



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 03:59 PM UTC

PDB ID : 9QF5 / pdb_00009qf5
EMDB ID : EMD-53099
Title : Structure of P. furiosus 70S ribosome grown at 102deg
Authors : Matzov, D.; Georgeson, J.; Westhof, E.; Schwartz, S.; Shalev-Benami, M.
Deposited on : 2025-03-11
Resolution : 2.84 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:

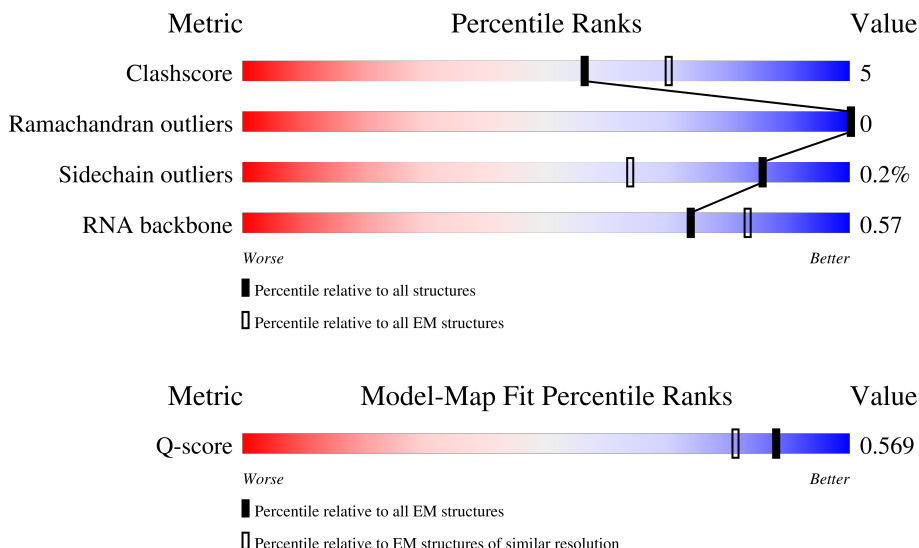
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.84 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11884 (2.34 - 3.34)

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	A1	1497	
2	Aa	202	
3	Ab	210	

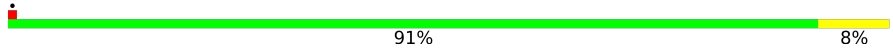
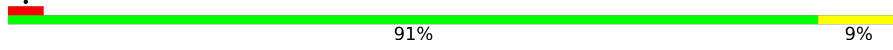
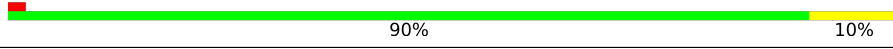
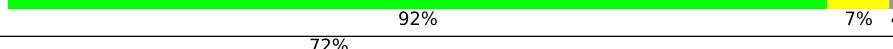
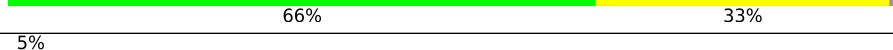
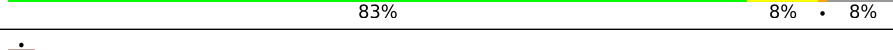
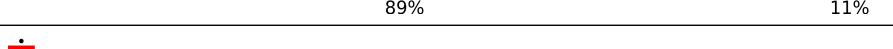
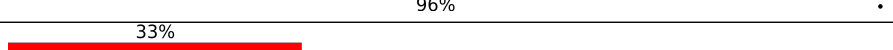
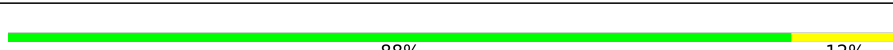
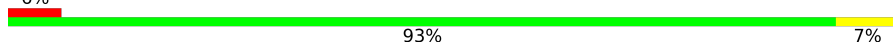
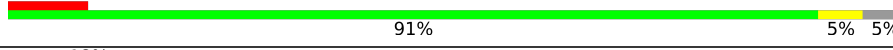
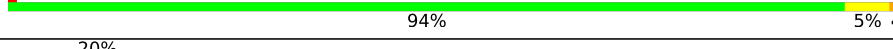
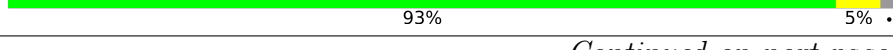
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Mol	Chain	Length	Quality of chain
4	Ac	198	
5	Ad	180	
6	Ae	243	
7	Af	236	
8	Ag	125	
9	Ah	215	
10	Ai	130	
11	Aj	127	
12	Ak	135	
13	Al	102	
14	Am	137	
15	An	147	
16	Ao	148	
17	Ap	56	
18	Aq	158	
19	Ar	113	
20	As	67	
21	At	132	
22	Au	150	
23	Av	99	
24	Aw	63	
25	Ax	71	
26	Ay	60	
27	B1	3051	
28	B2	125	

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Mol	Chain	Length	Quality of chain
29	BA	239	
30	BB	365	
31	BC	255	
32	BD	186	
33	BE	184	
34	BF	123	
34	BG	123	
35	BH	181	
36	BI	142	
37	BJ	141	
38	BK	83	
38	BL	83	
39	BM	147	
40	BN	194	
41	BO	203	
42	BP	120	
43	BQ	150	
44	BR	97	
45	BS	155	
46	BT	86	
47	BU	121	
48	BV	66	
49	BW	72	
50	BX	155	
51	BY	99	

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Mol	Chain	Length	Quality of chain
52	BZ	95	
53	Ba	130	
54	Bb	89	
55	Bc	87	
56	Bd	62	
57	Be	83	
58	Bf	51	
59	Bg	51	
60	Bh	37	
61	Bi	94	
62	Bj	77	
63	Bk	64	

2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 164122 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 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	1490	Total	C	N	O	P	S	0	0
			32256	14418	5942	10405	1490	1		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	5	4AC	C	modified residue	GB 18980902
A1	41	4AC	C	modified residue	GB 18980902
A1	87	4AC	C	modified residue	GB 18980902
A1	141	4AC	C	modified residue	GB 18980902
A1	195	4AC	C	modified residue	GB 18980902
A1	216	4AC	C	modified residue	GB 18980902
A1	220	4AC	C	modified residue	GB 18980902
A1	231	4AC	C	modified residue	GB 18980902
A1	274	4AC	C	modified residue	GB 18980902
A1	291	4AC	C	modified residue	GB 18980902
A1	307	4AC	C	modified residue	GB 18980902
A1	367	4AC	C	modified residue	GB 18980902
A1	382	4AC	C	modified residue	GB 18980902
A1	405	4AC	C	modified residue	GB 18980902
A1	427	4AC	C	modified residue	GB 18980902
A1	444	4AC	C	modified residue	GB 18980902
A1	467	4AC	C	modified residue	GB 18980902
A1	499	4AC	C	modified residue	GB 18980902
A1	534	4AC	C	modified residue	GB 18980902
A1	540	4AC	C	modified residue	GB 18980902
A1	546	4AC	C	modified residue	GB 18980902
A1	578	4AC	C	modified residue	GB 18980902
A1	614	4AC	C	modified residue	GB 18980902
A1	624	4AC	C	modified residue	GB 18980902
A1	636	4AC	C	modified residue	GB 18980902
A1	691	4AC	C	modified residue	GB 18980902
A1	706	4AC	C	modified residue	GB 18980902
A1	719	4AC	C	modified residue	GB 18980902

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Chain	Residue	Modelled	Actual	Comment	Reference
A1	739	4AC	C	modified residue	GB 18980902
A1	761	4AC	C	modified residue	GB 18980902
A1	810	4AC	C	modified residue	GB 18980902
A1	816	4AC	C	modified residue	GB 18980902
A1	827	4AC	C	modified residue	GB 18980902
A1	836	4AC	C	modified residue	GB 18980902
A1	839	4AC	C	modified residue	GB 18980902
A1	856	4AC	C	modified residue	GB 18980902
A1	1016	4AC	C	modified residue	GB 18980902
A1	1029	4AC	C	modified residue	GB 18980902
A1	1067	4AC	C	modified residue	GB 18980902
A1	1092	4AC	C	modified residue	GB 18980902
A1	1135	4AC	C	modified residue	GB 18980902
A1	1181	4AC	C	modified residue	GB 18980902
A1	1221	4AC	C	modified residue	GB 18980902
A1	1227	4AC	C	modified residue	GB 18980902
A1	1254	4AC	C	modified residue	GB 18980902
A1	1288	4AC	C	modified residue	GB 18980902
A1	1314	4AC	C	modified residue	GB 18980902
A1	1467	4AC	C	modified residue	GB 18980902

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Aa	196	Total	C	N	O	S	0	0
			1572	1017	270	281	4		

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ab	195	Total	C	N	O	S	0	0
			1529	979	282	265	3		

- Molecule 4 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ac	185	Total	C	N	O	S	0	0
			1520	983	265	267	5		

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ad	173	Total	C	N	O	S	0	0
			1452	913	280	255	4		

- Molecule 6 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ae	242	Total	C	N	O	S	0	0
			1981	1280	356	340	5		

- Molecule 7 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Af	228	Total	C	N	O	S	0	0
			1800	1139	336	318	7		

- Molecule 8 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ag	124	Total	C	N	O	S	0	0
			975	618	179	177	1		

- Molecule 9 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ah	214	Total	C	N	O	S	0	0
			1728	1095	325	301	7		

- Molecule 10 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Ai	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		

- Molecule 11 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Aj	125	Total	C	N	O		0	0
			982	610	205	167			

- Molecule 12 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Ak	134	Total	C	N	O	S	0	0
			1058	663	201	189	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Al	99	Total	C	N	O	S	0	0
			798	494	155	146	3		

- Molecule 14 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Am	128	Total	C	N	O	S	0	0
			963	597	192	172	2		

- Molecule 15 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	An	144	Total	C	N	O	S	0	0
			1124	715	215	191	3		

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ao	137	Total	C	N	O	S	0	0
			1096	690	216	185	5		

- Molecule 17 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ap	54	Total	C	N	O	S	0	0
			441	279	92	65	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Aq	157	Total	C	N	O	S	0	0
			1302	829	249	220	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ar	107	Total	C	N	O	S	0	0
			877	560	165	149	3		

- Molecule 20 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	As	64	Total	C	N	O	S	0	0
			527	333	101	91	2		

- Molecule 21 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	At	122	Total	C	N	O	S	0	0
			991	635	185	165	6		

- Molecule 22 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Au	149	Total	C	N	O		0	0
			1221	790	219	212			

- Molecule 23 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Av	95	Total	C	N	O	S	0	0
			787	511	128	145	3		

- Molecule 24 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Aw	61	Total	C	N	O	S	0	0
			460	295	82	78	5		

- Molecule 25 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Ax	64	Total	C	N	O		0	0
			508	311	101	96			

- Molecule 26 is a protein called Zn-ribbon RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Ay	56	Total	C	N	O	S	0	0
			434	272	78	76	8		

- Molecule 27 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	B1	2931	Total	C	N	O	P	S	0	0
			63533	28393	11737	20471	2931	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	B2	125	Total	C	N	O	P	0	0
			2689	1198	494	872	125		

- Molecule 29 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BA	238	Total	C	N	O	S	0	0
			1825	1161	345	315	4		

- Molecule 30 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BB	364	Total	C	N	O	S	0	0
			2900	1862	525	499	14		

- Molecule 31 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BC	255	Total	C	N	O	S	0	0
			2026	1288	391	342	5		

- Molecule 32 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BD	184	Total	C	N	O	S	0	0
			1442	905	275	254	8		

- Molecule 33 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BE	183	Total	C	N	O	S	0	0
			1468	951	251	265	1		

- Molecule 34 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BF	122	Total	C	N	O	S	0	0
			931	594	154	180	3		
34	BG	121	Total	C	N	O	S	0	0
			921	588	152	178	3		

- Molecule 35 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BH	167	Total	C	N	O	S	0	0
			1367	868	261	232	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BI	142	Total	C	N	O	S	0	0
			1150	737	215	195	3		

- Molecule 37 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BJ	140	Total	C	N	O	S	0	0
			1062	660	214	185	3		

- Molecule 38 is a protein called Large ribosomal subunit protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BK	81	Total	C	N	O	S	0	0
			614	386	119	108	1		
38	BL	82	Total	C	N	O	S	0	0
			621	391	120	109	1		

- Molecule 39 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BM	147	Total	C	N	O	S	0	0
			1154	727	227	195	5		

- Molecule 40 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BN	193	Total	C	N	O	S	0	0
			1587	1015	315	252	5		

- Molecule 41 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BO	196	Total	C	N	O	S	0	0
			1560	996	294	269	1		

- Molecule 42 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BP	120	Total	C	N	O	S	0	0
			966	606	186	171	3		

- Molecule 43 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BQ	148	Total	C	N	O	S	0	0
			1238	783	252	199	4		

- Molecule 44 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BR	96	Total	C	N	O	S	0	0
			794	506	161	126	1		

- Molecule 45 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BS	151	Total	C	N	O	S	0	0
			1204	770	228	202	4		

- Molecule 46 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BT	86	Total	C	N	O	S	0	0
			696	449	120	126	1		

- Molecule 47 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BU	120	Total	C	N	O	S	0	0
			1003	635	194	170	4		

- Molecule 48 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BV	63	Total	C	N	O	S	0	0
			527	336	100	85	6		

- Molecule 49 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BW	67	Total	C	N	O	S	0	0
			545	338	107	96	4		

- Molecule 50 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BX	154	Total	C	N	O	S	0	0
			1235	783	234	212	6		

- Molecule 51 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BY	97	Total	C	N	O	S	0	0
			730	475	115	139	1		

- Molecule 52 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	BZ	94	Total	C	N	O	0	0
			746	487	138	121		

- Molecule 53 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	Ba	127	Total	C	N	O	S	0	0
			1068	686	214	167	1		

- Molecule 54 is a protein called Large ribosomal subunit protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bb	87	Total	C	N	O	S	0	0
			725	454	156	104	11		

- Molecule 55 is a protein called Large ribosomal subunit protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Bc	86	Total	C	N	O	S	0	0
			677	429	131	116	1		

- Molecule 56 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	Bd	61	Total	C	N	O	S	0	0
			493	304	109	76	4		

- Molecule 57 is a protein called Large ribosomal subunit protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Be	81	Total	C	N	O	S	0	0
			606	378	126	97	5		

- Molecule 58 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	Bf	50	Total	C	N	O	0	0
			437	279	97	61		

- Molecule 59 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Bg	46	Total	C	N	O	S	0	0
			375	238	77	56	4		

- Molecule 60 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Bh	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 61 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Bi	94	Total	C	N	O	S	0	0
			787	499	161	122	5		

- Molecule 62 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bj	77	Total	C	N	O	S	0	0
			659	425	118	115	1		

- Molecule 63 is a protein called C2H2-type domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bk	61	Total	C	N	O	S	0	0
			508	327	102	76	3		

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
64	Af	1	Total	Zn	0
			1	1	
64	Ap	1	Total	Zn	0
			1	1	
64	Ar	1	Total	Zn	0
			1	1	
64	Aw	1	Total	Zn	0
			1	1	
64	Ay	2	Total	Zn	0
			2	2	
64	BV	1	Total	Zn	0
			1	1	
64	Bb	1	Total	Zn	0
			1	1	
64	Bd	1	Total	Zn	0
			1	1	
64	Be	1	Total	Zn	0
			1	1	
64	Bg	1	Total	Zn	0
			1	1	
64	Bi	1	Total	Zn	0
			1	1	
64	Bk	1	Total	Zn	0
			1	1	

- Molecule 65 is water.

Mol	Chain	Residues	Atoms		AltConf
65	A1	69	Total 69	O 69	0
65	Ac	1	Total 1	O 1	0
65	Ae	1	Total 1	O 1	0
65	Ah	1	Total 1	O 1	0
65	Aj	1	Total 1	O 1	0
65	Ak	1	Total 1	O 1	0
65	Aq	1	Total 1	O 1	0
65	B1	1221	Total 1221	O 1221	0
65	B2	9	Total 9	O 9	0
65	BA	16	Total 16	O 16	0
65	BB	12	Total 12	O 12	0
65	BC	14	Total 14	O 14	0
65	BE	2	Total 2	O 2	0
65	BH	7	Total 7	O 7	0
65	BI	5	Total 5	O 5	0
65	BJ	4	Total 4	O 4	0
65	BM	13	Total 13	O 13	0
65	BN	12	Total 12	O 12	0
65	BO	3	Total 3	O 3	0
65	BP	4	Total 4	O 4	0
65	BQ	4	Total 4	O 4	0

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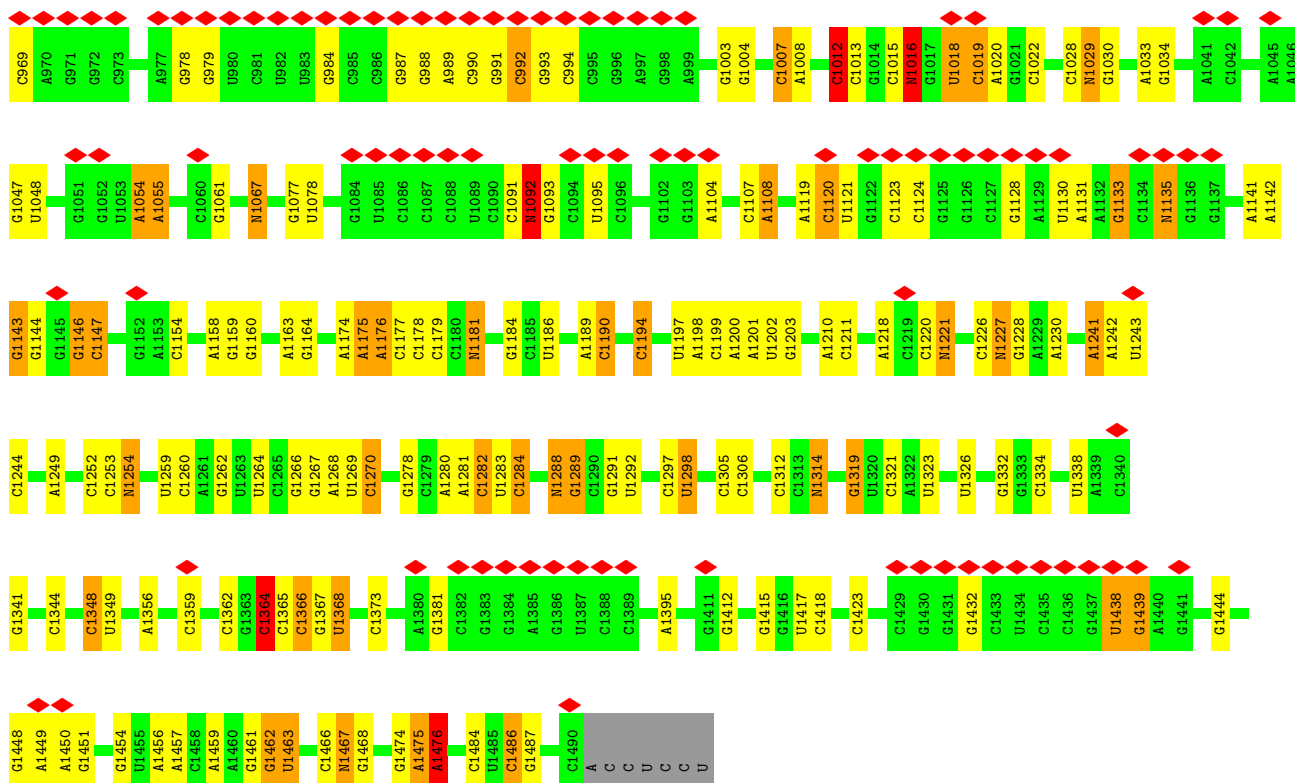
Mol	Chain	Residues	Atoms		AltConf
65	BR	5	Total 5	O 5	0
65	BS	14	Total 14	O 14	0
65	BT	5	Total 5	O 5	0
65	BU	8	Total 8	O 8	0
65	BV	4	Total 4	O 4	0
65	BX	2	Total 2	O 2	0
65	BY	1	Total 1	O 1	0
65	BZ	3	Total 3	O 3	0
65	Ba	11	Total 11	O 11	0
65	Bb	7	Total 7	O 7	0
65	Bc	2	Total 2	O 2	0
65	Bd	7	Total 7	O 7	0
65	Be	2	Total 2	O 2	0
65	Bf	8	Total 8	O 8	0
65	Bg	1	Total 1	O 1	0
65	Bi	1	Total 1	O 1	0
65	Bj	1	Total 1	O 1	0
65	Bk	4	Total 4	O 4	0

3 Residue-property plots

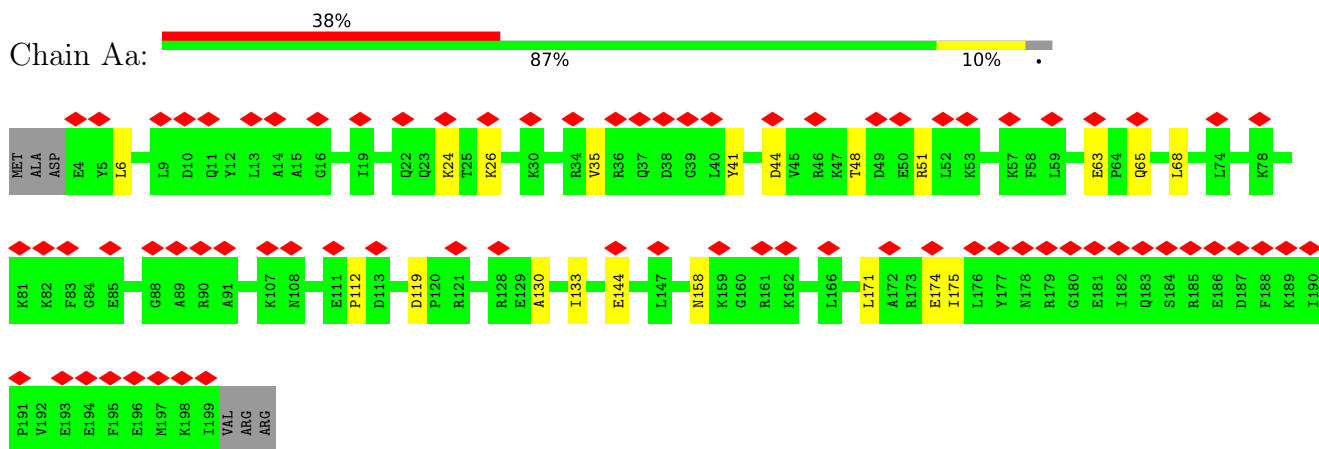
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 16S rRNA

