



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2023 – 10:36 am GMT

PDB ID : 7O7Z
EMDB ID : EMD-12757
Title : Rabbit 80S ribosome stalled close to the mutated SARS-CoV-2 slippery site
by a pseudoknot (classified for pseudoknot)
Authors : Bhatt, P.R.; Scaiola, A.; Leibundgut, M.A.; Atkins, J.F.; Ban, N.
Deposited on : 2021-04-14
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

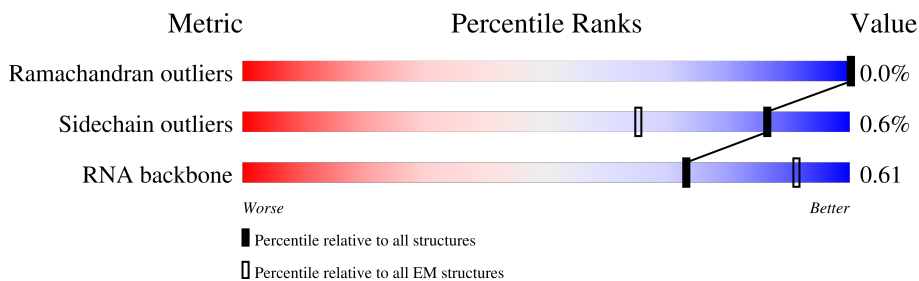
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 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 ≥ 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	A2	1870	
2	AA	84	
3	AB	69	
4	AC	156	
5	AD	133	
6	AE	115	
7	AF	317	
8	AG	56	

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Mol	Chain	Length	Quality of chain
9	AH	220	
10	AI	76	
11	AT	76	
12	AZ	295	
13	Aa	264	
14	Ab	293	
15	Ac	281	
16	Ad	263	
17	Ae	204	
18	Af	249	
19	Ag	432	
20	Ah	208	
21	Ai	194	
22	Aj	165	
23	Ak	158	
24	Al	132	
25	Am	151	
26	An	151	
27	Ao	145	
28	Ap	172	
29	Aq	135	
30	Ar	152	
31	As	145	
32	At	119	
33	Au	83	

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Mol	Chain	Length	Quality of chain
34	Av	130	99%
35	Aw	143	97%
36	Ax	130	96%
37	Ay	124	69% 31% 8%
38	Az	25	100%
39	B5	4808	66% 12% 22% 5%
40	B7	120	92% 8%
41	B8	158	85% 13%
42	BA	257	98%
43	BB	403	99%
44	BC	413	87% 12%
45	BD	297	99%
46	BE	291	84% 16% 8%
47	BF	247	91% 9%
48	BG	266	87% 12% 7%
49	BH	192	99%
50	BI	214	99%
51	BJ	178	95%
52	BK	1071	97%
53	BL	211	98%
54	BM	218	63% 37%
55	BN	204	100%
56	BO	203	98%
57	BP	184	86% 14%
58	BQ	188	99%

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Mol	Chain	Length	Quality of chain
59	BR	196	91% 8%
60	BS	176	100%
61	BT	160	99%
62	BU	128	77% 23%
63	BV	140	99% 6%
64	BW	157	76% 23% 38%
65	BX	156	76% 24%
66	BY	145	92% 8%
67	BZ	136	99%
68	Ba	148	98%
69	Bb	245	44% 56% 7%
70	Bc	115	94% 6% 11%
71	Bd	125	86% 14% 5%
72	Be	135	96%
73	Bf	110	100%
74	Bg	117	97%
75	Bh	123	99%
76	Bi	105	96%
77	Bj	97	89% 11%
78	Bk	70	99%
79	Bl	51	94%
80	Bm	128	41% 59%
81	Bo	106	98%
82	Bp	92	99%
83	Br	137	91% 8%

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Mol	Chain	Length	Quality of chain
84	Bs	318	<p>62% 38%</p>
85	Bt	165	<p>95% 5%</p>
86	Bv	217	<p>95%</p>

2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 229742 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A2	1770	37833	16911	6781	12371	1770	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1249	B8N	C	conflict	GB GBCT01000564.1
A2	1338	4AC	C	conflict	GB GBCT01000564.1
A2	1843	4AC	C	conflict	GB GBCT01000564.1

- Molecule 2 is a protein called 40S ribosomal protein S27.

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

- Molecule 3 is a protein called Ribosomal protein S28.

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

- Molecule 4 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AC	74	610	385	117	101	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein S30.

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

- Molecule 6 is a protein called Ribosomal protein eS26.

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

- Molecule 7 is a protein called RACK1.

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

- Molecule 8 is a protein called uS14.

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

- Molecule 9 is a RNA chain called mRNA containing SARS-CoV-2 sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	AH	95	2018	901	349	673	95	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AH	3466	U	A	conflict	GB NC_045512.2
AH	3468	A	C	conflict	GB NC_045512.2

- Molecule 10 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	AI	76	939	393	11	459	76	0	0

- Molecule 11 is a RNA chain called P-site Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
11	AT	76	1652	746	294	536	76	0	0

- Molecule 12 is a protein called 40S ribosomal protein SA.

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

- Molecule 13 is a protein called 40S ribosomal protein S3a.

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

- Molecule 14 is a protein called Ribosomal protein uS5.

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

- Molecule 15 is a protein called 40S ribosomal protein S3.

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

- Molecule 16 is a protein called Ribosomal protein eS4.

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

- Molecule 17 is a protein called Ribosomal protein S5.

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

- Molecule 18 is a protein called 40S ribosomal protein S6.

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

- Molecule 19 is a protein called 40S ribosomal protein S7.

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

- Molecule 20 is a protein called 40S ribosomal protein S8.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 21 is a protein called Ribosomal protein S9 (Predicted).

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

- Molecule 22 is a protein called eS10.

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

- Molecule 23 is a protein called 40S ribosomal protein S11.

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

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Al	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 25 is a protein called uS15.

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

- Molecule 26 is a protein called 40S ribosomal protein uS11.

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

- Molecule 27 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Ao	128	1048	665	197	179	7	0	0

- Molecule 28 is a protein called uS9.

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

- Molecule 29 is a protein called 40S ribosomal protein eS17.

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

- Molecule 30 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Ar	148	1217	763	245	208	1	0	0

- Molecule 31 is a protein called Ribosomal protein eS19.

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

- Molecule 32 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	At	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 33 is a protein called Ribosomal protein eS21.

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

- Molecule 34 is a protein called Ribosomal protein S15a.

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

- Molecule 35 is a protein called 40S ribosomal protein S23.

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

- Molecule 36 is a protein called 40S ribosomal protein S24.

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

- Molecule 37 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ay	85	Total	C	N	O	S	0	0
			683	439	128	115	1		

- Molecule 38 is a protein called 60s ribosomal protein l41.

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

- Molecule 39 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	B5	3764	80772	36003	14762	26243	3764	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 40 is a RNA chain called 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
40	B7	120	2570	1141	456	851	122	0	0

- Molecule 41 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
41	B8	156	3319	1481	585	1097	156	0	0

- Molecule 42 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	BA	253	1940	1214	396	324	6	0	0

- Molecule 43 is a protein called Ribosomal protein L3.

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

- Molecule 44 is a protein called 60S ribosomal protein L4.

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

- Molecule 45 is a protein called Ribosomal_L18_c domain-containing protein.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 46 is a protein called 60S ribosomal protein L6.

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

- Molecule 47 is a protein called Ribosomal Protein uL30.

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

- Molecule 48 is a protein called Ribosomal protein eL8.

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

- Molecule 49 is a protein called 60S ribosomal protein L9.

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

- Molecule 50 is a protein called 60S ribosomal protein L10.

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

- Molecule 51 is a protein called Ribosomal protein L11.

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

- Molecule 52 is a protein called Replicase polyprotein 1ab.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BK	35	Total	C	N	O	S	0	0
			265	163	45	51	6		

- Molecule 53 is a protein called Ribosomal protein eL13.

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

- Molecule 54 is a protein called Ribosomal protein L14.

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

- Molecule 55 is a protein called Ribosomal protein L15.

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

- Molecule 56 is a protein called Ribosomal protein uL13.

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

- Molecule 57 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BP	159	Total	C	N	O	S	0	0
			1289	809	249	222	9		

- Molecule 58 is a protein called Ribosomal Protein eL18.

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

- Molecule 59 is a protein called 60S ribosomal protein L19.

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

- Molecule 60 is a protein called Ribosomal protein eL20.

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

- Molecule 61 is a protein called eL21.

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

- Molecule 62 is a protein called Ribosomal protein eL22.

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

- Molecule 63 is a protein called Ribosomal protein L23.

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

- Molecule 64 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BW	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 65 is a protein called uL23.

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

- Molecule 66 is a protein called Ribosomal protein L26.

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

- Molecule 67 is a protein called 60S ribosomal protein L27.

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

- Molecule 68 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Ba	147	Total	C	N	O	S	0	0
			1163	734	239	186	4		

- Molecule 69 is a protein called 60S ribosomal protein L29.

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

- Molecule 70 is a protein called eL30.

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

- Molecule 71 is a protein called eL31.

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

- Molecule 72 is a protein called eL32.

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

- Molecule 73 is a protein called eL33.

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

- Molecule 74 is a protein called 60S ribosomal protein L34.

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

- Molecule 75 is a protein called uL29.

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

- Molecule 76 is a protein called 60S ribosomal protein L36.

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

- Molecule 77 is a protein called Ribosomal protein L37.

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

- Molecule 78 is a protein called eL38.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bk	24	LYS	ASN	conflict	UNP G1U001

- Molecule 79 is a protein called eL39.

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

- Molecule 80 is a protein called 60S ribosomal protein L40.

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

- Molecule 81 is a protein called eL42.

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

- Molecule 82 is a protein called eL43.

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

- Molecule 83 is a protein called Ribosomal protein eL28.

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

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	Bs	196	1507	959	263	276	9	0	0

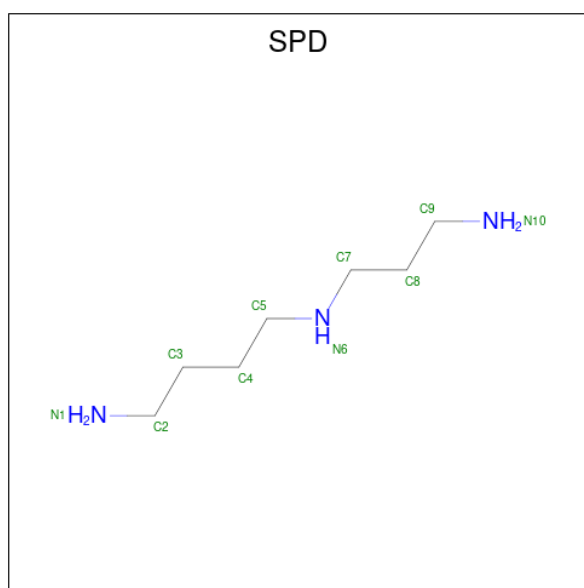
- Molecule 85 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	Bt	156	1178	733	221	220	4	0	0

- Molecule 86 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
86	Bv	212	1707	1092	308	299	8	0	0

- Molecule 87 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



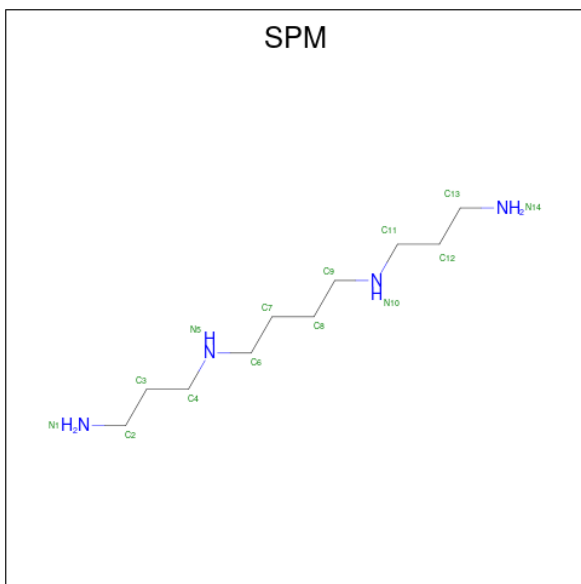
Mol	Chain	Residues	Atoms			AltConf
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
87	B5	1	10	7	3	0

- Molecule 88 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
88	A2	1	14	10	4	0
88	B5	1	14	10	4	0
88	B5	1	14	10	4	0

- Molecule 89 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
89	A2	109	109	109	0
89	AH	1	1	1	0
89	AT	3	3	3	0
89	Af	1	1	1	0
89	B5	284	284	284	0

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Mol	Chain	Residues	Atoms		AltConf
89	B7	9	Total 9	Mg 9	0
89	B8	9	Total 9	Mg 9	0
89	BP	1	Total 1	Mg 1	0
89	BR	1	Total 1	Mg 1	0
89	BV	1	Total 1	Mg 1	0
89	Ba	1	Total 1	Mg 1	0

- Molecule 90 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
90	A2	60	Total 60	X 60	0
90	AT	4	Total 4	X 4	0
90	Ae	1	Total 1	X 1	0
90	An	1	Total 1	X 1	0
90	Ar	1	Total 1	X 1	0
90	As	1	Total 1	X 1	0
90	B5	225	Total 225	X 225	0
90	B7	6	Total 6	X 6	0
90	B8	8	Total 8	X 8	0
90	BA	3	Total 3	X 3	0
90	BB	4	Total 4	X 4	0
90	BC	1	Total 1	X 1	0
90	BH	1	Total 1	X 1	0

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Mol	Chain	Residues	Atoms	AltConf
90	BI	1	Total X 1 1	0
90	BL	1	Total X 1 1	0
90	BN	1	Total X 1 1	0
90	BQ	2	Total X 2 2	0
90	BT	2	Total X 2 2	0
90	Bb	1	Total X 1 1	0
90	Be	1	Total X 1 1	0
90	Bf	1	Total X 1 1	0
90	Bg	1	Total X 1 1	0
90	Bl	1	Total X 1 1	0
90	Bo	1	Total X 1 1	0

- Molecule 91 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
91	AC	1	Total Zn 1 1	0
91	AE	1	Total Zn 1 1	0
91	AG	1	Total Zn 1 1	0
91	Bg	1	Total Zn 1 1	0
91	Bj	1	Total Zn 1 1	0
91	Bm	1	Total Zn 1 1	0
91	Bo	1	Total Zn 1 1	0
91	Bp	1	Total Zn 1 1	0

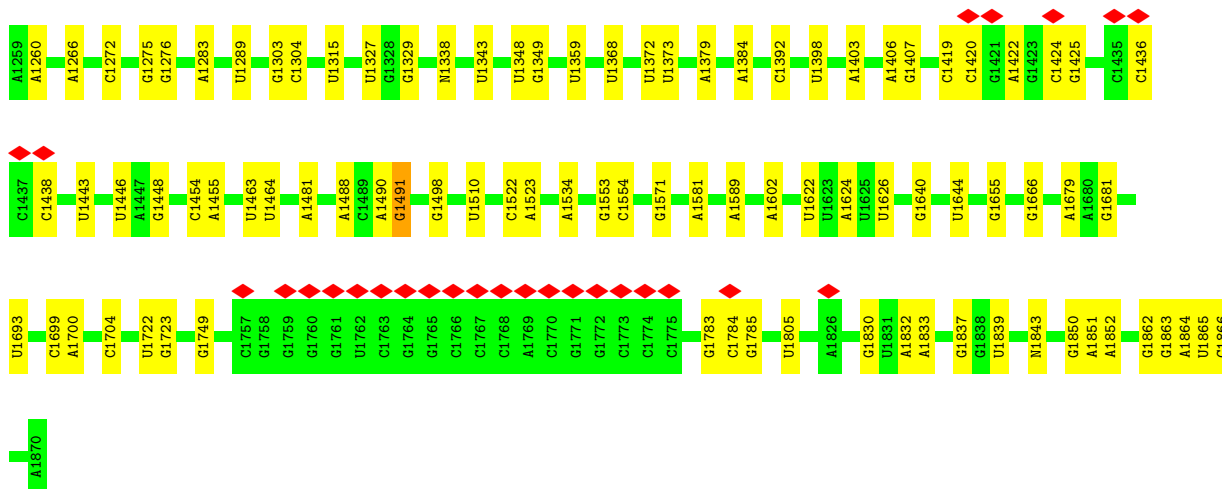
- Molecule 92 is water.

Mol	Chain	Residues	Atoms		AltConf
92	A2	526	Total 526	O 526	0
92	AH	9	Total 9	O 9	0
92	AI	1	Total 1	O 1	0
92	AT	12	Total 12	O 12	0
92	Aa	1	Total 1	O 1	0
92	Ac	1	Total 1	O 1	0
92	Af	3	Total 3	O 3	0
92	Ak	1	Total 1	O 1	0
92	Am	1	Total 1	O 1	0
92	An	2	Total 2	O 2	0
92	Ap	3	Total 3	O 3	0
92	As	2	Total 2	O 2	0
92	At	1	Total 1	O 1	0
92	Aw	3	Total 3	O 3	0
92	B5	1391	Total 1391	O 1391	0
92	B7	45	Total 45	O 45	0
92	B8	50	Total 50	O 50	0
92	BA	10	Total 10	O 10	0
92	BB	5	Total 5	O 5	0
92	BC	7	Total 7	O 7	0
92	BD	1	Total 1	O 1	0

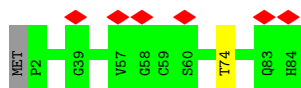
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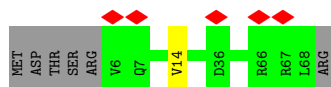
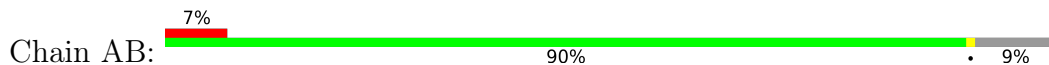
Mol	Chain	Residues	Atoms		AltConf
92	BF	1	Total 1	O 1	0
92	BH	1	Total 1	O 1	0
92	BI	4	Total 4	O 4	0
92	BL	3	Total 3	O 3	0
92	BN	3	Total 3	O 3	0
92	BO	1	Total 1	O 1	0
92	BP	2	Total 2	O 2	0
92	BR	5	Total 5	O 5	0
92	BV	2	Total 2	O 2	0
92	BX	2	Total 2	O 2	0
92	Ba	6	Total 6	O 6	0
92	Bd	1	Total 1	O 1	0
92	Be	4	Total 4	O 4	0
92	Bg	2	Total 2	O 2	0
92	Bj	3	Total 3	O 3	0
92	Bl	1	Total 1	O 1	0
92	Bo	1	Total 1	O 1	0



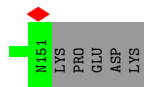
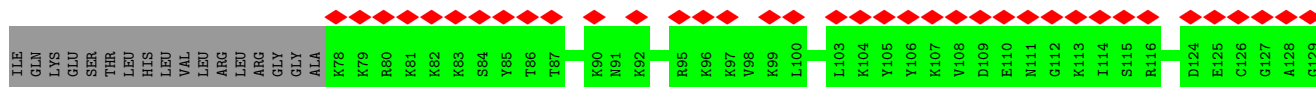
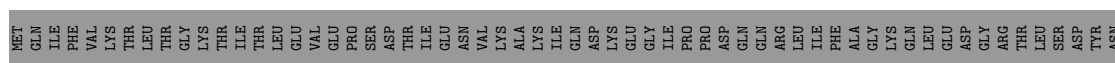
• Molecule 2: 40S ribosomal protein S27



