



## wwPDB EM Validation Summary Report ⓘ

Nov 29, 2025 – 08:22 am GMT

PDB ID : 9QF4 / pdb\_00009qf4  
EMDB ID : EMD-53098  
Title : Structure of P. furiosus 70S ribosome grown at 95 degC  
Authors : Matzov, D.; Georgeson, G.; Westhof, E.; Schwartz, S.; Shalev-Benami, M.  
Deposited on : 2025-03-11  
Resolution : 2.59 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:

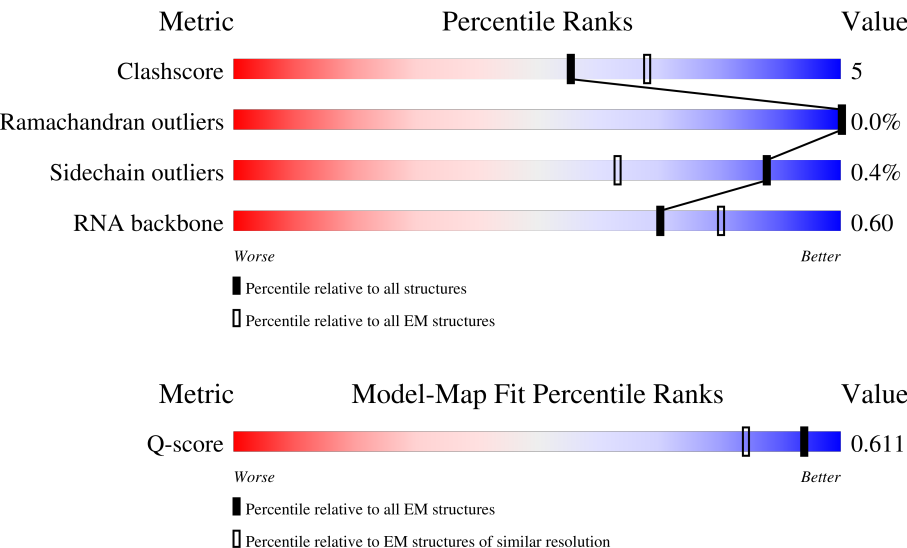
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 2.59 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.





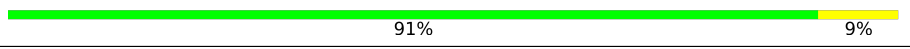


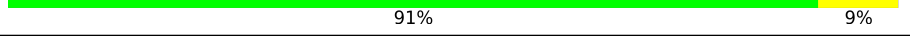
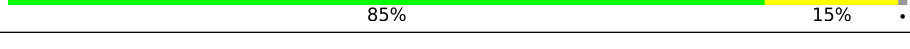
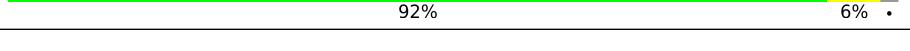
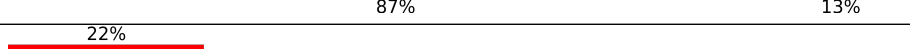
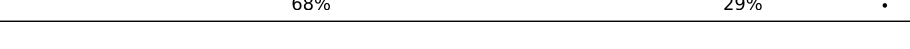
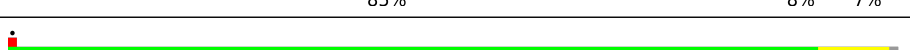
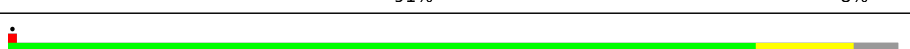
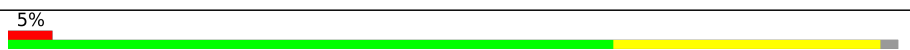

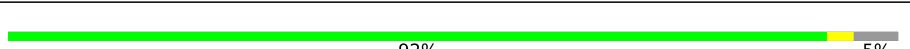





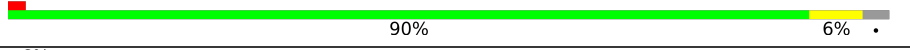
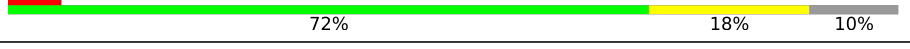



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	7741 ( 2.09 - 3.09 )

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	






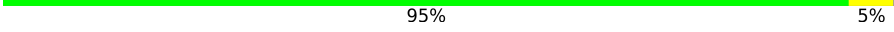
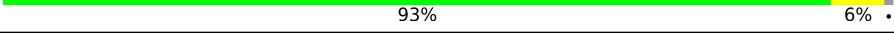


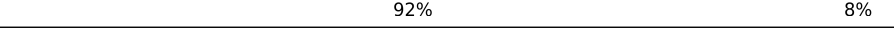
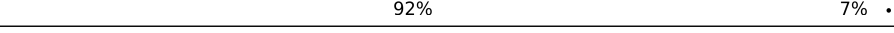
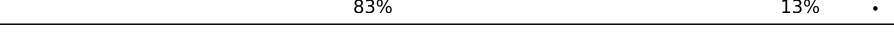
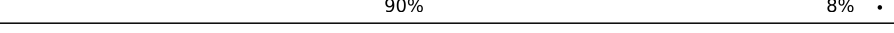


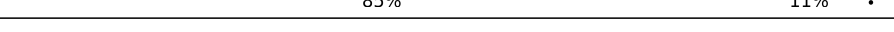


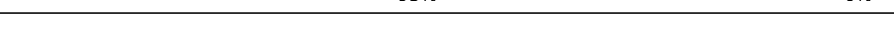






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Mol	Chain	Length	Quality of chain
4	Ac	198	
5	Ad	180	
6	Ae	243	
7	Af	236	
8	Ag	125	
9	Ah	215	
10	Ai	130	
11	Aj	127	
12	Ak	135	
13	Al	102	
14	Am	137	
15	An	147	
16	Ao	148	
17	Ap	56	
18	Aq	158	
19	Ar	113	
20	As	67	
21	At	132	
22	Au	150	
23	Av	99	
23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



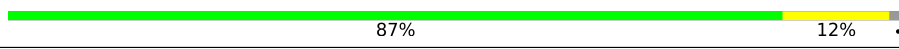
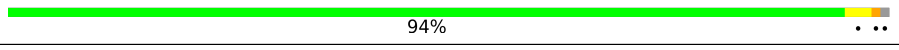
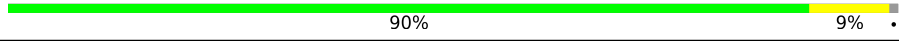

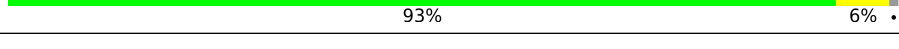
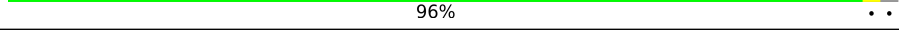
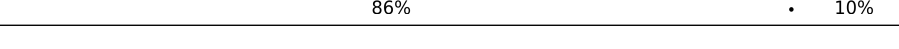
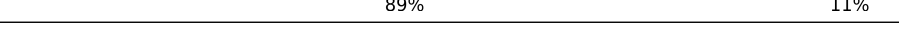
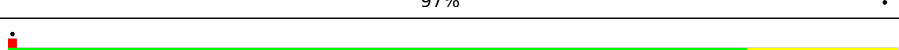
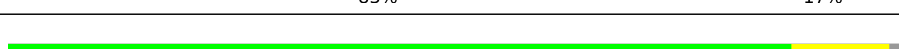
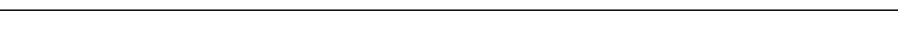
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Mol	Chain	Length	Quality of chain
28	B2	125	
29	BA	239	
30	BB	365	
31	BC	255	
32	BD	186	
33	BE	184	
34	BF	123	
34	BG	123	
35	BH	181	
36	BI	142	
37	BJ	141	
38	BK	83	
38	BL	83	
39	BM	147	
40	BN	194	
41	BO	203	
42	BP	120	
43	BQ	150	
44	BR	97	
45	BS	155	
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	 88% 10% .
52	BZ	95	 89% 9% .
53	Ba	130	 87% 12% .
54	Bb	89	 94% . .
55	Bc	87	 90% 9% .
56	Bd	62	 85% 13% .
57	Be	83	 93% 6% .
58	Bf	51	 96% . .
59	Bg	51	 86% . 10%
60	Bh	37	 89% 11%
61	Bi	94	 97% .
62	Bj	77	 83% 17%
63	Bk	64	 88% 11% .

## 2 Entry composition [i](#)

There are 65 unique types of molecules in this entry. The entry contains 165982 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
			32245	14415	5941	10398	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
			1568	1015	270	279	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
			1528	977	282	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
			1520	983	265	267	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ad	175	Total	C	N	O	S	0	0
			1470	924	284	258	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	226	Total	C	N	O	S	0	0
			1788	1131	334	316	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
			986	612	205	169			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Ak	135	Total	C	N	O	S	0	0
			1069	669	205	190	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	127	Total	C	N	O	S	0	0
			954	591	190	171	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	An	146	Total	C	N	O	S	0	0
			1141	724	220	194	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ao	141	Total	C	N	O	S	0	0
			1119	704	220	190	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
			451	286	93	67	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
			1296	826	246	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	123	Total	C	N	O	S	0	0
			996	638	186	166	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
			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
			63503	28372	11737	20462	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
			2695	1202	494	874	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
			1820	1158	344	314	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
			2904	1865	526	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	183	Total	C	N	O	S	0	0
			1420	891	274	247	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	120	Total	C	N	O	S	0	0
			913	583	151	177	2		

- 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
			1376	873	263	234	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	80	Total	C	N	O	S	0	0
			609	383	118	107	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
			794	506	161	126	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BS	152	Total	C	N	O	S	0	0
			1207	773	227	203	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
			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	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	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	37	Total	C	N	O	S	0	0
			348	221	85	40	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	63	Total	C	N	O	S	0	0
			523	335	105	80	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	607	Total	O	0
			607	607	
65	Aa	5	Total	O	0
			5	5	
65	Ac	3	Total	O	0
			3	3	
65	Ad	7	Total	O	0
			7	7	
65	Ae	15	Total	O	0
			15	15	

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Mol	Chain	Residues	Atoms		AltConf
65	Af	7	Total 7	O 7	0
65	Ag	1	Total 1	O 1	0
65	Ah	2	Total 2	O 2	0
65	Ai	10	Total 10	O 10	0
65	Aj	7	Total 7	O 7	0
65	Ak	3	Total 3	O 3	0
65	Al	5	Total 5	O 5	0
65	Am	4	Total 4	O 4	0
65	An	13	Total 13	O 13	0
65	Ap	1	Total 1	O 1	0
65	Aq	7	Total 7	O 7	0
65	Ar	7	Total 7	O 7	0
65	At	2	Total 2	O 2	0
65	Au	4	Total 4	O 4	0
65	Av	2	Total 2	O 2	0
65	Aw	3	Total 3	O 3	0
65	Ay	1	Total 1	O 1	0
65	B1	1513	Total 1513	O 1513	0
65	B2	17	Total 17	O 17	0
65	BA	25	Total 25	O 25	0
65	BB	20	Total 20	O 20	0

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Mol	Chain	Residues	Atoms		AltConf
65	BC	22	Total 22	O 22	0
65	BE	1	Total 1	O 1	0
65	BF	1	Total 1	O 1	0
65	BH	10	Total 10	O 10	0
65	BI	6	Total 6	O 6	0
65	BJ	5	Total 5	O 5	0
65	BM	22	Total 22	O 22	0
65	BN	26	Total 26	O 26	0
65	BO	3	Total 3	O 3	0
65	BP	4	Total 4	O 4	0
65	BQ	10	Total 10	O 10	0
65	BR	10	Total 10	O 10	0
65	BS	15	Total 15	O 15	0
65	BT	4	Total 4	O 4	0
65	BU	6	Total 6	O 6	0
65	BV	1	Total 1	O 1	0
65	BW	1	Total 1	O 1	0
65	BX	7	Total 7	O 7	0
65	BY	1	Total 1	O 1	0
65	BZ	2	Total 2	O 2	0
65	Ba	14	Total 14	O 14	0

