



## wwPDB EM Validation Summary Report ⓘ

Nov 29, 2025 – 07:47 am GMT

PDB ID : 9QF6 / pdb\_00009qf6  
EMDB ID : EMD-53100  
Title : Structure of P. furiosus 70S ribosome in RsmB deleted strain  
Authors : Matzov, D.; Georgeson, J.; Westhof, E.; Schwartz, S.; Shalev-Benami, M.  
Deposited on : 2025-03-11  
Resolution : 2.67 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

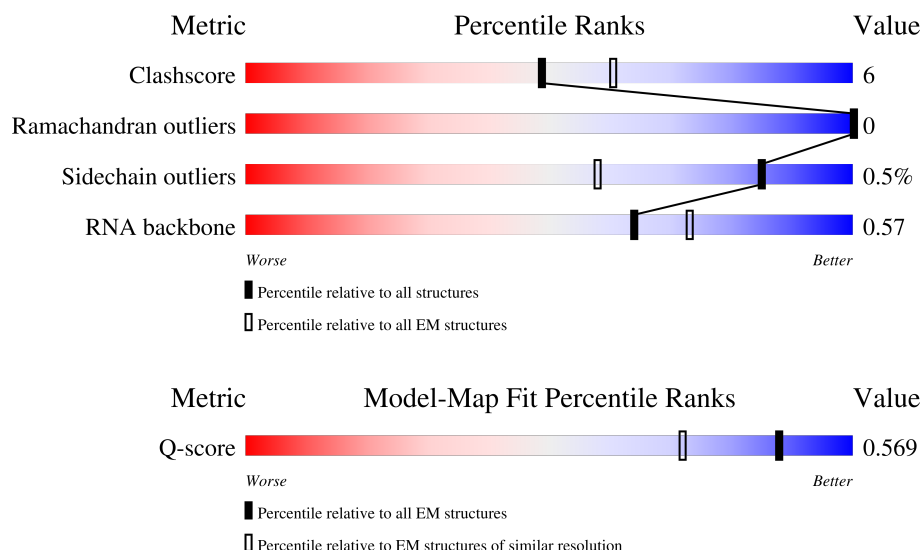
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 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 2.67 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.










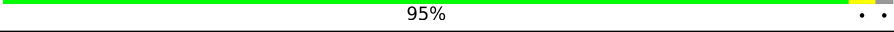



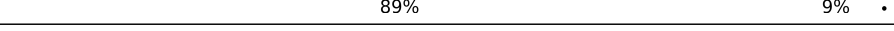







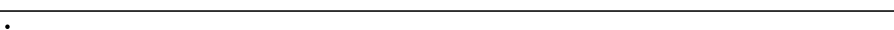

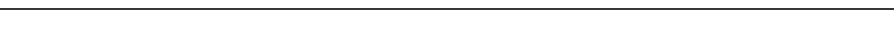
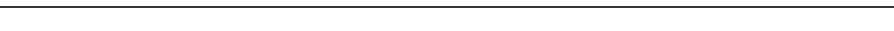


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	9182 ( 2.17 - 3.17 )

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

Mol	Chain	Length	Quality of chain
1	A1	1497	
2	Aa	202	
3	Ab	210	
























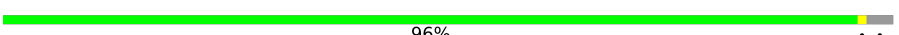

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Mol	Chain	Length	Quality of chain
4	Ac	198	
5	Ad	180	
6	Ae	243	
7	Af	236	
8	Ag	125	
9	Ah	215	
10	Ai	130	
11	Aj	127	
12	Ak	135	
13	Al	102	
14	Am	137	
15	An	147	
16	Ao	148	
17	Ap	56	
18	Aq	158	
19	Ar	113	
20	As	67	
21	At	132	
22	Au	150	
23	Av	99	
23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

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Mol	Chain	Length	Quality of chain
28	B2	125	
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	

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Mol	Chain	Length	Quality of chain
51	BY	99	 84%14% .
52	BZ	95	 96% . .
53	Ba	130	 95% . .
54	Bb	89	 91%8% .
55	Bc	87	 91%8% .
56	Bd	62	 87%10% .
57	Be	83	 84%14% .
58	Bf	51	 92%6% .
59	Bg	51	 84%6%10%
60	Bh	37	 84%14% .
61	Bi	94	 99% .
62	Bj	77	 94%6%
63	Bk	64	 81%16% .

## 2 Entry composition

There are 65 unique types of molecules in this entry. The entry contains 164601 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
			32212	14384	5942	10395	1490	1		

- 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
			1513	968	276	266	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
			1516	981	264	266	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
			1975	1277	353	340	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Af	226	Total	C	N	O	S	0	0
			1784	1129	333	315	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
			963	610	177	175	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
			1722	1089	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
			972	603	200	169			

- 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
			1048	657	200	186	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
			770	479	146	142	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
			1102	693	219	185	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ap	55	Total	C	N	O	S	0	0
			450	285	94	66	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Aq	156	Total	C	N	O	S	0	0
			1290	823	245	218	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	63	Total	C	N	O	S	0	0
			522	330	100	90	2		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
21	At	121	Total	C	N	O	S	0	0
			985	632	184	163	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
			791	514	129	145	3		
23	Bl	92	Total	C	N	O	S	0	0
			765	498	125	140	2		

- 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
			464	298	83	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
			495	305	98	92			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Az	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
			63424	28311	11737	20444	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	237	Total	C	N	O	S	0	0
			1814	1155	341	314	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BB	363	Total	C	N	O	S	0	0
			2888	1854	522	498	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	182	Total	C	N	O	S	0	0
			1415	886	272	249	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
			927	591	153	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	169	Total	C	N	O	S	0	0
			1383	879	263	235	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
			1058	657	213	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
			1564	999	295	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
			790	503	160	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
			1198	767	225	202	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
46	BT	84	Total	C	N	O	0	0
			674	434	118	122		

- 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
			533	339	103	85	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BW	70	Total	C	N	O	S	0	0
			565	351	111	99	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
			734	478	116	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	S	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	128	Total	C	N	O	S	0	0
			1082	693	218	170	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Bb	88	Total	C	N	O	S	0	0
			733	460	157	105	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	60	Total	C	N	O	S	0	0
			483	298	106	75	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
57	Be	82	Total	C	N	O	S	0	0
			616	383	127	101	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	S	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
			336	212	83	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
			652	420	118	113	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bk	62	Total	C	N	O	S	0	0
			514	330	103	78	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	Az	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	151	Total	O	0
			151	151	
65	Ae	3	Total	O	0
			3	3	
65	Ag	1	Total	O	0
			1	1	
65	Ah	1	Total	O	0
			1	1	
65	Aj	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
65	Ak	1	Total 1	O 1	0
65	Al	3	Total 3	O 3	0
65	Am	2	Total 2	O 2	0
65	Ao	2	Total 2	O 2	0
65	Ap	1	Total 1	O 1	0
65	Aq	2	Total 2	O 2	0
65	Au	1	Total 1	O 1	0
65	Av	1	Total 1	O 1	0
65	B1	1173	Total 1173	O 1173	0
65	B2	19	Total 19	O 19	0
65	BA	10	Total 10	O 10	0
65	BB	6	Total 6	O 6	0
65	BC	7	Total 7	O 7	0
65	BE	1	Total 1	O 1	0
65	BF	1	Total 1	O 1	0
65	BH	6	Total 6	O 6	0
65	BI	7	Total 7	O 7	0
65	BJ	2	Total 2	O 2	0
65	BM	11	Total 11	O 11	0
65	BN	14	Total 14	O 14	0
65	BO	2	Total 2	O 2	0

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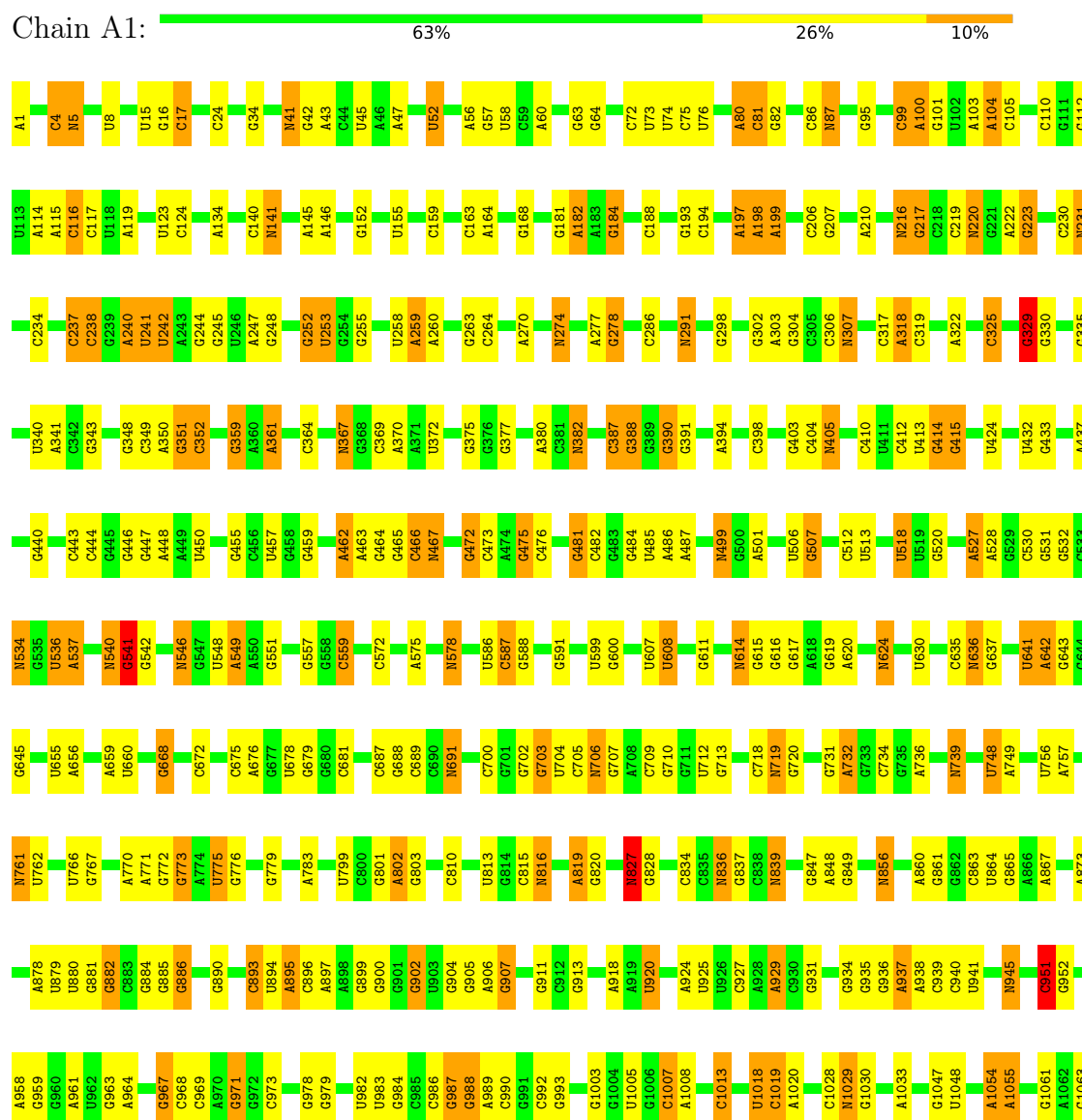
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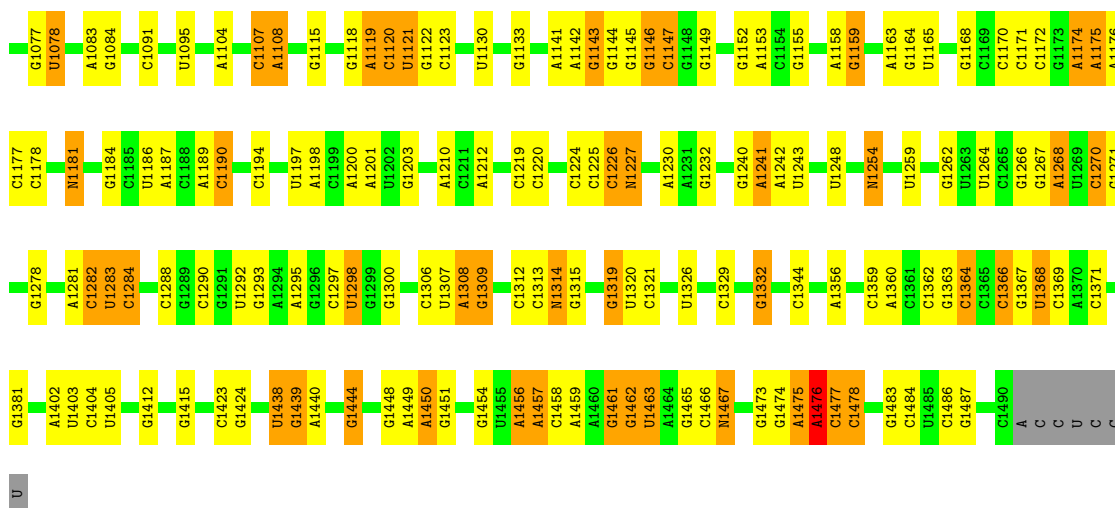
Mol	Chain	Residues	Atoms		AltConf
65	BP	8	Total 8	O 8	0
65	BQ	3	Total 3	O 3	0
65	BR	7	Total 7	O 7	0
65	BS	6	Total 6	O 6	0
65	BT	2	Total 2	O 2	0
65	BU	2	Total 2	O 2	0
65	BW	1	Total 1	O 1	0
65	BX	11	Total 11	O 11	0
65	BZ	2	Total 2	O 2	0
65	Ba	6	Total 6	O 6	0
65	Bb	3	Total 3	O 3	0
65	Bc	4	Total 4	O 4	0
65	Bd	5	Total 5	O 5	0
65	Bf	3	Total 3	O 3	0
65	Bi	3	Total 3	O 3	0
65	Bj	4	Total 4	O 4	0
65	Bk	2	Total 2	O 2	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

Chain Aa: 86% 11% .



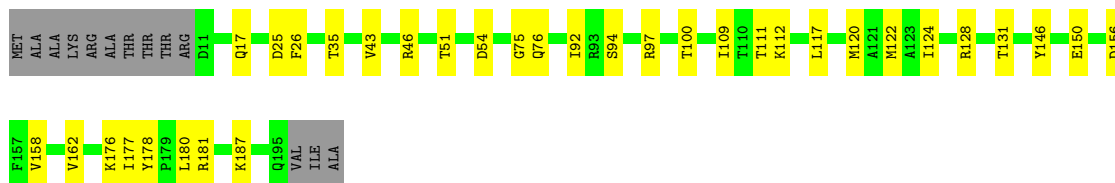
- Molecule 3: Small ribosomal subunit protein uS3

Chain Ab: 82% 10% 7%



- Molecule 4: Small ribosomal subunit protein eS1

Chain Ac: 76% 17% 7%



- Molecule 5: Small ribosomal subunit protein uS4

Chain Ad: 82% 14% .



- Molecule 6: Small ribosomal subunit protein eS4

Chain Ae: 87% 12%



- Molecule 7: Small ribosomal subunit protein uS5

Chain Af: 89% 7% .



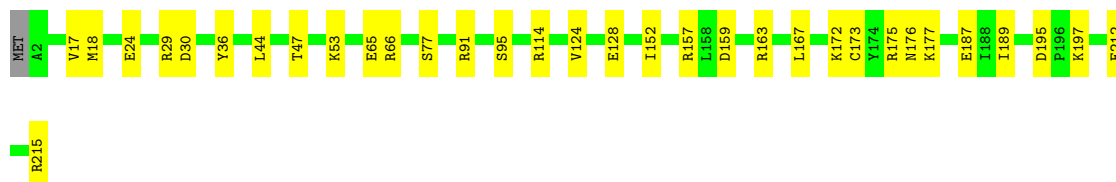
- Molecule 8: Small ribosomal subunit protein eS6

Chain Ag: 87% 12% .