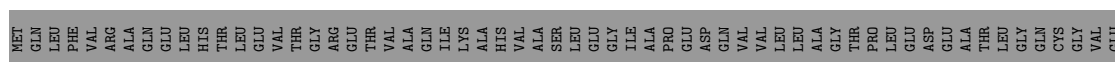
• Molecule 3: Ribosomal protein S28

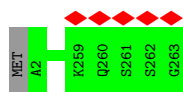


• Molecule 4: Ribosomal protein S27a

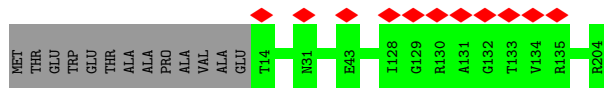


• Molecule 5: 40S ribosomal protein S30

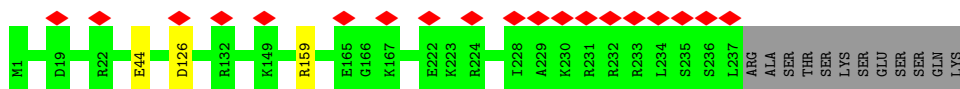




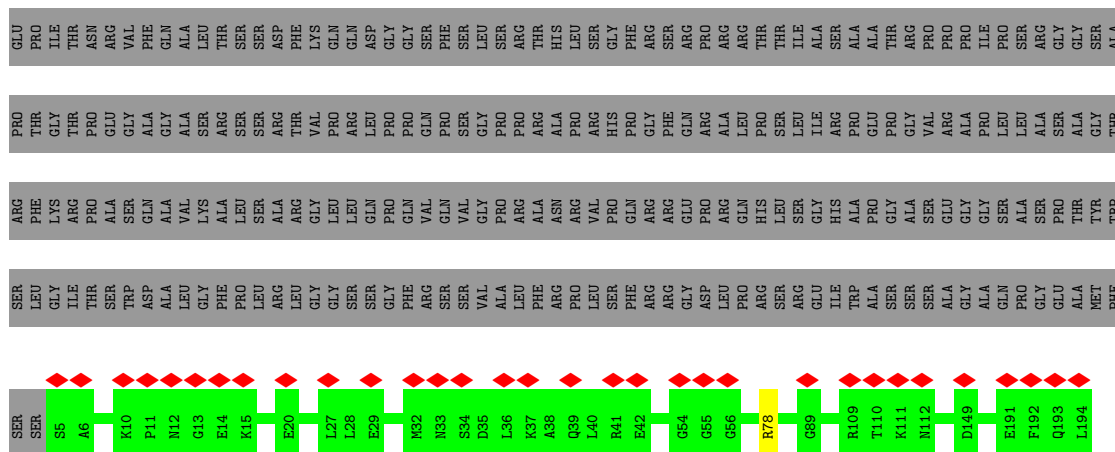
- Molecule 17: Ribosomal protein S5



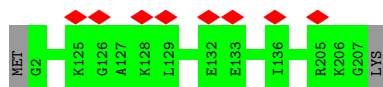
- Molecule 18: 40S ribosomal protein S6



- Molecule 19: 40S ribosomal protein S7

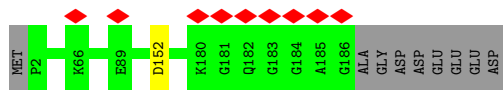


- Molecule 20: 40S ribosomal protein S8

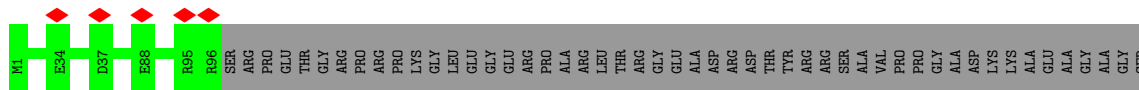


- Molecule 21: Ribosomal protein S9 (Predicted)

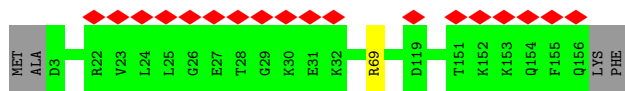




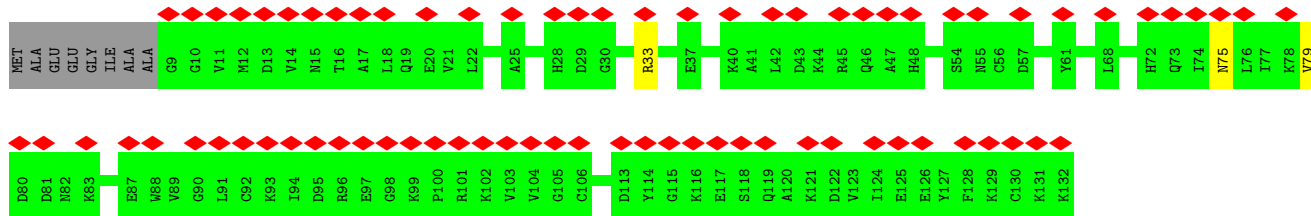
• Molecule 22: eS10



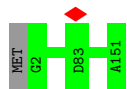
• Molecule 23: 40S ribosomal protein S11



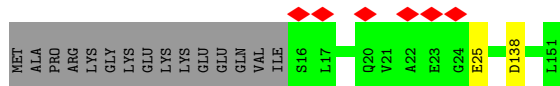
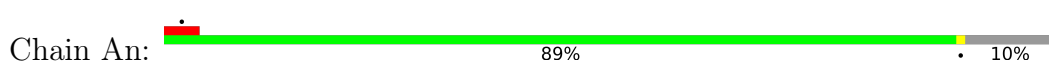
• Molecule 24: 40S ribosomal protein S12



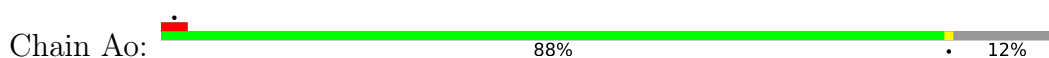
• Molecule 25: uS15

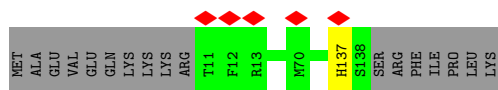


• Molecule 26: 40S ribosomal protein uS11

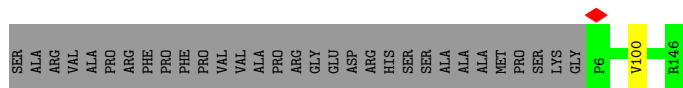
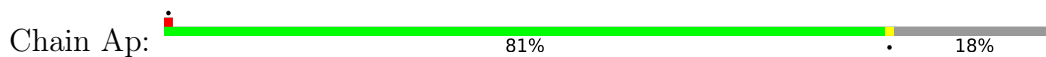


• Molecule 27: 40S ribosomal protein uS19

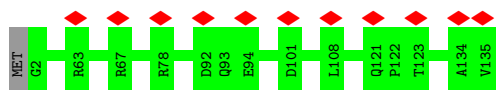




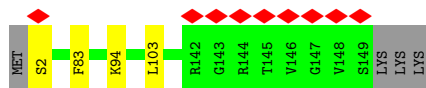
- Molecule 28: uS9



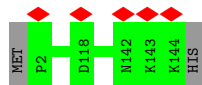
- Molecule 29: 40S ribosomal protein eS17



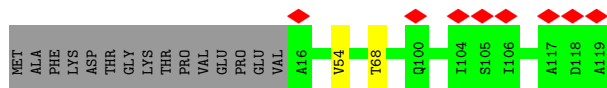
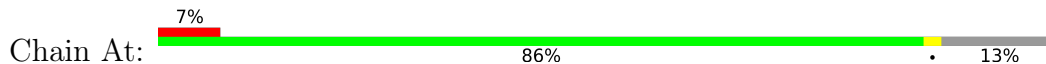
- Molecule 30: 40S ribosomal protein S18



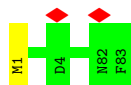
- Molecule 31: Ribosomal protein eS19



- Molecule 32: 40S ribosomal protein uS10



- Molecule 33: Ribosomal protein eS21



- Molecule 34: Ribosomal protein S15a

Chain Av:  99%



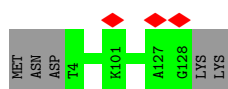
- Molecule 35: 40S ribosomal protein S23

Chain Aw:  97%



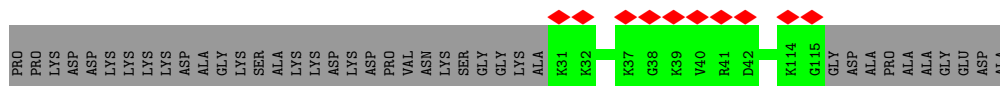
- Molecule 36: 40S ribosomal protein S24

Chain Ax:  96%



- Molecule 37: 40S ribosomal protein S25

Chain Ay:  8% 69% 31%



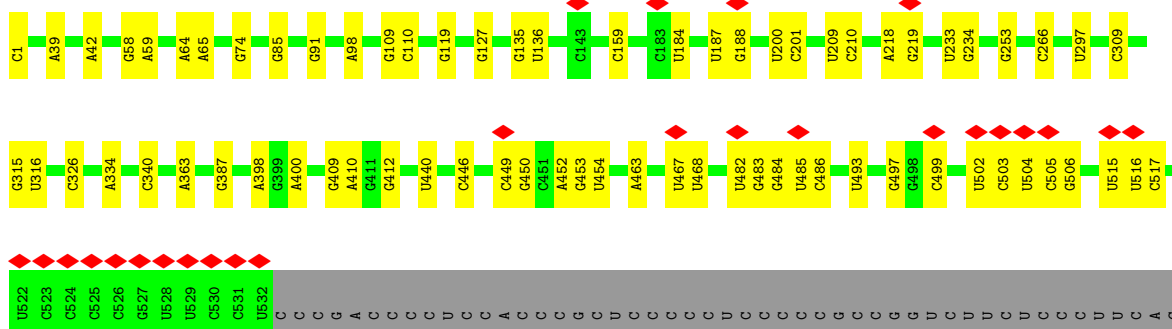
- Molecule 38: 60s ribosomal protein l41

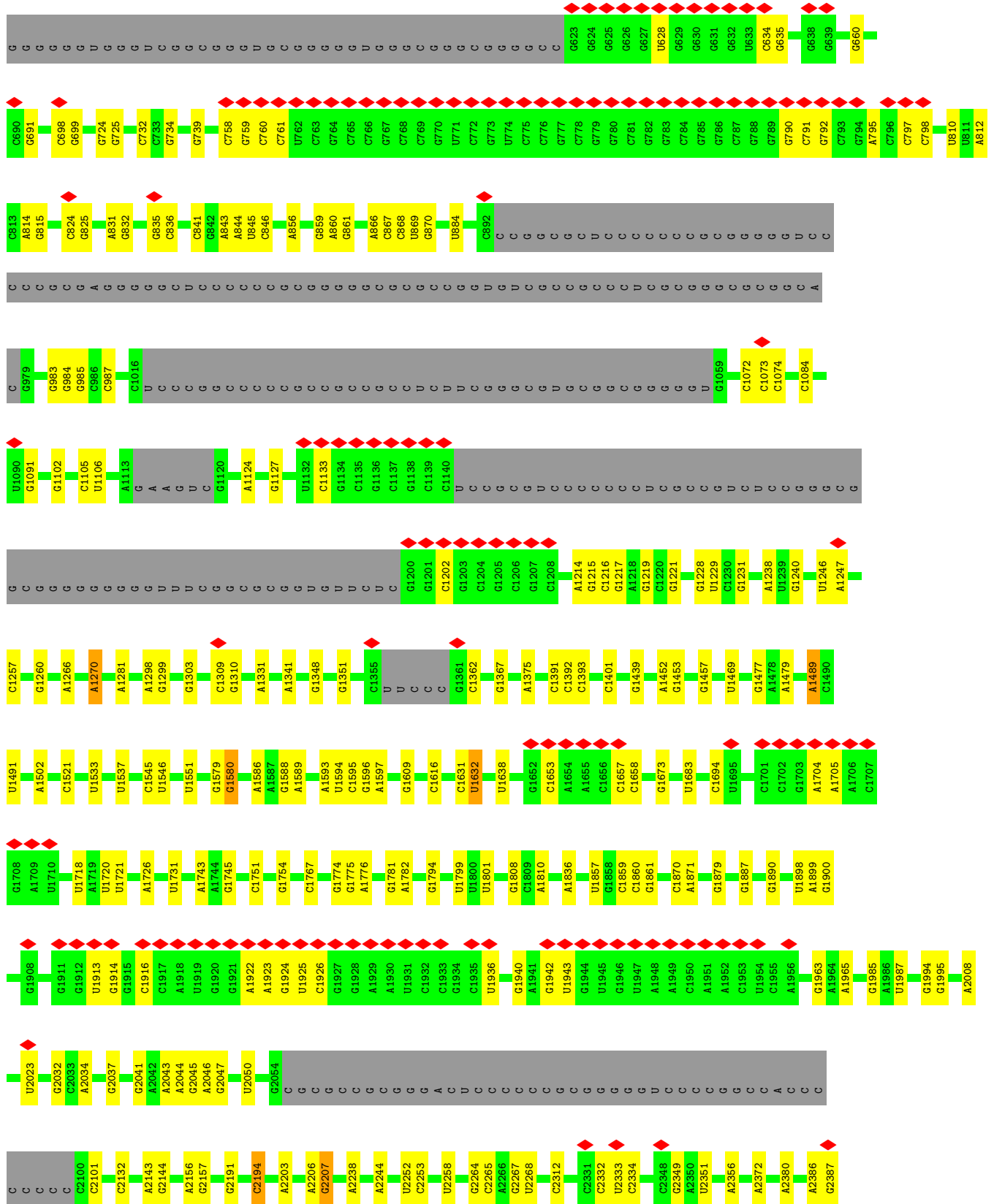
Chain Az:  100%

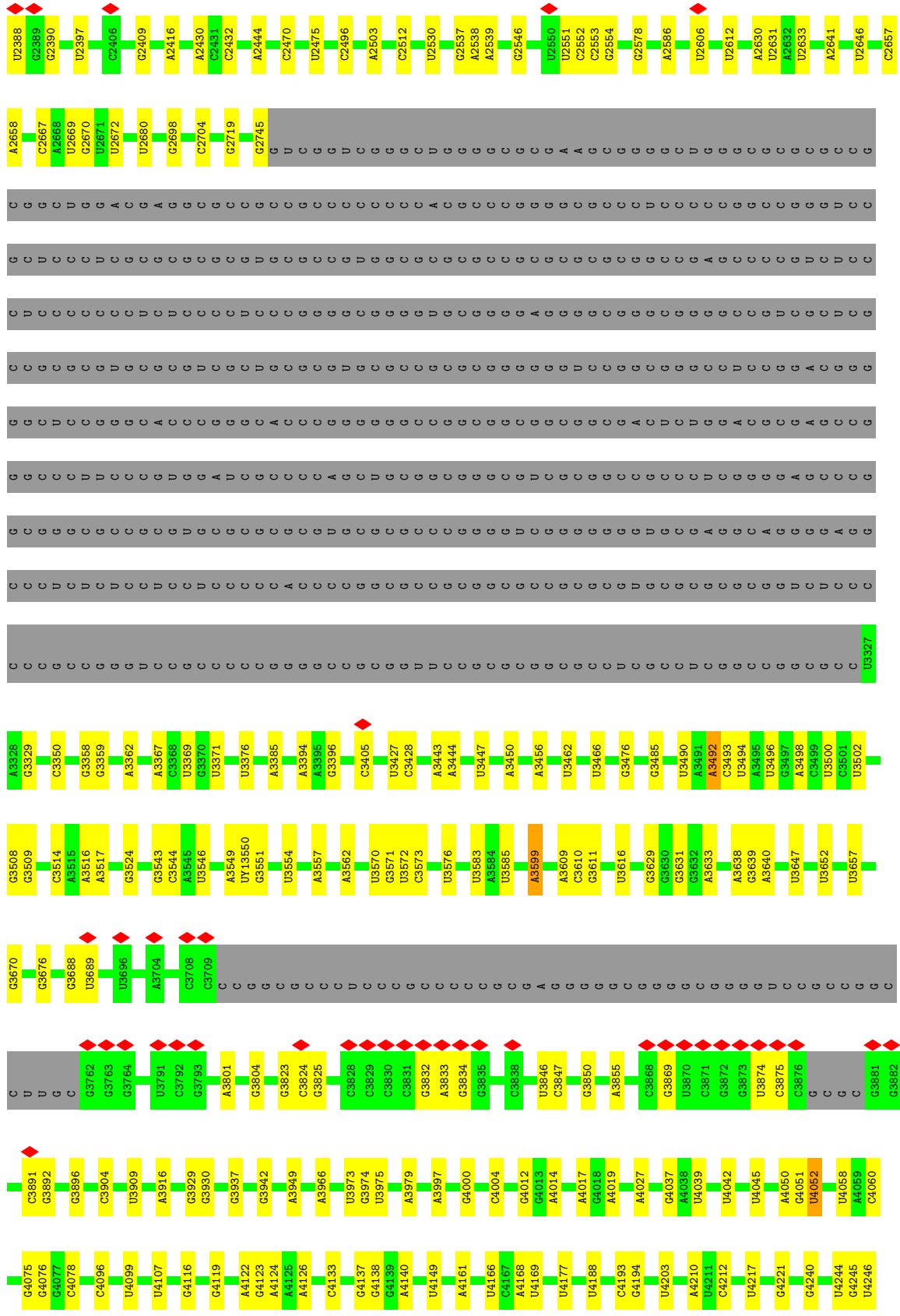
There are no outlier residues recorded for this chain.