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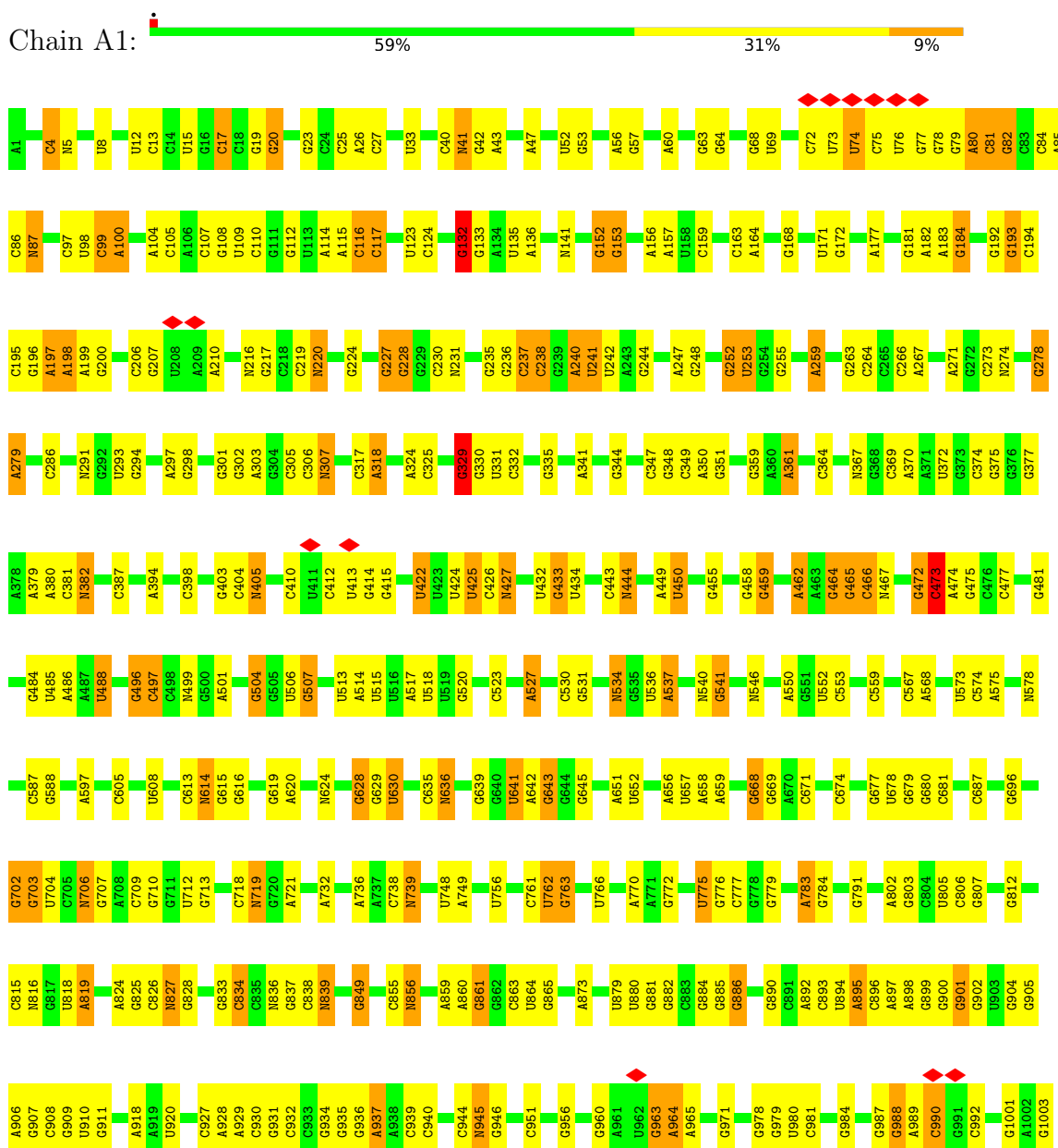
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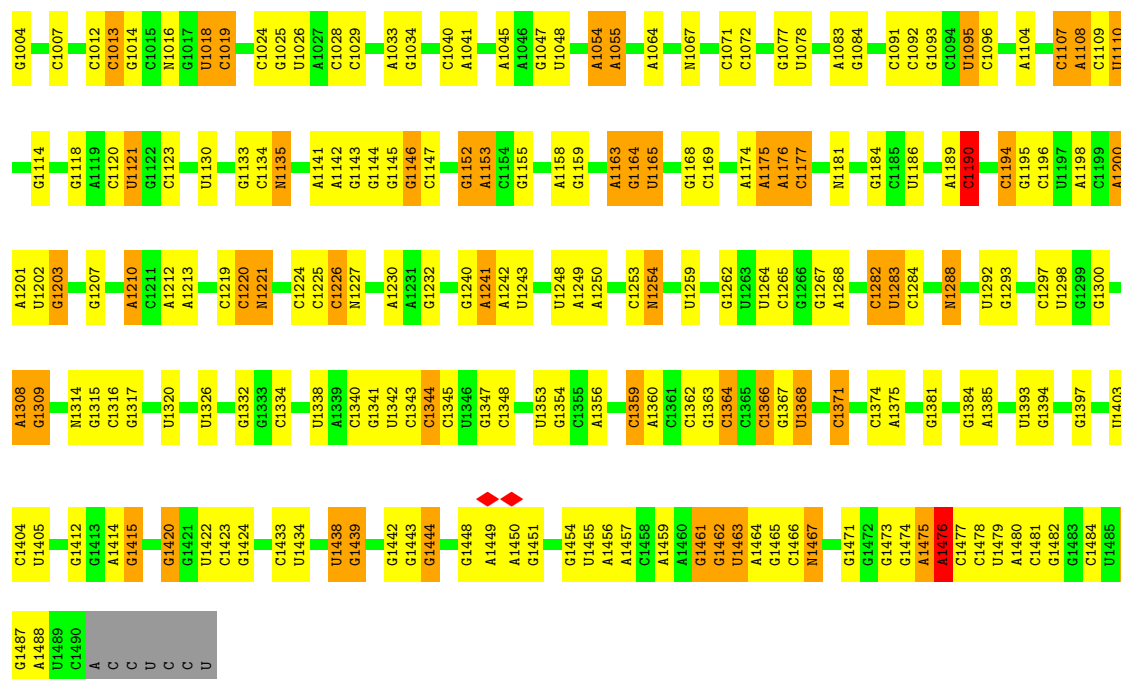
Mol	Chain	Residues	Atoms		AltConf
65	Bb	1	Total 1	O 1	0
65	Bc	5	Total 5	O 5	0
65	Bd	6	Total 6	O 6	0
65	Be	2	Total 2	O 2	0
65	Bf	8	Total 8	O 8	0
65	Bg	2	Total 2	O 2	0
65	Bh	2	Total 2	O 2	0
65	Bi	3	Total 3	O 3	0
65	Bk	4	Total 4	O 4	0

### 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





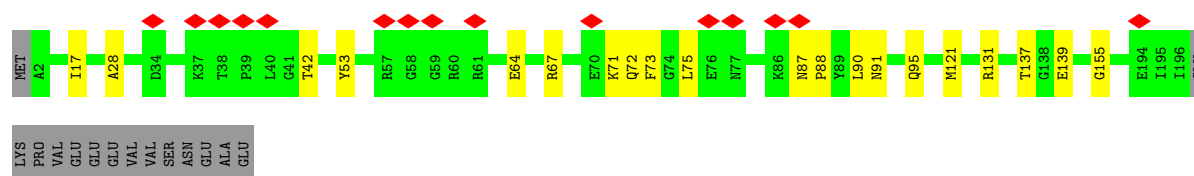
- Molecule 2: Small ribosomal subunit protein uS2

Chain Aa: 90% 7% .



- Molecule 3: Small ribosomal subunit protein uS3

Chain Ab: 7% 83% 10% 7%



- Molecule 4: Small ribosomal subunit protein eS1

Chain Ac: 85% 9% 7%



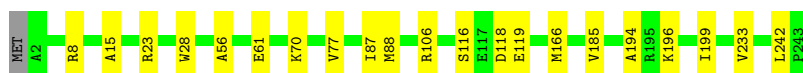
- Molecule 5: Small ribosomal subunit protein uS4

Chain Ad: 88% 9% .



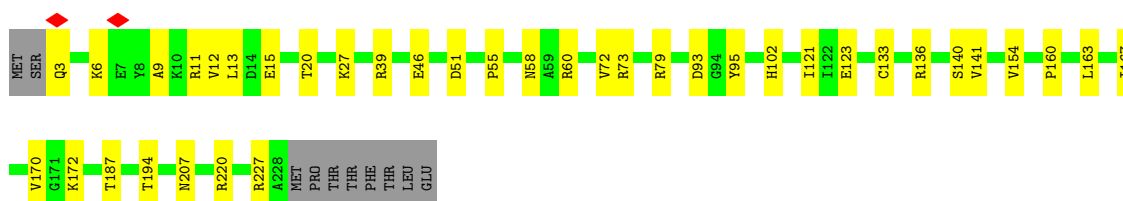
- Molecule 6: Small ribosomal subunit protein eS4

Chain Ae: 91% 9%



- Molecule 7: Small ribosomal subunit protein uS5

Chain Af: 80% 16%



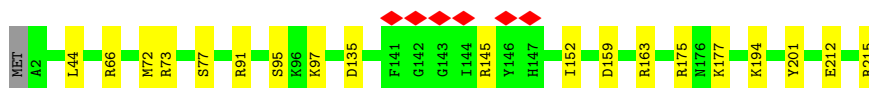
- Molecule 8: Small ribosomal subunit protein eS6

Chain Ag: 84% 15%



- Molecule 9: Small ribosomal subunit protein uS7

Chain Ah: 91% 9%



- Molecule 10: Small ribosomal subunit protein uS8

Chain Ai: 85% 15%



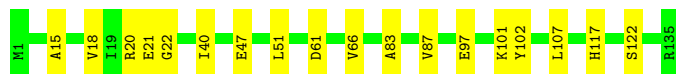
- Molecule 11: Small ribosomal subunit protein eS8

Chain Aj: 92% 6%



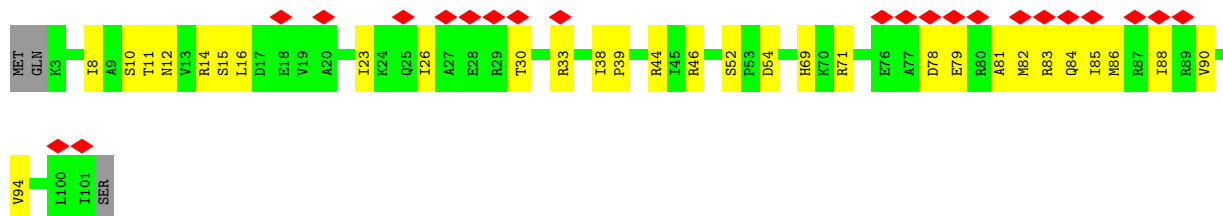
- Molecule 12: Small ribosomal subunit protein uS9

Chain Ak:  87% 13%




- Molecule 13: Small ribosomal subunit protein uS10

Chain Al:  22% 68% 29%



- Molecule 14: Small ribosomal subunit protein uS11

Chain Am:  85% 8% 7%




- Molecule 15: Small ribosomal subunit protein uS12

Chain An:  91% 8%



- Molecule 16: Small ribosomal subunit protein uS13

Chain Ao:  84% 11% 5%




- Molecule 17: Small ribosomal subunit protein uS14

Chain Ap:  5% 68% 30%



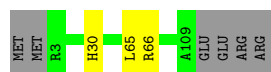
- Molecule 18: Small ribosomal subunit protein uS15

Chain Aq:  88% 11% .




- Molecule 19: Small ribosomal subunit protein uS17

Chain Ar:  92% . 5%




- Molecule 20: Small ribosomal subunit protein eS17

Chain As:  78% 18% .



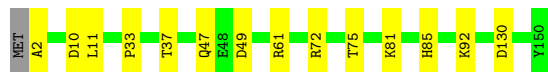
- Molecule 21: Small ribosomal subunit protein uS19

Chain At:  87% 6% 7%



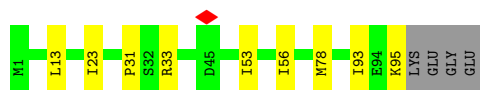
- Molecule 22: Small ribosomal subunit protein eS19

Chain Au:  90% 9% .




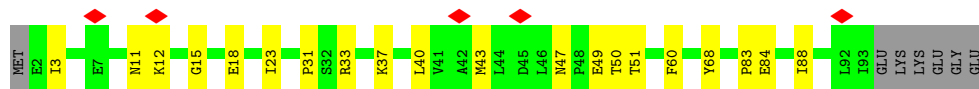
- Molecule 23: Small ribosomal subunit protein eS24

Chain Av:  87% 9% .



