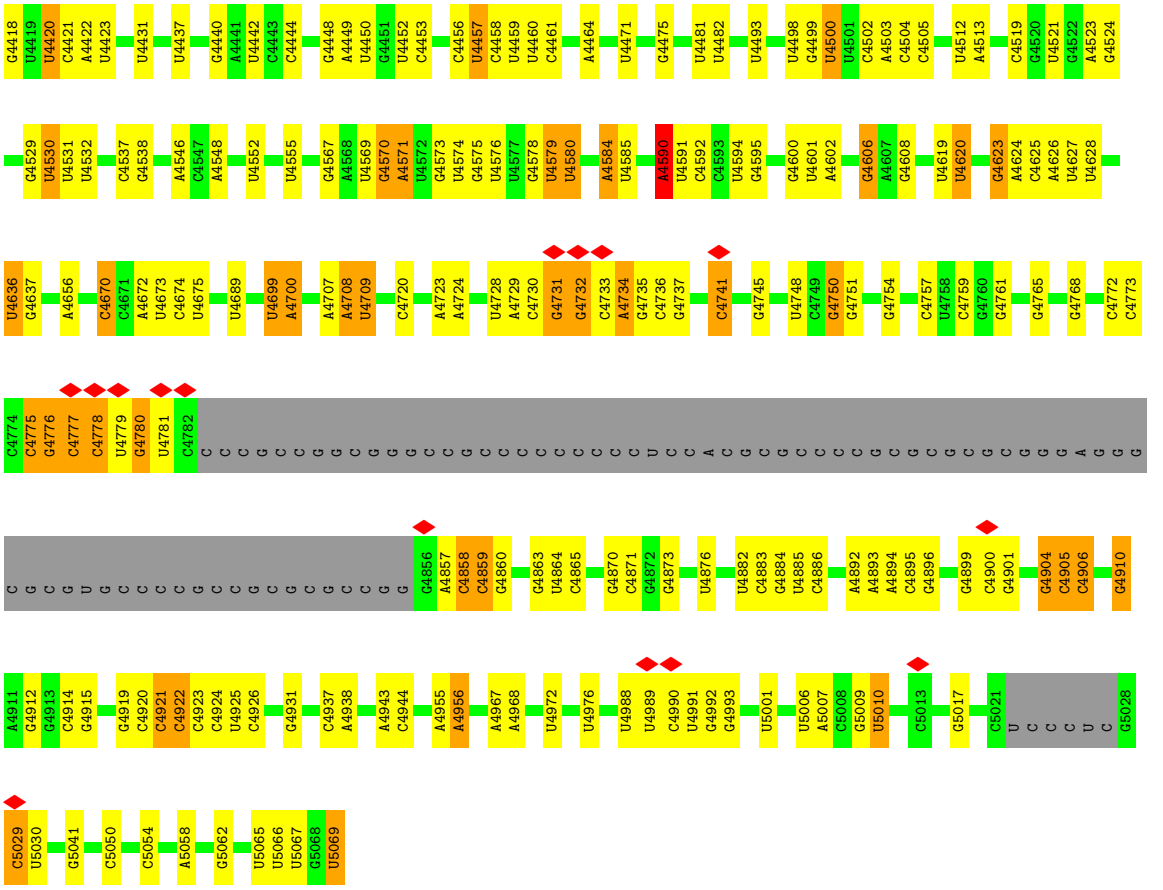








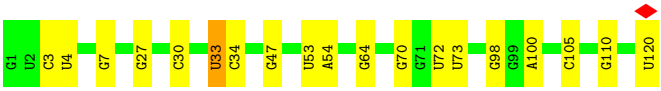




• Molecule 5: 5S rRNA

Chain L7:

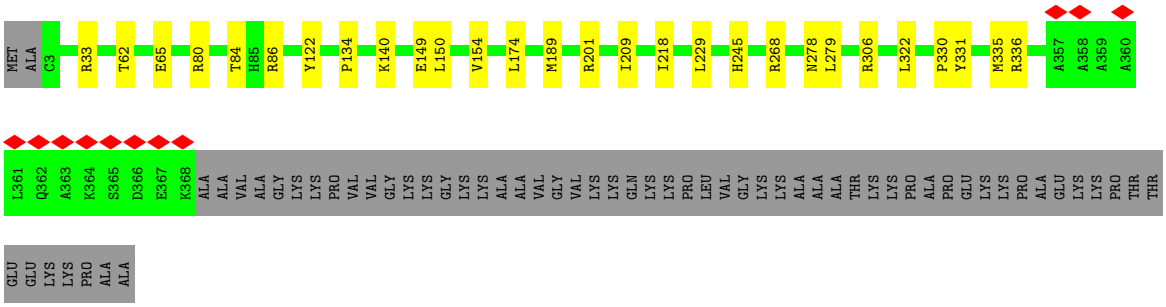




• Molecule 6: Large ribosomal subunit protein uL4

Chain LC:

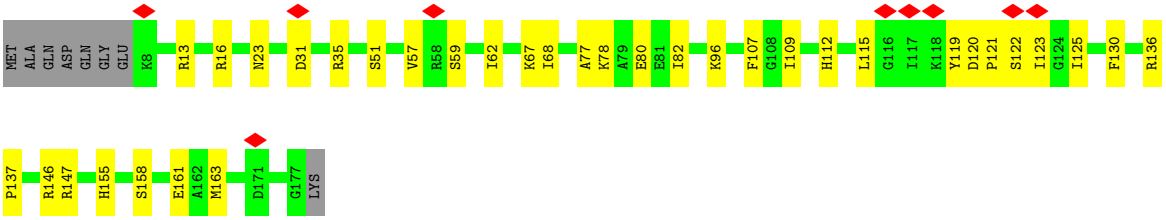




• Molecule 7: Large ribosomal subunit protein uL5

Chain LJ:

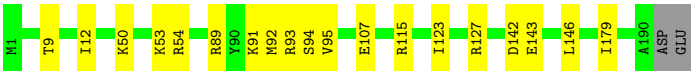




• Molecule 8: Large ribosomal subunit protein uL6

Chain LH:

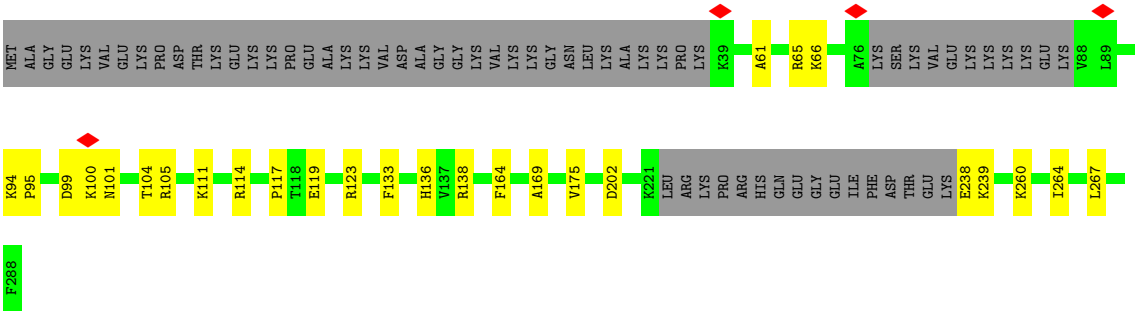




• Molecule 9: Large ribosomal subunit protein eL6

Chain LE:

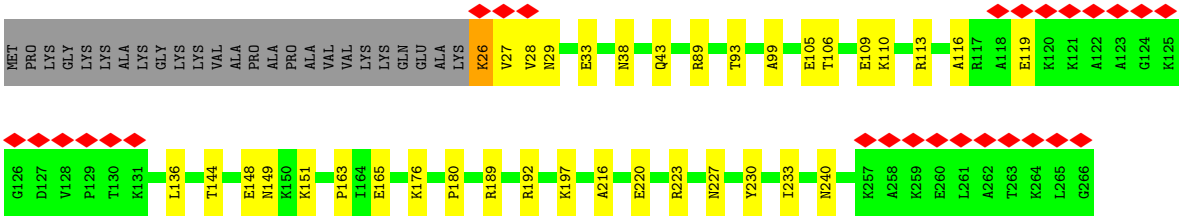




• Molecule 10: Large ribosomal subunit protein eL8

Chain LG:





• Molecule 11: Large ribosomal subunit protein uL13

Chain LO:

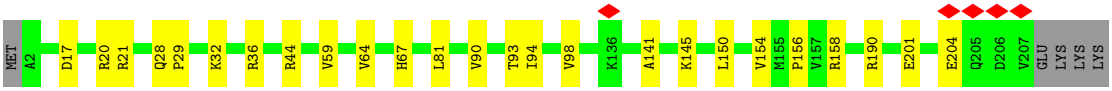




• Molecule 12: Large ribosomal subunit protein eL13

Chain LL:

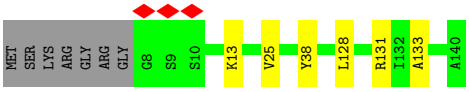




• Molecule 13: Large ribosomal subunit protein uL14

Chain LV:

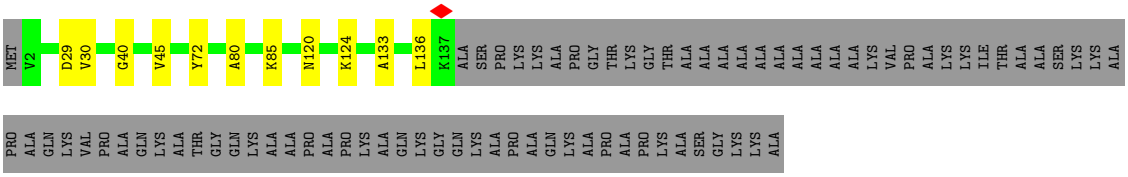




• Molecule 14: Large ribosomal subunit protein eL14

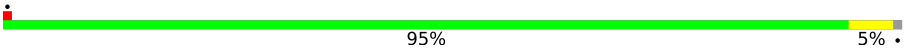
Chain LM:

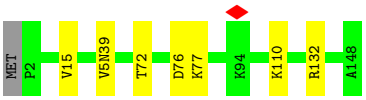




• Molecule 15: Large ribosomal subunit protein uL15

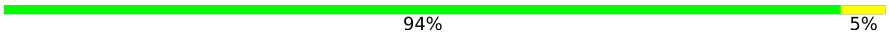
Chain La:





• Molecule 16: Large ribosomal subunit protein eL15

Chain LN:

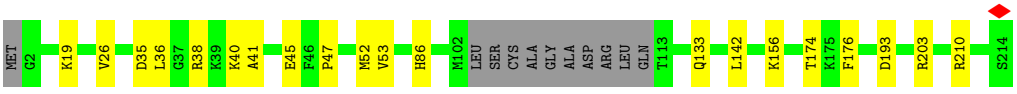




• Molecule 17: Large ribosomal subunit protein uL16

Chain LI:

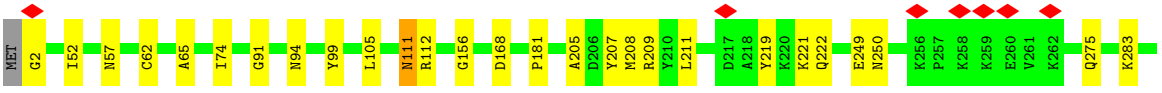


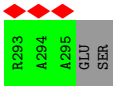


• Molecule 18: Large ribosomal subunit protein uL18

Chain LD:







• Molecule 19: Large ribosomal subunit protein eL18

Chain LQ:

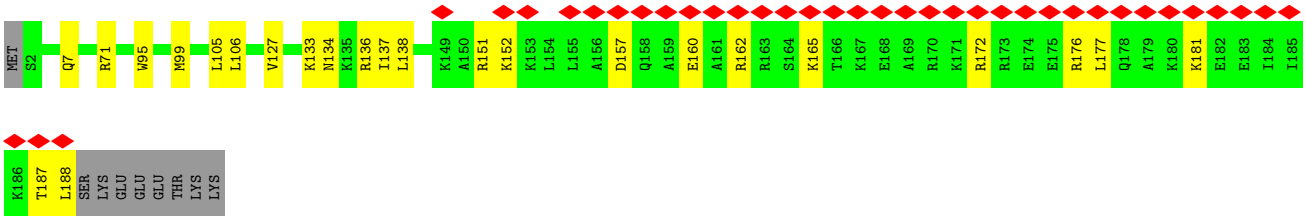




• Molecule 20: Large ribosomal subunit protein eL19

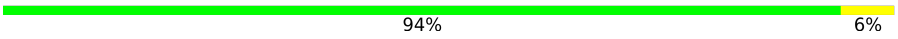
Chain LR:

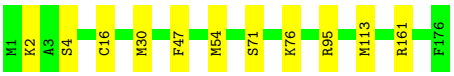




• Molecule 21: Large ribosomal subunit protein eL20

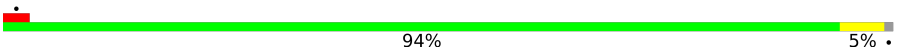
Chain LS:

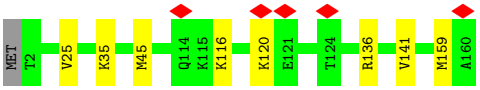




• Molecule 22: Large ribosomal subunit protein eL21

Chain LT:

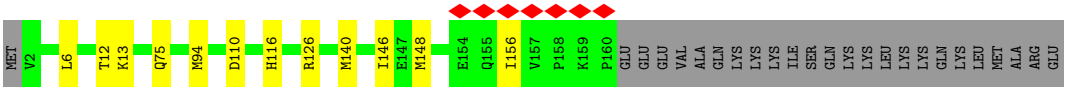




• Molecule 23: Large ribosomal subunit protein uL22

Chain LP:

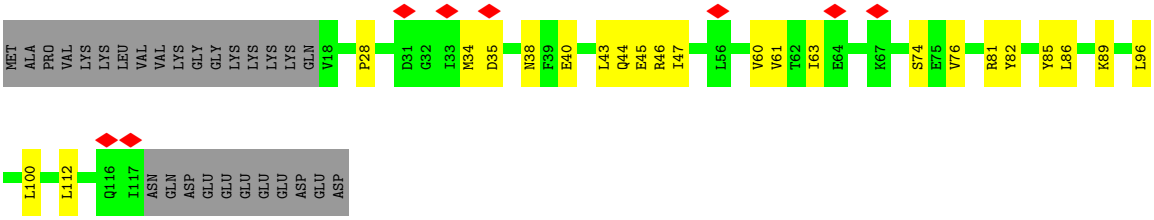




• Molecule 24: Large ribosomal subunit protein eL22

Chain LU:

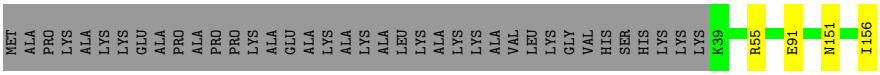




• Molecule 25: Large ribosomal subunit protein uL23

Chain LX:

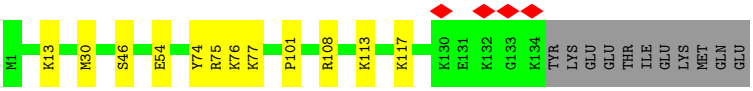




• Molecule 26: Large ribosomal subunit protein uL24

Chain LY:

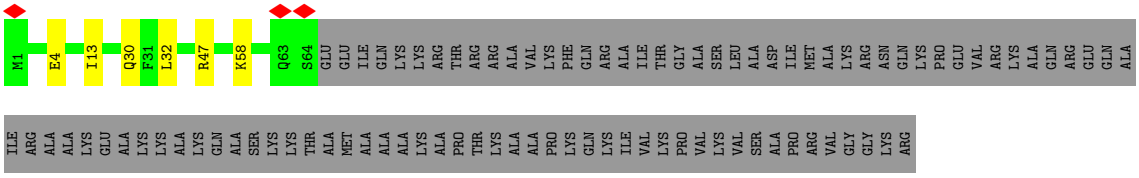




• Molecule 27: Large ribosomal subunit protein eL24

Chain LW:

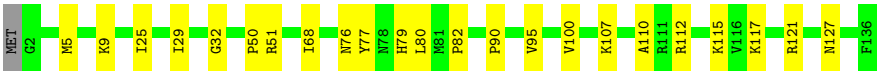




• Molecule 28: Large ribosomal subunit protein eL27

Chain LZ:

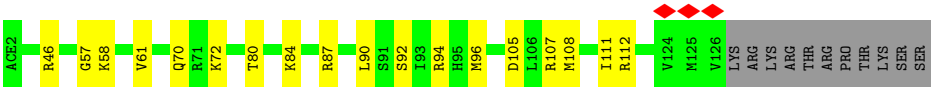




• Molecule 29: Large ribosomal subunit protein eL28

Chain Lr:





• Molecule 30: Large ribosomal subunit protein uL29

Chain Lh:

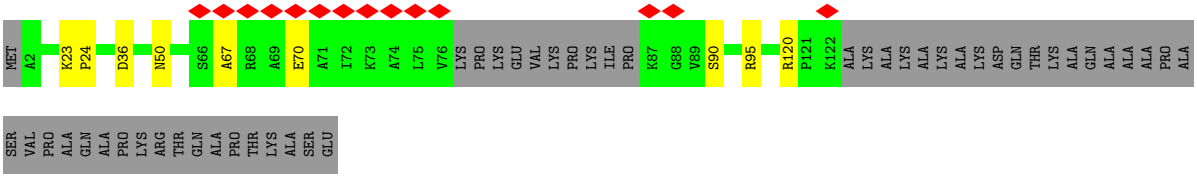




• Molecule 31: Large ribosomal subunit protein eL29

Chain Lb:

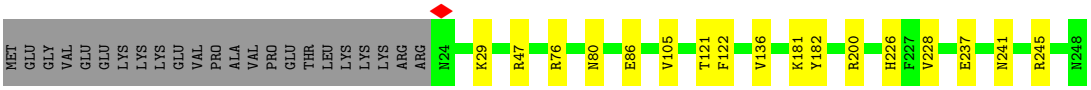




• Molecule 32: Large ribosomal subunit protein uL30

Chain LF:

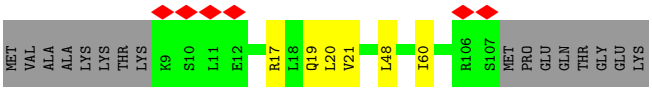




• Molecule 33: Large ribosomal subunit protein eL30

Chain Lc:

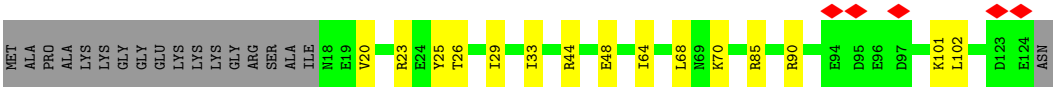




• Molecule 34: Large ribosomal subunit protein eL31

Chain Ld:





• Molecule 35: Large ribosomal subunit protein eL32

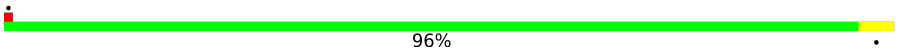
Chain Le:

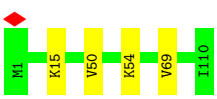




• Molecule 36: Large ribosomal subunit protein eL33

Chain Lf:

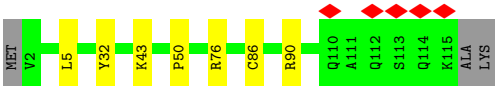




• Molecule 37: Large ribosomal subunit protein eL34

Chain Lg:





• Molecule 38: Large ribosomal subunit protein eL36

Chain Li:

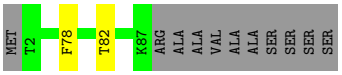




• Molecule 39: Large ribosomal subunit protein eL37

Chain Lj:

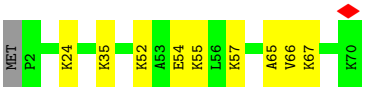




• Molecule 40: Large ribosomal subunit protein eL38

Chain Lk:

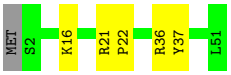




• Molecule 41: Large ribosomal subunit protein eL39

Chain Ll:

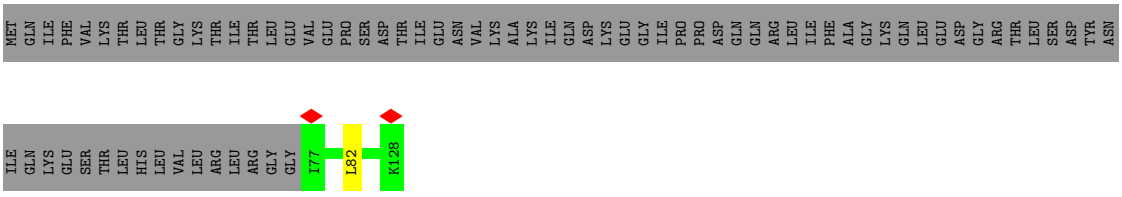




• Molecule 42: Ubiquitin-ribosomal protein eL40 fusion protein

Chain Lm:

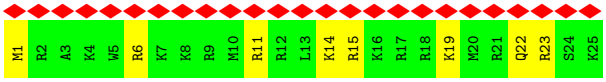




• Molecule 43: Small ribosomal subunit protein eS32

Chain Ln:

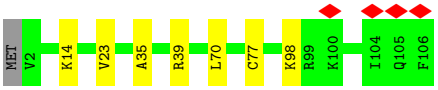




• Molecule 44: Large ribosomal subunit protein eL42

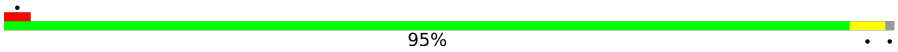
Chain Lo:

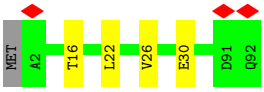




• Molecule 45: Large ribosomal subunit protein eL43

Chain Lp:

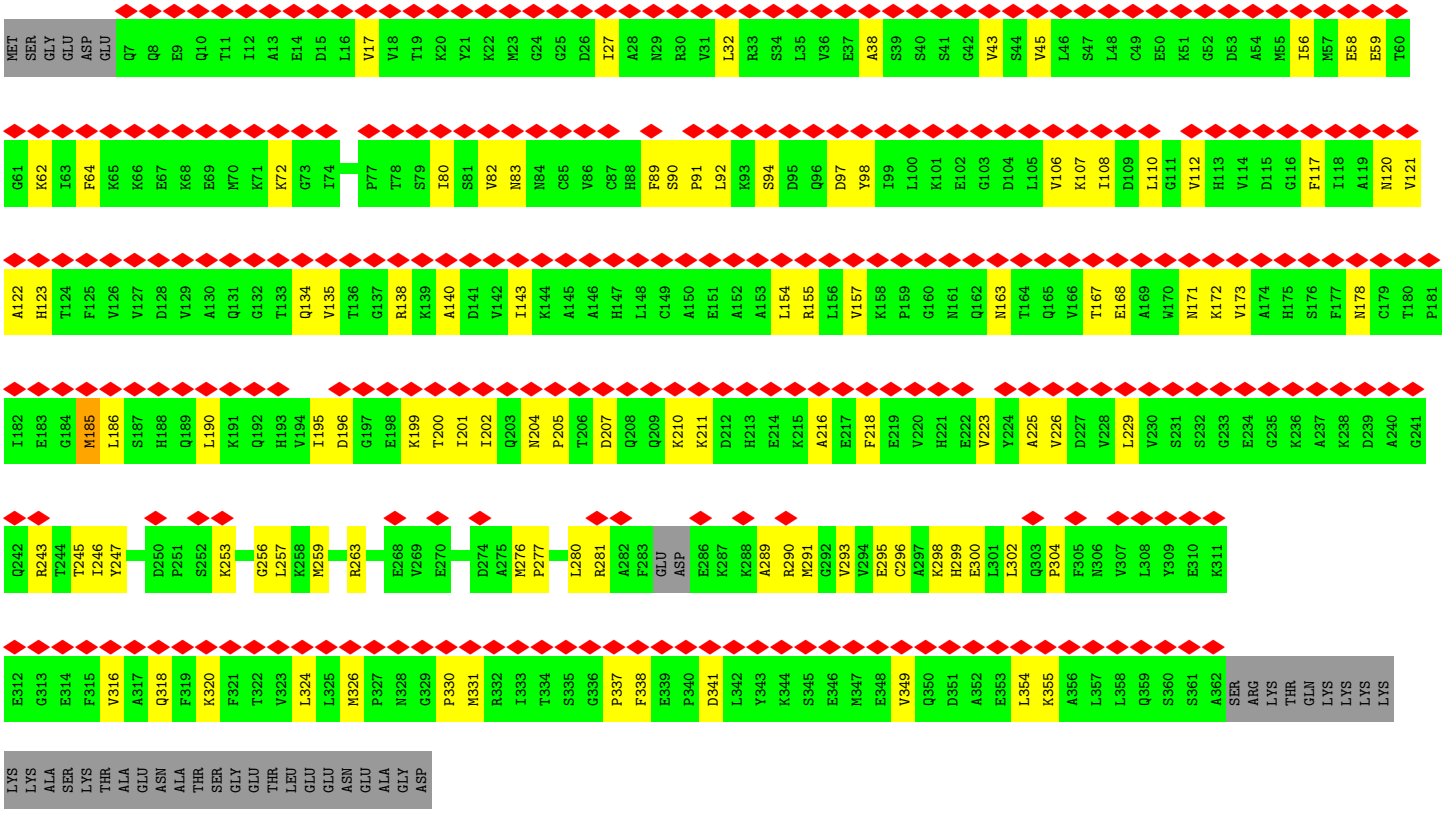




• Molecule 46: Proliferation-associated protein 2G4

Chain z:

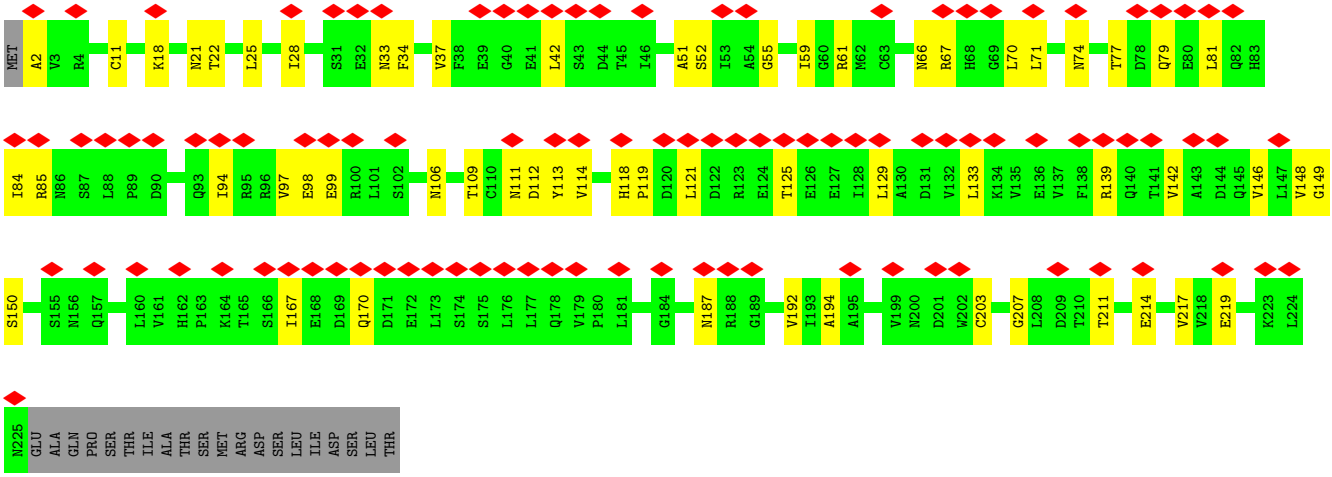




• Molecule 47: Eukaryotic translation initiation factor 6

Chain 6:




MET A2 V3 R4 C11 K18 N21 T22 L25 I28 S31 E32 N33 F34 V37 F38 E39 G40 E41 L42 S43 D44 T45 I46 A51 S52 I53 A54 G55 I59 G60 R61 M62 C63 N66 R67 H68 G69 L70 L71 N74 T77 D78 Q79 E80 L81 Q82 H83
I84 R85 N86 S87 L88 P89 D90 Q93 I94 R95 R96 V97 E98 E99 R100 L101 S102 N106 T109 C110 N111 D112 Y113 V114 H118 P119 D120 L121 D122 R123 E124 T125 E126 E127 I128 L129 A130 D131 V132 L133 K134 V135 E136 V137 F138 R139 Q140 T141 V142 A143 D144 Q145 V146 L147 V148 G149
S150 S155 N156 Q157 L160 V161 H162 P163 K164 T165 S166 I167 E168 D169 Q170 D171 E172 L173 S174 S175 L176 L177 Q178 V179 P180 L181 G184 N187 R188 G189 V192 I193 A194 A195 V199 N200 D201 W202 C203 G207 L208 D209 T210 T211 E214 V217 V218 E219 K223 L224
N225 GLU ALA GLN PRO SER THR ILE ALA THR SER MET ARG ASP SER LEU ILE ASP SER LEU THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67834	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	0.131	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0127	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, V5N, PSU, A1E6S, ZN, M3L, 1MA, UR3, ADP, OMC, ACE, SPM, 6MZ, A2M, 5MC, K, HIC, SPD, PUT, MLZ, UY1, OMG