- Molecule 9: Small ribosomal subunit protein uS7

Chain Ah: 84% 15%



- Molecule 10: Small ribosomal subunit protein uS8

Chain Ai: 87% 12% .



- Molecule 11: Small ribosomal subunit protein eS8

Chain Aj: 95% . .

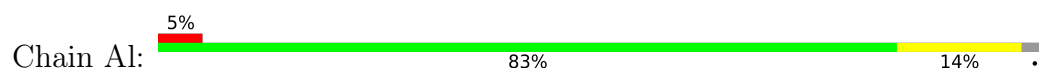


- Molecule 12: Small ribosomal subunit protein uS9

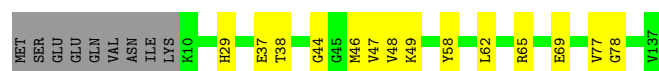
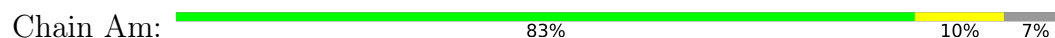
Chain Ak: 81% 19% .



- Molecule 13: Small ribosomal subunit protein uS10



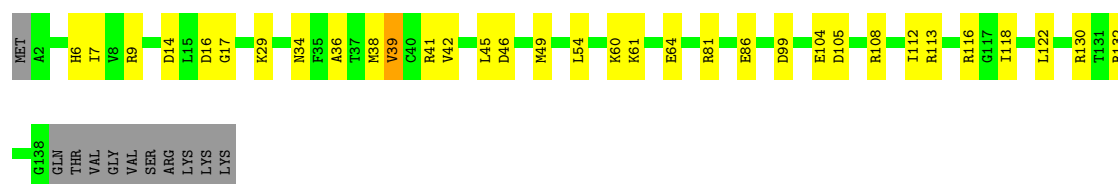
- Molecule 14: Small ribosomal subunit protein uS11



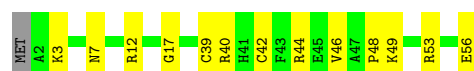
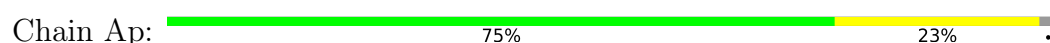
- Molecule 15: Small ribosomal subunit protein uS12



- Molecule 16: Small ribosomal subunit protein uS13



- Molecule 17: Small ribosomal subunit protein uS14



- Molecule 18: Small ribosomal subunit protein uS15



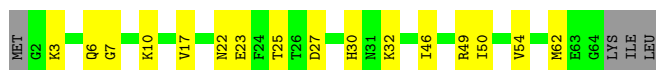
- Molecule 19: Small ribosomal subunit protein uS17





- Molecule 20: Small ribosomal subunit protein eS17

Chain As: 70% 24% 6%



- Molecule 21: Small ribosomal subunit protein uS19

Chain At: 80% 11% 8%



- Molecule 22: Small ribosomal subunit protein eS19

Chain Au: 87% 11% ..



- Molecule 23: Small ribosomal subunit protein eS24

Chain Av: 85% 11% .



- Molecule 23: Small ribosomal subunit protein eS24

Chain Bl: 82% 11% 7%



- Molecule 24: Small ribosomal subunit protein eS27

Chain Aw: 81% 16% .



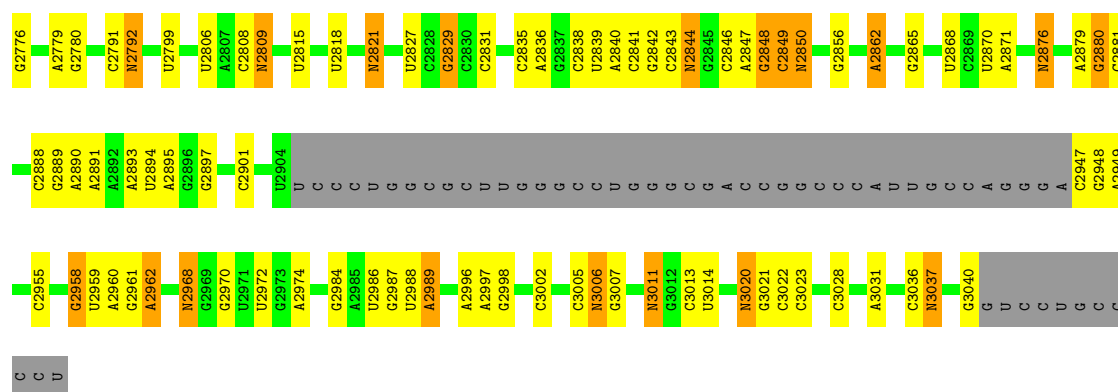
- Molecule 25: Small ribosomal subunit protein eS28

Chain Ax: 73% 17% 10%

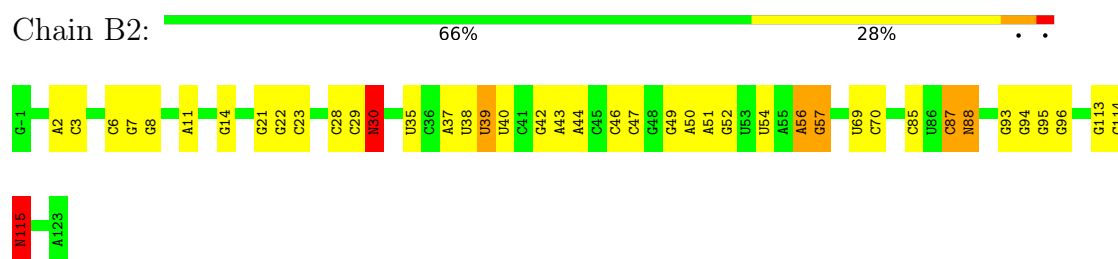


C9619	C2502	U2401	G2185	C2090	A2005	A1881	U1778	A1678	G1455	C1359	G1247	A1186
C9634	C2503	A2402	A2186	A2091	N2008	N1885	G1779	A1679	C1458	N1360	G1250	G1157
C2637	C2504	A2403	C2187	U2092	G2013	G1889	C1780	U1680	C1459	G1363	A1251	A1188
G9645	A2506	G2405	G2193	A2094	G2017	C1894	C1782	G1696	A1465	U1367	G1253	G1191
G2648	A2510	U2406	G2194	U2095	C2017	C1894	G1789	G1697	A1466	A1368	U1254	C
G2649	A2511	C2407	U2198	G2097	N2020	G1898	A1790	G1698	A1466	A1369	C1255	G
C2650	C2519	U2419	G2207	G2108	G2021	A1899	G1791	G1699	A1471	G1370	U1256	G
A2680	C2520	C2421	C2212	C2112	G2022	A1900	A1792	U1700	G1476	C1373	N1264	G
A2681	N2526	G2422	N2213	N2113	A2024	G1904	G1793	U1701	N1478	N1374	A1269	A
A2682	G2540	U2427	G2217	U2116	A2025	N1911	G1796	N1706	G1477	G1375	A1272	G
G2684	G2541	C2428	A2220	G2117	A2026	G1912	U1804	A1708	N1478	N1375	A1273	G
U2691	U2542	N2429	C2298	U2118	G2028	A1913	U1709	G1709	G1477	G1376	G1274	U
G2692	G2543	G2430	C2226	C2120	G2031	C1914	U1806	G1710	A1468	U1377	G1275	A
A2693	A2544	C2431	G2229	C2121	G2032	U1919	C1807	G1711	C1488	A1380	G1276	G
C2694	A2546	N2432	G2230	G2123	G2034	A1920	G1811	G1712	C1489	C1382	G1277	C
C2695	G2547	A2435	G2231	G2124	G2035	U1922	G1812	G1713	A1496	N1383	G1278	U
U2696	G2548	G2436	G2232	G2125	U2036	A1923	A1813	U1714	A1497	G1388	U1280	A
G2697	A2549	A2437	U2233	C2126	A2037	A1924	A1814	C1718	C1500	U1392	A1282	G
G2698	A2550	G2438	G2234	G2127	A2038	A1931	G1818	G1721	N1501	C1393	G1287	C
U2700	U2554	C2441	C2235	G2128	G2039	A1931	G1819	U1722	N1505	G1394	U1287	A
G2704	C2557	A2442	G2236	N2133	U2040	C1937	G1822	G1723	C1515	G1395	N1290	G
A2705	G2562	A2450	A2237	A2138	U2041	A1938	N1822	A1724	G1516	G1396	G1291	C
G2711	G2563	N2454	G2238	G2139	U2042	G1939	G1823	A1725	C1517	A1397	G1292	C
A2714	A2564	G2460	C2240	A2140	A2043	C1940	G1824	G1735	U1398	U1398	N1293	A
G2715	U2565	G2461	G2241	G2146	A2044	U1941	A1824	U1738	C1399	C1399	U1296	U
A2718	C2577	G2465	U2242	C2152	U2048	A1942	G1827	A1739	A1408	A1408	G1296	C
C2722	U2578	N2469	G2246	G2153	C2049	N1946	C1830	C1742	G1412	G1412	C1301	C
U2729	C2579	G2470	G2247	C2154	U2050	G1947	U1831	N1743	G1413	G1413	G1308	U
A2730	A2585	A2471	G2248	C2155	A2052	G1957	C1832	C1747	A1414	A1414	G1309	A
G2737	G2586	C2472	A2250	C2156	A2053	G1965	G1833	C1751	G1415	G1415	A1315	A
U2745	C2589	C2473	G2252	A2157	G2055	C1966	G1834	U1761	U1416	U1417	U1316	G
N2749	C2590	A2474	G2253	C2160	C2059	N1967	C1845	A1755	G1647	U1418	U1317	A
G2757	C2591	A2475	G2254	G2163	G2060	G1968	N1846	A1758	C1434	C1434	G1318	G
A2760	C2597	G2476	U2255	A2166	A2061	A1969	U1853	G1759	N1435	N1435	A1326	U
G2762	A2594	G2478	G2257	A2167	A2062	C1977	C1854	A1760	G1436	G1436	U1327	G
U2769	G2597	A2487	C2258	C2170	U2065	C1978	G1857	G1761	A1437	A1437	G1328	C
N2774	N2602	C2491	G2260	C2171	C2066	U1981	G1858	N1762	C1438	C1438	G1329	U
G2787	C2607	N2492	C2261	N2171	C2067	G1982	A1859	G1765	N1546	N1546	G1330	A
A2796	C2614	G2493	G2262	U2174	U2068	G1986	A1860	A1766	N1551	N1551	G1331	C
G2799	C2615	G2496	G2263	G2175	U2090	U1987	A1861	A1767	G1443	G1443	U1332	A
U2816	U2616	G2497	G2264	G2176	A2085	A1988	G1870	G1768	A1444	A1444	G1337	C
C2817	C2617	G2498	G2265	A2179	C2086	A1993	G1871	G1769	G1561	G1561	C1344	U
G2818	G2618	G2501	G2266	G2180	C2087	A2003	U1876	A1773	G1567	G1567	N1345	A
			G2267	A2183	U2088	C2004	G1877	C1774	A1569	C1450	G1355	C
			C2270	A2184	G2089				A1570			

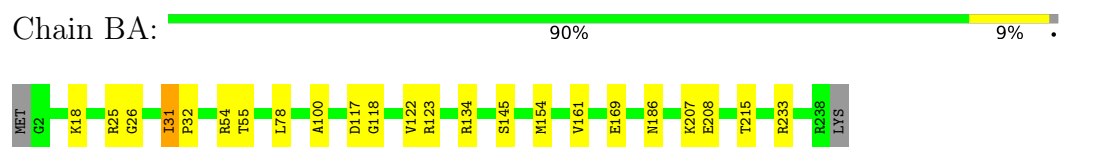




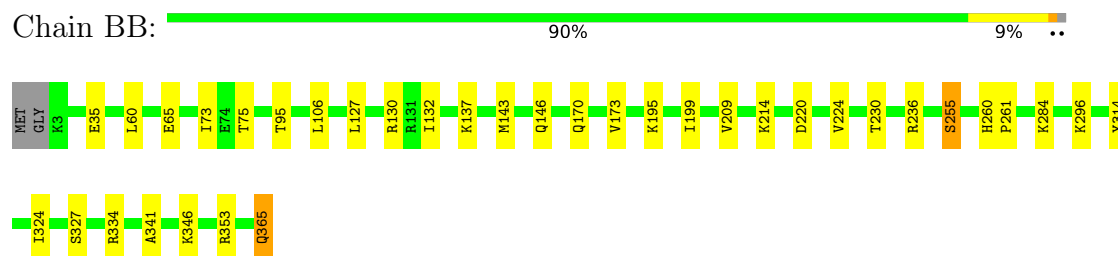
- Molecule 28: 5S rRNA



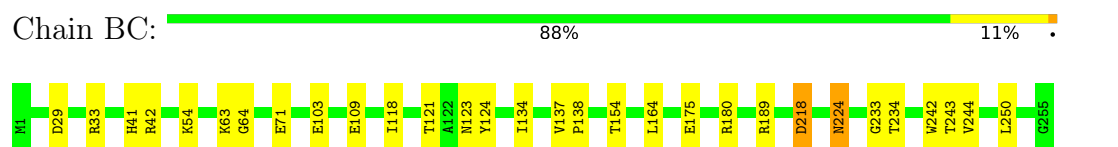
- Molecule 29: Large ribosomal subunit protein uL2



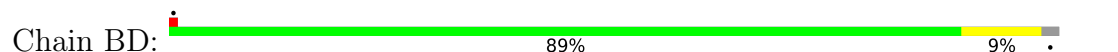
- Molecule 30: Large ribosomal subunit protein uL3

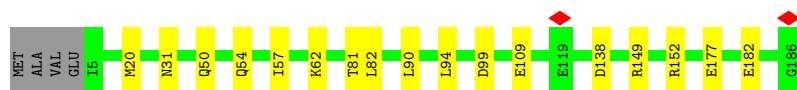


- Molecule 31: Large ribosomal subunit protein uL4



- Molecule 32: Large ribosomal subunit protein uL5





- Molecule 33: Large ribosomal subunit protein uL6

Chain BE: 92% 7%



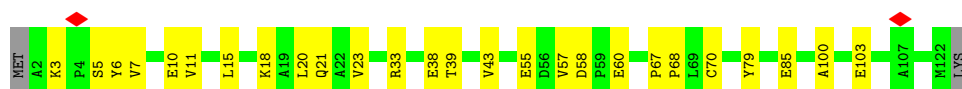
- Molecule 34: Large ribosomal subunit protein eL8

Chain BF: 85% 14%



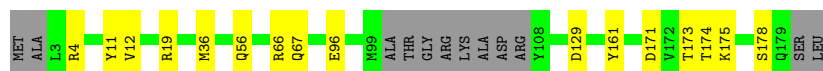
- Molecule 34: Large ribosomal subunit protein eL8

Chain BG: 77% 21%



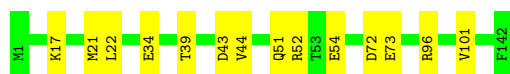
- Molecule 35: Large ribosomal subunit protein uL16

Chain BH: 85% 9% 7%



- Molecule 36: Large ribosomal subunit protein uL13

Chain BI: 90% 10%



- Molecule 37: Large ribosomal subunit protein uL14

Chain BJ: 93% 6%



- Molecule 38: Large ribosomal subunit protein eL14

Chain BK: 90% 7%



- Molecule 38: Large ribosomal subunit protein eL14

Chain BL: 72% 27%



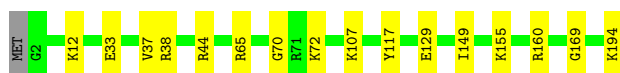
- Molecule 39: Large ribosomal subunit protein uL15

Chain BM: 82% 18%



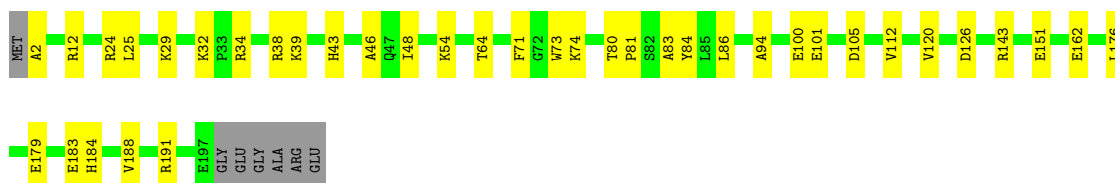
- Molecule 40: Large ribosomal subunit protein eL15

Chain BN: 91% 8%



- Molecule 41: Large ribosomal subunit protein uL18

Chain BO: 78% 19%



- Molecule 42: Large ribosomal subunit protein eL18

Chain BP: 88% 12%




- Molecule 43: Large ribosomal subunit protein eL19

Chain BQ: 89% 9%



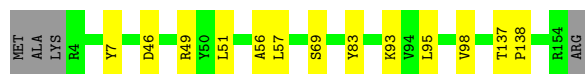
- Molecule 44: Large ribosomal subunit protein eL21

Chain BR:  87% 12% .