- Molecule 23: Small ribosomal subunit protein eS24

Chain Bl:  5% 73% 20% 7%




- Molecule 24: Small ribosomal subunit protein eS27

Chain Aw:  90% 6%




- Molecule 25: Small ribosomal subunit protein eS28

Chain Ax:  6% 72% 18% 10%



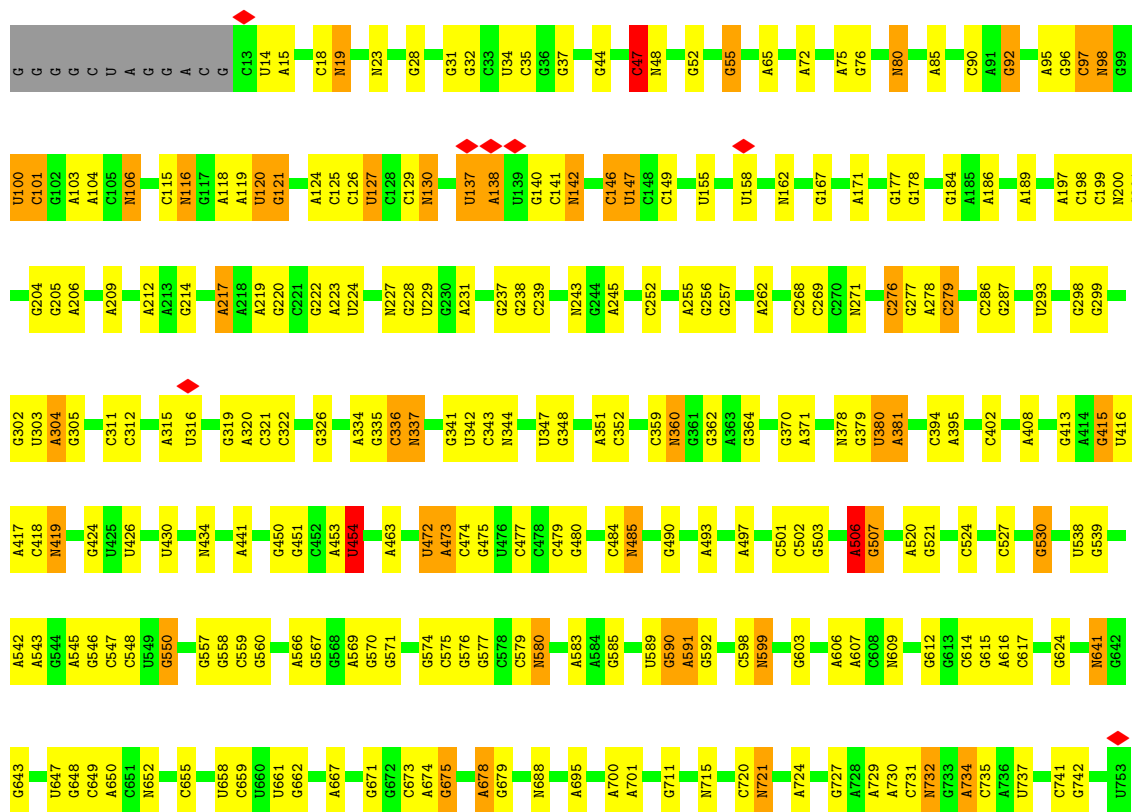
- Molecule 26: Zn-ribbon RNA-binding protein

Chain Ay:  82% 10% 7%



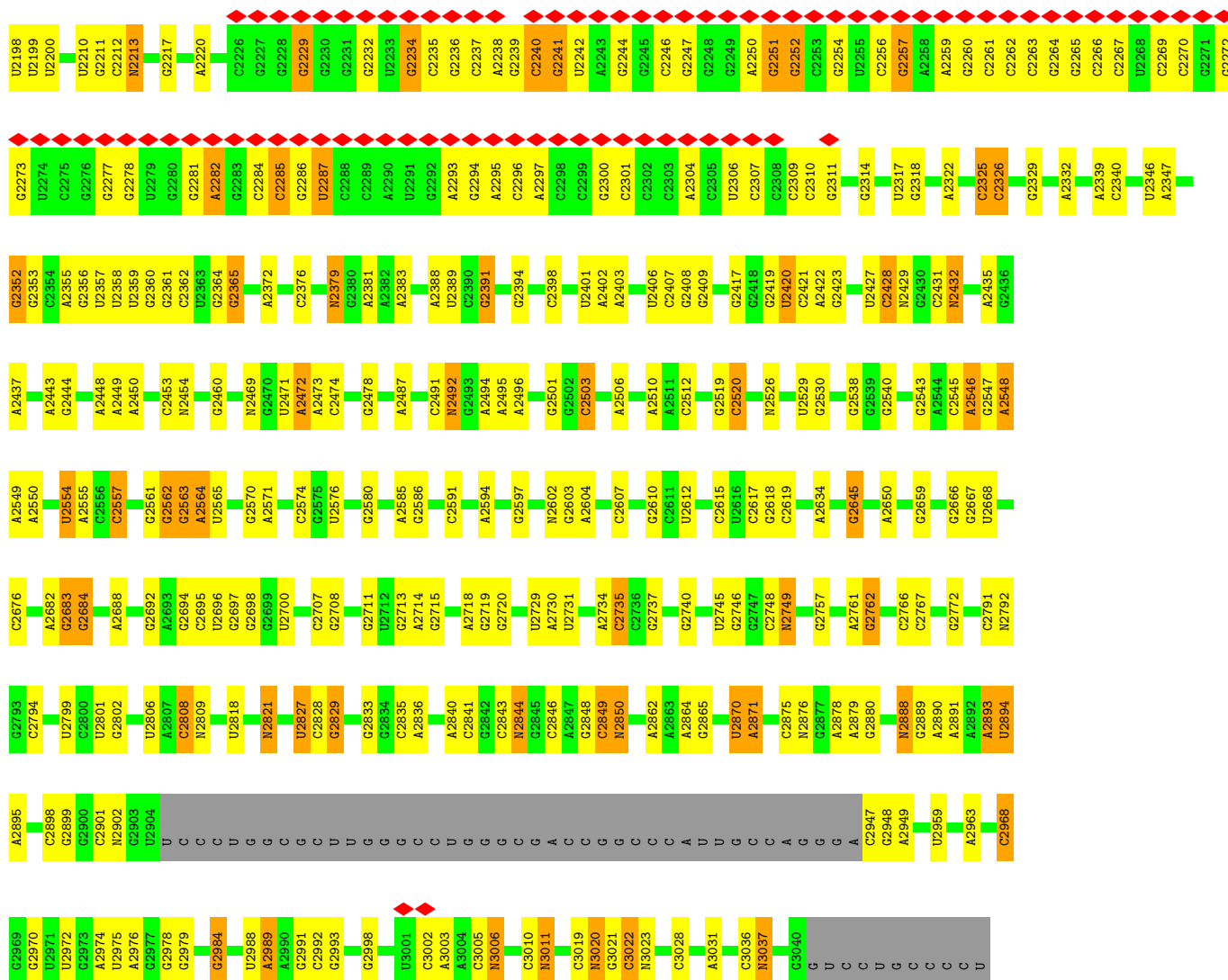
- Molecule 27: 23S rRNA

Chain B1:  60% 29% 7%



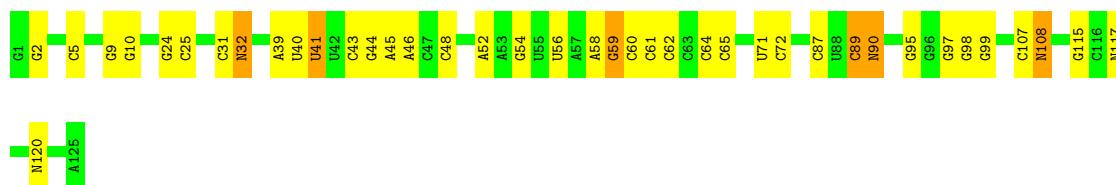


U2096	C2007	U1915	C1774	G1576	G1454	U1332	G1053	G860	U762
G2097	N2008	U1919	A1775	C1577	U1455	G1337	C1059	G863	G763
A2103	G2013	A1920	G1779	N1579	U1456	U1344	A1059	C864	A764
G2104	N2020	A1923	C1780	C1589	U1457	N1345	C1060	G865	G765
A2106	G2021	A1924	C1781	U1458	U1459	G1346	N1061	N866	G772
G2107	G2022	A1931	G1785	C1460	C1461	U1350	G1062	G867	G773
G2108	A2026	G1696	G1786	C1461	U1475	G1355	N1063	U875	U774
C2112	C2027	G1697	G1791	U1476	C1477	A1356	C1064	G876	G775
N2113	G2028	U1699	A1792	G1476	G1477	G1363	N1067	U877	A778
U2116	G2031	U1701	U1804	U1478	U1479	U1368	A1072	U878	A779
G2117	A1938	G1604	G1805	C1482	U1482	A1368	G1084	U879	A780
G2118	G1939	C1607	U1806	G1482	U1483	A1369	G1085	G781	G782
C2120	C2032	N1706	C1807	U1483	U1484	G1370	C1089	U883	G783
G2121	G2033	G1707	A1708	C1489	U1490	C1374	N1100	G887	N786
C2122	G2034	U1709	G1712	U1490	U1491	N1374	G1101	U888	U791
U2126	A2037	U1710	A1813	U1491	U1492	G1379	G1102	U889	C792
C2127	A2038	G1715	G1817	U1492	U1493	A1380	G1103	G891	A793
G2128	G1951	U1716	U1818	U1494	U1495	G1381	N1107	C895	C798
N2133	U1957	U1721	C1822	U1496	U1497	C1382	G1110	N896	G799
G2137	U1958	U1722	G1823	U1497	U1498	N1383	A1116	G899	N807
A2138	A2042	G1723	A1824	U1499	U1500	G1388	A1117	A900	G808
A2139	A2043	A1724	U1825	U1500	U1501	C1392	G1118	C904	A809
C2140	A2044	A1725	G1827	U1501	U1502	G1395	C1119	G911	A810
G2146	C2045	U1726	U1828	U1503	U1504	G1396	A1120	G912	A811
C2154	C2046	A1727	G1832	U1505	U1506	C1399	G1121	A918	C812
U2047	U2047	C1731	G1833	U1507	U1508	A1408	G1122	A919	N813
C2155	C2048	U1732	U1834	U1509	U1510	G1409	G1016	G920	U816
G2156	A2052	G1733	G1835	U1510	U1511	A1414	C1017	G921	A819
A2157	G2055	C1734	U1836	U1511	U1512	U1418	A1018	G922	U820
C2167	U2059	G1735	U1837	U1512	U1513	G1423	G1022	C923	G824
N2171	C2062	U1736	G1838	U1513	U1514	A1430	G1023	A924	C825
G2172	A2063	A1643	U1839	U1514	U1515	A1431	G1024	A925	C826
C2173	U2064	A1644	U1840	U1515	U1516	U1432	C1025	U926	N827
U2174	U2065	G1645	U1841	U1516	U1517	C1434	G1026	G928	U837
A2179	C2066	U1646	U1842	U1517	U1518	N1435	A1027	G931	A838
G2180	C2067	G1647	U1843	U1518	U1519	N1436	G1028	C932	A840
C2183	A2077	U1648	U1844	U1519	U1520	N1437	A1029	N933	C843
A2184	U2080	U1649	U1845	U1520	U1521	N1438	C1030	A938	A849
G2185	G2081	G1650	U1846	U1521	U1522	N1439	C1031	U939	A851
A2186	U2082	U1651	U1847	U1522	U1523	N1440	C1034	A940	C852
C2187	C2083	U1652	U1848	U1523	U1524	N1441	G1035	G945	A853
C2188	U2084	G1653	U1849	U1524	U1525	N1442	A1047	C948	A857
C2189	G2087	U1654	U1850	U1525	U1526	N1443	C1048	C949	
C2190	U2088	G1655	A1881	U1526	U1527	N1444	C1049		
G2193	G2089	U1656	U1885	U1527	U1528	N1445	C1051		
C2194	C2090	U1657	U1886	U1528	U1529	N1446	N1052		
A2195	A2091	A1768	U1887	U1529	U1530	N1447			
G2196	U2092	C1768	U1888	U1530	U1531	N1448			
C2197	A2095	N1769	U1889	U1531	U1532	N1449			
		G1770	U1890	U1532	U1533	N1450			
		A1771	U1891	U1533	U1534	N1451			
			U1892	U1534	U1535	N1452			
			U1893	U1535	U1536	N1453			
			U1894	U1536	U1537	N1454			
			U1895	U1537	U1538	N1455			
			U1896	U1538	U1539	N1456			
			U1897	U1539	U1540	N1457			
			U1898	U1540	U1541	N1458			
			U1899	U1541	U1542	N1459			
			U1900	U1542	U1543	N1460			
			U1901	U1543	U1544	N1461			
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			U1903	U1545	U1546	N1463			
			U1904	U1546	U1547	N1464			
			U1905	U1547	U1548	N1465			
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			U1907	U1549	U1550	N1467			
			U1908	U1550	U1551	N1468			
			U1909	U1551	U1552	N1469			
			U1910	U1552	U1553	N1470			
			U1911	U1553	U1554	N1471			
			U1912	U1554	U1555	N1472			
			U1913	U1555	U1556	N1473			
			U1914	U1556	U1557	N1474			
			U1915	U1557	U1558	N1475			
			U1916	U1558	U1559	N1476			
			U1917	U1559	U1560	N1477			
			U1918	U1560	U1561	N1478			
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			U1948	U1590	U1591	N1508			
			U1949	U1591	U1592	N1509			
			U1950	U1592	U1593	N1510			
			U1951	U1593	U1594	N1511			
			U1952	U1594	U1595	N1512			
			U1953	U1595	U1596	N1513			
			U1954	U1596	U1597	N1514			
			U1955	U1597	U1598	N1515			
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			U1969	U1611	U1612	N1529			
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			U1971	U1613	U1614	N1531			
			U1972	U1614	U1615	N1532			
			U1973	U1615	U1616	N1533			
			U1974	U1616	U1617	N1534			
			U1975	U1617	U1618	N1535			
			U1976	U1618	U1619	N1536			
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			U1980	U1622	U1623	N1540			
			U1981	U1623	U1624	N1541			
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			U1986	U1628	U1629	N1546			
			U1987	U1629	U1630	N1547			
			U1988	U1630	U1631	N1548			
			U1989	U1631	U1632	N1549			
			U1990	U1632	U1633	N1550			
			U1991	U1633	U1634	N1551			
			U1992	U1634	U1635	N1552			
			U1993	U1635	U1636	N1553			
			U1994	U1636	U1637	N1554			
			U1995	U1637	U1638	N1555			
			U1996	U1638	U1639	N1556			
			U1997	U1639	U1640	N1557			
			U1998	U1640	U1641	N1558			
			U1999	U1641	U1642	N1559			
			U2000	U1642	U1643	N1560			
			U2001	U1643	U1644	N1561			
			U2002	U1644	U1645	N1562			
			U2003	U1645	U1646	N1563		</	