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	LA	0.18	0/1958	0.44	0/2623
2	LB	0.19	0/3294	0.40	0/4406
3	L8	0.38	0/3609	0.86	4/5623 (0.1%)
4	L5	0.38	7/82526 (0.0%)	0.89	49/128745 (0.0%)
5	L7	0.33	0/2858	0.80	1/4455 (0.0%)
6	LC	0.18	0/2968	0.40	0/3985
7	LJ	0.18	0/1385	0.46	0/1852
8	LH	0.17	0/1537	0.38	0/2066
9	LE	0.19	0/1820	0.39	0/2442
10	LG	0.20	0/1959	0.42	0/2637
11	LO	0.22	0/1686	0.41	0/2257
12	LL	0.18	0/1706	0.43	0/2284
13	LV	0.17	0/1002	0.41	0/1345
14	LM	0.18	0/1142	0.39	0/1527
15	La	0.18	0/1178	0.41	0/1573
16	LN	0.19	0/1745	0.44	0/2338
17	LI	0.16	0/1683	0.39	0/2247
18	LD	0.16	0/2437	0.39	0/3263
19	LQ	0.18	0/1536	0.43	0/2052
20	LR	0.17	0/1582	0.40	0/2091
21	LS	0.19	0/1500	0.41	0/2013
22	LT	0.21	0/1345	0.41	0/1795
23	LP	0.21	0/1328	0.44	0/1784
24	LU	0.18	0/830	0.44	0/1114
25	LX	0.22	0/983	0.42	0/1323
26	LY	0.17	0/1132	0.38	0/1504
27	LW	0.17	0/547	0.39	0/728
28	LZ	0.18	0/1141	0.40	0/1521
29	Lr	0.22	0/1027	0.42	0/1377
30	Lh	0.17	0/1022	0.36	0/1351
31	Lb	0.20	0/900	0.44	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LF	0.20	0/1926	0.41	1/2567 (0.0%)
33	Lc	0.18	0/780	0.38	0/1046
34	Ld	0.19	0/903	0.44	0/1216
35	Le	0.18	0/1082	0.44	0/1443
36	Lf	0.19	0/902	0.39	0/1208
37	Lg	0.19	0/916	0.42	0/1220
38	Li	0.17	0/843	0.38	0/1115
39	Lj	0.19	0/731	0.45	0/967
40	Lk	0.17	0/574	0.38	0/761
41	Ll	0.18	0/453	0.36	0/599
42	Lm	0.17	0/433	0.44	0/575
43	Ln	0.19	0/240	0.43	0/305
44	Lo	0.16	0/877	0.42	0/1156
45	Lp	0.18	0/728	0.45	0/967
46	z	0.17	0/2911	0.46	1/3913 (0.0%)
47	6	0.19	0/1728	0.51	0/2352
All	All	0.32	7/147393 (0.0%)	0.75	56/216918 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L5	2787	A2M	O3'-P	5.27	1.61	1.56
4	L5	3830	A2M	O3'-P	5.26	1.61	1.56
4	L5	4523	A2M	O3'-P	5.25	1.61	1.56
4	L5	4571	A2M	O3'-P	5.13	1.61	1.56
4	L5	1326	A2M	O3'-P	5.12	1.61	1.56

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L8	126	C	C2-N1-C1'	8.09	127.70	118.80
4	L5	1501	C	C2-N1-C1'	7.94	127.53	118.80
4	L5	2469	C	C2-N1-C1'	7.32	126.86	118.80
4	L5	4778	C	C2-N1-C1'	7.19	126.71	118.80
4	L5	4778	C	N1-C2-O2	6.98	123.09	118.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	LA	1930	0	2028	9	0
2	LB	3239	0	3377	22	0
3	L8	3316	0	1687	18	0
4	L5	76516	0	38741	570	0
5	L7	2558	0	1296	9	0
6	LC	2914	0	3087	20	0
7	LJ	1362	0	1399	26	0
8	LH	1518	0	1601	11	0
9	LE	1786	0	1945	24	0
10	LG	1926	0	2074	21	0
11	LO	1654	0	1799	17	0
12	LL	1672	0	1786	22	0
13	LV	988	0	1047	5	0
14	LM	1120	0	1187	6	0
15	La	1162	0	1206	3	0
16	LN	1700	0	1749	6	0
17	LI	1645	0	1694	15	0
18	LD	2391	0	2426	21	0
19	LQ	1512	0	1628	11	0
20	LR	1566	0	1729	18	0
21	LS	1460	0	1502	6	0
22	LT	1311	0	1392	7	0
23	LP	1296	0	1331	7	0
24	LU	816	0	842	15	0
25	LX	966	0	1040	4	0
26	LY	1115	0	1205	12	0
27	LW	534	0	546	5	0
28	LZ	1115	0	1195	12	0
29	Lr	1011	0	1085	15	0
30	Lh	1014	0	1148	8	0
31	Lb	898	0	983	7	0
32	LF	1885	0	2022	11	0
33	Lc	770	0	809	3	0
34	Ld	888	0	930	9	0
35	Le	1061	0	1160	8	0
36	Lf	883	0	924	4	0
37	Lg	906	0	998	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Li	832	0	917	7	0
39	Lj	712	0	744	2	0
40	Lk	568	0	637	8	0
41	Ll	443	0	482	4	0
42	Lm	436	0	476	1	0
43	Ln	239	0	289	10	0
44	Lo	870	0	936	4	0
45	Lp	715	0	769	4	0
46	z	2837	0	2869	73	0
47	6	1704	0	1677	43	0
48	L5	111	0	0	0	0
48	L7	4	0	0	0	0
48	L8	2	0	0	0	0
48	LA	3	0	0	0	0
48	LB	1	0	0	0	0
48	LH	1	0	0	0	0
48	LI	1	0	0	0	0
48	LN	2	0	0	0	0
48	LQ	1	0	0	0	0
48	Lb	1	0	0	0	0
48	Le	1	0	0	0	0
48	Lf	2	0	0	0	0
48	Lg	1	0	0	0	0
48	Ll	1	0	0	0	0
49	L5	120	0	228	17	0
49	LN	10	0	19	0	0
50	L5	6	0	12	1	0
51	L5	29	0	0	0	0
52	L5	126	0	234	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
All	All	140215	0	102899	1029	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 4.

The worst 5 of 1029 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)
49:L5:5227:SPD:C2	49:L5:5227:SPD:N1	1.83	1.41
49:L5:5227:SPD:N10	49:L5:5227:SPD:C9	1.83	1.41
49:L5:5227:SPD:N6	49:L5:5227:SPD:C5	1.85	1.39
49:L5:5227:SPD:C9	49:L5:5227:SPD:C8	2.02	1.36
49:L5:5227:SPD:N6	49:L5:5227:SPD:C7	1.85	1.36

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	LA	249/252 (99%)	239 (96%)	10 (4%)	0	100	100
2	LB	399/403 (99%)	389 (98%)	10 (2%)	0	100	100
6	LC	364/427 (85%)	358 (98%)	6 (2%)	0	100	100
7	LJ	168/178 (94%)	162 (96%)	6 (4%)	0	100	100
8	LH	188/192 (98%)	184 (98%)	4 (2%)	0	100	100
9	LE	217/288 (75%)	205 (94%)	12 (6%)	0	100	100
10	LG	239/266 (90%)	230 (96%)	9 (4%)	0	100	100
11	LO	200/203 (98%)	197 (98%)	3 (2%)	0	100	100
12	LL	205/211 (97%)	200 (98%)	5 (2%)	0	100	100
13	LV	131/140 (94%)	130 (99%)	1 (1%)	0	100	100
14	LM	134/215 (62%)	131 (98%)	3 (2%)	0	100	100
15	La	144/148 (97%)	139 (96%)	4 (3%)	1 (1%)	18	34
16	LN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
17	LI	199/214 (93%)	195 (98%)	4 (2%)	0	100	100
18	LD	292/297 (98%)	281 (96%)	11 (4%)	0	100	100
19	LQ	185/188 (98%)	180 (97%)	5 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	LR	185/196 (94%)	184 (100%)	1 (0%)	0	100	100
21	LS	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
22	LT	159/160 (99%)	157 (99%)	2 (1%)	0	100	100
23	LP	158/184 (86%)	154 (98%)	4 (2%)	0	100	100
24	LU	98/128 (77%)	96 (98%)	2 (2%)	0	100	100
25	LX	116/156 (74%)	116 (100%)	0	0	100	100
26	LY	132/145 (91%)	132 (100%)	0	0	100	100
27	LW	62/157 (40%)	62 (100%)	0	0	100	100
28	LZ	134/136 (98%)	130 (97%)	4 (3%)	0	100	100
29	Lr	125/137 (91%)	121 (97%)	4 (3%)	0	100	100
30	Lh	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
31	Lb	106/159 (67%)	105 (99%)	1 (1%)	0	100	100
32	LF	225/248 (91%)	219 (97%)	6 (3%)	0	100	100
33	Lc	97/115 (84%)	95 (98%)	2 (2%)	0	100	100
34	Ld	105/125 (84%)	104 (99%)	1 (1%)	0	100	100
35	Le	127/135 (94%)	126 (99%)	1 (1%)	0	100	100
36	Lf	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
37	Lg	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
38	Li	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
39	Lj	85/97 (88%)	85 (100%)	0	0	100	100
40	Lk	67/70 (96%)	67 (100%)	0	0	100	100
41	Ll	48/51 (94%)	48 (100%)	0	0	100	100
42	Lm	50/128 (39%)	50 (100%)	0	0	100	100
43	Ln	23/25 (92%)	23 (100%)	0	0	100	100
44	Lo	103/106 (97%)	97 (94%)	6 (6%)	0	100	100
45	Lp	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
46	z	363/394 (92%)	356 (98%)	7 (2%)	0	100	100
47	6	222/245 (91%)	207 (93%)	15 (7%)	0	100	100
All	All	7009/7846 (89%)	6842 (98%)	166 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	La	15	VAL

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	LA	193/193 (100%)	193 (100%)	0	100 100
2	LB	347/348 (100%)	347 (100%)	0	100 100
6	LC	305/348 (88%)	305 (100%)	0	100 100
7	LJ	143/149 (96%)	143 (100%)	0	100 100
8	LH	169/171 (99%)	169 (100%)	0	100 100
9	LE	196/252 (78%)	196 (100%)	0	100 100
10	LG	203/223 (91%)	200 (98%)	3 (2%)	57 80
11	LO	173/174 (99%)	173 (100%)	0	100 100
12	LL	173/177 (98%)	173 (100%)	0	100 100
13	LV	102/107 (95%)	102 (100%)	0	100 100
14	LM	116/161 (72%)	116 (100%)	0	100 100
15	La	119/120 (99%)	119 (100%)	0	100 100
16	LN	171/172 (99%)	171 (100%)	0	100 100
17	LI	173/181 (96%)	173 (100%)	0	100 100
18	LD	247/250 (99%)	246 (100%)	1 (0%)	84 93
19	LQ	164/165 (99%)	164 (100%)	0	100 100
20	LR	166/175 (95%)	166 (100%)	0	100 100
21	LS	157/157 (100%)	157 (100%)	0	100 100
22	LT	141/140 (101%)	141 (100%)	0	100 100
23	LP	141/163 (86%)	141 (100%)	0	100 100
24	LU	90/115 (78%)	90 (100%)	0	100 100
25	LX	106/133 (80%)	106 (100%)	0	100 100
26	LY	124/135 (92%)	124 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	LW	56/126 (44%)	56 (100%)	0	100	100
28	LZ	118/118 (100%)	118 (100%)	0	100	100
29	Lr	110/120 (92%)	110 (100%)	0	100	100
30	Lh	109/110 (99%)	109 (100%)	0	100	100
31	Lb	90/125 (72%)	90 (100%)	0	100	100
32	LF	196/215 (91%)	196 (100%)	0	100	100
33	Lc	84/97 (87%)	84 (100%)	0	100	100
34	Ld	98/110 (89%)	98 (100%)	0	100	100
35	Le	115/121 (95%)	115 (100%)	0	100	100
36	Lf	89/89 (100%)	89 (100%)	0	100	100
37	Lg	98/100 (98%)	98 (100%)	0	100	100
38	Li	86/89 (97%)	86 (100%)	0	100	100
39	Lj	74/80 (92%)	74 (100%)	0	100	100
40	Lk	64/65 (98%)	64 (100%)	0	100	100
41	Ll	47/48 (98%)	47 (100%)	0	100	100
42	Lm	48/115 (42%)	48 (100%)	0	100	100
43	Ln	24/24 (100%)	24 (100%)	0	100	100
44	Lo	93/93 (100%)	93 (100%)	0	100	100
45	Lp	75/75 (100%)	75 (100%)	0	100	100
46	z	316/336 (94%)	314 (99%)	2 (1%)	78	91
47	6	194/213 (91%)	194 (100%)	0	100	100
All	All	6103/6678 (91%)	6097 (100%)	6 (0%)	87	96

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	LD	111	ASN
46	z	185[A]	MET
46	z	185[B]	MET
10	LG	27	VAL
10	LG	26	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
22	LT	127	GLN
47	6	156	ASN
26	LY	56	GLN
47	6	86	ASN
42	Lm	104	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L8	155/156 (99%)	17 (10%)	0
4	L5	3552/5069 (70%)	562 (15%)	23 (0%)
5	L7	119/120 (99%)	9 (7%)	0
All	All	3826/5345 (71%)	588 (15%)	23 (0%)

5 of 588 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L8	23	C
3	L8	34	U
3	L8	35	C
3	L8	59	A
3	L8	62	A

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	L5	2774	C
4	L5	4699	U
4	L5	4139	G
4	L5	4776	G
4	L5	975	C

