



## wwPDB EM Validation Summary Report ⓘ

Nov 7, 2023 – 07:20 am GMT

PDB ID : 7ZJX  
EMDB ID : EMD-14752  
Title : Rabbit 80S ribosome programmed with SECIS and SBP2  
Authors : Hilal, T.; Simonovic, M.; Spahn, C.M.T.  
Deposited on : 2022-04-12  
Resolution : 3.10 Å (reported)  
Based on initial model : 7O7Y

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev70  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

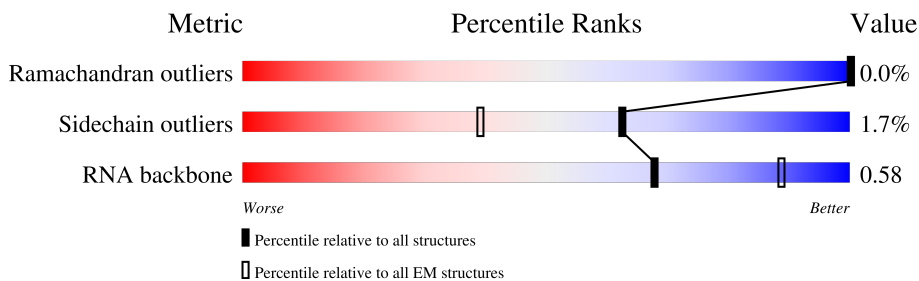
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	854	
2	I	163	
3	L5	4808	
4	L7	120	
5	L8	158	
6	LD	257	
7	LE	403	
8	LF	413	

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Mol	Chain	Length	Quality of chain
9	LG	297	97%
10	LH	291	5% 82% 16%
11	LI	247	91% 9%
12	LJ	266	86% 12%
13	LK	192	98%
14	LL	214	7% 99%
15	LM	178	95%
16	LO	211	98%
17	LP	218	61% 37%
18	LQ	204	98%
19	LR	203	95%
20	LS	184	86% 14%
21	LT	188	95%
22	LU	196	91% 8%
23	LV	176	98%
24	LW	160	99%
25	LX	128	77% 23%
26	LY	140	7% 99%
27	LZ	157	6% 59% 41%
28	La	156	76% 24%
29	Lb	145	91% 8%
30	Lc	136	99%
31	Ld	148	97%
32	Le	245	42% 56%
33	Lf	115	9% 91% 6%



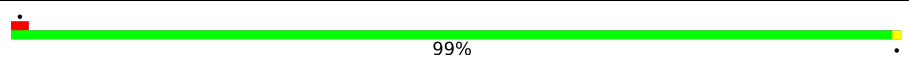
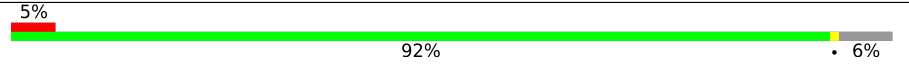
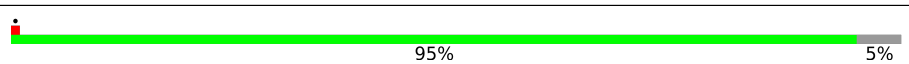
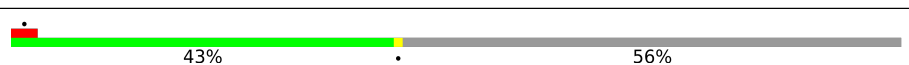
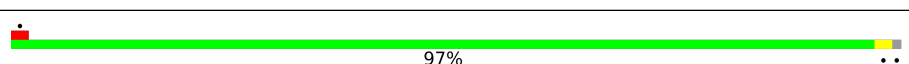
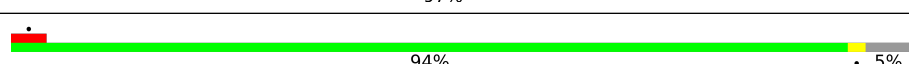
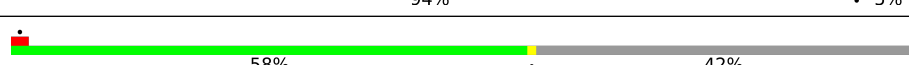
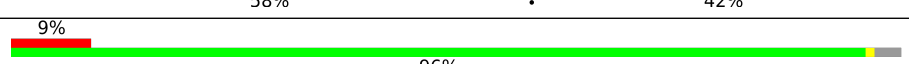
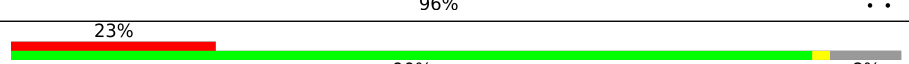
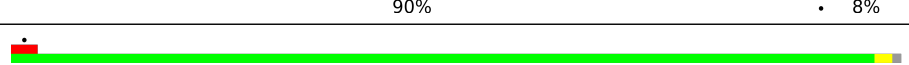
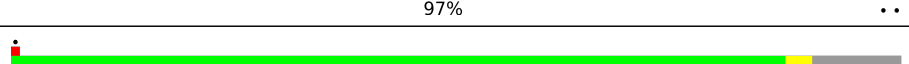
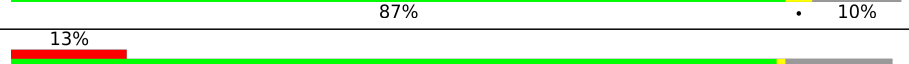


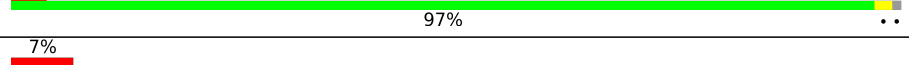
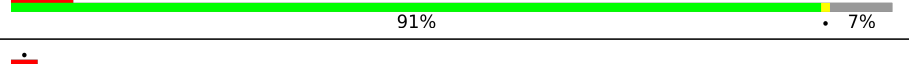
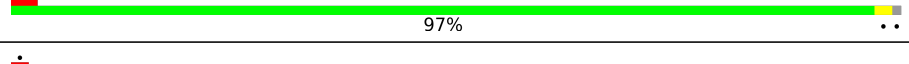
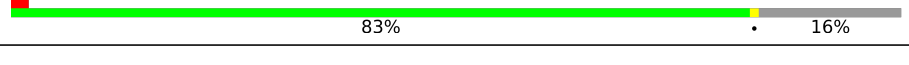
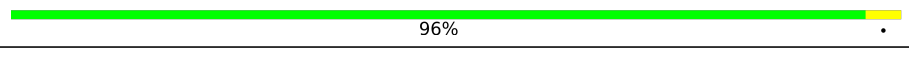
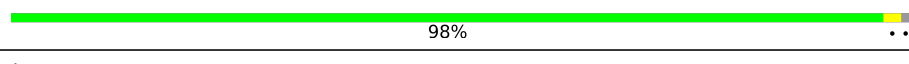
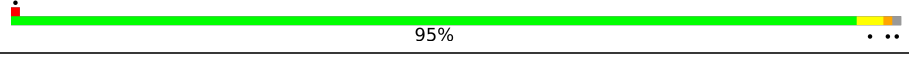
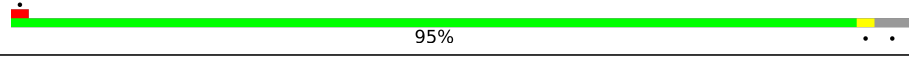

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Mol	Chain	Length	Quality of chain
34	Lg	125	82% 14%
35	Lh	135	94%
36	Li	110	99%
37	Lj	117	95%
38	Lk	123	98%
39	Ll	105	95%
40	Lm	97	89% 11%
41	Ln	70	97%
42	Lo	51	94%
43	Lp	128	41% 59%
44	Lq	106	7% 98%
45	Lr	92	97%
46	Ls	137	89% 8%
47	Lx	217	11% 77% 22%
48	S	855	95%
49	S2	1870	78% 17% 5%
50	SB	84	98%
51	SC	69	12% 91% 9%
52	SD	156	6% 43% 57%
53	SE	133	7% 42% 57%
54	SF	115	88% 12%
55	SG	317	7% 97%
56	SH	56	98%
57	SL	295	74% 25%
58	SM	264	5% 84% 15%

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Mol	Chain	Length	Quality of chain
59	SN	293	 75% 25%
60	SO	281	 79% 20% 5%
61	SP	263	 99%
62	SQ	204	 92% 6% 5%
63	SR	249	 95% 5%
64	SS	432	 43% 56%
65	ST	208	 97%
66	SU	194	 94% 5%
67	SV	165	 58% 42%
68	SW	158	 96% 9%
69	SX	132	 90% 8% 23%
70	SY	151	 97%
71	SZ	151	 87% 10%
72	Sa	145	 86% 12% 13%
73	Sb	172	 81% 18%
74	Sc	135	 97%
75	Sd	152	 91% 7% 7%
76	Se	145	 97%
77	Sf	119	 83% 16%
78	Sg	83	 96%
79	Sh	130	 98%
80	Si	143	 95%
81	Sj	130	 95%
82	Sk	124	 60% 40%
83	Sl	25	 100%

## 2 Entry composition

There are 84 unique types of molecules in this entry. The entry contains 222755 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 Selenocysteine insertion sequence-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	204	1379	881	257	238	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	687	ARG	LYS	conflict	UNP Q96T21
B	692	ILE	VAL	conflict	UNP Q96T21

- Molecule 2 is a RNA chain called CrPV IRES.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	I	163	3447	1544	588	1152	163	0	0

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	L5	3732	80089	35700	14644	26013	3732	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	L7	120	2570	1141	456	851	122	0	0

- Molecule 5 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	L8	156	3319	1481	585	1097	156	0	0

- Molecule 6 is a protein called 60S ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LD	253	Total	C	N	O	S	0	0
			1939	1214	396	323	6		

- Molecule 7 is a protein called 60S ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	LE	398	Total	C	N	O	S	0	0
			3206	2042	605	546	13		

- Molecule 8 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	LF	362	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

- Molecule 9 is a protein called Ribosomal\_L18\_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	LG	294	Total	C	N	O	S	0	0
			2398	1516	439	429	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LG	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 10 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LH	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 11 is a protein called 60S ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	LI	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LI	182	ASN	GLY	conflict	UNP A0A7J8C453
LI	199	HIS	ARG	conflict	UNP A0A7J8C453

- Molecule 12 is a protein called 60S ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LJ	233	1877	1197	361	315	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LJ	184	LEU	ILE	conflict	UNP P62424

- Molecule 13 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	LK	190	1516	954	284	272	6	0	0

- Molecule 14 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LL	213	1717	1086	332	285	14	0	0

- Molecule 15 is a protein called 60S ribosomal protein L11.

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

- Molecule 16 is a protein called 60S ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	LO	210	1702	1065	354	279	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LO	74	ARG	HIS	conflict	UNP G1TKB3

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Chain	Residue	Modelled	Actual	Comment	Reference
LO	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 17 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	LP	138	1137	727	221	182	7	0	0

- Molecule 18 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	LQ	203	1701	1072	359	266	4	0	0

- Molecule 19 is a protein called 60S ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	LR	199	1630	1051	319	255	5	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LR	174	LEU	ILE	conflict	UNP A0A0N8ETI8
LR	194	ASP	GLU	conflict	UNP A0A0N8ETI8

- Molecule 20 is a protein called 60S ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	LS	159	1288	808	249	222	9	0	0

- Molecule 21 is a protein called 60S ribosomal Protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	LT	187	1515	946	315	250	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LT	134	ARG	CYS	conflict	UNP F6QKI9

- Molecule 22 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	LU	180	1508	933	328	238	9	0	0

- Molecule 23 is a protein called 60S ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	LV	176	1457	924	288	234	11	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LV	36	ASN	ILE	conflict	UNP A0A1Z5LHJ5

- Molecule 24 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LW	159	1298	823	252	217	6	0	0

- Molecule 25 is a protein called 60S ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LX	99	806	516	141	147	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LX	60	ALA	VAL	conflict	UNP Q4R5I3

- Molecule 26 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LY	139	1034	648	199	182	5	0	0

- Molecule 27 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LZ	93	766	480	153	129	4	0	0

- Molecule 28 is a protein called Ribosomal\_L23eN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	La	118	967	618	181	167	1	0	0

- Molecule 29 is a protein called Ribosomal protein L26.

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

- Molecule 30 is a protein called 60S ribosomal protein L27.

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

- Molecule 31 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	Ld	147	1159	732	239	185	3	0	0

- Molecule 32 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Le	108	881	548	196	134	3	0	0

- Molecule 33 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Lf	108	836	530	148	151	7	0	0

- Molecule 34 is a protein called 60S ribosomal protein L31.

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

- Molecule 35 is a protein called Ribosomal protein L32.

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

- Molecule 36 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	Li	110	884	560	175	144	5	0	0

- Molecule 37 is a protein called 60S ribosomal protein L34.

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

- Molecule 38 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Lk	122	1013	640	204	168	1	0	0

- Molecule 39 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	Ll	102	830	520	176	129	5	0	0

- Molecule 40 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Lm	86	705	434	155	111	5	0	0

- Molecule 41 is a protein called 60S ribosomal protein L38.

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

- Molecule 42 is a protein called 60S ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Lo	50	447	286	96	64	1	0	0

- Molecule 43 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	Lp	52	432	269	90	67	6	0	0

- Molecule 44 is a protein called 60S ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Lq	105	863	543	175	139	6	0	0

- Molecule 45 is a protein called 60S ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	Lr	91	708	445	136	120	7	0	0

- Molecule 46 is a protein called 60S ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Ls	126	1014	629	209	170	6	0	0

- Molecule 47 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
47	Lx	169	840	502	169	169	0	0

- Molecule 48 is a RNA chain called GPX4 SECIS element.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
48	S	46	983	438	179	320	46	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1118	U	C	conflict	GB 25123295
S	1126	A	C	conflict	GB 25123295
S	1132	A	U	conflict	GB 25123295
S	1133	G	-	insertion	GB 25123295
S	1134	C	-	insertion	GB 25123295
S	1135	C	-	insertion	GB 25123295
S	1136	C	-	insertion	GB 25123295
S	1150	U	A	conflict	GB 25123295

- Molecule 49 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	S2	1770	37825	16906	6780	12369	1770	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	251	C	U	conflict	GB 37956930
S2	583	U	C	conflict	GB 37956930
S2	584	A	C	conflict	GB 37956930
S2	585	A	G	conflict	GB 37956930
S2	1338	4AC	C	conflict	GB 37956930
S2	1843	4AC	C	conflict	GB 37956930

- Molecule 50 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	SB	83	651	408	121	115	7	0	0

- Molecule 51 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	SC	63	495	302	98	93	2	0	0

- Molecule 52 is a protein called Ubiquitin carboxyl extension protein 80.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	SD	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 53 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	SE	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 54 is a protein called 40S ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	SF	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 55 is a protein called Guanine nucleotide-binding protein subunit beta-2-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	SG	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 56 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	SH	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 57 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	SL	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 58 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	SM	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 59 is a protein called 40S ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	SN	220	1706	1105	292	300	9	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SN	33	ILE	VAL	conflict	UNP O18789
SN	101	ALA	SER	conflict	UNP O18789

- Molecule 60 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	SO	225	1751	1116	315	313	7	0	0

- Molecule 61 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	SP	262	2076	1324	386	358	8	0	0

- Molecule 62 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	SQ	191	1509	943	286	273	7	0	0

- Molecule 63 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	SR	237	1923	1200	387	329	7	0	0

- Molecule 64 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	SS	190	1529	975	281	272	1	0	0

- Molecule 65 is a protein called 40S ribosomal protein S8.



Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	ST	206	1686	1058	332	291	5	0	0

- Molecule 66 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	SU	185	1525	969	306	248	2	0	0

- Molecule 67 is a protein called S10\_ plectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	SV	96	810	530	143	131	6	0	0

- Molecule 68 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	SW	154	1262	804	236	216	6	0	0

- Molecule 69 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	SX	121	943	591	167	176	9	0	0

- Molecule 70 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	SY	150	1208	773	229	205	1	0	0

- Molecule 71 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	SZ	136	1016	621	199	190	6	0	0

- Molecule 72 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Sa	127	Total	C	N	O	S	0	0
			1042	662	196	177	7		

- Molecule 73 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Sb	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 74 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Sc	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 75 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Sd	141	Total	C	N	O	S	0	0
			1171	736	235	199	1		

- Molecule 76 is a protein called 40S Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Se	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 77 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Sf	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 78 is a protein called 40S ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Sg	83	Total	C	N	O	S	0	0
			640	394	117	124	5		

- Molecule 79 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
79	Sh	129	1034	659	193	176	6	0	0

- Molecule 80 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
80	Si	141	1099	693	219	184	3	0	0

- Molecule 81 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
81	Sj	125	1015	642	199	169	5	0	0

- Molecule 82 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
82	Sk	75	598	382	111	104	1	0	0

- Molecule 83 is a protein called 60S ribosomal protein L41.

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

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
84	Lj	1	Total	Zn	0
			1	1	
84	Lm	1	Total	Zn	0
			1	1	
84	Lp	1	Total	Zn	0
			1	1	
84	Lq	1	Total	Zn	0
			1	1	
84	Lr	1	Total	Zn	0
			1	1	
84	SD	1	Total	Zn	0
			1	1	

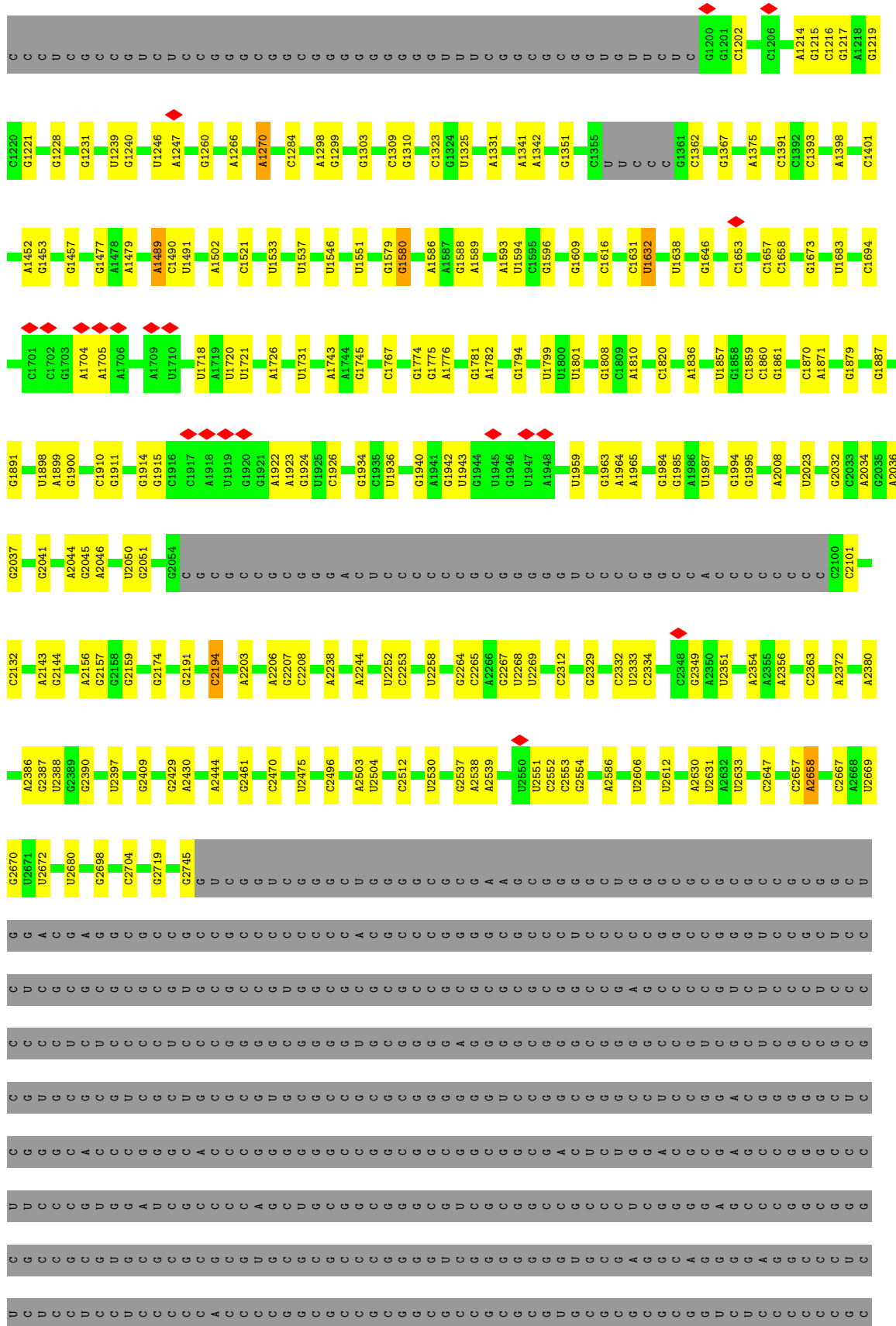
*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
84	SF	1	Total 1	Zn 1	0
84	SH	1	Total 1	Zn 1	0

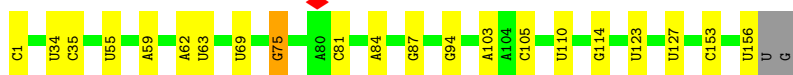
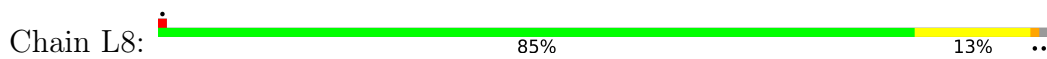












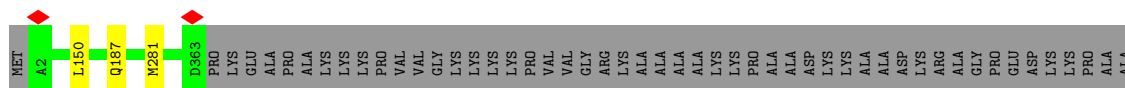
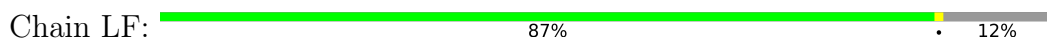
- Molecule 6: 60S ribosomal protein uL2



- Molecule 7: 60S ribosomal protein uL3



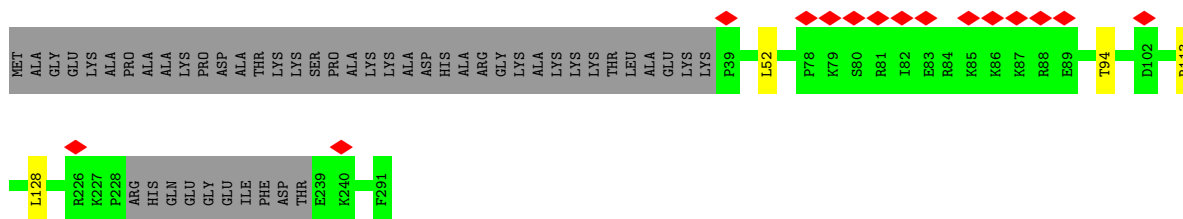
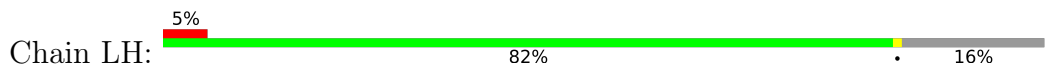
- Molecule 8: 60S ribosomal protein L4



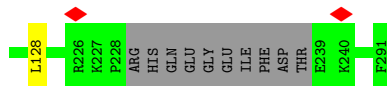
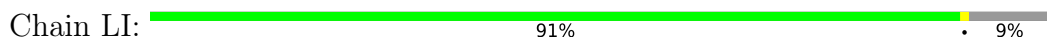
- Molecule 9: Ribosomal\_L18\_c domain-containing protein



- Molecule 10: 60S ribosomal protein L6



- Molecule 11: 60S ribosomal Protein uL30





- Molecule 18: Ribosomal protein L15

Chain LQ:  98%




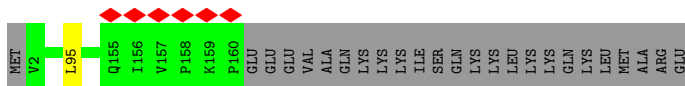
- Molecule 19: 60S ribosomal protein uL13

Chain LR:  95%



- Molecule 20: 60S ribosomal protein uL22

Chain LS:  86% 14%



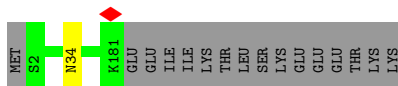
- Molecule 21: 60S ribosomal Protein eL18

Chain LT:  95%



- Molecule 22: 60S ribosomal protein L19

Chain LU:  91% 8%



- Molecule 23: 60S ribosomal protein eL20

Chain LV:  98%




- Molecule 24: 60S ribosomal protein L21

Chain LW:  99%



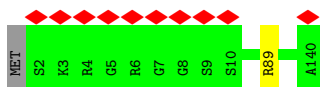
- Molecule 25: 60S ribosomal protein eL22

Chain LX:  77% 23%



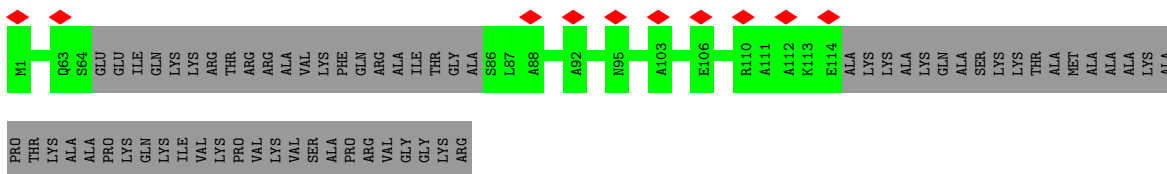
- Molecule 26: 60S ribosomal protein L23

Chain LY:  7% 99%




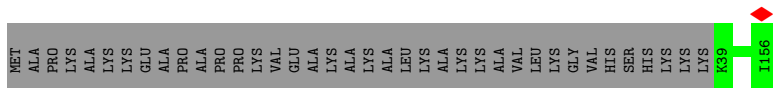
- Molecule 27: Ribosomal protein L24

Chain LZ:  6% 59% 41%



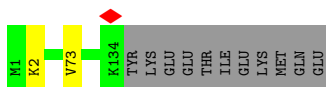
- Molecule 28: Ribosomal\_L23eN domain-containing protein

Chain La:  76% 24%



- Molecule 29: Ribosomal protein L26

Chain Lb:  91% 8%



- Molecule 30: 60S ribosomal protein L27

Chain Lc:  99%



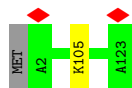
- Molecule 31: 60S ribosomal protein L27a

Chain Ld:  97%

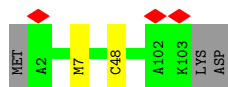




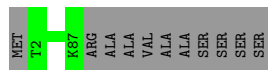
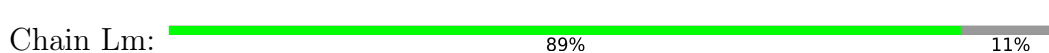
• Molecule 38: 60S ribosomal protein L35



• Molecule 39: 60S ribosomal protein L36



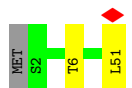
• Molecule 40: Ribosomal protein L37



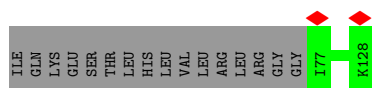
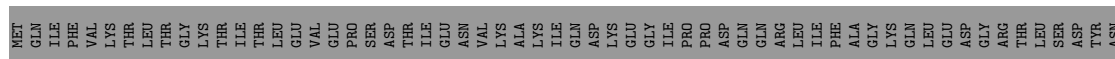
• Molecule 41: 60S ribosomal protein L38



• Molecule 42: 60S ribosomal protein eL39



• Molecule 43: 60S ribosomal protein L40











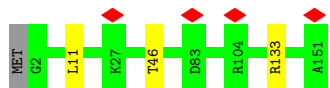




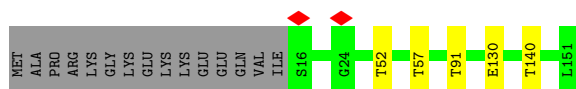




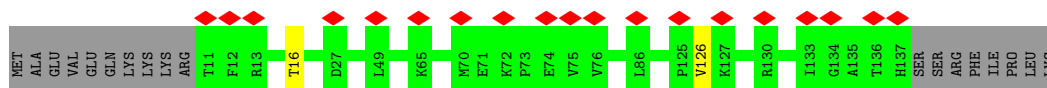
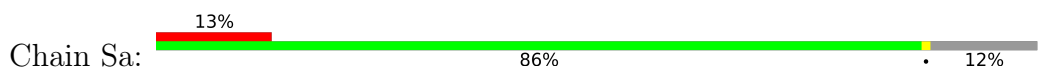
- Molecule 70: 40S ribosomal protein S13



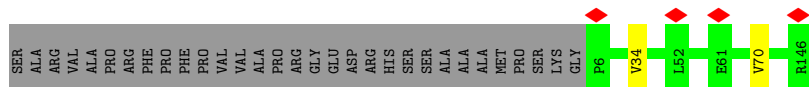
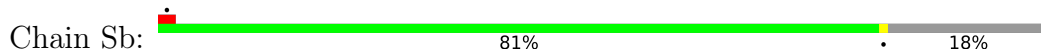
- Molecule 71: 40S ribosomal protein uS11



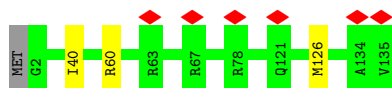
- Molecule 72: 40S ribosomal protein S15



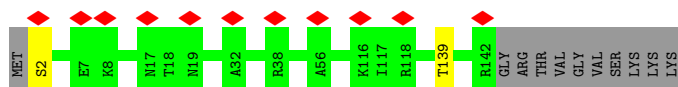
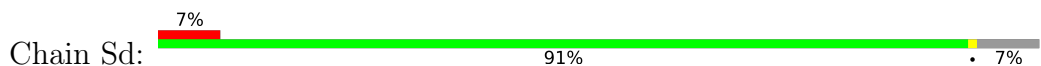
- Molecule 73: 40S ribosomal protein uS9



- Molecule 74: 40S ribosomal protein S17



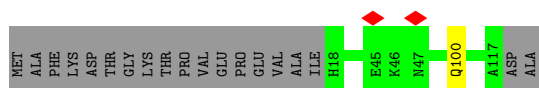
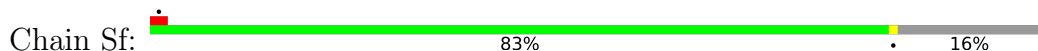
- Molecule 75: 40S ribosomal protein S18



- Molecule 76: 40S Ribosomal protein eS19



• Molecule 77: 40S ribosomal protein S20



• Molecule 78: 40S ribosomal protein eS21



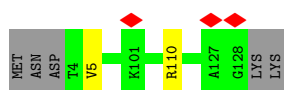
• Molecule 79: 40S ribosomal protein S15a



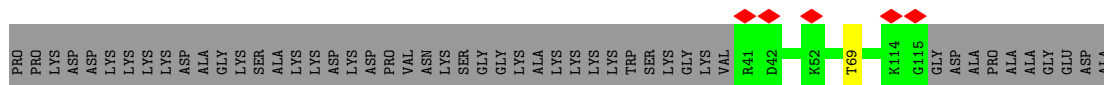
• Molecule 80: 40S ribosomal protein S23



• Molecule 81: 40S ribosomal protein S24



• Molecule 82: 40S ribosomal protein S25



- Molecule 83: 60S ribosomal protein L41

Chain SI:  100%

There are no outlier residues recorded for this chain.