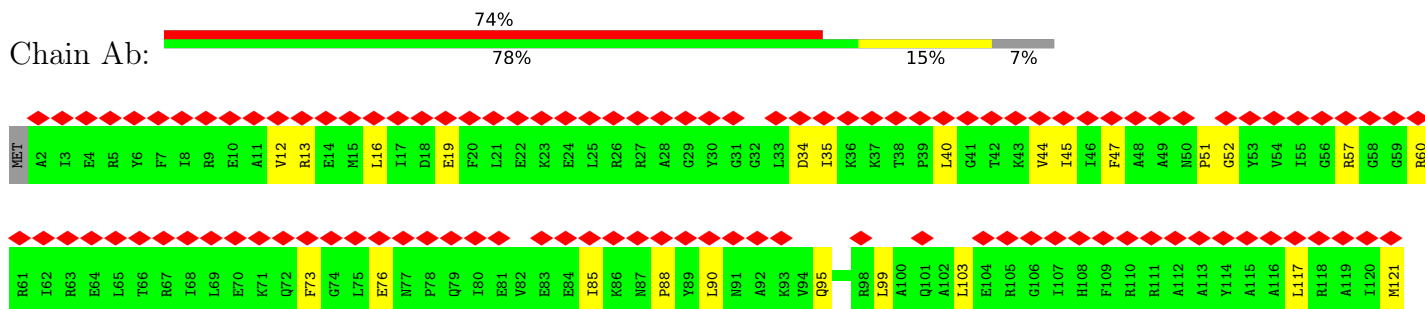


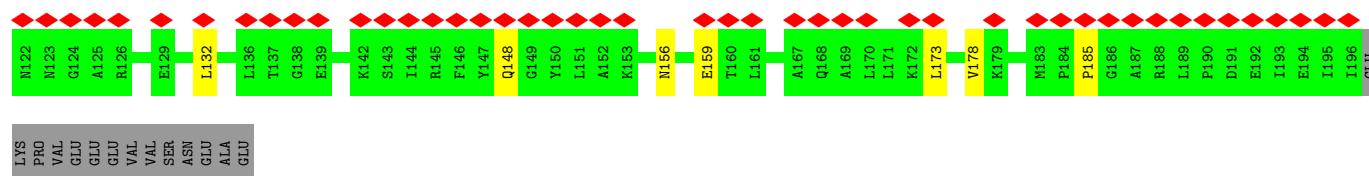


• Molecule 2: Small ribosomal subunit protein uS2



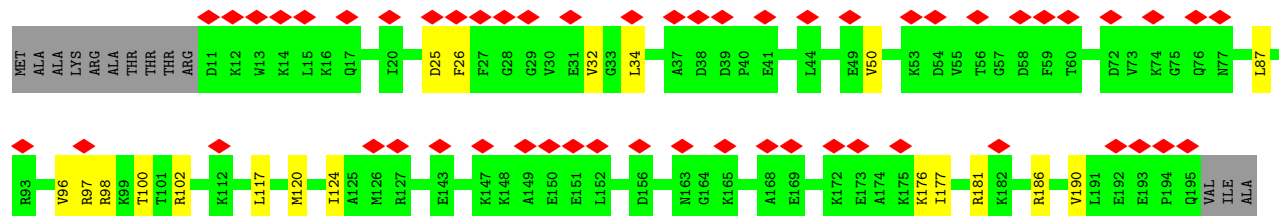
• Molecule 3: Small ribosomal subunit protein uS3





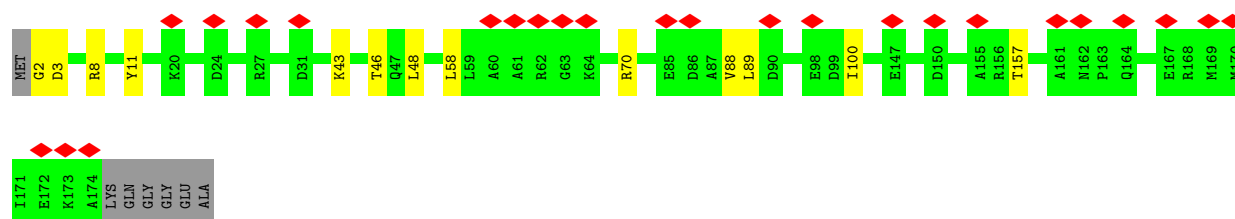
- Molecule 4: Small ribosomal subunit protein eS1

Chain Ac: 27% 84% 10% 7%



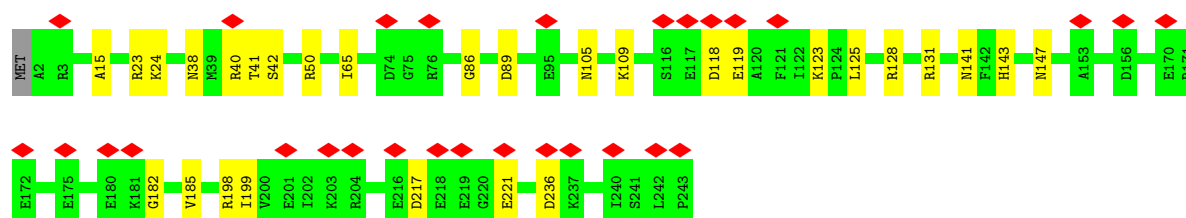
- Molecule 5: Small ribosomal subunit protein uS4

Chain Ad: 14% 89% 7%



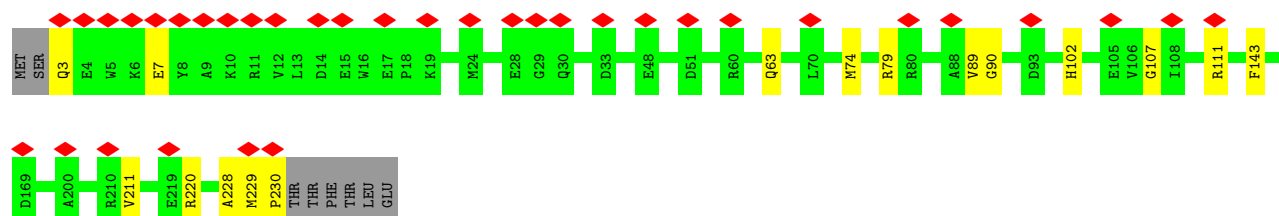
- Molecule 6: Small ribosomal subunit protein eS4

Chain Ae: 12% 88% 12%

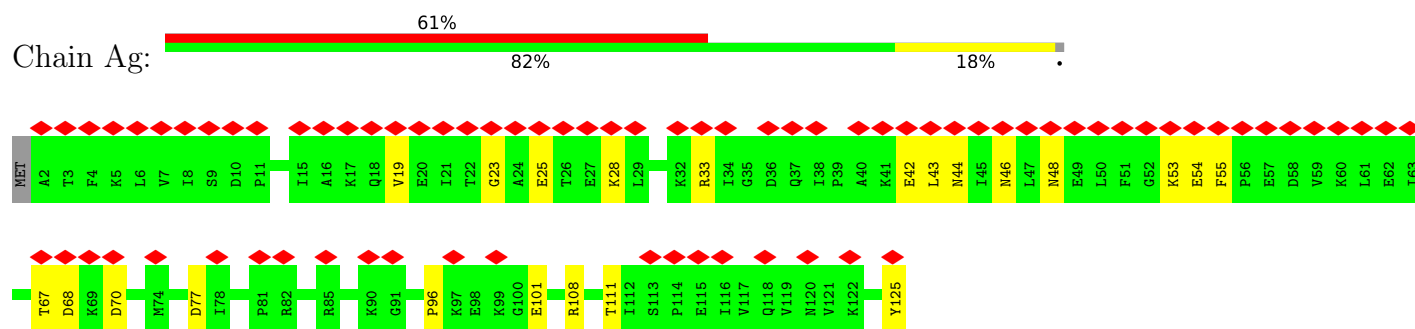


- Molecule 7: Small ribosomal subunit protein uS5

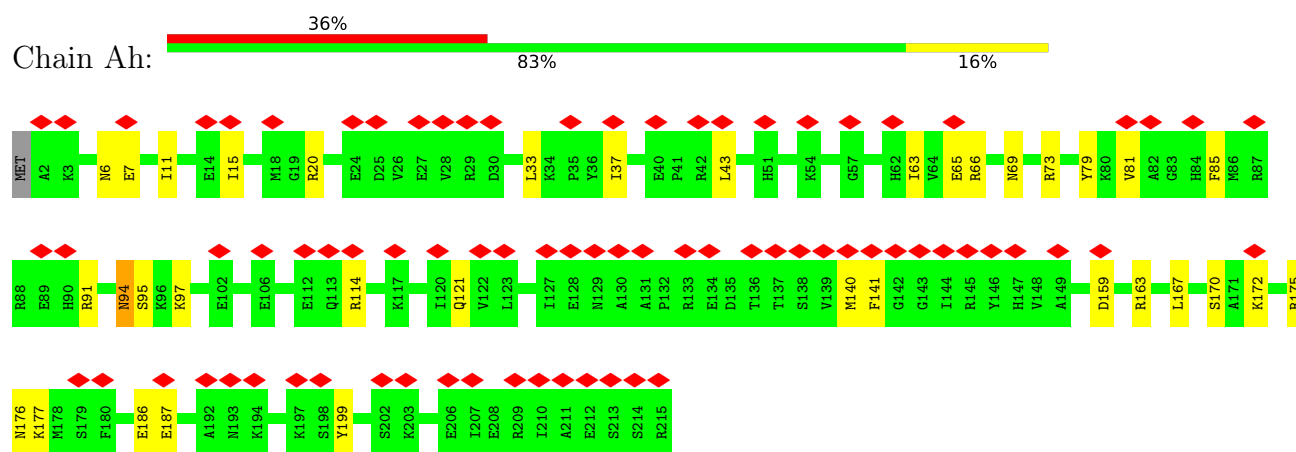
Chain Af: 15% 90% 7%



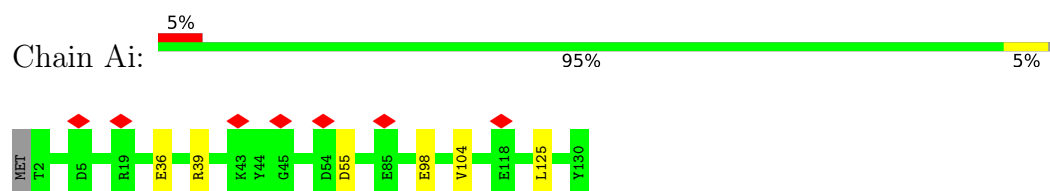
- Molecule 8: Small ribosomal subunit protein eS6



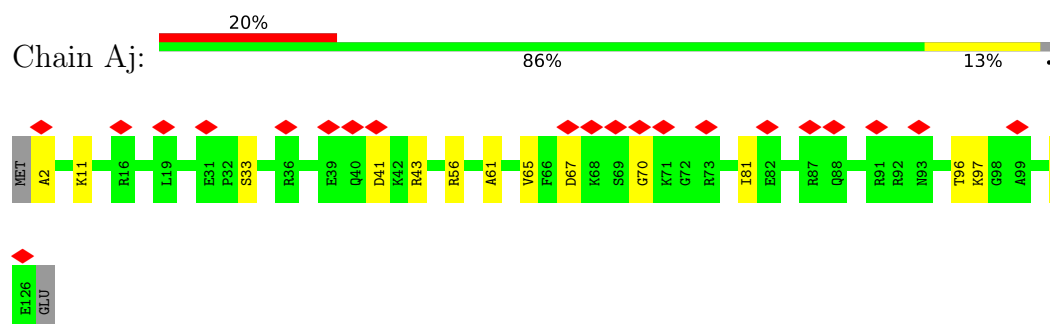
- Molecule 9: Small ribosomal subunit protein uS7



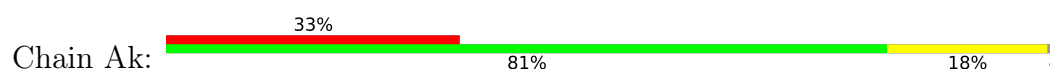
- Molecule 10: Small ribosomal subunit protein uS8

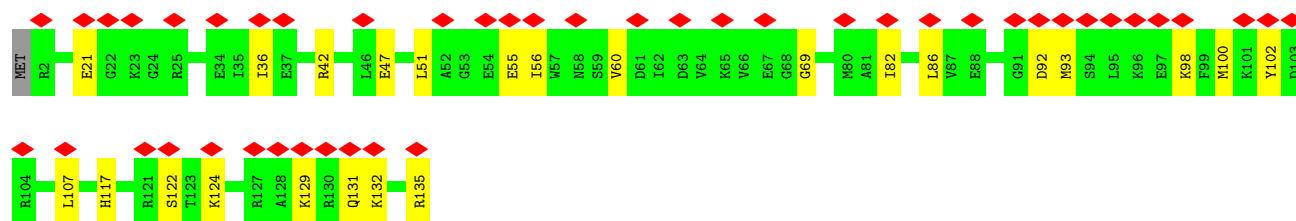


- Molecule 11: Small ribosomal subunit protein eS8

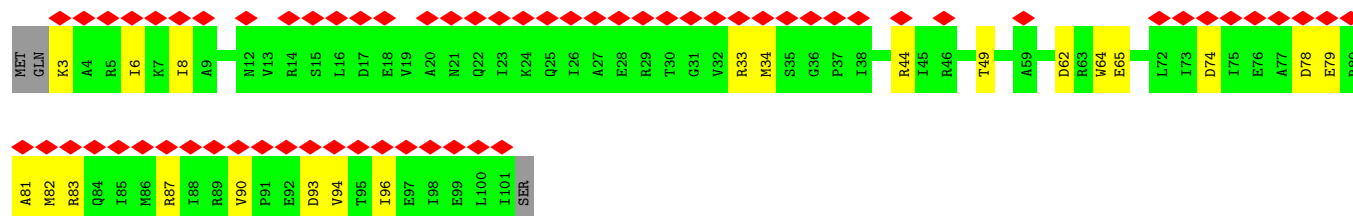
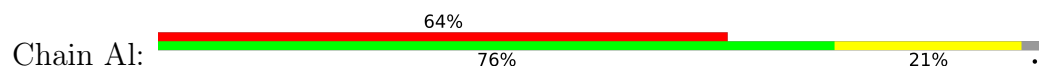


- Molecule 12: Small ribosomal subunit protein uS9

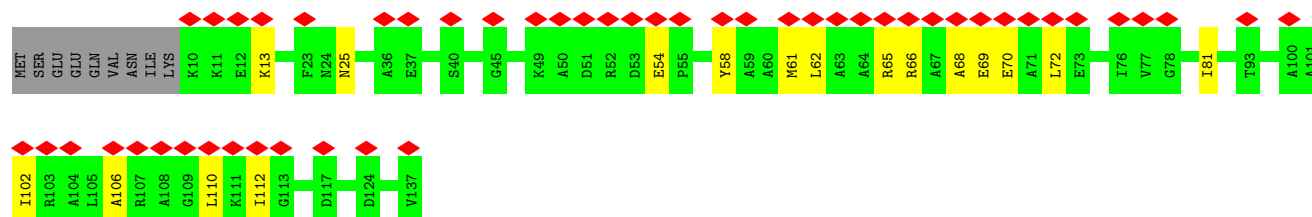
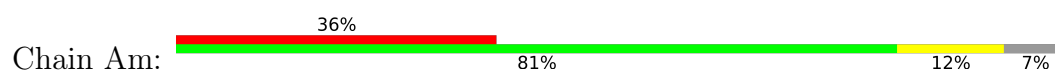




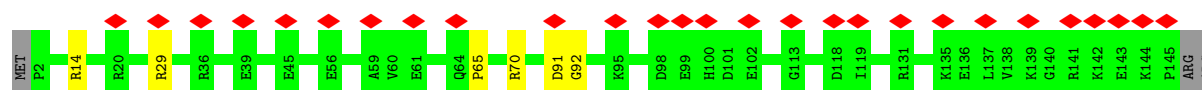
- Molecule 13: Small ribosomal subunit protein uS10



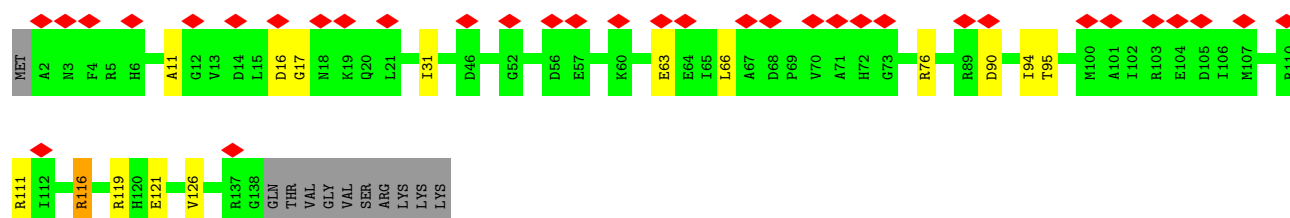
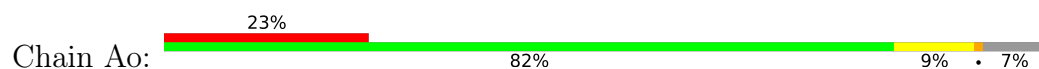
- Molecule 14: Small ribosomal subunit protein uS11



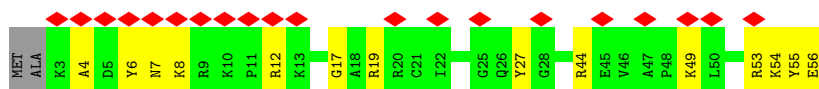
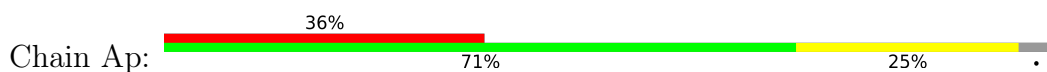
- Molecule 15: Small ribosomal subunit protein uS12



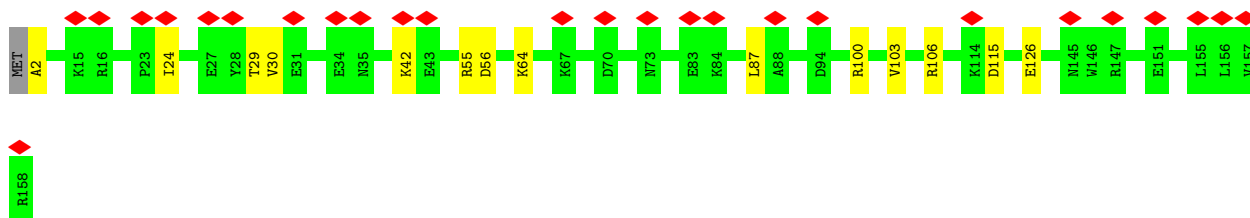
- Molecule 16: Small ribosomal subunit protein uS13



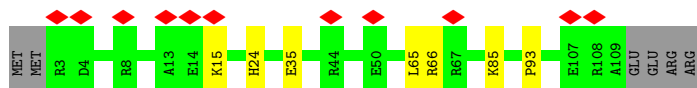
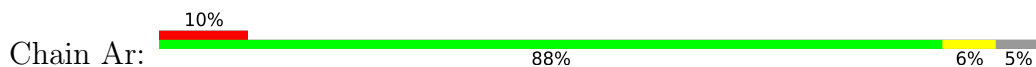
- Molecule 17: Small ribosomal subunit protein uS14



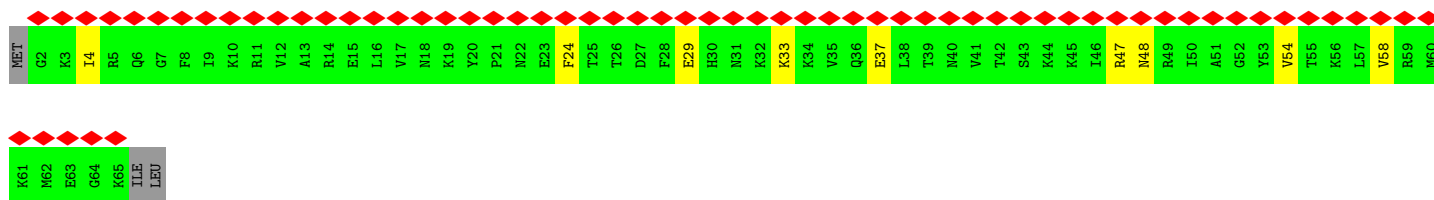
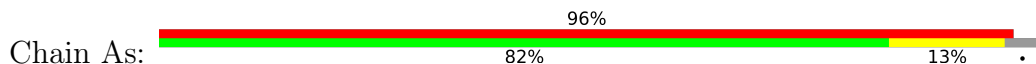
- Molecule 18: Small ribosomal subunit protein uS15



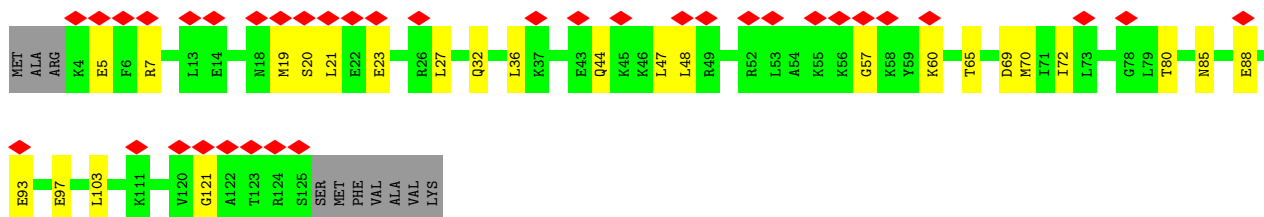
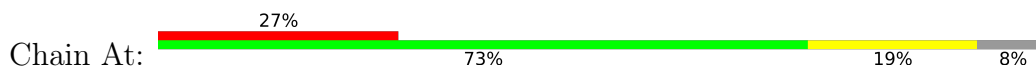
- Molecule 19: Small ribosomal subunit protein uS17



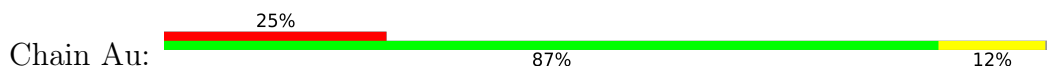
- Molecule 20: Small ribosomal subunit protein eS17