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

139 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	$\#\|Z\|>2$
4	PSU	L5	2839	4	18,21,22	1.08	1 (5%)	22,30,33	1.83	4 (18%)
4	PSU	L5	4403	4	18,21,22	1.11	1 (5%)	22,30,33	1.94	6 (27%)
4	PSU	L5	4471	4	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
4	OMU	L5	4227	4	19,22,23	3.02	8 (42%)	26,31,34	1.72	5 (19%)
4	PSU	L5	4431	4	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
4	PSU	L5	4457	4	18,21,22	1.09	1 (5%)	22,30,33	1.80	4 (18%)
4	PSU	L5	3695	4	18,21,22	1.03	1 (5%)	22,30,33	1.70	5 (22%)
4	A2M	L5	400	4	22,25,26	3.19	9 (40%)	31,36,39	2.90	10 (32%)
4	A2M	L5	3785	4	22,25,26	3.18	11 (50%)	31,36,39	3.07	13 (41%)
4	OMG	L5	4637	4,48	23,26,27	0.50	0	33,38,41	0.55	0
4	A2M	L5	3830	4	22,25,26	3.17	9 (40%)	31,36,39	2.97	10 (32%)
4	6MZ	L5	4220	4	22,25,26	1.40	4 (18%)	30,36,39	2.14	9 (30%)
4	PSU	L5	4689	4	18,21,22	1.01	1 (5%)	22,30,33	1.69	3 (13%)
4	OMC	L5	2422	4	19,22,23	0.63	0	26,31,34	0.74	0
4	PSU	L5	3715	4	18,21,22	1.05	1 (5%)	22,30,33	1.75	4 (18%)
4	PSU	L5	4673	4	18,21,22	1.09	1 (5%)	22,30,33	1.68	4 (18%)
4	A2M	L5	1534	4	22,25,26	3.21	9 (40%)	31,36,39	2.91	10 (32%)
15	V5N	La	39	15	9,11,12	2.70	2 (22%)	9,14,16	1.47	2 (22%)
4	OMG	L5	4494	4,48	23,26,27	0.54	0	33,38,41	0.52	0
4	PSU	L5	3762	4	18,21,22	1.09	1 (5%)	22,30,33	1.65	4 (18%)
4	OMC	L5	4536	4	19,22,23	0.55	0	26,31,34	0.68	0
4	PSU	L5	1779	4	18,21,22	0.99	1 (5%)	22,30,33	1.68	4 (18%)
4	OMG	L5	3899	4	23,26,27	0.54	0	33,38,41	0.62	0
4	UY1	L5	3818	4,48	19,22,23	1.38	3 (15%)	22,31,34	2.05	4 (18%)
4	OMC	L5	2365	4	19,22,23	0.60	0	26,31,34	0.65	0
4	PSU	L5	1862	4	18,21,22	1.06	1 (5%)	22,30,33	1.73	4 (18%)
4	UR3	L5	4530	4	19,22,23	2.85	6 (31%)	26,32,35	1.30	3 (11%)
4	PSU	L5	1582	4	18,21,22	1.07	1 (5%)	22,30,33	1.66	4 (18%)
31	MLZ	Lb	5	31,48	8,9,10	0.73	0	4,9,11	0.62	0
4	OMG	L5	4623	4	23,26,27	0.61	0	33,38,41	0.59	0
4	PSU	L5	4552	4	18,21,22	1.04	1 (5%)	22,30,33	1.75	4 (18%)
4	OMC	L5	1340	4	19,22,23	0.55	0	26,31,34	0.96	1 (3%)
4	OMG	L5	4618	4	23,26,27	0.52	0	33,38,41	0.52	0
4	PSU	L5	4636	4	18,21,22	1.03	1 (5%)	22,30,33	1.83	5 (22%)
4	PSU	L5	4972	4,48	18,21,22	1.04	1 (5%)	22,30,33	1.72	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OMC	L5	3841	4	19,22,23	0.52	0	26,31,34	0.68	0
4	OMU	L5	2837	4	19,22,23	3.02	8 (42%)	26,31,34	1.72	4 (15%)
4	OMG	L5	4196	4	23,26,27	0.51	0	33,38,41	0.47	0
4	PSU	L5	3637	4,48	18,21,22	1.06	1 (5%)	22,30,33	1.85	4 (18%)
4	A2M	L5	3718	4	22,25,26	3.22	9 (40%)	31,36,39	2.81	10 (32%)
4	PSU	L5	4442	4	18,21,22	1.05	1 (5%)	22,30,33	1.81	5 (22%)
4	PSU	L5	4569	4	18,21,22	1.13	1 (5%)	22,30,33	1.65	4 (18%)
4	PSU	L5	1860	4	18,21,22	1.05	1 (5%)	22,30,33	1.80	5 (22%)
4	PSU	L5	2632	4	18,21,22	1.05	1 (5%)	22,30,33	1.73	4 (18%)
3	OMG	L8	75	3	23,26,27	0.49	0	33,38,41	0.46	0
4	PSU	L5	4420	4	18,21,22	1.12	2 (11%)	22,30,33	1.71	5 (22%)
4	A2M	L5	3825	4	22,25,26	3.17	9 (40%)	31,36,39	3.01	10 (32%)
4	PSU	L5	4531	4	18,21,22	1.09	1 (5%)	22,30,33	1.72	4 (18%)
2	HIC	LB	245	2	10,11,12	1.53	2 (20%)	8,14,16	1.00	0
4	OMG	L5	3744	4	23,26,27	0.50	0	33,38,41	0.51	0
4	A2M	L5	4523	4	22,25,26	3.18	9 (40%)	31,36,39	2.99	11 (35%)
4	OMC	L5	3808	4	19,22,23	0.58	0	26,31,34	0.77	1 (3%)
4	PSU	L5	4532	4	18,21,22	1.01	1 (5%)	22,30,33	1.68	4 (18%)
4	OMU	L5	4620	4	19,22,23	2.97	8 (42%)	26,31,34	1.68	5 (19%)
4	OMC	L5	3887	4	19,22,23	0.62	0	26,31,34	0.65	0
4	A2M	L5	2401	4	22,25,26	3.19	9 (40%)	31,36,39	2.91	10 (32%)
4	PSU	L5	3764	4	18,21,22	1.08	1 (5%)	22,30,33	1.74	6 (27%)
4	OMC	L5	1881	4	19,22,23	0.55	0	26,31,34	0.69	0
4	PSU	L5	1683	4,48	18,21,22	1.07	1 (5%)	22,30,33	1.72	4 (18%)
4	OMG	L5	4499	4	23,26,27	0.52	0	33,38,41	0.51	0
4	OMC	L5	2351	4	19,22,23	0.57	0	26,31,34	1.01	2 (7%)
4	OMG	L5	2364	4	23,26,27	0.52	0	33,38,41	0.47	0
4	A2M	L5	3724	4	22,25,26	3.19	9 (40%)	31,36,39	2.95	11 (35%)
4	PSU	L5	3768	4	18,21,22	1.07	1 (5%)	22,30,33	1.66	3 (13%)
4	OMC	L5	3869	4	19,22,23	0.61	0	26,31,34	0.72	0
4	A2M	L5	2787	4	22,25,26	3.19	9 (40%)	31,36,39	2.84	10 (32%)
4	PSU	L5	4423	4	18,21,22	1.07	1 (5%)	22,30,33	1.78	4 (18%)
4	A2M	L5	2363	4	22,25,26	3.15	9 (40%)	31,36,39	2.97	10 (32%)
4	OMG	L5	3944	4	23,26,27	0.47	0	33,38,41	0.64	0
4	A2M	L5	398	4	22,25,26	3.19	9 (40%)	31,36,39	2.96	11 (35%)
4	PSU	L5	4312	4	18,21,22	1.01	1 (5%)	22,30,33	1.77	3 (13%)
4	PSU	L5	2508	4	18,21,22	1.01	1 (5%)	22,30,33	1.72	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	OMG	L5	3627	4	23,26,27	0.53	0	33,38,41	0.64	0
4	OMG	L5	3792	4	23,26,27	0.49	0	33,38,41	0.49	0
4	5MC	L5	4447	4,48	18,22,23	0.71	0	26,32,35	0.73	0
4	OMC	L5	3701	4,48	19,22,23	0.55	0	26,31,34	0.60	0
42	M3L	Lm	98	42	10,11,12	0.51	0	9,14,16	0.46	0
4	A2M	L5	1524	4	22,25,26	3.21	9 (40%)	31,36,39	3.02	10 (32%)
4	OMC	L5	2861	4	19,22,23	0.58	0	26,31,34	0.83	1 (3%)
4	PSU	L5	4500	4	18,21,22	1.06	1 (5%)	22,30,33	1.83	5 (22%)
4	OMG	L5	1316	4	23,26,27	0.53	0	33,38,41	0.67	0
4	5MC	L5	3782	4	18,22,23	0.61	0	26,32,35	0.58	0
4	PSU	L5	1677	4	18,21,22	1.11	2 (11%)	22,30,33	1.75	4 (18%)
4	OMU	L5	4306	4	19,22,23	3.03	8 (42%)	26,31,34	1.77	5 (19%)
4	OMU	L5	4498	4,48	19,22,23	2.99	8 (42%)	26,31,34	1.72	5 (19%)
4	PSU	L5	4521	4,48	18,21,22	1.04	1 (5%)	22,30,33	1.90	5 (22%)
4	PSU	L5	5010	4	18,21,22	1.08	1 (5%)	22,30,33	1.73	4 (18%)
4	OMG	L5	2424	4	23,26,27	0.50	0	33,38,41	0.49	0
4	PSU	L5	1792	4	18,21,22	1.03	1 (5%)	22,30,33	1.71	3 (13%)
4	PSU	L5	2843	4	18,21,22	1.10	1 (5%)	22,30,33	1.78	4 (18%)
4	PSU	L5	3920	4	18,21,22	1.10	1 (5%)	22,30,33	1.73	4 (18%)
4	A2M	L5	1871	4	22,25,26	3.16	10 (45%)	31,36,39	2.98	11 (35%)
4	PSU	L5	3884	4	18,21,22	1.07	1 (5%)	22,30,33	1.83	4 (18%)
4	A2M	L5	3867	4	22,25,26	3.19	10 (45%)	31,36,39	2.99	10 (32%)
1	V5N	LA	216	1	9,11,12	2.59	3 (33%)	9,14,16	1.18	1 (11%)
4	OMU	L5	2415	4	19,22,23	3.08	8 (42%)	26,31,34	1.71	5 (19%)
4	A2M	L5	3760	4	22,25,26	3.16	9 (40%)	31,36,39	2.96	10 (32%)
4	OMG	L5	4370	4	23,26,27	0.50	0	33,38,41	0.59	0
4	OMG	L5	1522	4	23,26,27	0.54	0	33,38,41	0.60	0
4	OMC	L5	2804	4	19,22,23	0.58	0	26,31,34	0.67	0
4	PSU	L5	3734	4	18,21,22	1.03	1 (5%)	22,30,33	1.68	4 (18%)
3	OMU	L8	14	3,4,48	19,22,23	3.04	8 (42%)	26,31,34	1.66	5 (19%)
4	OMG	L5	4228	4	23,26,27	0.48	0	33,38,41	0.61	0
4	PSU	L5	4628	4	18,21,22	1.02	1 (5%)	22,30,33	1.69	3 (13%)
4	PSU	L5	1782	4	18,21,22	1.07	1 (5%)	22,30,33	1.76	4 (18%)
4	A2M	L5	4590	4	22,25,26	3.16	9 (40%)	31,36,39	3.04	11 (35%)
4	OMG	L5	4392	4	23,26,27	0.46	0	33,38,41	0.50	0
44	MLZ	Lo	53	44	8,9,10	0.72	0	4,9,11	0.55	0
4	OMG	L5	1625	4,48	23,26,27	0.54	0	33,38,41	0.50	0
4	PSU	L5	3853	4	18,21,22	1.08	1 (5%)	22,30,33	1.61	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	PSU	L5	4296	4,48	18,21,22	1.03	1 (5%)	22,30,33	1.86	4 (18%)
4	1MA	L5	1322	4	21,25,26	0.46	0	31,37,40	0.76	1 (3%)
4	PSU	L5	1536	4	18,21,22	1.08	1 (5%)	22,30,33	1.71	4 (18%)
4	PSU	L5	4353	4	18,21,22	1.03	1 (5%)	22,30,33	1.82	4 (18%)
4	PSU	L5	4576	4	18,21,22	1.05	1 (5%)	22,30,33	1.81	5 (22%)
4	PSU	L5	4361	4	18,21,22	1.01	1 (5%)	22,30,33	1.70	3 (13%)
4	PSU	L5	3844	4	18,21,22	1.11	1 (5%)	22,30,33	1.77	4 (18%)
4	OMU	L5	3925	4	19,22,23	3.00	8 (42%)	26,31,34	1.70	4 (15%)
4	PSU	L5	3639	4	18,21,22	1.05	1 (5%)	22,30,33	1.70	4 (18%)
4	A2M	L5	1326	4	22,25,26	3.15	9 (40%)	31,36,39	2.94	10 (32%)
4	PSU	L5	1744	4,48	18,21,22	1.03	1 (5%)	22,30,33	1.70	4 (18%)
4	PSU	L5	3729	4	18,21,22	1.06	1 (5%)	22,30,33	1.72	4 (18%)
4	PSU	L5	3758	4	18,21,22	1.12	1 (5%)	22,30,33	1.78	4 (18%)
4	PSU	L5	4293	4	18,21,22	0.99	1 (5%)	22,30,33	1.67	4 (18%)
4	PSU	L5	4493	4,48	18,21,22	1.10	1 (5%)	22,30,33	1.87	5 (22%)
4	PSU	L5	4299	4	18,21,22	1.01	1 (5%)	22,30,33	1.76	4 (18%)
4	A2M	L5	3723	4	22,25,26	3.18	9 (40%)	31,36,39	2.94	10 (32%)
4	PSU	L5	3851	4	18,21,22	1.09	1 (5%)	22,30,33	1.73	4 (18%)
4	OMC	L5	2824	4	19,22,23	0.60	0	26,31,34	0.68	0
4	PSU	L5	1781	4	18,21,22	1.06	1 (5%)	22,30,33	1.60	4 (18%)
4	A2M	L5	4571	4	22,25,26	3.22	9 (40%)	31,36,39	3.00	12 (38%)
4	PSU	L5	4579	4	18,21,22	1.05	1 (5%)	22,30,33	1.74	4 (18%)
3	PSU	L8	69	3	18,21,22	1.04	1 (5%)	22,30,33	1.78	5 (22%)
4	OMC	L5	4456	4	19,22,23	0.57	0	26,31,34	0.71	1 (3%)
4	OMG	L5	2876	4	23,26,27	0.49	0	33,38,41	0.53	0
4	A2M	L5	2815	4	22,25,26	3.18	10 (45%)	31,36,39	2.98	11 (35%)
4	PSU	L5	5001	4	18,21,22	1.04	1 (5%)	22,30,33	1.74	4 (18%)
4	PSU	L5	3770	4	18,21,22	1.04	1 (5%)	22,30,33	1.71	5 (22%)
3	PSU	L8	55	3	18,21,22	1.07	1 (5%)	22,30,33	1.87	5 (22%)