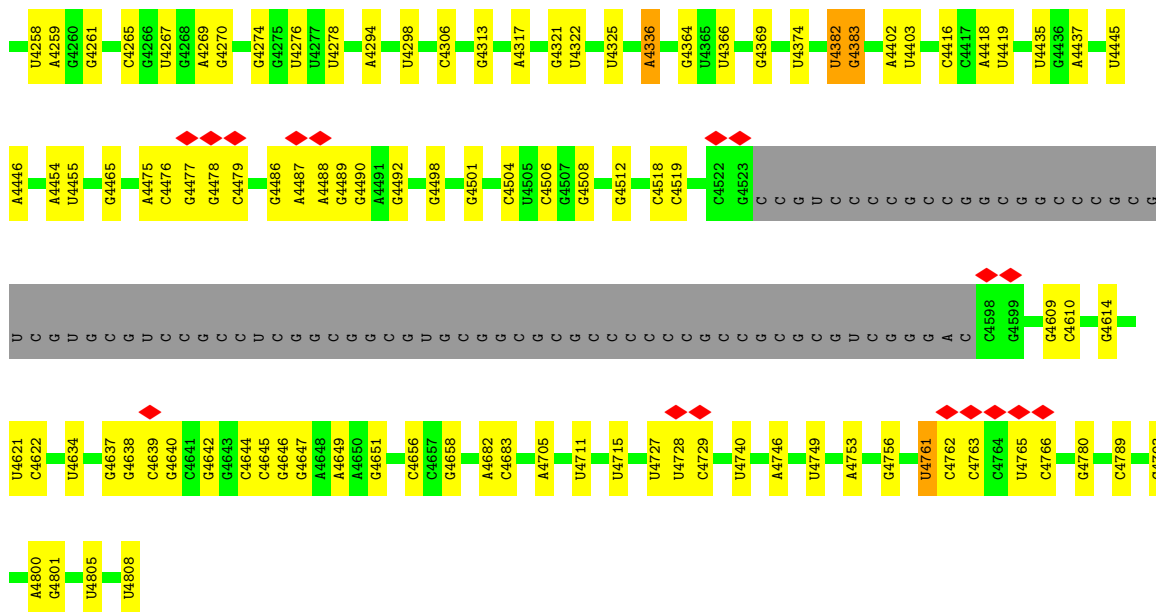
- Molecule 39: 28S rRNA

Chain B5:  5% 66% 12% 22%





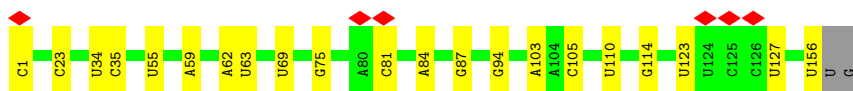
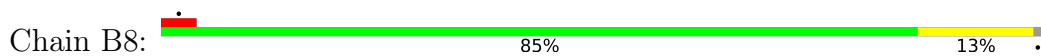




• Molecule 40: 5S



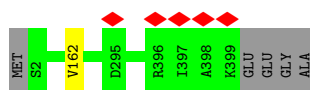
• Molecule 41: 5.8S rRNA



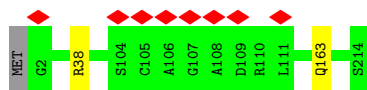
• Molecule 42: Ribosomal protein uL2



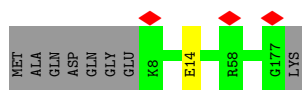
• Molecule 43: Ribosomal protein L3



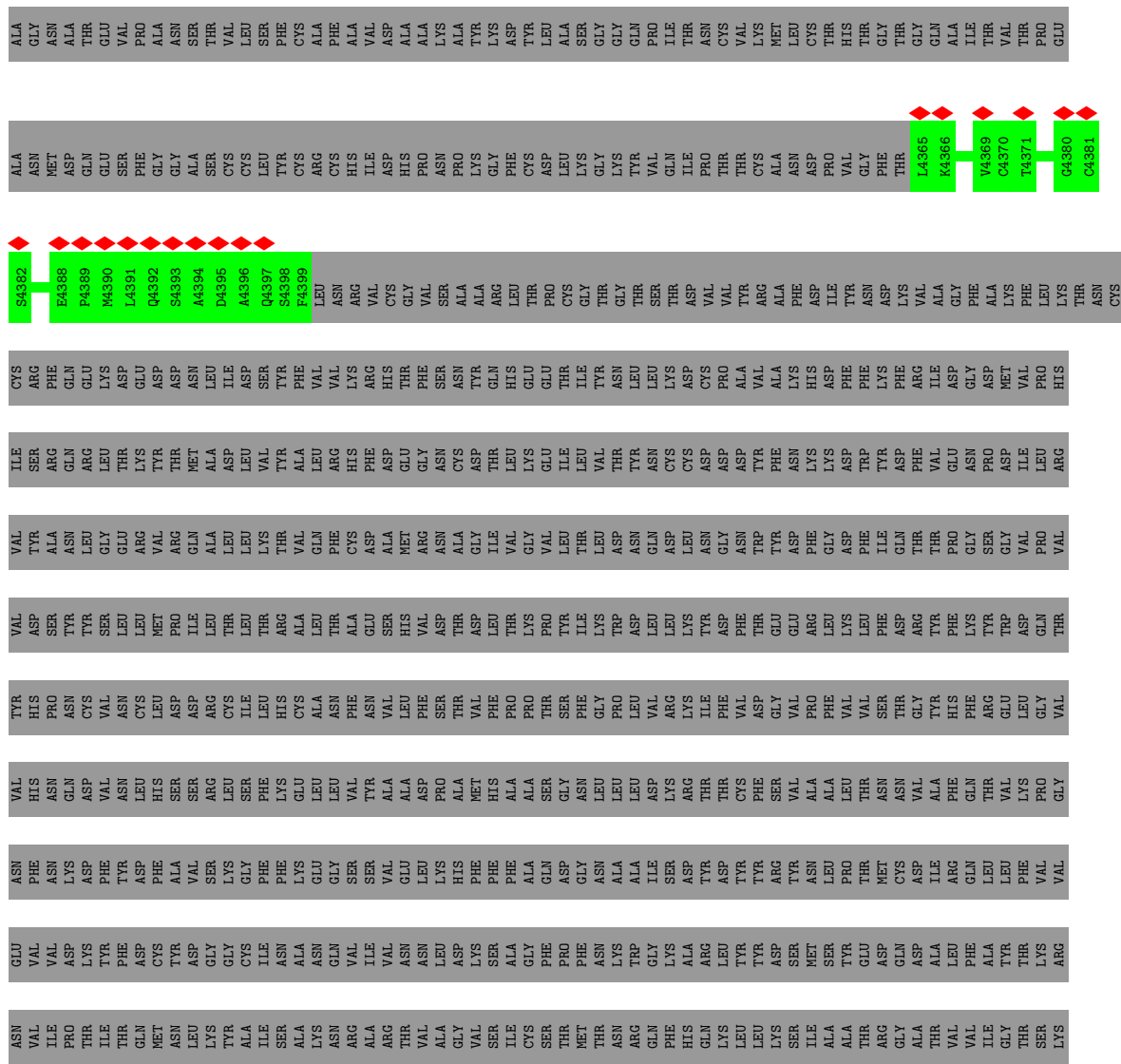
• Molecule 44: 60S ribosomal protein L4



- Molecule 51: Ribosomal protein L11

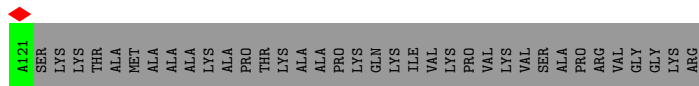


- Molecule 52: Replicase polyprotein 1ab

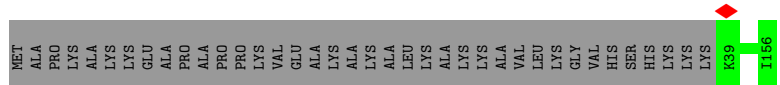
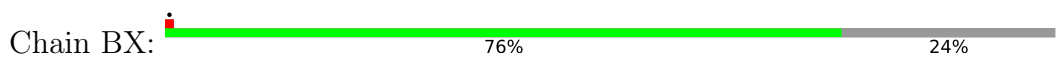



Highlighted residues in Chain BK:

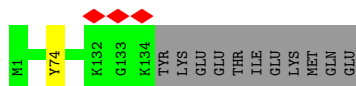
- S4382
- E4386
- M4389
- M4390
- L4391
- Q4392
- S4393
- A4394
- D4396
- A4396
- Q4397
- S4398
- F4399
- L4365
- K4366
- V4369
- C4370
- T4371
- G4380
- C4381



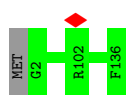
• Molecule 65: uL23



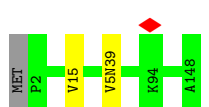
• Molecule 66: Ribosomal protein L26



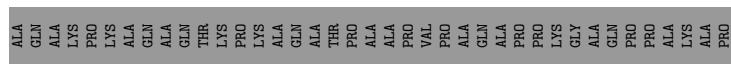
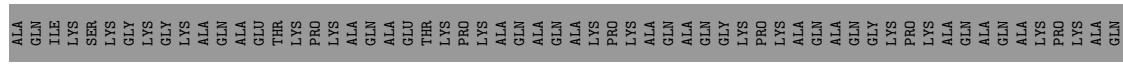
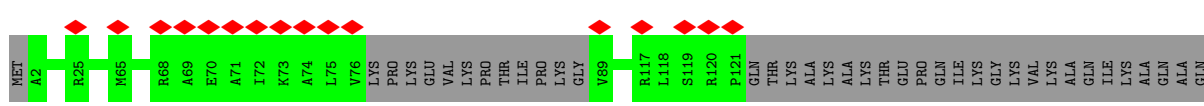
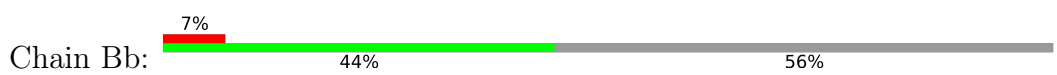
• Molecule 67: 60S ribosomal protein L27



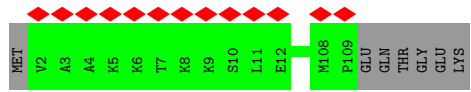
• Molecule 68: 60S ribosomal protein L27a



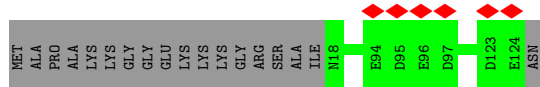
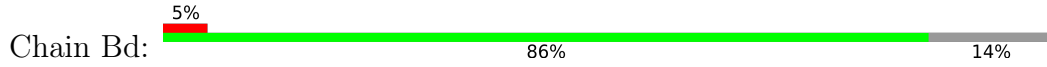
• Molecule 69: 60S ribosomal protein L29



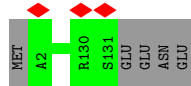
• Molecule 70: eL30



• Molecule 71: eL31



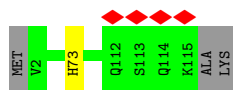
• Molecule 72: eL32



• Molecule 73: eL33



• Molecule 74: 60S ribosomal protein L34

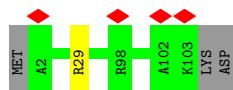


• Molecule 75: uL29

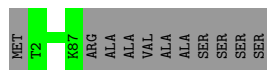
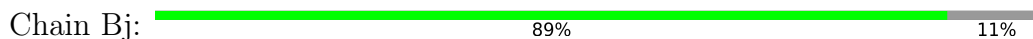


• Molecule 76: 60S ribosomal protein L36

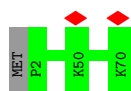




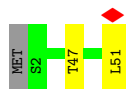
• Molecule 77: Ribosomal protein L37



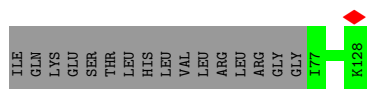
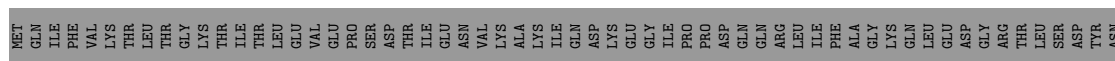
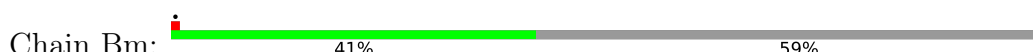
• Molecule 78: eL38



• Molecule 79: eL39



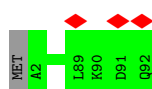
• Molecule 80: 60S ribosomal protein L40



• Molecule 81: eL42



• Molecule 82: eL43



MET	GLY	ASP	ILE	LEU	S6	R7	D8	T9	L10	Y11	E12	A13	V14	R15	E16	V17	L18	H19	G20	N21	Q22	R23	K24	R25	R26	K27	F28	L29	E30	T31	V32	E33	L34	Q35	I36	S37	L38	K39	M40	Y41	D42	K45	D46	K47	R48	F49	S50	G51	F110	T52	V53	R54	L55	K56	S57	T58	P59	R60	P61
K62	F63	S64	V65	C66	V67	L68	G69	D70	Q71	Q72	H73	C74	D75	E76	A77	K78	A79	V80	D81	I82	P83	H84	M85	D86	I87	E88	A89	L90	K91	K92	L93	N94	K95	N96	K97	K98	L99	V100	K101	K102	K103	A104	K105	K106	Y107	D108	A109	F110	L111	A112	S113	E114	S115	L116	I117	K118	Q119	I120	P121
R122	I123	L124	G125	P126	G127	L128	N129	K130	A131	G132	K133	F134	P135	S136	L137	L138	T139	H140	N141	E142	N143	M144	V145	A146	K147	V148	D149	E150	V151	K152	S153	T154	I155	K156	F157	Q158	M159	K160	K161	V162	L163	C164	L165	A166	V167	A168	V169	G170	H171	V172	K173	M174	T175	D176	D177	E178	L179	V180	Y181
N182	I183	H184	L185	A186	V187	N188	F189	L190	V191	S192	L193	L194	K195	K196	N197	W198	Q199	N200	V201	R202	A203	L204	Y205	I206	K207	S208	T209	M210	G211	K212	P213	Q214	R215	L216	Y217																								

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	171706	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	56604	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	45.454	Depositor
Minimum map value	-18.107	Depositor
Average map value	-0.006	Depositor
Map value standard deviation	0.952	Depositor
Recommended contour level	5.0	Depositor
Map size (\AA)	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	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: OMG, AYA, G7M, NMM, UY1, UNX, MG, V5N, 1MA, HIC, AAC, PSU, OMC, 5MC, SPM, AME, H2U, MA6, M3L, ZN, MLZ, 6MZ, GTP, SPD, UR3, B8N, A2M, 4AC, 5MU, M2G, HY3, 2MG, OMU, SAC, YYG

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	A2	0.22	1/40342 (0.0%)	0.70	11/62877 (0.0%)
2	AA	0.24	0/665	0.46	0/891
3	AB	0.25	0/497	0.56	0/666
4	AC	0.24	0/622	0.48	0/822
5	AD	0.25	0/462	0.53	0/607
6	AE	0.25	0/828	0.54	0/1109
7	AF	0.23	0/2493	0.46	0/3394
8	AG	0.24	0/470	0.52	0/623
9	AH	0.13	0/2253	0.69	3/3508 (0.1%)
10	AI	0.29	0/68	0.70	0/103
11	AT	0.36	1/1440 (0.1%)	0.68	0/2242
12	AZ	0.24	0/1771	0.47	0/2406
13	Aa	0.24	0/1841	0.46	0/2459
14	Ab	0.25	0/1742	0.46	0/2354
15	Ac	0.25	0/1779	0.49	0/2395
16	Ad	0.25	0/2118	0.51	0/2849
17	Ae	0.24	0/1531	0.48	0/2059
18	Af	0.24	0/1946	0.52	0/2590
19	Ag	0.25	0/1552	0.48	0/2079
20	Ah	0.24	0/1715	0.52	0/2287
21	Ai	0.24	0/1550	0.53	0/2069
22	Aj	0.24	0/834	0.43	0/1125
23	Ak	0.26	0/1284	0.51	0/1717
24	Al	0.22	0/968	0.42	0/1296
25	Am	0.23	0/1232	0.48	0/1656
26	An	0.25	0/1029	0.55	0/1380
27	Ao	0.25	0/1069	0.49	0/1429
28	Ap	0.24	0/1142	0.51	0/1528
29	Aq	0.23	0/1094	0.49	0/1469
30	Ar	0.24	0/1226	0.54	0/1643

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	As	0.23	0/1119	0.46	0/1498
32	At	0.23	0/831	0.52	0/1115
33	Au	0.25	0/636	0.49	0/852
34	Av	0.24	0/1051	0.49	0/1406
35	Aw	0.25	0/1107	0.51	0/1475
36	Ax	0.24	0/1032	0.51	0/1371
37	Ay	0.23	0/691	0.46	0/922
38	Az	0.22	0/240	0.66	0/305
39	B5	0.25	3/87403 (0.0%)	0.70	12/136359 (0.0%)
40	B7	0.24	0/2835	0.69	0/4418
41	B8	0.30	1/3635 (0.0%)	0.70	0/5661
42	BA	0.26	0/1965	0.55	0/2633
43	BB	0.25	0/3261	0.50	0/4364
44	BC	0.24	0/2932	0.51	0/3939
45	BD	0.25	0/2437	0.48	0/3264
46	BE	0.25	0/1998	0.50	0/2673
47	BF	0.25	0/1922	0.50	0/2563
48	BG	0.24	0/1908	0.48	0/2566
49	BH	0.24	0/1535	0.50	0/2063
50	BI	0.25	0/1756	0.51	0/2346
51	BJ	0.25	0/1385	0.51	0/1852
52	BK	0.25	0/269	0.46	0/361
53	BL	0.25	0/1733	0.54	0/2316
54	BM	0.24	0/1158	0.50	0/1547
55	BN	0.25	0/1746	0.55	0/2338
56	BO	0.25	0/1662	0.49	0/2222
57	BP	0.24	0/1317	0.49	0/1768
58	BQ	0.25	0/1539	0.56	0/2054
59	BR	0.23	0/1524	0.54	0/2013
60	BS	0.26	0/1497	0.53	0/2008
61	BT	0.26	0/1326	0.50	0/1770
62	BU	0.25	0/820	0.48	0/1100
63	BV	0.26	0/1048	0.53	0/1402
64	BW	0.25	0/1006	0.50	0/1334
65	BX	0.25	0/984	0.49	0/1323
66	BY	0.24	0/1132	0.52	0/1504
67	BZ	0.26	0/1130	0.49	0/1507
68	Ba	0.25	0/1179	0.50	0/1572
69	Bb	0.23	0/884	0.52	0/1169
70	Bc	0.24	0/847	0.44	0/1134
71	Bd	0.25	0/903	0.53	0/1216
72	Be	0.24	0/1088	0.53	0/1451
73	Bf	0.27	0/903	0.54	0/1208

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
74	Bg	0.25	0/916	0.55	0/1220
75	Bh	0.23	0/1021	0.49	0/1348
76	Bi	0.24	0/841	0.52	0/1112
77	Bj	0.25	0/720	0.56	0/952
78	Bk	0.25	0/575	0.45	0/761
79	Bl	0.23	0/459	0.50	0/608
80	Bm	0.23	0/426	0.51	0/564
81	Bo	0.26	0/866	0.52	0/1141
82	Bp	0.24	0/718	0.50	0/953
83	Br	0.24	0/1020	0.54	0/1366
84	Bs	0.24	0/1530	0.45	0/2064
85	Bt	0.23	0/1193	0.48	0/1609
86	Bv	0.23	0/1735	0.45	0/2328
All	All	0.24	6/236957 (0.0%)	0.63	26/347620 (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
81	Bo	0	1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4761	U	C4-O4	12.83	1.33	1.23
41	B8	1	C	OP3-P	-10.68	1.48	1.61
1	A2	1	U	OP3-P	-10.67	1.48	1.61
39	B5	1	C	OP3-P	-10.59	1.48	1.61
11	AT	1	G	OP3-P	-10.58	1.48	1.61