- Molecule 45: Large ribosomal subunit protein uL22

Chain BS:  89% 8% .




- Molecule 46: Large ribosomal subunit protein uL23

Chain BT:  85% 13% .



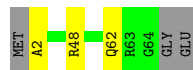
- Molecule 47: Large ribosomal subunit protein uL24

Chain BU:  79% 20% ..



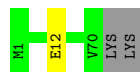
- Molecule 48: Large ribosomal subunit protein eL24

Chain BV:  91% 5% 5%




- Molecule 49: Large ribosomal subunit protein uL29

Chain BW:  96% ..




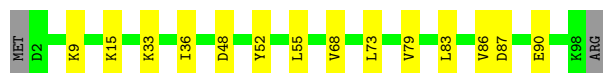
- Molecule 50: Large ribosomal subunit protein uL30

Chain BX:  86% 13% .



- Molecule 51: Large ribosomal subunit protein eL30

Chain BY:  84% 14% .



- Molecule 52: Large ribosomal subunit protein eL31

Chain BZ:  96% ..



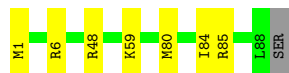
- Molecule 53: Large ribosomal subunit protein eL32

Chain Ba:  95% ..



- Molecule 54: Large ribosomal subunit protein eL34

Chain Bb:  91% 8% .




- Molecule 55: Large ribosomal subunit protein eL33

Chain Bc:  91% 8% .




- Molecule 56: Large ribosomal subunit protein eL37

Chain Bd:  87% 10% .



- Molecule 57: Large ribosomal subunit protein eL43

Chain Be:  84% 14% .




- Molecule 58: Large ribosomal subunit protein eL39

Chain Bf:  92% 6% .




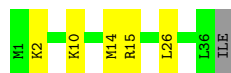
- Molecule 59: Large ribosomal subunit protein eL40

Chain Bg:  84% 6% 10%



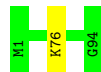
- Molecule 60: Small ribosomal subunit protein eS32

Chain Bh:  84% 14% .



- Molecule 61: Large ribosomal subunit protein eL42

Chain Bi:  99% .




- Molecule 62: Large ribosomal subunit protein eL20

Chain Bj:  94% 6%



- Molecule 63: C2H2-type domain-containing protein

Chain Bk:  81% 16% .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91960	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	2.600	Depositor
Minimum map value	-1.451	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.0083	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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.12	1/33844 (0.0%)	0.24	0/52748
2	Aa	0.10	0/1603	0.26	0/2167
3	Ab	0.10	0/1535	0.26	0/2065
4	Ac	0.10	0/1542	0.29	0/2067
5	Ad	0.11	0/1476	0.26	0/1980
6	Ae	0.10	0/2024	0.27	0/2732
7	Af	0.09	0/1814	0.25	0/2444
8	Ag	0.13	0/978	0.34	0/1311
9	Ah	0.12	0/1758	0.30	0/2362
10	Ai	0.11	0/1049	0.28	0/1408
11	Aj	0.07	0/981	0.21	0/1312
12	Ak	0.11	0/1064	0.29	0/1426
13	Al	0.10	0/778	0.28	0/1049
14	Am	0.10	0/981	0.27	0/1320
15	An	0.11	0/1141	0.27	0/1518
16	Ao	0.13	0/1121	0.33	0/1507
17	Ap	0.10	0/459	0.32	0/605
18	Aq	0.34	1/1318 (0.1%)	0.54	4/1773 (0.2%)
19	Ar	0.08	0/899	0.22	0/1215
20	As	0.15	0/528	0.36	0/701
21	At	0.09	0/1005	0.23	0/1343
22	Au	0.10	0/1251	0.25	0/1686
23	Av	0.11	0/807	0.27	0/1082
23	Bl	0.10	0/781	0.31	0/1049
24	Aw	0.12	0/471	0.34	0/634
25	Ax	0.10	0/497	0.28	0/668
26	Az	0.17	0/448	0.40	1/610 (0.2%)
27	B1	0.11	2/67034 (0.0%)	0.25	2/104432 (0.0%)
28	B2	0.08	0/2927	0.23	0/4559
29	BA	0.11	0/1859	0.27	0/2512
30	BB	0.10	0/2954	0.26	0/3976
31	BC	0.11	0/2068	0.26	0/2787



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	BD	0.11	0/1437	0.29	0/1925
33	BE	0.09	0/1499	0.24	0/2022
34	BF	0.10	0/939	0.26	0/1267
34	BG	0.13	0/933	0.34	0/1260
35	BH	0.09	0/1413	0.25	0/1897
36	BI	0.10	0/1168	0.23	0/1561
37	BJ	0.08	0/1071	0.23	0/1444
38	BK	0.11	0/618	0.25	0/829
38	BL	0.10	0/626	0.28	0/840
39	BM	0.11	0/1175	0.29	0/1563
40	BN	0.10	0/1626	0.25	0/2169
41	BO	0.09	0/1602	0.24	0/2158
42	BP	0.12	0/980	0.27	0/1313
43	BQ	0.09	0/1254	0.25	0/1655
44	BR	0.10	0/811	0.25	0/1086
45	BS	0.10	0/1225	0.31	0/1651
46	BT	0.11	0/682	0.30	0/915
47	BU	0.13	0/1019	0.31	0/1360
48	BV	0.09	0/548	0.21	0/731
49	BW	0.12	0/566	0.23	0/749
50	BX	0.10	0/1254	0.27	0/1677
51	BY	0.11	0/744	0.26	0/1004
52	BZ	0.10	0/760	0.25	0/1024
53	Ba	0.10	0/1107	0.26	0/1477
54	Bb	0.11	0/751	0.26	0/999
55	Bc	0.10	0/686	0.30	0/916
56	Bd	0.09	0/493	0.24	0/652
57	Be	0.12	0/625	0.30	0/832
58	Bf	0.10	0/445	0.25	0/593
59	Bg	0.08	0/384	0.23	0/509
60	Bh	0.16	0/342	0.33	0/443
61	Bi	0.10	0/805	0.22	0/1064
62	Bj	0.11	0/662	0.24	0/875
63	Bk	0.19	0/524	0.45	1/691 (0.1%)
All	All	0.11	4/169769 (0.0%)	0.26	8/250199 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Aq	89	PRO	CG-CD	-9.98	1.16	1.50
1	A1	775	OMU	O3'-P	5.13	1.61	1.56
27	B1	857	A2M	O3'-P	5.06	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	506	A2M	O3'-P	5.01	1.61	1.56

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Aq	89	PRO	N-CD-CG	-14.76	81.06	103.20
18	Aq	89	PRO	CA-N-CD	-9.29	98.99	112.00
18	Aq	89	PRO	CA-CB-CG	-7.79	89.69	104.50
63	Bk	11	ASP	CA-CB-CG	6.72	119.32	112.60
26	Az	60	PRO	CA-N-CD	-6.42	103.01	112.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	32212	0	16327	350	0
2	Aa	1572	0	1629	17	0
3	Ab	1513	0	1580	19	0
4	Ac	1516	0	1597	26	0
5	Ad	1452	0	1521	21	0
6	Ae	1975	0	2040	23	0
7	Af	1784	0	1836	12	0
8	Ag	963	0	1006	12	0
9	Ah	1722	0	1768	31	0
10	Ai	1028	0	1065	11	0
11	Aj	972	0	1037	4	0
12	Ak	1048	0	1085	19	0
13	Al	770	0	797	11	0
14	Am	963	0	994	9	0
15	An	1124	0	1217	12	0
16	Ao	1102	0	1143	24	0
17	Ap	450	0	473	15	0
18	Aq	1290	0	1367	10	0
19	Ar	877	0	898	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	As	522	0	557	12	0
21	At	985	0	1046	12	0
22	Au	1221	0	1263	13	0
23	Av	791	0	819	8	0
23	Bl	765	0	788	8	0
24	Aw	464	0	503	8	0
25	Ax	495	0	516	9	0
26	Az	434	0	402	3	0
27	B1	63424	0	32104	644	0
28	B2	2689	0	1367	33	0
29	BA	1814	0	1878	19	0
30	BB	2888	0	3025	28	0
31	BC	2026	0	2137	20	0
32	BD	1415	0	1433	15	0
33	BE	1468	0	1507	8	0
34	BF	927	0	971	10	0
34	BG	921	0	969	17	0
35	BH	1383	0	1410	11	0
36	BI	1150	0	1240	8	0
37	BJ	1058	0	1116	6	0
38	BK	614	0	670	4	0
38	BL	621	0	678	16	0
39	BM	1154	0	1219	27	0
40	BN	1587	0	1683	13	0
41	BO	1564	0	1572	31	0
42	BP	966	0	1019	8	0
43	BQ	1238	0	1365	12	0
44	BR	790	0	825	11	0
45	BS	1198	0	1242	10	0
46	BT	674	0	732	8	0
47	BU	1003	0	1074	20	0
48	BV	533	0	523	3	0
49	BW	565	0	618	1	0
50	BX	1235	0	1314	16	0
51	BY	734	0	779	9	0
52	BZ	746	0	803	2	0
53	Ba	1082	0	1172	3	0
54	Bb	733	0	800	7	0
55	Bc	677	0	729	8	0
56	Bd	483	0	495	5	0
57	Be	616	0	655	11	0
58	Bf	437	0	498	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	Bg	375	0	394	2	0
60	Bh	336	0	387	7	0
61	Bi	787	0	833	1	0
62	Bj	652	0	686	4	0
63	Bk	514	0	555	6	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	Az	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	151	0	0	34	0
65	Ae	3	0	0	0	0
65	Ag	1	0	0	1	0
65	Ah	1	0	0	0	0
65	Aj	1	0	0	0	0
65	Ak	1	0	0	0	0
65	Al	3	0	0	1	0
65	Am	2	0	0	0	0
65	Ao	2	0	0	0	0
65	Ap	1	0	0	0	0
65	Aq	2	0	0	0	0
65	Au	1	0	0	1	0
65	Av	1	0	0	0	0
65	B1	1173	0	0	153	0
65	B2	19	0	0	0	0
65	BA	10	0	0	1	0
65	BB	6	0	0	0	0
65	BC	7	0	0	2	0
65	BE	1	0	0	0	0
65	BF	1	0	0	0	0
65	BH	6	0	0	1	0
65	BI	7	0	0	0	0
65	BJ	2	0	0	1	0
65	BM	11	0	0	1	0
65	BN	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	BO	2	0	0	0	0
65	BP	8	0	0	0	0
65	BQ	3	0	0	0	0
65	BR	7	0	0	2	0
65	BS	6	0	0	0	0
65	BT	2	0	0	0	0
65	BU	2	0	0	0	0
65	BW	1	0	0	0	0
65	BX	11	0	0	2	0
65	BZ	2	0	0	0	0
65	Ba	6	0	0	0	0
65	Bb	3	0	0	0	0
65	Bc	4	0	0	0	0
65	Bd	5	0	0	1	0
65	Bf	3	0	0	1	0
65	Bi	3	0	0	0	0
65	Bj	4	0	0	0	0
65	Bk	2	0	0	0	0
All	All	164601	0	117751	1551	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 6.

The worst 5 of 1551 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)
1:A1:945:4AC:HM73	1:A1:1181:4AC:HM71	1.47	0.96
1:A1:302:G:HO2'	5:Ad:2:GLY:N	1.63	0.95
27:B1:574:G:N2	55:Bc:76:PRO:O	2.03	0.91
1:A1:1145:G:O2'	1:A1:1146:G:OP1	1.91	0.89
1:A1:1462:G:O2'	1:A1:1463:U:OP2	1.89	0.89