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
4	PSU	L5	2839	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4403	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4471	4	-	0/7/25/26	0/2/2/2
4	OMU	L5	4227	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	4431	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4457	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	3695	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	400	4	-	0/9/27/28	0/3/3/3
4	A2M	L5	3785	4	-	2/9/27/28	0/3/3/3
4	OMG	L5	4637	4,48	-	2/9/27/28	0/3/3/3
4	A2M	L5	3830	4	-	0/9/27/28	0/3/3/3
4	6MZ	L5	4220	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	4689	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	2422	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	3715	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4673	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	1534	4	-	2/9/27/28	0/3/3/3
15	V5N	La	39	15	-	1/9/10/12	0/1/1/1
4	OMG	L5	4494	4,48	-	1/9/27/28	0/3/3/3
4	PSU	L5	3762	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	4536	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	1779	4	-	0/7/25/26	0/2/2/2
4	OMG	L5	3899	4	-	0/9/27/28	0/3/3/3
4	UY1	L5	3818	4,48	-	2/9/27/28	0/2/2/2
4	OMC	L5	2365	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	1862	4	-	0/7/25/26	0/2/2/2
4	UR3	L5	4530	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	1582	4	-	0/7/25/26	0/2/2/2
31	MLZ	Lb	5	31,48	-	1/7/8/10	-
4	OMG	L5	4623	4	-	2/9/27/28	0/3/3/3
4	PSU	L5	4552	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	1340	4	-	0/9/27/28	0/2/2/2
4	OMG	L5	4618	4	-	2/9/27/28	0/3/3/3
4	PSU	L5	4636	4	-	2/7/25/26	0/2/2/2
4	PSU	L5	4972	4,48	-	0/7/25/26	0/2/2/2
4	OMC	L5	3841	4	-	0/9/27/28	0/2/2/2
4	OMU	L5	2837	4	-	0/9/27/28	0/2/2/2
4	OMG	L5	4196	4	-	1/9/27/28	0/3/3/3
4	PSU	L5	3637	4,48	-	0/7/25/26	0/2/2/2
4	A2M	L5	3718	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	4442	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4569	4	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	L5	1860	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	2632	4	-	0/7/25/26	0/2/2/2
3	OMG	L8	75	3	-	0/9/27/28	0/3/3/3
4	PSU	L5	4420	4	-	4/7/25/26	0/2/2/2
4	A2M	L5	3825	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	4531	4	-	2/7/25/26	0/2/2/2
2	HIC	LB	245	2	-	0/5/6/8	0/1/1/1
4	OMG	L5	3744	4	-	0/9/27/28	0/3/3/3
4	A2M	L5	4523	4	-	1/9/27/28	0/3/3/3
4	OMC	L5	3808	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	4532	4	-	0/7/25/26	0/2/2/2
4	OMU	L5	4620	4	-	0/9/27/28	0/2/2/2
4	OMC	L5	3887	4	-	0/9/27/28	0/2/2/2
4	A2M	L5	2401	4	-	1/9/27/28	0/3/3/3
4	PSU	L5	3764	4	-	2/7/25/26	0/2/2/2
4	OMC	L5	1881	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	1683	4,48	-	0/7/25/26	0/2/2/2
4	OMG	L5	4499	4	-	0/9/27/28	0/3/3/3
4	OMC	L5	2351	4	-	4/9/27/28	0/2/2/2
4	OMG	L5	2364	4	-	2/9/27/28	0/3/3/3
4	A2M	L5	3724	4	-	1/9/27/28	0/3/3/3
4	PSU	L5	3768	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	3869	4	-	0/9/27/28	0/2/2/2
4	A2M	L5	2787	4	-	4/9/27/28	0/3/3/3
4	PSU	L5	4423	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	2363	4	-	0/9/27/28	0/3/3/3
4	OMG	L5	3944	4	-	2/9/27/28	0/3/3/3
4	A2M	L5	398	4	-	3/9/27/28	0/3/3/3
4	PSU	L5	4312	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	2508	4	-	0/7/25/26	0/2/2/2
4	OMG	L5	3627	4	-	0/9/27/28	0/3/3/3
4	OMG	L5	3792	4	-	0/9/27/28	0/3/3/3
4	5MC	L5	4447	4,48	-	4/7/25/26	0/2/2/2
4	OMC	L5	3701	4,48	-	4/9/27/28	0/2/2/2
42	M3L	Lm	98	42	-	0/9/10/12	-
4	A2M	L5	1524	4	-	0/9/27/28	0/3/3/3
4	OMC	L5	2861	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	4500	4	-	1/7/25/26	0/2/2/2
4	OMG	L5	1316	4	-	0/9/27/28	0/3/3/3
4	5MC	L5	3782	4	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	L5	1677	4	-	0/7/25/26	0/2/2/2
4	OMU	L5	4306	4	-	0/9/27/28	0/2/2/2
4	OMU	L5	4498	4,48	-	0/9/27/28	0/2/2/2
4	PSU	L5	4521	4,48	-	0/7/25/26	0/2/2/2
4	PSU	L5	5010	4	-	0/7/25/26	0/2/2/2
4	OMG	L5	2424	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	1792	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	2843	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	3920	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	1871	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	3884	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	3867	4	-	0/9/27/28	0/3/3/3
1	V5N	LA	216	1	-	2/9/10/12	0/1/1/1
4	OMU	L5	2415	4	-	1/9/27/28	0/2/2/2
4	A2M	L5	3760	4	-	2/9/27/28	0/3/3/3
4	OMG	L5	4370	4	-	0/9/27/28	0/3/3/3
4	OMG	L5	1522	4	-	0/9/27/28	0/3/3/3
4	OMC	L5	2804	4	-	0/9/27/28	0/2/2/2
4	PSU	L5	3734	4	-	0/7/25/26	0/2/2/2
3	OMU	L8	14	3,4,48	-	1/9/27/28	0/2/2/2
4	OMG	L5	4228	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	4628	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	1782	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	4590	4	-	2/9/27/28	0/3/3/3
4	OMG	L5	4392	4	-	0/9/27/28	0/3/3/3
44	MLZ	Lo	53	44	-	1/7/8/10	-
4	OMG	L5	1625	4,48	-	1/9/27/28	0/3/3/3
4	PSU	L5	3853	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4296	4,48	-	0/7/25/26	0/2/2/2
4	1MA	L5	1322	4	-	0/7/25/26	0/3/3/3
4	PSU	L5	1536	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4353	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4576	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4361	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	3844	4	-	1/7/25/26	0/2/2/2
4	OMU	L5	3925	4	-	1/9/27/28	0/2/2/2
4	PSU	L5	3639	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	1326	4	-	1/9/27/28	0/3/3/3
4	PSU	L5	1744	4,48	-	0/7/25/26	0/2/2/2
4	PSU	L5	3729	4	-	2/7/25/26	0/2/2/2
4	PSU	L5	3758	4	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PSU	L5	4293	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	4493	4,48	-	0/7/25/26	0/2/2/2
4	PSU	L5	4299	4	-	0/7/25/26	0/2/2/2
4	A2M	L5	3723	4	-	2/9/27/28	0/3/3/3
4	PSU	L5	3851	4	-	0/7/25/26	0/2/2/2
4	OMC	L5	2824	4	-	1/9/27/28	0/2/2/2
4	PSU	L5	1781	4	-	2/7/25/26	0/2/2/2
4	A2M	L5	4571	4	-	0/9/27/28	0/3/3/3
4	PSU	L5	4579	4	-	0/7/25/26	0/2/2/2
3	PSU	L8	69	3	-	0/7/25/26	0/2/2/2
4	OMC	L5	4456	4	-	0/9/27/28	0/2/2/2
4	OMG	L5	2876	4	-	1/9/27/28	0/3/3/3
4	A2M	L5	2815	4	-	3/9/27/28	0/3/3/3
4	PSU	L5	5001	4	-	0/7/25/26	0/2/2/2
4	PSU	L5	3770	4	-	0/7/25/26	0/2/2/2
3	PSU	L8	55	3	-	0/7/25/26	0/2/2/2

The worst 5 of 342 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L5	1524	A2M	C3'-C4'	-8.95	1.30	1.53
4	L5	2815	A2M	C3'-C4'	-8.83	1.30	1.53
4	L5	398	A2M	C3'-C4'	-8.82	1.30	1.53
4	L5	3867	A2M	C3'-C4'	-8.77	1.30	1.53
4	L5	400	A2M	C3'-C4'	-8.75	1.30	1.53

The worst 5 of 539 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L5	3825	A2M	N6-C6-N1	-6.81	103.43	118.35
4	L5	4590	A2M	N6-C6-N1	-6.77	103.51	118.35
4	L5	3830	A2M	N6-C6-N1	-6.76	103.54	118.35
4	L5	2815	A2M	N6-C6-N1	-6.75	103.57	118.35
4	L5	1326	A2M	N6-C6-N1	-6.74	103.58	118.35

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L8	14	OMU	C1'-C2'-O2'-CM2
4	L5	398	A2M	C1'-C2'-O2'-CM'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	L5	2364	OMG	O4'-C4'-C5'-O5'
4	L5	2415	OMU	C1'-C2'-O2'-CM2
4	L5	2787	A2M	C2'-C1'-N9-C8

There are no ring outliers.

35 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L5	4457	PSU	1	0
4	L5	3830	A2M	1	0
4	L5	4220	6MZ	1	0
4	L5	3762	PSU	1	0
4	L5	4530	UR3	1	0
4	L5	4623	OMG	2	0
4	L5	1340	OMC	1	0
4	L5	4196	OMG	1	0
4	L5	3718	A2M	4	0
4	L5	2632	PSU	1	0
3	L8	75	OMG	1	0
4	L5	4620	OMU	2	0
4	L5	3764	PSU	2	0
4	L5	4499	OMG	1	0
4	L5	2351	OMC	1	0
4	L5	3724	A2M	1	0
4	L5	3869	OMC	4	0
4	L5	398	A2M	1	0
4	L5	2861	OMC	1	0
4	L5	5010	PSU	1	0
4	L5	2424	OMG	1	0
4	L5	1871	A2M	1	0
4	L5	3884	PSU	1	0
4	L5	3867	A2M	2	0
4	L5	2415	OMU	2	0
4	L5	3760	A2M	1	0
4	L5	4590	A2M	1	0
4	L5	3925	OMU	1	0
4	L5	4293	PSU	1	0
4	L5	3723	A2M	3	0
4	L5	2824	OMC	1	0
4	L5	4571	A2M	1	0
4	L5	4579	PSU	2	0
4	L5	2876	OMG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L5	2815	A2M	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 162 ligands modelled in this entry, 137 are monoatomic - leaving 25 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	$\#\|Z\| > 2$
52	SPM	L5	5231	-	13,13,13	0.36	0	12,12,12	0.98	0
53	ADP	L5	5235	-	27,29,29	1.34	4 (14%)	42,45,45	1.99	9 (21%)
49	SPD	L5	5103	-	9,9,9	0.30	0	8,8,8	0.89	0
49	SPD	L5	5226	-	9,9,9	0.34	0	8,8,8	0.81	0
52	SPM	L5	5230	-	13,13,13	0.35	0	12,12,12	0.97	0
51	A1E6S	L5	5223	-	26,33,33	5.21	12 (46%)	12,52,52	2.10	4 (33%)
49	SPD	LN	302	-	9,9,9	0.32	0	8,8,8	0.92	0
52	SPM	L5	5229	-	13,13,13	0.35	0	12,12,12	0.87	0
49	SPD	L5	5110	-	9,9,9	0.33	0	8,8,8	0.84	0
49	SPD	L5	5111	-	9,9,9	0.33	0	8,8,8	0.81	0
49	SPD	L5	5112	-	9,9,9	0.32	0	8,8,8	0.56	0
50	PUT	L5	5113	-	5,5,5	0.14	0	4,4,4	0.15	0
49	SPD	L5	5104	-	9,9,9	0.32	0	8,8,8	0.83	0
49	SPD	L5	5105	-	9,9,9	0.32	0	8,8,8	0.92	0
52	SPM	L5	5224	-	13,13,13	0.35	0	12,12,12	1.07	0
49	SPD	L5	5106	-	9,9,9	0.37	0	8,8,8	0.90	0
49	SPD	L5	5109	-	9,9,9	0.33	0	8,8,8	0.95	0
49	SPD	L5	5107	-	9,9,9	0.34	0	8,8,8	0.75	0
52	SPM	L5	5233	-	13,13,13	0.34	0	12,12,12	0.88	0
52	SPM	L5	5232	-	13,13,13	0.37	0	12,12,12	0.78	0
52	SPM	L5	5225	-	13,13,13	0.36	0	12,12,12	0.94	0
49	SPD	L5	5227	-	9,9,9	9.02	7 (77%)	8,8,8	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
52	SPM	L5	5228	-	13,13,13	0.35	0	12,12,12	1.09	0
52	SPM	L5	5234	-	13,13,13	0.35	0	12,12,12	0.93	0
49	SPD	L5	5108	-	9,9,9	0.34	0	8,8,8	0.94	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
52	SPM	L5	5231	-	-	5/11/11/11	-
53	ADP	L5	5235	-	-	0/16/32/32	0/3/3/3
49	SPD	L5	5103	-	-	1/7/7/7	-
49	SPD	L5	5226	-	-	2/7/7/7	-
52	SPM	L5	5230	-	-	4/11/11/11	-
51	A1E6S	L5	5223	-	-	3/7/76/76	0/3/5/5
49	SPD	LN	302	-	-	1/7/7/7	-
52	SPM	L5	5229	-	-	1/11/11/11	-
49	SPD	L5	5110	-	-	2/7/7/7	-
49	SPD	L5	5111	-	-	0/7/7/7	-
49	SPD	L5	5112	-	-	3/7/7/7	-
50	PUT	L5	5113	-	-	1/3/3/3	-
49	SPD	L5	5104	-	-	3/7/7/7	-
49	SPD	L5	5105	-	-	2/7/7/7	-
52	SPM	L5	5224	-	-	6/11/11/11	-
49	SPD	L5	5106	-	-	3/7/7/7	-
49	SPD	L5	5109	-	-	2/7/7/7	-
49	SPD	L5	5107	-	-	3/7/7/7	-
52	SPM	L5	5233	-	-	6/11/11/11	-
52	SPM	L5	5232	-	-	5/11/11/11	-
52	SPM	L5	5225	-	-	7/11/11/11	-
49	SPD	L5	5227	-	-	2/7/7/7	-
52	SPM	L5	5228	-	-	0/11/11/11	-
52	SPM	L5	5234	-	-	3/11/11/11	-
49	SPD	L5	5108	-	-	3/7/7/7	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	L5	5223	A1E6S	C17-C18	23.16	1.52	1.33
49	L5	5227	SPD	C8-C7	12.55	2.02	1.51
49	L5	5227	SPD	C4-C5	12.46	2.01	1.51
49	L5	5227	SPD	C7-N6	11.48	1.85	1.46
49	L5	5227	SPD	C5-N6	11.44	1.85	1.46

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	L5	5235	ADP	C5-C4-N3	-6.53	118.23	126.75
51	L5	5223	A1E6S	C02-C03-C04	5.46	108.27	100.64
53	L5	5235	ADP	N3-C4-N9	5.06	135.43	127.08
53	L5	5235	ADP	C2-N3-C4	3.96	121.11	111.75
53	L5	5235	ADP	PA-O3A-PB	-3.62	120.42	132.83

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	L5	5226	SPD	C7-C8-C9-N10
49	L5	5227	SPD	C4-C5-N6-C7
51	L5	5223	A1E6S	C17-C18-C21-C22
51	L5	5223	A1E6S	C19-C18-C21-C22
49	L5	5104	SPD	C3-C4-C5-N6

There are no ring outliers.

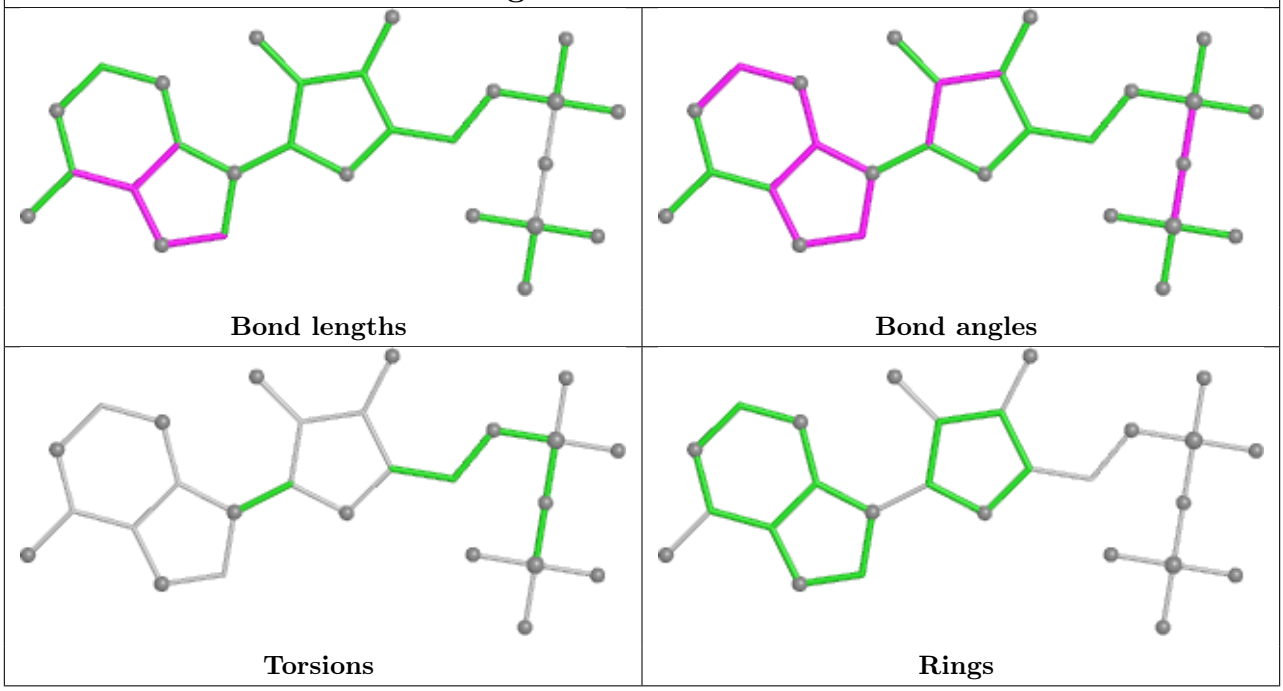
10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	L5	5112	SPD	5	0
50	L5	5113	PUT	1	0
52	L5	5224	SPM	2	0
49	L5	5109	SPD	1	0
49	L5	5107	SPD	1	0
52	L5	5225	SPM	1	0
49	L5	5227	SPD	9	0
52	L5	5228	SPM	2	0
52	L5	5234	SPM	1	0
49	L5	5108	SPD	1	0