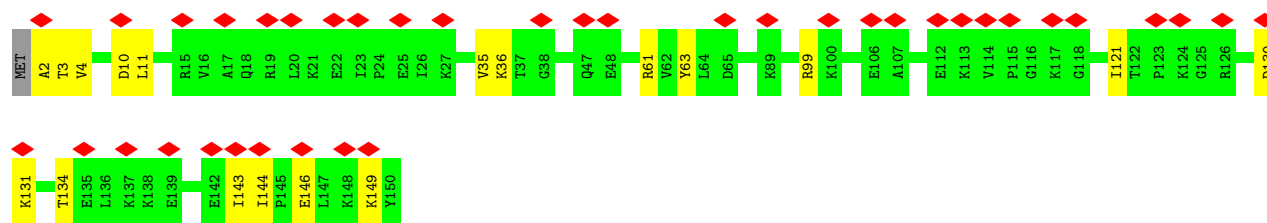


- Molecule 21: Small ribosomal subunit protein uS19

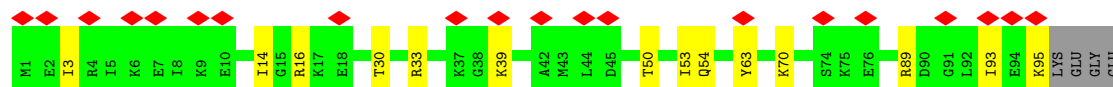
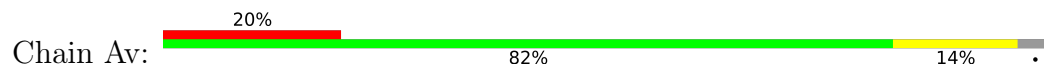


- Molecule 22: Small ribosomal subunit protein eS19

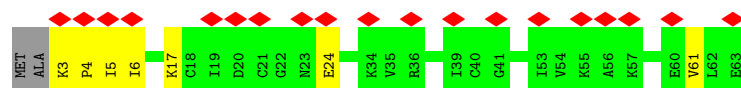
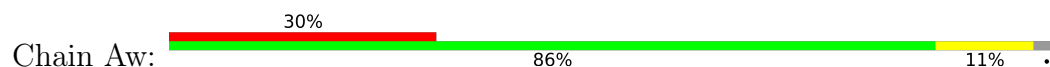




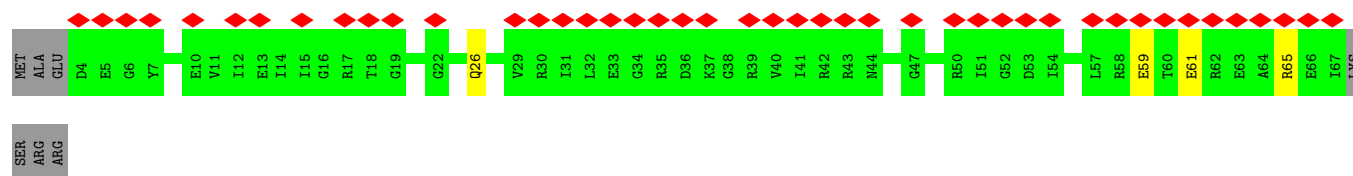
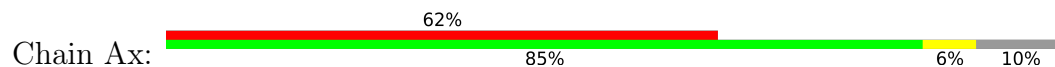
- Molecule 23: Small ribosomal subunit protein eS24



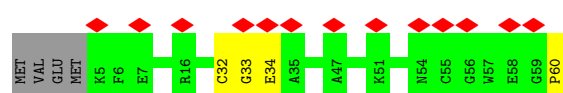
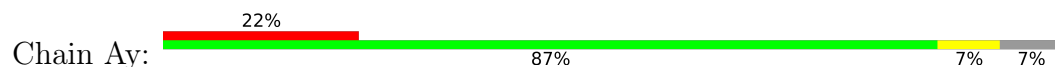
- Molecule 24: Small ribosomal subunit protein eS27



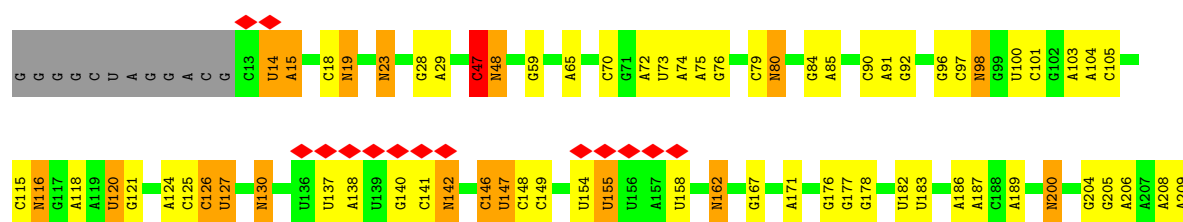
- Molecule 25: Small ribosomal subunit protein eS28



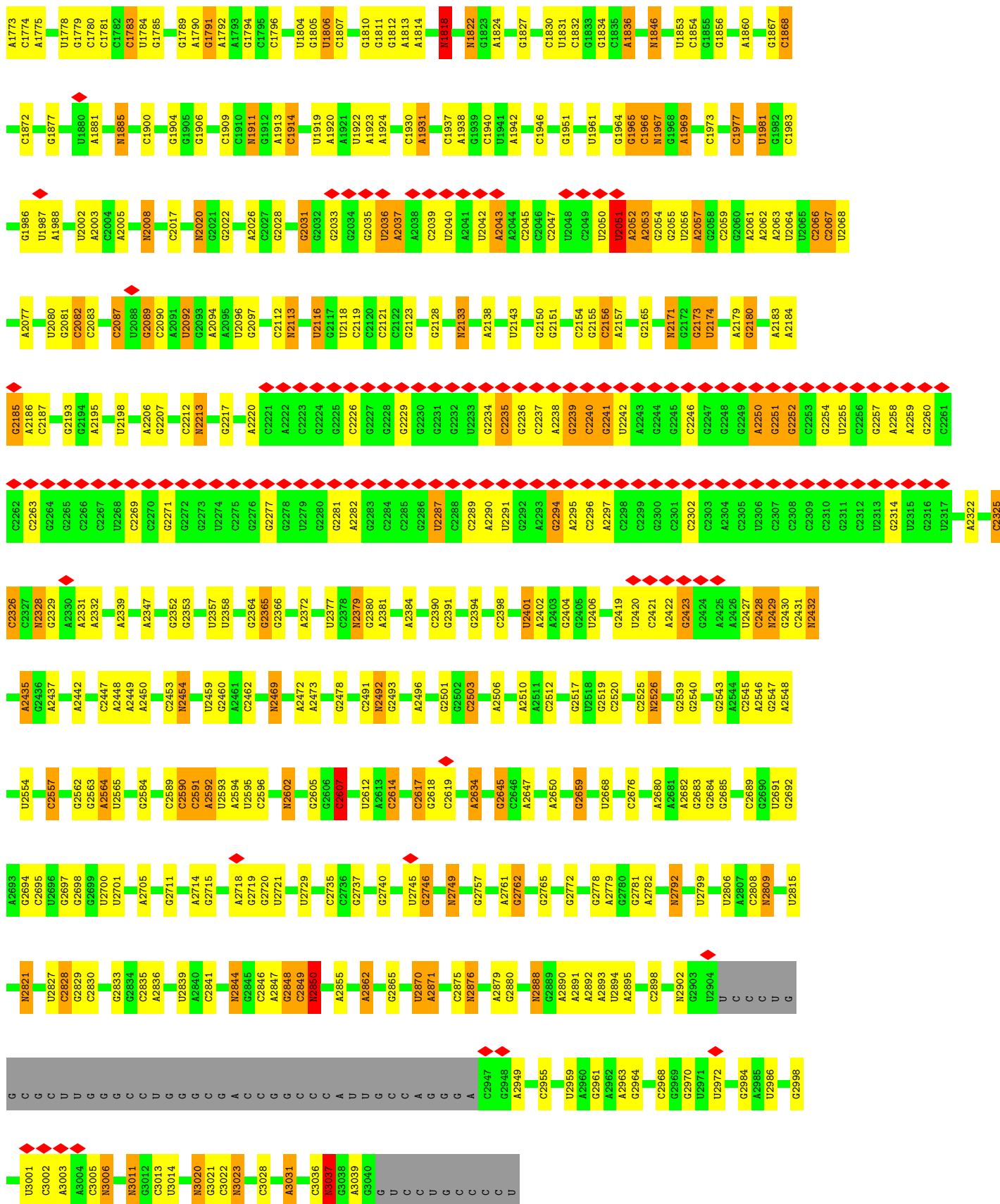
- Molecule 26: Zn-ribbon RNA-binding protein



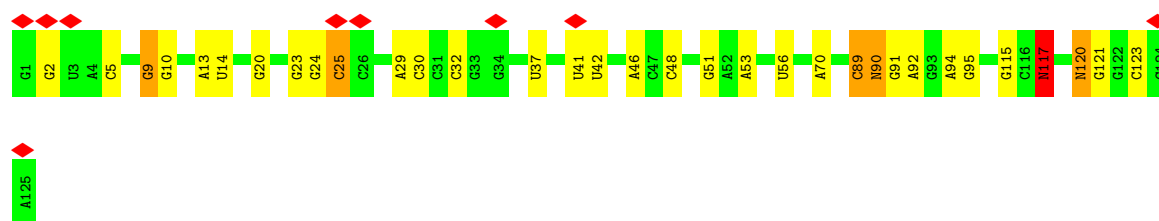
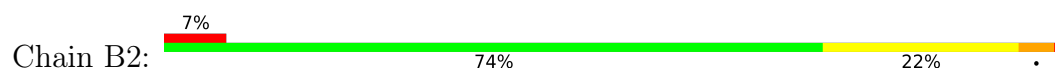
- Molecule 27: 23S rRNA



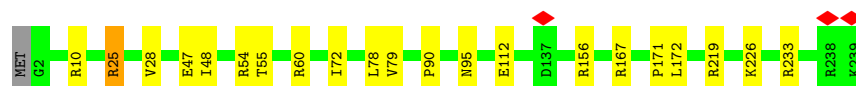




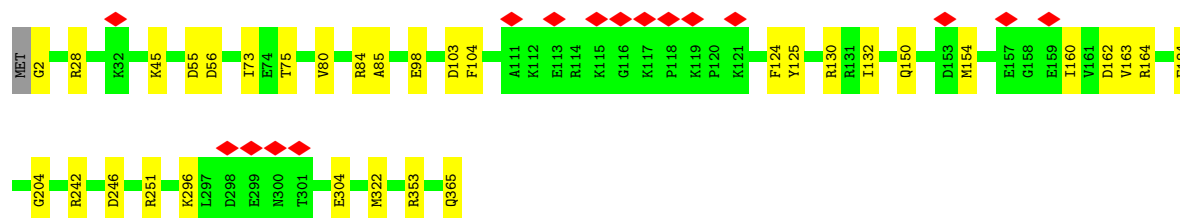
• Molecule 28: 5S rRNA



- Molecule 29: Large ribosomal subunit protein uL2



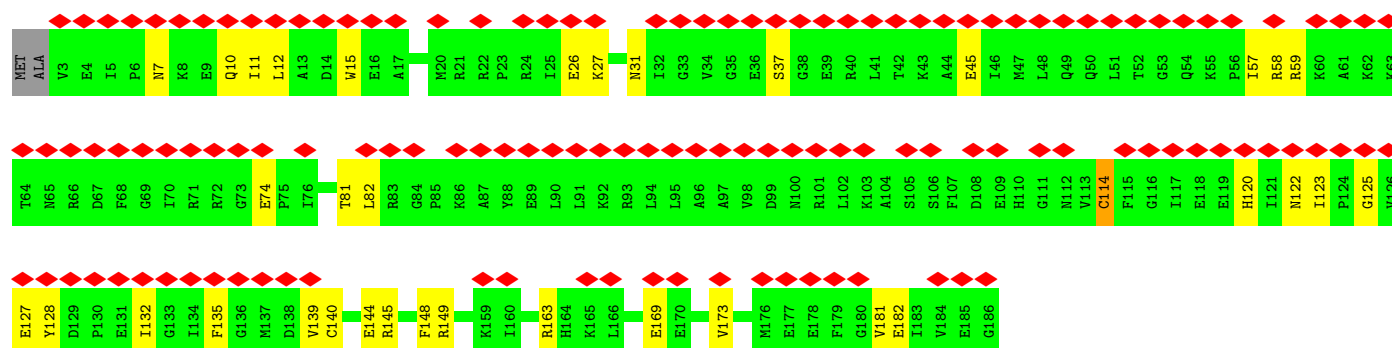
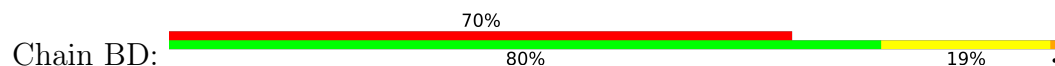
- Molecule 30: Large ribosomal subunit protein uL3



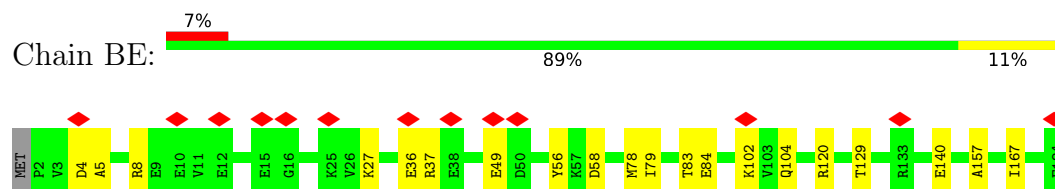
- Molecule 31: Large ribosomal subunit protein uL4



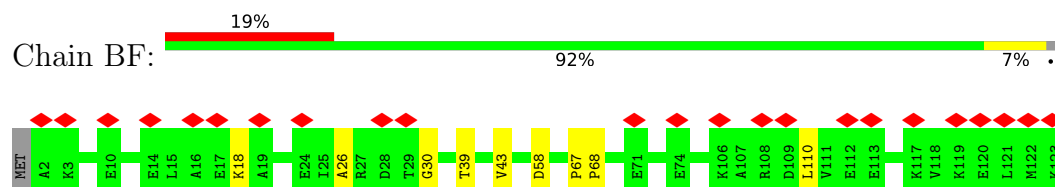
- Molecule 32: Large ribosomal subunit protein uL5



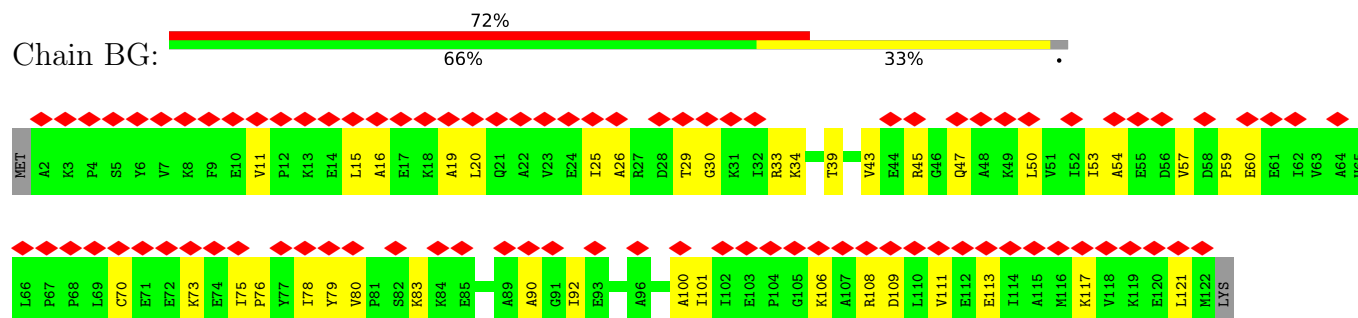
- Molecule 33: Large ribosomal subunit protein uL6



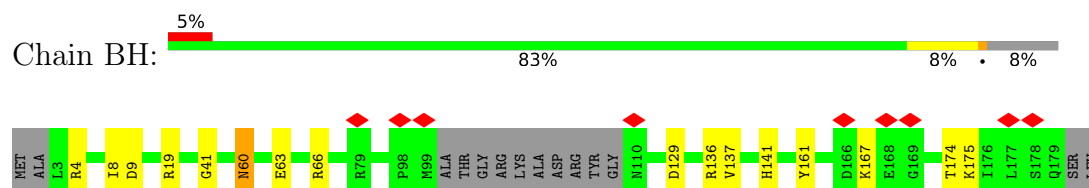
- Molecule 34: Large ribosomal subunit protein eL8



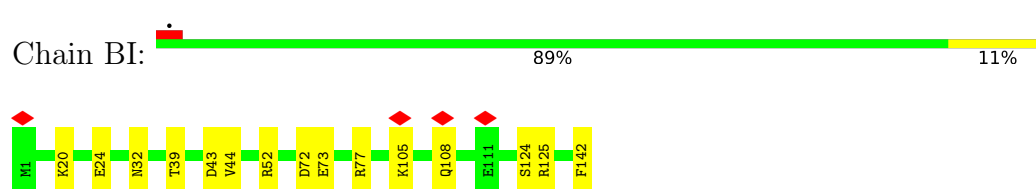
- Molecule 34: Large ribosomal subunit protein eL8



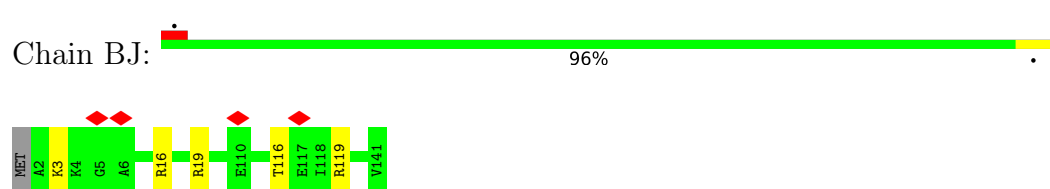
- Molecule 35: Large ribosomal subunit protein uL16



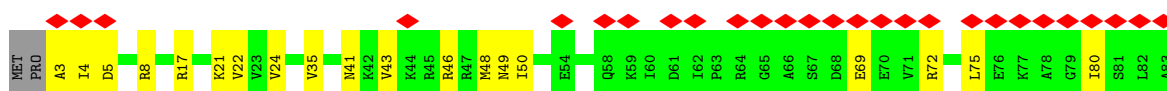
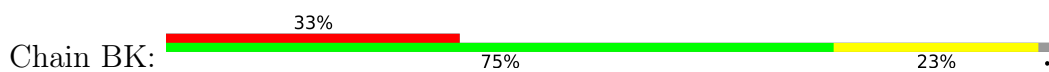
- Molecule 36: Large ribosomal subunit protein uL13



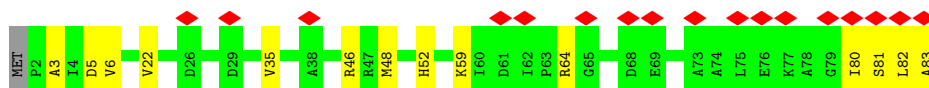
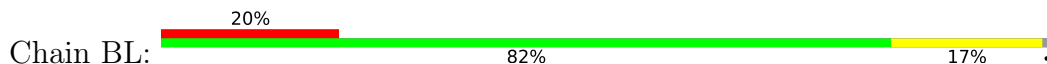
- Molecule 37: Large ribosomal subunit protein uL14



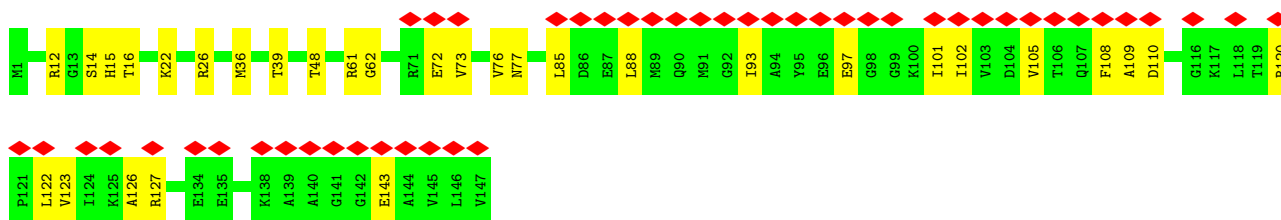
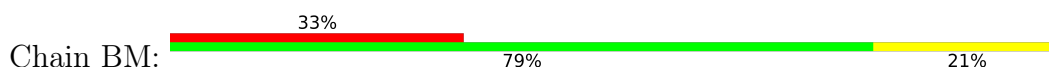
- Molecule 38: Large ribosomal subunit protein eL14



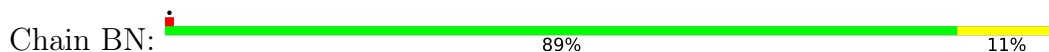
- Molecule 38: Large ribosomal subunit protein eL14



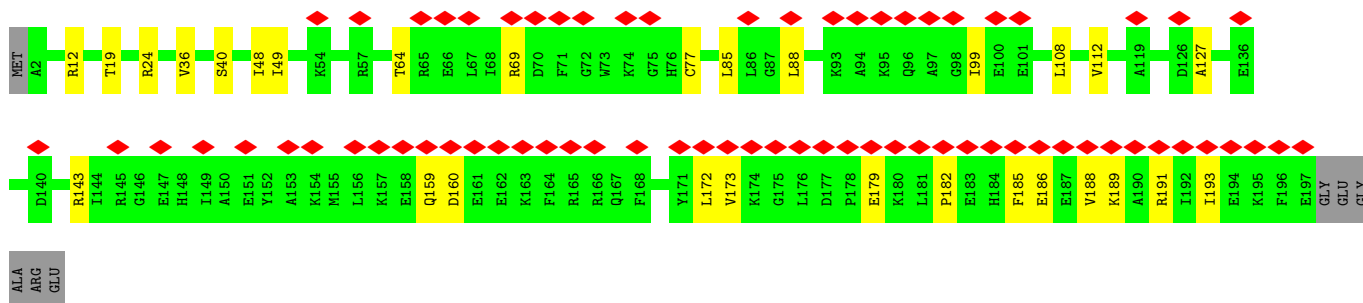
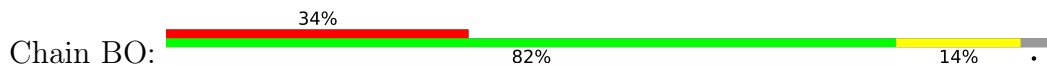
- Molecule 39: Large ribosomal subunit protein uL15



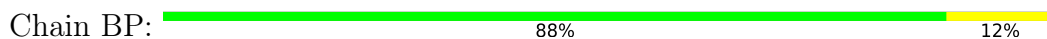
- Molecule 40: Large ribosomal subunit protein eL15



- Molecule 41: Large ribosomal subunit protein uL18

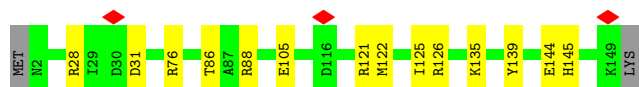


- Molecule 42: Large ribosomal subunit protein eL18





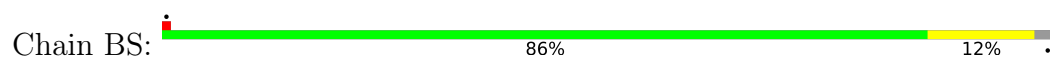
- Molecule 43: Large ribosomal subunit protein eL19