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39295	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.751	Depositor
Minimum map value	0.000	Depositor
Average map value	0.026	Depositor
Map value standard deviation	0.102	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	409.2, 409.2, 409.2	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	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: AAC, PSU, MA6, GTP, OMC, ZN, AME, MLZ, OMU, NMM, 4AC, SAC, 7MG, HY3, AYA, OMG, 5MC, 6MZ, 1MA, A2M, UR3, M3L, HIC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	B	0.27	0/1398	0.46	0/1905
2	I	0.17	0/3847	0.77	4/5981 (0.1%)
3	L5	0.26	1/86665 (0.0%)	0.69	8/135207 (0.0%)
4	L7	0.27	0/2835	0.68	1/4418 (0.0%)
5	L8	0.31	1/3635 (0.0%)	0.68	0/5661
6	LD	0.27	0/1977	0.55	0/2651
7	LE	0.26	0/3261	0.50	0/4364
8	LF	0.26	0/2932	0.52	0/3939
9	LG	0.26	0/2437	0.48	0/3264
10	LH	0.26	0/1998	0.51	0/2673
11	LI	0.27	0/1922	0.50	0/2563
12	LJ	0.25	0/1908	0.49	0/2566
13	LK	0.26	0/1535	0.50	0/2063
14	LL	0.26	0/1756	0.51	0/2346
15	LM	0.25	0/1385	0.53	0/1852
16	LO	0.25	0/1733	0.55	0/2316
17	LP	0.26	0/1158	0.50	0/1547
18	LQ	0.26	0/1746	0.55	0/2338
19	LR	0.26	0/1662	0.50	0/2222
20	LS	0.26	0/1315	0.49	0/1763
21	LT	0.26	0/1539	0.56	0/2054
22	LU	0.24	0/1524	0.54	0/2013
23	LV	0.27	0/1497	0.54	0/2008
24	LW	0.26	0/1326	0.50	0/1770
25	LX	0.26	0/820	0.48	0/1100
26	LY	0.27	0/1048	0.51	0/1402
27	LZ	0.26	0/779	0.50	0/1034
28	La	0.25	0/984	0.49	0/1323
29	Lb	0.25	0/1132	0.53	0/1504
30	Lc	0.27	0/1130	0.50	0/1507
31	Ld	0.26	0/1188	0.51	0/1587

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	Le	0.24	0/884	0.52	0/1169
33	Lf	0.25	0/847	0.45	0/1134
34	Lg	0.25	0/903	0.52	0/1216
35	Lh	0.26	0/1088	0.52	0/1451
36	Li	0.28	0/903	0.54	0/1208
37	Lj	0.26	0/916	0.55	0/1220
38	Lk	0.24	0/1021	0.50	0/1348
39	Ll	0.25	0/841	0.53	0/1112
40	Lm	0.25	0/720	0.57	0/952
41	Ln	0.25	0/575	0.46	0/761
42	Lo	0.24	0/459	0.53	0/608
43	Lp	0.24	0/426	0.52	0/564
44	Lq	0.25	0/866	0.51	0/1141
45	Lr	0.25	0/718	0.51	0/953
46	Ls	0.25	0/1020	0.54	0/1366
47	Lx	0.23	0/836	0.40	0/1161
48	S	0.25	0/1098	0.80	1/1710 (0.1%)
49	S2	0.23	1/40365 (0.0%)	0.69	7/62915 (0.0%)
50	SB	0.25	0/665	0.48	0/891
51	SC	0.24	0/497	0.57	0/666
52	SD	0.25	0/560	0.49	0/745
53	SE	0.25	0/462	0.55	0/607
54	SF	0.25	0/828	0.54	0/1109
55	SG	0.24	0/2493	0.48	0/3394
56	SH	0.25	0/470	0.51	0/623
57	SL	0.25	0/1771	0.47	0/2406
58	SM	0.25	0/1841	0.46	0/2459
59	SN	0.26	0/1742	0.47	0/2354
60	SO	0.25	0/1779	0.49	0/2395
61	SP	0.25	0/2118	0.51	0/2849
62	SQ	0.24	0/1531	0.49	0/2059
63	SR	0.25	0/1946	0.54	0/2590
64	SS	0.25	0/1552	0.49	0/2079
65	ST	0.25	0/1715	0.52	0/2287
66	SU	0.24	0/1550	0.53	0/2069
67	SV	0.25	0/834	0.44	0/1125
68	SW	0.26	0/1284	0.52	0/1717
69	SX	0.23	0/953	0.44	0/1276
70	SY	0.24	0/1232	0.49	0/1656
71	SZ	0.26	0/1029	0.54	0/1380
72	Sa	0.25	0/1063	0.49	0/1421
73	Sb	0.24	0/1142	0.52	0/1528
74	Sc	0.23	0/1094	0.48	0/1469

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
75	Sd	0.23	0/1180	0.54	0/1581
76	Se	0.24	0/1119	0.47	0/1498
77	Sf	0.24	0/805	0.52	0/1081
78	Sg	0.26	0/636	0.50	0/852
79	Sh	0.25	0/1051	0.50	0/1406
80	Si	0.25	0/1107	0.50	0/1475
81	Sj	0.25	0/1032	0.52	0/1371
82	Sk	0.24	0/604	0.49	0/810
83	Sl	0.22	0/240	0.65	0/305
All	All	0.25	3/234483 (0.0%)	0.63	21/344463 (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
47	Lx	0	1
80	Si	0	3
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	S2	1	U	OP3-P	-10.60	1.48	1.61
3	L5	1	C	OP3-P	-10.58	1.48	1.61
5	L8	1	C	OP3-P	-10.57	1.48	1.61

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	219	A	OP1-P-O3'	-10.62	81.84	105.20
2	I	219	A	OP2-P-O3'	-10.56	81.96	105.20
49	S2	1454	C	C2-N1-C1'	8.73	128.40	118.80
49	S2	1454	C	N1-C2-O2	8.72	124.13	118.90
2	I	220	G	OP1-P-OP2	7.42	130.73	119.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
47	Lx	60	ARG	Peptide
80	Si	61	GLN	Mainchain,Peptide
80	Si	62	HY3	Mainchain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	200/854 (23%)	171 (86%)	28 (14%)	1 (0%)	29	64
6	LD	251/257 (98%)	238 (95%)	13 (5%)	0	100	100
7	LE	395/403 (98%)	386 (98%)	9 (2%)	0	100	100
8	LF	360/413 (87%)	354 (98%)	6 (2%)	0	100	100
9	LG	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
10	LH	239/291 (82%)	231 (97%)	8 (3%)	0	100	100
11	LI	224/247 (91%)	218 (97%)	6 (3%)	0	100	100
12	LJ	229/266 (86%)	228 (100%)	1 (0%)	0	100	100
13	LK	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
14	LL	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
15	LM	168/178 (94%)	164 (98%)	4 (2%)	0	100	100
16	LO	208/211 (99%)	203 (98%)	5 (2%)	0	100	100
17	LP	136/218 (62%)	133 (98%)	3 (2%)	0	100	100
18	LQ	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
19	LR	197/203 (97%)	197 (100%)	0	0	100	100
20	LS	157/184 (85%)	155 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	LT	185/188 (98%)	180 (97%)	5 (3%)	0	100	100
22	LU	178/196 (91%)	178 (100%)	0	0	100	100
23	LV	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
24	LW	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
25	LX	97/128 (76%)	95 (98%)	2 (2%)	0	100	100
26	LY	137/140 (98%)	137 (100%)	0	0	100	100
27	LZ	89/157 (57%)	89 (100%)	0	0	100	100
28	La	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
29	Lb	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
30	Lc	133/136 (98%)	133 (100%)	0	0	100	100
31	Ld	145/148 (98%)	136 (94%)	8 (6%)	1 (1%)	22	57
32	Le	103/245 (42%)	98 (95%)	5 (5%)	0	100	100
33	Lf	106/115 (92%)	106 (100%)	0	0	100	100
34	Lg	105/125 (84%)	105 (100%)	0	0	100	100
35	Lh	128/135 (95%)	127 (99%)	1 (1%)	0	100	100
36	Li	108/110 (98%)	108 (100%)	0	0	100	100
37	Lj	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
38	Lk	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
39	Ll	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
40	Lm	84/97 (87%)	84 (100%)	0	0	100	100
41	Ln	67/70 (96%)	67 (100%)	0	0	100	100
42	Lo	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
43	Lp	49/128 (38%)	49 (100%)	0	0	100	100
44	Lq	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
45	Lr	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
46	Ls	124/137 (90%)	121 (98%)	3 (2%)	0	100	100
47	Lx	161/217 (74%)	143 (89%)	18 (11%)	0	100	100
50	SB	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
51	SC	61/69 (88%)	61 (100%)	0	0	100	100
52	SD	65/156 (42%)	64 (98%)	1 (2%)	0	100	100
53	SE	55/133 (41%)	55 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	SF	99/115 (86%)	97 (98%)	2 (2%)	0	100	100
55	SG	311/317 (98%)	300 (96%)	11 (4%)	0	100	100
56	SH	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
57	SL	219/295 (74%)	214 (98%)	5 (2%)	0	100	100
58	SM	220/264 (83%)	216 (98%)	4 (2%)	0	100	100
59	SN	218/293 (74%)	212 (97%)	6 (3%)	0	100	100
60	SO	223/281 (79%)	220 (99%)	3 (1%)	0	100	100
61	SP	260/263 (99%)	255 (98%)	5 (2%)	0	100	100
62	SQ	189/204 (93%)	183 (97%)	6 (3%)	0	100	100
63	SR	235/249 (94%)	233 (99%)	2 (1%)	0	100	100
64	SS	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
65	ST	204/208 (98%)	203 (100%)	1 (0%)	0	100	100
66	SU	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
67	SV	94/165 (57%)	92 (98%)	2 (2%)	0	100	100
68	SW	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
69	SX	119/132 (90%)	115 (97%)	4 (3%)	0	100	100
70	SY	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
71	SZ	134/151 (89%)	128 (96%)	6 (4%)	0	100	100
72	Sa	125/145 (86%)	124 (99%)	1 (1%)	0	100	100
73	Sb	139/172 (81%)	132 (95%)	7 (5%)	0	100	100
74	Sc	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
75	Sd	139/152 (91%)	136 (98%)	3 (2%)	0	100	100
76	Se	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
77	Sf	98/119 (82%)	94 (96%)	4 (4%)	0	100	100
78	Sg	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
79	Sh	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
80	Si	138/143 (96%)	137 (99%)	1 (1%)	0	100	100
81	Sj	123/130 (95%)	123 (100%)	0	0	100	100
82	Sk	73/124 (59%)	71 (97%)	2 (3%)	0	100	100
83	Sl	23/25 (92%)	23 (100%)	0	0	100	100
All	All	11653/14208 (82%)	11397 (98%)	254 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	703	SER
31	Ld	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	B	102/761 (13%)	99 (97%)	3 (3%)	42	72
6	LD	195/199 (98%)	191 (98%)	4 (2%)	53	79
7	LE	344/347 (99%)	336 (98%)	8 (2%)	50	77
8	LF	302/337 (90%)	299 (99%)	3 (1%)	76	90
9	LG	247/250 (99%)	240 (97%)	7 (3%)	43	73
10	LH	216/251 (86%)	212 (98%)	4 (2%)	57	81
11	LI	197/215 (92%)	195 (99%)	2 (1%)	76	90
12	LJ	199/223 (89%)	196 (98%)	3 (2%)	65	85
13	LK	169/171 (99%)	167 (99%)	2 (1%)	71	88
14	LL	180/181 (99%)	178 (99%)	2 (1%)	73	89
15	LM	143/149 (96%)	142 (99%)	1 (1%)	84	93
16	LO	175/176 (99%)	172 (98%)	3 (2%)	60	83
17	LP	117/161 (73%)	113 (97%)	4 (3%)	37	69
18	LQ	171/172 (99%)	168 (98%)	3 (2%)	59	82
19	LR	171/173 (99%)	164 (96%)	7 (4%)	30	64
20	LS	139/163 (85%)	138 (99%)	1 (1%)	84	93
21	LT	164/165 (99%)	156 (95%)	8 (5%)	25	57
22	LU	159/175 (91%)	158 (99%)	1 (1%)	86	94
23	LV	154/154 (100%)	151 (98%)	3 (2%)	57	81
24	LW	139/140 (99%)	139 (100%)	0	100	100
25	LX	88/113 (78%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	LY	106/107 (99%)	105 (99%)	1 (1%)	78	91
27	LZ	79/126 (63%)	79 (100%)	0	100	100
28	La	106/134 (79%)	106 (100%)	0	100	100
29	Lb	124/135 (92%)	122 (98%)	2 (2%)	62	84
30	Lc	117/118 (99%)	116 (99%)	1 (1%)	78	91
31	Ld	118/120 (98%)	116 (98%)	2 (2%)	60	83
32	Le	87/183 (48%)	83 (95%)	4 (5%)	27	59
33	Lf	92/98 (94%)	89 (97%)	3 (3%)	38	69
34	Lg	98/110 (89%)	94 (96%)	4 (4%)	30	64
35	Lh	116/121 (96%)	113 (97%)	3 (3%)	46	74
36	Li	89/89 (100%)	88 (99%)	1 (1%)	73	89
37	Lj	98/100 (98%)	95 (97%)	3 (3%)	40	70
38	Lk	109/110 (99%)	108 (99%)	1 (1%)	78	91
39	Ll	86/89 (97%)	84 (98%)	2 (2%)	50	77
40	Lm	73/80 (91%)	73 (100%)	0	100	100
41	Ln	64/65 (98%)	63 (98%)	1 (2%)	62	84
42	Lo	47/48 (98%)	45 (96%)	2 (4%)	29	62
43	Lp	47/115 (41%)	47 (100%)	0	100	100
44	Lq	92/93 (99%)	91 (99%)	1 (1%)	73	89
45	Lr	74/75 (99%)	72 (97%)	2 (3%)	44	74
46	Ls	109/120 (91%)	106 (97%)	3 (3%)	43	73
50	SB	75/76 (99%)	74 (99%)	1 (1%)	69	87
51	SC	56/62 (90%)	56 (100%)	0	100	100
52	SD	60/140 (43%)	60 (100%)	0	100	100
53	SE	47/106 (44%)	46 (98%)	1 (2%)	53	79
54	SF	88/98 (90%)	88 (100%)	0	100	100
55	SG	272/275 (99%)	268 (98%)	4 (2%)	65	85
56	SH	48/49 (98%)	48 (100%)	0	100	100
57	SL	182/243 (75%)	180 (99%)	2 (1%)	73	89
58	SM	203/231 (88%)	202 (100%)	1 (0%)	88	94
59	SN	185/223 (83%)	184 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
60	SO	189/232 (82%)	187 (99%)	2 (1%)	73	89
61	SP	224/225 (100%)	222 (99%)	2 (1%)	78	91
62	SQ	161/170 (95%)	158 (98%)	3 (2%)	57	81
63	SR	207/218 (95%)	206 (100%)	1 (0%)	88	94
64	SS	170/360 (47%)	167 (98%)	3 (2%)	59	82
65	ST	178/180 (99%)	174 (98%)	4 (2%)	52	78
66	SU	161/168 (96%)	158 (98%)	3 (2%)	57	81
67	SV	87/136 (64%)	86 (99%)	1 (1%)	73	89
68	SW	139/142 (98%)	137 (99%)	2 (1%)	67	86
69	SX	103/108 (95%)	101 (98%)	2 (2%)	57	81
70	SY	130/131 (99%)	127 (98%)	3 (2%)	50	77
71	SZ	106/119 (89%)	101 (95%)	5 (5%)	26	59
72	Sa	113/130 (87%)	111 (98%)	2 (2%)	59	82
73	Sb	117/140 (84%)	115 (98%)	2 (2%)	60	83
74	Sc	120/121 (99%)	117 (98%)	3 (2%)	47	75
75	Sd	122/131 (93%)	121 (99%)	1 (1%)	81	92
76	Se	112/114 (98%)	110 (98%)	2 (2%)	59	82
77	Sf	92/107 (86%)	91 (99%)	1 (1%)	73	89
78	Sg	67/67 (100%)	65 (97%)	2 (3%)	41	71
79	Sh	112/113 (99%)	110 (98%)	2 (2%)	59	82
80	Si	112/114 (98%)	109 (97%)	3 (3%)	44	74
81	Sj	107/112 (96%)	105 (98%)	2 (2%)	57	81
82	Sk	66/102 (65%)	65 (98%)	1 (2%)	65	85
83	Sl	24/24 (100%)	24 (100%)	0	100	100
All	All	9937/11879 (84%)	9770 (98%)	167 (2%)	62	83