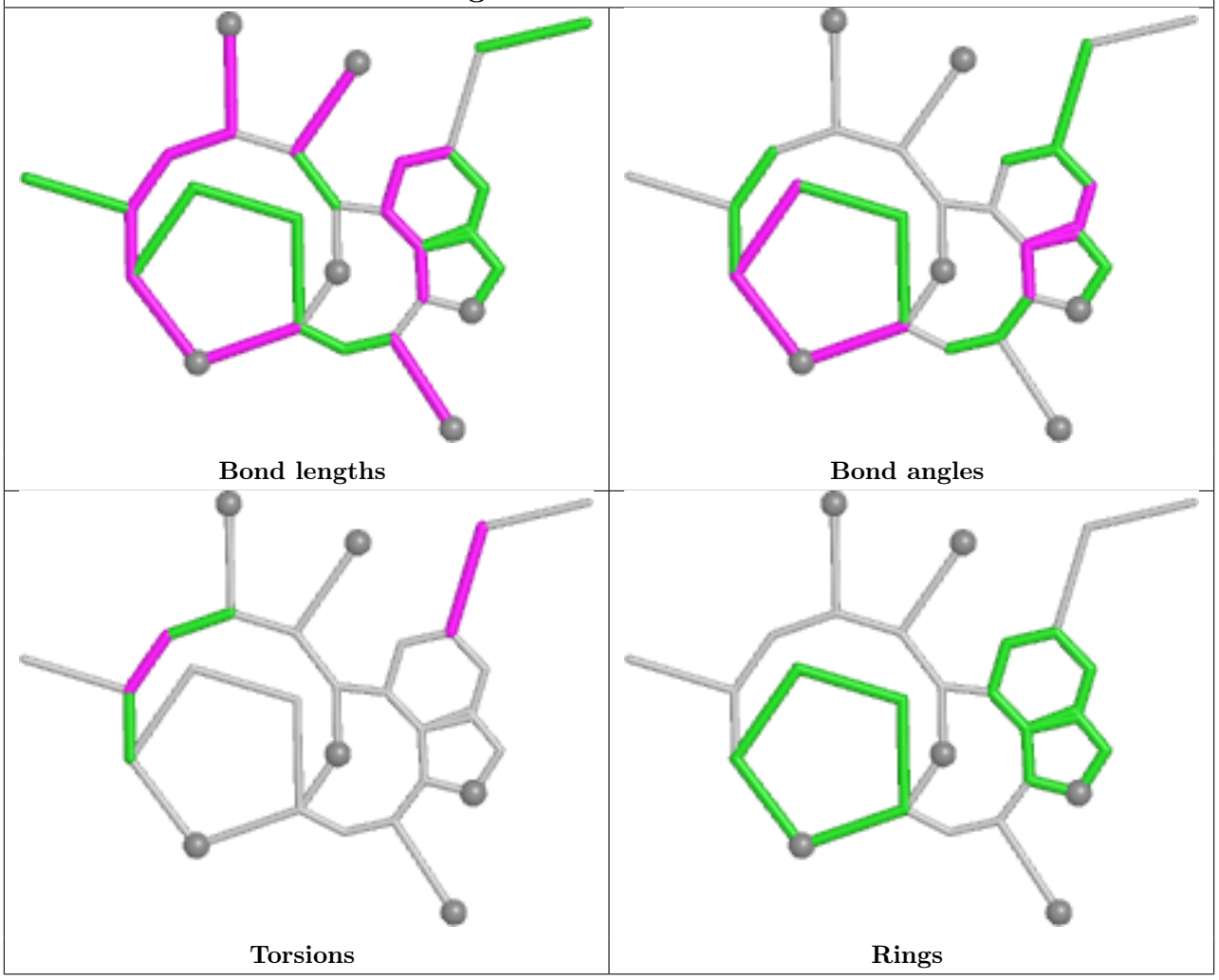
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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 5235



Ligand A1E6S L5 5223



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.

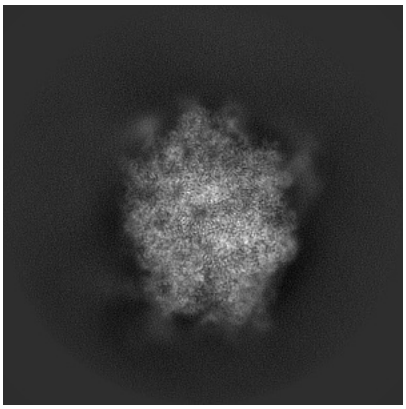
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-66933. These allow visual inspection of the internal detail of the map and identification of artifacts.

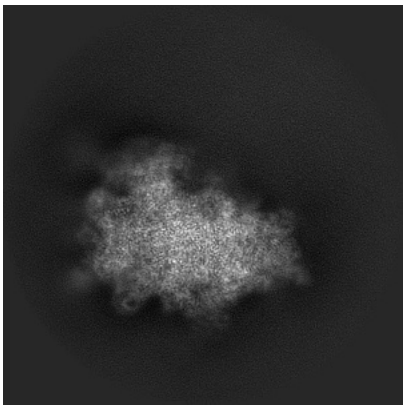
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

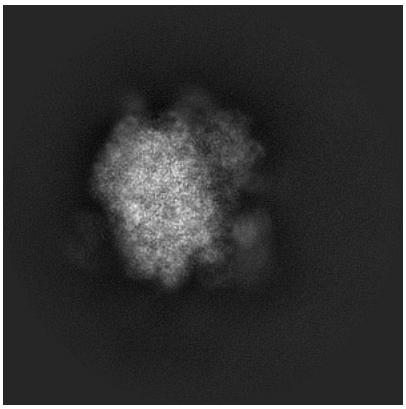
6.1.1 Primary map



X

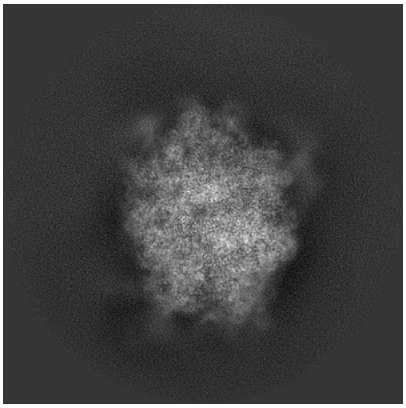


Y

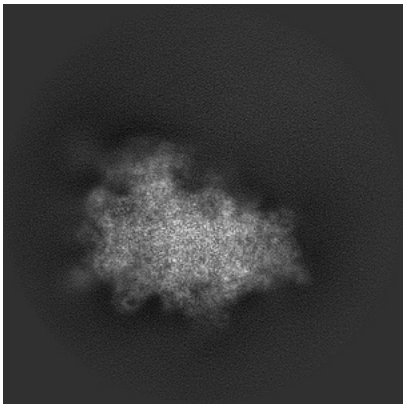


Z

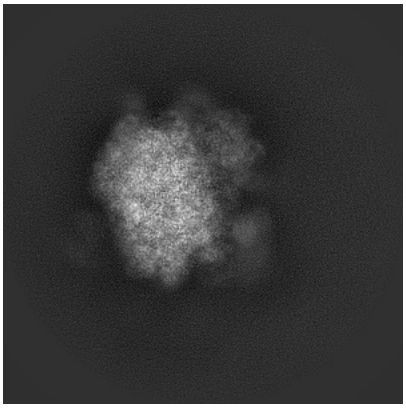
6.1.2 Raw map



X



Y

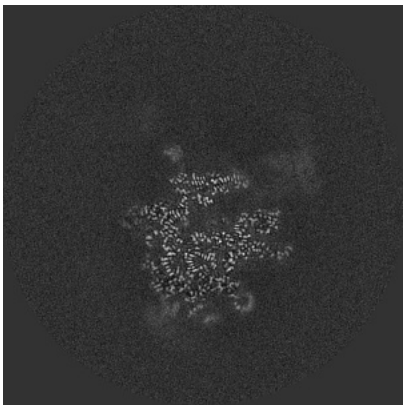


Z

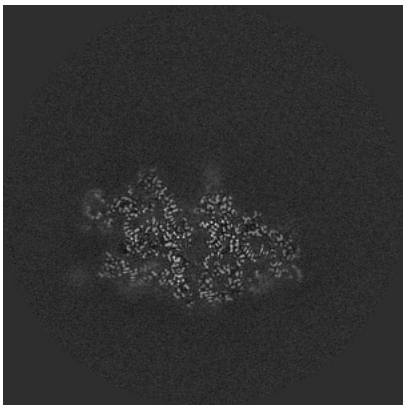
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

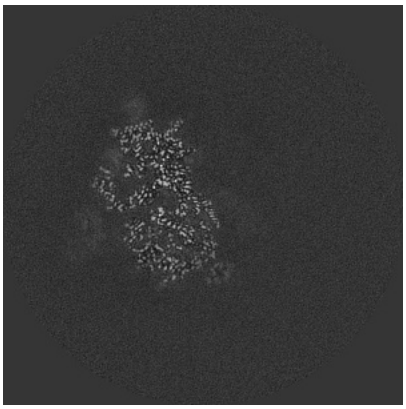
6.2.1 Primary map



X Index: 240

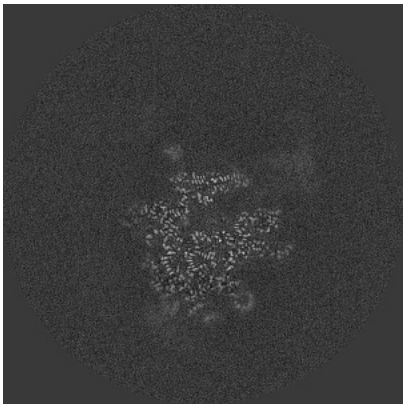


Y Index: 240

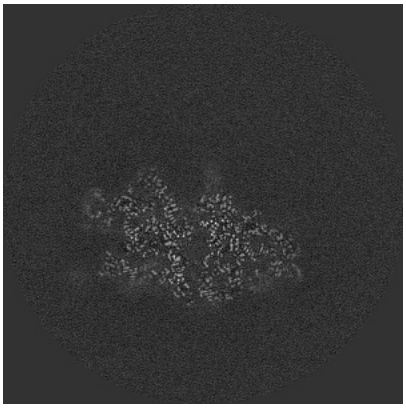


Z Index: 240

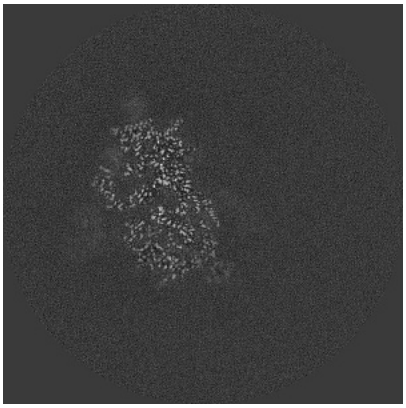
6.2.2 Raw map



X Index: 240



Y Index: 240

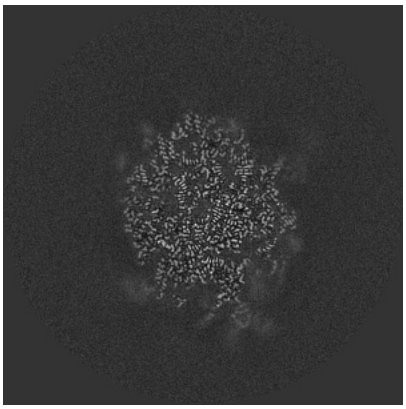


Z Index: 240

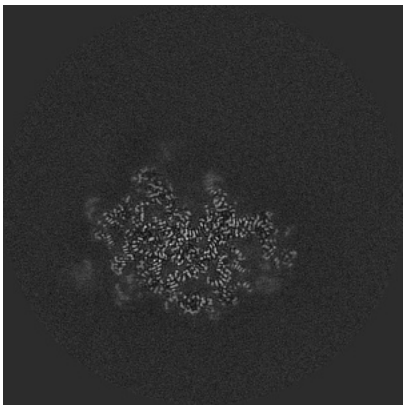
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

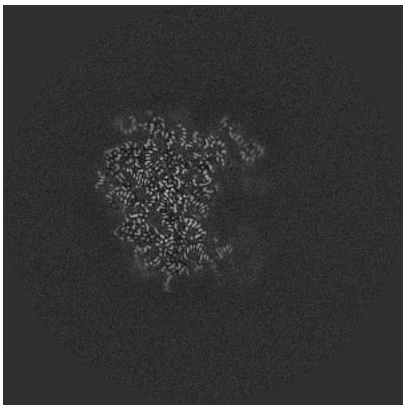
6.3.1 Primary map



X Index: 207

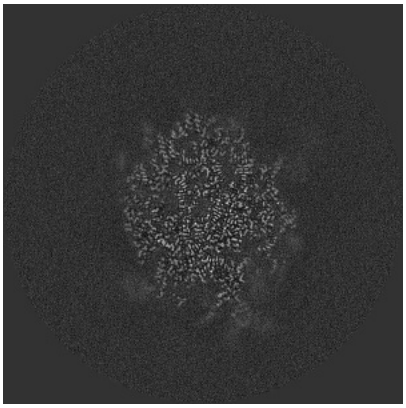


Y Index: 254

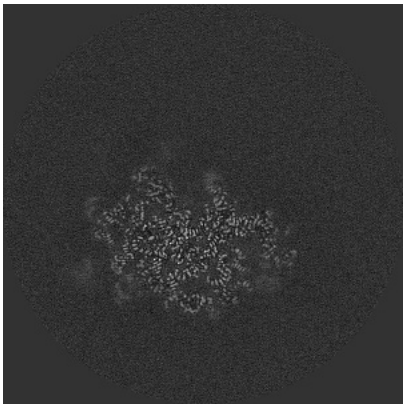


Z Index: 204

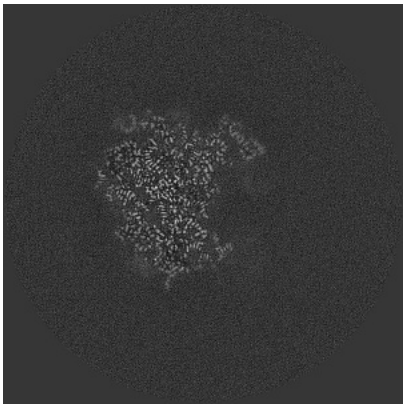
6.3.2 Raw map



X Index: 207



Y Index: 254

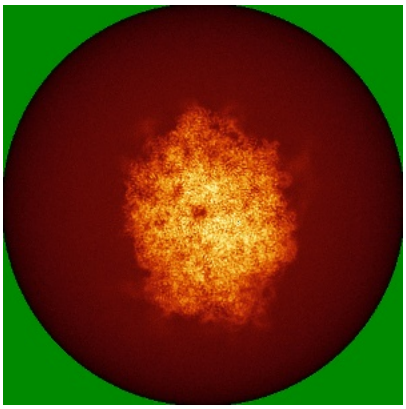


Z Index: 203

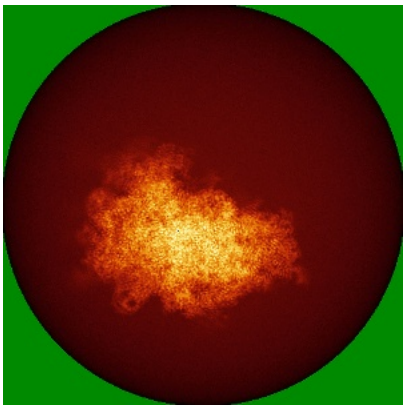
The images above show the largest variance slices of the map in three orthogonal directions.