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Aa	194/202 (96%)	190 (98%)	4 (2%)	0	100	100
3	Ab	193/210 (92%)	189 (98%)	4 (2%)	0	100	100
4	Ac	183/198 (92%)	179 (98%)	4 (2%)	0	100	100
5	Ad	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
6	Ae	240/243 (99%)	232 (97%)	8 (3%)	0	100	100
7	Af	224/236 (95%)	215 (96%)	9 (4%)	0	100	100
8	Ag	122/125 (98%)	110 (90%)	12 (10%)	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%)	118 (96%)	5 (4%)	0	100	100
12	Ak	132/135 (98%)	126 (96%)	6 (4%)	0	100	100
13	Al	97/102 (95%)	93 (96%)	4 (4%)	0	100	100
14	Am	126/137 (92%)	118 (94%)	8 (6%)	0	100	100
15	An	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
16	Ao	135/148 (91%)	134 (99%)	1 (1%)	0	100	100
17	Ap	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
18	Aq	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
19	Ar	105/113 (93%)	104 (99%)	1 (1%)	0	100	100
20	As	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
21	At	119/132 (90%)	117 (98%)	2 (2%)	0	100	100
22	Au	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
23	Av	93/99 (94%)	92 (99%)	1 (1%)	0	100	100
23	Bl	90/99 (91%)	89 (99%)	1 (1%)	0	100	100
24	Aw	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
25	Ax	62/71 (87%)	61 (98%)	1 (2%)	0	100	100
26	Az	54/60 (90%)	53 (98%)	1 (2%)	0	100	100
29	BA	235/239 (98%)	223 (95%)	12 (5%)	0	100	100
30	BB	361/365 (99%)	348 (96%)	13 (4%)	0	100	100
31	BC	253/255 (99%)	247 (98%)	6 (2%)	0	100	100
32	BD	180/186 (97%)	163 (91%)	17 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	BE	181/184 (98%)	178 (98%)	3 (2%)	0	100	100
34	BF	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
34	BG	119/123 (97%)	116 (98%)	3 (2%)	0	100	100
35	BH	165/181 (91%)	161 (98%)	4 (2%)	0	100	100
36	BI	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
37	BJ	138/141 (98%)	138 (100%)	0	0	100	100
38	BK	79/83 (95%)	72 (91%)	7 (9%)	0	100	100
38	BL	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
39	BM	145/147 (99%)	136 (94%)	9 (6%)	0	100	100
40	BN	191/194 (98%)	183 (96%)	8 (4%)	0	100	100
41	BO	194/203 (96%)	190 (98%)	4 (2%)	0	100	100
42	BP	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
43	BQ	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
44	BR	94/97 (97%)	94 (100%)	0	0	100	100
45	BS	149/155 (96%)	144 (97%)	5 (3%)	0	100	100
46	BT	82/86 (95%)	80 (98%)	2 (2%)	0	100	100
47	BU	118/121 (98%)	116 (98%)	2 (2%)	0	100	100
48	BV	61/66 (92%)	61 (100%)	0	0	100	100
49	BW	68/72 (94%)	67 (98%)	1 (2%)	0	100	100
50	BX	152/155 (98%)	149 (98%)	3 (2%)	0	100	100
51	BY	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
52	BZ	92/95 (97%)	90 (98%)	2 (2%)	0	100	100
53	Ba	126/130 (97%)	125 (99%)	1 (1%)	0	100	100
54	Bb	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
55	Bc	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
56	Bd	58/62 (94%)	55 (95%)	3 (5%)	0	100	100
57	Be	80/83 (96%)	73 (91%)	7 (9%)	0	100	100
58	Bf	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
59	Bg	44/51 (86%)	44 (100%)	0	0	100	100
60	Bh	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
61	Bi	92/94 (98%)	92 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	Bj	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
63	Bk	60/64 (94%)	59 (98%)	1 (2%)	0	100	100
All	All	7961/8293 (96%)	7729 (97%)	232 (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%)	168 (100%)	0	100	100
3	Ab	149/167 (89%)	148 (99%)	1 (1%)	81	92
4	Ac	161/171 (94%)	161 (100%)	0	100	100
5	Ad	156/160 (98%)	156 (100%)	0	100	100
6	Ae	211/213 (99%)	210 (100%)	1 (0%)	86	95
7	Af	186/197 (94%)	185 (100%)	1 (0%)	86	95
8	Ag	103/108 (95%)	103 (100%)	0	100	100
9	Ah	182/184 (99%)	181 (100%)	1 (0%)	86	95
10	Ai	107/108 (99%)	106 (99%)	1 (1%)	75	89
11	Aj	98/103 (95%)	98 (100%)	0	100	100
12	Ak	106/111 (96%)	106 (100%)	0	100	100
13	Al	82/91 (90%)	82 (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	112/122 (92%)	111 (99%)	1 (1%)	75	89
17	Ap	44/46 (96%)	44 (100%)	0	100	100
18	Aq	141/143 (99%)	141 (100%)	0	100	100
19	Ar	96/102 (94%)	96 (100%)	0	100	100
20	As	57/61 (93%)	55 (96%)	2 (4%)	31	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	At	104/114 (91%)	103 (99%)	1 (1%)	73	88
22	Au	126/127 (99%)	125 (99%)	1 (1%)	79	91
23	Av	86/89 (97%)	86 (100%)	0	100	100
23	Bl	83/89 (93%)	83 (100%)	0	100	100
24	Aw	53/54 (98%)	53 (100%)	0	100	100
25	Ax	51/60 (85%)	51 (100%)	0	100	100
26	Az	48/53 (91%)	48 (100%)	0	100	100
29	BA	186/189 (98%)	185 (100%)	1 (0%)	86	95
30	BB	308/312 (99%)	306 (99%)	2 (1%)	84	93
31	BC	213/213 (100%)	209 (98%)	4 (2%)	52	77
32	BD	142/158 (90%)	141 (99%)	1 (1%)	81	92
33	BE	155/156 (99%)	154 (99%)	1 (1%)	84	93
34	BF	97/99 (98%)	97 (100%)	0	100	100
34	BG	97/99 (98%)	95 (98%)	2 (2%)	48	74
35	BH	143/152 (94%)	143 (100%)	0	100	100
36	BI	122/122 (100%)	122 (100%)	0	100	100
37	BJ	106/108 (98%)	105 (99%)	1 (1%)	75	89
38	BK	64/66 (97%)	64 (100%)	0	100	100
38	BL	65/66 (98%)	64 (98%)	1 (2%)	60	82
39	BM	117/117 (100%)	116 (99%)	1 (1%)	75	89
40	BN	161/162 (99%)	160 (99%)	1 (1%)	84	93
41	BO	158/169 (94%)	158 (100%)	0	100	100
42	BP	101/101 (100%)	99 (98%)	2 (2%)	50	76
43	BQ	128/130 (98%)	127 (99%)	1 (1%)	79	91
44	BR	85/87 (98%)	83 (98%)	2 (2%)	44	70
45	BS	125/130 (96%)	125 (100%)	0	100	100
46	BT	74/77 (96%)	73 (99%)	1 (1%)	62	82
47	BU	110/110 (100%)	109 (99%)	1 (1%)	75	89
48	BV	54/56 (96%)	54 (100%)	0	100	100
49	BW	60/66 (91%)	60 (100%)	0	100	100
50	BX	132/133 (99%)	132 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	BY	78/80 (98%)	77 (99%)	1 (1%)	65	84
52	BZ	76/83 (92%)	76 (100%)	0	100	100
53	Ba	115/117 (98%)	115 (100%)	0	100	100
54	Bb	80/81 (99%)	80 (100%)	0	100	100
55	Bc	73/74 (99%)	73 (100%)	0	100	100
56	Bd	48/51 (94%)	47 (98%)	1 (2%)	48	74
57	Be	60/61 (98%)	60 (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	32/35 (91%)	32 (100%)	0	100	100
61	Bi	82/83 (99%)	82 (100%)	0	100	100
62	Bj	70/72 (97%)	70 (100%)	0	100	100
63	Bk	53/55 (96%)	53 (100%)	0	100	100
All	All	6775/7027 (96%)	6741 (100%)	34 (0%)	85	95

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
44	BR	7	SER
44	BR	94	ARG
51	BY	55	LEU
30	BB	365	GLN
30	BB	255	SER

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

Mol	Chain	Res	Type
29	BA	7	GLN
29	BA	229	HIS
30	BB	365	GLN
34	BG	21	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1487/1497 (99%)	247 (16%)	17 (1%)
27	B1	2928/3051 (95%)	437 (14%)	29 (0%)
28	B2	124/125 (99%)	16 (12%)	0
All	All	4539/4673 (97%)	700 (15%)	46 (1%)

5 of 700 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	4	C
1	A1	17	5MC
1	A1	34	G
1	A1	42	G
1	A1	43	A

5 of 46 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	B1	920	OMG
27	B1	1696	G
27	B1	982	A
27	B1	1368	A
27	B1	1940	C

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

243 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	$\# Z  > 2$
27	4AC	B1	23	27	21,24,25	3.25	9 (42%)	29,34,37	1.06	4 (13%)
27	4AC	B1	866	27	21,24,25	3.26	10 (47%)	29,34,37	1.04	4 (13%)
1	4AC	A1	761	1	21,24,25	3.29	9 (42%)	29,34,37	1.08	4 (13%)
27	OMG	B1	808	27	18,26,27	2.59	8 (44%)	19,38,41	1.53	4 (21%)
27	5MC	B1	1344	27	18,22,23	3.17	7 (38%)	26,32,35	1.00	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMC	A1	1226	1	19,22,23	3.07	8 (42%)	26,31,34	0.72	0
27	4AC	B1	360	27	21,24,25	3.27	10 (47%)	29,34,37	1.04	4 (13%)
1	5MU	A1	1110	1	19,22,23	0.41	0	28,32,35	0.55	0
1	4AC	A1	499	1	21,24,25	3.27	9 (42%)	29,34,37	1.05	4 (13%)
27	OMC	B1	2557	27	19,22,23	3.13	8 (42%)	26,31,34	1.02	2 (7%)
1	4AC	A1	231	1	21,24,25	3.28	9 (42%)	29,34,37	1.07	4 (13%)
27	4AC	B1	200	27	21,24,25	3.26	9 (42%)	29,34,37	1.04	4 (13%)
27	OMG	B1	2022	27	18,26,27	2.60	8 (44%)	19,38,41	1.53	5 (26%)
1	LHH	A1	238	1	22,25,26	2.93	6 (27%)	29,35,38	1.51	4 (13%)
27	4AC	B1	580	27	21,24,25	3.25	9 (42%)	29,34,37	1.02	4 (13%)
27	OMG	B1	2028	27	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)
1	4AC	A1	945	1	21,24,25	3.30	9 (42%)	29,34,37	1.12	4 (13%)
27	4AC	B1	2821	27	21,24,25	3.29	9 (42%)	29,34,37	1.06	4 (13%)
27	4AC	B1	227	27	21,24,25	3.29	10 (47%)	29,34,37	1.07	4 (13%)
1	OMG	A1	459	1	18,26,27	2.59	8 (44%)	19,38,41	1.48	4 (21%)
1	5MC	A1	1190	1	18,22,23	3.18	7 (38%)	26,32,35	0.96	2 (7%)
1	5MC	A1	473	1	18,22,23	3.19	7 (38%)	26,32,35	0.99	2 (7%)
1	G7M	A1	481	1	20,26,27	4.09	10 (50%)	17,39,42	0.98	1 (5%)
27	4AC	B1	130	27	21,24,25	3.26	10 (47%)	29,34,37	1.03	4 (13%)
27	A2M	B1	506	27	18,25,26	4.22	7 (38%)	18,36,39	2.28	4 (22%)
27	4AC	B1	1911	27	21,24,25	3.25	9 (42%)	29,34,37	1.03	4 (13%)
27	5MC	B1	1977	27	18,22,23	3.18	7 (38%)	26,32,35	1.00	2 (7%)
27	4AC	B1	979	27	21,24,25	3.26	9 (42%)	29,34,37	1.05	4 (13%)
1	OMC	A1	1364	1	19,22,23	3.13	8 (42%)	26,31,34	0.71	0
1	4AC	A1	540	1	21,24,25	3.26	10 (47%)	29,34,37	1.04	4 (13%)
1	4AC	A1	836	1	21,24,25	3.26	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	1052	27	21,24,25	3.28	9 (42%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1501	27	21,24,25	3.28	9 (42%)	29,34,37	1.10	4 (13%)
27	OMG	B1	530	27	18,26,27	2.61	8 (44%)	19,38,41	1.48	4 (21%)
1	OMC	A1	834	1	19,22,23	3.10	8 (42%)	26,31,34	0.66	0
27	OMG	B1	921	27	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)
27	A2M	B1	880	27	18,25,26	4.24	7 (38%)	18,36,39	2.20	4 (22%)
1	4AC	A1	624	1	21,24,25	3.31	9 (42%)	29,34,37	1.13	4 (13%)
27	OMG	B1	887	27	18,26,27	2.61	8 (44%)	19,38,41	1.51	4 (21%)
27	4AC	B1	1064	27	21,24,25	3.25	10 (47%)	29,34,37	1.07	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	OMU	B1	926	27	19,22,23	3.32	7 (36%)	26,31,34	2.04	8 (30%)
27	OMG	B1	1904	27	18,26,27	2.58	8 (44%)	19,38,41	1.52	4 (21%)
1	4AC	A1	87	1	21,24,25	3.28	9 (42%)	29,34,37	1.45	6 (20%)
1	OMG	A1	1115	1	18,26,27	2.61	8 (44%)	19,38,41	1.53	4 (21%)
27	4AC	B1	162	27	21,24,25	3.28	10 (47%)	29,34,37	1.08	4 (13%)
27	4AC	B1	378	27	21,24,25	3.25	10 (47%)	29,34,37	1.43	6 (20%)
27	OMG	B1	856	27	18,26,27	2.60	8 (44%)	19,38,41	1.53	4 (21%)
27	4AC	B1	1100	27	21,24,25	3.25	9 (42%)	29,34,37	1.04	4 (13%)
27	UR3	B1	2700	27	19,22,23	3.17	7 (36%)	26,32,35	1.41	3 (11%)
27	4AC	B1	2792	27	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
27	OMG	B1	1965	27	18,26,27	2.60	8 (44%)	19,38,41	1.56	4 (21%)
1	OMG	A1	1003	1	18,26,27	2.61	8 (44%)	19,38,41	1.52	4 (21%)
27	OMG	B1	214	27	18,26,27	2.61	8 (44%)	19,38,41	1.55	4 (21%)
27	4AC	B1	2602	27	21,24,25	3.25	10 (47%)	29,34,37	1.03	4 (13%)
1	OMU	A1	1165	1	19,22,23	3.30	7 (36%)	26,31,34	1.68	5 (19%)
27	4AC	B1	1067	27	21,24,25	3.25	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1293	27	21,24,25	3.30	9 (42%)	29,34,37	1.34	6 (20%)
27	4AC	B1	527	27	21,24,25	3.26	9 (42%)	29,34,37	1.07	4 (13%)
27	4AC	B1	2454	27	21,24,25	3.29	10 (47%)	29,34,37	1.06	4 (13%)
1	5MC	A1	681	1	18,22,23	3.16	7 (38%)	26,32,35	1.20	4 (15%)
27	OMG	B1	55	27	18,26,27	2.59	8 (44%)	19,38,41	1.51	4 (21%)
1	OMC	A1	1270	1	19,22,23	3.13	8 (42%)	26,31,34	0.72	0
1	4AC	A1	1314	1	21,24,25	3.27	9 (42%)	29,34,37	1.04	4 (13%)
28	4AC	B2	115	28	21,24,25	3.30	10 (47%)	29,34,37	1.41	6 (20%)
1	5MC	A1	927	1	18,22,23	3.21	7 (38%)	26,32,35	0.99	2 (7%)
1	5MC	A1	687	1	18,22,23	3.20	7 (38%)	26,32,35	0.98	2 (7%)
1	4AC	A1	1254	1	21,24,25	3.26	9 (42%)	29,34,37	1.26	6 (20%)
27	4AC	B1	1546	27	21,24,25	3.26	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	2379	27	21,24,25	3.22	10 (47%)	29,34,37	1.03	3 (10%)
27	4AC	B1	1751	27	21,24,25	3.28	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	2526	27	21,24,25	3.26	10 (47%)	29,34,37	1.27	6 (20%)
1	4AC	A1	839	1	21,24,25	3.25	9 (42%)	29,34,37	1.06	4 (13%)
1	OMC	A1	1371	1	19,22,23	3.14	8 (42%)	26,31,34	0.72	0
1	4AC	A1	719	1	21,24,25	3.24	9 (42%)	29,34,37	1.06	4 (13%)
1	OMG	A1	645	1	18,26,27	2.60	8 (44%)	19,38,41	1.46	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMG	A1	668	1	18,26,27	2.61	8 (44%)	19,38,41	1.49	4 (21%)
1	4AC	A1	1467	1	21,24,25	3.29	9 (42%)	29,34,37	1.45	5 (17%)
27	4AC	B1	1178	27	21,24,25	3.27	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	2749	27	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	3037	27	21,24,25	3.28	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	2213	27	21,24,25	3.24	9 (42%)	29,34,37	1.05	4 (13%)
1	5MC	A1	352	1	18,22,23	3.18	7 (38%)	26,32,35	0.99	2 (7%)
27	4AC	B1	337	27	21,24,25	3.25	10 (47%)	29,34,37	1.03	4 (13%)
27	5MU	B1	2401	27	19,22,23	0.41	0	28,32,35	0.71	0
27	OMC	B1	2607	27	19,22,23	3.13	8 (42%)	26,31,34	0.72	0
27	4AC	B1	1107	27	21,24,25	3.22	10 (47%)	29,34,37	1.04	4 (13%)
1	4AC	A1	220	1	21,24,25	3.26	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	3006	27	21,24,25	3.27	9 (42%)	29,34,37	1.07	4 (13%)
27	OMC	B1	2119	27	19,22,23	3.10	8 (42%)	26,31,34	0.73	0
27	4AC	B1	2876	27	21,24,25	3.27	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	1383	27	21,24,25	3.26	10 (47%)	29,34,37	1.07	4 (13%)
1	OMG	A1	507	1	18,26,27	2.59	8 (44%)	19,38,41	1.52	4 (21%)
27	4AC	B1	2429	27	21,24,25	3.25	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	1442	27	21,24,25	3.24	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	2020	27	21,24,25	3.25	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	80	27	21,24,25	3.26	10 (47%)	29,34,37	1.06	4 (13%)
27	A2M	B1	2506	27	18,25,26	4.23	7 (38%)	18,36,39	2.25	4 (22%)
1	5MC	A1	1013	1	18,22,23	3.19	7 (38%)	26,32,35	0.99	2 (7%)
27	4AC	B1	48	27	21,24,25	3.21	10 (47%)	29,34,37	0.98	3 (10%)
1	4AC	A1	41	1	21,24,25	3.26	10 (47%)	29,34,37	1.41	6 (20%)
27	4AC	B1	2844	27	21,24,25	3.26	10 (47%)	29,34,37	1.03	4 (13%)
1	5MC	A1	863	1	18,22,23	3.19	7 (38%)	26,32,35	1.01	2 (7%)
27	4AC	B1	479	27	21,24,25	3.28	9 (42%)	29,34,37	1.10	4 (13%)
27	4AC	B1	732	27	21,24,25	3.27	9 (42%)	29,34,37	1.06	4 (13%)
27	4AC	B1	953	27	21,24,25	3.26	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1374	27	21,24,25	3.30	10 (47%)	29,34,37	1.11	4 (13%)
1	4AC	A1	382	1	21,24,25	3.26	10 (47%)	29,34,37	1.02	4 (13%)
1	4AC	A1	636	1	21,24,25	3.27	9 (42%)	29,34,37	1.09	4 (13%)
27	4AC	B1	1579	27	21,24,25	3.29	9 (42%)	29,34,37	1.08	4 (13%)
27	4AC	B1	3011	27	21,24,25	3.27	9 (42%)	29,34,37	1.03	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	A2M	B1	857	27	18,25,26	4.21	7 (38%)	18,36,39	2.22	4 (22%)
27	OMG	B1	2540	27	18,26,27	2.60	8 (44%)	19,38,41	1.50	4 (21%)
1	OMU	A1	775	1	19,22,23	3.29	7 (36%)	26,31,34	1.73	5 (19%)
27	4AC	B1	1706	27	21,24,25	3.27	9 (42%)	29,34,37	1.05	4 (13%)
27	5MC	B1	2617	27	18,22,23	3.19	7 (38%)	26,32,35	1.06	1 (3%)
27	4AC	B1	2171	27	21,24,25	3.24	10 (47%)	29,34,37	1.23	6 (20%)
27	4AC	B1	1360	27	21,24,25	3.31	9 (42%)	29,34,37	1.48	5 (17%)
27	5MC	B1	2067	27	18,22,23	3.20	7 (38%)	26,32,35	1.00	2 (7%)
27	4AC	B1	98	27	21,24,25	3.27	10 (47%)	29,34,37	1.03	4 (13%)
27	5MC	B1	336	27	18,22,23	3.17	7 (38%)	26,32,35	1.02	2 (7%)
27	4AC	B1	485	27	21,24,25	3.23	10 (47%)	29,34,37	1.02	3 (10%)
27	OMG	B1	920	27	18,26,27	2.61	8 (44%)	19,38,41	1.51	4 (21%)
27	4AC	B1	933	27	21,24,25	3.27	10 (47%)	29,34,37	1.09	4 (13%)
27	A2M	B1	940	27	18,25,26	4.26	7 (38%)	18,36,39	2.26	4 (22%)
1	5MC	A1	1484	1	18,22,23	3.16	7 (38%)	26,32,35	0.99	2 (7%)
27	4AC	B1	1264	27	21,24,25	3.27	10 (47%)	29,34,37	1.06	4 (13%)
1	4AC	A1	367	1	21,24,25	3.24	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	1345	27	21,24,25	3.24	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	1885	27	21,24,25	3.25	10 (47%)	29,34,37	1.02	4 (13%)
27	5MC	B1	2087	27	18,22,23	3.17	7 (38%)	26,32,35	0.99	2 (7%)
27	4AC	B1	1128	27	21,24,25	3.25	10 (47%)	29,34,37	1.02	4 (13%)
1	4AC	A1	1181	1	21,24,25	3.26	10 (47%)	29,34,37	1.26	5 (17%)
1	OMC	A1	1194	1	19,22,23	3.12	8 (42%)	26,31,34	0.71	0
27	4AC	B1	688	27	21,24,25	3.27	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	786	27	21,24,25	3.26	9 (42%)	29,34,37	1.05	4 (13%)
27	OMG	B1	2180	27	18,26,27	2.60	8 (44%)	19,38,41	1.54	4 (21%)
27	OMC	B1	1489	27	19,22,23	3.10	8 (42%)	26,31,34	0.74	0
27	4AC	B1	243	27	21,24,25	3.25	10 (47%)	29,34,37	1.03	4 (13%)
1	5MC	A1	951	1	18,22,23	3.21	7 (38%)	26,32,35	1.06	2 (7%)
1	4AC	A1	546	1	21,24,25	3.28	9 (42%)	29,34,37	1.06	4 (13%)
28	4AC	B2	30	28	21,24,25	3.30	10 (47%)	29,34,37	1.06	4 (13%)
27	OMG	B1	2562	27	18,26,27	2.60	8 (44%)	19,38,41	1.52	4 (21%)
1	4AC	A1	816	1	21,24,25	3.27	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1478	27	21,24,25	3.24	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	1639	27	21,24,25	3.27	10 (47%)	29,34,37	1.05	4 (13%)