### • Molecule 28: 5S rRNA

Chain B2: 68% 27% 5%




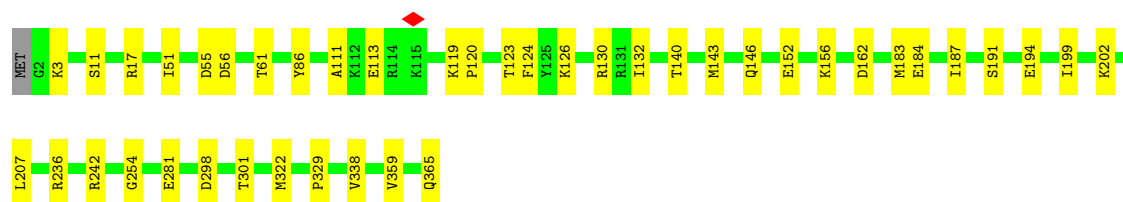
### • Molecule 29: Large ribosomal subunit protein uL2

Chain BA: 88% 11%



### • Molecule 30: Large ribosomal subunit protein uL3

Chain BB:  88% 12%



- Molecule 31: Large ribosomal subunit protein uL4

Chain BC:  90% 9%



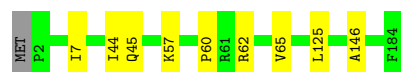
- Molecule 32: Large ribosomal subunit protein uL5

Chain BD:  87% 12%



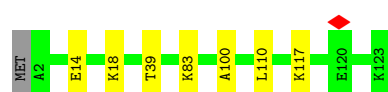
- Molecule 33: Large ribosomal subunit protein uL6

Chain BE:  95% 5%




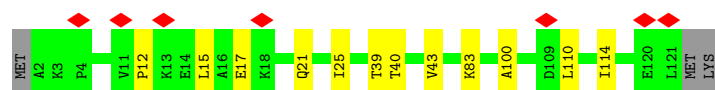
- Molecule 34: Large ribosomal subunit protein eL8

Chain BF:  93% 6%




- Molecule 34: Large ribosomal subunit protein eL8

Chain BG:  88% 10% 6%



- Molecule 35: Large ribosomal subunit protein uL16

Chain BH:  82% 12% 7%



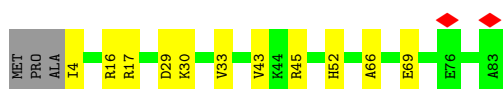
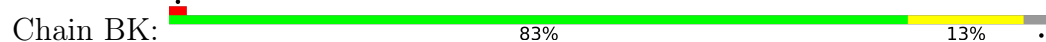
- Molecule 36: Large ribosomal subunit protein uL13



- Molecule 37: Large ribosomal subunit protein uL14



- Molecule 38: Large ribosomal subunit protein eL14



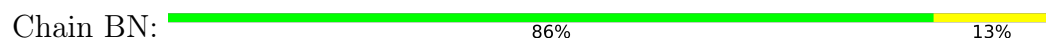
- Molecule 38: Large ribosomal subunit protein eL14



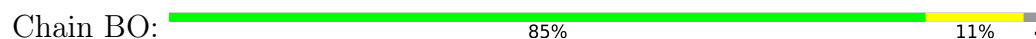
- Molecule 39: Large ribosomal subunit protein uL15



- Molecule 40: Large ribosomal subunit protein eL15



- Molecule 41: Large ribosomal subunit protein uL18





- Molecule 42: Large ribosomal subunit protein eL18

Chain BP: 87% 12% .



- Molecule 43: Large ribosomal subunit protein eL19

Chain BQ: 91% 7% .



- Molecule 44: Large ribosomal subunit protein eL21

Chain BR: 93% 6% .



- Molecule 45: Large ribosomal subunit protein uL22

Chain BS: 86% 12% .



- Molecule 46: Large ribosomal subunit protein uL23

Chain BT: 94% 6% .



- Molecule 47: Large ribosomal subunit protein uL24

Chain BU: 81% 18% .

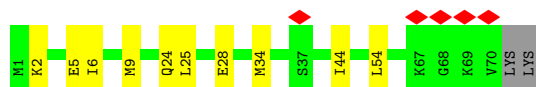
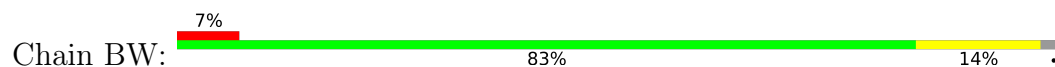


- Molecule 48: Large ribosomal subunit protein eL24

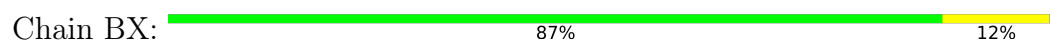
Chain BV: 76% 20% 5% .



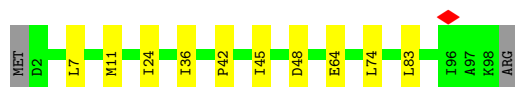
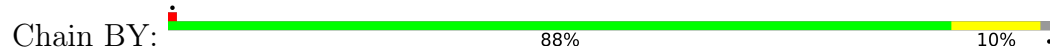
- Molecule 49: Large ribosomal subunit protein uL29



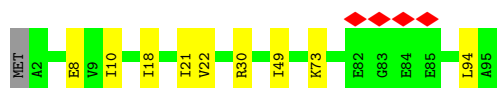
- Molecule 50: Large ribosomal subunit protein uL30



- Molecule 51: Large ribosomal subunit protein eL30



- Molecule 52: Large ribosomal subunit protein eL31



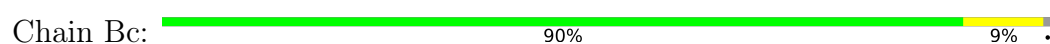
- Molecule 53: Large ribosomal subunit protein eL32



- Molecule 54: Large ribosomal subunit protein eL34



- Molecule 55: Large ribosomal subunit protein eL33





- Molecule 56: Large ribosomal subunit protein eL37

Chain Bd: 85% 13%



- Molecule 57: Large ribosomal subunit protein eL43

Chain Be: 93% 6%



- Molecule 58: Large ribosomal subunit protein eL39

Chain Bf: 96%



- Molecule 59: Large ribosomal subunit protein eL40

Chain Bg: 86% 10%



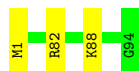
- Molecule 60: Small ribosomal subunit protein eS32

Chain Bh: 89% 11%



- Molecule 61: Large ribosomal subunit protein eL42

Chain Bi: 97%

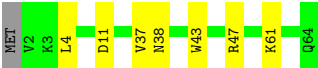
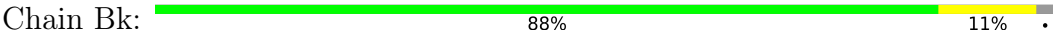


- Molecule 62: Large ribosomal subunit protein eL20

Chain Bj: 83% 17%



• 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	169992	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	3.282	Depositor
Minimum map value	-1.916	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.18	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: UR3, ZN, 4SU, 4AC, OMU, LV2, 5MC, OMG, OMC, 2MG, LHH, 5MU, MA6, 7MG, A2M

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	0.15	1/33222 (0.0%)	0.26	1/51763 (0.0%)
2	Aa	0.11	0/1599	0.25	0/2162
3	Ab	0.13	0/1550	0.32	0/2083
4	Ac	0.10	0/1546	0.27	0/2072
5	Ad	0.11	0/1494	0.24	0/2003
6	Ae	0.11	0/2030	0.27	0/2739
7	Af	0.12	0/1818	0.30	0/2449
8	Ag	0.13	0/990	0.38	0/1327
9	Ah	0.11	0/1765	0.27	0/2371
10	Ai	0.12	0/1049	0.28	0/1408
11	Aj	0.11	0/995	0.25	0/1327
12	Ak	0.12	0/1085	0.28	0/1452
13	Al	0.17	0/806	0.42	0/1083
14	Am	0.11	0/972	0.24	0/1309
15	An	0.11	0/1158	0.29	0/1539
16	Ao	0.11	0/1138	0.27	0/1532
17	Ap	0.12	0/460	0.32	0/606
18	Aq	0.12	0/1324	0.29	0/1780
19	Ar	0.12	0/899	0.25	0/1215
20	As	0.12	0/533	0.35	0/708
21	At	0.10	0/1016	0.24	0/1358
22	Au	0.10	0/1251	0.24	0/1686
23	Av	0.11	0/807	0.29	0/1082
23	Bl	0.44	2/781 (0.3%)	0.71	3/1049 (0.3%)
24	Aw	0.12	0/471	0.31	0/634
25	Ax	0.13	0/510	0.41	0/684
26	Ay	0.11	0/448	0.28	0/610
27	B1	0.14	1/66129 (0.0%)	0.25	0/102990
28	B2	0.10	0/2881	0.21	0/4483
29	BA	0.12	0/1865	0.30	0/2519
30	BB	0.12	0/2970	0.31	0/3993
31	BC	0.12	0/2068	0.28	0/2787