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
60	SO	46	THR
71	SZ	91	THR
62	SQ	103	LEU
66	SU	5	ARG
74	Sc	40	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
46	Ls	6	GLN
58	SM	40	ASN
61	SP	179	ASN
57	SL	50	ASN
58	SM	118	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	160/163 (98%)	90 (56%)	6 (3%)
3	L5	3718/4808 (77%)	532 (14%)	3 (0%)
4	L7	118/120 (98%)	8 (6%)	0
48	S	45/855 (5%)	19 (42%)	4 (8%)
49	S2	1759/1870 (94%)	243 (13%)	2 (0%)
5	L8	155/158 (98%)	18 (11%)	0
All	All	5955/7974 (74%)	910 (15%)	15 (0%)

5 of 910 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	I	33	A
2	I	37	U
2	I	39	A
2	I	44	G
2	I	46	U

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	3549	A
49	S2	191	A
3	L5	4445	U
49	S2	1485	A
48	S	1113	G

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

219 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
57	SAC	SL	2	57	7,8,9	0.52	0	8,9,11	0.89	1 (12%)
3	OMU	L5	2258	3	19,22,23	1.01	2 (10%)	26,31,34	1.75	5 (19%)
3	A2M	L5	3492	3,49	18,25,26	2.03	5 (27%)	18,36,39	2.55	6 (33%)
49	A2M	S2	513	49	18,25,26	1.96	5 (27%)	18,36,39	2.17	5 (27%)
49	A2M	S2	469	49	18,25,26	1.98	5 (27%)	18,36,39	2.19	5 (27%)
3	PSU	L5	1683	3	18,21,22	1.40	3 (16%)	22,30,33	1.80	5 (22%)
3	A2M	L5	2630	3	18,25,26	1.99	5 (27%)	18,36,39	2.29	6 (33%)
49	A2M	S2	27	49	18,25,26	1.93	5 (27%)	18,36,39	2.22	4 (22%)
3	A2M	L5	3450	3	18,25,26	1.94	5 (27%)	18,36,39	2.17	5 (27%)
49	OMC	S2	518	49	19,22,23	1.15	2 (10%)	26,31,34	0.92	1 (3%)
3	OMC	L5	2265	3	19,22,23	1.15	2 (10%)	26,31,34	0.89	0
49	PSU	S2	864	49	18,21,22	1.43	3 (16%)	22,30,33	1.81	4 (18%)
3	PSU	L5	1718	3	18,21,22	1.39	3 (16%)	22,30,33	1.84	5 (22%)
49	OMG	S2	437	49	18,26,27	1.94	2 (11%)	19,38,41	1.71	4 (21%)
49	A2M	S2	485	49	18,25,26	1.92	5 (27%)	18,36,39	2.17	5 (27%)
3	PSU	L5	4382	3	18,21,22	1.38	3 (16%)	22,30,33	1.76	4 (18%)
3	A2M	L5	3456	3	18,25,26	2.00	5 (27%)	18,36,39	2.13	4 (22%)
3	OMG	L5	4364	3	18,26,27	1.96	2 (11%)	19,38,41	1.70	4 (21%)
3	OMU	L5	2680	3	19,22,23	1.01	2 (10%)	26,31,34	1.81	6 (23%)
3	OMU	L5	3657	44,3	19,22,23	0.99	2 (10%)	26,31,34	1.85	5 (19%)
3	A2M	L5	4317	3	18,25,26	1.98	5 (27%)	18,36,39	2.13	4 (22%)
3	PSU	L5	4278	3	18,21,22	1.48	2 (11%)	22,30,33	1.65	3 (13%)
3	PSU	L5	3500	3	18,21,22	1.42	3 (16%)	22,30,33	1.84	5 (22%)
3	OMG	L5	1477	3	18,26,27	1.96	2 (11%)	19,38,41	1.72	5 (26%)
49	PSU	S2	1239	49	18,21,22	1.42	3 (16%)	22,30,33	1.80	4 (18%)
49	MA6	S2	1852	49	19,26,27	0.98	1 (5%)	18,38,41	1.75	5 (27%)
3	OMC	L5	1820	3	19,22,23	1.16	2 (10%)	26,31,34	0.93	0
3	OMU	L5	4052	3	19,22,23	0.99	2 (10%)	26,31,34	1.78	4 (15%)
5	OMG	L8	75	5	18,26,27	1.99	2 (11%)	19,38,41	1.67	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMG	L5	4116	3	18,26,27	1.98	2 (11%)	19,38,41	1.70	4 (21%)
3	A2M	L5	1270	3	18,25,26	1.95	5 (27%)	18,36,39	2.20	5 (27%)
3	5MC	L5	4193	3	18,22,23	1.29	3 (16%)	26,32,35	1.48	4 (15%)
3	PSU	L5	4217	3	18,21,22	1.40	3 (16%)	22,30,33	1.80	4 (18%)
49	PSU	S2	573	49	18,21,22	1.42	3 (16%)	22,30,33	1.81	4 (18%)
49	PSU	S2	682	49	18,21,22	1.41	3 (16%)	22,30,33	1.85	4 (18%)
49	PSU	S2	1233	49	18,21,22	1.42	3 (16%)	22,30,33	1.82	5 (22%)
3	PSU	L5	3462	3	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
49	PSU	S2	1046	49	18,21,22	1.39	3 (16%)	22,30,33	1.87	4 (18%)
49	OMU	S2	1289	49	19,22,23	0.98	2 (10%)	26,31,34	1.74	5 (19%)
3	PSU	L5	3652	3	18,21,22	1.37	3 (16%)	22,30,33	1.88	5 (22%)
49	PSU	S2	105	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	5 (22%)
3	A2M	L5	4269	3	18,25,26	1.97	5 (27%)	18,36,39	2.24	6 (33%)
49	OMU	S2	1805	49	19,22,23	0.99	2 (10%)	26,31,34	1.76	4 (15%)
3	PSU	L5	4058	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	5 (22%)
49	OMU	S2	172	49	19,22,23	0.99	2 (10%)	26,31,34	1.82	4 (15%)
3	PSU	L5	2475	3	18,21,22	1.41	3 (16%)	22,30,33	1.87	4 (18%)
3	PSU	L5	3466	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
3	OMG	L5	3974	3	18,26,27	1.96	2 (11%)	19,38,41	1.72	5 (26%)
49	OMG	S2	602	49	18,26,27	1.97	2 (11%)	19,38,41	1.69	4 (21%)
3	PSU	L5	1731	3	18,21,22	1.37	3 (16%)	22,30,33	1.84	4 (18%)
3	PSU	L5	4039	3	18,21,22	1.39	3 (16%)	22,30,33	1.82	5 (22%)
49	A2M	S2	99	49	18,25,26	1.99	5 (27%)	18,36,39	2.20	5 (27%)
3	OMC	L5	3433	3	19,22,23	1.17	2 (10%)	26,31,34	0.98	1 (3%)
49	OMG	S2	684	49	18,26,27	1.96	2 (11%)	19,38,41	1.69	5 (26%)
49	4AC	S2	1338	49	21,24,25	1.10	2 (9%)	29,34,37	1.19	3 (10%)
3	PSU	L5	4435	3	18,21,22	1.39	3 (16%)	22,30,33	1.89	5 (22%)
3	PSU	L5	2351	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)
3	PSU	L5	3585	3	18,21,22	1.39	3 (16%)	22,30,33	1.81	5 (22%)
3	A2M	L5	1489	3	18,25,26	1.95	5 (27%)	18,36,39	2.11	4 (22%)
3	PSU	L5	3369	3	18,21,22	1.35	3 (16%)	22,30,33	1.85	4 (18%)
3	OMU	L5	3973	3	19,22,23	1.00	2 (10%)	26,31,34	1.83	6 (23%)
3	OMG	L5	4383	3	18,26,27	1.98	2 (11%)	19,38,41	1.70	4 (21%)
49	OMU	S2	121	49	19,22,23	1.01	2 (10%)	26,31,34	1.77	6 (23%)
3	PSU	L5	4246	3	18,21,22	1.39	3 (16%)	22,30,33	1.85	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	L5	4045	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	5 (22%)
49	A2M	S2	159	49	18,25,26	1.95	5 (27%)	18,36,39	2.14	5 (27%)
49	A2M	S2	1679	49	18,25,26	2.01	5 (27%)	18,36,39	2.16	5 (27%)
3	PSU	L5	3490	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	5 (22%)
3	OMC	L5	4202	3	19,22,23	1.16	2 (10%)	26,31,34	0.91	1 (3%)
3	A2M	L5	398	3	18,25,26	2.00	5 (27%)	18,36,39	2.15	5 (27%)
49	OMG	S2	1448	49	18,26,27	1.93	2 (11%)	19,38,41	1.68	4 (21%)
49	MA6	S2	1851	49	19,26,27	0.95	1 (5%)	18,38,41	1.78	6 (33%)
32	MLZ	Le	5	32	8,9,10	0.49	0	4,9,11	0.19	0
3	PSU	L5	1491	3	18,21,22	1.40	3 (16%)	22,30,33	1.85	4 (18%)
49	PSU	S2	1626	49	18,21,22	1.42	3 (16%)	22,30,33	1.77	4 (18%)
3	PSU	L5	1799	3	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
3	5MC	L5	3514	3	18,22,23	1.34	3 (16%)	26,32,35	1.24	3 (11%)
3	OMG	L5	1260	3	18,26,27	1.98	2 (11%)	19,38,41	1.71	4 (21%)
3	OMG	L5	3676	3	18,26,27	1.94	2 (11%)	19,38,41	1.76	5 (26%)
3	OMG	L5	4240	3	18,26,27	1.98	2 (11%)	19,38,41	1.69	5 (26%)
3	PSU	L5	3583	3	18,21,22	1.39	3 (16%)	22,30,33	1.82	4 (18%)
49	PSU	S2	93	49	18,21,22	1.41	3 (16%)	22,30,33	1.79	4 (18%)
49	OMU	S2	355	49	19,22,23	0.99	2 (10%)	26,31,34	1.78	5 (19%)
49	OMU	S2	1443	49	19,22,23	0.99	2 (10%)	26,31,34	1.74	4 (15%)
3	A2M	L5	3557	3	18,25,26	1.96	5 (27%)	18,36,39	2.17	4 (22%)
49	PSU	S2	407	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	4 (18%)
49	PSU	S2	1446	49	18,21,22	1.44	3 (16%)	22,30,33	1.81	4 (18%)
3	OMU	L5	4244	3	19,22,23	1.02	2 (10%)	26,31,34	1.79	5 (19%)
3	PSU	L5	4740	3	18,21,22	1.40	3 (16%)	22,30,33	1.85	5 (22%)
49	PSU	S2	1005	49	18,21,22	1.43	3 (16%)	22,30,33	1.82	4 (18%)
3	PSU	L5	1537	3	18,21,22	1.40	3 (16%)	22,30,33	1.84	5 (22%)
78	AME	Sg	1	78	9,10,11	0.67	0	9,11,13	1.07	1 (11%)
49	PSU	S2	1175	49	18,21,22	1.41	3 (16%)	22,30,33	1.80	4 (18%)
3	PSU	L5	4107	3	18,21,22	1.38	3 (16%)	22,30,33	1.80	4 (18%)
76	NMM	Se	67	76	9,11,12	1.57	1 (11%)	6,12,14	3.46	2 (33%)
3	PSU	L5	4374	3	18,21,22	1.40	3 (16%)	22,30,33	1.88	5 (22%)
3	PSU	L5	4711	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
3	PSU	L5	3502	3	18,21,22	1.43	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	1632	3	18,21,22	1.44	4 (22%)	22,30,33	1.70	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	PSU	S2	1348	49	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
49	A2M	S2	1384	49	18,25,26	2.02	5 (27%)	18,36,39	2.17	4 (22%)
49	PSU	S2	1644	49	18,21,22	1.43	3 (16%)	22,30,33	1.83	4 (18%)
3	PSU	L5	4099	3	18,21,22	1.39	3 (16%)	22,30,33	1.86	4 (18%)
3	OMG	L5	3631	3	18,26,27	2.00	2 (11%)	19,38,41	1.68	4 (21%)
49	OMU	S2	1327	49	19,22,23	1.00	2 (10%)	26,31,34	1.81	5 (19%)
49	PSU	S2	119	49	18,21,22	1.43	3 (16%)	22,30,33	1.84	4 (18%)
3	PSU	L5	4267	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)
49	PSU	S2	210	49	18,21,22	1.45	3 (16%)	22,30,33	1.80	5 (22%)
49	PSU	S2	1047	49	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
3	PSU	L5	1801	3	18,21,22	1.38	3 (16%)	22,30,33	1.86	4 (18%)
3	OMC	L5	2208	3	19,22,23	1.16	2 (10%)	26,31,34	0.95	1 (3%)
49	6MZ	S2	1833	49	18,25,26	0.89	1 (5%)	16,36,39	1.79	4 (25%)
3	OMG	L5	2267	3	18,26,27	1.95	2 (11%)	19,38,41	1.68	4 (21%)
3	A2M	L5	1810	3	18,25,26	1.97	5 (27%)	18,36,39	2.20	6 (33%)
49	OMG	S2	645	49	18,26,27	1.96	2 (11%)	19,38,41	1.73	5 (26%)
3	PSU	L5	3371	3	18,21,22	1.38	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	4325	3	18,21,22	1.37	3 (16%)	22,30,33	1.85	5 (22%)
49	PSU	S2	109	49	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
3	PSU	L5	1721	3	18,21,22	1.41	3 (16%)	22,30,33	1.84	4 (18%)
49	OMC	S2	174	49	19,22,23	1.17	2 (10%)	26,31,34	0.90	0
49	4AC	S2	1843	49	21,24,25	1.12	2 (9%)	29,34,37	1.30	3 (10%)
49	A2M	S2	591	49	18,25,26	1.99	5 (27%)	18,36,39	2.30	5 (27%)
49	PSU	S2	650	49	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)
3	OMC	L5	3540	3	19,22,23	1.14	2 (10%)	26,31,34	0.88	1 (3%)
49	PSU	S2	1693	49	18,21,22	1.41	3 (16%)	22,30,33	1.84	5 (22%)
43	M3L	Lp	98	43	10,11,12	0.51	0	9,14,16	0.47	0
49	OMG	S2	1491	49	18,26,27	1.95	2 (11%)	19,38,41	1.67	4 (21%)
3	OMC	L5	2667	3	19,22,23	1.17	2 (10%)	26,31,34	0.87	0
3	OMG	L5	2719	3	18,26,27	1.94	2 (11%)	19,38,41	1.69	4 (21%)
49	7MG	S2	1640	49	22,26,27	1.18	2 (9%)	29,39,42	2.13	9 (31%)
3	OMG	L5	1580	3	18,26,27	1.95	2 (11%)	19,38,41	1.75	5 (26%)
3	OMC	L5	3573	3	19,22,23	1.14	2 (10%)	26,31,34	0.90	0
3	OMC	L5	4282	3	19,22,23	1.16	2 (10%)	26,31,34	0.94	1 (3%)
49	OMG	S2	1329	49	18,26,27	1.94	2 (11%)	19,38,41	1.71	4 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	PSU	S2	218	49	18,21,22	1.40	3 (16%)	22,30,33	1.86	4 (18%)
3	OMG	L5	3476	3	18,26,27	1.97	2 (11%)	19,38,41	1.70	4 (21%)
49	PSU	S2	816	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	4 (18%)
3	OMG	L5	3359	3	18,26,27	1.97	2 (11%)	19,38,41	1.72	5 (26%)
3	6MZ	L5	3966	3	18,25,26	0.85	1 (5%)	16,36,39	2.10	4 (25%)
3	PSU	L5	3496	3	18,21,22	1.43	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	4042	3	18,21,22	1.39	3 (16%)	22,30,33	1.86	5 (22%)
3	OMG	L5	3942	3	18,26,27	1.96	2 (11%)	19,38,41	1.69	4 (21%)
3	A2M	L5	2658	3	18,25,26	1.98	5 (27%)	18,36,39	2.10	3 (16%)
3	OMC	L5	3601	3	19,22,23	1.14	2 (10%)	26,31,34	0.96	2 (7%)
75	SAC	Sd	2	75	7,8,9	0.54	0	8,9,11	0.85	1 (12%)
49	PSU	S2	867	49	18,21,22	1.42	3 (16%)	22,30,33	1.84	4 (18%)
80	HY3	Si	62	80	6,8,9	1.30	1 (16%)	5,10,12	1.40	1 (20%)
3	OMG	L5	3524	3	18,26,27	1.97	2 (11%)	19,38,41	1.67	4 (21%)
3	PSU	L5	4149	3	18,21,22	1.36	3 (16%)	22,30,33	1.90	4 (18%)
49	PSU	S2	815	49	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
3	OMC	L5	2194	3	19,22,23	1.15	2 (10%)	26,31,34	0.94	1 (3%)
3	PSU	L5	4298	3	18,21,22	1.36	3 (16%)	22,30,33	1.86	5 (22%)
49	A2M	S2	1032	49	18,25,26	1.97	5 (27%)	18,36,39	2.17	4 (22%)
49	PSU	S2	1245	49	18,21,22	1.42	3 (16%)	22,30,33	1.80	4 (18%)
3	PSU	L5	4177	3	18,21,22	1.40	3 (16%)	22,30,33	1.85	5 (22%)
3	A2M	L5	3517	3	18,25,26	1.89	5 (27%)	18,36,39	2.23	5 (27%)
5	PSU	L8	55	5	18,21,22	1.40	3 (16%)	22,30,33	1.84	4 (18%)
49	PSU	S2	1057	49	18,21,22	1.40	3 (16%)	22,30,33	1.86	4 (18%)
7	HIC	LE	245	7	8,11,12	0.89	0	6,14,16	0.84	0
3	A2M	L5	400	3	18,25,26	1.99	5 (27%)	18,36,39	2.13	4 (22%)
3	1MA	L5	1266	3	16,25,26	2.58	3 (18%)	18,37,40	2.30	3 (16%)
49	PSU	S2	967	49	18,21,22	1.41	3 (16%)	22,30,33	1.82	4 (18%)
49	A2M	S2	166	49	18,25,26	2.02	5 (27%)	18,36,39	2.16	5 (27%)
3	A2M	L5	2206	3	18,25,26	1.97	5 (27%)	18,36,39	2.11	5 (27%)
3	A2M	L5	1479	3	18,25,26	1.97	5 (27%)	18,36,39	2.19	4 (22%)
3	PSU	L5	3576	3	18,21,22	1.39	3 (16%)	22,30,33	1.71	4 (18%)
3	UR3	L5	4276	3	19,22,23	1.29	3 (15%)	26,32,35	1.24	2 (7%)
49	PSU	S2	610	49	18,21,22	1.41	3 (16%)	22,30,33	1.82	5 (22%)
49	PSU	S2	823	49	18,21,22	1.39	3 (16%)	22,30,33	1.80	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
49	OMC	S2	463	49	19,22,23	1.18	2 (10%)	26,31,34	0.88	0
3	PSU	L5	3494	3	18,21,22	1.42	3 (16%)	22,30,33	1.80	5 (22%)
3	OMC	L5	3619	19,3	19,22,23	1.17	2 (10%)	26,31,34	0.87	0
3	OMG	L5	4138	3	18,26,27	1.96	2 (11%)	19,38,41	1.73	5 (26%)
3	PSU	L5	4322	3	18,21,22	1.39	3 (16%)	22,30,33	1.85	4 (18%)
3	PSU	L5	4188	3	18,21,22	1.37	3 (16%)	22,30,33	1.90	4 (18%)
49	PSU	S2	687	49	18,21,22	1.41	3 (16%)	22,30,33	1.81	5 (22%)
49	PSU	S2	1368	49	18,21,22	1.40	3 (16%)	22,30,33	1.84	5 (22%)
3	A2M	L5	3599	3	18,25,26	1.99	5 (27%)	18,36,39	2.21	5 (27%)
4	GTP	L7	1	4	26,34,34	0.97	1 (3%)	32,54,54	1.24	2 (6%)
3	OMC	L5	2704	3	19,22,23	1.15	2 (10%)	26,31,34	0.87	1 (3%)
3	OMG	L5	4245	3	18,26,27	1.96	2 (11%)	19,38,41	1.67	4 (21%)
3	A2M	L5	3562	3	18,25,26	1.98	5 (27%)	18,36,39	2.18	5 (27%)
49	OMU	S2	116	49	19,22,23	1.00	2 (10%)	26,31,34	1.73	6 (23%)
49	PSU	S2	1178	49	18,21,22	1.43	3 (16%)	22,30,33	1.81	4 (18%)
3	OMG	L5	4369	3	18,26,27	1.98	2 (11%)	19,38,41	1.69	4 (21%)
3	PSU	L5	4749	3	18,21,22	1.42	3 (16%)	22,30,33	1.82	4 (18%)
49	OMG	S2	510	49	18,26,27	1.94	2 (11%)	19,38,41	1.73	5 (26%)
8	AYA	LF	2	8	6,7,8	0.73	0	5,8,10	0.33	0
49	OMG	S2	868	49	18,26,27	1.95	2 (11%)	19,38,41	1.67	4 (21%)
3	OMG	L5	2207	3	18,26,27	1.98	2 (11%)	19,38,41	1.62	4 (21%)
3	PSU	L5	3427	3	18,21,22	1.39	3 (16%)	22,30,33	1.84	5 (22%)
49	OMU	S2	429	49	19,22,23	1.01	2 (10%)	26,31,34	1.82	6 (23%)
3	PSU	L5	1720	3	18,21,22	1.38	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	3616	3	18,21,22	1.38	3 (16%)	22,30,33	1.90	5 (22%)
49	PSU	S2	34	49	18,21,22	1.41	3 (16%)	22,30,33	1.85	4 (18%)
49	PSU	S2	652	49	18,21,22	1.42	3 (16%)	22,30,33	1.85	5 (22%)
49	OMC	S2	1704	49	19,22,23	1.17	2 (10%)	26,31,34	0.88	1 (3%)
49	PSU	S2	1082	49	18,21,22	1.36	3 (16%)	22,30,33	1.84	4 (18%)
49	PSU	S2	36	49	18,21,22	1.41	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	1638	3	18,21,22	1.38	3 (16%)	22,30,33	1.84	5 (22%)
5	PSU	L8	69	5	18,21,22	1.38	3 (16%)	22,30,33	1.85	4 (18%)
49	A2M	S2	577	49	18,25,26	1.97	5 (27%)	18,36,39	2.15	5 (27%)
3	OMC	L5	1284	3	19,22,23	1.18	2 (10%)	26,31,34	0.89	0
46	SAC	Ls	2	46	7,8,9	0.52	0	8,9,11	0.84	1 (12%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OMU	L5	4366	3	19,22,23	0.99	2 (10%)	26,31,34	1.80	5 (19%)
3	A2M	L5	2244	3	18,25,26	2.01	5 (27%)	18,36,39	2.19	5 (27%)
3	A2M	L5	4336	3	18,25,26	1.98	5 (27%)	18,36,39	2.16	5 (27%)
44	MLZ	Lq	53	44	8,9,10	0.48	0	4,9,11	0.16	0
49	PSU	S2	802	49	18,21,22	1.43	3 (16%)	22,30,33	1.80	5 (22%)
3	PSU	L5	3447	3	18,21,22	1.40	3 (16%)	22,30,33	1.81	4 (18%)
49	OMC	S2	1392	49	19,22,23	1.17	2 (10%)	26,31,34	0.96	1 (3%)
49	OMU	S2	628	49	19,22,23	1.01	1 (5%)	26,31,34	1.84	5 (19%)
3	PSU	L5	4419	3	18,21,22	1.40	3 (16%)	22,30,33	1.82	5 (22%)
3	PSU	L5	3554	3	18,21,22	1.40	3 (16%)	22,30,33	1.82	5 (22%)
3	OMC	L5	2647	3	19,22,23	1.15	2 (10%)	26,31,34	1.01	1 (3%)
3	PSU	L5	4166	3	18,21,22	1.40	3 (16%)	22,30,33	1.83	4 (18%)
3	PSU	L5	4203	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)
3	PSU	L5	4169	3	18,21,22	1.39	3 (16%)	22,30,33	1.83	5 (22%)
49	A2M	S2	669	49	18,25,26	1.87	4 (22%)	18,36,39	2.37	5 (27%)