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	3.15	10 (47%)	29,34,37	0.94	2 (6%)
27	LHH	B1	1439	27	22,25,26	2.92	6 (27%)	29,35,38	1.33	2 (6%)
27	4AC	B1	2850	27	21,24,25	3.25	10 (47%)	29,34,37	1.03	4 (13%)
1	4AC	A1	5	1	21,24,25	3.27	9 (42%)	29,34,37	1.07	4 (13%)
1	4AC	A1	1029	1	21,24,25	3.26	9 (42%)	29,34,37	1.05	4 (13%)
27	OMC	B1	2735	27	19,22,23	3.13	8 (42%)	26,31,34	0.73	0
27	4AC	B1	1762	27	21,24,25	3.25	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	2008	27	21,24,25	3.27	10 (47%)	29,34,37	1.02	4 (13%)
27	4AC	B1	1846	27	21,24,25	3.28	10 (47%)	29,34,37	1.06	4 (13%)
1	5MC	A1	230	1	18,22,23	3.17	7 (38%)	26,32,35	0.99	2 (7%)
1	4AC	A1	578	1	21,24,25	3.27	9 (42%)	29,34,37	1.29	6 (20%)
1	OMG	A1	861	1	18,26,27	2.58	8 (44%)	19,38,41	1.50	4 (21%)
27	4AC	B1	715	27	21,24,25	3.26	10 (47%)	29,34,37	1.03	4 (13%)
1	OMC	A1	1028	1	19,22,23	3.12	8 (42%)	26,31,34	0.72	0
27	OMU	B1	1488	27	19,22,23	3.29	7 (36%)	26,31,34	1.69	4 (15%)
27	OMU	B1	2554	27	19,22,23	3.29	7 (36%)	26,31,34	1.69	4 (15%)
27	4AC	B1	344	27	21,24,25	3.29	9 (42%)	29,34,37	1.06	4 (13%)
27	4AC	B1	896	27	21,24,25	3.25	9 (42%)	29,34,37	1.03	3 (10%)
27	OMG	B1	2757	27	18,26,27	2.59	8 (44%)	19,38,41	1.59	5 (26%)
27	4AC	B1	116	27	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
1	A2M	A1	819	1	18,25,26	4.27	7 (38%)	18,36,39	2.27	4 (22%)
1	4AC	A1	141	1	21,24,25	3.30	9 (42%)	29,34,37	1.08	4 (13%)
1	OMU	A1	762	1	19,22,23	3.31	7 (36%)	26,31,34	1.70	5 (19%)
27	4AC	B1	1608	27	21,24,25	3.30	9 (42%)	29,34,37	1.29	6 (20%)
27	4AC	B1	2469	27	21,24,25	3.25	10 (47%)	29,34,37	1.06	4 (13%)
1	OMG	A1	455	1	18,26,27	2.59	8 (44%)	19,38,41	1.54	5 (26%)
27	OMG	B1	2391	27	18,26,27	2.56	8 (44%)	19,38,41	1.53	5 (26%)
1	5MC	A1	17	1	18,22,23	3.16	7 (38%)	26,32,35	0.98	2 (7%)
1	OMC	A1	117	1	19,22,23	3.11	8 (42%)	26,31,34	0.70	0
27	4AC	B1	652	27	21,24,25	3.24	10 (47%)	29,34,37	1.06	4 (13%)
1	4AC	A1	691	1	21,24,25	3.28	10 (47%)	29,34,37	1.09	4 (13%)
27	4AC	B1	2432	27	21,24,25	3.27	10 (47%)	29,34,37	1.05	4 (13%)
1	4AC	A1	216	1	21,24,25	3.30	10 (47%)	29,34,37	1.09	4 (13%)
27	4AC	B1	1505	27	21,24,25	3.26	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	1061	27	21,24,25	3.27	9 (42%)	29,34,37	1.04	4 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	OMC	B1	1832	27	19,22,23	3.13	8 (42%)	26,31,34	0.69	0
27	4AC	B1	434	27	21,24,25	3.25	10 (47%)	29,34,37	1.43	6 (20%)
1	OMU	A1	1368	1	19,22,23	3.29	7 (36%)	26,31,34	1.72	5 (19%)
1	MA6	A1	1475	1	18,26,27	0.98	1 (5%)	19,38,41	4.49	3 (15%)
1	4AC	A1	614	1	21,24,25	3.26	10 (47%)	29,34,37	1.05	4 (13%)
1	4AC	A1	307	1	21,24,25	3.24	10 (47%)	29,34,37	1.06	4 (13%)
27	4AC	B1	1769	27	21,24,25	3.23	9 (42%)	29,34,37	1.02	3 (10%)
1	4SU	A1	756	1	18,21,22	3.89	8 (44%)	26,30,33	2.22	5 (19%)
1	4AC	A1	534	1	21,24,25	3.28	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1822	27	21,24,25	3.26	9 (42%)	29,34,37	1.08	4 (13%)
1	5MC	A1	466	1	18,22,23	3.12	7 (38%)	26,32,35	1.09	2 (7%)
1	OMG	A1	541	1	18,26,27	2.61	8 (44%)	19,38,41	1.98	6 (31%)
27	OMC	B1	501	27	19,22,23	3.12	8 (42%)	26,31,34	0.74	0
27	OMG	B1	2684	27	18,26,27	2.61	8 (44%)	19,38,41	1.48	4 (21%)
27	4AC	B1	1649	27	21,24,25	3.28	9 (42%)	29,34,37	1.09	4 (13%)
27	OMC	B1	2808	27	19,22,23	3.12	8 (42%)	26,31,34	0.72	0
1	4AC	A1	706	1	21,24,25	3.26	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	1743	27	21,24,25	3.29	9 (42%)	29,34,37	1.06	4 (13%)
27	4SU	B1	2565	27	18,21,22	3.87	8 (44%)	26,30,33	2.23	5 (19%)
27	4AC	B1	19	27	21,24,25	3.28	9 (42%)	29,34,37	1.07	4 (13%)
1	MA6	A1	1476	1	18,26,27	1.00	1 (5%)	19,38,41	4.37	3 (15%)
27	4AC	B1	950	27	21,24,25	3.24	10 (47%)	29,34,37	1.04	4 (13%)
27	4AC	B1	1967	27	21,24,25	3.23	9 (42%)	29,34,37	1.01	4 (13%)
27	OMG	B1	2365	27	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)
27	OMU	B1	454	27	19,22,23	3.32	7 (36%)	26,31,34	2.02	7 (26%)
1	OMG	A1	329	1	18,26,27	2.61	8 (44%)	19,38,41	1.58	5 (26%)
27	OMG	B1	2108	27	18,26,27	2.58	8 (44%)	19,38,41	1.53	4 (21%)
27	4AC	B1	419	27	21,24,25	3.26	9 (42%)	29,34,37	1.05	4 (13%)
27	OMC	B1	2059	27	19,22,23	3.13	8 (42%)	26,31,34	0.76	0
1	A1I59	A1	1366	1	22,27,28	2.57	6 (27%)	29,39,42	1.07	2 (6%)
1	A2M	A1	361	1	18,25,26	0.63	1 (5%)	18,36,39	0.91	1 (5%)
27	4AC	B1	2492	27	21,24,25	3.27	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	1818	27	21,24,25	3.24	10 (47%)	29,34,37	1.03	4 (13%)
27	4AC	B1	721	27	21,24,25	3.24	9 (42%)	29,34,37	1.03	4 (13%)
1	4AC	A1	856	1	21,24,25	3.24	10 (47%)	29,34,37	1.05	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4AC	A1	274	1	21,24,25	3.27	9 (42%)	29,34,37	1.05	4 (13%)
27	OMG	B1	841	27	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)
27	4AC	B1	2133	27	21,24,25	3.24	9 (42%)	29,34,37	1.04	4 (13%)
27	LHH	B1	502	27	22,25,26	2.93	6 (27%)	29,35,38	1.33	2 (6%)
27	5MU	B1	888	27	19,22,23	0.45	0	28,32,35	0.82	1 (3%)
1	MA6	A1	1457	1	18,26,27	1.03	1 (5%)	19,38,41	4.23	3 (15%)
27	4AC	B1	1435	27	21,24,25	3.24	10 (47%)	29,34,37	1.06	4 (13%)
28	4AC	B2	88	28	21,24,25	3.28	9 (42%)	29,34,37	1.06	4 (13%)
27	4AC	B1	1551	27	21,24,25	3.26	10 (47%)	29,34,37	1.04	4 (13%)
27	OMG	B1	2984	27	18,26,27	2.59	8 (44%)	19,38,41	1.51	4 (21%)
1	5MC	A1	1362	1	18,22,23	3.19	7 (38%)	26,32,35	1.01	2 (7%)
1	OMU	A1	8	1	19,22,23	3.31	7 (36%)	26,31,34	1.78	6 (23%)
27	OMC	B1	1099	27	19,22,23	3.11	8 (42%)	26,31,34	0.69	0
27	4AC	B1	1150	27	21,24,25	3.27	10 (47%)	29,34,37	1.08	4 (13%)
1	4AC	A1	405	1	21,24,25	3.27	10 (47%)	29,34,37	1.05	4 (13%)
27	4AC	B1	2809	27	21,24,25	3.26	10 (47%)	29,34,37	1.05	4 (13%)
1	4AC	A1	291	1	21,24,25	3.25	10 (47%)	29,34,37	1.01	4 (13%)
1	4AC	A1	827	1	21,24,25	3.28	10 (47%)	29,34,37	1.07	4 (13%)
27	4AC	B1	2968	27	21,24,25	3.25	10 (47%)	29,34,37	1.27	6 (20%)
1	4AC	A1	1227	1	21,24,25	3.13	10 (47%)	29,34,37	0.96	1 (3%)
27	4AC	B1	1946	27	21,24,25	3.24	9 (42%)	29,34,37	1.42	6 (20%)
27	4AC	B1	2113	27	21,24,25	3.25	10 (47%)	29,34,37	1.04	4 (13%)
27	OMG	B1	1557	27	18,26,27	2.60	8 (44%)	19,38,41	1.49	4 (21%)
1	4AC	A1	739	1	21,24,25	3.30	9 (42%)	29,34,37	1.06	4 (13%)
27	4AC	B1	3020	27	21,24,25	3.27	9 (42%)	29,34,37	1.06	4 (13%)
1	OMU	A1	52	1	19,22,23	3.31	7 (36%)	26,31,34	1.68	5 (19%)
27	4AC	B1	1290	27	21,24,25	3.25	9 (42%)	29,34,37	1.02	4 (13%)
27	OMC	B1	1914	27	19,22,23	3.09	8 (42%)	26,31,34	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	23	27	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	866	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	761	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	808	27	-	0/5/27/28	0/3/3/3
27	5MC	B1	1344	27	-	0/7/25/26	0/2/2/2
1	OMC	A1	1226	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	360	27	-	0/11/29/30	0/2/2/2
1	5MU	A1	1110	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	499	1	-	2/11/29/30	0/2/2/2
27	OMC	B1	2557	27	-	2/9/27/28	0/2/2/2
1	4AC	A1	231	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	200	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2022	27	-	1/5/27/28	0/3/3/3
1	LHH	A1	238	1	-	4/13/31/32	0/2/2/2
27	4AC	B1	580	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2028	27	-	1/5/27/28	0/3/3/3
1	4AC	A1	945	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	2821	27	-	3/11/29/30	0/2/2/2
27	4AC	B1	227	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	459	1	-	0/5/27/28	0/3/3/3
1	5MC	A1	1190	1	-	2/7/25/26	0/2/2/2
1	5MC	A1	473	1	-	0/7/25/26	0/2/2/2
1	G7M	A1	481	1	-	2/3/25/26	0/3/3/3
27	4AC	B1	130	27	-	0/11/29/30	0/2/2/2
27	A2M	B1	506	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	1911	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	1977	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	979	27	-	3/11/29/30	0/2/2/2
1	OMC	A1	1364	1	-	0/9/27/28	0/2/2/2
1	4AC	A1	540	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	836	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1052	27	-	1/11/29/30	0/2/2/2
27	4AC	B1	1501	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	530	27	-	0/5/27/28	0/3/3/3
1	OMC	A1	834	1	-	0/9/27/28	0/2/2/2
27	OMG	B1	921	27	-	1/5/27/28	0/3/3/3
27	A2M	B1	880	27	-	0/5/27/28	0/3/3/3
1	4AC	A1	624	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	887	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	1064	27	-	0/11/29/30	0/2/2/2
27	OMU	B1	926	27	-	4/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMG	B1	1904	27	-	0/5/27/28	0/3/3/3
1	4AC	A1	87	1	-	3/11/29/30	0/2/2/2
1	OMG	A1	1115	1	-	0/5/27/28	0/3/3/3
27	4AC	B1	162	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	378	27	-	1/11/29/30	0/2/2/2
27	OMG	B1	856	27	-	2/5/27/28	0/3/3/3
27	4AC	B1	1100	27	-	0/11/29/30	0/2/2/2
27	UR3	B1	2700	27	-	2/7/25/26	0/2/2/2
27	4AC	B1	2792	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	1965	27	-	0/5/27/28	0/3/3/3
1	OMG	A1	1003	1	-	0/5/27/28	0/3/3/3
27	OMG	B1	214	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	2602	27	-	0/11/29/30	0/2/2/2
1	OMU	A1	1165	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	1067	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1293	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	527	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2454	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	681	1	-	0/7/25/26	0/2/2/2
27	OMG	B1	55	27	-	2/5/27/28	0/3/3/3
1	OMC	A1	1270	1	-	2/9/27/28	0/2/2/2
1	4AC	A1	1314	1	-	0/11/29/30	0/2/2/2
28	4AC	B2	115	28	-	3/11/29/30	0/2/2/2
1	5MC	A1	927	1	-	0/7/25/26	0/2/2/2
1	5MC	A1	687	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	1254	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1546	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2379	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1751	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2526	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	839	1	-	2/11/29/30	0/2/2/2
1	OMC	A1	1371	1	-	0/9/27/28	0/2/2/2
1	4AC	A1	719	1	-	2/11/29/30	0/2/2/2
1	OMG	A1	645	1	-	0/5/27/28	0/3/3/3
1	OMG	A1	668	1	-	0/5/27/28	0/3/3/3
1	4AC	A1	1467	1	-	2/11/29/30	0/2/2/2
27	4AC	B1	1178	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2749	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	3037	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2213	27	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A1	352	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	337	27	-	0/11/29/30	0/2/2/2
27	5MU	B1	2401	27	-	3/7/25/26	0/2/2/2
27	OMC	B1	2607	27	-	2/9/27/28	0/2/2/2
27	4AC	B1	1107	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	220	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	3006	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2119	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	2876	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1383	27	-	2/11/29/30	0/2/2/2
1	OMG	A1	507	1	-	0/5/27/28	0/3/3/3
27	4AC	B1	2429	27	-	3/11/29/30	0/2/2/2
27	4AC	B1	1442	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2020	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	80	27	-	0/11/29/30	0/2/2/2
27	A2M	B1	2506	27	-	0/5/27/28	0/3/3/3
1	5MC	A1	1013	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	48	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	2844	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	479	27	-	3/11/29/30	0/2/2/2
27	4AC	B1	732	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	953	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1374	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	382	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	636	1	-	1/11/29/30	0/2/2/2
27	4AC	B1	1579	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	3011	27	-	0/11/29/30	0/2/2/2
27	A2M	B1	857	27	-	2/5/27/28	0/3/3/3
27	OMG	B1	2540	27	-	0/5/27/28	0/3/3/3
1	OMU	A1	775	1	-	5/9/27/28	0/2/2/2
27	4AC	B1	1706	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	2617	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	2171	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1360	27	-	2/11/29/30	0/2/2/2
27	5MC	B1	2067	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	98	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	336	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	485	27	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	OMG	B1	920	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	933	27	-	0/11/29/30	0/2/2/2
27	A2M	B1	940	27	-	0/5/27/28	0/3/3/3
1	5MC	A1	1484	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	1264	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	367	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1345	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1885	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	2087	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1128	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1181	1	-	0/11/29/30	0/2/2/2
1	OMC	A1	1194	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	688	27	-	3/11/29/30	0/2/2/2
27	4AC	B1	786	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2180	27	-	0/5/27/28	0/3/3/3
27	OMC	B1	1489	27	-	2/9/27/28	0/2/2/2
27	4AC	B1	243	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	951	1	-	1/7/25/26	0/2/2/2
1	4AC	A1	546	1	-	0/11/29/30	0/2/2/2
28	4AC	B2	30	28	-	0/11/29/30	0/2/2/2
27	OMG	B1	2562	27	-	0/5/27/28	0/3/3/3
1	4AC	A1	816	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1478	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1639	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	467	1	-	0/11/29/30	0/2/2/2
27	LHH	B1	1439	27	-	2/13/31/32	0/2/2/2
27	4AC	B1	2850	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	5	1	-	2/11/29/30	0/2/2/2
1	4AC	A1	1029	1	-	0/11/29/30	0/2/2/2
27	OMC	B1	2735	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	1762	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2008	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1846	27	-	1/11/29/30	0/2/2/2
1	5MC	A1	230	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	578	1	-	0/11/29/30	0/2/2/2
1	OMG	A1	861	1	-	1/5/27/28	0/3/3/3
27	4AC	B1	715	27	-	2/11/29/30	0/2/2/2
1	OMC	A1	1028	1	-	0/9/27/28	0/2/2/2
27	OMU	B1	1488	27	-	0/9/27/28	0/2/2/2
27	OMU	B1	2554	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	344	27	-	2/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	896	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2757	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	116	27	-	2/11/29/30	0/2/2/2
1	A2M	A1	819	1	-	2/5/27/28	0/3/3/3
1	4AC	A1	141	1	-	0/11/29/30	0/2/2/2
1	OMU	A1	762	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	1608	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	2469	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	455	1	-	1/5/27/28	0/3/3/3
27	OMG	B1	2391	27	-	3/5/27/28	0/3/3/3
1	5MC	A1	17	1	-	2/7/25/26	0/2/2/2
1	OMC	A1	117	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	652	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	691	1	-	2/11/29/30	0/2/2/2
27	4AC	B1	2432	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	216	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1505	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1061	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	1832	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	434	27	-	0/11/29/30	0/2/2/2
1	OMU	A1	1368	1	-	0/9/27/28	0/2/2/2
1	MA6	A1	1475	1	-	0/7/29/30	0/3/3/3
1	4AC	A1	614	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	307	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1769	27	-	0/11/29/30	0/2/2/2
1	4SU	A1	756	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	534	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1822	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	466	1	-	3/7/25/26	0/2/2/2
1	OMG	A1	541	1	-	2/5/27/28	0/3/3/3
27	OMC	B1	501	27	-	2/9/27/28	0/2/2/2
27	OMG	B1	2684	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	1649	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2808	27	-	0/9/27/28	0/2/2/2
1	4AC	A1	706	1	-	1/11/29/30	0/2/2/2
27	4AC	B1	1743	27	-	0/11/29/30	0/2/2/2
27	4SU	B1	2565	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	19	27	-	0/11/29/30	0/2/2/2
1	MA6	A1	1476	1	-	2/7/29/30	0/3/3/3
27	4AC	B1	950	27	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	1967	27	-	2/11/29/30	0/2/2/2
27	OMG	B1	2365	27	-	0/5/27/28	0/3/3/3
27	OMU	B1	454	27	-	0/9/27/28	0/2/2/2
1	OMG	A1	329	1	-	3/5/27/28	0/3/3/3
27	OMG	B1	2108	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	419	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2059	27	-	0/9/27/28	0/2/2/2
1	A1I59	A1	1366	1	-	1/11/33/34	0/2/2/2
1	A2M	A1	361	1	-	2/5/27/28	0/3/3/3
27	4AC	B1	2492	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1818	27	-	0/11/29/30	0/2/2/2
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
1	4AC	A1	274	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	841	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	2133	27	-	0/11/29/30	0/2/2/2
27	LHH	B1	502	27	-	1/13/31/32	0/2/2/2
27	5MU	B1	888	27	-	0/7/25/26	0/2/2/2
1	MA6	A1	1457	1	-	0/7/29/30	0/3/3/3
27	4AC	B1	1435	27	-	0/11/29/30	0/2/2/2
28	4AC	B2	88	28	-	0/11/29/30	0/2/2/2
27	4AC	B1	1551	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2984	27	-	0/5/27/28	0/3/3/3
1	5MC	A1	1362	1	-	2/7/25/26	0/2/2/2
1	OMU	A1	8	1	-	4/9/27/28	0/2/2/2
27	OMC	B1	1099	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	1150	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	405	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	2809	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	291	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	827	1	-	2/11/29/30	0/2/2/2
27	4AC	B1	2968	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1227	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1946	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2113	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	1557	27	-	4/5/27/28	0/3/3/3
1	4AC	A1	739	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	3020	27	-	0/11/29/30	0/2/2/2
1	OMU	A1	52	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	1290	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	1914	27	-	1/9/27/28	0/2/2/2