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	BD	0.16	0/1442	0.37	0/1933
33	BE	0.11	0/1499	0.24	0/2022
34	BF	0.12	0/939	0.30	0/1267
34	BG	0.14	0/925	0.41	0/1250
35	BH	0.12	0/1405	0.26	0/1886
36	BI	0.11	0/1168	0.25	0/1561
37	BJ	0.11	0/1075	0.27	0/1448
38	BK	0.12	0/613	0.34	0/822
38	BL	0.10	0/626	0.25	0/840
39	BM	0.15	0/1175	0.40	0/1563
40	BN	0.12	0/1626	0.26	0/2169
41	BO	0.11	0/1602	0.26	0/2158
42	BP	0.12	0/980	0.24	0/1313
43	BQ	0.11	0/1254	0.23	0/1655
44	BR	0.11	0/815	0.24	0/1090
45	BS	0.12	0/1234	0.28	0/1662
46	BT	0.13	0/705	0.32	0/946
47	BU	0.12	0/1019	0.29	0/1360
48	BV	0.13	0/548	0.29	0/731
49	BW	0.14	0/566	0.31	0/749
50	BX	0.12	0/1254	0.30	0/1677
51	BY	0.12	0/744	0.27	0/1004
52	BZ	0.13	0/760	0.28	0/1024
53	Ba	0.11	0/1107	0.26	0/1477
54	Bb	0.11	0/751	0.24	0/999
55	Bc	0.11	0/686	0.32	0/916
56	Bd	0.11	0/504	0.25	0/667
57	Be	0.11	0/625	0.25	0/832
58	Bf	0.13	0/445	0.25	0/593
59	Bg	0.10	0/384	0.25	0/509
60	Bh	0.12	0/354	0.24	0/458
61	Bi	0.10	0/805	0.24	0/1064
62	Bj	0.12	0/669	0.32	0/884
63	Bk	0.11	0/533	0.26	0/703
All	All	0.14	4/168467 (0.0%)	0.27	4/248035 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Bl	83	PRO	CG-CD	-8.20	1.22	1.50
23	Bl	83	PRO	N-CD	5.25	1.55	1.47
1	A1	775	OMU	O3'-P	5.07	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	857	A2M	O3'-P	5.00	1.61	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B1	83	PRO	CA-N-CD	-11.89	95.35	112.00
23	B1	83	PRO	N-CD-CG	-11.30	86.25	103.20
1	A1	237	C	C4'-C3'-O3'	6.67	123.01	113.00
23	B1	83	PRO	CA-CB-CG	-6.52	92.12	104.50

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	32245	0	16371	313	0
2	Aa	1568	0	1625	10	0
3	Ab	1528	0	1611	14	0
4	Ac	1520	0	1603	14	0
5	Ad	1470	0	1542	12	0
6	Ae	1981	0	2051	13	0
7	Af	1788	0	1842	25	0
8	Ag	975	0	1032	14	0
9	Ah	1728	0	1775	15	0
10	Ai	1028	0	1065	14	0
11	Aj	986	0	1070	5	0
12	Ak	1069	0	1121	12	0
13	Al	798	0	845	26	0
14	Am	954	0	981	9	0
15	An	1141	0	1232	9	0
16	Ao	1119	0	1153	11	0
17	Ap	451	0	472	11	0
18	Aq	1296	0	1369	13	0
19	Ar	877	0	898	3	0
20	As	527	0	559	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	At	996	0	1053	6	0
22	Au	1221	0	1263	12	0
23	Av	791	0	819	7	0
23	Bl	765	0	788	15	0
24	Aw	464	0	503	4	0
25	Ax	508	0	533	10	0
26	Ay	434	0	402	5	0
27	B1	63503	0	32151	530	0
28	B2	2695	0	1371	27	0
29	BA	1820	0	1889	20	0
30	BB	2904	0	3061	29	0
31	BC	2026	0	2137	18	0
32	BD	1420	0	1441	15	0
33	BE	1468	0	1507	5	0
34	BF	927	0	971	4	0
34	BG	913	0	960	8	0
35	BH	1376	0	1403	12	0
36	BI	1150	0	1240	9	0
37	BJ	1062	0	1127	8	0
38	BK	609	0	665	7	0
38	BL	621	0	678	4	0
39	BM	1154	0	1219	21	0
40	BN	1587	0	1683	17	0
41	BO	1564	0	1572	18	0
42	BP	966	0	1019	11	0
43	BQ	1238	0	1365	9	0
44	BR	794	0	836	5	0
45	BS	1207	0	1255	12	0
46	BT	696	0	754	5	0
47	BU	1003	0	1074	19	0
48	BV	533	0	523	10	0
49	BW	565	0	618	6	0
50	BX	1235	0	1314	15	0
51	BY	734	0	779	7	0
52	BZ	746	0	803	6	0
53	Ba	1082	0	1172	10	0
54	Bb	733	0	800	3	0
55	Bc	677	0	731	5	0
56	Bd	493	0	502	8	0
57	Be	616	0	655	4	0
58	Bf	437	0	498	1	0
59	Bg	375	0	394	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	Bh	348	0	409	4	0
61	Bi	787	0	833	3	0
62	Bj	659	0	699	8	0
63	Bk	523	0	563	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	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	607	0	0	7	0
65	Aa	5	0	0	0	0
65	Ac	3	0	0	0	0
65	Ad	7	0	0	0	0
65	Ae	15	0	0	1	0
65	Af	7	0	0	0	0
65	Ag	1	0	0	0	0
65	Ah	2	0	0	0	0
65	Ai	10	0	0	0	0
65	Aj	7	0	0	0	0
65	Ak	3	0	0	0	0
65	Al	5	0	0	0	0
65	Am	4	0	0	0	0
65	An	13	0	0	1	0
65	Ap	1	0	0	0	0
65	Aq	7	0	0	1	0
65	Ar	7	0	0	0	0
65	At	2	0	0	0	0
65	Au	4	0	0	0	0
65	Av	2	0	0	0	0
65	Aw	3	0	0	0	0
65	Ay	1	0	0	0	0
65	B1	1513	0	0	43	0
65	B2	17	0	0	0	0
65	BA	25	0	0	0	0
65	BB	20	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	BC	22	0	0	2	0
65	BE	1	0	0	0	0
65	BF	1	0	0	0	0
65	BH	10	0	0	0	0
65	BI	6	0	0	1	0
65	BJ	5	0	0	0	0
65	BM	22	0	0	0	0
65	BN	26	0	0	0	0
65	BO	3	0	0	0	0
65	BP	4	0	0	0	0
65	BQ	10	0	0	1	0
65	BR	10	0	0	1	0
65	BS	15	0	0	1	0
65	BT	4	0	0	0	0
65	BU	6	0	0	0	0
65	BV	1	0	0	0	0
65	BW	1	0	0	0	0
65	BX	7	0	0	0	0
65	BY	1	0	0	0	0
65	BZ	2	0	0	0	0
65	Ba	14	0	0	0	0
65	Bb	1	0	0	0	0
65	Bc	5	0	0	0	0
65	Bd	6	0	0	0	0
65	Be	2	0	0	0	0
65	Bf	8	0	0	0	0
65	Bg	2	0	0	0	0
65	Bh	2	0	0	0	0
65	Bi	3	0	0	0	0
65	Bk	4	0	0	0	0
All	All	165982	0	118249	1324	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 1324 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)
8:Ag:46:ASN:ND2	8:Ag:49:GLU:HG2	1.58	1.18
8:Ag:46:ASN:HD21	8:Ag:49:GLU:HG2	0.95	1.05
8:Ag:46:ASN:HD21	8:Ag:49:GLU:CG	1.81	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Al:26:ILE:HD11	13:Al:84:GLN:HB3	1.52	0.91
25:Ax:18:THR:O	25:Ax:24:VAL:HG12	1.70	0.91

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%)	193 (100%)	1 (0%)	0	100	100
3	Ab	193/210 (92%)	188 (97%)	5 (3%)	0	100	100
4	Ac	183/198 (92%)	182 (100%)	1 (0%)	0	100	100
5	Ad	173/180 (96%)	171 (99%)	2 (1%)	0	100	100
6	Ae	240/243 (99%)	232 (97%)	8 (3%)	0	100	100
7	Af	224/236 (95%)	217 (97%)	7 (3%)	0	100	100
8	Ag	122/125 (98%)	115 (94%)	7 (6%)	0	100	100
9	Ah	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
10	Ai	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
11	Aj	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
12	Ak	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
13	Al	97/102 (95%)	92 (95%)	5 (5%)	0	100	100
14	Am	125/137 (91%)	121 (97%)	4 (3%)	0	100	100
15	An	144/147 (98%)	141 (98%)	3 (2%)	0	100	100
16	Ao	139/148 (94%)	133 (96%)	6 (4%)	0	100	100
17	Ap	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
18	Aq	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
19	Ar	105/113 (93%)	103 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	As	62/67 (92%)	59 (95%)	3 (5%)	0	100	100
21	At	121/132 (92%)	120 (99%)	1 (1%)	0	100	100
22	Au	147/150 (98%)	145 (99%)	2 (1%)	0	100	100
23	Av	93/99 (94%)	91 (98%)	2 (2%)	0	100	100
23	Bl	90/99 (91%)	85 (94%)	5 (6%)	0	100	100
24	Aw	59/63 (94%)	59 (100%)	0	0	100	100
25	Ax	62/71 (87%)	58 (94%)	4 (6%)	0	100	100
26	Ay	54/60 (90%)	51 (94%)	3 (6%)	0	100	100
29	BA	235/239 (98%)	224 (95%)	11 (5%)	0	100	100
30	BB	362/365 (99%)	347 (96%)	15 (4%)	0	100	100
31	BC	253/255 (99%)	246 (97%)	7 (3%)	0	100	100
32	BD	181/186 (97%)	172 (95%)	9 (5%)	0	100	100
33	BE	181/184 (98%)	177 (98%)	4 (2%)	0	100	100
34	BF	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
34	BG	118/123 (96%)	117 (99%)	1 (1%)	0	100	100
35	BH	165/181 (91%)	163 (99%)	2 (1%)	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	78/83 (94%)	74 (95%)	4 (5%)	0	100	100
38	BL	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
39	BM	145/147 (99%)	135 (93%)	9 (6%)	1 (1%)	19	38
40	BN	191/194 (98%)	190 (100%)	1 (0%)	0	100	100
41	BO	194/203 (96%)	192 (99%)	2 (1%)	0	100	100
42	BP	118/120 (98%)	118 (100%)	0	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	150/155 (97%)	146 (97%)	4 (3%)	0	100	100
46	BT	84/86 (98%)	84 (100%)	0	0	100	100
47	BU	118/121 (98%)	117 (99%)	1 (1%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	BX	152/155 (98%)	150 (99%)	2 (1%)	0	100	100
51	BY	95/99 (96%)	93 (98%)	2 (2%)	0	100	100
52	BZ	92/95 (97%)	89 (97%)	3 (3%)	0	100	100
53	Ba	126/130 (97%)	125 (99%)	1 (1%)	0	100	100
54	Bb	86/89 (97%)	86 (100%)	0	0	100	100
55	Bc	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
56	Bd	59/62 (95%)	54 (92%)	5 (8%)	0	100	100
57	Be	80/83 (96%)	79 (99%)	1 (1%)	0	100	100
58	Bf	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
59	Bg	44/51 (86%)	44 (100%)	0	0	100	100
60	Bh	35/37 (95%)	35 (100%)	0	0	100	100
61	Bi	92/94 (98%)	92 (100%)	0	0	100	100
62	Bj	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
63	Bk	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
All	All	7979/8293 (96%)	7783 (98%)	195 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	BM	56	ASP

### 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	167/173 (96%)	167 (100%)	0	100	100
3	Ab	152/167 (91%)	149 (98%)	3 (2%)	50	74
4	Ac	162/171 (95%)	162 (100%)	0	100	100
5	Ad	158/160 (99%)	158 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Ae	212/213 (100%)	211 (100%)	1 (0%)	86	95
7	Af	187/197 (95%)	185 (99%)	2 (1%)	70	86
8	Ag	107/108 (99%)	107 (100%)	0	100	100
9	Ah	183/184 (100%)	183 (100%)	0	100	100
10	Ai	107/108 (99%)	107 (100%)	0	100	100
11	Aj	101/103 (98%)	101 (100%)	0	100	100
12	Ak	110/111 (99%)	110 (100%)	0	100	100
13	Al	88/91 (97%)	88 (100%)	0	100	100
14	Am	94/104 (90%)	94 (100%)	0	100	100
15	An	118/121 (98%)	117 (99%)	1 (1%)	79	91
16	Ao	113/122 (93%)	112 (99%)	1 (1%)	75	90
17	Ap	44/46 (96%)	43 (98%)	1 (2%)	45	71
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%)	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	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	54/60 (90%)	54 (100%)	0	100	100
26	Ay	48/53 (91%)	47 (98%)	1 (2%)	48	73
29	BA	187/189 (99%)	187 (100%)	0	100	100
30	BB	311/312 (100%)	310 (100%)	1 (0%)	91	97
31	BC	213/213 (100%)	211 (99%)	2 (1%)	75	90
32	BD	142/158 (90%)	141 (99%)	1 (1%)	81	93
33	BE	155/156 (99%)	154 (99%)	1 (1%)	84	94
34	BF	97/99 (98%)	97 (100%)	0	100	100
34	BG	96/99 (97%)	96 (100%)	0	100	100
35	BH	142/152 (93%)	141 (99%)	1 (1%)	81	93
36	BI	122/122 (100%)	122 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	64 (98%)	1 (2%)	60	81
39	BM	117/117 (100%)	116 (99%)	1 (1%)	75	90
40	BN	161/162 (99%)	159 (99%)	2 (1%)	67	85
41	BO	158/169 (94%)	158 (100%)	0	100	100
42	BP	101/101 (100%)	100 (99%)	1 (1%)	73	88
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%)	125 (99%)	1 (1%)	79	91
46	BT	77/77 (100%)	77 (100%)	0	100	100
47	BU	110/110 (100%)	110 (100%)	0	100	100
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%)	130 (98%)	2 (2%)	60	81
51	BY	78/80 (98%)	78 (100%)	0	100	100
52	BZ	76/83 (92%)	75 (99%)	1 (1%)	65	84
53	Ba	115/117 (98%)	114 (99%)	1 (1%)	75	90
54	Bb	80/81 (99%)	79 (99%)	1 (1%)	65	84
55	Bc	73/74 (99%)	72 (99%)	1 (1%)	62	82
56	Bd	49/51 (96%)	49 (100%)	0	100	100
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	34/35 (97%)	34 (100%)	0	100	100
61	Bi	82/83 (99%)	82 (100%)	0	100	100
62	Bj	72/72 (100%)	71 (99%)	1 (1%)	62	82
63	Bk	54/55 (98%)	54 (100%)	0	100	100
All	All	6819/7027 (97%)	6790 (100%)	29 (0%)	88	96