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
57	SAC	SL	2	57	-	1/7/8/10	-
3	OMU	L5	2258	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	3492	3,49	-	0/5/27/28	0/3/3/3
49	A2M	S2	513	49	-	0/5/27/28	0/3/3/3
49	A2M	S2	469	49	-	0/5/27/28	0/3/3/3
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2630	3	-	0/5/27/28	0/3/3/3
49	A2M	S2	27	49	-	0/5/27/28	0/3/3/3
3	A2M	L5	3450	3	-	0/5/27/28	0/3/3/3
49	OMC	S2	518	49	-	2/9/27/28	0/2/2/2
3	OMC	L5	2265	3	-	2/9/27/28	0/2/2/2
49	PSU	S2	864	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	1718	3	-	0/7/25/26	0/2/2/2
49	OMG	S2	437	49	-	0/5/27/28	0/3/3/3
49	A2M	S2	485	49	-	0/5/27/28	0/3/3/3
3	PSU	L5	4382	3	-	4/7/25/26	0/2/2/2
3	A2M	L5	3456	3	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMG	L5	4364	3	-	0/5/27/28	0/3/3/3
3	OMU	L5	2680	3	-	0/9/27/28	0/2/2/2
3	OMU	L5	3657	44,3	-	0/9/27/28	0/2/2/2
3	A2M	L5	4317	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4278	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3500	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1477	3	-	0/5/27/28	0/3/3/3
49	PSU	S2	1239	49	-	0/7/25/26	0/2/2/2
49	MA6	S2	1852	49	-	2/7/29/30	0/3/3/3
3	OMC	L5	1820	3	-	0/9/27/28	0/2/2/2
3	OMU	L5	4052	3	-	0/9/27/28	0/2/2/2
5	OMG	L8	75	5	-	0/5/27/28	0/3/3/3
3	OMG	L5	4116	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	1270	3	-	1/5/27/28	0/3/3/3
3	5MC	L5	4193	3	-	4/7/25/26	0/2/2/2
3	PSU	L5	4217	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	573	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	682	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	1233	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	3462	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1046	49	-	2/7/25/26	0/2/2/2
49	OMU	S2	1289	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	3652	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	105	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	4269	3	-	1/5/27/28	0/3/3/3
49	OMU	S2	1805	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	4058	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	172	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	2475	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	3466	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3974	3	-	0/5/27/28	0/3/3/3
49	OMG	S2	602	49	-	0/5/27/28	0/3/3/3
3	PSU	L5	1731	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4039	3	-	0/7/25/26	0/2/2/2
49	A2M	S2	99	49	-	1/5/27/28	0/3/3/3
3	OMC	L5	3433	3	-	4/9/27/28	0/2/2/2
49	OMG	S2	684	49	-	2/5/27/28	0/3/3/3
49	4AC	S2	1338	49	-	4/11/29/30	0/2/2/2
3	PSU	L5	4435	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	2351	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3585	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	1489	3	-	3/5/27/28	0/3/3/3
3	PSU	L5	3369	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	3973	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4383	3	-	2/5/27/28	0/3/3/3
49	OMU	S2	121	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	4246	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4045	3	-	0/7/25/26	0/2/2/2
49	A2M	S2	159	49	-	0/5/27/28	0/3/3/3
49	A2M	S2	1679	49	-	0/5/27/28	0/3/3/3
3	PSU	L5	3490	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	4202	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	398	3	-	1/5/27/28	0/3/3/3
49	OMG	S2	1448	49	-	1/5/27/28	0/3/3/3
49	MA6	S2	1851	49	-	1/7/29/30	0/3/3/3
32	MLZ	Le	5	32	-	1/7/8/10	-
3	PSU	L5	1491	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1626	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	1799	3	-	0/7/25/26	0/2/2/2
3	5MC	L5	3514	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	1260	3	-	1/5/27/28	0/3/3/3
3	OMG	L5	3676	3	-	0/5/27/28	0/3/3/3
3	OMG	L5	4240	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3583	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	93	49	-	0/7/25/26	0/2/2/2
49	OMU	S2	355	49	-	0/9/27/28	0/2/2/2
49	OMU	S2	1443	49	-	0/9/27/28	0/2/2/2
3	A2M	L5	3557	3	-	0/5/27/28	0/3/3/3
49	PSU	S2	407	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	1446	49	-	0/7/25/26	0/2/2/2
3	OMU	L5	4244	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4740	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	1005	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	1537	3	-	0/7/25/26	0/2/2/2
78	AME	Sg	1	78	-	2/9/10/12	-
49	PSU	S2	1175	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4107	3	-	0/7/25/26	0/2/2/2
76	NMM	Se	67	76	-	2/9/11/13	-
3	PSU	L5	4374	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4711	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3502	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1632	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	PSU	S2	1348	49	-	0/7/25/26	0/2/2/2
49	A2M	S2	1384	49	-	0/5/27/28	0/3/3/3
49	PSU	S2	1644	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4099	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3631	3	-	0/5/27/28	0/3/3/3
49	OMU	S2	1327	49	-	0/9/27/28	0/2/2/2
49	PSU	S2	119	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4267	3	-	2/7/25/26	0/2/2/2
49	PSU	S2	210	49	-	2/7/25/26	0/2/2/2
49	PSU	S2	1047	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	1801	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2208	3	-	0/9/27/28	0/2/2/2
49	6MZ	S2	1833	49	-	0/5/27/28	0/3/3/3
3	OMG	L5	2267	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	1810	3	-	0/5/27/28	0/3/3/3
49	OMG	S2	645	49	-	3/5/27/28	0/3/3/3
3	PSU	L5	3371	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4325	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	109	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	1721	3	-	0/7/25/26	0/2/2/2
49	OMC	S2	174	49	-	0/9/27/28	0/2/2/2
49	4AC	S2	1843	49	-	2/11/29/30	0/2/2/2
49	A2M	S2	591	49	-	0/5/27/28	0/3/3/3
49	PSU	S2	650	49	-	0/7/25/26	0/2/2/2
3	OMC	L5	3540	3	-	0/9/27/28	0/2/2/2
49	PSU	S2	1693	49	-	0/7/25/26	0/2/2/2
43	M3L	Lp	98	43	-	0/9/10/12	-
49	OMG	S2	1491	49	-	1/5/27/28	0/3/3/3
3	OMC	L5	2667	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	2719	3	-	0/5/27/28	0/3/3/3
49	7MG	S2	1640	49	-	0/7/37/38	0/3/3/3
3	OMG	L5	1580	3	-	2/5/27/28	0/3/3/3
3	OMC	L5	3573	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	4282	3	-	0/9/27/28	0/2/2/2
49	OMG	S2	1329	49	-	0/5/27/28	0/3/3/3
49	PSU	S2	218	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	3476	3	-	0/5/27/28	0/3/3/3
49	PSU	S2	816	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	3359	3	-	0/5/27/28	0/3/3/3
3	6MZ	L5	3966	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3496	3	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4042	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3942	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	2658	3	-	1/5/27/28	0/3/3/3
3	OMC	L5	3601	3	-	0/9/27/28	0/2/2/2
75	SAC	Sd	2	75	-	0/7/8/10	-
49	PSU	S2	867	49	-	0/7/25/26	0/2/2/2
80	HY3	Si	62	80	-	0/1/12/14	0/1/1/1
3	OMG	L5	3524	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4149	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	815	49	-	0/7/25/26	0/2/2/2
3	OMC	L5	2194	3	-	2/9/27/28	0/2/2/2
3	PSU	L5	4298	3	-	0/7/25/26	0/2/2/2
49	A2M	S2	1032	49	-	0/5/27/28	0/3/3/3
49	PSU	S2	1245	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	4177	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3517	3	-	2/5/27/28	0/3/3/3
5	PSU	L8	55	5	-	0/7/25/26	0/2/2/2
49	PSU	S2	1057	49	-	0/7/25/26	0/2/2/2
7	HIC	LE	245	7	-	2/5/6/8	0/1/1/1
3	A2M	L5	400	3	-	0/5/27/28	0/3/3/3
3	1MA	L5	1266	3	-	0/3/25/26	0/3/3/3
49	PSU	S2	967	49	-	0/7/25/26	0/2/2/2
49	A2M	S2	166	49	-	0/5/27/28	0/3/3/3
3	A2M	L5	2206	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	1479	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3576	3	-	2/7/25/26	0/2/2/2
3	UR3	L5	4276	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	610	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	823	49	-	2/7/25/26	0/2/2/2
49	OMC	S2	463	49	-	0/9/27/28	0/2/2/2
3	PSU	L5	3494	3	-	2/7/25/26	0/2/2/2
3	OMC	L5	3619	19,3	-	1/9/27/28	0/2/2/2
3	OMG	L5	4138	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4322	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4188	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	687	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	1368	49	-	0/7/25/26	0/2/2/2
3	A2M	L5	3599	3	-	1/5/27/28	0/3/3/3
4	GTP	L7	1	4	-	0/18/38/38	0/3/3/3
3	OMC	L5	2704	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4245	3	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A2M	L5	3562	3	-	0/5/27/28	0/3/3/3
49	OMU	S2	116	49	-	0/9/27/28	0/2/2/2
49	PSU	S2	1178	49	-	0/7/25/26	0/2/2/2
3	OMG	L5	4369	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	4749	3	-	0/7/25/26	0/2/2/2
49	OMG	S2	510	49	-	0/5/27/28	0/3/3/3
8	AYA	LF	2	8	-	2/4/6/8	-
49	OMG	S2	868	49	-	0/5/27/28	0/3/3/3
3	OMG	L5	2207	3	-	0/5/27/28	0/3/3/3
3	PSU	L5	3427	3	-	0/7/25/26	0/2/2/2
49	OMU	S2	429	49	-	4/9/27/28	0/2/2/2
3	PSU	L5	1720	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3616	3	-	0/7/25/26	0/2/2/2
49	PSU	S2	34	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	652	49	-	0/7/25/26	0/2/2/2
49	OMC	S2	1704	49	-	0/9/27/28	0/2/2/2
49	PSU	S2	1082	49	-	0/7/25/26	0/2/2/2
49	PSU	S2	36	49	-	0/7/25/26	0/2/2/2
3	PSU	L5	1638	3	-	0/7/25/26	0/2/2/2
5	PSU	L8	69	5	-	0/7/25/26	0/2/2/2
49	A2M	S2	577	49	-	2/5/27/28	0/3/3/3
3	OMC	L5	1284	3	-	0/9/27/28	0/2/2/2
46	SAC	Ls	2	46	-	0/7/8/10	-
3	OMU	L5	4366	3	-	0/9/27/28	0/2/2/2
3	A2M	L5	2244	3	-	0/5/27/28	0/3/3/3
3	A2M	L5	4336	3	-	1/5/27/28	0/3/3/3
44	MLZ	Lq	53	44	-	0/7/8/10	-
49	PSU	S2	802	49	-	2/7/25/26	0/2/2/2
3	PSU	L5	3447	3	-	0/7/25/26	0/2/2/2
49	OMC	S2	1392	49	-	1/9/27/28	0/2/2/2
49	OMU	S2	628	49	-	2/9/27/28	0/2/2/2
3	PSU	L5	4419	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3554	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2647	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4166	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4203	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4169	3	-	0/7/25/26	0/2/2/2
49	A2M	S2	669	49	-	3/5/27/28	0/3/3/3