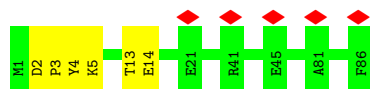
- Molecule 44: Large ribosomal subunit protein eL21



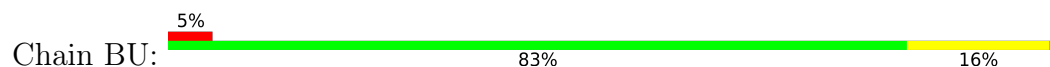
- Molecule 45: Large ribosomal subunit protein uL22



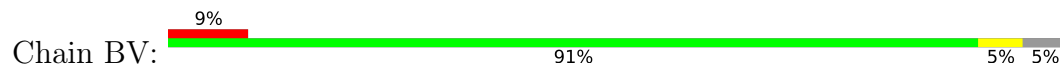
- Molecule 46: Large ribosomal subunit protein uL23



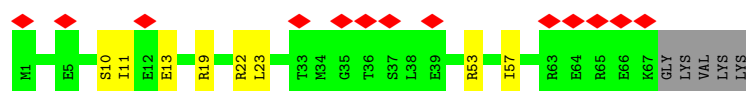
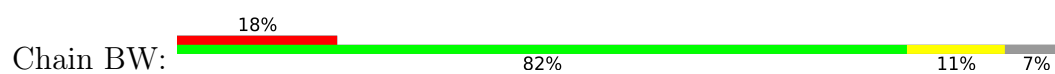
- Molecule 47: Large ribosomal subunit protein uL24



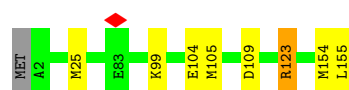
- Molecule 48: Large ribosomal subunit protein eL24



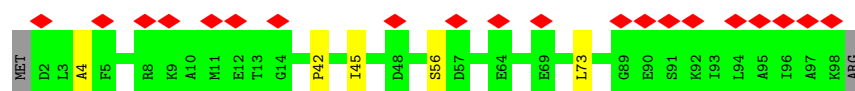
- Molecule 49: Large ribosomal subunit protein uL29



- Molecule 50: Large ribosomal subunit protein uL30



- Molecule 51: Large ribosomal subunit protein eL30



- Molecule 52: Large ribosomal subunit protein eL31



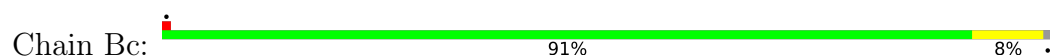
- Molecule 53: Large ribosomal subunit protein eL32



- Molecule 54: Large ribosomal subunit protein eL34



- Molecule 55: Large ribosomal subunit protein eL33

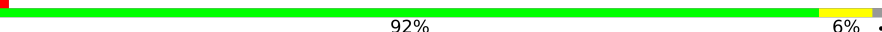


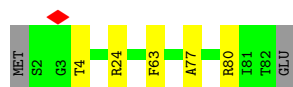
- Molecule 56: Large ribosomal subunit protein eL37

Chain Bd:  94% 5%



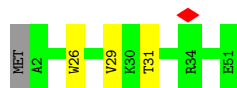
- Molecule 57: Large ribosomal subunit protein eL43

Chain Be:  92% 6%



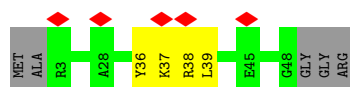
- Molecule 58: Large ribosomal subunit protein eL39

Chain Bf:  92% 6%



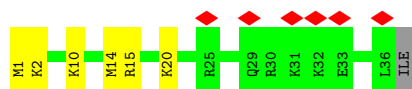
- Molecule 59: Large ribosomal subunit protein eL40

Chain Bg:  10% 82% 8% 10%



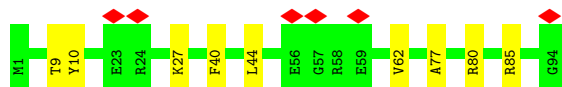
- Molecule 60: Small ribosomal subunit protein eS32

Chain Bh:  16% 81% 16%

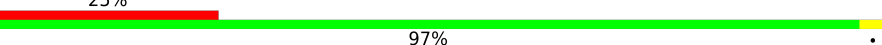


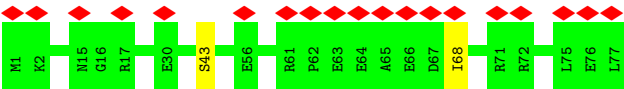
- Molecule 61: Large ribosomal subunit protein eL42

Chain Bi:  6% 90% 10%

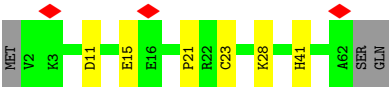
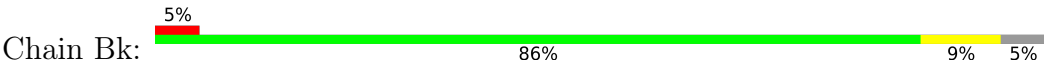


- Molecule 62: Large ribosomal subunit protein eL20

Chain Bj:  25% 97%



- Molecule 63: C2H2-type domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37459	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.01	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.452	Depositor
Minimum map value	-1.201	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.38	Depositor
Map size (Å)	443.52002, 443.52002, 443.52002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.99000007, 0.99000007, 0.99000007	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, ZN, 4SU, OMC, 2MG, A2M, MA6, LHH, 4AC, OMU, G7M, 5MC, A1I59, 5MU, OMG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A1	0.14	0/33307	0.23	0/51887
2	Aa	0.12	0/1603	0.27	0/2167
3	Ab	0.10	0/1551	0.25	0/2083
4	Ac	0.09	0/1546	0.23	0/2072
5	Ad	0.10	0/1476	0.22	0/1980
6	Ae	0.11	0/2030	0.25	0/2739
7	Af	0.20	0/1831	0.33	0/2468
8	Ag	0.11	0/990	0.27	0/1327
9	Ah	0.11	0/1765	0.27	0/2371
10	Ai	0.12	0/1049	0.26	0/1408
11	Aj	0.12	0/991	0.26	0/1322
12	Ak	0.12	0/1074	0.27	0/1438
13	Al	0.11	0/806	0.28	0/1083
14	Am	0.11	0/981	0.28	0/1320
15	An	0.10	0/1141	0.25	0/1518
16	Ao	0.14	0/1115	0.33	0/1500
17	Ap	0.38	0/450	0.66	1/594 (0.2%)
18	Aq	0.14	0/1330	0.30	0/1787
19	Ar	0.13	0/899	0.27	0/1215
20	As	0.09	0/533	0.25	0/708
21	At	0.10	0/1011	0.23	0/1351
22	Au	0.10	0/1251	0.24	0/1686
23	Av	0.11	0/803	0.27	0/1078
24	Aw	0.09	0/467	0.25	0/630
25	Ax	0.11	0/510	0.32	0/684
26	Ay	0.11	0/448	0.26	0/610
27	B1	0.16	0/65902	0.25	1/102618 (0.0%)
28	B2	0.10	0/2927	0.20	0/4559
29	BA	0.14	0/1870	0.29	0/2526
30	BB	0.16	0/2966	0.31	0/3989
31	BC	0.14	0/2068	0.30	0/2787
32	BD	0.25	0/1465	0.39	1/1962 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BE	0.13	0/1499	0.30	0/2022
34	BF	0.11	0/943	0.26	0/1271
34	BG	0.15	0/933	0.39	0/1260
35	BH	0.18	0/1396	0.34	0/1874
36	BI	0.17	0/1168	0.30	0/1561
37	BJ	0.15	0/1075	0.25	0/1448
38	BK	0.10	0/618	0.26	0/829
38	BL	0.12	0/626	0.27	0/840
39	BM	0.17	0/1175	0.34	0/1563
40	BN	0.13	0/1626	0.26	0/2169
41	BO	0.14	0/1598	0.29	0/2154
42	BP	0.14	0/980	0.29	0/1313
43	BQ	0.12	0/1254	0.25	0/1655
44	BR	0.15	0/815	0.29	0/1090
45	BS	0.16	0/1231	0.32	0/1658
46	BT	0.25	0/705	0.54	2/946 (0.2%)
47	BU	0.15	0/1019	0.27	0/1360
48	BV	0.12	0/542	0.25	0/724
49	BW	0.15	0/546	0.28	0/723
50	BX	0.14	0/1254	0.33	0/1677
51	BY	0.12	0/740	0.25	0/1000
52	BZ	0.14	0/760	0.34	0/1024
53	Ba	0.13	0/1093	0.27	0/1459
54	Bb	0.18	0/743	0.38	0/988
55	Bc	0.13	0/686	0.32	0/916
56	Bd	0.22	0/504	0.33	0/667
57	Be	0.13	0/615	0.30	0/820
58	Bf	0.15	0/445	0.26	0/593
59	Bg	0.10	0/384	0.25	0/509
60	Bh	0.18	0/349	0.45	0/451
61	Bi	0.13	0/805	0.24	0/1064
62	Bj	0.14	0/669	0.33	0/884
63	Bk	0.14	0/518	0.32	0/683
All	All	0.15	0/167470	0.27	5/246662 (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
12	Ak	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
29	BA	0	1
31	BC	0	1
45	BS	0	1
50	BX	0	1
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	BT	5	LYS	N-CA-CB	-7.40	98.99	111.27
46	BT	5	LYS	CB-CA-C	6.64	121.59	110.44
27	B1	2051	U	C4'-C3'-O3'	5.38	121.08	113.00
32	BD	114	CYS	CA-CB-SG	5.22	126.42	114.40
17	Ap	4	ALA	N-CA-C	-5.11	106.63	112.92

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	Ak	135	ARG	Sidechain
29	BA	25	ARG	Sidechain
31	BC	128	ARG	Sidechain
45	BS	65	ARG	Sidechain
50	BX	123	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	32256	0	16364	265	0
2	Aa	1572	0	1629	13	0
3	Ab	1529	0	1618	18	0
4	Ac	1520	0	1603	14	0
5	Ad	1452	0	1521	11	0
6	Ae	1981	0	2051	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Af	1800	0	1851	11	0
8	Ag	975	0	1032	18	0
9	Ah	1728	0	1775	30	0
10	Ai	1028	0	1065	5	0
11	Aj	982	0	1066	11	0
12	Ak	1058	0	1105	15	0
13	Al	798	0	845	16	0
14	Am	963	0	994	12	0
15	An	1124	0	1217	5	0
16	Ao	1096	0	1132	9	0
17	Ap	441	0	456	12	0
18	Aq	1302	0	1380	10	0
19	Ar	877	0	898	5	0
20	As	527	0	559	6	0
21	At	991	0	1051	16	0
22	Au	1221	0	1263	15	0
23	Av	787	0	808	10	0
24	Aw	460	0	492	6	0
25	Ax	508	0	533	2	0
26	Ay	434	0	402	3	0
27	B1	63533	0	32139	575	0
28	B2	2689	0	1367	19	0
29	BA	1825	0	1891	15	0
30	BB	2900	0	3050	21	0
31	BC	2026	0	2137	20	0
32	BD	1442	0	1464	29	0
33	BE	1468	0	1507	11	0
34	BF	931	0	982	6	0
34	BG	921	0	969	29	0
35	BH	1367	0	1398	10	0
36	BI	1150	0	1240	9	0
37	BJ	1062	0	1127	4	0
38	BK	614	0	670	10	0
38	BL	621	0	678	10	0
39	BM	1154	0	1219	23	0
40	BN	1587	0	1683	17	0
41	BO	1560	0	1561	26	0
42	BP	966	0	1019	11	0
43	BQ	1238	0	1365	9	0
44	BR	794	0	836	5	0
45	BS	1204	0	1253	17	0
46	BT	696	0	754	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BU	1003	0	1074	15	0
48	BV	527	0	512	2	0
49	BW	545	0	593	6	0
50	BX	1235	0	1314	6	0
51	BY	730	0	768	4	0
52	BZ	746	0	803	4	0
53	Ba	1068	0	1157	10	0
54	Bb	725	0	789	5	0
55	Bc	677	0	731	6	0
56	Bd	493	0	502	2	0
57	Be	606	0	649	4	0
58	Bf	437	0	498	2	0
59	Bg	375	0	394	3	0
60	Bh	343	0	407	7	0
61	Bi	787	0	834	7	0
62	Bj	659	0	699	2	0
63	Bk	508	0	550	4	0
64	Af	1	0	0	0	0
64	Ap	1	0	0	0	0
64	Ar	1	0	0	0	0
64	Aw	1	0	0	0	0
64	Ay	2	0	0	0	0
64	BV	1	0	0	0	0
64	Bb	1	0	0	0	0
64	Bd	1	0	0	0	0
64	Be	1	0	0	0	0
64	Bg	1	0	0	0	0
64	Bi	1	0	0	0	0
64	Bk	1	0	0	0	0
65	A1	69	0	0	19	0
65	Ac	1	0	0	0	0
65	Ae	1	0	0	0	0
65	Ah	1	0	0	0	0
65	Aj	1	0	0	0	0
65	Ak	1	0	0	0	0
65	Aq	1	0	0	0	0
65	B1	1221	0	0	101	0
65	B2	9	0	0	0	0
65	BA	16	0	0	1	0
65	BB	12	0	0	1	0
65	BC	14	0	0	1	0
65	BE	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	BH	7	0	0	0	0
65	BI	5	0	0	0	0
65	BJ	4	0	0	0	0
65	BM	13	0	0	1	0
65	BN	12	0	0	0	0
65	BO	3	0	0	0	0
65	BP	4	0	0	0	0
65	BQ	4	0	0	0	0
65	BR	5	0	0	1	0
65	BS	14	0	0	3	0
65	BT	5	0	0	0	0
65	BU	8	0	0	0	0
65	BV	4	0	0	0	0
65	BX	2	0	0	1	0
65	BY	1	0	0	0	0
65	BZ	3	0	0	0	0
65	Ba	11	0	0	0	0
65	Bb	7	0	0	1	0
65	Bc	2	0	0	1	0
65	Bd	7	0	0	0	0
65	Be	2	0	0	0	0
65	Bf	8	0	0	0	0
65	Bg	1	0	0	0	0
65	Bi	1	0	0	0	0
65	Bj	1	0	0	0	0
65	Bk	4	0	0	0	0
All	All	164122	0	117293	1344	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 1344 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BO:85:LEU:HD11	41:BO:185:PHE:CE1	1.73	1.23
41:BO:85:LEU:CD1	41:BO:185:PHE:CE1	2.27	1.18
41:BO:85:LEU:CD1	41:BO:185:PHE:HE1	1.56	1.18
27:B1:85:A:OP2	47:BU:47:ARG:NH2	1.94	1.00
1:A1:302:G:HO2'	5:Ad:2:GLY:N	1.63	0.96

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	194/202 (96%)	191 (98%)	3 (2%)	0	100	100
3	Ab	193/210 (92%)	191 (99%)	2 (1%)	0	100	100
4	Ac	183/198 (92%)	183 (100%)	0	0	100	100
5	Ad	171/180 (95%)	168 (98%)	3 (2%)	0	100	100
6	Ae	240/243 (99%)	232 (97%)	8 (3%)	0	100	100
7	Af	226/236 (96%)	215 (95%)	11 (5%)	0	100	100
8	Ag	122/125 (98%)	117 (96%)	5 (4%)	0	100	100
9	Ah	212/215 (99%)	202 (95%)	10 (5%)	0	100	100
10	Ai	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
11	Aj	123/127 (97%)	120 (98%)	3 (2%)	0	100	100
12	Ak	132/135 (98%)	125 (95%)	7 (5%)	0	100	100
13	Al	97/102 (95%)	94 (97%)	3 (3%)	0	100	100
14	Am	126/137 (92%)	122 (97%)	4 (3%)	0	100	100
15	An	142/147 (97%)	141 (99%)	1 (1%)	0	100	100
16	Ao	135/148 (91%)	131 (97%)	4 (3%)	0	100	100
17	Ap	52/56 (93%)	45 (86%)	7 (14%)	0	100	100
18	Aq	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
19	Ar	105/113 (93%)	104 (99%)	1 (1%)	0	100	100
20	As	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
21	At	120/132 (91%)	119 (99%)	1 (1%)	0	100	100
22	Au	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
23	Av	93/99 (94%)	89 (96%)	4 (4%)	0	100	100
24	Aw	59/63 (94%)	59 (100%)	0	0	100	100
25	Ax	62/71 (87%)	59 (95%)	3 (5%)	0	100	100
26	Ay	54/60 (90%)	53 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BA	236/239 (99%)	226 (96%)	10 (4%)	0	100	100
30	BB	362/365 (99%)	351 (97%)	11 (3%)	0	100	100
31	BC	253/255 (99%)	247 (98%)	6 (2%)	0	100	100
32	BD	182/186 (98%)	167 (92%)	15 (8%)	0	100	100
33	BE	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
34	BF	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
34	BG	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
35	BH	163/181 (90%)	154 (94%)	9 (6%)	0	100	100
36	BI	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
37	BJ	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
38	BK	79/83 (95%)	71 (90%)	8 (10%)	0	100	100
38	BL	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
39	BM	145/147 (99%)	132 (91%)	13 (9%)	0	100	100
40	BN	191/194 (98%)	187 (98%)	4 (2%)	0	100	100
41	BO	194/203 (96%)	190 (98%)	4 (2%)	0	100	100
42	BP	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
43	BQ	146/150 (97%)	142 (97%)	4 (3%)	0	100	100
44	BR	94/97 (97%)	93 (99%)	1 (1%)	0	100	100
45	BS	149/155 (96%)	145 (97%)	4 (3%)	0	100	100
46	BT	84/86 (98%)	84 (100%)	0	0	100	100
47	BU	118/121 (98%)	114 (97%)	4 (3%)	0	100	100
48	BV	61/66 (92%)	61 (100%)	0	0	100	100
49	BW	65/72 (90%)	65 (100%)	0	0	100	100
50	BX	152/155 (98%)	148 (97%)	4 (3%)	0	100	100
51	BY	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
52	BZ	92/95 (97%)	89 (97%)	3 (3%)	0	100	100
53	Ba	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
54	Bb	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
55	Bc	84/87 (97%)	80 (95%)	4 (5%)	0	100	100
56	Bd	59/62 (95%)	55 (93%)	4 (7%)	0	100	100
57	Be	79/83 (95%)	72 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	Bf	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
59	Bg	44/51 (86%)	42 (96%)	2 (4%)	0	100	100
60	Bh	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
61	Bi	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
62	Bj	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
63	Bk	59/64 (92%)	58 (98%)	1 (2%)	0	100	100
All	All	7873/8194 (96%)	7633 (97%)	240 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	168/173 (97%)	167 (99%)	1 (1%)	78	89
3	Ab	152/167 (91%)	152 (100%)	0	100	100
4	Ac	162/171 (95%)	162 (100%)	0	100	100
5	Ad	156/160 (98%)	156 (100%)	0	100	100
6	Ae	212/213 (100%)	212 (100%)	0	100	100
7	Af	188/197 (95%)	188 (100%)	0	100	100
8	Ag	107/108 (99%)	106 (99%)	1 (1%)	70	84
9	Ah	183/184 (100%)	182 (100%)	1 (0%)	81	90
10	Ai	107/108 (99%)	107 (100%)	0	100	100
11	Aj	100/103 (97%)	100 (100%)	0	100	100
12	Ak	109/111 (98%)	109 (100%)	0	100	100
13	Al	88/91 (97%)	88 (100%)	0	100	100
14	Am	95/104 (91%)	95 (100%)	0	100	100
15	An	117/121 (97%)	117 (100%)	0	100	100
16	Ao	111/122 (91%)	110 (99%)	1 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Ap	43/46 (94%)	43 (100%)	0	100	100
18	Aq	142/143 (99%)	142 (100%)	0	100	100
19	Ar	96/102 (94%)	96 (100%)	0	100	100
20	As	57/61 (93%)	57 (100%)	0	100	100
21	At	105/114 (92%)	105 (100%)	0	100	100
22	Au	126/127 (99%)	126 (100%)	0	100	100
23	Av	85/89 (96%)	85 (100%)	0	100	100
24	Aw	52/54 (96%)	52 (100%)	0	100	100
25	Ax	54/60 (90%)	54 (100%)	0	100	100
26	Ay	48/53 (91%)	48 (100%)	0	100	100
29	BA	187/189 (99%)	186 (100%)	1 (0%)	81	90
30	BB	310/312 (99%)	310 (100%)	0	100	100
31	BC	213/213 (100%)	212 (100%)	1 (0%)	81	90
32	BD	146/158 (92%)	146 (100%)	0	100	100
33	BE	155/156 (99%)	155 (100%)	0	100	100
34	BF	98/99 (99%)	98 (100%)	0	100	100
34	BG	97/99 (98%)	97 (100%)	0	100	100
35	BH	142/152 (93%)	140 (99%)	2 (1%)	59	78
36	BI	122/122 (100%)	119 (98%)	3 (2%)	42	66
37	BJ	107/108 (99%)	107 (100%)	0	100	100
38	BK	64/66 (97%)	64 (100%)	0	100	100
38	BL	65/66 (98%)	65 (100%)	0	100	100
39	BM	117/117 (100%)	116 (99%)	1 (1%)	70	84
40	BN	161/162 (99%)	161 (100%)	0	100	100
41	BO	157/169 (93%)	157 (100%)	0	100	100
42	BP	101/101 (100%)	101 (100%)	0	100	100
43	BQ	128/130 (98%)	128 (100%)	0	100	100
44	BR	86/87 (99%)	86 (100%)	0	100	100
45	BS	126/130 (97%)	126 (100%)	0	100	100
46	BT	77/77 (100%)	77 (100%)	0	100	100
47	BU	110/110 (100%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BV	53/56 (95%)	53 (100%)	0	100	100
49	BW	58/66 (88%)	58 (100%)	0	100	100
50	BX	132/133 (99%)	132 (100%)	0	100	100
51	BY	77/80 (96%)	77 (100%)	0	100	100
52	BZ	76/83 (92%)	76 (100%)	0	100	100
53	Ba	113/117 (97%)	113 (100%)	0	100	100
54	Bb	79/81 (98%)	79 (100%)	0	100	100
55	Bc	73/74 (99%)	73 (100%)	0	100	100
56	Bd	49/51 (96%)	49 (100%)	0	100	100
57	Be	59/61 (97%)	59 (100%)	0	100	100
58	Bf	46/47 (98%)	46 (100%)	0	100	100
59	Bg	37/39 (95%)	37 (100%)	0	100	100
60	Bh	34/35 (97%)	34 (100%)	0	100	100
61	Bi	82/83 (99%)	82 (100%)	0	100	100
62	Bj	72/72 (100%)	72 (100%)	0	100	100
63	Bk	52/55 (94%)	52 (100%)	0	100	100
All	All	6724/6938 (97%)	6712 (100%)	12 (0%)	85	95