The worst 5 of 2073 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A1	819	A2M	O4'-C1'	15.43	1.62	1.41
27	B1	940	A2M	O4'-C1'	15.36	1.62	1.41
27	B1	880	A2M	O4'-C1'	15.27	1.62	1.41
27	B1	857	A2M	O4'-C1'	15.21	1.62	1.41
27	B1	506	A2M	O4'-C1'	15.18	1.62	1.41

The worst 5 of 874 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	1475	MA6	N1-C6-N6	-13.53	102.81	117.06
1	A1	1476	MA6	N1-C6-N6	-13.49	102.85	117.06
1	A1	1475	MA6	C1'-N9-C4	12.76	149.06	126.64
1	A1	1457	MA6	C1'-N9-C4	12.36	148.36	126.64
1	A1	1457	MA6	N1-C6-N6	-12.27	104.14	117.06

There are no chirality outliers.

5 of 138 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A1	8	OMU	C1'-C2'-O2'-CM2
1	A1	238	LHH	C5-C4-N4-C7
1	A1	238	LHH	N3-C4-N4-C7
1	A1	238	LHH	C3'-C4'-C5'-O5'
1	A1	238	LHH	O4'-C4'-C5'-O5'

There are no ring outliers.

176 monomers are involved in 268 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	23	4AC	1	0
27	B1	866	4AC	1	0
1	A1	761	4AC	1	0
1	A1	1226	OMC	1	0
27	B1	360	4AC	1	0
1	A1	499	4AC	2	0
1	A1	231	4AC	1	0
27	B1	200	4AC	1	0
27	B1	580	4AC	1	0
1	A1	945	4AC	4	0
27	B1	2821	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	227	4AC	1	0
27	B1	130	4AC	1	0
27	B1	506	A2M	1	0
27	B1	1911	4AC	1	0
27	B1	1977	5MC	1	0
27	B1	979	4AC	2	0
1	A1	1364	OMC	1	0
1	A1	540	4AC	1	0
1	A1	836	4AC	1	0
27	B1	1052	4AC	3	0
27	B1	1501	4AC	2	0
27	B1	530	OMG	1	0
27	B1	921	OMG	1	0
1	A1	624	4AC	4	0
27	B1	887	OMG	1	0
27	B1	1064	4AC	2	0
27	B1	926	OMU	1	0
1	A1	87	4AC	2	0
27	B1	162	4AC	1	0
27	B1	378	4AC	2	0
27	B1	856	OMG	1	0
27	B1	1100	4AC	1	0
27	B1	2792	4AC	1	0
27	B1	2602	4AC	1	0
27	B1	1067	4AC	2	0
27	B1	1293	4AC	2	0
27	B1	527	4AC	1	0
27	B1	2454	4AC	1	0
27	B1	55	OMG	1	0
1	A1	1314	4AC	4	0
28	B2	115	4AC	2	0
1	A1	1254	4AC	1	0
27	B1	1546	4AC	2	0
27	B1	2379	4AC	2	0
27	B1	1751	4AC	1	0
27	B1	2526	4AC	1	0
1	A1	839	4AC	2	0
1	A1	719	4AC	2	0
1	A1	668	OMG	1	0
1	A1	1467	4AC	2	0
27	B1	1178	4AC	2	0
27	B1	2749	4AC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	3037	4AC	2	0
27	B1	2213	4AC	2	0
1	A1	352	5MC	1	0
27	B1	337	4AC	3	0
27	B1	2401	5MU	1	0
27	B1	1107	4AC	3	0
1	A1	220	4AC	2	0
27	B1	3006	4AC	3	0
27	B1	2876	4AC	1	0
27	B1	1383	4AC	1	0
1	A1	507	OMG	1	0
27	B1	2429	4AC	2	0
27	B1	1442	4AC	1	0
27	B1	2020	4AC	1	0
27	B1	80	4AC	1	0
1	A1	1013	5MC	1	0
27	B1	48	4AC	2	0
1	A1	41	4AC	1	0
27	B1	2844	4AC	2	0
27	B1	479	4AC	1	0
27	B1	732	4AC	1	0
27	B1	953	4AC	1	0
27	B1	1374	4AC	3	0
1	A1	382	4AC	1	0
1	A1	636	4AC	3	0
27	B1	1579	4AC	2	0
27	B1	3011	4AC	1	0
27	B1	857	A2M	1	0
1	A1	775	OMU	1	0
27	B1	1706	4AC	1	0
27	B1	2617	5MC	6	0
27	B1	2171	4AC	2	0
27	B1	1360	4AC	7	0
27	B1	2067	5MC	1	0
27	B1	98	4AC	1	0
27	B1	485	4AC	3	0
27	B1	920	OMG	2	0
27	B1	933	4AC	2	0
27	B1	1264	4AC	1	0
1	A1	367	4AC	1	0
27	B1	1345	4AC	1	0
27	B1	1885	4AC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	1128	4AC	1	0
1	A1	1181	4AC	4	0
27	B1	688	4AC	1	0
27	B1	786	4AC	1	0
27	B1	1489	OMC	2	0
27	B1	243	4AC	2	0
1	A1	951	5MC	4	0
1	A1	546	4AC	1	0
28	B2	30	4AC	3	0
27	B1	2562	OMG	2	0
1	A1	816	4AC	2	0
27	B1	1478	4AC	2	0
27	B1	1639	4AC	1	0
1	A1	467	4AC	1	0
27	B1	2850	4AC	1	0
1	A1	5	4AC	1	0
1	A1	1029	4AC	1	0
27	B1	1762	4AC	1	0
27	B1	2008	4AC	1	0
27	B1	1846	4AC	2	0
1	A1	578	4AC	2	0
27	B1	715	4AC	1	0
27	B1	1488	OMU	1	0
27	B1	344	4AC	1	0
27	B1	896	4AC	2	0
27	B1	116	4AC	1	0
1	A1	141	4AC	1	0
27	B1	1608	4AC	1	0
27	B1	2469	4AC	1	0
27	B1	652	4AC	1	0
1	A1	691	4AC	4	0
27	B1	2432	4AC	2	0
1	A1	216	4AC	1	0
27	B1	1505	4AC	1	0
27	B1	1061	4AC	1	0
27	B1	434	4AC	1	0
1	A1	1368	OMU	1	0
1	A1	1475	MA6	3	0
1	A1	614	4AC	1	0
1	A1	307	4AC	2	0
27	B1	1769	4AC	4	0
1	A1	534	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	1822	4AC	1	0
1	A1	541	OMG	1	0
27	B1	2684	OMG	1	0
27	B1	1649	4AC	1	0
1	A1	706	4AC	2	0
27	B1	1743	4AC	2	0
27	B1	19	4AC	1	0
1	A1	1476	MA6	3	0
27	B1	950	4AC	2	0
27	B1	1967	4AC	1	0
27	B1	454	OMU	1	0
1	A1	329	OMG	1	0
27	B1	419	4AC	2	0
1	A1	1366	A1I59	2	0
27	B1	2492	4AC	4	0
27	B1	1818	4AC	2	0
27	B1	721	4AC	1	0
1	A1	856	4AC	1	0
1	A1	274	4AC	1	0
27	B1	2133	4AC	1	0
27	B1	888	5MU	1	0
1	A1	1457	MA6	2	0
27	B1	1435	4AC	2	0
28	B2	88	4AC	2	0
27	B1	1551	4AC	1	0
27	B1	1150	4AC	1	0
1	A1	405	4AC	2	0
27	B1	2809	4AC	2	0
1	A1	291	4AC	1	0
1	A1	827	4AC	1	0
27	B1	2968	4AC	1	0
1	A1	1227	4AC	1	0
27	B1	1946	4AC	1	0
27	B1	2113	4AC	2	0
1	A1	739	4AC	1	0
27	B1	3020	4AC	1	0
1	A1	52	OMU	1	0
27	B1	1290	4AC	1	0
27	B1	1914	OMC	2	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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

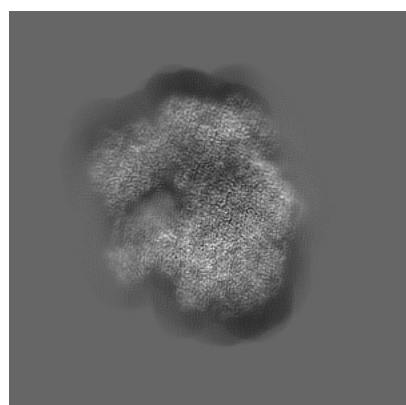
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53100. These allow visual inspection of the internal detail of the map and identification of artifacts.