The worst 5 of 610 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1266	1MA	C2-N3	8.88	1.39	1.29
3	L5	2207	OMG	C5-C6	-7.10	1.33	1.47
3	L5	3631	OMG	C5-C6	-7.06	1.33	1.47
3	L5	3524	OMG	C5-C6	-7.05	1.33	1.47
3	L5	4116	OMG	C5-C6	-7.04	1.33	1.47

The worst 5 of 869 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
76	Se	67	NMM	NE-CZ-NH2	-7.43	112.67	119.48
3	L5	1266	1MA	N1-C2-N3	-7.18	117.65	126.02
3	L5	4269	A2M	N3-C2-N1	-6.89	117.91	128.68
3	L5	1270	A2M	N3-C2-N1	-6.85	117.97	128.68
3	L5	2630	A2M	N3-C2-N1	-6.85	117.97	128.68

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	LE	245	HIC	CA-CB-CG-ND1
49	S2	429	OMU	C2'-C1'-N1-C2
49	S2	429	OMU	C2'-C1'-N1-C6
49	S2	577	A2M	C3'-C4'-C5'-O5'
49	S2	645	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	181:C	O3'	199:A	P	24.04
1	I	202:C	O3'	216:U	P	23.09



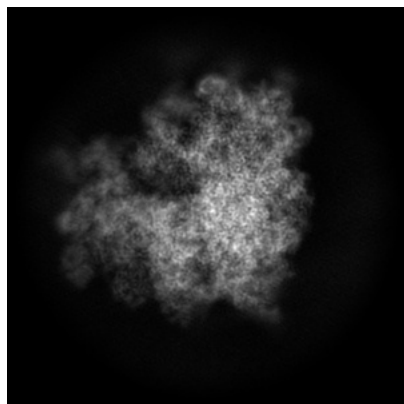
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14752. These allow visual inspection of the internal detail of the map and identification of artifacts.

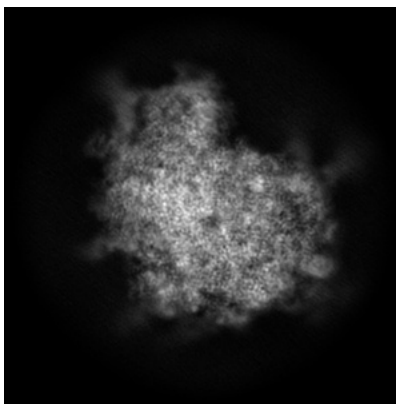
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

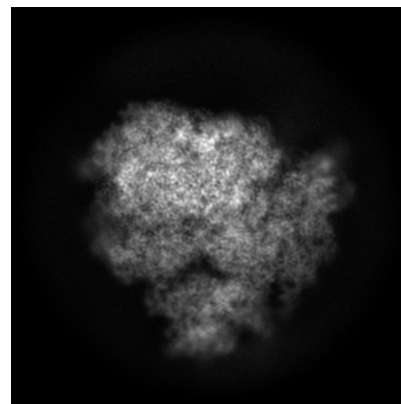
#### 6.1.1 Primary map



X

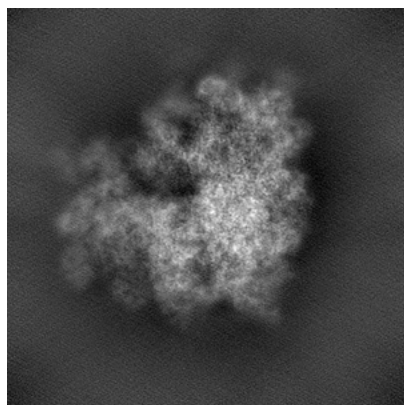


Y

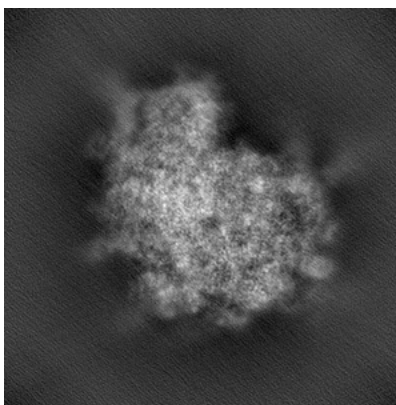


Z

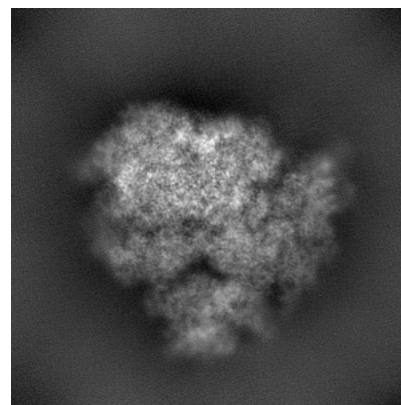
#### 6.1.2 Raw map



X



Y

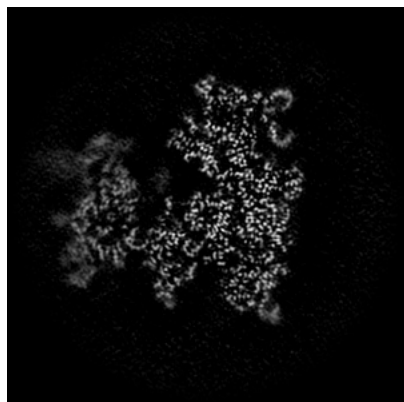


Z

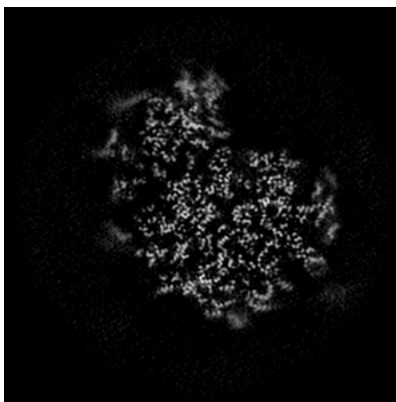
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

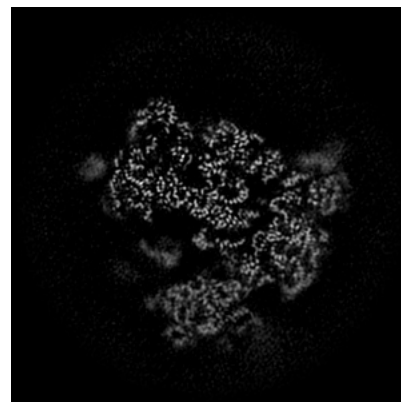
### 6.2.1 Primary map



X Index: 165

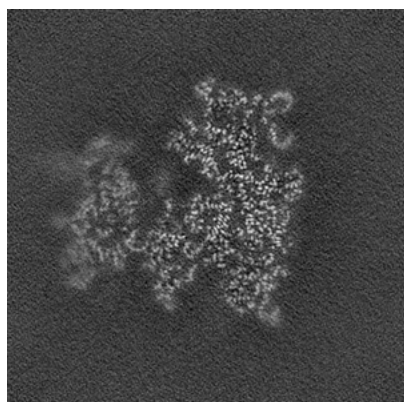


Y Index: 165

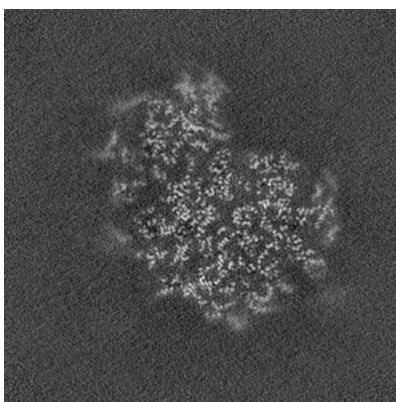


Z Index: 165

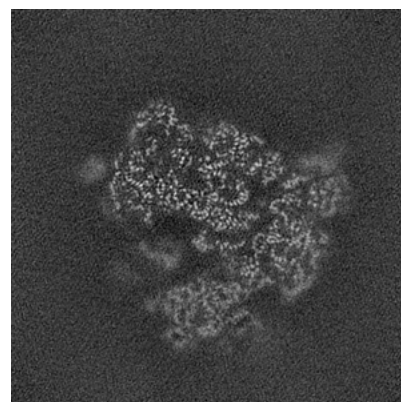
### 6.2.2 Raw map



X Index: 165



Y Index: 165

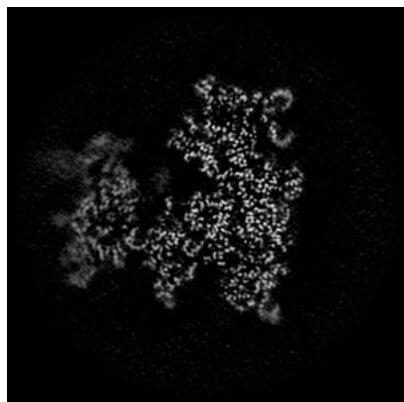


Z Index: 165

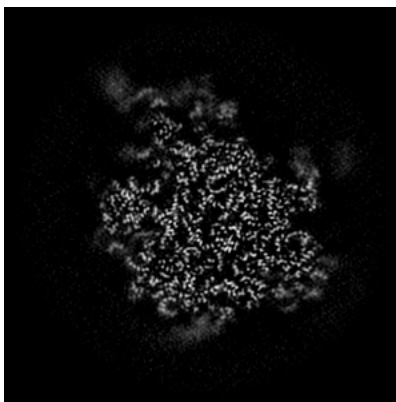
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