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	BE	45	GLN
55	Bc	47	SER
39	BM	61	ARG
52	BZ	8	GLU
38	BL	5	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	Ac	153	ASN
31	BC	204	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1489/1497 (99%)	233 (15%)	16 (1%)
27	B1	2928/3051 (95%)	409 (13%)	28 (0%)
28	B2	124/125 (99%)	11 (8%)	0
All	All	4541/4673 (97%)	653 (14%)	44 (0%)

5 of 653 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	4	C
1	A1	17	5MC
1	A1	20	G
1	A1	27	C
1	A1	33	U

5 of 44 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	B1	1186	A
27	B1	2166	A
27	B1	1368	A
27	B1	1765	G
27	B1	2251	G

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

311 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	274	1	21,24,25	3.26	10 (47%)	29,34,37	1.08	4 (13%)
27	OMC	B1	1832	27	19,22,23	3.12	8 (42%)	26,31,34	0.73	0
27	OMG	B1	2562	27	18,26,27	2.56	8 (44%)	19,38,41	1.51	4 (21%)
27	OMG	B1	2391	27	18,26,27	2.54	8 (44%)	19,38,41	1.52	5 (26%)
1	4AC	A1	945	1	21,24,25	3.39	10 (47%)	29,34,37	1.76	6 (20%)
27	4AC	B1	1762	27	21,24,25	3.21	10 (47%)	29,34,37	1.03	3 (10%)
1	5MC	A1	1190	1	18,22,23	3.17	7 (38%)	26,32,35	0.99	2 (7%)
27	4AC	B1	360	27	21,24,25	3.25	10 (47%)	29,34,37	1.08	4 (13%)
27	4AC	B1	950	27	21,24,25	3.23	10 (47%)	29,34,37	1.07	3 (10%)
1	5MC	A1	466	1	18,22,23	3.19	7 (38%)	26,32,35	1.01	2 (7%)
1	5MC	A1	681	1	18,22,23	3.16	7 (38%)	26,32,35	1.01	2 (7%)
27	4AC	B1	786	27	21,24,25	3.27	9 (42%)	29,34,37	1.11	4 (13%)
27	4AC	B1	2888	27	21,24,25	3.25	10 (47%)	29,34,37	1.10	4 (13%)
27	4AC	B1	1639	27	21,24,25	3.30	9 (42%)	29,34,37	1.27	5 (17%)
27	OMG	B1	1904	27	18,26,27	2.53	8 (44%)	19,38,41	1.51	5 (26%)
27	5MC	B1	932	27	18,22,23	3.12	7 (38%)	26,32,35	0.99	2 (7%)
27	4AC	B1	1885	27	21,24,25	3.26	10 (47%)	29,34,37	1.08	4 (13%)
27	4AC	B1	200	27	21,24,25	3.25	10 (47%)	29,34,37	1.08	3 (10%)
27	OMG	B1	1533	27	18,26,27	2.55	8 (44%)	19,38,41	1.48	4 (21%)
27	OMG	B1	2365	27	18,26,27	2.57	8 (44%)	19,38,41	1.50	4 (21%)
27	OMU	B1	2554	27	19,22,23	3.27	7 (36%)	26,31,34	1.70	5 (19%)
1	4AC	A1	1227	1	21,24,25	3.30	10 (47%)	29,34,37	1.12	4 (13%)
27	4AC	B1	162	27	21,24,25	3.26	9 (42%)	29,34,37	1.09	4 (13%)
27	4AC	B1	609	27	21,24,25	3.27	9 (42%)	29,34,37	1.10	3 (10%)
1	4AC	A1	467	1	21,24,25	3.28	9 (42%)	29,34,37	1.12	3 (10%)
27	4AC	B1	485	27	21,24,25	3.24	10 (47%)	29,34,37	1.06	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	4AC	B1	1150	27	21,24,25	3.20	10 (47%)	29,34,37	1.16	3 (10%)
27	4AC	B1	933	27	21,24,25	3.16	10 (47%)	29,34,37	1.02	2 (6%)
27	4AC	B1	130	27	21,24,25	3.25	10 (47%)	29,34,37	1.05	3 (10%)
27	4AC	B1	1649	27	21,24,25	3.23	10 (47%)	29,34,37	1.08	4 (13%)
27	4AC	B1	896	27	21,24,25	3.24	10 (47%)	29,34,37	1.02	2 (6%)
1	OMU	A1	488	1	19,22,23	3.29	7 (36%)	26,31,34	1.68	5 (19%)
27	OMU	B1	926	27	19,22,23	3.25	7 (36%)	26,31,34	1.72	5 (19%)
1	LV2	A1	927	1	20,23,24	3.33	7 (35%)	26,33,36	0.61	0
27	OMC	B1	2735	27	19,22,23	3.10	8 (42%)	26,31,34	0.81	0
27	4AC	B1	2083	27	21,24,25	3.26	9 (42%)	29,34,37	1.08	4 (13%)
27	4AC	B1	1757	27	21,24,25	3.25	10 (47%)	29,34,37	1.15	4 (13%)
27	4AC	B1	2792	27	21,24,25	3.25	10 (47%)	29,34,37	1.09	4 (13%)
1	5MC	A1	1484	1	18,22,23	3.14	7 (38%)	26,32,35	0.98	2 (7%)
27	5MC	B1	2047	27	18,22,23	3.18	7 (38%)	26,32,35	1.04	2 (7%)
27	OMG	B1	887	27	18,26,27	2.58	8 (44%)	19,38,41	1.52	4 (21%)
27	OMG	B1	675	27	18,26,27	2.56	8 (44%)	19,38,41	1.57	5 (26%)
27	4AC	B1	2020	27	21,24,25	3.27	9 (42%)	29,34,37	1.10	3 (10%)
1	OMC	A1	1194	1	19,22,23	3.12	8 (42%)	26,31,34	0.72	0
1	4AC	A1	367	1	21,24,25	3.26	10 (47%)	29,34,37	1.07	3 (10%)
27	4AC	B1	2492	27	21,24,25	3.28	10 (47%)	29,34,37	1.11	4 (13%)
27	OMC	B1	47	27	19,22,23	3.13	8 (42%)	26,31,34	0.95	2 (7%)
1	A2M	A1	361	1	18,25,26	4.23	7 (38%)	18,36,39	2.36	4 (22%)
1	4AC	A1	1221	1	21,24,25	3.28	9 (42%)	29,34,37	1.11	4 (13%)
1	4AC	A1	1467	1	21,24,25	3.26	10 (47%)	29,34,37	1.13	4 (13%)
27	OMG	B1	921	27	18,26,27	2.58	8 (44%)	19,38,41	1.57	4 (21%)
1	5MC	A1	605	1	18,22,23	3.14	7 (38%)	26,32,35	1.05	2 (7%)
27	4AC	B1	827	27	21,24,25	3.24	9 (42%)	29,34,37	1.10	4 (13%)
27	OMG	B1	920	27	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)
28	4AC	B2	90	28	21,24,25	3.26	9 (42%)	29,34,37	1.11	4 (13%)
27	4AC	B1	337	27	21,24,25	3.25	10 (47%)	29,34,37	1.10	4 (13%)
27	OMC	B1	2059	27	19,22,23	3.11	8 (42%)	26,31,34	0.81	0
1	4SU	A1	756	1	18,21,22	3.87	8 (44%)	26,30,33	2.18	4 (15%)
27	4AC	B1	2876	27	21,24,25	3.27	10 (47%)	29,34,37	1.13	5 (17%)
1	4AC	A1	427	1	21,24,25	3.33	9 (42%)	29,34,37	1.27	5 (17%)
27	4AC	B1	1383	27	21,24,25	3.26	9 (42%)	29,34,37	1.07	3 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A1	951	1	18,22,23	3.18	7 (38%)	26,32,35	0.99	2 (7%)
1	4AC	A1	739	1	21,24,25	3.29	9 (42%)	29,34,37	1.10	3 (10%)
27	4AC	B1	1478	27	21,24,25	3.23	10 (47%)	29,34,37	1.08	4 (13%)
1	4AC	A1	827	1	21,24,25	3.27	10 (47%)	29,34,37	1.06	3 (10%)
1	OMG	A1	504	1	18,26,27	2.59	8 (44%)	19,38,41	1.50	4 (21%)
27	4AC	B1	2602	27	21,24,25	3.26	9 (42%)	29,34,37	1.08	4 (13%)
1	OMC	A1	761	1	19,22,23	3.11	8 (42%)	26,31,34	0.88	0
27	4AC	B1	2429	27	21,24,25	3.27	9 (42%)	29,34,37	1.06	3 (10%)
1	4AC	A1	231	1	21,24,25	3.26	9 (42%)	29,34,37	1.10	4 (13%)
1	A2M	A1	819	1	18,25,26	4.25	7 (38%)	18,36,39	2.28	4 (22%)
1	4AC	A1	5	1	21,24,25	3.27	10 (47%)	29,34,37	1.08	3 (10%)
27	5MC	B1	1973	27	18,22,23	3.15	7 (38%)	26,32,35	1.06	2 (7%)
27	4AC	B1	732	27	21,24,25	3.27	9 (42%)	29,34,37	1.10	3 (10%)
1	OMC	A1	1028	1	19,22,23	0.47	0	26,31,34	0.84	1 (3%)
1	4AC	A1	856	1	21,24,25	3.25	10 (47%)	29,34,37	1.10	3 (10%)
27	OMC	B1	2607	27	19,22,23	3.12	8 (42%)	26,31,34	0.71	0
1	OMU	A1	425	1	19,22,23	3.31	7 (36%)	26,31,34	1.67	4 (15%)
27	OMC	B1	2557	27	19,22,23	3.11	8 (42%)	26,31,34	0.80	0
27	OMG	B1	2180	27	18,26,27	2.57	8 (44%)	19,38,41	1.54	4 (21%)
27	4AC	B1	98	27	21,24,25	3.24	9 (42%)	29,34,37	1.07	3 (10%)
1	4AC	A1	1314	1	21,24,25	3.22	9 (42%)	29,34,37	1.04	2 (6%)
1	4AC	A1	836	1	21,24,25	3.26	10 (47%)	29,34,37	1.07	3 (10%)
27	4AC	B1	142	27	21,24,25	3.30	9 (42%)	29,34,37	1.11	4 (13%)
1	4AC	A1	499	1	21,24,25	3.26	9 (42%)	29,34,37	1.09	4 (13%)
27	OMC	B1	1099	27	19,22,23	3.07	8 (42%)	26,31,34	0.71	0
1	4AC	A1	706	1	21,24,25	3.27	10 (47%)	29,34,37	1.09	4 (13%)
1	OMG	A1	329	1	18,26,27	2.59	8 (44%)	19,38,41	1.56	4 (21%)
27	4AC	B1	1128	27	21,24,25	3.29	10 (47%)	29,34,37	1.23	5 (17%)
27	5MC	B1	2087	27	18,22,23	3.13	7 (38%)	26,32,35	1.02	2 (7%)
27	5MC	B1	1966	27	18,22,23	3.14	7 (38%)	26,32,35	1.03	2 (7%)
1	OMC	A1	1371	1	19,22,23	3.14	8 (42%)	26,31,34	0.82	0
1	OMG	A1	1420	1	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)
1	OMG	A1	541	1	18,26,27	2.57	8 (44%)	19,38,41	1.52	4 (21%)
1	OMG	A1	833	1	18,26,27	2.56	8 (44%)	19,38,41	1.52	4 (21%)
27	4AC	B1	116	27	21,24,25	3.22	10 (47%)	29,34,37	1.05	3 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MA6	A1	1457	1	18,26,27	1.02	1 (5%)	19,38,41	4.60	3 (15%)