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	4761	U	N3-C4-C5	12.53	122.12	114.60
39	B5	4761	U	C2-N3-C4	-11.85	119.89	127.00
39	B5	4761	U	C5-C4-O4	-9.84	120.00	125.90
1	A2	1454	C	C2-N1-C1'	7.45	126.99	118.80
39	B5	4761	U	N1-C2-N3	7.12	119.17	114.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
81	Bo	53	MLZ	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	
2	AA	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
3	AB	61/69 (88%)	61 (100%)	0	0	100	100
4	AC	72/156 (46%)	70 (97%)	2 (3%)	0	100	100
5	AD	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
6	AE	99/115 (86%)	99 (100%)	0	0	100	100
7	AF	311/317 (98%)	302 (97%)	9 (3%)	0	100	100
8	AG	53/56 (95%)	53 (100%)	0	0	100	100
12	AZ	219/295 (74%)	214 (98%)	5 (2%)	0	100	100
13	Aa	220/264 (83%)	218 (99%)	2 (1%)	0	100	100
14	Ab	218/293 (74%)	217 (100%)	1 (0%)	0	100	100
15	Ac	223/281 (79%)	222 (100%)	1 (0%)	0	100	100
16	Ad	260/263 (99%)	257 (99%)	3 (1%)	0	100	100
17	Ae	189/204 (93%)	186 (98%)	3 (2%)	0	100	100
18	Af	235/249 (94%)	234 (100%)	1 (0%)	0	100	100
19	Ag	188/432 (44%)	186 (99%)	2 (1%)	0	100	100
20	Ah	204/208 (98%)	201 (98%)	3 (2%)	0	100	100
21	Ai	183/194 (94%)	180 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	Aj	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
23	Ak	152/158 (96%)	149 (98%)	3 (2%)	0	100	100
24	Al	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
25	Am	148/151 (98%)	148 (100%)	0	0	100	100
26	An	134/151 (89%)	131 (98%)	3 (2%)	0	100	100
27	Ao	126/145 (87%)	125 (99%)	0	1 (1%)	19	29
28	Ap	139/172 (81%)	135 (97%)	3 (2%)	1 (1%)	22	32
29	Aq	132/135 (98%)	132 (100%)	0	0	100	100
30	Ar	146/152 (96%)	143 (98%)	3 (2%)	0	100	100
31	As	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
32	At	102/119 (86%)	101 (99%)	1 (1%)	0	100	100
33	Au	81/83 (98%)	81 (100%)	0	0	100	100
34	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
35	Aw	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
36	Ax	123/130 (95%)	123 (100%)	0	0	100	100
37	Ay	83/124 (67%)	81 (98%)	2 (2%)	0	100	100
38	Az	23/25 (92%)	23 (100%)	0	0	100	100
42	BA	250/257 (97%)	242 (97%)	8 (3%)	0	100	100
43	BB	395/403 (98%)	391 (99%)	4 (1%)	0	100	100
44	BC	360/413 (87%)	356 (99%)	4 (1%)	0	100	100
45	BD	291/297 (98%)	289 (99%)	2 (1%)	0	100	100
46	BE	239/291 (82%)	233 (98%)	6 (2%)	0	100	100
47	BF	224/247 (91%)	218 (97%)	6 (3%)	0	100	100
48	BG	229/266 (86%)	228 (100%)	1 (0%)	0	100	100
49	BH	188/192 (98%)	188 (100%)	0	0	100	100
50	BI	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
51	BJ	168/178 (94%)	168 (100%)	0	0	100	100
52	BK	33/1071 (3%)	33 (100%)	0	0	100	100
53	BL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
54	BM	136/218 (62%)	134 (98%)	2 (2%)	0	100	100
55	BN	201/204 (98%)	197 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	BO	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
57	BP	157/184 (85%)	155 (99%)	2 (1%)	0	100	100
58	BQ	185/188 (98%)	182 (98%)	3 (2%)	0	100	100
59	BR	178/196 (91%)	178 (100%)	0	0	100	100
60	BS	174/176 (99%)	174 (100%)	0	0	100	100
61	BT	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
62	BU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
63	BV	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
64	BW	119/157 (76%)	119 (100%)	0	0	100	100
65	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
66	BY	132/145 (91%)	131 (99%)	1 (1%)	0	100	100
67	BZ	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
68	Ba	144/148 (97%)	138 (96%)	5 (4%)	1 (1%)	22	32
69	Bb	103/245 (42%)	99 (96%)	4 (4%)	0	100	100
70	Bc	106/115 (92%)	106 (100%)	0	0	100	100
71	Bd	105/125 (84%)	105 (100%)	0	0	100	100
72	Be	128/135 (95%)	128 (100%)	0	0	100	100
73	Bf	108/110 (98%)	108 (100%)	0	0	100	100
74	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
75	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
76	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
77	Bj	84/97 (87%)	84 (100%)	0	0	100	100
78	Bk	67/70 (96%)	67 (100%)	0	0	100	100
79	Bl	48/51 (94%)	48 (100%)	0	0	100	100
80	Bm	49/128 (38%)	49 (100%)	0	0	100	100
81	Bo	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
82	Bp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
83	Br	124/137 (90%)	122 (98%)	2 (2%)	0	100	100
84	Bs	194/318 (61%)	189 (97%)	5 (3%)	0	100	100
85	Bt	154/165 (93%)	152 (99%)	2 (1%)	0	100	100
86	Bv	210/217 (97%)	197 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	11943/14908 (80%)	11780 (99%)	160 (1%)	3 (0%)	100 100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	Ao	137	HIS
28	Ap	100	VAL
68	Ba	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
2	AA	75/76 (99%)	74 (99%)	1 (1%)	69 84
3	AB	56/62 (90%)	55 (98%)	1 (2%)	59 76
4	AC	67/140 (48%)	67 (100%)	0	100 100
5	AD	47/106 (44%)	46 (98%)	1 (2%)	53 72
6	AE	88/98 (90%)	87 (99%)	1 (1%)	73 87
7	AF	272/275 (99%)	268 (98%)	4 (2%)	65 80
8	AG	48/49 (98%)	48 (100%)	0	100 100
12	AZ	182/243 (75%)	177 (97%)	5 (3%)	44 65
13	Aa	203/231 (88%)	202 (100%)	1 (0%)	88 95
14	Ab	185/223 (83%)	182 (98%)	3 (2%)	62 79
15	Ac	189/232 (82%)	187 (99%)	2 (1%)	73 87
16	Ad	224/225 (100%)	224 (100%)	0	100 100
17	Ae	161/170 (95%)	161 (100%)	0	100 100
18	Af	207/218 (95%)	204 (99%)	3 (1%)	67 82
19	Ag	170/360 (47%)	169 (99%)	1 (1%)	86 94
20	Ah	178/180 (99%)	178 (100%)	0	100 100
21	Ai	161/168 (96%)	160 (99%)	1 (1%)	86 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	Aj	87/136 (64%)	87 (100%)	0	100	100
23	Ak	139/142 (98%)	138 (99%)	1 (1%)	84	92
24	Al	104/108 (96%)	101 (97%)	3 (3%)	42	62
25	Am	130/131 (99%)	130 (100%)	0	100	100
26	An	106/119 (89%)	104 (98%)	2 (2%)	57	75
27	Ao	114/130 (88%)	114 (100%)	0	100	100
28	Ap	117/140 (84%)	117 (100%)	0	100	100
29	Aq	120/121 (99%)	120 (100%)	0	100	100
30	Ar	127/131 (97%)	124 (98%)	3 (2%)	49	68
31	As	112/114 (98%)	112 (100%)	0	100	100
32	At	94/107 (88%)	92 (98%)	2 (2%)	53	72
33	Au	67/67 (100%)	67 (100%)	0	100	100
34	Av	112/113 (99%)	112 (100%)	0	100	100
35	Aw	112/114 (98%)	111 (99%)	1 (1%)	78	90
36	Ax	107/112 (96%)	107 (100%)	0	100	100
37	Ay	75/102 (74%)	75 (100%)	0	100	100
38	Az	24/24 (100%)	24 (100%)	0	100	100
42	BA	194/198 (98%)	193 (100%)	1 (0%)	88	95
43	BB	344/347 (99%)	343 (100%)	1 (0%)	92	97
44	BC	302/337 (90%)	301 (100%)	1 (0%)	92	97
45	BD	247/250 (99%)	247 (100%)	0	100	100
46	BE	216/251 (86%)	216 (100%)	0	100	100
47	BF	197/215 (92%)	197 (100%)	0	100	100
48	BG	199/223 (89%)	197 (99%)	2 (1%)	76	88
49	BH	169/171 (99%)	169 (100%)	0	100	100
50	BI	180/181 (99%)	178 (99%)	2 (1%)	73	87
51	BJ	143/149 (96%)	142 (99%)	1 (1%)	84	92
52	BK	30/936 (3%)	30 (100%)	0	100	100
53	BL	175/176 (99%)	172 (98%)	3 (2%)	60	78
54	BM	117/161 (73%)	117 (100%)	0	100	100
55	BN	171/172 (99%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	BO	171/173 (99%)	171 (100%)	0	100	100
57	BP	140/163 (86%)	140 (100%)	0	100	100
58	BQ	164/165 (99%)	163 (99%)	1 (1%)	86	94
59	BR	159/175 (91%)	158 (99%)	1 (1%)	86	94
60	BS	154/154 (100%)	154 (100%)	0	100	100
61	BT	139/140 (99%)	139 (100%)	0	100	100
62	BU	88/113 (78%)	88 (100%)	0	100	100
63	BV	106/107 (99%)	106 (100%)	0	100	100
64	BW	100/126 (79%)	99 (99%)	1 (1%)	76	88
65	BX	106/134 (79%)	106 (100%)	0	100	100
66	BY	124/135 (92%)	123 (99%)	1 (1%)	81	91
67	BZ	117/118 (99%)	117 (100%)	0	100	100
68	Ba	118/119 (99%)	118 (100%)	0	100	100
69	Bb	87/183 (48%)	87 (100%)	0	100	100
70	Bc	92/98 (94%)	92 (100%)	0	100	100
71	Bd	98/110 (89%)	98 (100%)	0	100	100
72	Be	116/121 (96%)	116 (100%)	0	100	100
73	Bf	89/89 (100%)	89 (100%)	0	100	100
74	Bg	98/100 (98%)	97 (99%)	1 (1%)	76	88
75	Bh	109/110 (99%)	109 (100%)	0	100	100
76	Bi	86/89 (97%)	85 (99%)	1 (1%)	71	85
77	Bj	73/80 (91%)	73 (100%)	0	100	100
78	Bk	64/65 (98%)	64 (100%)	0	100	100
79	Bl	47/48 (98%)	45 (96%)	2 (4%)	29	46
80	Bm	47/115 (41%)	47 (100%)	0	100	100
81	Bo	92/93 (99%)	92 (100%)	0	100	100
82	Bp	74/75 (99%)	74 (100%)	0	100	100
83	Br	109/120 (91%)	109 (100%)	0	100	100
84	Bs	164/258 (64%)	164 (100%)	0	100	100
85	Bt	128/137 (93%)	127 (99%)	1 (1%)	81	91
86	Bv	191/195 (98%)	185 (97%)	6 (3%)	40	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	10394/12642 (82%)	10332 (99%)	62 (1%)	86 94

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	An	25	GLU
85	Bt	74	VAL
35	Aw	105	PHE
79	Bl	51	LEU
86	Bv	96	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
84	Bs	34	ASN
84	Bs	179	ASN
28	Ap	114	GLN
28	Ap	97	GLN
84	Bs	191	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1758/1870 (94%)	225 (12%)	0
10	AI	2/76 (2%)	1 (50%)	0
11	AT	75/76 (98%)	10 (13%)	0
39	B5	3750/4808 (77%)	489 (13%)	3 (0%)
40	B7	118/120 (98%)	8 (6%)	0
41	B8	155/158 (98%)	17 (10%)	0
9	AH	94/220 (42%)	29 (30%)	0
All	All	5952/7328 (81%)	779 (13%)	3 (0%)

5 of 779 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	3	C
1	A2	4	C
1	A2	33	G
1	A2	41	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
39	B5	1545	C
39	B5	1588	G
39	B5	4445	U