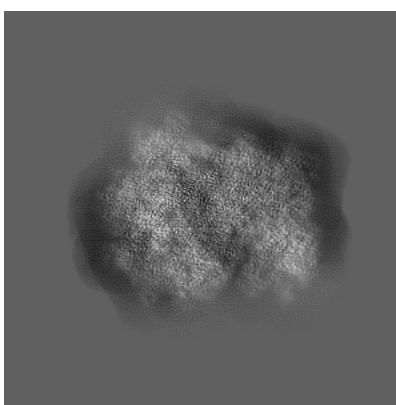
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

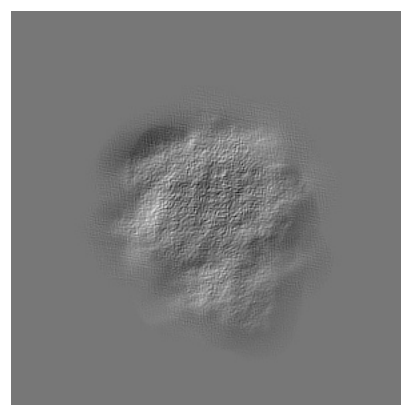
#### 6.1.1 Primary map



X



Y

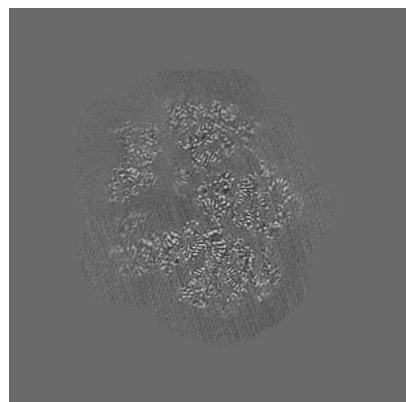


Z

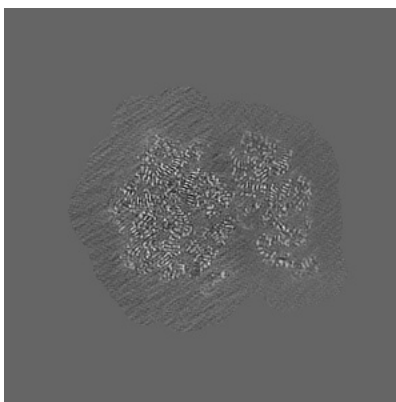
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

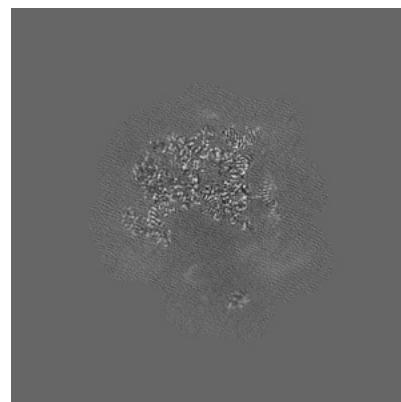
#### 6.2.1 Primary map



X Index: 224



Y Index: 224

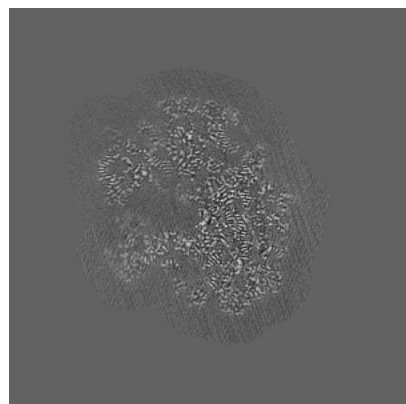


Z Index: 224

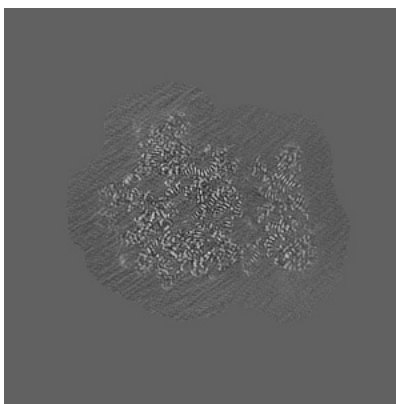
The images above show central slices of the map in three orthogonal directions.

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

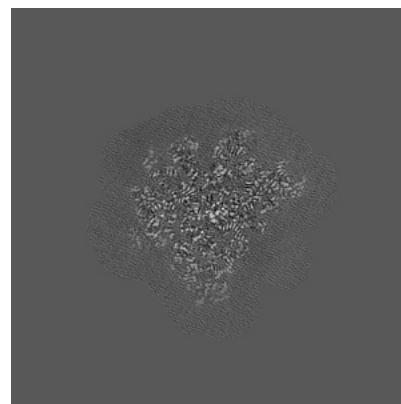
### 6.3.1 Primary map



X Index: 238



Y Index: 242

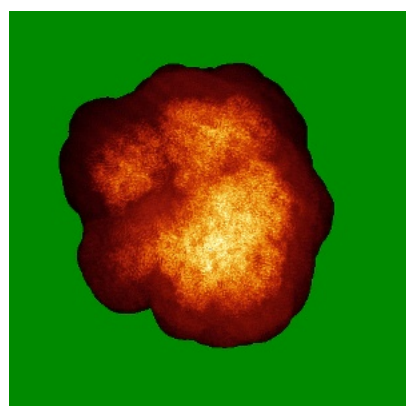


Z Index: 182

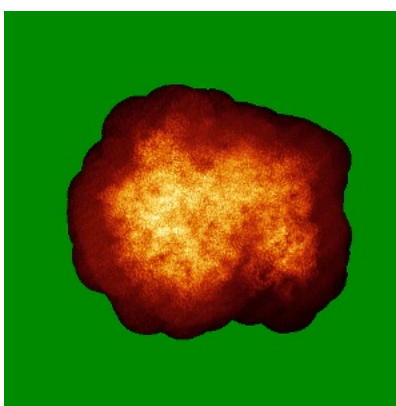
The images above show the largest variance slices of the map in three orthogonal directions.

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

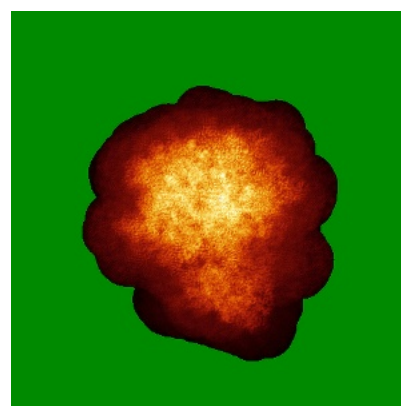
### 6.4.1 Primary map



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.

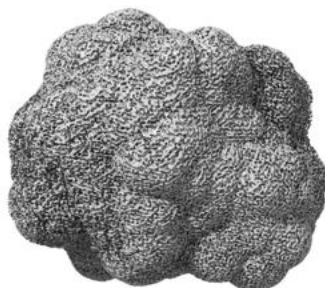


## 6.5 Orthogonal surface views [i](#)

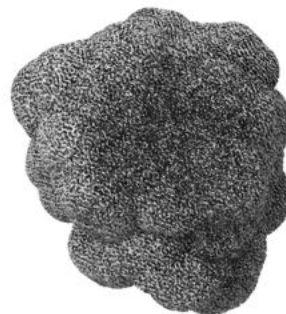
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0083. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

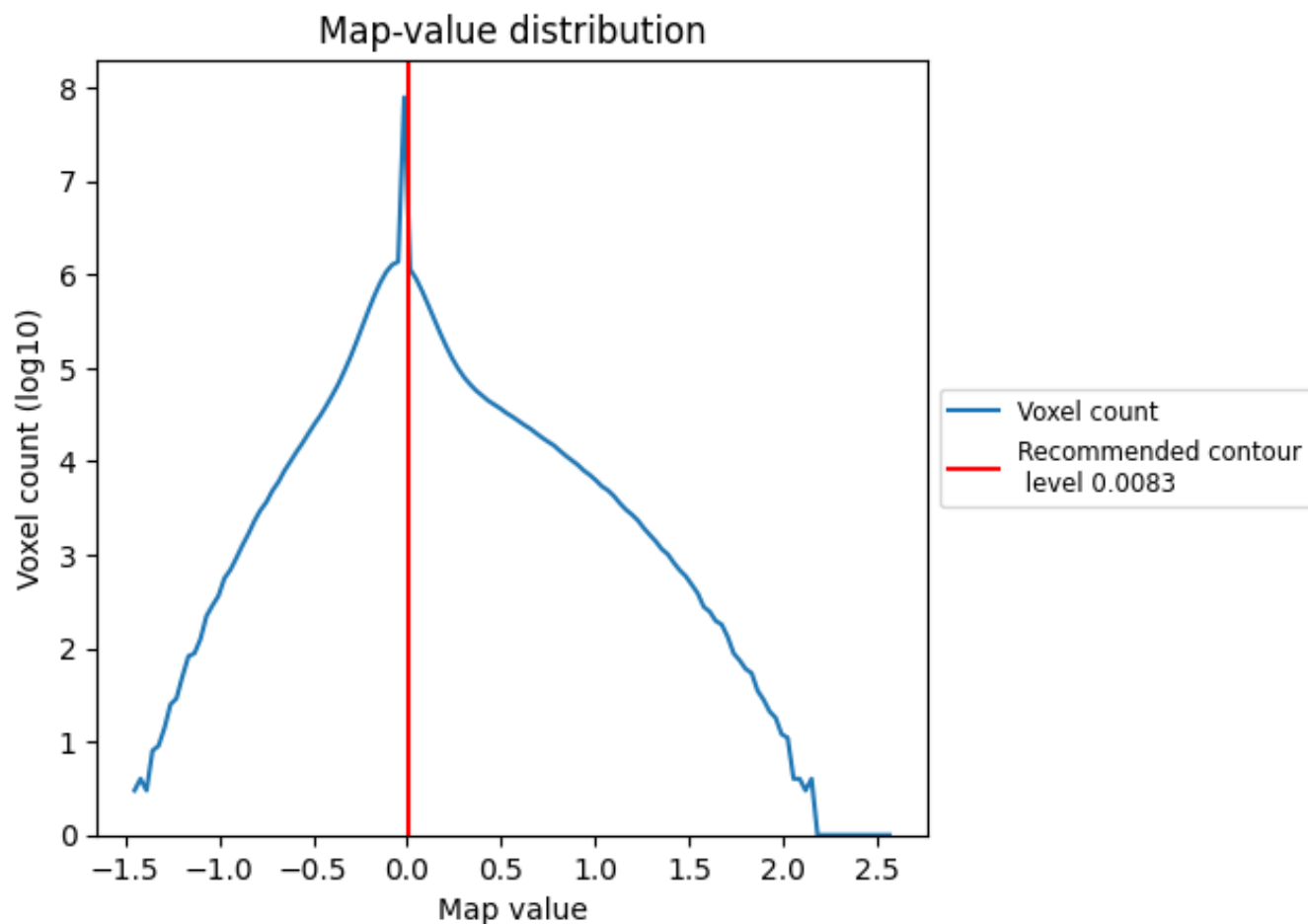
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

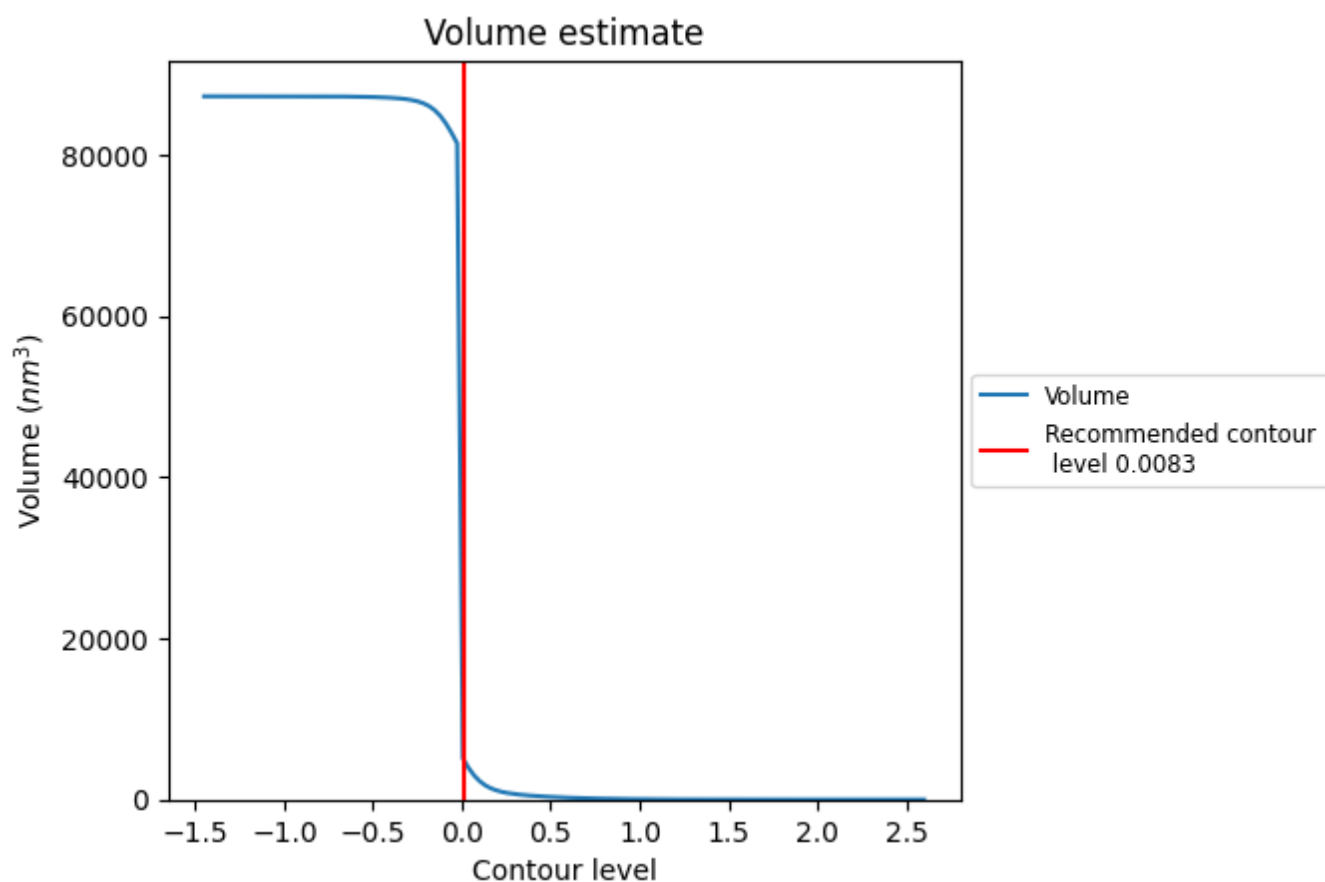
This section contains the results of statistical analysis of the map.