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	BH	167	LYS
36	BI	32	ASN
39	BM	120	ARG
36	BI	125	ARG
16	Ao	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	Ab	148	GLN
4	Ac	133	GLN
32	BD	120	HIS
40	BN	174	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1487/1497 (99%)	238 (16%)	14 (0%)
27	B1	2928/3051 (95%)	421 (14%)	28 (0%)
28	B2	124/125 (99%)	15 (12%)	0
All	All	4539/4673 (97%)	674 (14%)	42 (0%)

5 of 674 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	4	C
1	A1	8	OMU
1	A1	17	5MC
1	A1	20	G
1	A1	33	U

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	B1	1186	A
27	B1	2052	A
27	B1	1368	A
27	B1	1914	OMC
27	B1	2251	G

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

316 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	4AC	A1	810	1	21,24,25	3.25	10 (47%)	28,34,37	1.11	4 (14%)
27	4AC	B1	786	27	21,24,25	3.21	10 (47%)	28,34,37	1.07	4 (14%)
27	OMC	B1	2059	27	19,22,23	3.13	8 (42%)	25,31,34	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	OMG	B1	2684	27	23,26,27	2.44	9 (39%)	32,38,41	2.43	10 (31%)
27	OMG	B1	2540	27	23,26,27	2.44	9 (39%)	32,38,41	2.47	10 (31%)
1	5MC	A1	623	1	19,22,23	3.61	8 (42%)	26,32,35	0.97	1 (3%)
1	4AC	A1	141	1	21,24,25	3.29	10 (47%)	28,34,37	1.16	4 (14%)
27	OMG	B1	808	27	23,26,27	2.42	9 (39%)	32,38,41	2.48	10 (31%)
27	OMU	B1	2593	27	19,22,23	3.32	7 (36%)	25,31,34	1.74	5 (20%)
27	4AC	B1	2429	27	21,24,25	3.25	10 (47%)	28,34,37	1.10	4 (14%)
1	5MC	A1	473	1	19,22,23	3.65	8 (42%)	26,32,35	1.00	2 (7%)
1	4AC	A1	231	1	21,24,25	3.22	10 (47%)	28,34,37	1.08	4 (14%)
1	5MC	A1	273	1	19,22,23	3.58	8 (42%)	26,32,35	1.00	1 (3%)
27	4AC	B1	1639	27	21,24,25	3.26	9 (42%)	28,34,37	1.14	4 (14%)
1	5MC	A1	1484	1	19,22,23	3.55	8 (42%)	26,32,35	0.95	2 (7%)
27	4AC	B1	142	27	21,24,25	3.29	10 (47%)	28,34,37	1.12	4 (14%)
1	4AC	A1	1092	1	21,24,25	3.27	10 (47%)	28,34,37	1.12	4 (14%)
27	4AC	B1	1439	27	21,24,25	3.21	10 (47%)	28,34,37	1.09	4 (14%)
27	4AC	B1	1404	27	21,24,25	3.16	10 (47%)	28,34,37	1.27	6 (21%)
27	OMC	B1	2735	27	19,22,23	3.11	8 (42%)	25,31,34	0.73	0
1	OMU	A1	762	1	19,22,23	3.32	7 (36%)	25,31,34	2.13	7 (28%)
1	4AC	A1	624	1	21,24,25	3.26	10 (47%)	28,34,37	1.21	5 (17%)
27	5MC	B1	97	27	19,22,23	3.61	8 (42%)	26,32,35	0.97	2 (7%)
27	4AC	B1	130	27	21,24,25	3.23	10 (47%)	28,34,37	1.48	6 (21%)
28	4AC	B2	90	28	21,24,25	3.23	10 (47%)	28,34,37	1.08	4 (14%)
27	4AC	B1	688	27	21,24,25	3.21	10 (47%)	28,34,37	1.12	4 (14%)
27	5MC	B1	2617	27	19,22,23	3.57	8 (42%)	26,32,35	1.03	2 (7%)
27	4AC	B1	116	27	21,24,25	3.18	10 (47%)	28,34,37	1.06	4 (14%)
27	OMC	B1	1099	27	19,22,23	3.09	8 (42%)	25,31,34	0.69	0
1	G7M	A1	481	1	23,26,27	3.70	12 (52%)	34,39,42	1.74	6 (17%)
27	4AC	B1	2171	27	21,24,25	3.19	10 (47%)	28,34,37	1.07	4 (14%)
27	4AC	B1	1769	27	21,24,25	3.16	10 (47%)	28,34,37	1.08	4 (14%)
27	4AC	B1	2902	27	21,24,25	0.37	0	28,34,37	0.60	0
1	OMG	A1	227	1	23,26,27	2.43	9 (39%)	32,38,41	2.44	11 (34%)
27	4AC	B1	3037	27	21,24,25	3.27	10 (47%)	28,34,37	1.54	7 (25%)
27	4AC	B1	1664	27	21,24,25	3.23	10 (47%)	28,34,37	1.07	4 (14%)
28	4AC	B2	120	28	21,24,25	3.25	10 (47%)	28,34,37	1.07	4 (14%)
27	4AC	B1	1846	27	21,24,25	3.21	10 (47%)	28,34,37	1.06	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	A1	467	1	21,24,25	3.27	10 (47%)	28,34,37	1.12	4 (14%)
27	OMG	B1	2022	27	23,26,27	2.44	9 (39%)	32,38,41	2.38	10 (31%)
27	OMG	B1	841	27	23,26,27	2.44	9 (39%)	32,38,41	2.67	12 (37%)
27	OMC	B1	1832	27	19,22,23	3.15	8 (42%)	25,31,34	0.74	0
27	A2M	B1	2506	27	22,25,26	3.46	9 (40%)	30,36,39	2.62	13 (43%)
27	A2M	B1	857	27	22,25,26	3.47	9 (40%)	30,36,39	2.62	13 (43%)
1	5MC	A1	1486	1	19,22,23	3.61	8 (42%)	26,32,35	1.03	2 (7%)
27	4AC	B1	732	27	21,24,25	3.23	10 (47%)	28,34,37	1.11	4 (14%)
1	4AC	A1	691	1	21,24,25	3.20	10 (47%)	28,34,37	1.09	4 (14%)
1	4SU	A1	756	1	18,21,22	3.98	8 (44%)	25,30,33	2.26	5 (20%)
27	OMG	B1	921	27	23,26,27	2.44	9 (39%)	32,38,41	2.38	10 (31%)
1	5MC	A1	533	1	19,22,23	3.59	8 (42%)	26,32,35	0.95	2 (7%)
1	4AC	A1	291	1	21,24,25	3.22	10 (47%)	28,34,37	1.27	6 (21%)
27	4AC	B1	3020	27	21,24,25	3.22	10 (47%)	28,34,37	1.08	4 (14%)
27	OMG	B1	920	27	23,26,27	2.45	8 (34%)	32,38,41	2.53	10 (31%)
27	4AC	B1	1286	27	21,24,25	3.18	10 (47%)	28,34,37	1.18	4 (14%)
27	4AC	B1	392	27	21,24,25	3.24	10 (47%)	28,34,37	1.10	4 (14%)
27	4SU	B1	2565	27	18,21,22	3.96	8 (44%)	25,30,33	2.29	5 (20%)
1	OMC	A1	1252	1	19,22,23	3.14	8 (42%)	25,31,34	0.70	0
27	5MC	B1	2067	27	19,22,23	3.60	8 (42%)	26,32,35	1.44	5 (19%)
27	4AC	B1	23	27	21,24,25	3.20	10 (47%)	28,34,37	1.10	4 (14%)
27	OMG	B1	2180	27	23,26,27	2.43	9 (39%)	32,38,41	2.43	10 (31%)
27	4AC	B1	1505	27	21,24,25	3.18	10 (47%)	28,34,37	1.08	4 (14%)
1	5MC	A1	523	1	19,22,23	3.61	8 (42%)	26,32,35	0.96	2 (7%)
27	OMG	B1	675	27	23,26,27	2.43	9 (39%)	32,38,41	2.38	12 (37%)
27	4AC	B1	2432	27	21,24,25	3.22	10 (47%)	28,34,37	1.07	4 (14%)
27	OMG	B1	2757	27	23,26,27	2.43	9 (39%)	32,38,41	2.38	13 (40%)
27	4AC	B1	2526	27	21,24,25	3.21	10 (47%)	28,34,37	1.09	4 (14%)
27	4AC	B1	434	27	21,24,25	3.15	10 (47%)	28,34,37	1.08	4 (14%)
27	4AC	B1	1734	27	21,24,25	3.25	10 (47%)	28,34,37	1.14	4 (14%)
27	4AC	B1	479	27	21,24,25	3.21	10 (47%)	28,34,37	1.05	4 (14%)
27	4AC	B1	953	27	21,24,25	3.20	10 (47%)	28,34,37	1.09	4 (14%)
1	OMG	A1	645	1	23,26,27	2.47	8 (34%)	32,38,41	2.54	10 (31%)
1	5MC	A1	826	1	19,22,23	3.61	8 (42%)	26,32,35	0.98	2 (7%)
27	4AC	B1	2492	27	21,24,25	3.19	10 (47%)	28,34,37	1.44	6 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	A1	1067	1	21,24,25	3.25	10 (47%)	28,34,37	1.11	4 (14%)
27	4AC	B1	19	27	21,24,25	3.21	10 (47%)	28,34,37	1.07	4 (14%)
27	4AC	B1	1290	27	21,24,25	3.21	10 (47%)	28,34,37	1.07	4 (14%)
27	4AC	B1	715	27	21,24,25	3.23	10 (47%)	28,34,37	1.10	4 (14%)
1	4AC	A1	636	1	21,24,25	3.26	10 (47%)	28,34,37	1.12	4 (14%)
1	4AC	A1	614	1	21,24,25	3.22	10 (47%)	28,34,37	1.14	4 (14%)
1	MA6	A1	1475	1	23,26,27	1.35	3 (13%)	33,38,41	4.07	14 (42%)
1	4AC	A1	534	1	21,24,25	3.23	10 (47%)	28,34,37	1.08	4 (14%)
27	4AC	B1	276	27	21,24,25	3.23	10 (47%)	28,34,37	1.08	4 (14%)
27	4AC	B1	1546	27	21,24,25	3.21	10 (47%)	28,34,37	1.07	4 (14%)
27	4AC	B1	1178	27	21,24,25	3.23	10 (47%)	28,34,37	1.10	4 (14%)
27	OMG	B1	2365	27	23,26,27	2.45	9 (39%)	32,38,41	2.43	10 (31%)
1	OMU	A1	52	1	19,22,23	3.34	7 (36%)	25,31,34	1.80	5 (20%)
1	MA6	A1	1476	1	23,26,27	1.33	3 (13%)	33,38,41	3.96	14 (42%)
27	4AC	B1	1386	27	21,24,25	3.20	10 (47%)	28,34,37	1.04	4 (14%)
1	4AC	A1	216	1	21,24,25	3.25	10 (47%)	28,34,37	1.50	6 (21%)
27	4AC	B1	1383	27	21,24,25	3.19	10 (47%)	28,34,37	1.08	4 (14%)
1	OMC	A1	1270	1	19,22,23	3.13	8 (42%)	25,31,34	0.73	0
27	4AC	B1	2749	27	21,24,25	3.21	10 (47%)	28,34,37	1.36	6 (21%)
1	4AC	A1	307	1	21,24,25	3.21	10 (47%)	28,34,37	1.11	4 (14%)
1	4AC	A1	1221	1	21,24,25	3.26	10 (47%)	28,34,37	1.11	4 (14%)
27	5MC	B1	1966	27	19,22,23	3.55	8 (42%)	26,32,35	1.00	2 (7%)
27	4AC	B1	1612	27	21,24,25	3.28	10 (47%)	28,34,37	1.11	4 (14%)
1	4AC	A1	836	1	21,24,25	3.24	10 (47%)	28,34,37	1.07	4 (14%)
27	OMG	B1	887	27	23,26,27	2.45	9 (39%)	32,38,41	2.46	11 (34%)
1	2MG	A1	1004	1	23,26,27	2.87	9 (39%)	33,38,41	3.07	13 (39%)
27	4AC	B1	2328	27	21,24,25	3.23	10 (47%)	28,34,37	1.06	4 (14%)
1	4AC	A1	41	1	21,24,25	3.22	10 (47%)	28,34,37	1.06	4 (14%)
27	4AC	B1	652	27	21,24,25	3.22	10 (47%)	28,34,37	1.08	4 (14%)
27	4AC	B1	2809	27	21,24,25	3.19	10 (47%)	28,34,37	1.05	4 (14%)
27	4AC	B1	2821	27	21,24,25	3.24	9 (42%)	28,34,37	1.05	4 (14%)
27	A2M	B1	880	27	22,25,26	3.46	9 (40%)	30,36,39	3.34	16 (53%)
27	5MC	B1	2082	27	19,22,23	3.55	8 (42%)	26,32,35	0.95	1 (3%)
27	LHH	B1	904	27	22,25,26	2.89	6 (27%)	28,35,38	1.45	2 (7%)
27	LHH	B1	502	27	22,25,26	2.83	6 (27%)	28,35,38	1.45	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	3011	27	21,24,25	3.18	10 (47%)	28,34,37	1.05	4 (14%)
27	4AC	B1	337	27	21,24,25	3.19	10 (47%)	28,34,37	1.16	4 (14%)
27	4AC	B1	1751	27	21,24,25	3.22	10 (47%)	28,34,37	1.07	4 (14%)
27	5MC	B1	18	27	19,22,23	3.57	8 (42%)	26,32,35	1.00	2 (7%)
1	OMC	A1	426	1	19,22,23	3.16	8 (42%)	25,31,34	0.73	0
27	OMC	B1	1914	27	19,22,23	3.11	8 (42%)	25,31,34	1.35	2 (8%)
1	4AC	A1	1181	1	21,24,25	3.22	10 (47%)	28,34,37	1.09	4 (14%)
27	5MC	B1	2453	27	19,22,23	3.61	8 (42%)	26,32,35	0.96	1 (3%)
27	4AC	B1	1501	27	21,24,25	3.19	10 (47%)	28,34,37	1.05	4 (14%)
27	OMG	B1	2659	27	23,26,27	2.45	9 (39%)	32,38,41	2.42	10 (31%)
27	A2M	B1	940	27	22,25,26	3.50	9 (40%)	30,36,39	2.62	12 (40%)
1	4AC	A1	367	1	21,24,25	3.24	10 (47%)	28,34,37	1.11	4 (14%)
1	4AC	A1	1288	1	21,24,25	3.24	10 (47%)	28,34,37	1.14	4 (14%)
27	4AC	B1	979	27	21,24,25	3.23	10 (47%)	28,34,37	1.58	7 (25%)
27	5MC	B1	336	27	19,22,23	3.55	8 (42%)	26,32,35	1.10	2 (7%)
27	4AC	B1	1967	27	21,24,25	3.17	10 (47%)	28,34,37	1.03	3 (10%)
1	4AC	A1	427	1	21,24,25	3.30	10 (47%)	28,34,37	1.22	5 (17%)
27	4AC	B1	896	27	21,24,25	3.24	10 (47%)	28,34,37	1.06	4 (14%)
27	4AC	B1	759	27	21,24,25	3.25	10 (47%)	28,34,37	1.11	4 (14%)
27	LHH	B1	641	27	22,25,26	2.88	6 (27%)	28,35,38	1.43	2 (7%)
1	OMG	A1	455	1	23,26,27	2.45	9 (39%)	32,38,41	2.42	10 (31%)
27	4AC	B1	2850	27	21,24,25	3.22	10 (47%)	28,34,37	1.12	4 (14%)
28	4AC	B2	117	28	21,24,25	3.23	10 (47%)	28,34,37	1.06	4 (14%)
27	OMG	B1	2391	27	23,26,27	2.40	9 (39%)	32,38,41	2.35	11 (34%)
27	4AC	B1	1621	27	21,24,25	3.22	10 (47%)	28,34,37	1.23	5 (17%)
27	4AC	B1	580	27	21,24,25	3.23	10 (47%)	28,34,37	1.09	4 (14%)
27	5MC	B1	2087	27	19,22,23	3.59	8 (42%)	26,32,35	0.98	2 (7%)
1	4AC	A1	706	1	21,24,25	3.23	10 (47%)	28,34,37	1.10	4 (14%)
27	OMU	B1	2668	27	19,22,23	3.31	8 (42%)	25,31,34	1.80	5 (20%)
27	4AC	B1	599	27	21,24,25	3.21	10 (47%)	28,34,37	1.07	4 (14%)
27	4AC	B1	2844	27	21,24,25	3.19	10 (47%)	28,34,37	1.05	4 (14%)
27	OMC	B1	501	27	19,22,23	3.09	8 (42%)	25,31,34	0.74	0
27	4AC	B1	378	27	21,24,25	3.40	10 (47%)	28,34,37	1.26	4 (14%)
1	5MC	A1	863	1	19,22,23	3.61	8 (42%)	26,32,35	0.98	2 (7%)
27	4AC	B1	2133	27	21,24,25	3.17	10 (47%)	28,34,37	1.06	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A1I59	A1	1366	1	22,27,28	2.54	6 (27%)	26,39,42	0.77	1 (3%)
1	5MC	A1	681	1	19,22,23	3.61	8 (42%)	26,32,35	0.99	2 (7%)
1	4AC	A1	1314	1	21,24,25	3.25	10 (47%)	28,34,37	1.41	6 (21%)
1	4AC	A1	1016	1	21,24,25	3.26	10 (47%)	28,34,37	1.11	4 (14%)
1	5MC	A1	718	1	19,22,23	3.62	8 (42%)	26,32,35	0.96	1 (3%)
27	4AC	B1	98	27	21,24,25	3.20	10 (47%)	28,34,37	1.05	4 (14%)
27	4AC	B1	1442	27	21,24,25	3.19	10 (47%)	28,34,37	1.07	4 (14%)
27	4AC	B1	80	27	21,24,25	3.22	10 (47%)	28,34,37	1.08	4 (14%)
1	OMU	A1	8	1	19,22,23	3.32	7 (36%)	25,31,34	1.82	5 (20%)
27	4AC	B1	1743	27	21,24,25	3.25	10 (47%)	28,34,37	1.11	4 (14%)
27	OMG	B1	2028	27	23,26,27	2.43	9 (39%)	32,38,41	2.41	10 (31%)
1	4AC	A1	274	1	21,24,25	3.22	10 (47%)	28,34,37	1.08	4 (14%)
27	4AC	B1	2469	27	21,24,25	3.20	10 (47%)	28,34,37	1.09	4 (14%)
27	OMC	B1	2428	27	19,22,23	3.17	8 (42%)	25,31,34	1.05	2 (8%)
27	5MC	B1	2875	27	19,22,23	3.62	8 (42%)	26,32,35	0.98	2 (7%)
27	OMC	B1	2557	27	19,22,23	3.11	8 (42%)	25,31,34	0.71	0
27	4AC	B1	1067	27	21,24,25	3.22	10 (47%)	28,34,37	1.06	4 (14%)
27	5MC	B1	359	27	19,22,23	3.60	8 (42%)	26,32,35	1.00	2 (7%)
1	OMC	A1	834	1	19,22,23	3.12	8 (42%)	25,31,34	0.73	0
1	OMU	A1	775	1	19,22,23	3.34	7 (36%)	25,31,34	1.92	7 (28%)
27	5MC	B1	47	27	19,22,23	3.57	8 (42%)	26,32,35	1.00	2 (7%)
27	4AC	B1	950	27	21,24,25	3.20	10 (47%)	28,34,37	1.06	4 (14%)
1	4AC	A1	839	1	21,24,25	3.22	10 (47%)	28,34,37	1.11	4 (14%)
1	4AC	A1	405	1	21,24,25	3.26	10 (47%)	28,34,37	1.08	4 (14%)
1	OMG	A1	861	1	23,26,27	2.43	9 (39%)	32,38,41	2.37	10 (31%)
27	4AC	B1	1061	27	21,24,25	3.23	10 (47%)	28,34,37	1.33	6 (21%)
27	5MC	B1	1620	27	19,22,23	3.61	8 (42%)	26,32,35	0.95	1 (3%)
27	4AC	B1	1762	27	21,24,25	3.19	10 (47%)	28,34,37	1.11	4 (14%)
1	4AC	A1	87	1	21,24,25	3.23	10 (47%)	28,34,37	1.10	4 (14%)
27	4AC	B1	1374	27	21,24,25	3.22	10 (47%)	28,34,37	1.25	5 (17%)
27	4AC	B1	3023	27	21,24,25	3.21	10 (47%)	28,34,37	1.06	4 (14%)
27	5MC	B1	275	27	19,22,23	3.64	8 (42%)	26,32,35	0.97	2 (7%)
1	4AC	A1	499	1	21,24,25	3.23	10 (47%)	28,34,37	1.10	4 (14%)
27	5MC	B1	1149	27	19,22,23	3.55	8 (42%)	26,32,35	0.97	2 (7%)
27	OMG	B1	2562	27	23,26,27	2.42	9 (39%)	32,38,41	2.41	11 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	721	27	21,24,25	3.22	10 (47%)	28,34,37	1.11	4 (14%)
1	4AC	A1	856	1	21,24,25	3.22	10 (47%)	28,34,37	1.09	4 (14%)
27	4AC	B1	243	27	21,24,25	3.22	10 (47%)	28,34,37	1.12	4 (14%)
1	OMG	A1	507	1	23,26,27	2.45	9 (39%)	32,38,41	2.40	10 (31%)
27	4AC	B1	1052	27	21,24,25	3.22	10 (47%)	28,34,37	1.11	4 (14%)
1	5MC	A1	687	1	19,22,23	3.59	8 (42%)	26,32,35	0.95	1 (3%)
1	4AC	A1	382	1	21,24,25	3.23	10 (47%)	28,34,37	1.08	4 (14%)
27	4AC	B1	2888	27	21,24,25	3.21	10 (47%)	28,34,37	1.08	4 (14%)
1	5MC	A1	951	1	19,22,23	3.62	8 (42%)	26,32,35	0.98	2 (7%)
27	OMC	B1	2808	27	19,22,23	3.11	8 (42%)	25,31,34	0.75	0
27	5MC	B1	1648	27	19,22,23	3.57	8 (42%)	26,32,35	0.96	3 (11%)
1	5MU	A1	926	1	19,22,23	0.26	0	27,32,35	0.34	0
27	4AC	B1	1551	27	21,24,25	3.21	10 (47%)	28,34,37	1.03	4 (14%)
27	LHH	B1	527	27	22,25,26	2.82	6 (27%)	28,35,38	1.59	3 (10%)
27	LHH	B1	1365	27	22,25,26	2.86	6 (27%)	28,35,38	1.51	3 (10%)
27	OMC	B1	2119	27	19,22,23	3.10	8 (42%)	25,31,34	0.74	0
27	4AC	B1	2020	27	21,24,25	3.24	10 (47%)	28,34,37	1.05	4 (14%)
27	OMU	B1	2401	27	19,22,23	3.33	7 (36%)	25,31,34	1.82	5 (20%)
27	OMC	B1	1489	27	19,22,23	3.12	8 (42%)	25,31,34	0.69	0
27	4AC	B1	609	27	21,24,25	3.27	10 (47%)	28,34,37	1.11	4 (14%)
27	A2M	B1	506	27	22,25,26	3.48	9 (40%)	30,36,39	2.58	12 (40%)
27	OMC	B1	2607	27	19,22,23	3.11	8 (42%)	25,31,34	0.69	0
27	4AC	B1	1822	27	21,24,25	3.19	10 (47%)	28,34,37	1.30	6 (21%)
27	LHH	B1	2968	27	22,25,26	2.82	6 (27%)	28,35,38	1.57	3 (10%)
27	4AC	B1	1478	27	21,24,25	3.22	10 (47%)	28,34,37	1.14	4 (14%)
1	5MC	A1	466	1	19,22,23	3.66	8 (42%)	26,32,35	0.98	2 (7%)
27	OMG	B1	214	27	23,26,27	2.44	9 (39%)	32,38,41	2.43	10 (31%)
27	OMU	B1	454	27	19,22,23	3.33	8 (42%)	25,31,34	1.79	5 (20%)
27	4AC	B1	1264	27	21,24,25	3.23	10 (47%)	28,34,37	1.08	4 (14%)
1	4AC	A1	444	1	21,24,25	3.24	10 (47%)	28,34,37	1.11	4 (14%)
27	A2M	B1	262	27	22,25,26	0.25	0	30,36,39	0.54	0
27	5MC	B1	1977	27	19,22,23	3.60	8 (42%)	26,32,35	0.96	2 (7%)
27	4AC	B1	933	27	21,24,25	3.11	10 (47%)	28,34,37	1.42	4 (14%)
27	4AC	B1	741	27	21,24,25	3.25	10 (47%)	28,34,37	1.14	4 (14%)
1	OMC	A1	1194	1	19,22,23	3.15	8 (42%)	25,31,34	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4AC	A1	1135	1	21,24,25	3.28	10 (47%)	28,34,37	1.07	4 (14%)
27	5MC	B1	1451	27	19,22,23	3.55	8 (42%)	26,32,35	1.04	2 (7%)
1	OMG	A1	459	1	23,26,27	2.46	8 (34%)	32,38,41	2.47	10 (31%)
27	OMC	B1	977	27	19,22,23	3.09	8 (42%)	25,31,34	0.75	0
27	OMU	B1	1488	27	19,22,23	3.31	8 (42%)	25,31,34	1.90	7 (28%)
1	4AC	A1	816	1	21,24,25	3.24	10 (47%)	28,34,37	1.10	4 (14%)
27	5MC	B1	1868	27	19,22,23	3.55	8 (42%)	26,32,35	0.96	2 (7%)
27	4AC	B1	1322	27	21,24,25	3.22	10 (47%)	28,34,37	1.08	4 (14%)
1	4AC	A1	1254	1	21,24,25	3.24	10 (47%)	28,34,37	1.14	4 (14%)
1	MA6	A1	1457	1	23,26,27	1.32	3 (13%)	33,38,41	4.06	14 (42%)
27	4AC	B1	1128	27	21,24,25	3.17	10 (47%)	28,34,37	1.04	4 (14%)
27	4AC	B1	3006	27	21,24,25	3.25	10 (47%)	28,34,37	1.11	4 (14%)
27	4AC	B1	1911	27	21,24,25	3.22	10 (47%)	28,34,37	1.06	4 (14%)
27	OMU	B1	1981	27	19,22,23	3.34	7 (36%)	25,31,34	1.82	5 (20%)
27	4AC	B1	1608	27	21,24,25	3.24	10 (47%)	28,34,37	1.31	5 (17%)
1	4AC	A1	546	1	21,24,25	3.26	10 (47%)	28,34,37	1.10	4 (14%)
1	OMG	A1	763	1	23,26,27	2.45	9 (39%)	32,38,41	2.44	10 (31%)
1	4AC	A1	1467	1	21,24,25	3.22	10 (47%)	28,34,37	1.47	6 (21%)
27	4AC	B1	1885	27	21,24,25	3.21	10 (47%)	28,34,37	1.03	4 (14%)
1	OMG	A1	153	1	23,26,27	2.48	8 (34%)	32,38,41	2.46	10 (31%)
27	4AC	B1	2213	27	21,24,25	3.18	10 (47%)	28,34,37	1.09	4 (14%)
27	4AC	B1	2602	27	21,24,25	3.22	10 (47%)	28,34,37	1.07	4 (14%)
1	4AC	A1	195	1	21,24,25	3.30	10 (47%)	28,34,37	1.15	4 (14%)
1	4AC	A1	578	1	21,24,25	3.23	10 (47%)	28,34,37	1.09	4 (14%)
1	5MC	A1	855	1	19,22,23	3.60	8 (42%)	26,32,35	0.96	2 (7%)
27	OMG	B1	1533	27	23,26,27	2.43	9 (39%)	32,38,41	2.38	10 (31%)
1	OMG	A1	329	1	23,26,27	2.46	9 (39%)	32,38,41	2.38	11 (34%)
27	4AC	B1	1703	27	21,24,25	3.25	10 (47%)	28,34,37	1.11	4 (14%)
27	4AC	B1	419	27	21,24,25	3.18	10 (47%)	28,34,37	1.07	4 (14%)
27	A2M	B1	2057	27	22,25,26	3.48	9 (40%)	30,36,39	2.62	12 (40%)
27	5MC	B1	932	27	19,22,23	3.56	8 (42%)	26,32,35	0.97	2 (7%)
27	4AC	B1	1293	27	21,24,25	3.22	10 (47%)	28,34,37	1.06	4 (14%)
27	4AC	B1	1313	27	21,24,25	3.24	10 (47%)	28,34,37	1.12	4 (14%)
27	4AC	B1	271	27	21,24,25	3.24	10 (47%)	28,34,37	1.11	4 (14%)
1	5MC	A1	605	1	19,22,23	3.61	8 (42%)	26,32,35	0.99	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	2876	27	21,24,25	3.23	10 (47%)	28,34,37	1.10	4 (14%)
1	5MC	A1	1190	1	19,22,23	3.63	8 (42%)	26,32,35	0.96	2 (7%)
1	OMG	A1	668	1	23,26,27	2.45	8 (34%)	32,38,41	2.48	10 (31%)
1	4AC	A1	540	1	21,24,25	3.24	10 (47%)	28,34,37	1.10	4 (14%)
27	4AC	B1	1107	27	21,24,25	3.19	10 (47%)	28,34,37	1.05	4 (14%)
27	4AC	B1	1100	27	21,24,25	3.21	10 (47%)	28,34,37	1.08	4 (14%)
1	OMU	A1	425	1	19,22,23	3.29	7 (36%)	25,31,34	1.81	5 (20%)
27	4AC	B1	360	27	21,24,25	3.24	10 (47%)	28,34,37	1.29	6 (21%)
27	OMC	B1	1783	27	19,22,23	3.10	8 (42%)	25,31,34	0.72	0
27	4AC	B1	2008	27	21,24,25	3.19	10 (47%)	28,34,37	1.06	4 (14%)
27	4AC	B1	813	27	21,24,25	3.25	10 (47%)	28,34,37	1.38	5 (17%)
27	4AC	B1	1435	27	21,24,25	3.22	10 (47%)	28,34,37	1.10	4 (14%)
27	4AC	B1	1064	27	21,24,25	3.24	10 (47%)	28,34,37	1.57	5 (17%)
27	4AC	B1	227	27	21,24,25	3.23	10 (47%)	28,34,37	1.10	4 (14%)
1	4AC	A1	220	1	21,24,25	3.24	10 (47%)	28,34,37	1.10	4 (14%)
1	OMG	A1	901	1	23,26,27	2.46	9 (39%)	32,38,41	2.45	10 (31%)
27	4AC	B1	1818	27	21,24,25	3.20	10 (47%)	28,34,37	1.48	6 (21%)
27	UR3	B1	2700	27	19,22,23	3.19	8 (42%)	26,32,35	1.66	4 (15%)
27	4AC	B1	2113	27	21,24,25	3.17	10 (47%)	28,34,37	1.29	6 (21%)
27	4AC	B1	1706	27	21,24,25	3.24	10 (47%)	28,34,37	1.10	4 (14%)
1	OMC	A1	117	1	19,22,23	3.13	8 (42%)	25,31,34	0.94	1 (4%)
27	5MC	B1	226	27	19,22,23	3.58	8 (42%)	26,32,35	0.96	2 (7%)
1	OMU	A1	1368	1	19,22,23	3.32	7 (36%)	25,31,34	1.82	5 (20%)