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

239 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
39	PSU	B5	4045	39	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
41	OMG	B8	75	41	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	A2	967	1	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	4138	39	18,26,27	0.91	1 (5%)	19,38,41	1.09	2 (10%)
39	A2M	B5	1810	89,39	18,25,26	1.01	1 (5%)	18,36,39	1.34	2 (11%)
39	PSU	B5	4267	89,39	18,21,22	1.37	2 (11%)	22,30,33	1.89	5 (22%)
39	OMC	B5	3619	39	19,22,23	0.81	0	26,31,34	0.84	0
39	PSU	B5	1491	39	18,21,22	1.37	2 (11%)	22,30,33	1.93	4 (18%)
1	A2M	A2	669	1,89	18,25,26	0.93	1 (5%)	18,36,39	1.34	2 (11%)
1	PSU	A2	1178	1	18,21,22	1.36	2 (11%)	22,30,33	1.94	3 (13%)
39	PSU	B5	1683	39	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	A2	34	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
1	OMG	A2	1491	1,89	18,26,27	0.90	1 (5%)	19,38,41	1.17	3 (15%)
11	5MC	AT	49	11	18,22,23	0.95	2 (11%)	26,32,35	1.13	2 (7%)
1	PSU	A2	1082	1	18,21,22	1.39	3 (16%)	22,30,33	1.85	3 (13%)
39	PSU	B5	1537	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	3447	39	18,21,22	1.36	2 (11%)	22,30,33	1.92	3 (13%)
1	OMU	A2	1443	1,89	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
39	PSU	B5	3616	39	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
39	A2M	B5	2206	89,39	18,25,26	0.99	1 (5%)	18,36,39	1.19	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	A2	1327	1,89	19,22,23	1.19	2 (10%)	26,31,34	1.71	5 (19%)
1	PSU	A2	1626	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
39	UR3	B5	4276	39	19,22,23	0.99	1 (5%)	26,32,35	1.42	1 (3%)
11	YYG	AT	37	11	31,42,43	1.68	4 (12%)	33,62,65	2.12	10 (30%)
1	A2M	A2	1032	1	18,25,26	0.97	1 (5%)	18,36,39	1.27	2 (11%)
39	PSU	B5	3496	39	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
39	A2M	B5	4336	39	18,25,26	1.03	1 (5%)	18,36,39	1.25	2 (11%)
39	PSU	B5	4749	39	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
11	G7M	AT	46	11	20,26,27	2.63	4 (20%)	17,39,42	0.95	1 (5%)
1	OMG	A2	1329	1	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
1	PSU	A2	1057	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
39	OMU	B5	2680	39	19,22,23	1.22	2 (10%)	26,31,34	1.74	5 (19%)
11	H2U	AT	16	11	18,21,22	0.99	2 (11%)	21,30,33	1.38	2 (9%)
1	OMG	A2	684	1	18,26,27	0.92	1 (5%)	19,38,41	1.12	2 (10%)
39	PSU	B5	3494	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
39	5MC	B5	4193	39	18,22,23	1.00	2 (11%)	26,32,35	1.24	2 (7%)
11	PSU	AT	28	11	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)
39	PSU	B5	3652	89,39	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
11	PSU	AT	27	11	18,21,22	1.35	2 (11%)	22,30,33	1.92	3 (13%)
39	OMC	B5	2194	89,39	19,22,23	0.81	0	26,31,34	0.94	2 (7%)
39	OMG	B5	3631	39	18,26,27	0.92	1 (5%)	19,38,41	1.13	2 (10%)
39	OMG	B5	3974	39	18,26,27	0.89	1 (5%)	19,38,41	1.13	2 (10%)
39	OMC	B5	3433	39	19,22,23	0.79	0	26,31,34	0.76	0
39	PSU	B5	4169	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	OMG	B5	4245	39	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
39	A2M	B5	1270	39	18,25,26	0.94	1 (5%)	18,36,39	1.26	2 (11%)
39	OMG	B5	3476	39	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
1	OMU	A2	1805	1	19,22,23	1.23	3 (15%)	26,31,34	1.71	4 (15%)
35	HY3	Aw	62	35	6,8,9	1.90	1 (16%)	5,10,12	1.13	1 (20%)
39	PSU	B5	3466	39	18,21,22	1.35	2 (11%)	22,30,33	1.91	4 (18%)
39	A2M	B5	4269	89,39	18,25,26	1.01	1 (5%)	18,36,39	1.28	2 (11%)
11	H2U	AT	17	11	18,21,22	1.00	2 (11%)	21,30,33	1.72	2 (9%)
1	MA6	A2	1851	1	19,26,27	0.92	1 (5%)	18,38,41	1.53	3 (16%)
39	OMC	B5	2265	89,39	19,22,23	0.82	0	26,31,34	0.86	1 (3%)
1	OMU	A2	355	1	19,22,23	1.24	3 (15%)	26,31,34	1.74	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	A2	27	1,89	18,25,26	1.00	1 (5%)	18,36,39	1.22	2 (11%)
1	PSU	A2	210	1	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	573	1	18,21,22	1.33	2 (11%)	22,30,33	1.91	4 (18%)
1	PSU	A2	687	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
39	PSU	B5	4177	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	5MC	B5	3514	89,39	18,22,23	0.94	2 (11%)	26,32,35	1.18	3 (11%)
39	OMU	B5	4366	39	19,22,23	1.23	3 (15%)	26,31,34	1.71	4 (15%)
1	MA6	A2	1852	1	19,26,27	0.94	1 (5%)	18,38,41	1.45	3 (16%)
11	2MG	AT	10	11	18,26,27	0.90	1 (5%)	16,38,41	1.10	2 (12%)
1	PSU	A2	652	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
1	OMC	A2	1392	1	19,22,23	0.84	0	26,31,34	0.95	1 (3%)
39	PSU	B5	4149	39	18,21,22	1.36	2 (11%)	22,30,33	1.94	4 (18%)
1	B8N	A2	1249	1	24,29,30	1.29	3 (12%)	29,42,45	1.26	3 (10%)
39	OMG	B5	4369	39	18,26,27	0.94	1 (5%)	19,38,41	1.13	2 (10%)
39	PSU	B5	1801	39	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
39	OMG	B5	4240	39	18,26,27	0.92	1 (5%)	19,38,41	1.07	2 (10%)
39	PSU	B5	4374	39	18,21,22	1.37	2 (11%)	22,30,33	1.93	3 (13%)
39	PSU	B5	3502	39	18,21,22	1.37	2 (11%)	22,30,33	1.95	4 (18%)
1	PSU	A2	1047	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	OMG	A2	510	1,89	18,26,27	0.93	1 (5%)	19,38,41	1.08	2 (10%)
39	PSU	B5	4278	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	OMU	B5	2258	39	19,22,23	1.22	2 (10%)	26,31,34	1.68	4 (15%)
39	OMU	B5	4244	39	19,22,23	1.21	2 (10%)	26,31,34	1.70	4 (15%)
1	PSU	A2	109	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	A2M	B5	1479	39	18,25,26	0.98	1 (5%)	18,36,39	1.27	2 (11%)
1	A2M	A2	99	1,89	18,25,26	1.02	1 (5%)	18,36,39	1.26	2 (11%)
39	PSU	B5	4099	39	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
39	PSU	B5	1799	39	18,21,22	1.38	2 (11%)	22,30,33	1.90	3 (13%)
39	A2M	B5	3450	39	18,25,26	1.00	1 (5%)	18,36,39	1.19	2 (11%)
39	OMG	B5	2719	39	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
39	OMC	B5	4282	89,39	19,22,23	0.82	0	26,31,34	0.83	0
39	PSU	B5	4419	39	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
39	A2M	B5	3599	39	18,25,26	0.96	1 (5%)	18,36,39	1.23	2 (11%)
1	A2M	A2	485	1	18,25,26	0.98	1 (5%)	18,36,39	1.27	2 (11%)
1	OMC	A2	1704	1	19,22,23	0.81	0	26,31,34	0.83	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	PSU	B5	3427	39	18,21,22	1.34	2 (11%)	22,30,33	1.92	3 (13%)
39	A2M	B5	4317	39	18,25,26	1.01	1 (5%)	18,36,39	1.23	2 (11%)
1	OMC	A2	518	1	19,22,23	0.81	0	26,31,34	0.80	0
39	PSU	B5	2351	39	18,21,22	1.36	2 (11%)	22,30,33	1.92	4 (18%)
1	PSU	A2	218	1	18,21,22	1.35	2 (11%)	22,30,33	1.91	3 (13%)
11	5MU	AT	54	11	19,22,23	1.41	6 (31%)	28,32,35	2.05	7 (25%)
1	A2M	A2	166	1	18,25,26	1.04	1 (5%)	18,36,39	1.27	2 (11%)
39	PSU	B5	3554	39	18,21,22	1.36	2 (11%)	22,30,33	1.86	3 (13%)
1	PSU	A2	1693	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	4 (18%)
1	A2M	A2	591	1	18,25,26	1.03	1 (5%)	18,36,39	1.19	2 (11%)
39	OMC	B5	1820	89,39	19,22,23	0.81	0	26,31,34	0.84	0
39	PSU	B5	3500	39	18,21,22	1.37	2 (11%)	22,30,33	1.91	3 (13%)
11	PSU	AT	39	11	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	A2	650	1	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
1	OMU	A2	116	1	19,22,23	1.21	3 (15%)	26,31,34	1.69	5 (19%)
39	PSU	B5	4322	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
44	AYA	BC	2	44	6,7,8	0.75	0	5,8,10	0.24	0
1	OMG	A2	602	1	18,26,27	0.94	1 (5%)	19,38,41	1.07	2 (10%)
1	A2M	A2	1384	1	18,25,26	1.03	1 (5%)	18,36,39	1.23	2 (11%)
39	PSU	B5	1720	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
80	M3L	Bm	98	80	10,11,12	0.82	0	9,14,16	0.50	0
11	PSU	AT	55	11	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
1	OMU	A2	172	1	19,22,23	1.20	3 (15%)	26,31,34	1.72	4 (15%)
39	OMG	B5	3942	11,39	18,26,27	0.94	1 (5%)	19,38,41	1.10	2 (10%)
1	OMU	A2	121	1	19,22,23	1.22	3 (15%)	26,31,34	1.69	4 (15%)
39	PSU	B5	3371	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4711	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
39	A2M	B5	3492	1,39	18,25,26	1.01	1 (5%)	18,36,39	1.28	2 (11%)
41	PSU	B8	69	41	18,21,22	1.38	2 (11%)	22,30,33	1.93	4 (18%)
39	A2M	B5	2244	89,39	18,25,26	0.99	1 (5%)	18,36,39	1.24	2 (11%)
39	PSU	B5	3462	39	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
39	PSU	B5	4058	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
11	OMC	AT	32	11	19,22,23	0.81	0	26,31,34	0.80	0
1	PSU	A2	407	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
39	OMG	B5	1580	39	18,26,27	0.94	1 (5%)	19,38,41	1.08	2 (10%)
39	OMG	B5	2207	39	18,26,27	0.92	1 (5%)	19,38,41	1.08	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	A2M	B5	3517	39	18,25,26	0.93	1 (5%)	18,36,39	1.37	2 (11%)
39	PSU	B5	4039	39	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4107	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	3 (13%)
39	OMG	B5	4116	39	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
39	PSU	B5	4203	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4298	39	18,21,22	1.37	2 (11%)	22,30,33	1.94	4 (18%)
31	NMM	As	67	31	9,11,12	0.59	0	6,12,14	0.46	0
39	A2M	B5	1489	89,39	18,25,26	1.00	1 (5%)	18,36,39	1.37	2 (11%)
39	A2M	B5	3557	39	18,25,26	1.00	1 (5%)	18,36,39	1.23	2 (11%)
1	PSU	A2	1245	1	18,21,22	1.34	2 (11%)	22,30,33	1.88	3 (13%)
1	G7M	A2	1640	1,11	20,26,27	2.64	4 (20%)	17,39,42	0.91	1 (5%)
81	MLZ	B ₀	53	81	8,9,10	0.48	0	4,9,11	0.10	0
39	OMC	B5	2667	39	19,22,23	0.81	0	26,31,34	0.82	1 (3%)
39	PSU	B5	4188	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
1	4AC	A2	1338	1	21,24,25	1.09	2 (9%)	29,34,37	1.31	3 (10%)
39	PSU	B5	1731	39	18,21,22	1.35	2 (11%)	22,30,33	1.85	4 (18%)
1	OMC	A2	174	1,89	19,22,23	0.80	0	26,31,34	0.78	0
39	PSU	B5	4325	39	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
42	V5N	BA	216	42	4,11,12	0.77	0	5,14,16	1.55	1 (20%)
39	OMG	B5	2267	39	18,26,27	0.94	1 (5%)	19,38,41	1.03	2 (10%)
39	PSU	B5	3576	39	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
1	PSU	A2	1644	1,89	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
11	M2G	AT	26	11	20,27,28	1.40	3 (15%)	22,40,43	0.98	2 (9%)
1	PSU	A2	1368	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	3 (13%)
1	PSU	A2	1233	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)
1	OMG	A2	437	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
1	PSU	A2	1348	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
39	A2M	B5	400	39	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
39	A2M	B5	2630	89,39	18,25,26	0.97	1 (5%)	18,36,39	1.27	2 (11%)
1	OMG	A2	1448	1	18,26,27	0.94	1 (5%)	19,38,41	1.09	2 (10%)
39	OMG	B5	3676	39	18,26,27	0.93	1 (5%)	19,38,41	1.11	2 (10%)
1	PSU	A2	1175	1	18,21,22	1.36	2 (11%)	22,30,33	1.88	3 (13%)
39	A2M	B5	398	39	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
1	PSU	A2	36	1	18,21,22	1.35	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	4042	39	18,21,22	1.35	2 (11%)	22,30,33	1.93	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
68	V5N	Ba	39	68	4,11,12	0.76	0	5,14,16	1.56	1 (20%)
1	PSU	A2	815	1	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	4AC	A2	1843	1	21,24,25	1.01	1 (4%)	29,34,37	1.04	3 (10%)
1	PSU	A2	119	1	18,21,22	1.35	2 (11%)	22,30,33	1.86	3 (13%)
1	A2M	A2	577	1	18,25,26	1.00	1 (5%)	18,36,39	1.24	2 (11%)
39	6MZ	B5	3966	39	18,25,26	0.86	1 (5%)	16,36,39	2.01	4 (25%)
40	GTP	B7	1	40	26,34,34	0.94	2 (7%)	32,54,54	0.80	0
39	PSU	B5	1718	39	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
11	OMG	AT	34	11,9	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
39	PSU	B5	4217	39	18,21,22	1.39	2 (11%)	22,30,33	1.87	3 (13%)
39	OMU	B5	4052	39	19,22,23	1.23	3 (15%)	26,31,34	1.71	5 (19%)
39	OMG	B5	1260	39	18,26,27	0.94	1 (5%)	19,38,41	1.17	2 (10%)
1	PSU	A2	864	1	18,21,22	1.36	2 (11%)	22,30,33	1.91	3 (13%)
39	OMG	B5	3524	39	18,26,27	0.90	1 (5%)	19,38,41	1.06	2 (10%)
39	PSU	B5	4246	39	18,21,22	1.35	2 (11%)	22,30,33	1.93	3 (13%)
39	PSU	B5	4435	39	18,21,22	1.38	2 (11%)	22,30,33	1.91	3 (13%)
39	OMG	B5	3359	39	18,26,27	0.94	1 (5%)	19,38,41	1.11	2 (10%)
12	SAC	AZ	2	12	7,8,9	0.52	0	8,9,11	0.86	1 (12%)
39	OMC	B5	4202	39	19,22,23	0.81	0	26,31,34	0.80	0
1	OMU	A2	1289	1	19,22,23	1.24	3 (15%)	26,31,34	1.69	5 (19%)
1	PSU	A2	1046	1	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)
39	1MA	B5	1266	89,39	16,25,26	1.52	2 (12%)	18,37,40	1.06	3 (16%)
39	PSU	B5	2475	39	18,21,22	1.36	2 (11%)	22,30,33	1.87	3 (13%)
39	A2M	B5	3456	39	18,25,26	1.02	1 (5%)	18,36,39	1.25	2 (11%)
43	HIC	BB	245	43	8,11,12	0.85	0	6,14,16	0.82	0
39	A2M	B5	3562	39	18,25,26	1.01	1 (5%)	18,36,39	1.27	2 (11%)
39	OMG	B5	4364	39	18,26,27	0.92	1 (5%)	19,38,41	1.10	2 (10%)
39	PSU	B5	3583	39	18,21,22	1.38	2 (11%)	22,30,33	1.93	3 (13%)
11	1MA	AT	14	11	16,25,26	1.56	2 (12%)	18,37,40	1.03	3 (16%)
1	PSU	A2	93	1	18,21,22	1.37	2 (11%)	22,30,33	1.90	3 (13%)
39	OMC	B5	3540	39	19,22,23	0.79	0	26,31,34	0.77	0
1	PSU	A2	867	1	18,21,22	1.35	2 (11%)	22,30,33	1.92	4 (18%)
39	OMC	B5	1284	39	19,22,23	0.80	0	26,31,34	0.77	0
39	OMC	B5	3601	39	19,22,23	0.81	0	26,31,34	0.80	0
1	PSU	A2	1446	1	18,21,22	1.35	2 (11%)	22,30,33	1.90	3 (13%)
39	OMG	B5	4383	39	18,26,27	0.95	1 (5%)	19,38,41	1.10	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	A2	159	1	18,25,26	1.00	1 (5%)	18,36,39	1.25	2 (11%)
41	PSU	B8	55	41	18,21,22	1.36	2 (11%)	22,30,33	1.93	4 (18%)
39	OMC	B5	2208	89,39	19,22,23	0.79	0	26,31,34	0.78	0
1	OMC	A2	463	1	19,22,23	0.81	0	26,31,34	0.81	0
1	A2M	A2	1679	1	18,25,26	1.01	1 (5%)	18,36,39	1.25	2 (11%)
39	OMG	B5	1477	39	18,26,27	0.92	1 (5%)	19,38,41	1.09	2 (10%)
39	PSU	B5	3585	89,39	18,21,22	1.39	2 (11%)	22,30,33	1.89	3 (13%)
30	SAC	Ar	2	30	7,8,9	0.53	0	8,9,11	0.89	1 (12%)
39	OMC	B5	3573	39	19,22,23	0.81	0	26,31,34	0.87	1 (3%)
1	A2M	A2	469	1	18,25,26	1.03	1 (5%)	18,36,39	1.30	2 (11%)
11	1MA	AT	58	11	16,25,26	1.58	2 (12%)	18,37,40	1.05	2 (11%)
39	PSU	B5	4740	39	18,21,22	1.36	2 (11%)	22,30,33	1.89	3 (13%)
1	A2M	A2	513	1	18,25,26	1.02	1 (5%)	18,36,39	1.23	2 (11%)
39	PSU	B5	3490	39	18,21,22	1.36	2 (11%)	22,30,33	1.88	4 (18%)
39	PSU	B5	1721	39	18,21,22	1.36	2 (11%)	22,30,33	1.91	4 (18%)
39	UY1	B5	3550	39	19,22,23	1.31	3 (15%)	22,31,34	2.02	5 (22%)
1	OMU	A2	429	1	19,22,23	1.19	2 (10%)	26,31,34	1.69	5 (19%)
1	PSU	A2	105	1	18,21,22	1.37	2 (11%)	22,30,33	1.92	3 (13%)
39	PSU	B5	4382	39	18,21,22	1.37	2 (11%)	22,30,33	1.89	4 (18%)
33	AME	Au	1	33	9,10,11	0.47	0	9,11,13	0.88	1 (11%)
1	PSU	A2	682	1	18,21,22	1.38	2 (11%)	22,30,33	1.89	3 (13%)
1	OMG	A2	868	1	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
39	PSU	B5	4166	39	18,21,22	1.37	2 (11%)	22,30,33	1.86	4 (18%)
83	SAC	Br	2	83	7,8,9	0.51	0	8,9,11	0.86	1 (12%)
39	A2M	B5	2658	89,39	18,25,26	1.00	1 (5%)	18,36,39	1.24	2 (11%)
69	MLZ	Bb	5	69	8,9,10	0.48	0	4,9,11	0.07	0
1	PSU	A2	816	1	18,21,22	1.34	2 (11%)	22,30,33	1.91	4 (18%)
1	OMU	A2	628	1	19,22,23	1.18	2 (10%)	26,31,34	1.70	5 (19%)
1	6MZ	A2	1833	1,89	18,25,26	0.94	1 (5%)	16,36,39	1.77	3 (18%)
39	PSU	B5	1638	39	18,21,22	1.38	2 (11%)	22,30,33	1.90	3 (13%)
39	OMC	B5	2647	39	19,22,23	0.81	0	26,31,34	0.82	0
39	OMU	B5	3973	39	19,22,23	1.24	3 (15%)	26,31,34	1.69	4 (15%)
1	PSU	A2	1239	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	4 (18%)
1	PSU	A2	1005	1	18,21,22	1.38	2 (11%)	22,30,33	1.87	3 (13%)
39	OMC	B5	2704	39	19,22,23	0.81	0	26,31,34	0.83	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	OMU	B5	3657	39	19,22,23	1.24	2 (10%)	26,31,34	1.76	5 (19%)
1	PSU	A2	802	1	18,21,22	1.37	2 (11%)	22,30,33	1.88	3 (13%)
39	PSU	B5	3369	39	18,21,22	1.38	3 (16%)	22,30,33	1.94	4 (18%)
39	PSU	B5	1632	39	18,21,22	1.38	2 (11%)	22,30,33	1.89	4 (18%)
1	PSU	A2	610	1	18,21,22	1.36	2 (11%)	22,30,33	1.90	3 (13%)