1	5MC	A1	17	1	18,22,23	3.14	7 (38%)	26,32,35	0.99	2 (7%)
27	4AC	B1	2379	27	21,24,25	3.21	10 (47%)	29,34,37	1.07	2 (6%)
27	4AC	B1	1439	27	21,24,25	3.23	9 (42%)	29,34,37	1.07	4 (13%)
1	OMC	A1	117	1	19,22,23	3.11	8 (42%)	26,31,34	0.73	0
27	4AC	B1	721	27	21,24,25	3.24	10 (47%)	29,34,37	1.12	4 (13%)
27	4AC	B1	1178	27	21,24,25	3.27	9 (42%)	29,34,37	1.04	3 (10%)
1	4AC	A1	624	1	21,24,25	3.27	10 (47%)	29,34,37	1.10	4 (13%)
1	4AC	A1	291	1	21,24,25	3.25	10 (47%)	29,34,37	1.05	3 (10%)
27	4AC	B1	243	27	21,24,25	3.24	10 (47%)	29,34,37	1.08	3 (10%)
27	OMG	B1	1965	27	18,26,27	2.58	8 (44%)	19,38,41	1.50	4 (21%)
1	5MC	A1	273	1	18,22,23	3.16	7 (38%)	26,32,35	1.01	2 (7%)
1	5MU	A1	926	1	19,22,23	0.47	0	28,32,35	0.66	0
27	4AC	B1	1290	27	21,24,25	3.23	9 (42%)	29,34,37	1.07	3 (10%)
1	OMU	A1	1110	1	19,22,23	3.29	7 (36%)	26,31,34	1.67	4 (15%)
1	5MC	A1	230	1	18,22,23	3.15	7 (38%)	26,32,35	1.03	2 (7%)
1	2MG	A1	1004	1	18,26,27	2.53	7 (38%)	16,38,41	1.45	4 (25%)
27	4AC	B1	1664	27	21,24,25	3.20	10 (47%)	29,34,37	1.00	2 (6%)
27	4AC	B1	2850	27	21,24,25	3.25	9 (42%)	29,34,37	1.08	3 (10%)
27	4SU	B1	2565	27	18,21,22	3.83	8 (44%)	26,30,33	2.22	5 (19%)
1	OMG	A1	901	1	18,26,27	2.59	8 (44%)	19,38,41	1.54	4 (21%)
1	7MG	A1	481	1	22,26,27	3.82	10 (45%)	29,39,42	2.04	9 (31%)
27	4AC	B1	1286	27	21,24,25	3.34	9 (42%)	29,34,37	1.42	5 (17%)
28	4AC	B2	120	28	21,24,25	3.28	9 (42%)	29,34,37	1.10	3 (10%)
1	4AC	A1	614	1	21,24,25	3.26	10 (47%)	29,34,37	1.09	4 (13%)
1	OMC	A1	426	1	19,22,23	3.13	8 (42%)	26,31,34	0.82	0
27	4AC	B1	2454	27	21,24,25	3.28	10 (47%)	29,34,37	1.09	4 (13%)
1	4AC	A1	220	1	21,24,25	3.28	10 (47%)	29,34,37	1.15	3 (10%)
1	OMG	A1	464	1	18,26,27	2.56	8 (44%)	19,38,41	1.58	5 (26%)
27	5MC	B1	2453	27	18,22,23	3.16	7 (38%)	26,32,35	0.99	2 (7%)
1	4AC	A1	546	1	21,24,25	3.27	9 (42%)	29,34,37	1.10	3 (10%)
27	OMU	B1	2401	27	19,22,23	3.27	7 (36%)	26,31,34	1.72	5 (19%)
1	OMG	A1	668	1	18,26,27	2.58	8 (44%)	19,38,41	1.52	4 (21%)
1	4AC	A1	307	1	21,24,25	3.25	9 (42%)	29,34,37	1.11	4 (13%)
27	4AC	B1	1818	27	21,24,25	3.24	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	4AC	B1	271	27	21,24,25	3.29	9 (42%)	29,34,37	1.14	4 (13%)
27	4AC	B1	1822	27	21,24,25	3.24	10 (47%)	29,34,37	1.14	3 (10%)
27	4AC	B1	1743	27	21,24,25	3.29	9 (42%)	29,34,37	1.12	4 (13%)
1	4AC	A1	382	1	21,24,25	3.28	10 (47%)	29,34,37	1.10	4 (13%)
27	4AC	B1	1608	27	21,24,25	3.27	10 (47%)	29,34,37	1.09	4 (13%)
27	4AC	B1	1706	27	21,24,25	3.28	9 (42%)	29,34,37	1.10	4 (13%)
27	A2M	B1	880	27	18,25,26	4.26	8 (44%)	18,36,39	2.30	4 (22%)
27	4AC	B1	1769	27	21,24,25	3.22	10 (47%)	29,34,37	1.03	3 (10%)
27	5MC	B1	2067	27	18,22,23	3.16	7 (38%)	26,32,35	1.00	1 (3%)
27	5MC	B1	97	27	18,22,23	3.15	7 (38%)	26,32,35	1.02	2 (7%)
1	5MC	A1	1366	1	18,22,23	3.17	7 (38%)	26,32,35	0.95	1 (3%)
27	4AC	B1	1345	27	21,24,25	3.23	9 (42%)	29,34,37	1.06	3 (10%)
1	4AC	A1	534	1	21,24,25	3.27	10 (47%)	29,34,37	1.06	4 (13%)
1	OMG	A1	763	1	18,26,27	2.61	8 (44%)	19,38,41	1.56	4 (21%)
1	4AC	A1	1181	1	21,24,25	3.20	9 (42%)	29,34,37	1.01	2 (6%)
1	5MC	A1	687	1	18,22,23	3.15	7 (38%)	26,32,35	0.99	2 (7%)
27	LHH	B1	2968	27	22,25,26	1.95	7 (31%)	29,35,38	1.17	3 (10%)
27	4AC	B1	1435	27	21,24,25	3.22	10 (47%)	29,34,37	1.09	4 (13%)
27	OMC	B1	2808	27	19,22,23	3.11	8 (42%)	26,31,34	0.74	0
27	4AC	B1	2821	27	21,24,25	3.27	9 (42%)	29,34,37	1.06	3 (10%)
1	4AC	A1	578	1	21,24,25	3.28	10 (47%)	29,34,37	1.09	3 (10%)
1	LHH	A1	238	1	22,25,26	1.89	5 (22%)	29,35,38	1.45	5 (17%)
27	OMC	B1	2428	27	19,22,23	3.14	8 (42%)	26,31,34	0.74	0
27	4AC	B1	19	27	21,24,25	3.22	10 (47%)	29,34,37	1.09	3 (10%)
27	OMC	B1	904	27	19,22,23	3.10	8 (42%)	26,31,34	0.75	0
27	4AC	B1	1551	27	21,24,25	3.25	10 (47%)	29,34,37	1.03	3 (10%)
28	4AC	B2	32	28	21,24,25	3.30	9 (42%)	29,34,37	1.07	3 (10%)
27	4AC	B1	688	27	21,24,25	3.25	10 (47%)	29,34,37	1.08	3 (10%)
27	4AC	B1	1264	27	21,24,25	3.27	9 (42%)	29,34,37	1.11	4 (13%)
27	OMG	B1	2028	27	18,26,27	2.56	8 (44%)	19,38,41	1.49	4 (21%)
1	OMU	A1	1165	1	19,22,23	3.28	7 (36%)	26,31,34	1.70	5 (19%)
28	4AC	B2	108	28	21,24,25	3.26	9 (42%)	29,34,37	1.15	4 (13%)
1	OMG	A1	132	1	18,26,27	2.59	8 (44%)	19,38,41	1.51	4 (21%)
27	A2M	B1	506	27	18,25,26	4.25	8 (44%)	18,36,39	2.44	6 (33%)
27	OMG	B1	2022	27	18,26,27	2.56	8 (44%)	19,38,41	1.50	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	4AC	B1	2469	27	21,24,25	3.25	10 (47%)	29,34,37	1.10	4 (13%)
1	4AC	A1	719	1	21,24,25	3.25	10 (47%)	29,34,37	1.07	3 (10%)
27	4AC	B1	1052	27	21,24,25	3.23	9 (42%)	29,34,37	1.09	3 (10%)
27	4AC	B1	1322	27	21,24,25	3.27	10 (47%)	29,34,37	1.18	5 (17%)
1	OMG	A1	153	1	18,26,27	2.59	8 (44%)	19,38,41	1.52	4 (21%)
27	4AC	B1	344	27	21,24,25	3.28	10 (47%)	29,34,37	1.09	4 (13%)
27	OMU	B1	2668	27	19,22,23	3.26	7 (36%)	26,31,34	1.72	5 (19%)
27	4AC	B1	1100	27	21,24,25	3.24	10 (47%)	29,34,37	1.07	3 (10%)
27	OMC	B1	1914	27	19,22,23	3.09	8 (42%)	26,31,34	0.89	1 (3%)
27	4AC	B1	1067	27	21,24,25	3.26	9 (42%)	29,34,37	1.08	4 (13%)
27	4AC	B1	1911	27	21,24,25	3.25	10 (47%)	29,34,37	1.05	3 (10%)
1	4AC	A1	1016	1	21,24,25	3.28	9 (42%)	29,34,37	1.07	3 (10%)
27	4AC	B1	2113	27	21,24,25	3.22	10 (47%)	29,34,37	1.09	4 (13%)
1	OMU	A1	8	1	19,22,23	3.26	7 (36%)	26,31,34	1.71	5 (19%)
1	OMG	A1	507	1	18,26,27	2.58	8 (44%)	19,38,41	1.54	4 (21%)
27	5MC	B1	1983	27	18,22,23	3.16	7 (38%)	26,32,35	0.99	1 (3%)
27	LHH	B1	276	27	22,25,26	1.94	6 (27%)	29,35,38	1.26	4 (13%)
1	4AC	A1	1288	1	21,24,25	3.26	9 (42%)	29,34,37	1.09	3 (10%)
27	OMU	B1	1981	27	19,22,23	3.27	7 (36%)	26,31,34	1.66	5 (19%)
27	OMG	B1	2740	27	18,26,27	2.58	8 (44%)	19,38,41	1.53	4 (21%)
27	LHH	B1	527	27	22,25,26	1.92	6 (27%)	29,35,38	1.22	4 (13%)
27	4AC	B1	434	27	21,24,25	3.24	9 (42%)	29,34,37	1.09	3 (10%)
1	MA6	A1	1476	1	18,26,27	1.01	1 (5%)	19,38,41	4.59	3 (15%)
1	OMC	A1	1364	1	19,22,23	3.10	8 (42%)	26,31,34	0.73	0
1	4AC	A1	141	1	21,24,25	3.30	9 (42%)	29,34,37	1.13	3 (10%)
27	4AC	B1	2171	27	21,24,25	3.24	10 (47%)	29,34,37	1.08	4 (13%)
27	4AC	B1	2213	27	21,24,25	3.26	9 (42%)	29,34,37	1.09	3 (10%)
27	4AC	B1	48	27	21,24,25	3.20	10 (47%)	29,34,37	1.01	3 (10%)
27	OMG	B1	2540	27	18,26,27	2.57	8 (44%)	19,38,41	1.51	4 (21%)
27	OMG	B1	2684	27	18,26,27	2.57	8 (44%)	19,38,41	1.52	4 (21%)
1	OMG	A1	227	1	18,26,27	2.57	8 (44%)	19,38,41	1.52	4 (21%)
1	4AC	A1	816	1	21,24,25	3.26	10 (47%)	29,34,37	1.07	3 (10%)
27	4AC	B1	866	27	21,24,25	3.23	10 (47%)	29,34,37	1.04	3 (10%)
27	4AC	B1	2133	27	21,24,25	3.22	10 (47%)	29,34,37	1.07	3 (10%)
1	OMG	A1	1003	1	18,26,27	2.59	8 (44%)	19,38,41	1.49	4 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMU	A1	775	1	19,22,23	3.27	7 (36%)	26,31,34	1.71	5 (19%)
1	4AC	A1	41	1	21,24,25	3.26	9 (42%)	29,34,37	1.06	3 (10%)
27	OMG	B1	2984	27	18,26,27	2.57	8 (44%)	19,38,41	1.55	4 (21%)