1	OMG	A1	1003	1	23,26,27	2.47	9 (39%)	32,38,41	2.44	10 (31%)
27	4AC	B1	1757	27	21,24,25	3.21	10 (47%)	28,34,37	1.09	4 (14%)
27	4AC	B1	48	27	21,24,25	3.18	10 (47%)	28,34,37	1.01	3 (10%)
27	4AC	B1	807	27	21,24,25	3.21	10 (47%)	28,34,37	1.09	4 (14%)
27	4AC	B1	344	27	21,24,25	0.39	0	28,34,37	0.54	0
1	4AC	A1	827	1	21,24,25	3.24	10 (47%)	28,34,37	1.07	4 (14%)
27	4AC	B1	2379	27	21,24,25	3.17	10 (47%)	28,34,37	1.11	4 (14%)
27	OMG	B1	2984	27	23,26,27	2.44	9 (39%)	32,38,41	2.40	11 (34%)
1	5MC	A1	1362	1	19,22,23	3.66	8 (42%)	26,32,35	1.00	2 (7%)
1	OMG	A1	228	1	23,26,27	2.43	9 (39%)	32,38,41	2.39	10 (31%)
27	4AC	B1	1649	27	21,24,25	3.21	10 (47%)	28,34,37	1.08	4 (14%)
1	5MC	A1	17	1	19,22,23	3.60	8 (42%)	26,32,35	0.95	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	4AC	B1	798	27	21,24,25	3.19	10 (47%)	28,34,37	1.09	4 (14%)
27	OMG	B1	1557	27	23,26,27	2.45	9 (39%)	32,38,41	2.45	10 (31%)
27	4AC	B1	162	27	21,24,25	3.21	10 (47%)	28,34,37	1.06	4 (14%)
1	5MC	A1	230	1	19,22,23	3.61	8 (42%)	26,32,35	0.98	2 (7%)
27	4AC	B1	866	27	21,24,25	3.22	10 (47%)	28,34,37	1.06	4 (14%)
1	4AC	A1	1029	1	21,24,25	3.28	9 (42%)	28,34,37	1.57	5 (17%)
1	OMG	A1	833	1	23,26,27	2.46	8 (34%)	32,38,41	2.51	10 (31%)
1	5MC	A1	1015	1	19,22,23	3.64	8 (42%)	26,32,35	0.98	2 (7%)
1	4AC	A1	739	1	21,24,25	3.26	10 (47%)	28,34,37	1.13	4 (14%)
1	5MC	A1	1012	1	19,22,23	3.64	8 (42%)	26,32,35	0.99	2 (7%)
27	OMU	B1	2554	27	19,22,23	3.30	8 (42%)	25,31,34	1.80	5 (20%)
27	4AC	B1	1360	27	21,24,25	3.18	10 (47%)	28,34,37	1.17	5 (17%)
27	4AC	B1	200	27	21,24,25	3.19	10 (47%)	28,34,37	1.07	4 (14%)
1	4AC	A1	719	1	21,24,25	3.22	10 (47%)	28,34,37	1.07	4 (14%)
1	A2M	A1	819	1	22,25,26	3.50	9 (40%)	30,36,39	2.64	13 (43%)
27	4AC	B1	1150	27	21,24,25	3.22	10 (47%)	28,34,37	1.32	5 (17%)
1	4AC	A1	1227	1	21,24,25	3.23	10 (47%)	28,34,37	1.09	4 (14%)
1	5MC	A1	1013	1	19,22,23	3.64	8 (42%)	26,32,35	0.97	2 (7%)
1	4AC	A1	5	1	21,24,25	3.25	10 (47%)	28,34,37	1.06	4 (14%)
27	OMG	B1	1601	27	23,26,27	2.44	9 (39%)	32,38,41	2.53	10 (31%)
1	5MC	A1	1348	1	19,22,23	3.65	8 (42%)	26,32,35	1.43	4 (15%)
27	5MC	B1	877	27	19,22,23	3.58	8 (42%)	26,32,35	1.01	2 (7%)
1	LHH	A1	238	1	22,25,26	2.86	6 (27%)	28,35,38	1.58	3 (10%)
27	OMG	B1	2740	27	23,26,27	2.45	9 (39%)	32,38,41	2.44	10 (31%)
27	OMG	B1	1965	27	23,26,27	2.45	8 (34%)	32,38,41	2.66	12 (37%)
27	4AC	B1	2792	27	21,24,25	3.21	10 (47%)	28,34,37	1.09	4 (14%)
27	LHH	B1	1946	27	22,25,26	2.82	6 (27%)	28,35,38	1.41	3 (10%)
1	A2M	A1	361	1	22,25,26	3.48	9 (40%)	30,36,39	2.63	13 (43%)
1	LHH	A1	1364	1	22,25,26	2.90	5 (22%)	28,35,38	1.67	4 (14%)
1	4AC	A1	761	1	21,24,25	3.25	10 (47%)	28,34,37	1.11	4 (14%)
27	4AC	B1	485	27	21,24,25	3.19	10 (47%)	28,34,37	1.07	4 (14%)
27	5MC	B1	1983	27	19,22,23	3.53	8 (42%)	26,32,35	0.92	2 (7%)
27	4AC	B1	2454	27	21,24,25	3.24	10 (47%)	28,34,37	1.09	4 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	A1	810	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	786	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2059	27	-	0/9/27/28	0/2/2/2
27	OMG	B1	2684	27	-	0/9/27/28	0/3/3/3
27	OMG	B1	2540	27	-	0/9/27/28	0/3/3/3
1	5MC	A1	623	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	141	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	808	27	-	0/9/27/28	0/3/3/3
27	OMU	B1	2593	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	2429	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	473	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	231	1	-	0/11/29/30	0/2/2/2
1	5MC	A1	273	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	1639	27	-	3/11/29/30	0/2/2/2
1	5MC	A1	1484	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	142	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1092	1	-	2/11/29/30	0/2/2/2
27	4AC	B1	1439	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1404	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2735	27	-	0/9/27/28	0/2/2/2
1	OMU	A1	762	1	-	0/9/27/28	0/2/2/2
1	4AC	A1	624	1	-	0/11/29/30	0/2/2/2
27	5MC	B1	97	27	-	1/7/25/26	0/2/2/2
27	4AC	B1	130	27	-	0/11/29/30	0/2/2/2
28	4AC	B2	90	28	-	0/11/29/30	0/2/2/2
27	4AC	B1	688	27	-	3/11/29/30	0/2/2/2
27	5MC	B1	2617	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	116	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	1099	27	-	0/9/27/28	0/2/2/2
1	G7M	A1	481	1	-	2/7/25/26	0/3/3/3
27	4AC	B1	2171	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1769	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2902	27	-	4/11/29/30	0/2/2/2
1	OMG	A1	227	1	-	0/9/27/28	0/3/3/3
27	4AC	B1	3037	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1664	27	-	0/11/29/30	0/2/2/2
28	4AC	B2	120	28	-	1/11/29/30	0/2/2/2
27	4AC	B1	1846	27	-	2/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	A1	467	1	-	2/11/29/30	0/2/2/2
27	OMG	B1	2022	27	-	0/9/27/28	0/3/3/3
27	OMG	B1	841	27	-	0/9/27/28	0/3/3/3
27	OMC	B1	1832	27	-	0/9/27/28	0/2/2/2
27	A2M	B1	2506	27	-	0/9/27/28	0/3/3/3
27	A2M	B1	857	27	-	1/9/27/28	0/3/3/3
1	5MC	A1	1486	1	-	3/7/25/26	0/2/2/2
27	4AC	B1	732	27	-	2/11/29/30	0/2/2/2
1	4AC	A1	691	1	-	0/11/29/30	0/2/2/2
1	4SU	A1	756	1	-	0/7/25/26	0/2/2/2
27	OMG	B1	921	27	-	1/9/27/28	0/3/3/3
1	5MC	A1	533	1	-	2/7/25/26	0/2/2/2
1	4AC	A1	291	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	3020	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	920	27	-	1/9/27/28	0/3/3/3
27	4AC	B1	1286	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	392	27	-	2/11/29/30	0/2/2/2
27	4SU	B1	2565	27	-	0/7/25/26	0/2/2/2
1	OMC	A1	1252	1	-	0/9/27/28	0/2/2/2
27	5MC	B1	2067	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	23	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2180	27	-	2/9/27/28	0/3/3/3
27	4AC	B1	1505	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	523	1	-	0/7/25/26	0/2/2/2
27	OMG	B1	675	27	-	2/9/27/28	0/3/3/3
27	4AC	B1	2432	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2757	27	-	1/9/27/28	0/3/3/3
27	4AC	B1	2526	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	434	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1734	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	479	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	953	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	645	1	-	0/9/27/28	0/3/3/3
1	5MC	A1	826	1	-	1/7/25/26	0/2/2/2
27	4AC	B1	2492	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1067	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	19	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1290	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	715	27	-	2/11/29/30	0/2/2/2
1	4AC	A1	636	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	A1	614	1	-	0/11/29/30	0/2/2/2
1	MA6	A1	1475	1	-	0/11/29/30	0/3/3/3
1	4AC	A1	534	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	276	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1546	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1178	27	-	2/11/29/30	0/2/2/2
27	OMG	B1	2365	27	-	2/9/27/28	0/3/3/3
1	OMU	A1	52	1	-	0/9/27/28	0/2/2/2
1	MA6	A1	1476	1	-	1/11/29/30	0/3/3/3
27	4AC	B1	1386	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	216	1	-	1/11/29/30	0/2/2/2
27	4AC	B1	1383	27	-	2/11/29/30	0/2/2/2
1	OMC	A1	1270	1	-	2/9/27/28	0/2/2/2
27	4AC	B1	2749	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	307	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	1221	1	-	0/11/29/30	0/2/2/2
27	5MC	B1	1966	27	-	2/7/25/26	0/2/2/2
27	4AC	B1	1612	27	-	3/11/29/30	0/2/2/2
1	4AC	A1	836	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	887	27	-	2/9/27/28	0/3/3/3
1	2MG	A1	1004	1	-	0/9/27/28	0/3/3/3
27	4AC	B1	2328	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	41	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	652	27	-	1/11/29/30	0/2/2/2
27	4AC	B1	2809	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2821	27	-	0/11/29/30	0/2/2/2
27	A2M	B1	880	27	-	0/9/27/28	0/3/3/3
27	5MC	B1	2082	27	-	0/7/25/26	0/2/2/2
27	LHH	B1	904	27	-	2/13/31/32	0/2/2/2
27	LHH	B1	502	27	-	2/13/31/32	0/2/2/2
27	4AC	B1	3011	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	337	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1751	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	18	27	-	0/7/25/26	0/2/2/2
1	OMC	A1	426	1	-	0/9/27/28	0/2/2/2
27	OMC	B1	1914	27	-	3/9/27/28	0/2/2/2
1	4AC	A1	1181	1	-	0/11/29/30	0/2/2/2
27	5MC	B1	2453	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1501	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2659	27	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	A2M	B1	940	27	-	0/9/27/28	0/3/3/3
1	4AC	A1	367	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	1288	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	979	27	-	4/11/29/30	0/2/2/2
27	5MC	B1	336	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1967	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	427	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	896	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	759	27	-	0/11/29/30	0/2/2/2
27	LHH	B1	641	27	-	2/13/31/32	0/2/2/2
1	OMG	A1	455	1	-	2/9/27/28	0/3/3/3
27	4AC	B1	2850	27	-	2/11/29/30	0/2/2/2
28	4AC	B2	117	28	-	2/11/29/30	0/2/2/2
27	OMG	B1	2391	27	-	2/9/27/28	0/3/3/3
27	4AC	B1	1621	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	580	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	2087	27	-	0/7/25/26	0/2/2/2
1	4AC	A1	706	1	-	2/11/29/30	0/2/2/2
27	OMU	B1	2668	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	599	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2844	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	501	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	378	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	863	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	2133	27	-	0/11/29/30	0/2/2/2
1	A1I59	A1	1366	1	-	5/11/33/34	0/2/2/2
1	5MC	A1	681	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	1314	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	1016	1	-	2/11/29/30	0/2/2/2
1	5MC	A1	718	1	-	1/7/25/26	0/2/2/2
27	4AC	B1	98	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1442	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	80	27	-	0/11/29/30	0/2/2/2
1	OMU	A1	8	1	-	3/9/27/28	0/2/2/2
27	4AC	B1	1743	27	-	2/11/29/30	0/2/2/2
27	OMG	B1	2028	27	-	0/9/27/28	0/3/3/3
1	4AC	A1	274	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	2469	27	-	1/11/29/30	0/2/2/2
27	OMC	B1	2428	27	-	0/9/27/28	0/2/2/2
27	5MC	B1	2875	27	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMC	B1	2557	27	-	1/9/27/28	0/2/2/2
27	4AC	B1	1067	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	359	27	-	0/7/25/26	0/2/2/2
1	OMC	A1	834	1	-	0/9/27/28	0/2/2/2
1	OMU	A1	775	1	-	5/9/27/28	0/2/2/2
27	5MC	B1	47	27	-	1/7/25/26	0/2/2/2
27	4AC	B1	950	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	839	1	-	1/11/29/30	0/2/2/2
1	4AC	A1	405	1	-	0/11/29/30	0/2/2/2
1	OMG	A1	861	1	-	2/9/27/28	0/3/3/3
27	4AC	B1	1061	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	1620	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1762	27	-	1/11/29/30	0/2/2/2
1	4AC	A1	87	1	-	3/11/29/30	0/2/2/2
27	4AC	B1	1374	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	3023	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	275	27	-	2/7/25/26	0/2/2/2
1	4AC	A1	499	1	-	1/11/29/30	0/2/2/2
27	5MC	B1	1149	27	-	0/7/25/26	0/2/2/2
27	OMG	B1	2562	27	-	0/9/27/28	0/3/3/3
27	4AC	B1	721	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	856	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	243	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	507	1	-	0/9/27/28	0/3/3/3
27	4AC	B1	1052	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	687	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	382	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	2888	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	951	1	-	2/7/25/26	0/2/2/2
27	OMC	B1	2808	27	-	0/9/27/28	0/2/2/2
27	5MC	B1	1648	27	-	3/7/25/26	0/2/2/2
1	5MU	A1	926	1	-	2/7/25/26	0/2/2/2
27	4AC	B1	1551	27	-	0/11/29/30	0/2/2/2
27	LHH	B1	527	27	-	2/13/31/32	0/2/2/2
27	LHH	B1	1365	27	-	4/13/31/32	0/2/2/2
27	OMC	B1	2119	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	2020	27	-	0/11/29/30	0/2/2/2
27	OMU	B1	2401	27	-	4/9/27/28	0/2/2/2
27	OMC	B1	1489	27	-	2/9/27/28	0/2/2/2
27	4AC	B1	609	27	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	A2M	B1	506	27	-	0/9/27/28	0/3/3/3
27	OMC	B1	2607	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	1822	27	-	0/11/29/30	0/2/2/2
27	LHH	B1	2968	27	-	2/13/31/32	0/2/2/2
27	4AC	B1	1478	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	466	1	-	2/7/25/26	0/2/2/2
27	OMG	B1	214	27	-	0/9/27/28	0/3/3/3
27	OMU	B1	454	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	1264	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	444	1	-	0/11/29/30	0/2/2/2
27	A2M	B1	262	27	-	0/9/27/28	0/3/3/3
27	5MC	B1	1977	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	933	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	741	27	-	2/11/29/30	0/2/2/2
1	OMC	A1	1194	1	-	0/9/27/28	0/2/2/2
1	4AC	A1	1135	1	-	0/11/29/30	0/2/2/2
27	5MC	B1	1451	27	-	2/7/25/26	0/2/2/2
1	OMG	A1	459	1	-	1/9/27/28	0/3/3/3
27	OMC	B1	977	27	-	0/9/27/28	0/2/2/2
27	OMU	B1	1488	27	-	1/9/27/28	0/2/2/2
1	4AC	A1	816	1	-	0/11/29/30	0/2/2/2
27	5MC	B1	1868	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1322	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1254	1	-	0/11/29/30	0/2/2/2
1	MA6	A1	1457	1	-	3/11/29/30	0/3/3/3
27	4AC	B1	1128	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	3006	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1911	27	-	0/11/29/30	0/2/2/2
27	OMU	B1	1981	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	1608	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	546	1	-	0/11/29/30	0/2/2/2
1	OMG	A1	763	1	-	3/9/27/28	0/3/3/3
1	4AC	A1	1467	1	-	2/11/29/30	0/2/2/2
27	4AC	B1	1885	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	153	1	-	0/9/27/28	0/3/3/3
27	4AC	B1	2213	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2602	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	195	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	578	1	-	0/11/29/30	0/2/2/2
1	5MC	A1	855	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMG	B1	1533	27	-	2/9/27/28	0/3/3/3
1	OMG	A1	329	1	-	1/9/27/28	0/3/3/3
27	4AC	B1	1703	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	419	27	-	0/11/29/30	0/2/2/2
27	A2M	B1	2057	27	-	2/9/27/28	0/3/3/3
27	5MC	B1	932	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1293	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1313	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	271	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	605	1	-	1/7/25/26	0/2/2/2
27	4AC	B1	2876	27	-	1/11/29/30	0/2/2/2
1	5MC	A1	1190	1	-	2/7/25/26	0/2/2/2
1	OMG	A1	668	1	-	0/9/27/28	0/3/3/3
1	4AC	A1	540	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1107	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1100	27	-	0/11/29/30	0/2/2/2
1	OMU	A1	425	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	360	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	1783	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	2008	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	813	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1435	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1064	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	227	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	220	1	-	0/11/29/30	0/2/2/2
1	OMG	A1	901	1	-	0/9/27/28	0/3/3/3
27	4AC	B1	1818	27	-	2/11/29/30	0/2/2/2
27	UR3	B1	2700	27	-	2/7/25/26	0/2/2/2
27	4AC	B1	2113	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1706	27	-	0/11/29/30	0/2/2/2
1	OMC	A1	117	1	-	0/9/27/28	0/2/2/2
27	5MC	B1	226	27	-	0/7/25/26	0/2/2/2
1	OMU	A1	1368	1	-	0/9/27/28	0/2/2/2
1	OMG	A1	1003	1	-	0/9/27/28	0/3/3/3
27	4AC	B1	1757	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	48	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	807	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	344	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	827	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	2379	27	-	1/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMG	B1	2984	27	-	0/9/27/28	0/3/3/3
1	5MC	A1	1362	1	-	1/7/25/26	0/2/2/2
1	OMG	A1	228	1	-	1/9/27/28	0/3/3/3
27	4AC	B1	1649	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	17	1	-	2/7/25/26	0/2/2/2
27	4AC	B1	798	27	-	1/11/29/30	0/2/2/2
27	OMG	B1	1557	27	-	0/9/27/28	0/3/3/3
27	4AC	B1	162	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	230	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	866	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1029	1	-	2/11/29/30	0/2/2/2
1	OMG	A1	833	1	-	0/9/27/28	0/3/3/3
1	5MC	A1	1015	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	739	1	-	0/11/29/30	0/2/2/2
1	5MC	A1	1012	1	-	2/7/25/26	0/2/2/2
27	OMU	B1	2554	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	1360	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	200	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	719	1	-	0/11/29/30	0/2/2/2
1	A2M	A1	819	1	-	0/9/27/28	0/3/3/3
27	4AC	B1	1150	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1227	1	-	0/11/29/30	0/2/2/2
1	5MC	A1	1013	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	5	1	-	2/11/29/30	0/2/2/2
27	OMG	B1	1601	27	-	1/9/27/28	0/3/3/3
1	5MC	A1	1348	1	-	2/7/25/26	0/2/2/2
27	5MC	B1	877	27	-	0/7/25/26	0/2/2/2
1	LHH	A1	238	1	-	2/13/31/32	0/2/2/2
27	OMG	B1	2740	27	-	0/9/27/28	0/3/3/3
27	OMG	B1	1965	27	-	2/9/27/28	0/3/3/3
27	4AC	B1	2792	27	-	0/11/29/30	0/2/2/2
27	LHH	B1	1946	27	-	2/13/31/32	0/2/2/2
1	A2M	A1	361	1	-	0/9/27/28	0/3/3/3
1	LHH	A1	1364	1	-	4/13/31/32	0/2/2/2
1	4AC	A1	761	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	485	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	1983	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	2454	27	-	0/11/29/30	0/2/2/2