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
39	PSU	B5	4045	39	-	0/7/25/26	0/2/2/2
41	OMG	B8	75	41	-	0/5/27/28	0/3/3/3
1	PSU	A2	967	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	4138	39	-	0/5/27/28	0/3/3/3
39	A2M	B5	1810	89,39	-	0/5/27/28	0/3/3/3
39	PSU	B5	4267	89,39	-	0/7/25/26	0/2/2/2
39	OMC	B5	3619	39	-	2/9/27/28	0/2/2/2
39	PSU	B5	1491	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	669	1,89	-	2/5/27/28	0/3/3/3
1	PSU	A2	1178	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	1683	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	34	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	1491	1,89	-	2/5/27/28	0/3/3/3
11	5MC	AT	49	11	-	0/7/25/26	0/2/2/2
1	PSU	A2	1082	1	-	1/7/25/26	0/2/2/2
39	PSU	B5	1537	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3447	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	1443	1,89	-	1/9/27/28	0/2/2/2
39	PSU	B5	3616	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	2206	89,39	-	0/5/27/28	0/3/3/3
1	OMU	A2	1327	1,89	-	0/9/27/28	0/2/2/2
1	PSU	A2	1626	1	-	0/7/25/26	0/2/2/2
39	UR3	B5	4276	39	-	0/7/25/26	0/2/2/2
11	YYG	AT	37	11	-	0/20/42/43	0/3/4/4
1	A2M	A2	1032	1	-	0/5/27/28	0/3/3/3
39	PSU	B5	3496	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	4336	39	-	1/5/27/28	0/3/3/3
39	PSU	B5	4749	39	-	0/7/25/26	0/2/2/2
11	G7M	AT	46	11	-	1/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	A2	1329	1	-	1/5/27/28	0/3/3/3
1	PSU	A2	1057	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	2680	39	-	1/9/27/28	0/2/2/2
11	H2U	AT	16	11	-	1/7/38/39	0/2/2/2
1	OMG	A2	684	1	-	4/5/27/28	0/3/3/3
39	PSU	B5	3494	39	-	1/7/25/26	0/2/2/2
39	5MC	B5	4193	39	-	4/7/25/26	0/2/2/2
11	PSU	AT	28	11	-	0/7/25/26	0/2/2/2
39	PSU	B5	3652	89,39	-	0/7/25/26	0/2/2/2
11	PSU	AT	27	11	-	0/7/25/26	0/2/2/2
39	OMC	B5	2194	89,39	-	2/9/27/28	0/2/2/2
39	OMG	B5	3631	39	-	0/5/27/28	0/3/3/3
39	OMG	B5	3974	39	-	0/5/27/28	0/3/3/3
39	OMC	B5	3433	39	-	4/9/27/28	0/2/2/2
39	PSU	B5	4169	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	4245	39	-	0/5/27/28	0/3/3/3
39	A2M	B5	1270	39	-	0/5/27/28	0/3/3/3
39	OMG	B5	3476	39	-	0/5/27/28	0/3/3/3
1	OMU	A2	1805	1	-	2/9/27/28	0/2/2/2
35	HY3	Aw	62	35	-	0/1/12/14	0/1/1/1
39	PSU	B5	3466	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	4269	89,39	-	0/5/27/28	0/3/3/3
11	H2U	AT	17	11	-	6/7/38/39	0/2/2/2
1	MA6	A2	1851	1	-	0/7/29/30	0/3/3/3
39	OMC	B5	2265	89,39	-	1/9/27/28	0/2/2/2
1	OMU	A2	355	1	-	0/9/27/28	0/2/2/2
1	A2M	A2	27	1,89	-	2/5/27/28	0/3/3/3
1	PSU	A2	210	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	573	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	687	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4177	39	-	0/7/25/26	0/2/2/2
39	5MC	B5	3514	89,39	-	0/7/25/26	0/2/2/2
39	OMU	B5	4366	39	-	0/9/27/28	0/2/2/2
1	MA6	A2	1852	1	-	2/7/29/30	0/3/3/3
11	2MG	AT	10	11	-	0/5/27/28	0/3/3/3
1	PSU	A2	652	1	-	0/7/25/26	0/2/2/2
1	OMC	A2	1392	1	-	1/9/27/28	0/2/2/2
39	PSU	B5	4149	39	-	0/7/25/26	0/2/2/2
1	B8N	A2	1249	1	-	4/16/34/35	0/2/2/2
39	OMG	B5	4369	39	-	1/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PSU	B5	1801	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	4240	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	4374	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3502	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1047	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	510	1,89	-	0/5/27/28	0/3/3/3
39	PSU	B5	4278	39	-	0/7/25/26	0/2/2/2
39	OMU	B5	2258	39	-	0/9/27/28	0/2/2/2
39	OMU	B5	4244	39	-	0/9/27/28	0/2/2/2
1	PSU	A2	109	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	1479	39	-	0/5/27/28	0/3/3/3
1	A2M	A2	99	1,89	-	2/5/27/28	0/3/3/3
39	PSU	B5	4099	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1799	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3450	39	-	1/5/27/28	0/3/3/3
39	OMG	B5	2719	39	-	0/5/27/28	0/3/3/3
39	OMC	B5	4282	89,39	-	0/9/27/28	0/2/2/2
39	PSU	B5	4419	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3599	39	-	2/5/27/28	0/3/3/3
1	A2M	A2	485	1	-	0/5/27/28	0/3/3/3
1	OMC	A2	1704	1	-	2/9/27/28	0/2/2/2
39	PSU	B5	3427	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	4317	39	-	0/5/27/28	0/3/3/3
1	OMC	A2	518	1	-	0/9/27/28	0/2/2/2
39	PSU	B5	2351	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	218	1	-	0/7/25/26	0/2/2/2
11	5MU	AT	54	11	-	0/7/25/26	0/2/2/2
1	A2M	A2	166	1	-	0/5/27/28	0/3/3/3
39	PSU	B5	3554	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1693	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	591	1	-	0/5/27/28	0/3/3/3
39	OMC	B5	1820	89,39	-	1/9/27/28	0/2/2/2
39	PSU	B5	3500	39	-	0/7/25/26	0/2/2/2
11	PSU	AT	39	11	-	0/7/25/26	0/2/2/2
1	PSU	A2	650	1	-	0/7/25/26	0/2/2/2
1	OMU	A2	116	1	-	1/9/27/28	0/2/2/2
39	PSU	B5	4322	39	-	0/7/25/26	0/2/2/2
44	AYA	BC	2	44	-	0/4/6/8	-
1	OMG	A2	602	1	-	0/5/27/28	0/3/3/3
1	A2M	A2	1384	1	-	0/5/27/28	0/3/3/3
39	PSU	B5	1720	39	-	0/7/25/26	0/2/2/2
80	M3L	Bm	98	80	-	0/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PSU	AT	55	11	-	0/7/25/26	0/2/2/2
1	OMU	A2	172	1	-	0/9/27/28	0/2/2/2
39	OMG	B5	3942	11,39	-	0/5/27/28	0/3/3/3
1	OMU	A2	121	1	-	1/9/27/28	0/2/2/2
39	PSU	B5	3371	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4711	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3492	1,39	-	2/5/27/28	0/3/3/3
41	PSU	B8	69	41	-	0/7/25/26	0/2/2/2
39	A2M	B5	2244	89,39	-	0/5/27/28	0/3/3/3
39	PSU	B5	3462	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4058	39	-	0/7/25/26	0/2/2/2
11	OMC	AT	32	11	-	0/9/27/28	0/2/2/2
1	PSU	A2	407	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	1580	39	-	0/5/27/28	0/3/3/3
39	OMG	B5	2207	39	-	2/5/27/28	0/3/3/3
39	A2M	B5	3517	39	-	2/5/27/28	0/3/3/3
39	PSU	B5	4039	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4107	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	4116	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	4203	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4298	39	-	0/7/25/26	0/2/2/2
31	NMM	As	67	31	-	1/9/11/13	-
39	A2M	B5	1489	89,39	-	1/5/27/28	0/3/3/3
39	A2M	B5	3557	39	-	1/5/27/28	0/3/3/3
1	PSU	A2	1245	1	-	0/7/25/26	0/2/2/2
1	G7M	A2	1640	1,11	-	0/3/25/26	0/3/3/3
81	MLZ	B _o	53	81	-	0/7/8/10	-
39	OMC	B5	2667	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	4188	39	-	0/7/25/26	0/2/2/2
1	4AC	A2	1338	1	-	4/11/29/30	0/2/2/2
39	PSU	B5	1731	39	-	0/7/25/26	0/2/2/2
1	OMC	A2	174	1,89	-	0/9/27/28	0/2/2/2
39	PSU	B5	4325	39	-	0/7/25/26	0/2/2/2
42	V5N	BA	216	42	-	1/5/10/12	0/1/1/1
39	OMG	B5	2267	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	3576	39	-	1/7/25/26	0/2/2/2
1	PSU	A2	1644	1,89	-	0/7/25/26	0/2/2/2
11	M2G	AT	26	11	-	0/7/29/30	0/3/3/3
1	PSU	A2	1368	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1233	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	437	1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A2	1348	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	400	39	-	0/5/27/28	0/3/3/3
39	A2M	B5	2630	89,39	-	0/5/27/28	0/3/3/3
1	OMG	A2	1448	1	-	2/5/27/28	0/3/3/3
39	OMG	B5	3676	39	-	1/5/27/28	0/3/3/3
1	PSU	A2	1175	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	398	39	-	2/5/27/28	0/3/3/3
1	PSU	A2	36	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4042	39	-	0/7/25/26	0/2/2/2
68	V5N	Ba	39	68	-	0/5/10/12	0/1/1/1
1	PSU	A2	815	1	-	0/7/25/26	0/2/2/2
1	4AC	A2	1843	1	-	2/11/29/30	0/2/2/2
1	PSU	A2	119	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	577	1	-	2/5/27/28	0/3/3/3
39	6MZ	B5	3966	39	-	0/5/27/28	0/3/3/3
40	GTP	B7	1	40	-	0/18/38/38	0/3/3/3
39	PSU	B5	1718	39	-	0/7/25/26	0/2/2/2
11	OMG	AT	34	11,9	-	0/5/27/28	0/3/3/3
39	PSU	B5	4217	39	-	0/7/25/26	0/2/2/2
39	OMU	B5	4052	39	-	0/9/27/28	0/2/2/2
39	OMG	B5	1260	39	-	1/5/27/28	0/3/3/3
1	PSU	A2	864	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	3524	39	-	1/5/27/28	0/3/3/3
39	PSU	B5	4246	39	-	1/7/25/26	0/2/2/2
39	PSU	B5	4435	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3359	39	-	0/5/27/28	0/3/3/3
12	SAC	AZ	2	12	-	2/7/8/10	-
39	OMC	B5	4202	39	-	1/9/27/28	0/2/2/2
1	OMU	A2	1289	1	-	0/9/27/28	0/2/2/2
1	PSU	A2	1046	1	-	0/7/25/26	0/2/2/2
39	1MA	B5	1266	89,39	-	0/3/25/26	0/3/3/3
39	PSU	B5	2475	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	3456	39	-	0/5/27/28	0/3/3/3
43	HIC	BB	245	43	-	1/5/6/8	0/1/1/1
39	A2M	B5	3562	39	-	0/5/27/28	0/3/3/3
39	OMG	B5	4364	39	-	0/5/27/28	0/3/3/3
39	PSU	B5	3583	39	-	1/7/25/26	0/2/2/2
11	1MA	AT	14	11	-	0/3/25/26	0/3/3/3
1	PSU	A2	93	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	3540	39	-	0/9/27/28	0/2/2/2
1	PSU	A2	867	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	OMC	B5	1284	39	-	2/9/27/28	0/2/2/2
39	OMC	B5	3601	39	-	0/9/27/28	0/2/2/2
1	PSU	A2	1446	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	4383	39	-	0/5/27/28	0/3/3/3
1	A2M	A2	159	1	-	0/5/27/28	0/3/3/3
41	PSU	B8	55	41	-	0/7/25/26	0/2/2/2
39	OMC	B5	2208	89,39	-	0/9/27/28	0/2/2/2
1	OMC	A2	463	1	-	0/9/27/28	0/2/2/2
1	A2M	A2	1679	1	-	0/5/27/28	0/3/3/3
39	OMG	B5	1477	39	-	1/5/27/28	0/3/3/3
39	PSU	B5	3585	89,39	-	0/7/25/26	0/2/2/2
30	SAC	Ar	2	30	-	0/7/8/10	-
39	OMC	B5	3573	39	-	0/9/27/28	0/2/2/2
1	A2M	A2	469	1	-	1/5/27/28	0/3/3/3
11	1MA	AT	58	11	-	0/3/25/26	0/3/3/3
39	PSU	B5	4740	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	513	1	-	4/5/27/28	0/3/3/3
39	PSU	B5	3490	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1721	39	-	0/7/25/26	0/2/2/2
39	UY1	B5	3550	39	-	4/9/27/28	0/2/2/2
1	OMU	A2	429	1	-	4/9/27/28	0/2/2/2
1	PSU	A2	105	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4382	39	-	3/7/25/26	0/2/2/2
33	AME	Au	1	33	-	2/9/10/12	-
1	PSU	A2	682	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	868	1	-	0/5/27/28	0/3/3/3
39	PSU	B5	4166	39	-	0/7/25/26	0/2/2/2
83	SAC	Br	2	83	-	0/7/8/10	-
39	A2M	B5	2658	89,39	-	0/5/27/28	0/3/3/3
69	MLZ	Bb	5	69	-	2/7/8/10	-
1	PSU	A2	816	1	-	0/7/25/26	0/2/2/2
1	OMU	A2	628	1	-	2/9/27/28	0/2/2/2
1	6MZ	A2	1833	1,89	-	2/5/27/28	0/3/3/3
39	PSU	B5	1638	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	2647	39	-	1/9/27/28	0/2/2/2
39	OMU	B5	3973	39	-	1/9/27/28	0/2/2/2
1	PSU	A2	1239	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1005	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	2704	39	-	1/9/27/28	0/2/2/2
39	OMU	B5	3657	39	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A2	802	1	-	2/7/25/26	0/2/2/2
39	PSU	B5	3369	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1632	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	610	1	-	0/7/25/26	0/2/2/2

The worst 5 of 362 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1640	G7M	C8-N9	7.54	1.47	1.33
11	AT	46	G7M	C8-N9	7.45	1.46	1.33
11	AT	46	G7M	C8-N7	7.17	1.46	1.33
1	A2	1640	G7M	C8-N7	7.15	1.46	1.33
11	AT	37	YYG	O23-C21	6.57	1.45	1.34

The worst 5 of 616 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AT	17	H2U	C4-N3-C2	-7.02	119.97	125.79
39	B5	3369	PSU	N1-C2-N3	6.25	122.21	115.13
39	B5	4374	PSU	N1-C2-N3	6.22	122.18	115.13
39	B5	3502	PSU	N1-C2-N3	6.20	122.16	115.13
39	B5	4298	PSU	N1-C2-N3	6.19	122.14	115.13

There are no chirality outliers.

5 of 121 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A2	429	OMU	C2'-C1'-N1-C2
1	A2	429	OMU	C2'-C1'-N1-C6
1	A2	1833	6MZ	N1-C6-N6-C9
39	B5	3433	OMC	C2'-C1'-N1-C2
39	B5	3433	OMC	C2'-C1'-N1-C6

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 790 ligands modelled in this entry, 428 are monoatomic and 329 are unknown - leaving 33 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
87	SPD	A2	1902	-	9,9,9	0.15	0	8,8,8	0.15	0
87	SPD	B5	4906	-	9,9,9	0.15	0	8,8,8	0.16	0
87	SPD	B5	4901	-	9,9,9	0.14	0	8,8,8	0.15	0
87	SPD	A2	1906	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	B5	4917	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	B5	4919	-	9,9,9	0.15	0	8,8,8	0.21	0
87	SPD	B5	4914	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	B5	4908	-	9,9,9	0.16	0	8,8,8	0.16	0
87	SPD	B5	4910	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	B5	4909	-	9,9,9	0.16	0	8,8,8	0.19	0
88	SPM	B5	4915	-	13,13,13	0.16	0	12,12,12	0.22	0
87	SPD	A2	1907	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	A2	1901	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	B5	4920	-	9,9,9	0.15	0	8,8,8	0.23	0
87	SPD	B5	4905	-	9,9,9	0.16	0	8,8,8	0.21	0
87	SPD	B5	4924	-	9,9,9	0.16	0	8,8,8	0.14	0
88	SPM	A2	1909	-	13,13,13	0.14	0	12,12,12	0.18	0
87	SPD	B5	4913	-	9,9,9	0.16	0	8,8,8	0.17	0
87	SPD	B5	4903	-	9,9,9	0.16	0	8,8,8	0.20	0
87	SPD	B5	4921	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	B5	4904	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	B5	4923	-	9,9,9	0.15	0	8,8,8	0.20	0
87	SPD	A2	1903	-	9,9,9	0.15	0	8,8,8	0.19	0
88	SPM	B5	4912	-	13,13,13	0.15	0	12,12,12	0.23	0
87	SPD	B5	4907	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	B5	4911	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	A2	1904	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	B5	4918	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	B5	4922	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	B5	4902	-	9,9,9	0.15	0	8,8,8	0.23	0
87	SPD	A2	1905	-	9,9,9	0.16	0	8,8,8	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
87	SPD	B5	4916	-	9,9,9	0.15	0	8,8,8	0.22	0
87	SPD	A2	1908	-	9,9,9	0.15	0	8,8,8	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	A2	1902	-	-	0/7/7/7	-
87	SPD	B5	4906	-	-	1/7/7/7	-
87	SPD	B5	4901	-	-	1/7/7/7	-
87	SPD	A2	1906	-	-	1/7/7/7	-
87	SPD	B5	4917	-	-	0/7/7/7	-
87	SPD	B5	4919	-	-	0/7/7/7	-
87	SPD	B5	4914	-	-	0/7/7/7	-
87	SPD	B5	4908	-	-	0/7/7/7	-
87	SPD	B5	4910	-	-	1/7/7/7	-
87	SPD	B5	4909	-	-	0/7/7/7	-
88	SPM	B5	4915	-	-	0/11/11/11	-
87	SPD	A2	1907	-	-	1/7/7/7	-
87	SPD	A2	1901	-	-	1/7/7/7	-
87	SPD	B5	4920	-	-	0/7/7/7	-
87	SPD	B5	4905	-	-	0/7/7/7	-
87	SPD	B5	4924	-	-	1/7/7/7	-
88	SPM	A2	1909	-	-	1/11/11/11	-
87	SPD	B5	4913	-	-	0/7/7/7	-
87	SPD	B5	4903	-	-	2/7/7/7	-
87	SPD	B5	4921	-	-	1/7/7/7	-
87	SPD	B5	4904	-	-	0/7/7/7	-
87	SPD	B5	4923	-	-	0/7/7/7	-
87	SPD	A2	1903	-	-	0/7/7/7	-
88	SPM	B5	4912	-	-	1/11/11/11	-
87	SPD	B5	4907	-	-	0/7/7/7	-
87	SPD	B5	4911	-	-	0/7/7/7	-
87	SPD	A2	1904	-	-	0/7/7/7	-
87	SPD	B5	4918	-	-	0/7/7/7	-
87	SPD	B5	4922	-	-	1/7/7/7	-
87	SPD	B5	4902	-	-	1/7/7/7	-
87	SPD	A2	1905	-	-	0/7/7/7	-
87	SPD	B5	4916	-	-	0/7/7/7	-
87	SPD	A2	1908	-	-	0/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	A2	1909	SPM	C12-C11-N10-C9
87	B5	4901	SPD	C4-C5-N6-C7
87	B5	4902	SPD	C2-C3-C4-C5
87	B5	4924	SPD	C2-C3-C4-C5
87	B5	4903	SPD	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

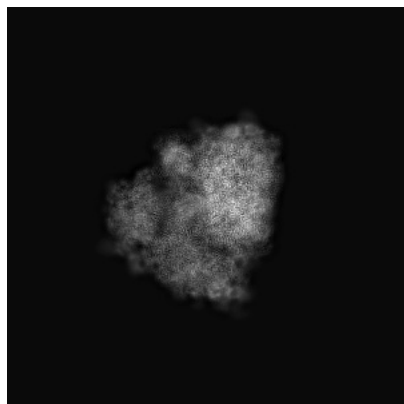
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12757. These allow visual inspection of the internal detail of the map and identification of artifacts.

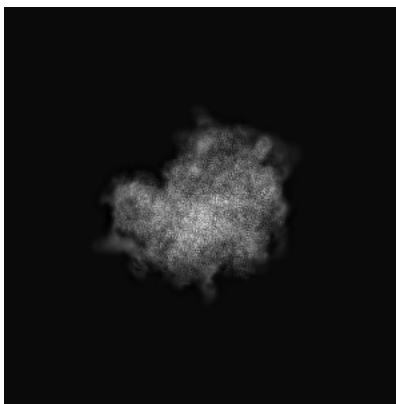
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

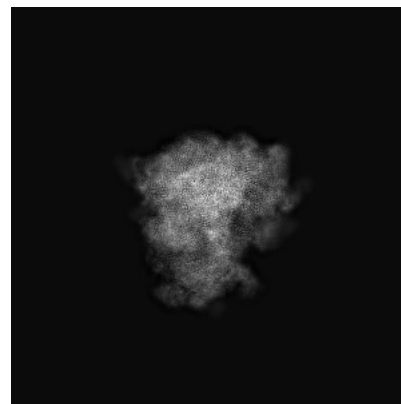
6.1.1 Primary map



X

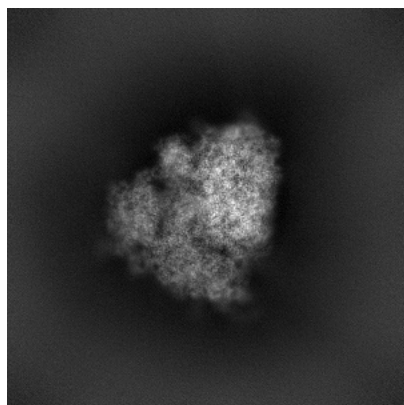


Y

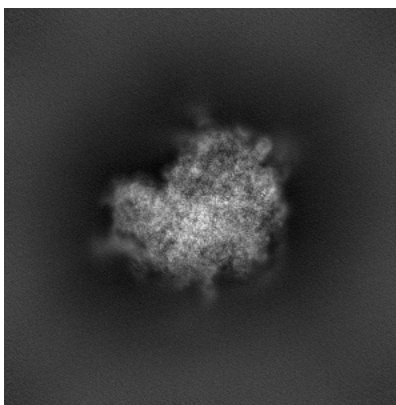


Z

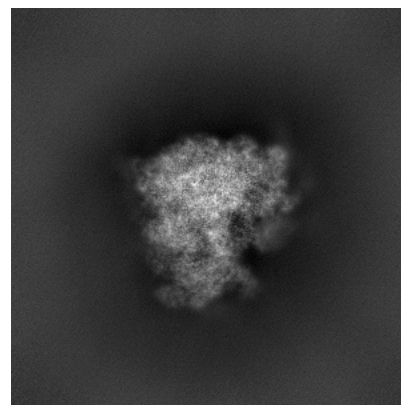
6.1.2 Raw map



X



Y

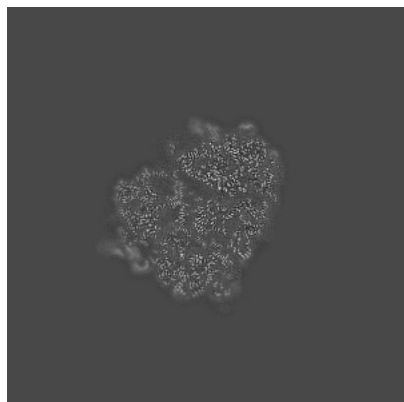


Z

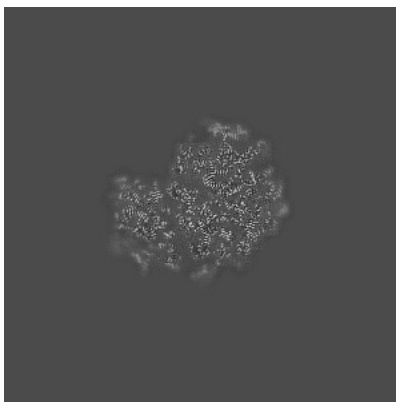
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

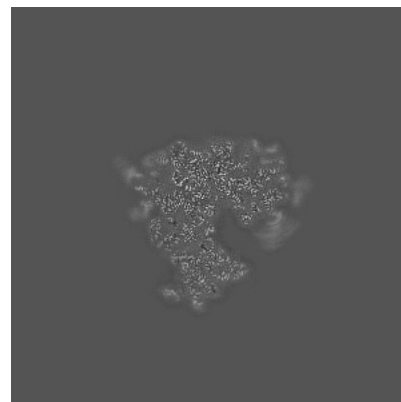
6.2.1 Primary map



X Index: 280

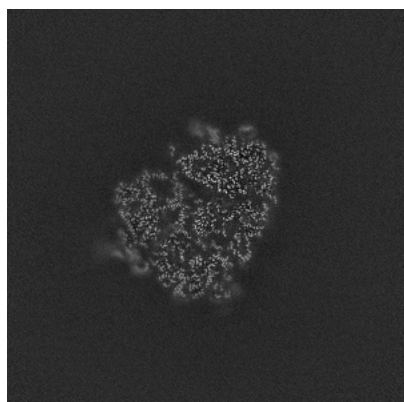


Y Index: 280

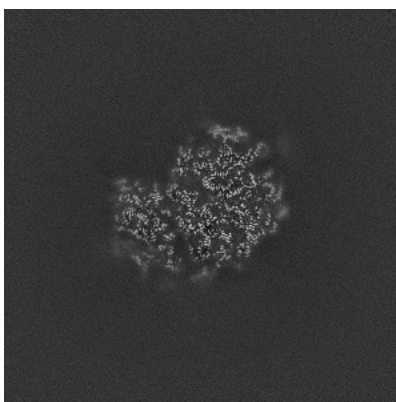


Z Index: 280

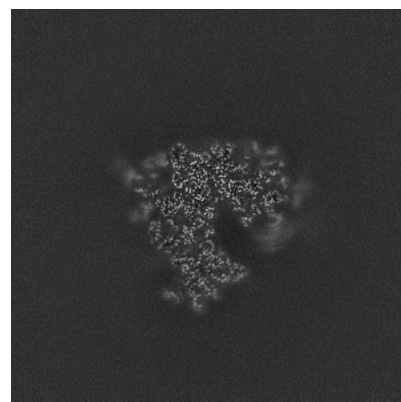
6.2.2 Raw map



X Index: 280



Y Index: 280

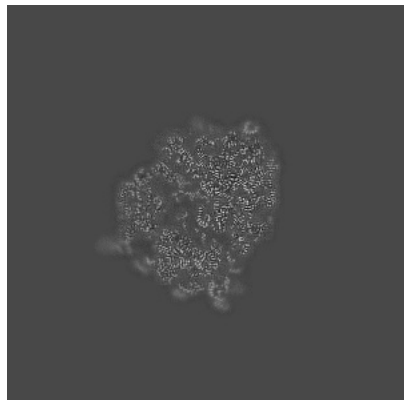


Z Index: 280

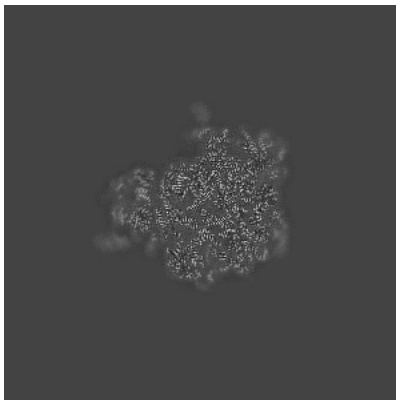
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