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

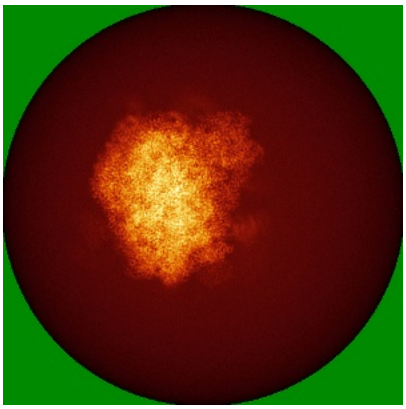
6.4.1 Primary map



X

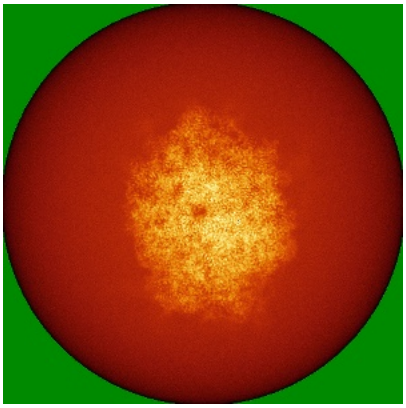


Y

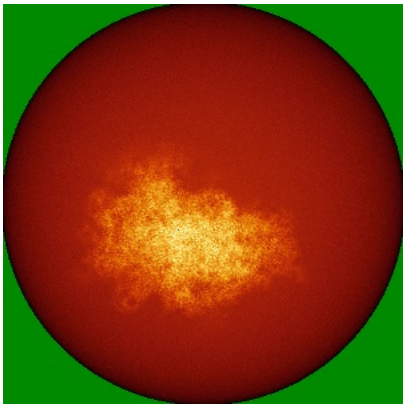


Z

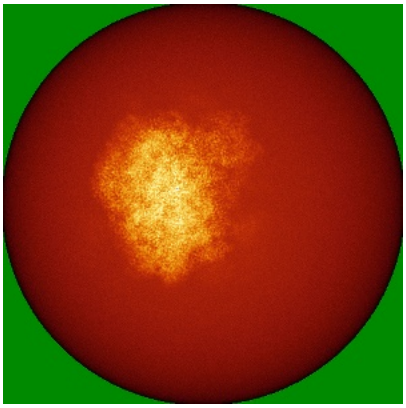
6.4.2 Raw map



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)

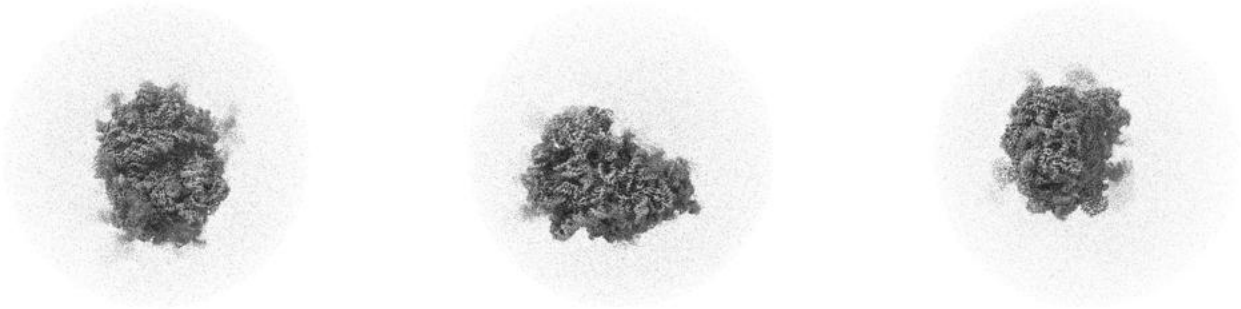
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0127. 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.

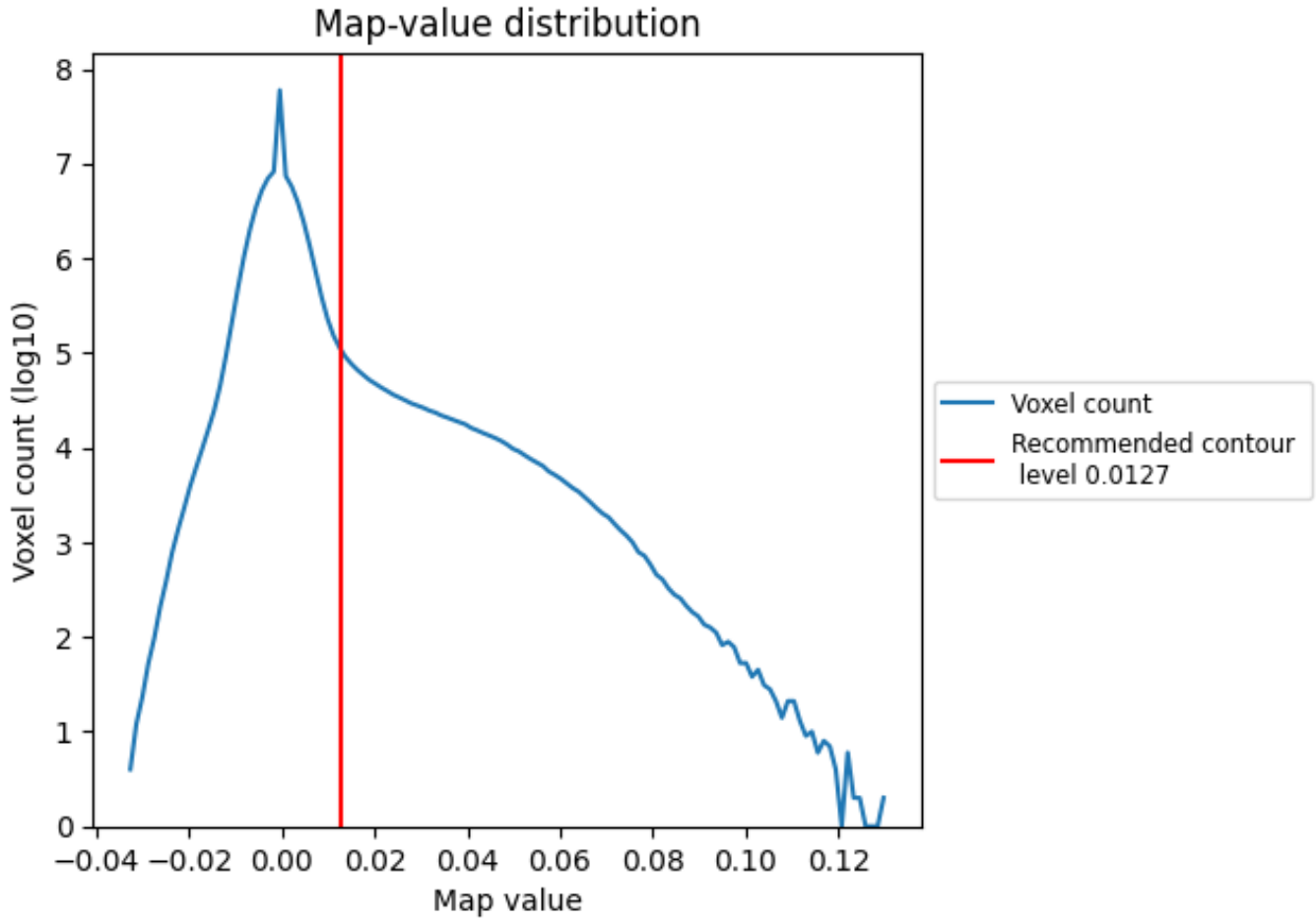
6.6 Mask visualisation (i)

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

7 Map analysis

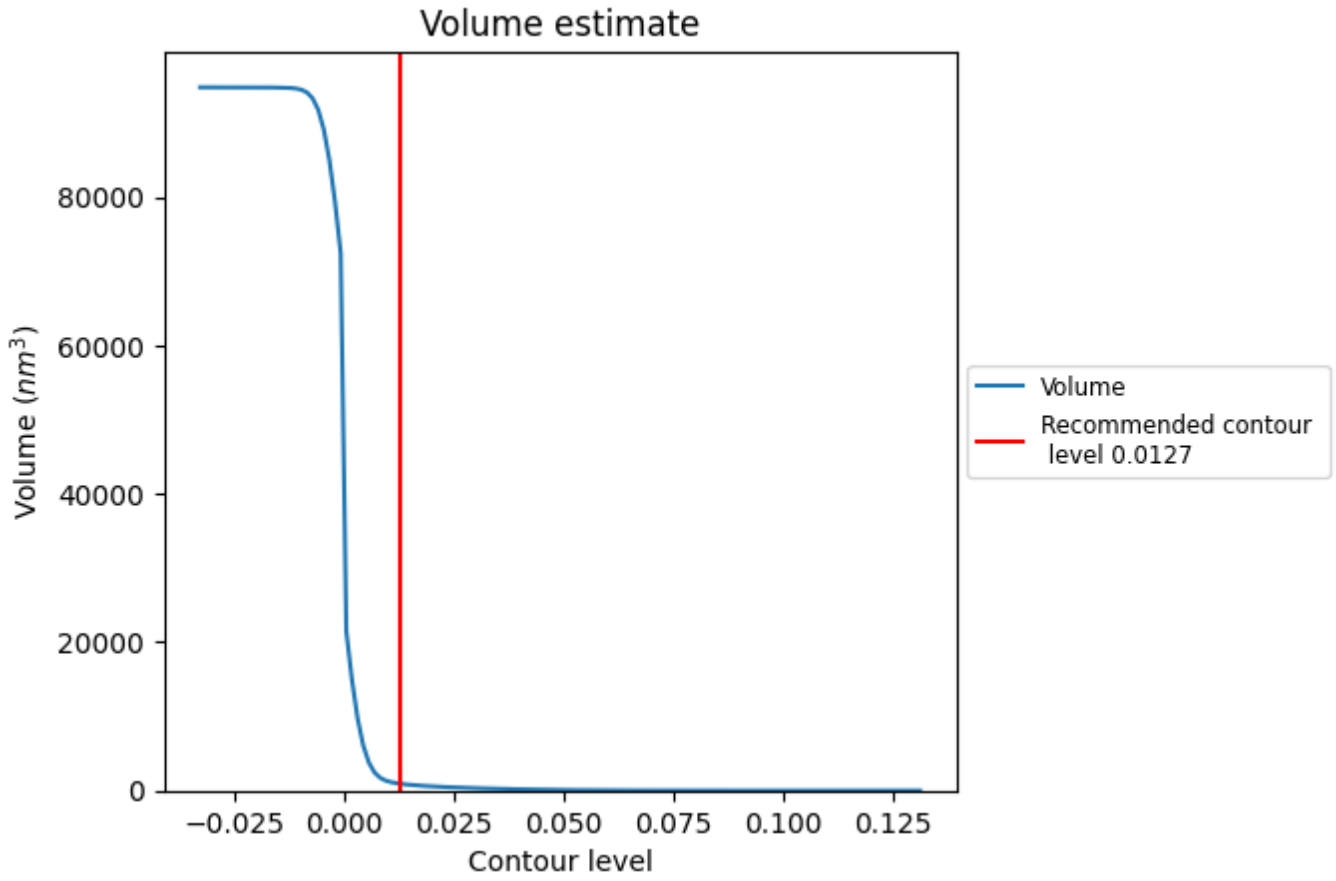
This section contains the results of statistical analysis of the map.

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.

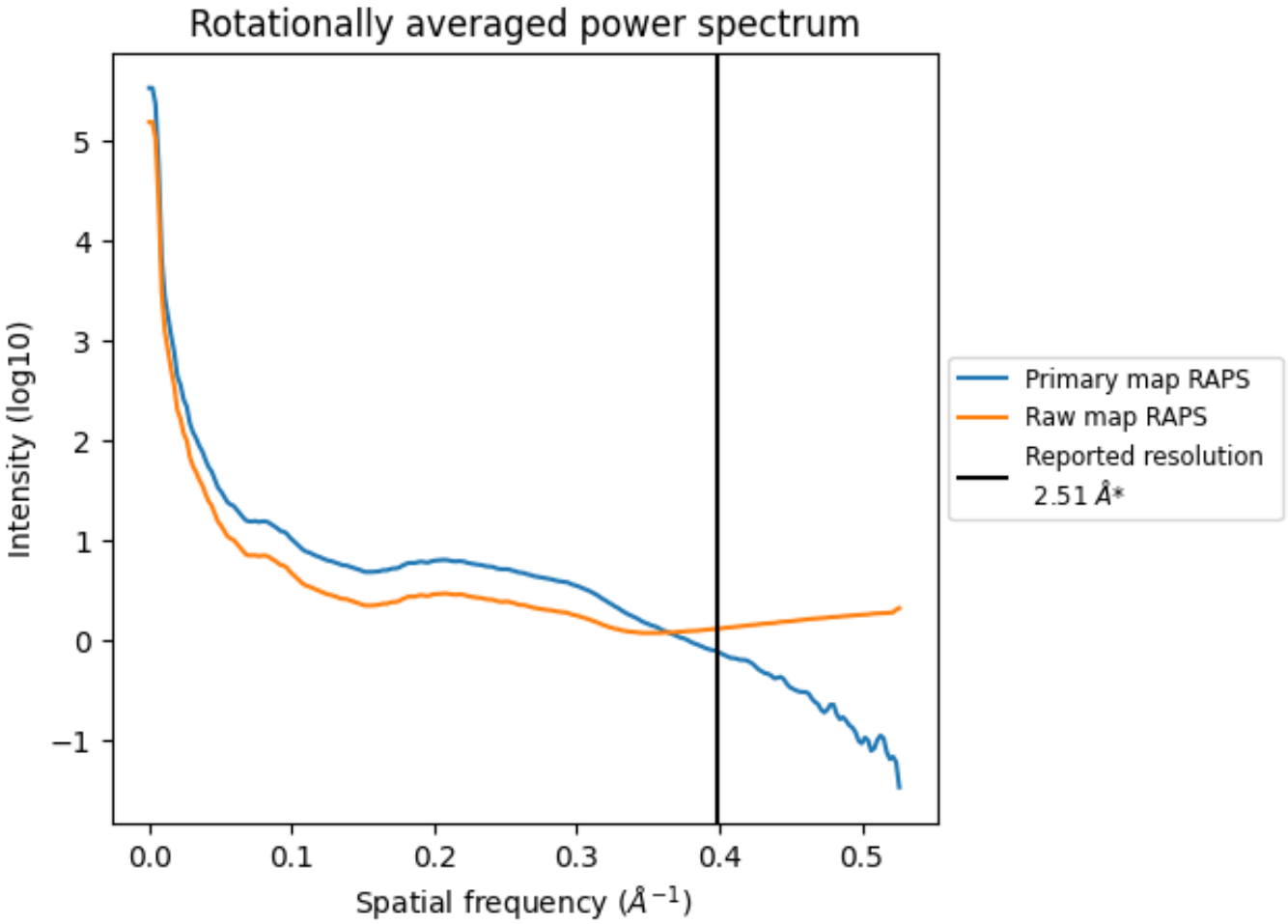
7.2 Volume estimate (i)