The worst 5 of 2829 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	481	G7M	C8-N7	10.84	1.51	1.33
27	B1	880	A2M	C2'-C1'	-9.13	1.30	1.53
1	A1	819	A2M	C2'-C1'	-8.99	1.31	1.53
27	B1	2565	4SU	C4-N3	8.97	1.46	1.37
27	B1	940	A2M	C2'-C1'	-8.96	1.31	1.53

The worst 5 of 1476 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	1457	MA6	N1-C6-N6	-11.71	102.58	116.86
1	A1	1476	MA6	N1-C6-N6	-11.49	102.85	116.86
1	A1	1475	MA6	N1-C6-N6	-11.40	102.97	116.86
1	A1	1475	MA6	C1'-N9-C8	-10.76	103.21	127.09
1	A1	1457	MA6	C1'-N9-C8	-10.18	104.51	127.09

There are no chirality outliers.

5 of 201 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A1	238	LHH	C5-C4-N4-C7
1	A1	238	LHH	N3-C4-N4-C7
1	A1	466	5MC	C3'-C4'-C5'-O5'
1	A1	481	G7M	O4'-C4'-C5'-O5'
1	A1	775	OMU	C1'-C2'-O2'-CM2

There are no ring outliers.

208 monomers are involved in 320 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A1	810	4AC	1	0
27	B1	786	4AC	1	0
1	A1	141	4AC	1	0
27	B1	2429	4AC	1	0
1	A1	231	4AC	1	0
1	A1	273	5MC	2	0
27	B1	1639	4AC	4	0
27	B1	142	4AC	1	0
1	A1	1092	4AC	1	0
27	B1	1439	4AC	2	0
27	B1	1404	4AC	2	0
1	A1	624	4AC	4	0
27	B1	130	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B2	90	4AC	2	0
27	B1	688	4AC	1	0
27	B1	2617	5MC	1	0
27	B1	116	4AC	1	0
27	B1	2171	4AC	1	0
27	B1	1769	4AC	3	0
27	B1	3037	4AC	4	0
27	B1	1664	4AC	2	0
28	B2	120	4AC	1	0
27	B1	1846	4AC	1	0
1	A1	467	4AC	1	0
27	B1	732	4AC	1	0
1	A1	691	4AC	5	0
27	B1	921	OMG	2	0
1	A1	291	4AC	1	0
27	B1	3020	4AC	1	0
27	B1	920	OMG	2	0
27	B1	1286	4AC	4	0
27	B1	392	4AC	1	0
27	B1	2067	5MC	1	0
27	B1	23	4AC	1	0
27	B1	1505	4AC	1	0
27	B1	2432	4AC	2	0
27	B1	2526	4AC	1	0
27	B1	434	4AC	1	0
27	B1	1734	4AC	1	0
27	B1	479	4AC	2	0
27	B1	953	4AC	1	0
1	A1	645	OMG	2	0
27	B1	2492	4AC	3	0
1	A1	1067	4AC	1	0
27	B1	19	4AC	1	0
27	B1	1290	4AC	1	0
27	B1	715	4AC	1	0
1	A1	636	4AC	1	0
1	A1	614	4AC	2	0
1	A1	1475	MA6	2	0
1	A1	534	4AC	1	0
27	B1	276	4AC	1	0
27	B1	1546	4AC	1	0
27	B1	1178	4AC	1	0
1	A1	1476	MA6	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	1386	4AC	1	0
1	A1	216	4AC	1	0
27	B1	1383	4AC	1	0
27	B1	2749	4AC	3	0
1	A1	307	4AC	2	0
1	A1	1221	4AC	1	0
27	B1	1612	4AC	1	0
1	A1	836	4AC	1	0
27	B1	2328	4AC	1	0
1	A1	41	4AC	1	0
27	B1	652	4AC	1	0
27	B1	2809	4AC	2	0
27	B1	2821	4AC	2	0
27	B1	2082	5MC	1	0
27	B1	3011	4AC	1	0
27	B1	337	4AC	1	0
27	B1	1751	4AC	1	0
1	A1	1181	4AC	1	0
27	B1	1501	4AC	1	0
27	B1	2659	OMG	1	0
1	A1	367	4AC	1	0
1	A1	1288	4AC	3	0
27	B1	979	4AC	5	0
27	B1	336	5MC	3	0
27	B1	1967	4AC	1	0
1	A1	427	4AC	4	0
27	B1	896	4AC	2	0
27	B1	759	4AC	1	0
27	B1	2850	4AC	2	0
28	B2	117	4AC	1	0
27	B1	1621	4AC	6	0
27	B1	580	4AC	1	0
27	B1	2087	5MC	1	0
1	A1	706	4AC	2	0
27	B1	599	4AC	2	0
27	B1	2844	4AC	1	0
27	B1	378	4AC	1	0
27	B1	2133	4AC	2	0
1	A1	1366	A1I59	1	0
1	A1	1314	4AC	2	0
1	A1	1016	4AC	2	0
27	B1	98	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	1442	4AC	1	0
27	B1	80	4AC	2	0
27	B1	1743	4AC	1	0
1	A1	274	4AC	1	0
27	B1	2469	4AC	1	0
27	B1	2428	OMC	3	0
27	B1	1067	4AC	1	0
27	B1	47	5MC	1	0
27	B1	950	4AC	1	0
1	A1	839	4AC	1	0
1	A1	405	4AC	1	0
27	B1	1061	4AC	1	0
27	B1	1762	4AC	2	0
1	A1	87	4AC	2	0
27	B1	1374	4AC	6	0
27	B1	3023	4AC	1	0
1	A1	499	4AC	1	0
27	B1	1149	5MC	4	0
27	B1	721	4AC	1	0
1	A1	856	4AC	1	0
27	B1	243	4AC	1	0
27	B1	1052	4AC	2	0
1	A1	687	5MC	1	0
1	A1	382	4AC	2	0
27	B1	2888	4AC	2	0
27	B1	1551	4AC	2	0
27	B1	527	LHH	1	0
27	B1	2020	4AC	1	0
27	B1	609	4AC	1	0
27	B1	2607	OMC	2	0
27	B1	1822	4AC	1	0
27	B1	1478	4AC	4	0
27	B1	214	OMG	1	0
27	B1	454	OMU	1	0
27	B1	1264	4AC	1	0
1	A1	444	4AC	3	0
27	B1	262	A2M	2	0
27	B1	1977	5MC	1	0
27	B1	933	4AC	6	0
27	B1	741	4AC	1	0
1	A1	1194	OMC	1	0
1	A1	1135	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	1451	5MC	1	0
27	B1	1488	OMU	1	0
1	A1	816	4AC	1	0
27	B1	1868	5MC	1	0
27	B1	1322	4AC	2	0
1	A1	1254	4AC	2	0
27	B1	1128	4AC	1	0
27	B1	3006	4AC	2	0
27	B1	1911	4AC	1	0
27	B1	1981	OMU	1	0
27	B1	1608	4AC	6	0
1	A1	546	4AC	1	0
1	A1	1467	4AC	1	0
27	B1	1885	4AC	3	0
27	B1	2213	4AC	2	0
27	B1	2602	4AC	1	0
1	A1	195	4AC	1	0
1	A1	578	4AC	1	0
1	A1	329	OMG	1	0
27	B1	1703	4AC	1	0
27	B1	419	4AC	2	0
27	B1	1293	4AC	1	0
27	B1	1313	4AC	4	0
27	B1	271	4AC	1	0
27	B1	2876	4AC	1	0
1	A1	668	OMG	1	0
1	A1	540	4AC	1	0
27	B1	1107	4AC	2	0
27	B1	1100	4AC	1	0
1	A1	425	OMU	1	0
27	B1	360	4AC	1	0
27	B1	1783	OMC	2	0
27	B1	2008	4AC	1	0
27	B1	813	4AC	3	0
27	B1	1435	4AC	1	0
27	B1	1064	4AC	4	0
27	B1	227	4AC	1	0
1	A1	220	4AC	1	0
27	B1	1818	4AC	1	0
27	B1	2113	4AC	2	0
27	B1	1706	4AC	3	0
1	A1	1368	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	1757	4AC	1	0
27	B1	48	4AC	1	0
27	B1	807	4AC	1	0
1	A1	827	4AC	1	0
27	B1	2379	4AC	1	0
27	B1	1649	4AC	1	0
27	B1	798	4AC	1	0
27	B1	162	4AC	1	0
27	B1	866	4AC	1	0
1	A1	1029	4AC	4	0
1	A1	739	4AC	1	0
1	A1	1012	5MC	1	0
27	B1	1360	4AC	6	0
27	B1	200	4AC	1	0
1	A1	719	4AC	1	0
1	A1	819	A2M	1	0
27	B1	1150	4AC	5	0
1	A1	1227	4AC	4	0
1	A1	5	4AC	1	0
27	B1	1601	OMG	3	0
27	B1	877	5MC	1	0
27	B1	2792	4AC	2	0
1	A1	361	A2M	1	0
1	A1	1364	LHH	1	0
1	A1	761	4AC	1	0
27	B1	485	4AC	4	0
27	B1	2454	4AC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

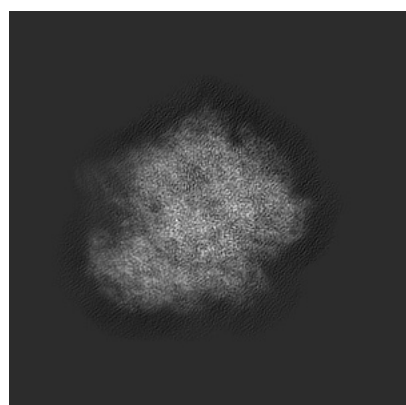
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53099. These allow visual inspection of the internal detail of the map and identification of artifacts.

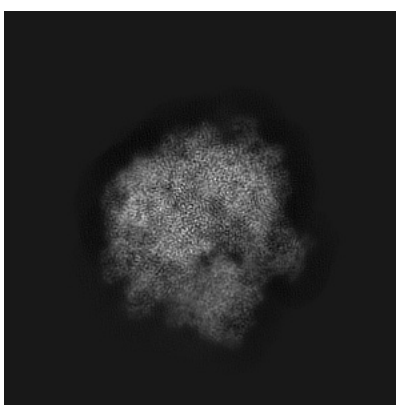
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

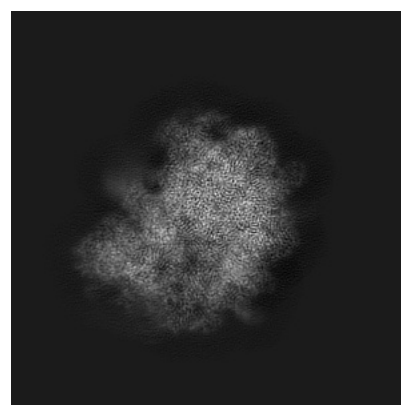
6.1.1 Primary map



X



Y

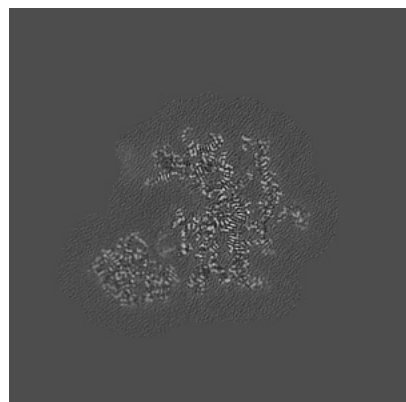


Z

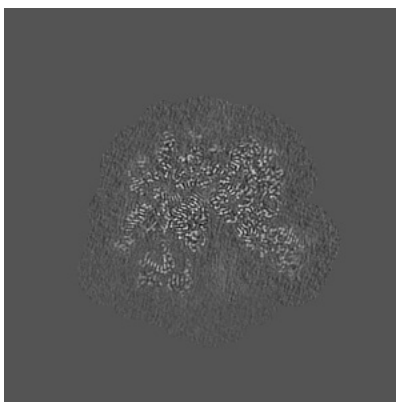
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

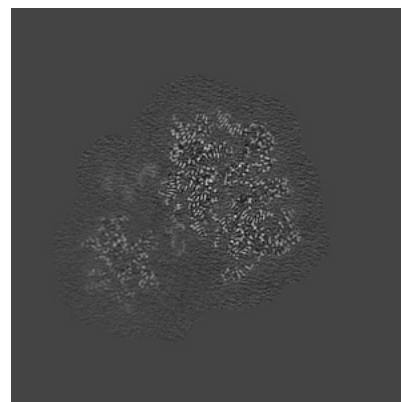
6.2.1 Primary map



X Index: 224



Y Index: 224

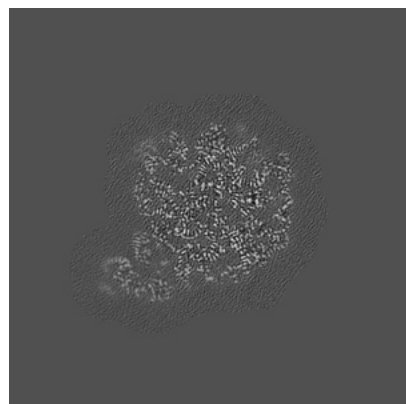


Z Index: 224

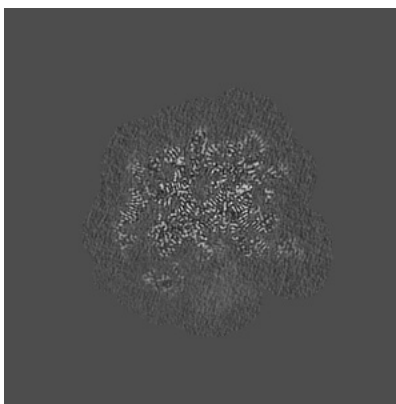
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

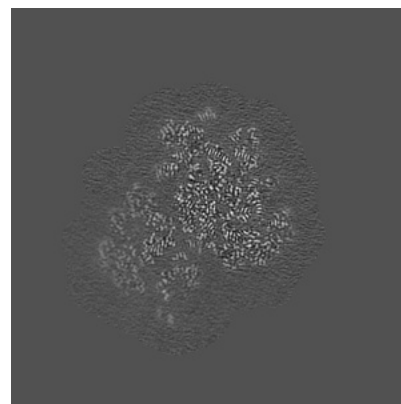
6.3.1 Primary map



X Index: 257



Y Index: 243

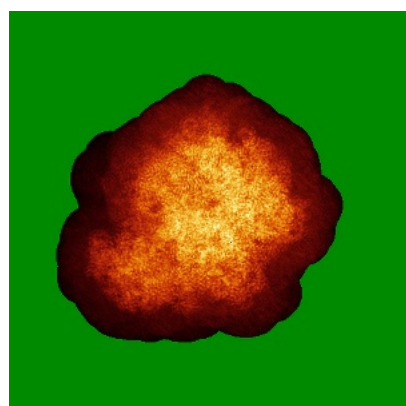


Z Index: 202

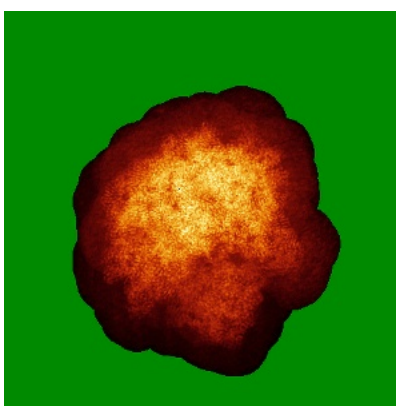
The images above show the largest variance slices of the map in three orthogonal directions.