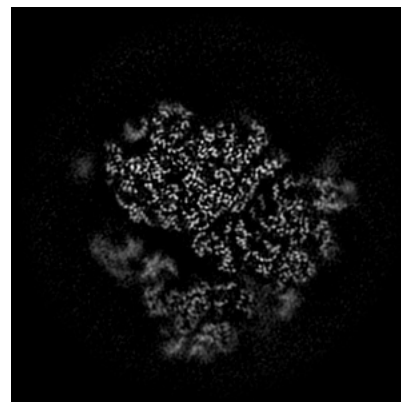
### 6.3.1 Primary map



X Index: 165

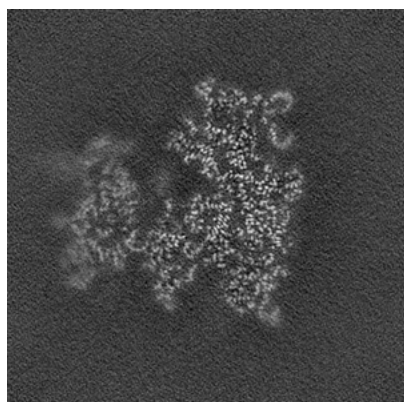


Y Index: 194

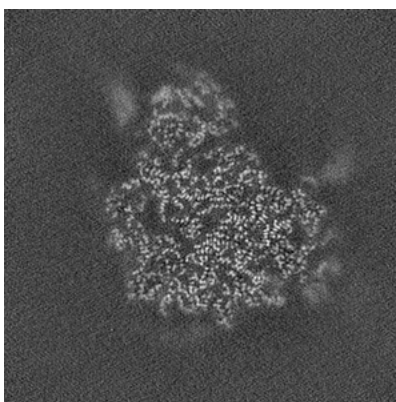


Z Index: 150

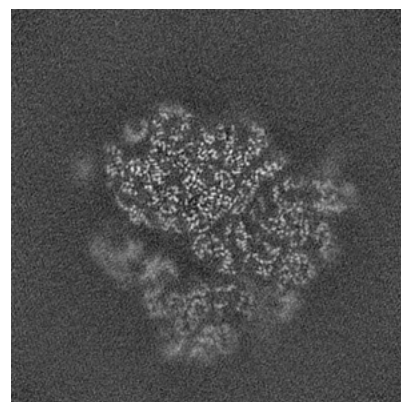
### 6.3.2 Raw map



X Index: 165



Y Index: 186



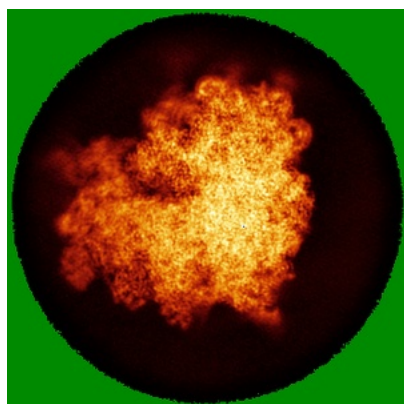
Z Index: 150

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

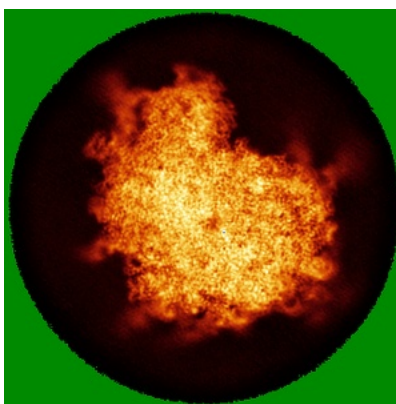


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

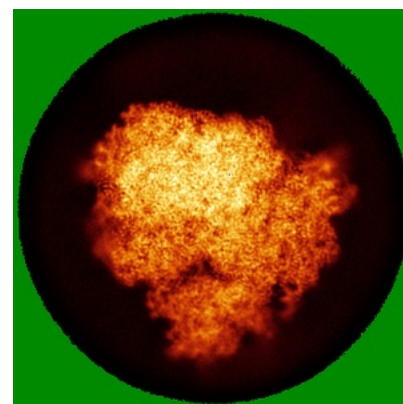
### 6.4.1 Primary map



X

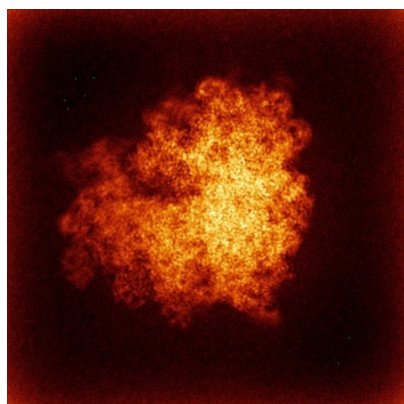


Y

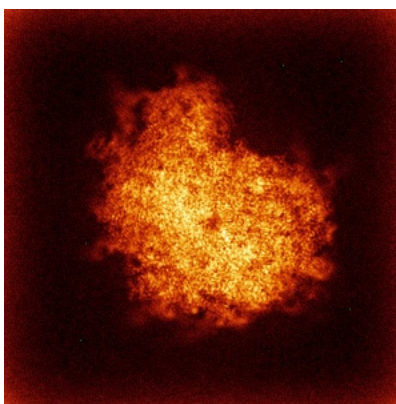


Z

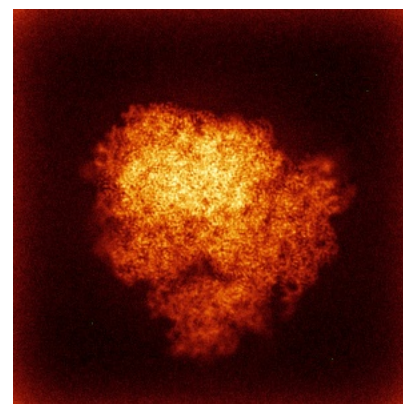
### 6.4.2 Raw map



X



Y

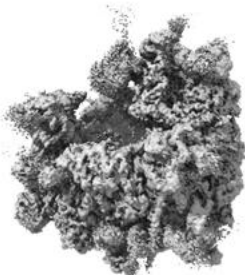


Z

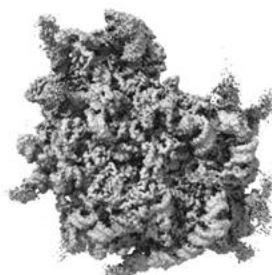
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



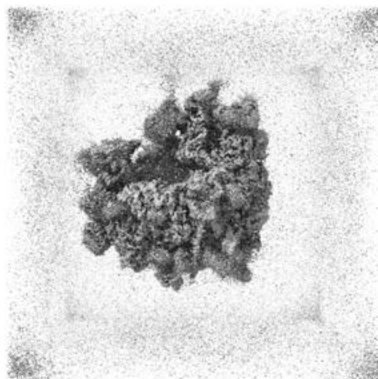
Y



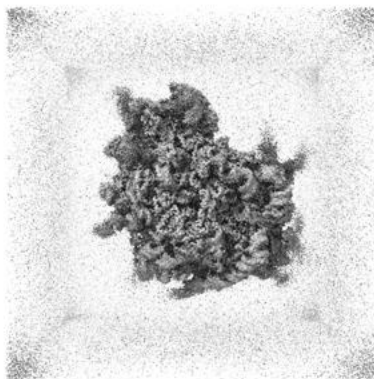
Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

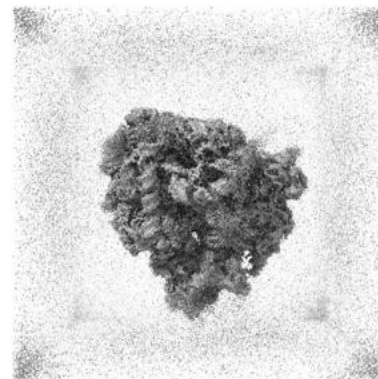
### 6.5.2 Raw map



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.

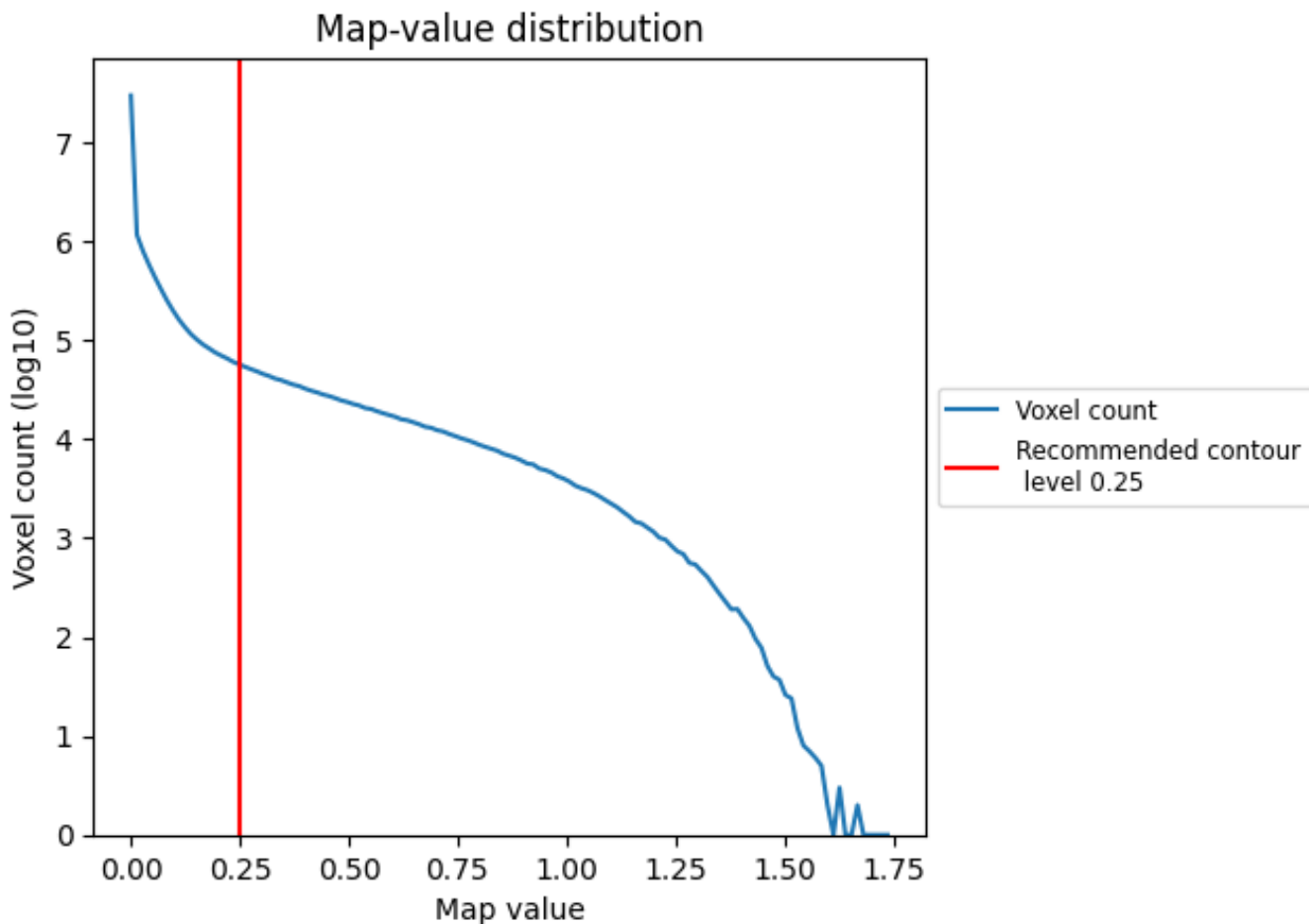
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

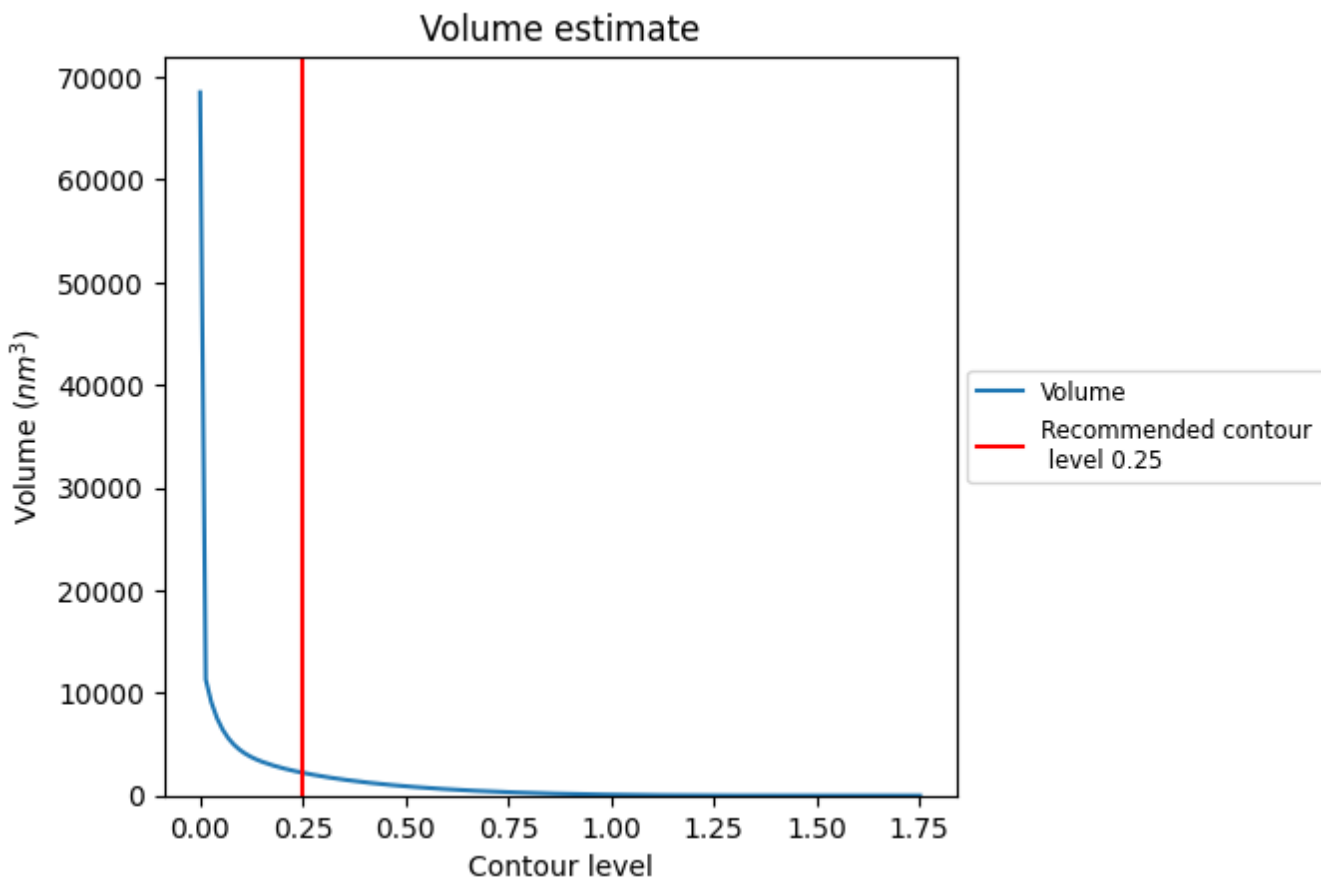
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

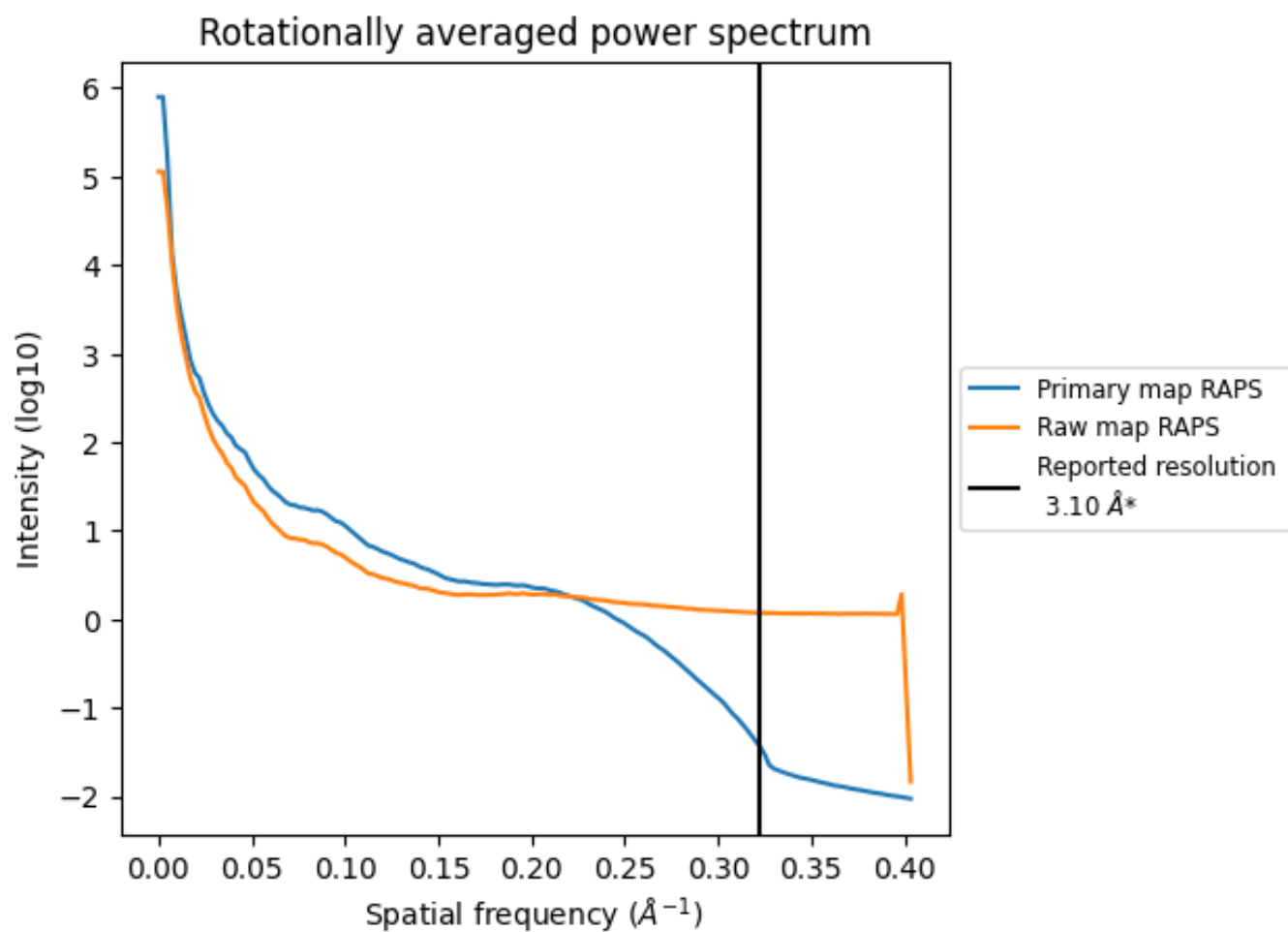
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2219 nm<sup>3</sup>; this corresponds to an approximate mass of 2005 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