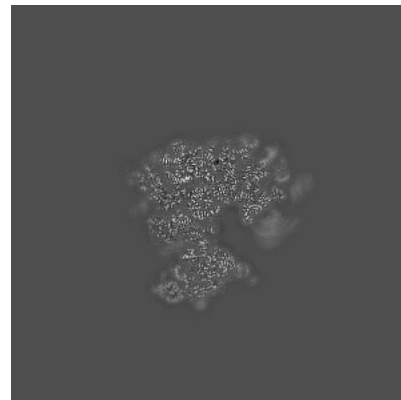
6.3.1 Primary map



X Index: 287

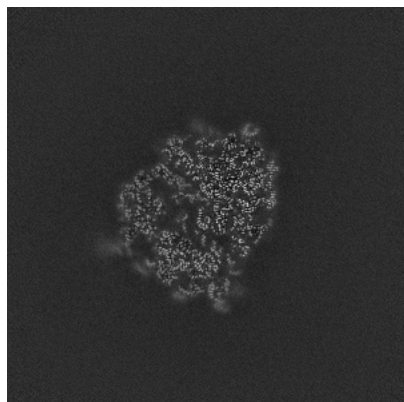


Y Index: 313

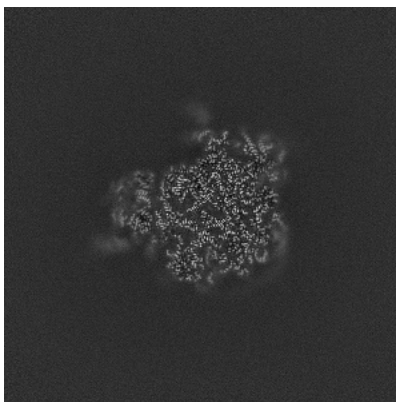


Z Index: 272

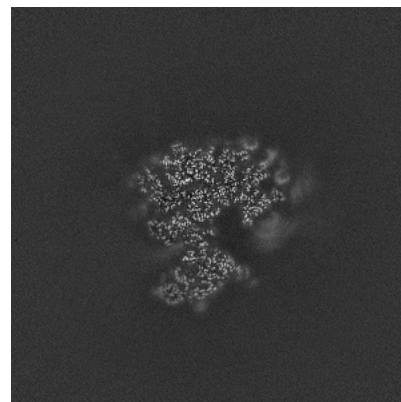
6.3.2 Raw map



X Index: 287



Y Index: 313

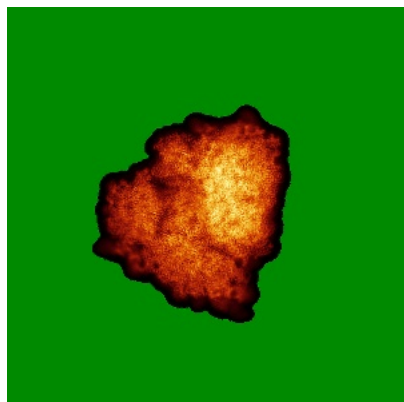


Z Index: 272

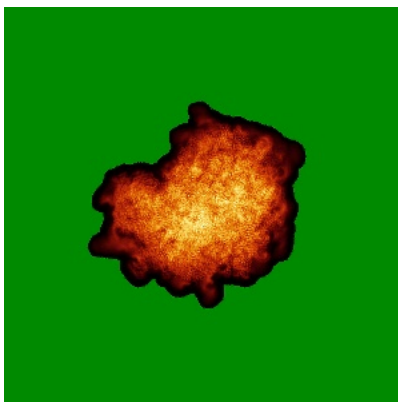
The images above show the largest variance slices of the map in three orthogonal directions.

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

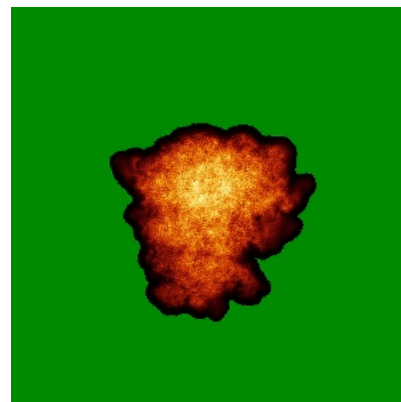
6.4.1 Primary map



X

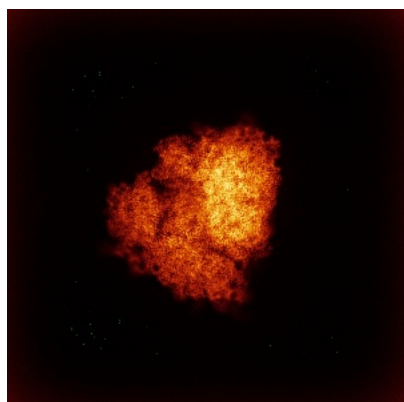


Y

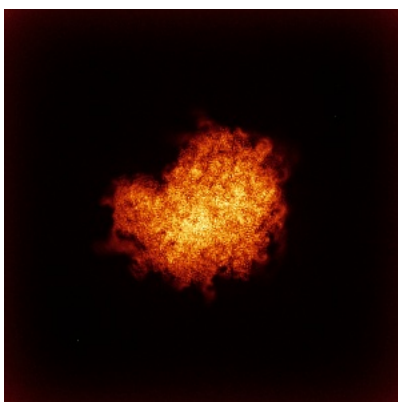


Z

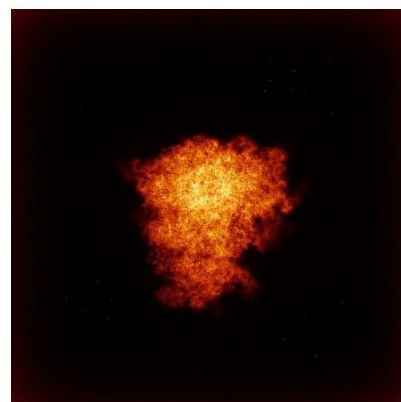
6.4.2 Raw map



X



Y

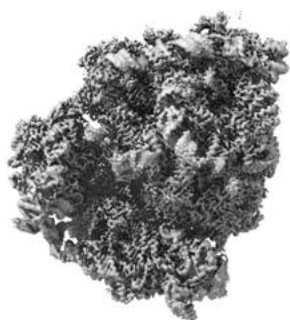


Z

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



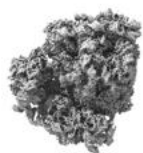
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

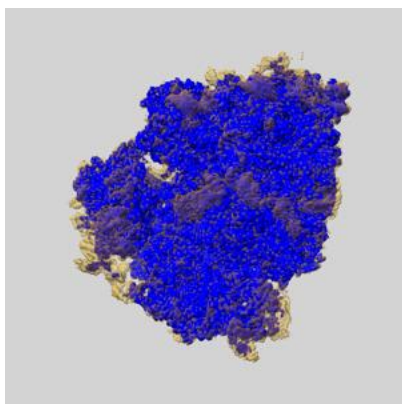
6.6 Mask visualisation [i](#)

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

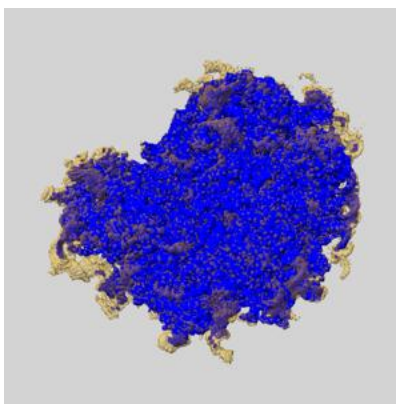
A mask typically either:

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

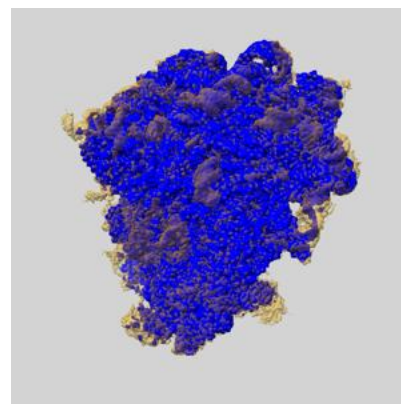
6.6.1 emd_12757_msk_1.map [i](#)



X

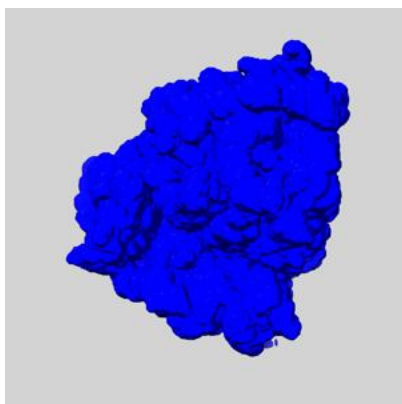


Y

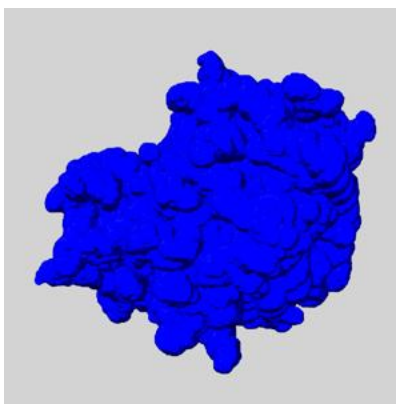


Z

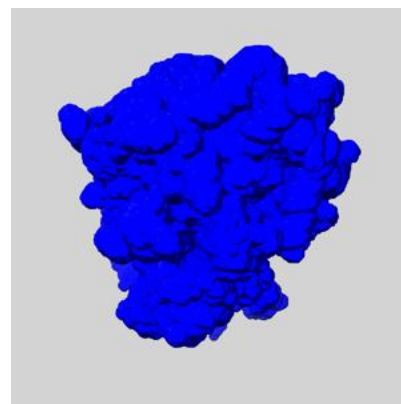
6.6.2 emd_12757_msk_2.map [i](#)



X



Y

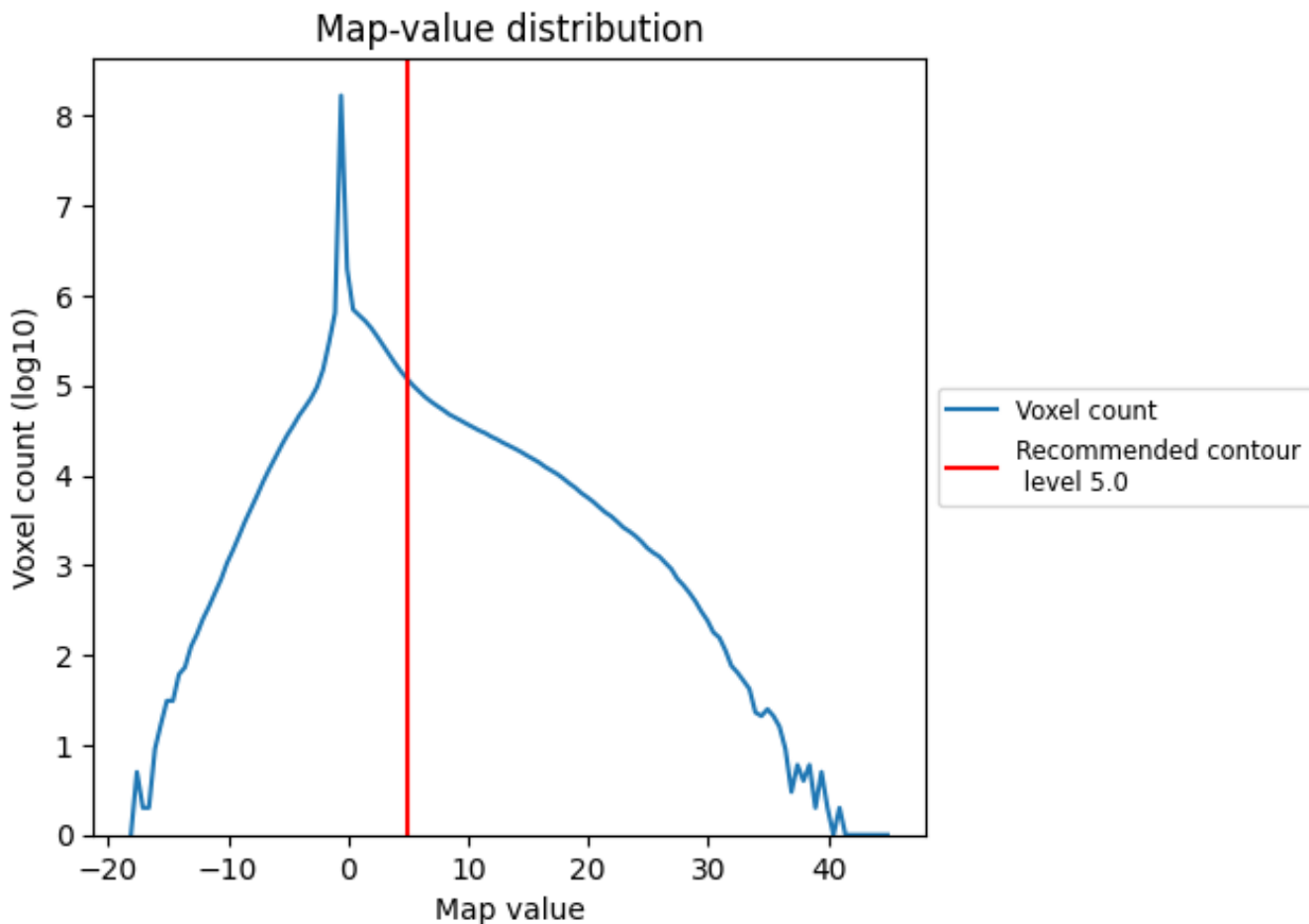


Z

7 Map analysis [i](#)

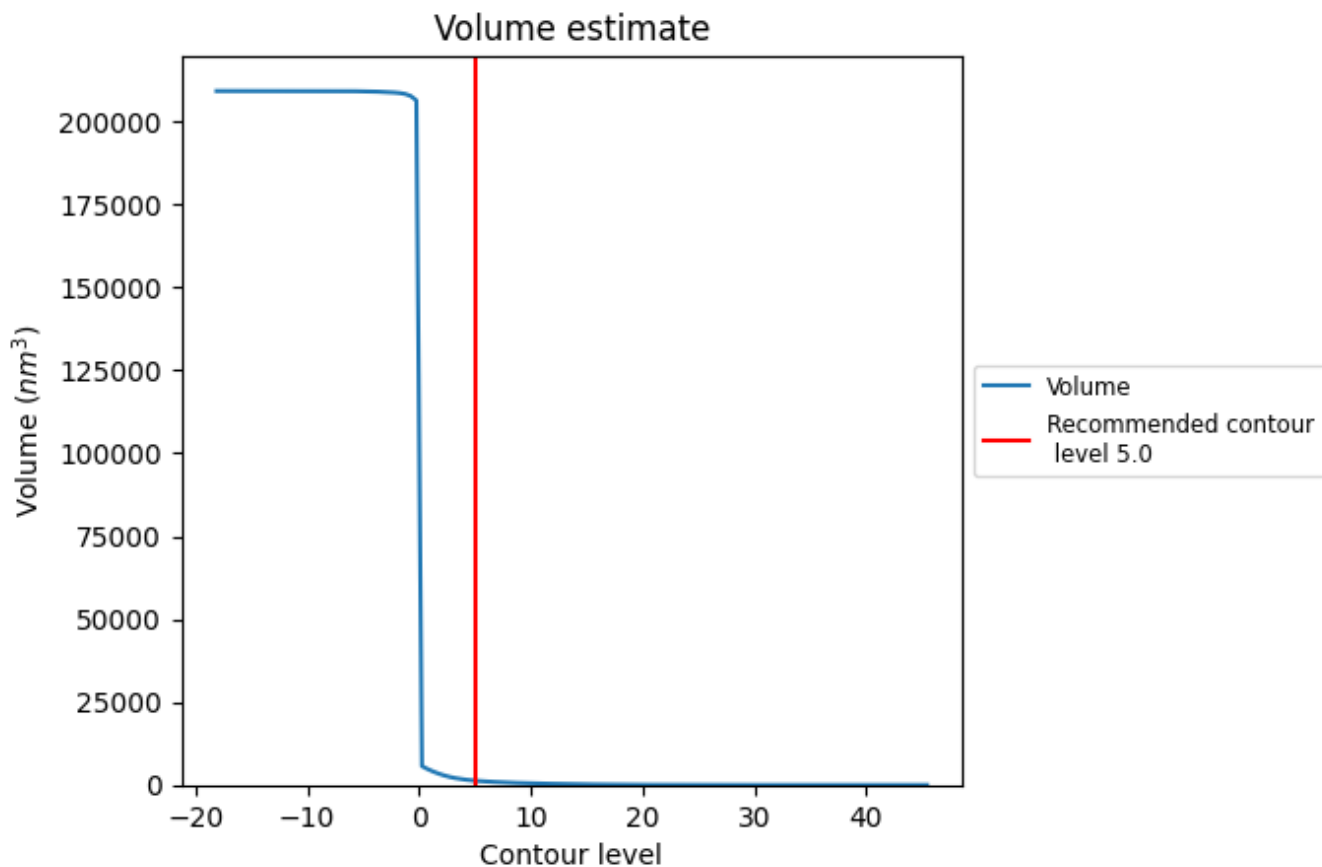
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