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

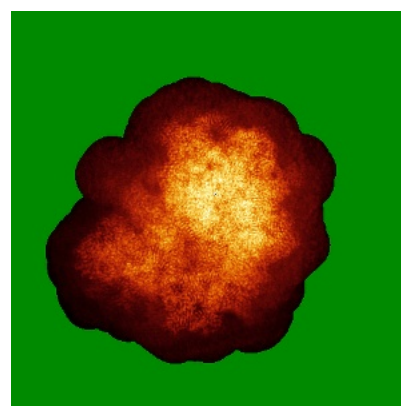
6.4.1 Primary map



X



Y



Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

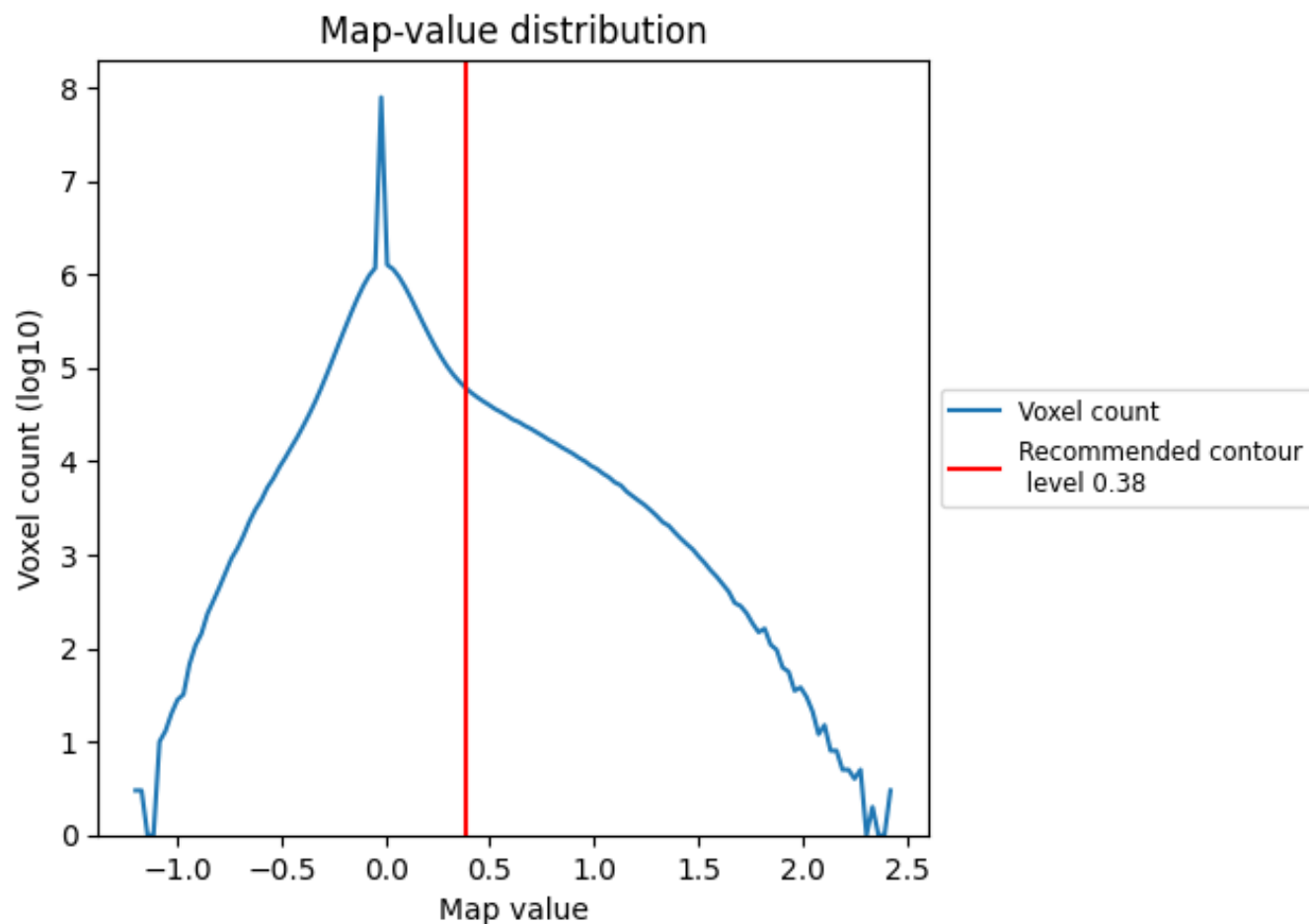
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

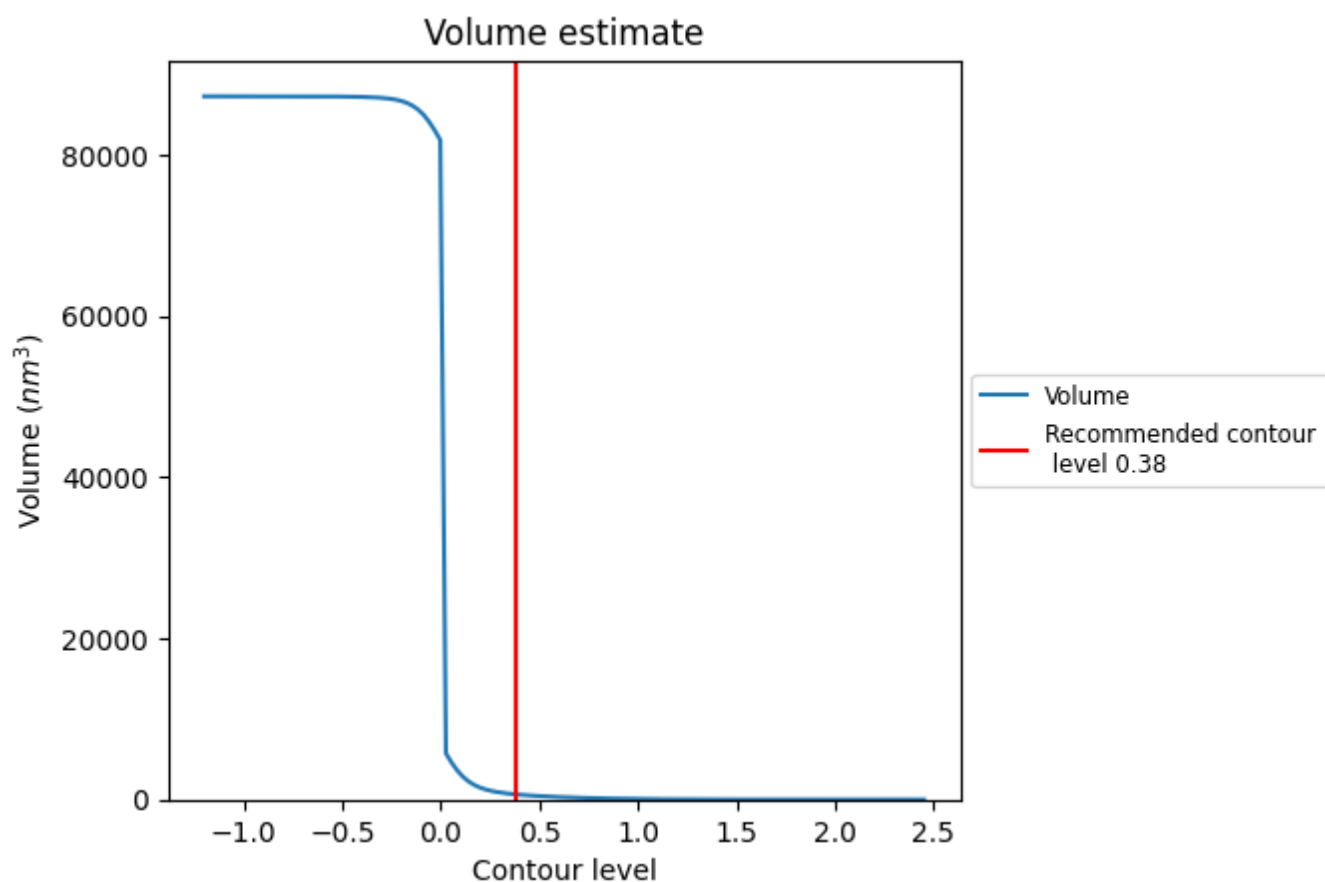
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

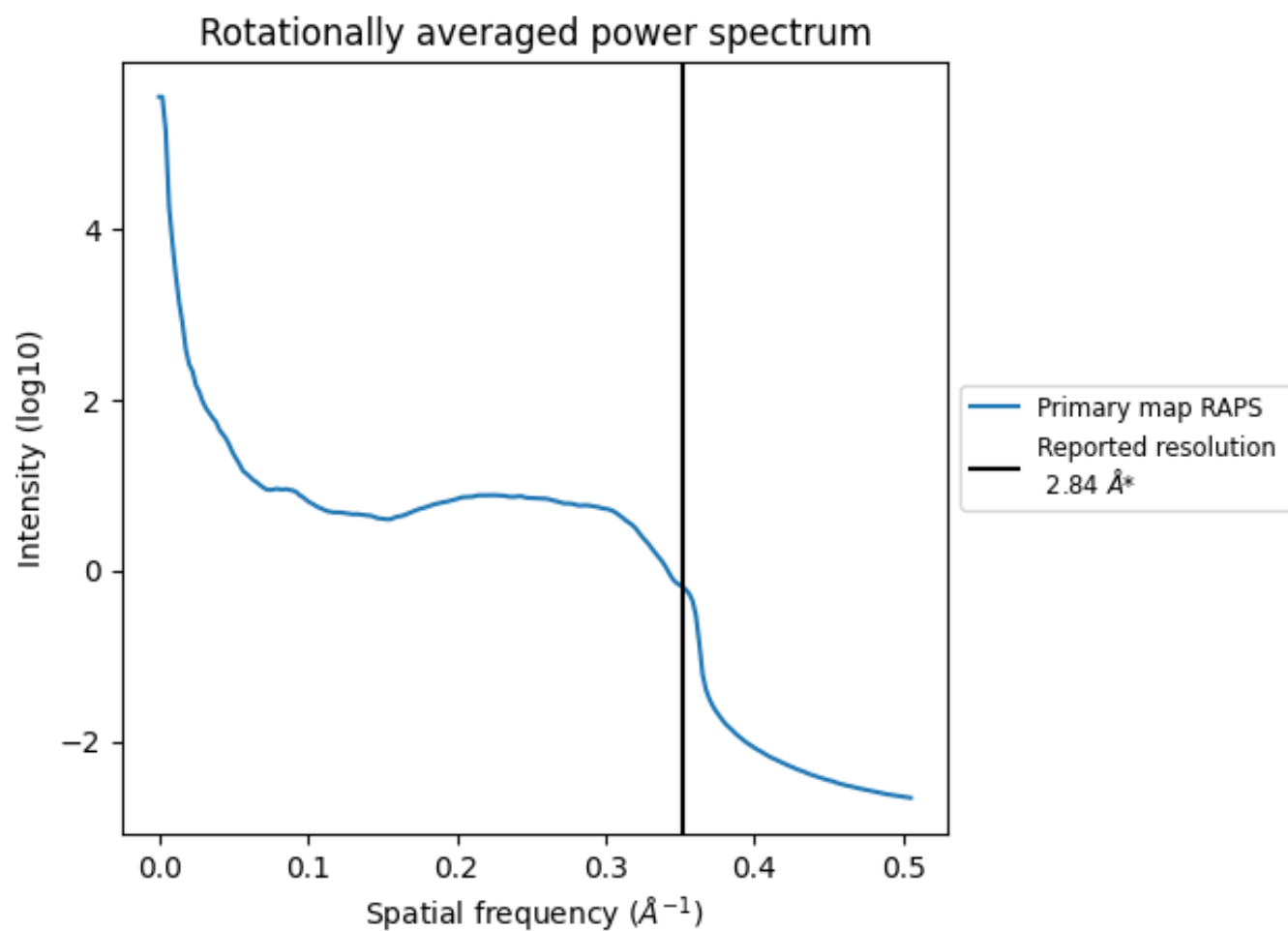
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 646 nm³; this corresponds to an approximate mass of 583 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.352 Å⁻¹

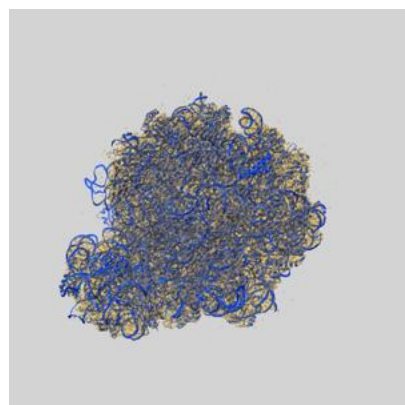
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

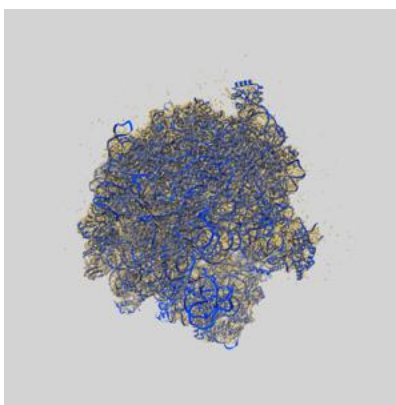
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53099 and PDB model 9QF5. Per-residue inclusion information can be found in [section 3](#) on [page 19](#).

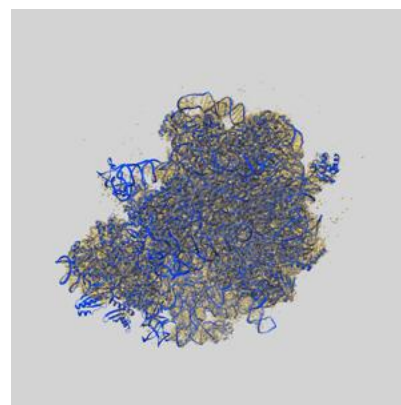
9.1 Map-model overlay [i](#)



X



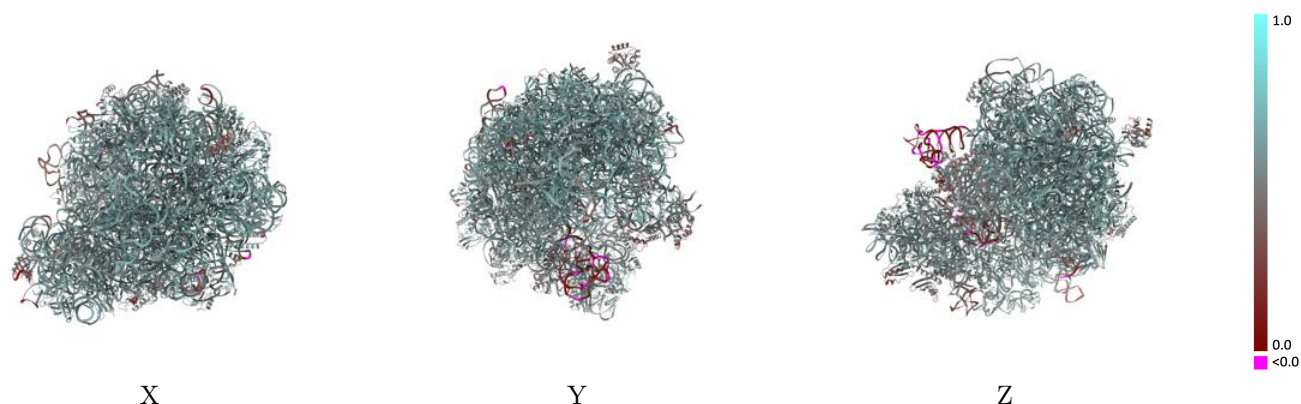
Y



Z

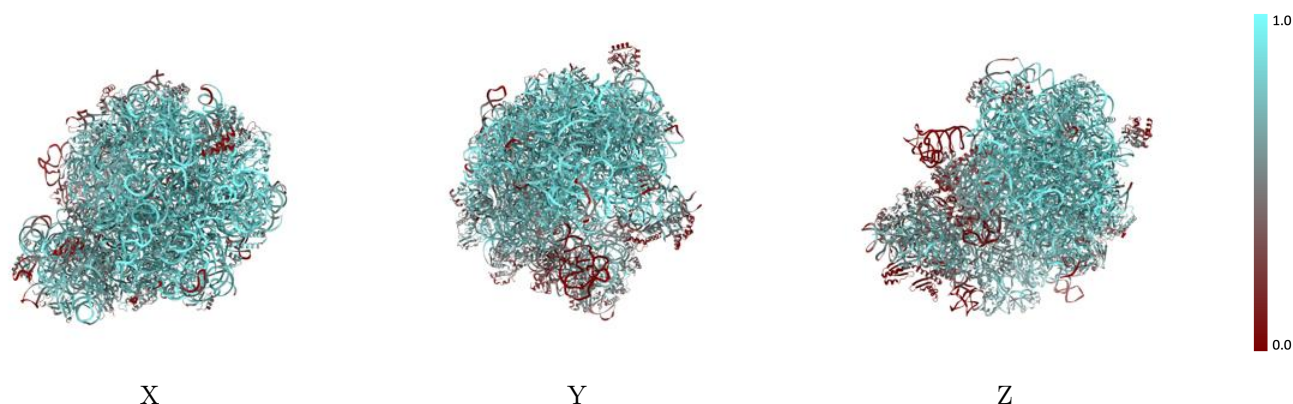
The images above show the 3D surface view of the map at the recommended contour level 0.38 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



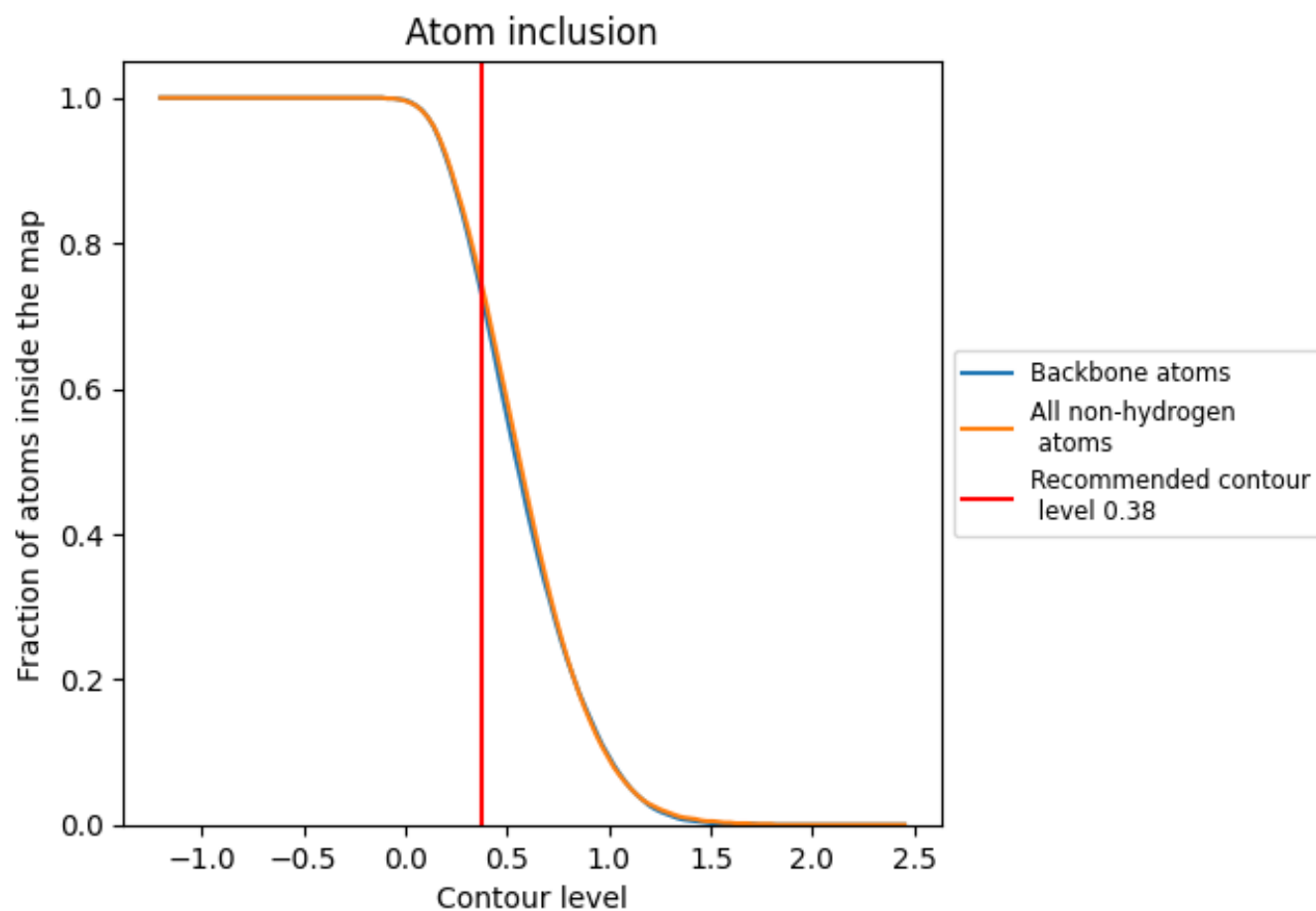
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.38).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7390	 0.5690
A1	 0.7140	 0.5590
Aa	 0.4590	 0.5340
Ab	 0.2300	 0.4740
Ac	 0.5110	 0.5470
Ad	 0.6540	 0.5750
Ae	 0.6820	 0.5790
Af	 0.6220	 0.5660
Ag	 0.3420	 0.5060
Ah	 0.4780	 0.5210
Ai	 0.6960	 0.5910
Aj	 0.6300	 0.5690
Ak	 0.5180	 0.5470
Al	 0.2630	 0.4380
Am	 0.4870	 0.5200
An	 0.5890	 0.5720
Ao	 0.5540	 0.5490
Ap	 0.5040	 0.5390
Aq	 0.6180	 0.5590
Ar	 0.6780	 0.5880
As	 0.0310	 0.4100
At	 0.5460	 0.5440
Au	 0.5770	 0.5630
Av	 0.5630	 0.5490
Aw	 0.5390	 0.5530
Ax	 0.3070	 0.4810
Ay	 0.5480	 0.5570
B1	 0.8510	 0.5820
B2	 0.7310	 0.5440
BA	 0.8650	 0.6210
BB	 0.7960	 0.6040
BC	 0.8090	 0.6050
BD	 0.2950	 0.4130
BE	 0.6810	 0.5670
BF	 0.6210	 0.5480



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Chain	Atom inclusion	Q-score
BG	 0.2570	 0.4080
BH	 0.7990	 0.5980
BI	 0.8190	 0.6070
BJ	 0.8200	 0.6160
BK	 0.5700	 0.5410
BL	 0.6200	 0.5530
BM	 0.6070	 0.5220
BN	 0.8970	 0.6300
BO	 0.5130	 0.4990
BP	 0.7820	 0.5920
BQ	 0.7830	 0.5860
BR	 0.8290	 0.6140
BS	 0.8590	 0.6150
BT	 0.7750	 0.5850
BU	 0.7930	 0.5950
BV	 0.7900	 0.6090
BW	 0.6760	 0.5350
BX	 0.8020	 0.6010
BY	 0.6140	 0.5520
BZ	 0.7410	 0.5810
Ba	 0.8350	 0.6050
Bb	 0.8260	 0.5940
Bc	 0.8150	 0.6050
Bd	 0.9170	 0.6290
Be	 0.8200	 0.6020
Bf	 0.8740	 0.6170
Bg	 0.6600	 0.5690
Bh	 0.6980	 0.5900
Bi	 0.7930	 0.5970
Bj	 0.6060	 0.5380
Bk	 0.7930	 0.5950