The volume at the recommended contour level is 933 nm^3; this corresponds to an approximate mass of 843 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)

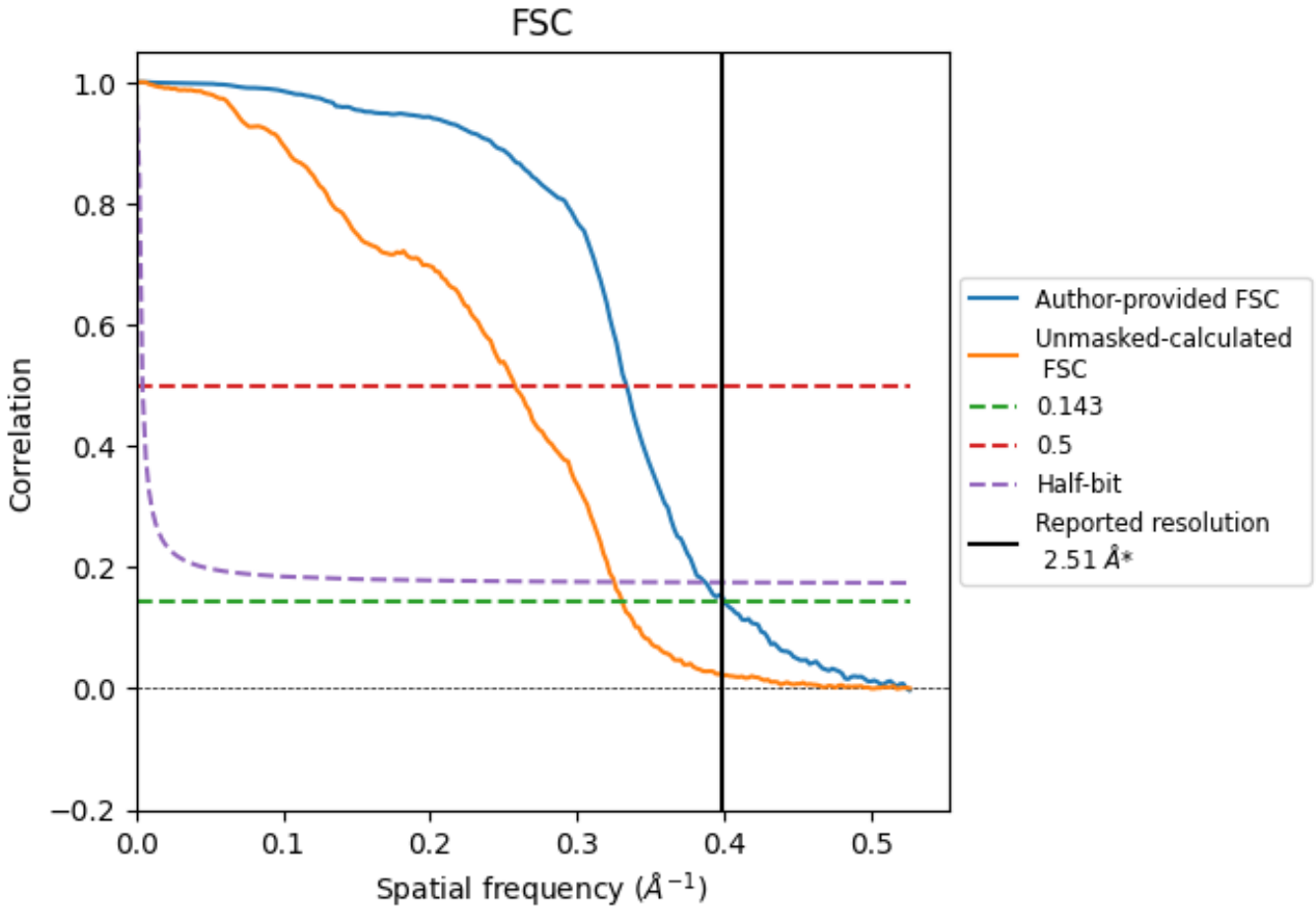


*Reported resolution corresponds to spatial frequency of 0.398 Å^{-1}

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 0.398 Å^{-1}

8.2 Resolution estimates (i)

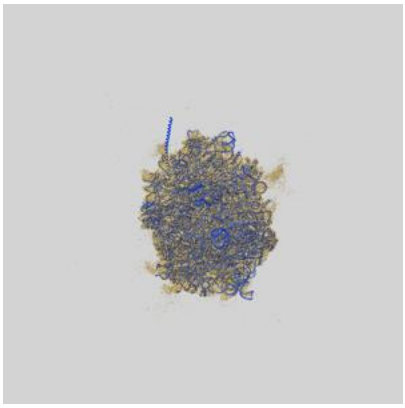
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.51	-	-
Author-provided FSC curve	2.50	3.00	2.58
Unmasked-calculated*	3.02	3.88	3.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.02 differs from the reported value 2.51 by more than 10 %

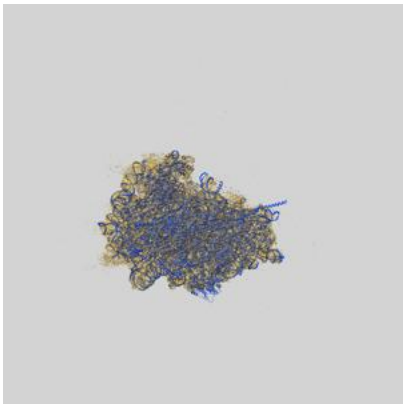
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-66933 and PDB model 9XJA. Per-residue inclusion information can be found in section 3 on page 17.

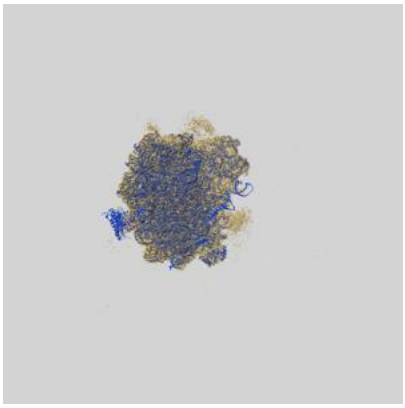
9.1 Map-model overlay



X



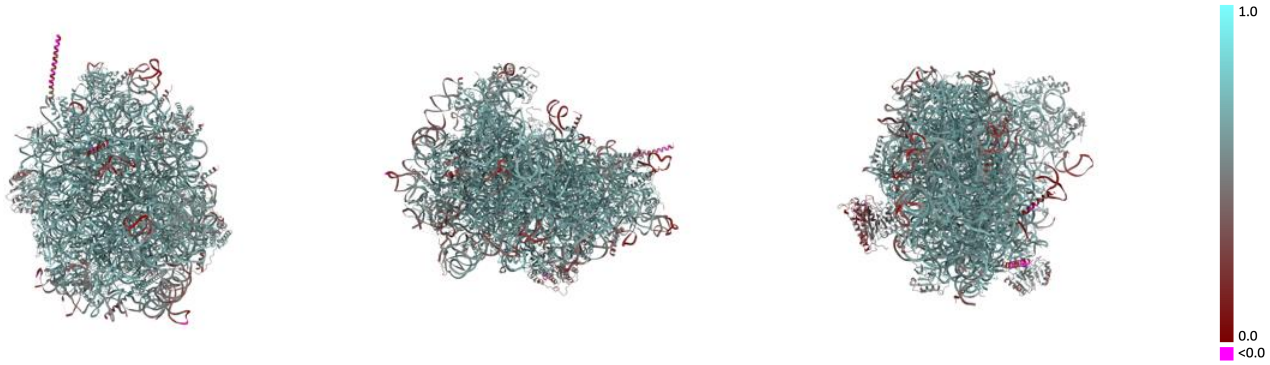
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0127 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.

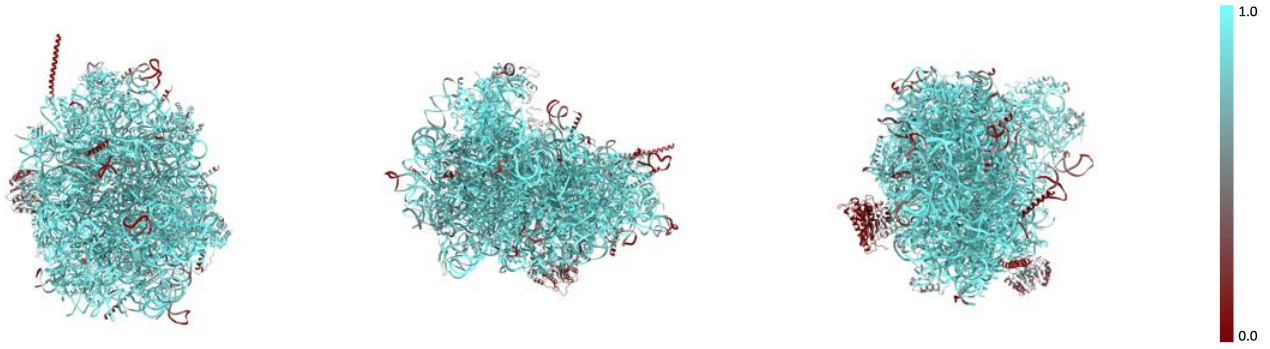
9.2 Q-score mapped to coordinate model (i)



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.

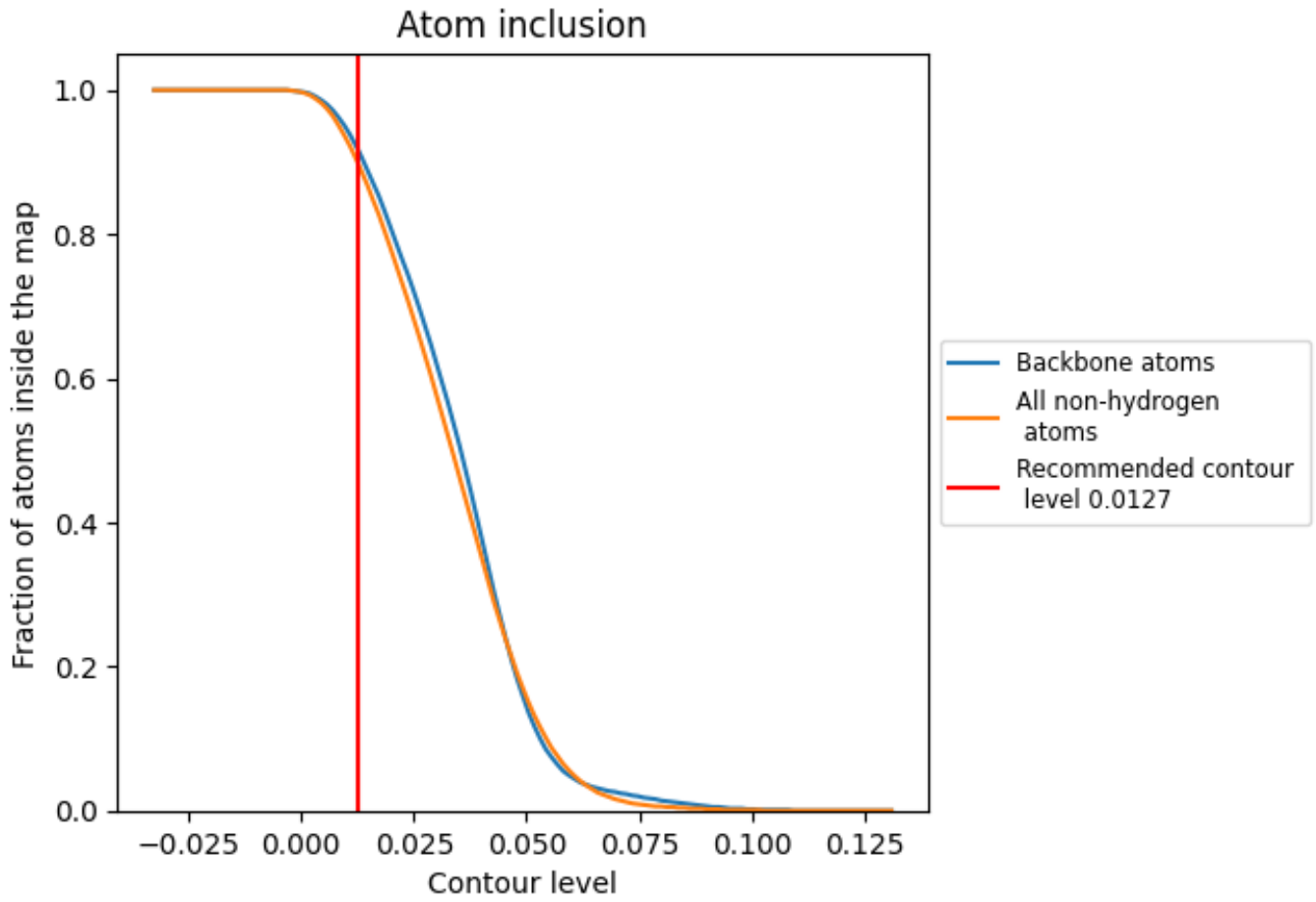
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0127).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (0.0127) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8970	0.6110
6	0.4330	0.4840
L5	0.9240	0.6070
L7	0.9840	0.6270
L8	0.9650	0.6420
LA	0.9540	0.6660
LB	0.9180	0.6480
LC	0.9390	0.6560
LD	0.8660	0.5920
LE	0.8930	0.6070
LF	0.9470	0.6620
LG	0.8240	0.5890
LH	0.9100	0.6290
LI	0.9200	0.6470
LJ	0.7600	0.5330
LL	0.9160	0.6390
LM	0.9320	0.6300
LN	0.9900	0.6920
LO	0.9420	0.6550
LP	0.9140	0.6530
LQ	0.9730	0.6810
LR	0.7520	0.5350
LS	0.9650	0.6620
LT	0.9060	0.6380
LU	0.7110	0.5170
LV	0.9310	0.6480
LW	0.8890	0.6290
LX	0.9250	0.6430
LY	0.8980	0.6260
LZ	0.9000	0.6160
La	0.9660	0.6820
Lb	0.7910	0.5760
Lc	0.8510	0.6020
Ld	0.8940	0.6260
Le	0.9660	0.6760



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lf	0.9660	0.6820
Lg	0.9140	0.6270
Lh	0.8870	0.6280
Li	0.9000	0.6200
Lj	0.9810	0.6910
Lk	0.7900	0.5590
Ll	0.9550	0.6560
Lm	0.9160	0.6300
Ln	0.0050	0.1640
Lo	0.8950	0.6410
Lp	0.9130	0.6430
Lr	0.9500	0.6500
z	0.1450	0.3510