### 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.

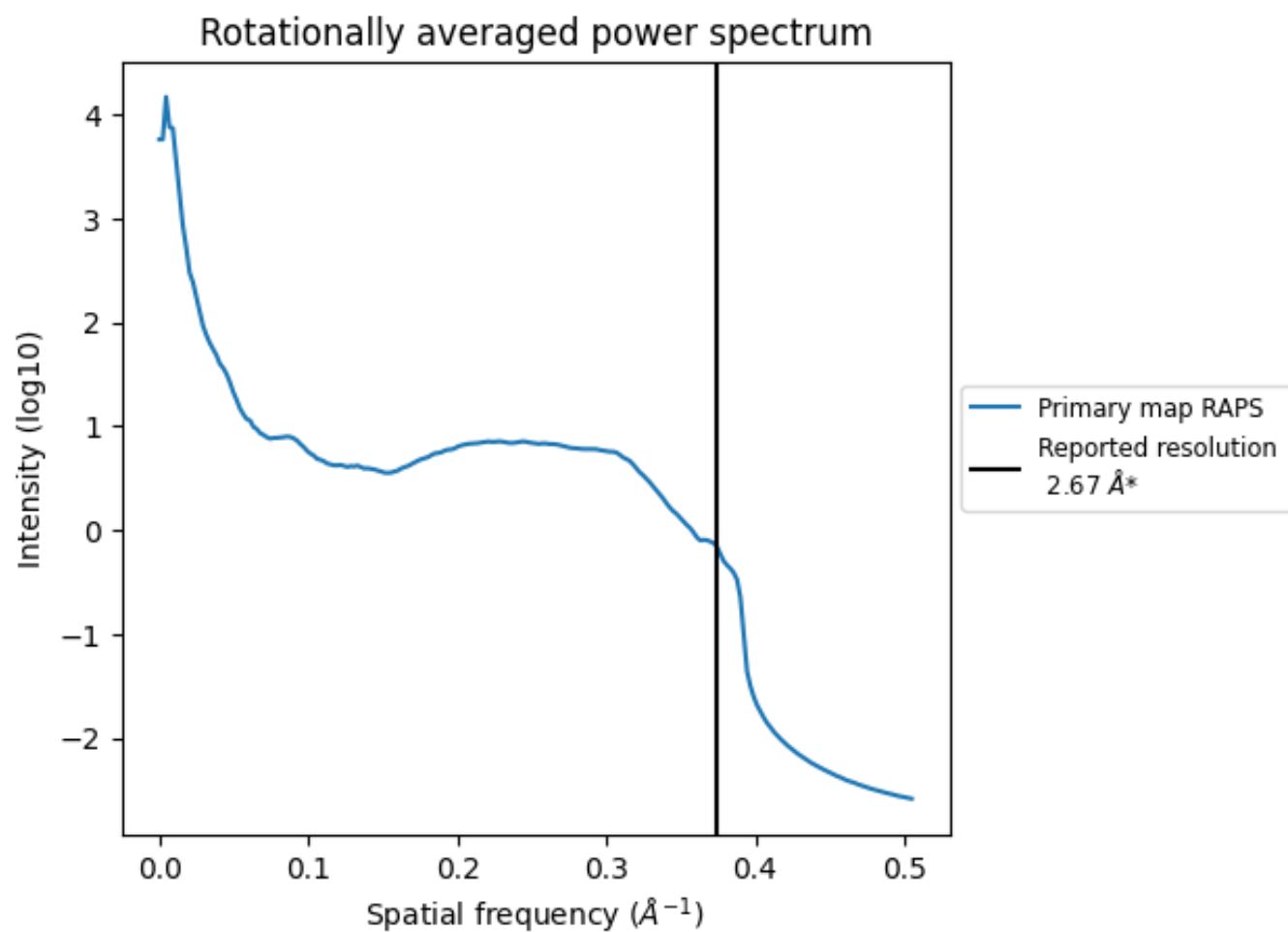
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5004 nm<sup>3</sup>; this corresponds to an approximate mass of 4520 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 0.375 Å<sup>-1</sup>

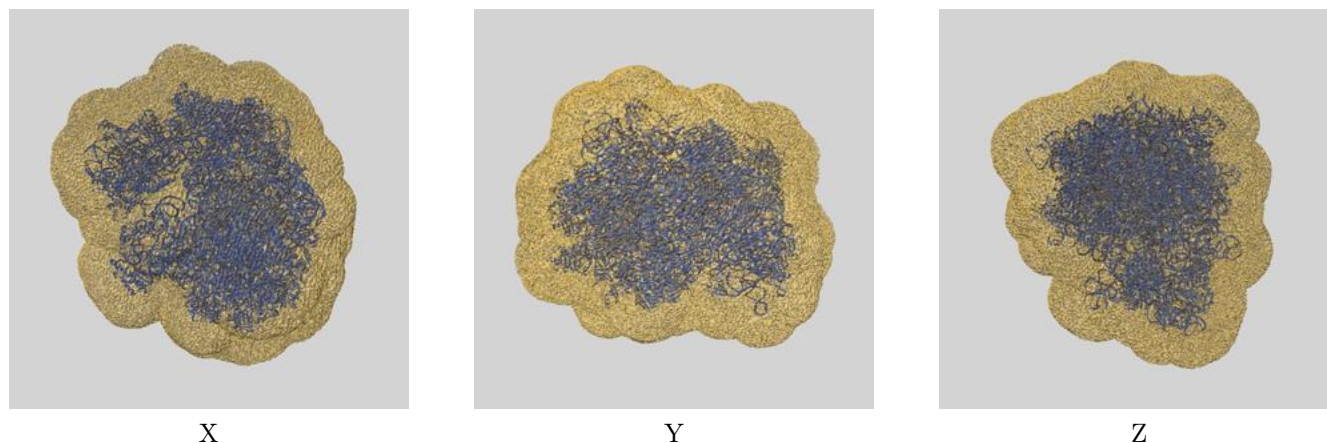
## 8 Fourier-Shell correlation

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

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

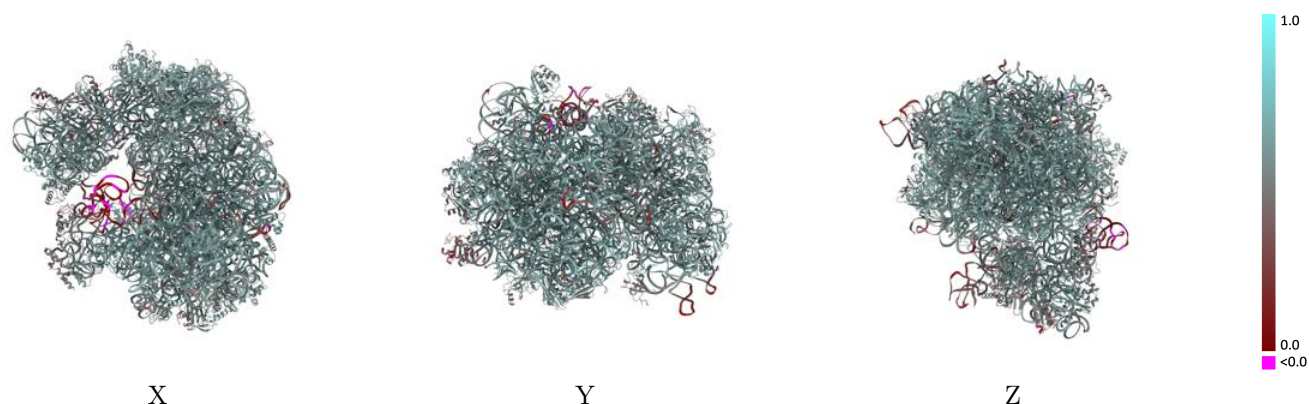
This section contains information regarding the fit between EMDB map EMD-53100 and PDB model 9QF6. Per-residue inclusion information can be found in section [3](#) on page [18](#).

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



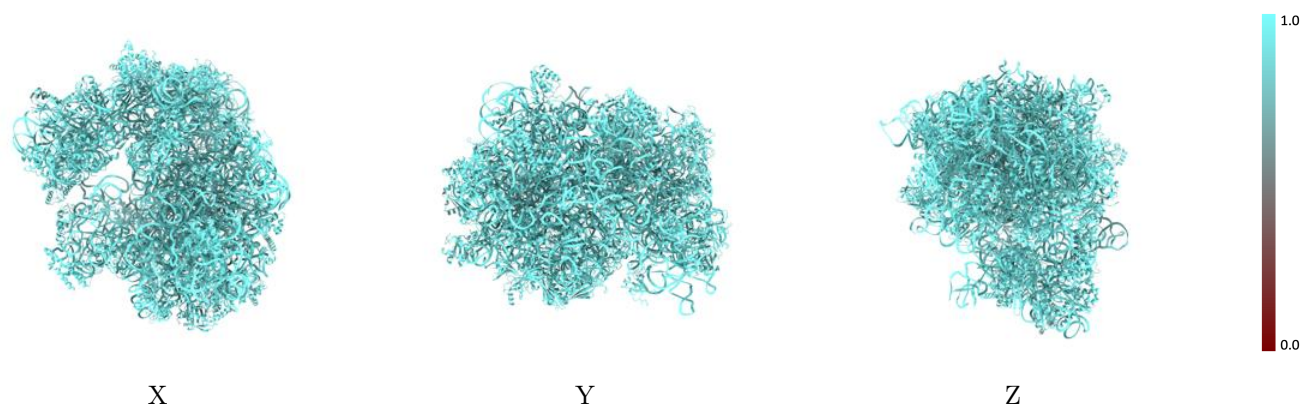
The images above show the 3D surface view of the map at the recommended contour level 0.0083 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



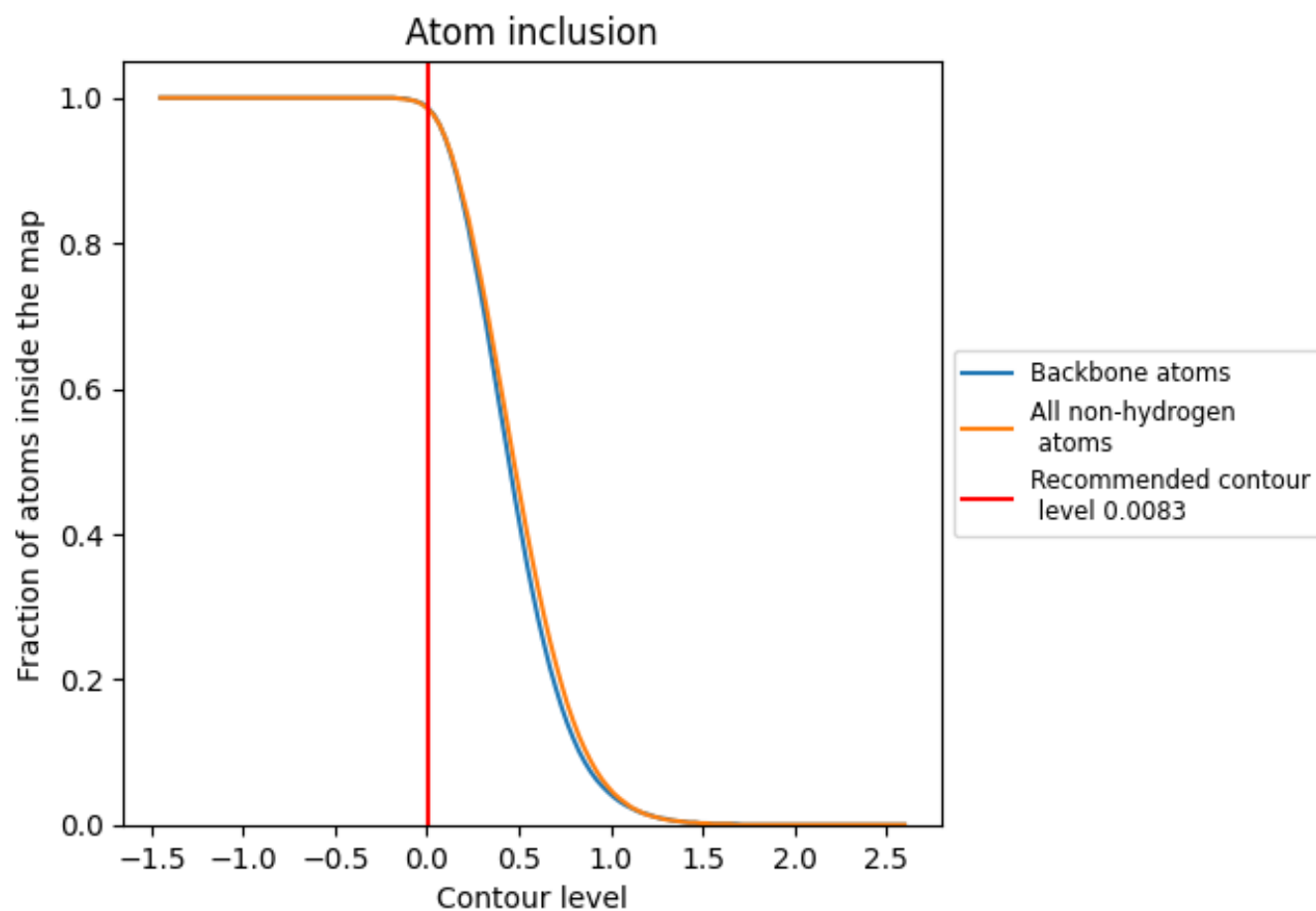
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0083).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.0083) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9840	 0.5690
A1	 0.9880	 0.5630
Aa	 0.9810	 0.5580
Ab	 0.9620	 0.5110
Ac	 0.9730	 0.5520
Ad	 0.9910	 0.5850
Ae	 0.9900	 0.5930
Af	 0.9880	 0.5880
Ag	 0.9770	 0.5140
Ah	 0.9860	 0.5650
Ai	 0.9920	 0.6050
Aj	 0.9940	 0.5990
Ak	 0.9870	 0.5790
Al	 0.8880	 0.4620
Am	 0.9810	 0.5600
An	 0.9890	 0.6010
Ao	 0.9650	 0.5540
Ap	 0.9840	 0.5460
Aq	 0.9740	 0.5820
Ar	 0.9920	 0.6050
As	 0.9740	 0.5080
At	 0.9960	 0.5600
Au	 0.9850	 0.5780
Av	 0.9990	 0.5600
Aw	 0.9870	 0.5730
Ax	 0.9790	 0.5220
Az	 0.9860	 0.5780
B1	 0.9840	 0.5690
B2	 0.9930	 0.5440
BA	 0.9920	 0.6240
BB	 0.9900	 0.6090
BC	 0.9840	 0.5930
BD	 0.9480	 0.4400
BE	 0.9970	 0.5700
BF	 0.9960	 0.5660



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Chain	Atom inclusion	Q-score
BG	 0.8910	 0.3840
BH	 0.9920	 0.5980
BI	 0.9930	 0.6140
BJ	 0.9880	 0.6170
BK	 0.9780	 0.5220
BL	 0.9870	 0.5280
BM	 0.9920	 0.5460
BN	 0.9970	 0.6370
BO	 0.9970	 0.5240
BP	 0.9960	 0.5850
BQ	 0.9930	 0.5950
BR	 0.9990	 0.6280
BS	 0.9920	 0.6100
BT	 0.9940	 0.6050
BU	 0.9880	 0.5820
BV	 0.9900	 0.6100
BW	 0.9870	 0.5300
BX	 0.9930	 0.6070
BY	 0.9780	 0.5370
BZ	 0.9900	 0.5870
Ba	 0.9880	 0.6060
Bb	 0.9910	 0.6070
Bc	 0.9920	 0.6030
Bd	 0.9940	 0.6380
Be	 0.9850	 0.6060
Bf	 0.9930	 0.6160
Bg	 1.0000	 0.5950
Bh	 0.9840	 0.6080
Bi	 0.9960	 0.6220
Bj	 0.9870	 0.5520
Bk	 0.9980	 0.6030
Bl	 0.8800	 0.4330