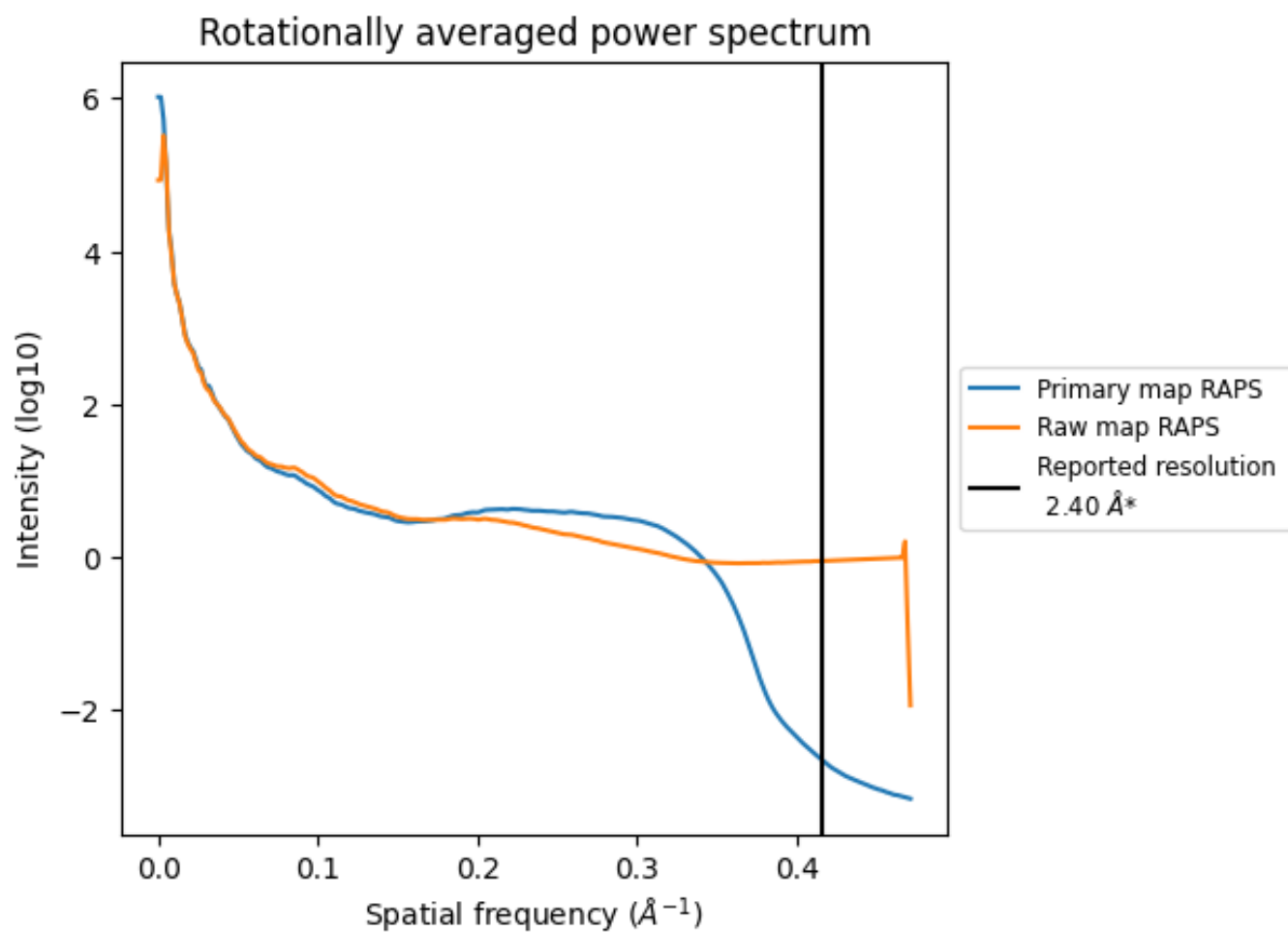
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1298 nm^3 ; this corresponds to an approximate mass of 1172 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

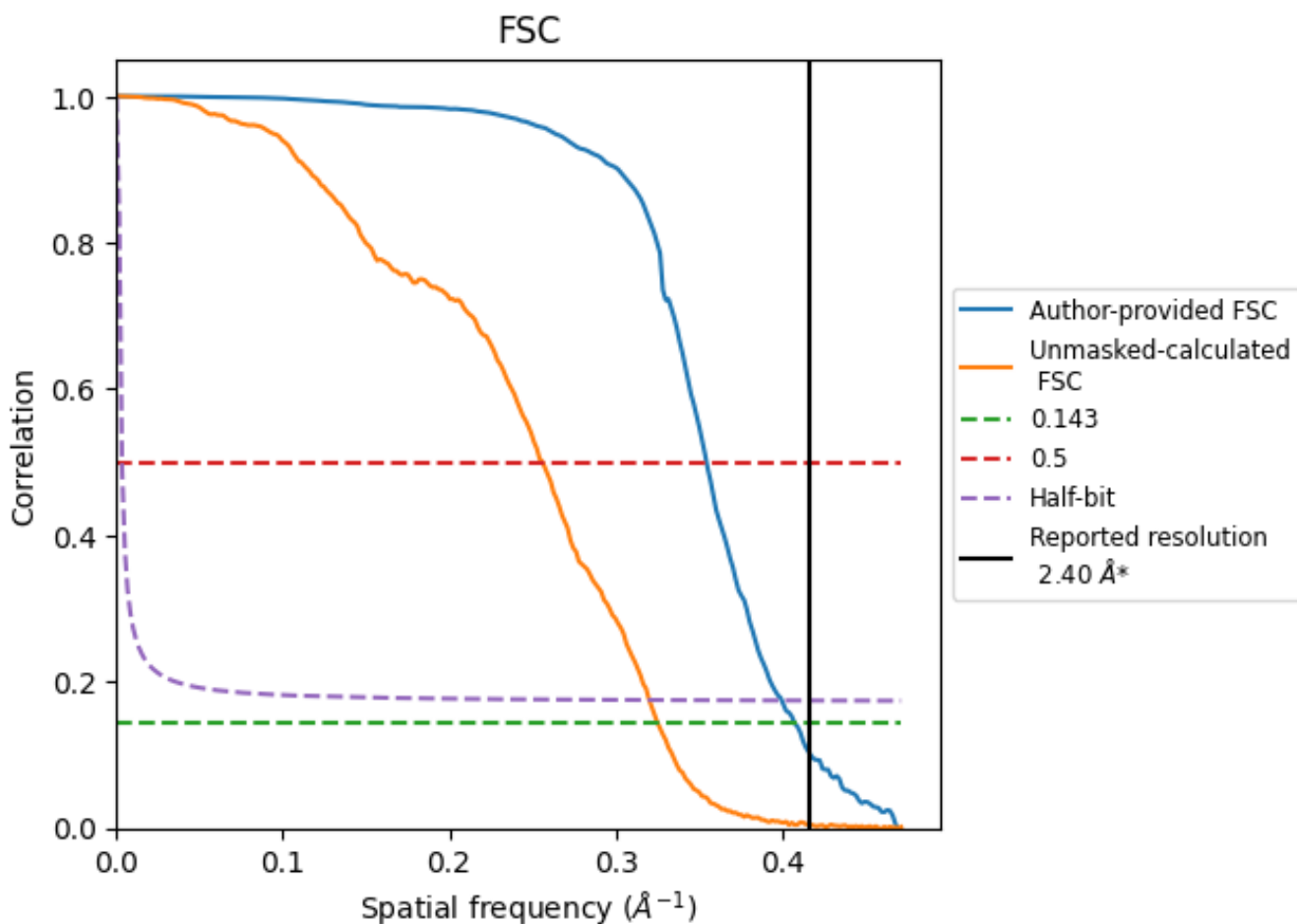


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

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 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

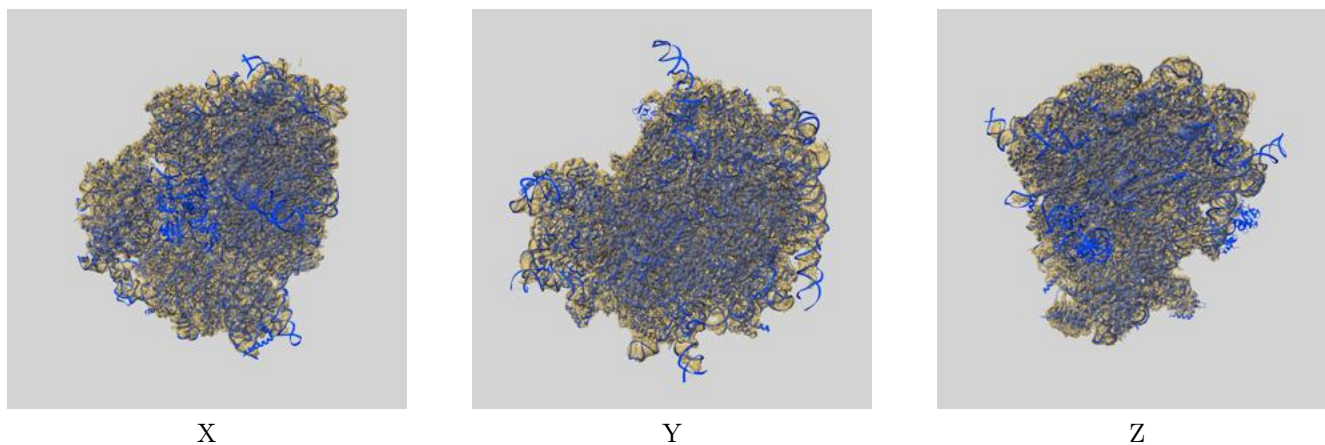
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.45	2.82	2.50
Unmasked-calculated*	3.07	3.90	3.12

*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 3.07 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

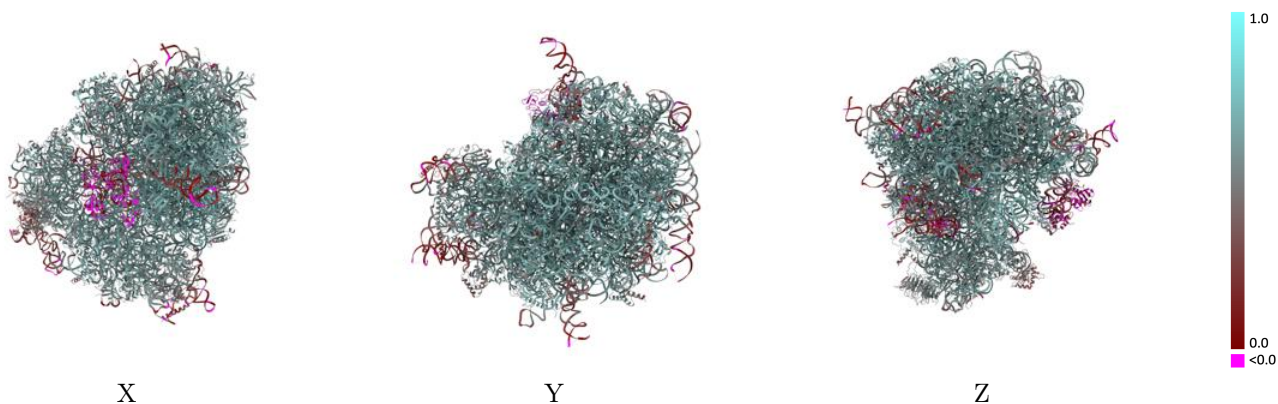
This section contains information regarding the fit between EMDB map EMD-12757 and PDB model 7O7Z. Per-residue inclusion information can be found in section 3 on page 27.

9.1 Map-model overlay [i](#)



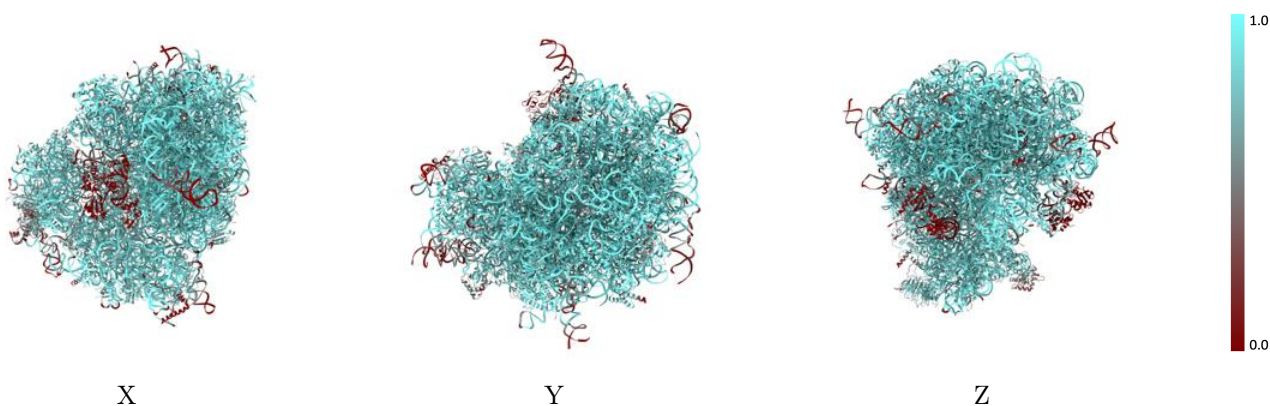
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



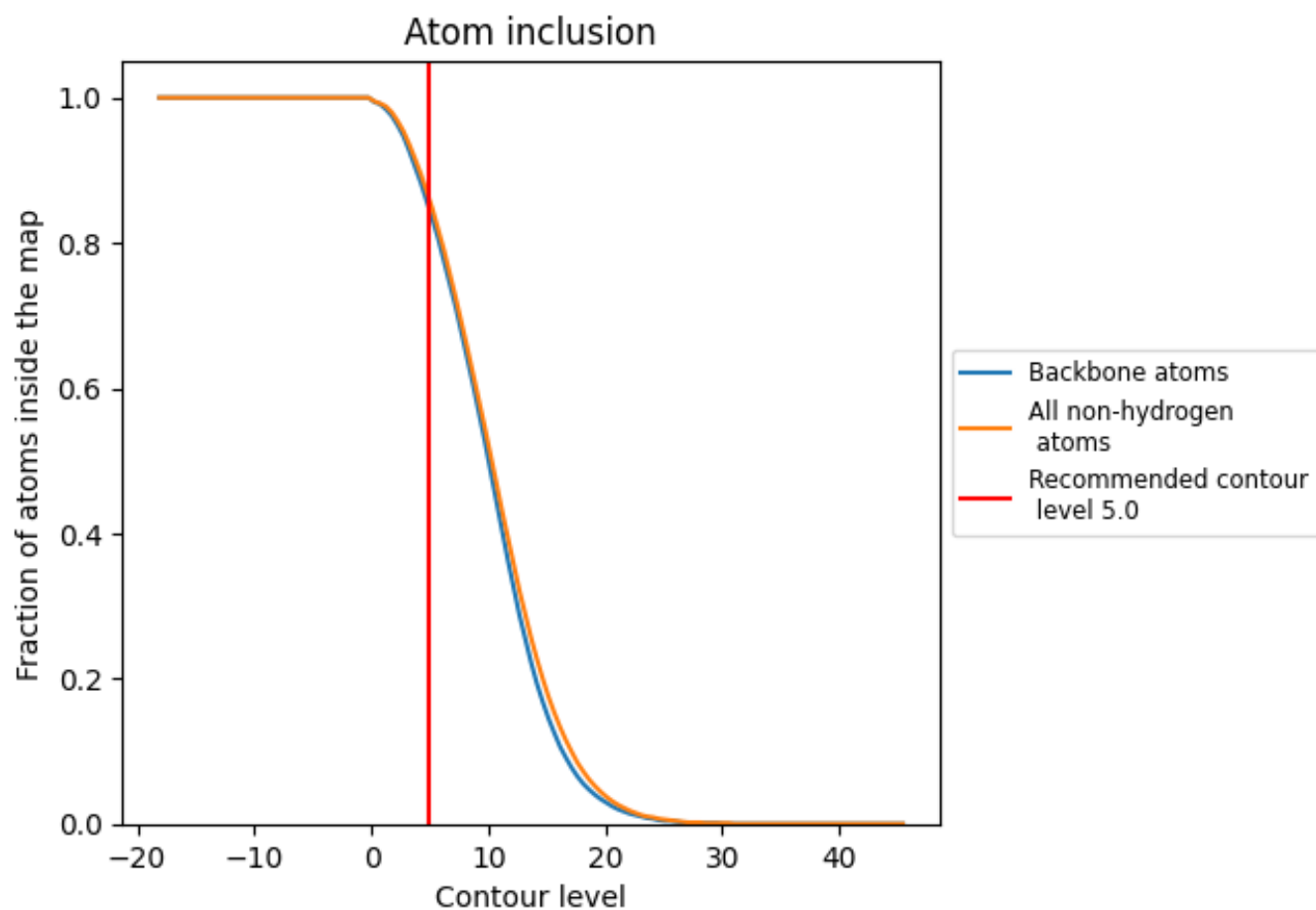
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





















































































The table lists the average atom inclusion at the recommended contour level (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8580	 0.5760
A2	 0.9060	 0.5760
AA	 0.7930	 0.5730
AB	 0.7670	 0.5800
AC	 0.4040	 0.3600
AD	 0.7460	 0.5580
AE	 0.8720	 0.6130
AF	 0.7090	 0.4910
AG	 0.9050	 0.6280
AH	 0.4400	 0.2140
AI	 0.4400	 0.3250
AT	 0.8960	 0.6030
AZ	 0.8340	 0.6010
Aa	 0.8400	 0.6110
Ab	 0.8900	 0.6230
Ac	 0.7440	 0.5600
Ad	 0.8750	 0.5940
Ae	 0.8290	 0.6050
Af	 0.7430	 0.4900
Ag	 0.6430	 0.5080
Ah	 0.8560	 0.5960
Ai	 0.8690	 0.6040
Aj	 0.7680	 0.5230
Ak	 0.8180	 0.5960
Al	 0.3160	 0.2940
Am	 0.8860	 0.6270
An	 0.8800	 0.6310
Ao	 0.7990	 0.5420
Ap	 0.8460	 0.5760
Aq	 0.7250	 0.5510
Ar	 0.8200	 0.5650
As	 0.8520	 0.5830
At	 0.7390	 0.5270
Au	 0.8530	 0.6110
Av	 0.9430	 0.6510























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Chain	Atom inclusion	Q-score
Aw	 0.9120	 0.6380
Ax	 0.8280	 0.5500
Ay	 0.7210	 0.5460
Az	 0.8850	 0.6340
B5	 0.9010	 0.5820
B7	 0.9860	 0.6500
B8	 0.9430	 0.6250
BA	 0.9330	 0.6500
BB	 0.9210	 0.6470
BC	 0.9370	 0.6460
BD	 0.9080	 0.6190
BE	 0.8130	 0.5770
BF	 0.9430	 0.6560
BG	 0.8290	 0.5900
BH	 0.8980	 0.6340
BI	 0.8850	 0.6430
BJ	 0.8680	 0.6220
BK	 0.4100	 0.4710
BL	 0.8760	 0.6160
BM	 0.9080	 0.6220
BN	 0.9750	 0.6620
BO	 0.9420	 0.6520
BP	 0.8990	 0.6400
BQ	 0.9400	 0.6520
BR	 0.8630	 0.6040
BS	 0.9460	 0.6560
BT	 0.8890	 0.6210
BU	 0.8210	 0.5660
BV	 0.8840	 0.6410
BW	 0.5050	 0.4500
BX	 0.9030	 0.6360
BY	 0.9010	 0.6330
BZ	 0.9090	 0.6370
Ba	 0.9630	 0.6560
Bb	 0.7560	 0.5580
Bc	 0.8070	 0.5920
Bd	 0.8820	 0.6290
Be	 0.9380	 0.6460
Bf	 0.9500	 0.6570
Bg	 0.9060	 0.6290
Bh	 0.8920	 0.6290
Bi	 0.8670	 0.6150

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Chain	Atom inclusion	Q-score
Bj	 0.9640	 0.6530
Bk	 0.7850	 0.5750
Bl	 0.9280	 0.6400
Bm	 0.9240	 0.6420
Bo	 0.8970	 0.6490
Bp	 0.8950	 0.6420
Br	 0.9360	 0.6430
Bs	 0.0060	 0.0310
Bt	 0.0020	 0.0450
Bv	 0.0720	 0.1750