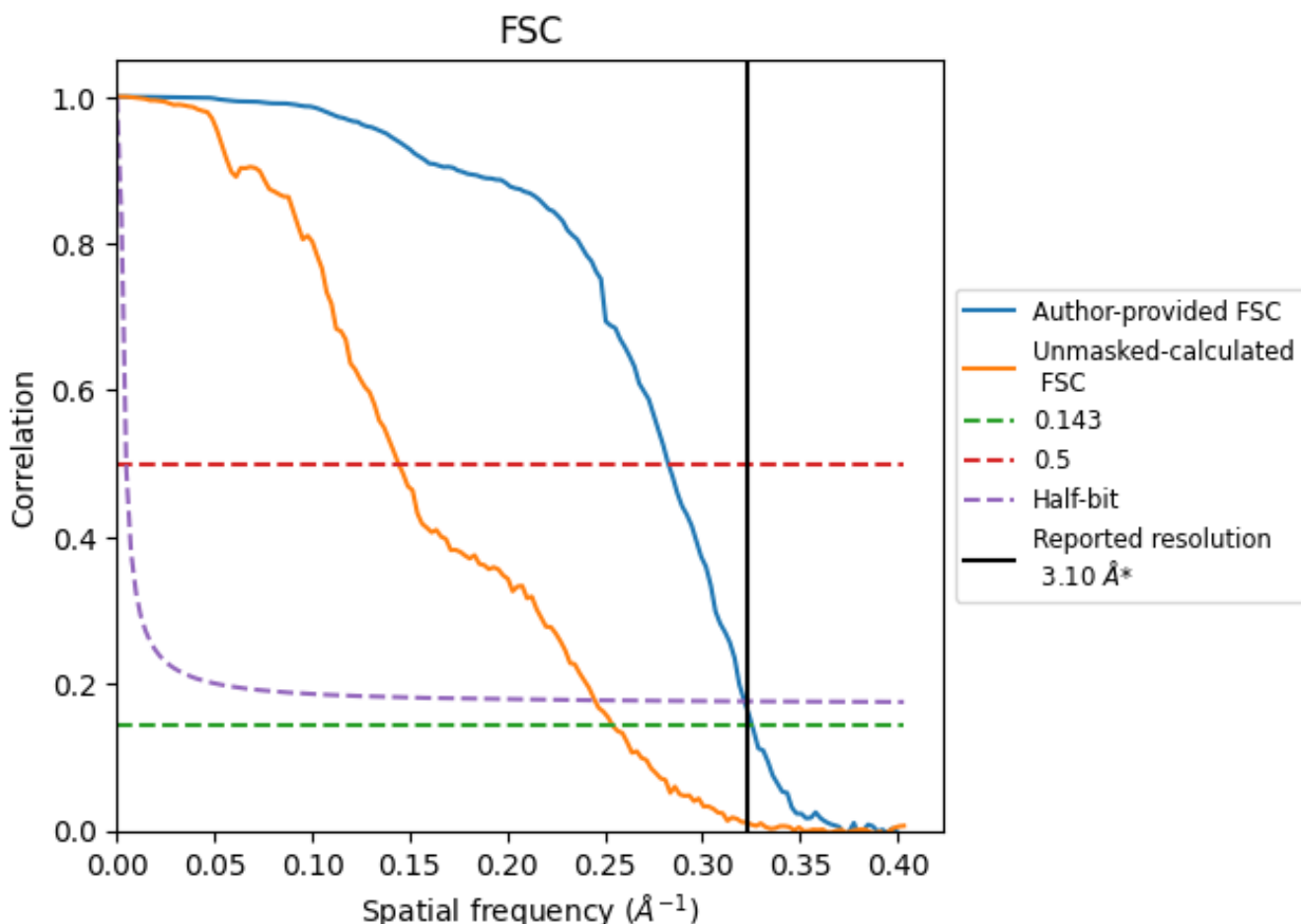
\*Reported resolution corresponds to spatial frequency of  $0.323 \text{ \AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

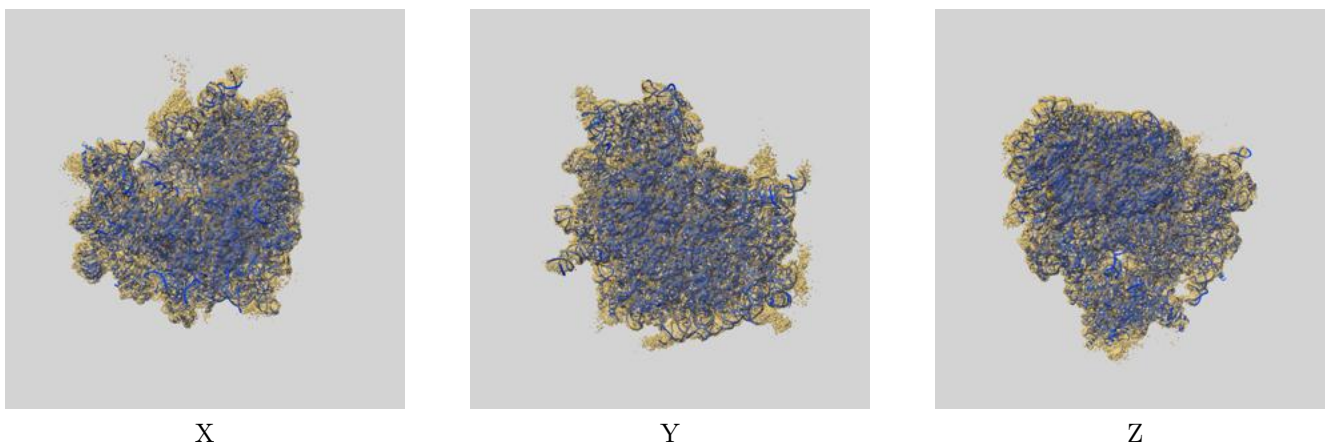
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.54	3.11
Unmasked-calculated*	3.94	6.93	4.08

\*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 3.94 differs from the reported value 3.1 by more than 10 %

## 9 Map-model fit [i](#)

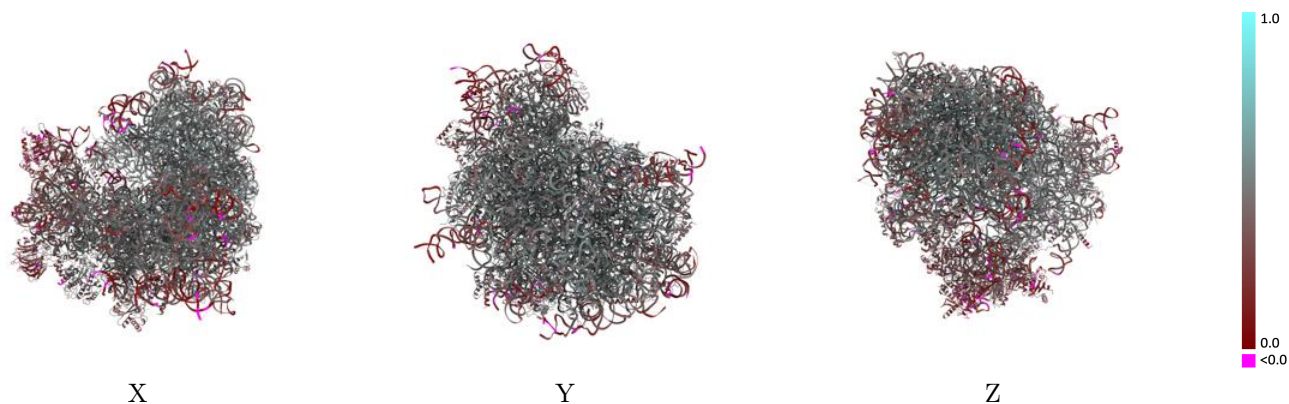
This section contains information regarding the fit between EMDB map EMD-14752 and PDB model 7ZJX. Per-residue inclusion information can be found in section 3 on page 21.

### 9.1 Map-model overlay [i](#)



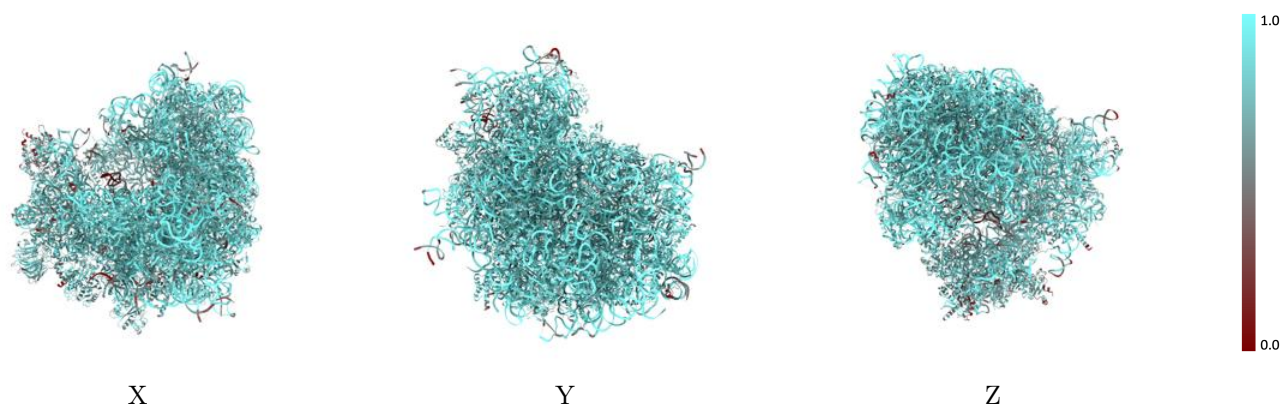
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



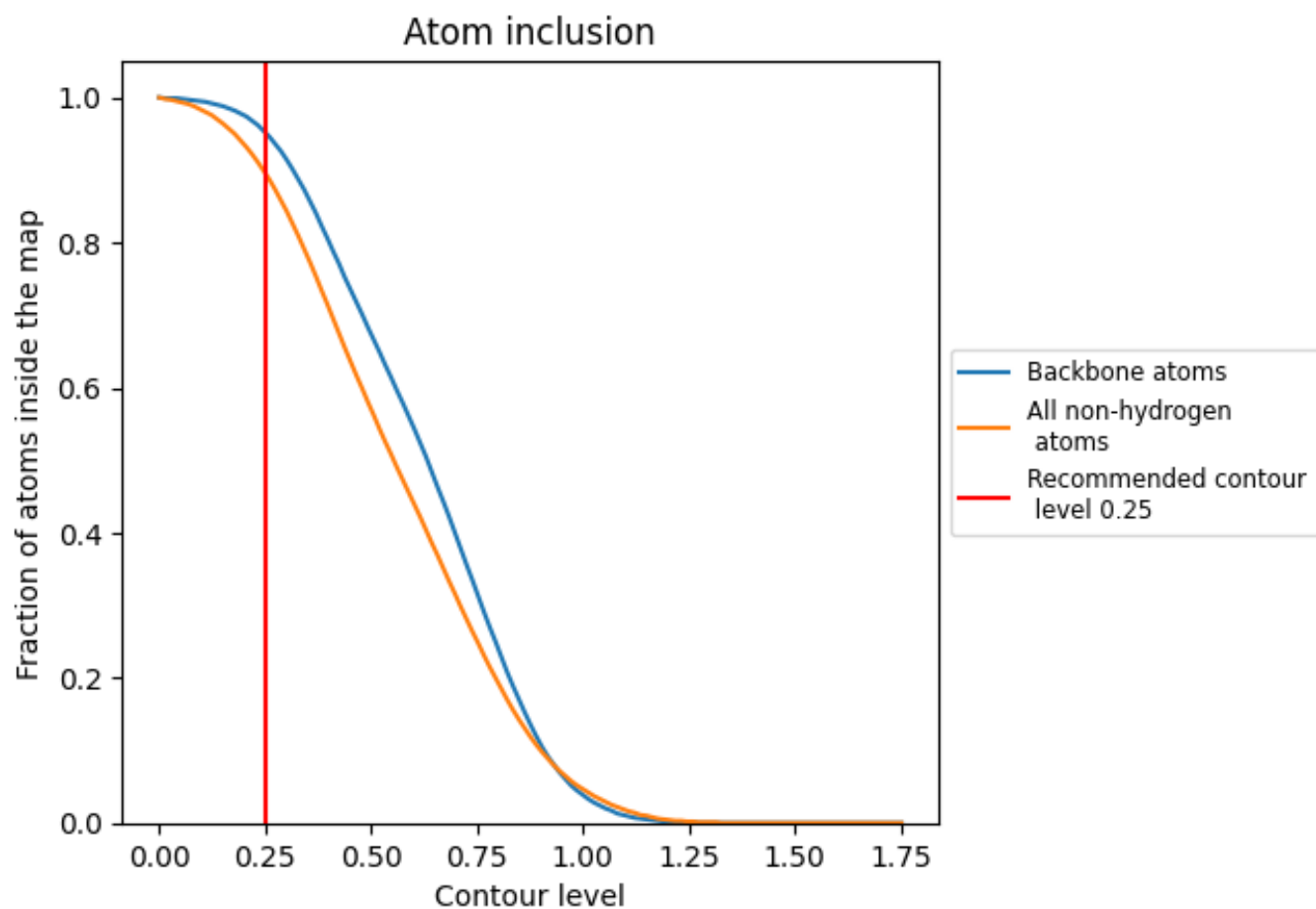
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.25).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8960	 0.4280
B	 0.5320	 0.1750
I	 0.6960	 0.1580
L5	 0.9580	 0.4480
L7	 0.9920	 0.4880
L8	 0.9680	 0.4730
LD	 0.8600	 0.5080
LE	 0.8940	 0.4970
LF	 0.8860	 0.4920
LG	 0.8860	 0.4490
LH	 0.8290	 0.4210
LI	 0.8610	 0.4830
LJ	 0.8620	 0.4420
LK	 0.8690	 0.4790
LL	 0.8030	 0.4740
LM	 0.8070	 0.4090
LO	 0.8570	 0.4520
LP	 0.8970	 0.4600
LQ	 0.9190	 0.5190
LR	 0.8740	 0.4890
LS	 0.8720	 0.4930
LT	 0.8770	 0.4920
LU	 0.8710	 0.4630
LV	 0.8880	 0.5030
LW	 0.8370	 0.4790
LX	 0.8900	 0.4380
LY	 0.8280	 0.4910
LZ	 0.7810	 0.3950
La	 0.8560	 0.4730
Lb	 0.8720	 0.4800
Lc	 0.9230	 0.4830
Ld	 0.9300	 0.5100
Le	 0.7920	 0.3950
Lf	 0.7950	 0.4400
Lg	 0.8910	 0.4910

















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Chain	Atom inclusion	Q-score
Lh	 0.8630	 0.4970
Li	 0.8920	 0.5140
Lj	 0.8630	 0.4790
Lk	 0.8660	 0.4640
Ll	 0.8440	 0.4370
Lm	 0.9050	 0.5140
Ln	 0.8420	 0.4420
Lo	 0.8530	 0.4670
Lp	 0.8740	 0.4850
Lq	 0.7960	 0.4680
Lr	 0.8240	 0.4830
Ls	 0.8960	 0.4910
Lx	 0.8010	 0.1730
S	 0.7810	 0.1380
S2	 0.9450	 0.4130
SB	 0.8330	 0.4410
SC	 0.6650	 0.3490
SD	 0.6800	 0.2290
SE	 0.7000	 0.3620
SF	 0.8240	 0.4520
SG	 0.7540	 0.2530
SH	 0.8170	 0.3830
SL	 0.8010	 0.4180
SM	 0.8140	 0.4400
SN	 0.8200	 0.4540
SO	 0.7080	 0.3550
SP	 0.8460	 0.4500
SQ	 0.7410	 0.3230
SR	 0.8400	 0.3770
SS	 0.7700	 0.3820
ST	 0.8460	 0.4560
SU	 0.8380	 0.4240
SV	 0.7630	 0.3430
SW	 0.7640	 0.4440
SX	 0.5510	 0.1750
SY	 0.8290	 0.4600
SZ	 0.8410	 0.4580
Sa	 0.6580	 0.3070
Sb	 0.7780	 0.3230
Sc	 0.7350	 0.3580
Sd	 0.6990	 0.2790
Se	 0.8020	 0.3240

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Chain	Atom inclusion	Q-score
Sf	 0.7700	 0.3470
Sg	 0.8360	 0.4270
Sh	 0.8330	 0.4650
Si	 0.8390	 0.4840
Sj	 0.8450	 0.3800
Sk	 0.7560	 0.2420
Sl	 0.8490	 0.4840