27	OMC	B1	2007	27	19,22,23	3.11	8 (42%)	26,31,34	0.76	0
1	4AC	A1	216	1	21,24,25	3.30	10 (47%)	29,34,37	1.11	4 (13%)
27	5MC	B1	2901	27	18,22,23	3.14	7 (38%)	26,32,35	1.02	2 (7%)
27	4AC	B1	378	27	21,24,25	3.24	10 (47%)	29,34,37	1.08	3 (10%)
27	A2M	B1	940	27	18,25,26	4.26	7 (38%)	18,36,39	2.27	4 (22%)
27	4AC	B1	807	27	21,24,25	3.26	10 (47%)	29,34,37	1.15	4 (13%)
1	4AC	A1	839	1	21,24,25	3.22	10 (47%)	29,34,37	1.08	3 (10%)
27	4AC	B1	2902	27	21,24,25	3.26	9 (42%)	29,34,37	1.10	3 (10%)
27	4AC	B1	3023	27	21,24,25	3.25	9 (42%)	29,34,37	1.09	3 (10%)
1	4AC	A1	540	1	21,24,25	3.27	9 (42%)	29,34,37	1.10	4 (13%)
27	4AC	B1	1846	27	21,24,25	3.27	10 (47%)	29,34,37	1.12	4 (13%)
27	4AC	B1	1751	27	21,24,25	3.28	9 (42%)	29,34,37	1.10	4 (13%)
27	4AC	B1	3020	27	21,24,25	3.27	9 (42%)	29,34,37	1.10	4 (13%)
1	OMC	A1	834	1	19,22,23	3.09	8 (42%)	26,31,34	0.76	0
27	4AC	B1	1967	27	21,24,25	3.20	10 (47%)	29,34,37	1.06	3 (10%)
27	4AC	B1	715	27	21,24,25	3.24	10 (47%)	29,34,37	1.07	3 (10%)
27	4AC	B1	1313	27	21,24,25	3.29	9 (42%)	29,34,37	1.16	4 (13%)
27	4AC	B1	1301	27	21,24,25	3.27	10 (47%)	29,34,37	1.67	5 (17%)
27	4AC	B1	23	27	21,24,25	3.24	9 (42%)	29,34,37	1.08	3 (10%)
27	5MC	B1	336	27	18,22,23	3.13	7 (38%)	26,32,35	1.06	2 (7%)
27	OMC	B1	2046	27	19,22,23	3.15	8 (42%)	26,31,34	0.82	0
1	MA6	A1	1475	1	18,26,27	0.99	1 (5%)	19,38,41	4.64	3 (15%)
27	5MC	B1	1648	27	18,22,23	3.18	7 (38%)	26,32,35	1.08	3 (11%)
27	OMU	B1	1488	27	19,22,23	3.24	7 (36%)	26,31,34	1.70	5 (19%)
1	5MC	A1	777	1	18,22,23	3.14	7 (38%)	26,32,35	1.03	2 (7%)
27	OMC	B1	1489	27	19,22,23	3.10	8 (42%)	26,31,34	0.77	0
27	4AC	B1	1501	27	21,24,25	3.25	9 (42%)	29,34,37	1.09	4 (13%)
1	5MC	A1	1362	1	18,22,23	3.17	7 (38%)	26,32,35	1.02	2 (7%)
27	5MC	B1	2617	27	18,22,23	3.16	7 (38%)	26,32,35	1.03	2 (7%)
27	4AC	B1	1064	27	21,24,25	3.26	10 (47%)	29,34,37	1.11	4 (13%)
27	4AC	B1	1442	27	21,24,25	3.24	10 (47%)	29,34,37	1.05	3 (10%)
27	4AC	B1	3037	27	21,24,25	3.27	9 (42%)	29,34,37	1.14	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	5MC	B1	2875	27	18,22,23	3.14	7 (38%)	26,32,35	1.02	2 (7%)
1	5MC	A1	473	1	18,22,23	3.16	7 (38%)	26,32,35	0.98	2 (7%)
1	4AC	A1	1135	1	21,24,25	3.29	9 (42%)	29,34,37	1.11	3 (10%)
27	OMC	B1	501	27	19,22,23	3.12	8 (42%)	26,31,34	0.89	1 (3%)
27	5MU	B1	883	27	19,22,23	0.45	0	28,32,35	0.74	0
27	OMG	B1	55	27	18,26,27	2.55	8 (44%)	19,38,41	1.50	4 (21%)
27	4AC	B1	599	27	21,24,25	3.29	9 (42%)	29,34,37	1.14	4 (13%)
1	OMG	A1	152	1	18,26,27	2.60	8 (44%)	19,38,41	1.55	4 (21%)
1	5MC	A1	815	1	18,22,23	3.15	7 (38%)	26,32,35	1.01	2 (7%)
27	4AC	B1	1546	27	21,24,25	3.23	10 (47%)	29,34,37	1.07	3 (10%)
27	UR3	B1	2700	27	19,22,23	3.22	7 (36%)	26,32,35	1.56	4 (15%)
1	4AC	A1	1254	1	21,24,25	3.28	9 (42%)	29,34,37	1.14	4 (13%)
27	OMG	B1	2108	27	18,26,27	2.55	8 (44%)	19,38,41	1.53	4 (21%)
1	OMG	A1	228	1	18,26,27	2.56	8 (44%)	19,38,41	1.53	4 (21%)
1	5MC	A1	863	1	18,22,23	3.16	7 (38%)	26,32,35	1.04	2 (7%)
27	4AC	B1	1374	27	21,24,25	3.27	9 (42%)	29,34,37	1.06	3 (10%)
27	4AC	B1	419	27	21,24,25	3.27	10 (47%)	29,34,37	1.12	4 (13%)
1	5MC	A1	1123	1	18,22,23	3.19	7 (38%)	26,32,35	1.04	2 (7%)
27	5MC	B1	2082	27	18,22,23	3.16	7 (38%)	26,32,35	0.98	1 (3%)
1	5MC	A1	1012	1	18,22,23	3.17	7 (38%)	26,32,35	0.97	2 (7%)
27	5MU	B1	888	27	19,22,23	0.47	0	28,32,35	0.66	0
27	OMG	B1	214	27	18,26,27	2.59	8 (44%)	19,38,41	1.57	4 (21%)
27	4AC	B1	580	27	21,24,25	3.27	10 (47%)	29,34,37	1.04	3 (10%)
1	5MC	A1	1486	1	18,22,23	3.17	7 (38%)	26,32,35	1.11	2 (7%)
1	OMG	A1	459	1	18,26,27	2.58	8 (44%)	19,38,41	1.51	4 (21%)
1	4AC	A1	444	1	21,24,25	3.25	9 (42%)	29,34,37	1.11	3 (10%)
1	OMU	A1	762	1	19,22,23	3.27	7 (36%)	26,31,34	1.72	4 (15%)
1	5MC	A1	523	1	18,22,23	3.16	7 (38%)	26,32,35	1.00	2 (7%)
27	5MC	B1	877	27	18,22,23	3.11	7 (38%)	26,32,35	1.05	2 (7%)
27	OMG	B1	530	27	18,26,27	2.59	8 (44%)	19,38,41	1.50	4 (21%)
27	4AC	B1	2749	27	21,24,25	3.25	10 (47%)	29,34,37	1.08	4 (13%)
27	4AC	B1	641	27	21,24,25	3.26	9 (42%)	29,34,37	1.08	3 (10%)
27	OMG	B1	2659	27	18,26,27	2.58	8 (44%)	19,38,41	1.54	4 (21%)
27	A2M	B1	857	27	18,25,26	4.18	7 (38%)	18,36,39	2.25	4 (22%)
27	LHH	B1	1946	27	22,25,26	1.96	7 (31%)	29,35,38	1.15	4 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	A2M	B1	2506	27	18,25,26	4.23	7 (38%)	18,36,39	2.33	4 (22%)
27	4AC	B1	80	27	21,24,25	3.24	10 (47%)	29,34,37	1.09	3 (10%)
27	4AC	B1	2809	27	21,24,25	3.23	10 (47%)	29,34,37	1.04	3 (10%)
27	4AC	B1	106	27	21,24,25	3.32	9 (42%)	29,34,37	1.28	5 (17%)
27	4AC	B1	953	27	21,24,25	3.24	10 (47%)	29,34,37	1.05	3 (10%)
1	4AC	A1	405	1	21,24,25	3.27	9 (42%)	29,34,37	1.12	4 (13%)
27	4AC	B1	2844	27	21,24,25	3.23	9 (42%)	29,34,37	1.06	3 (10%)
27	4AC	B1	813	27	21,24,25	3.33	9 (42%)	29,34,37	1.41	5 (17%)
27	4AC	B1	3006	27	21,24,25	3.27	9 (42%)	29,34,37	1.10	4 (13%)
28	4AC	B2	117	28	21,24,25	3.27	10 (47%)	29,34,37	1.08	3 (10%)
27	4AC	B1	2432	27	21,24,25	3.27	10 (47%)	29,34,37	1.10	4 (13%)
27	4AC	B1	979	27	21,24,25	3.29	9 (42%)	29,34,37	1.25	5 (17%)
1	OMG	A1	861	1	18,26,27	2.57	8 (44%)	19,38,41	1.52	4 (21%)
1	LHH	A1	1029	1	22,25,26	1.90	5 (22%)	29,35,38	1.24	4 (13%)
27	LHH	B1	502	27	22,25,26	1.91	7 (31%)	29,35,38	1.20	4 (13%)
27	4AC	B1	1579	27	21,24,25	3.28	9 (42%)	29,34,37	1.12	4 (13%)
27	OMG	B1	808	27	18,26,27	2.56	8 (44%)	19,38,41	1.52	4 (21%)
27	4AC	B1	1061	27	21,24,25	3.27	9 (42%)	29,34,37	1.11	4 (13%)
27	OMU	B1	454	27	19,22,23	3.31	7 (36%)	26,31,34	1.69	5 (19%)
1	4AC	A1	87	1	21,24,25	3.28	10 (47%)	29,34,37	1.12	3 (10%)
1	OMG	A1	455	1	18,26,27	2.58	8 (44%)	19,38,41	1.54	4 (21%)
1	OMC	A1	1226	1	19,22,23	3.12	8 (42%)	26,31,34	0.77	0
27	4AC	B1	652	27	21,24,25	3.23	9 (42%)	29,34,37	1.10	3 (10%)
27	4AC	B1	2526	27	21,24,25	3.25	9 (42%)	29,34,37	1.11	4 (13%)
27	4AC	B1	227	27	21,24,25	3.26	10 (47%)	29,34,37	1.07	3 (10%)
27	4AC	B1	1107	27	21,24,25	3.23	10 (47%)	29,34,37	1.02	3 (10%)
27	5MC	B1	1344	27	18,22,23	3.14	7 (38%)	26,32,35	1.04	2 (7%)
27	OMG	B1	550	27	18,26,27	2.57	8 (44%)	19,38,41	1.62	4 (21%)
1	OMU	A1	1368	1	19,22,23	3.31	7 (36%)	26,31,34	1.70	4 (15%)
1	4AC	A1	1067	1	21,24,25	3.28	10 (47%)	29,34,37	1.09	3 (10%)
27	4AC	B1	1505	27	21,24,25	3.26	9 (42%)	29,34,37	1.10	3 (10%)
27	4AC	B1	2008	27	21,24,25	3.26	9 (42%)	29,34,37	1.07	3 (10%)
27	5MC	B1	252	27	18,22,23	3.14	7 (38%)	26,32,35	1.04	2 (7%)
27	OMG	B1	2757	27	18,26,27	2.58	8 (44%)	19,38,41	1.57	4 (21%)
1	5MC	A1	1013	1	18,22,23	3.15	7 (38%)	26,32,35	0.98	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
27	5MC	B1	1977	27	18,22,23	3.15	7 (38%)	26,32,35	0.98	2 (7%)
1	OMG	A1	645	1	18,26,27	2.57	8 (44%)	19,38,41	1.47	4 (21%)
1	4AC	A1	636	1	21,24,25	3.28	9 (42%)	29,34,37	1.13	5 (17%)
27	4AC	B1	1293	27	21,24,25	3.26	9 (42%)	29,34,37	1.05	3 (10%)
27	4AC	B1	3011	27	21,24,25	3.25	9 (42%)	29,34,37	1.07	3 (10%)

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	274	1	-	0/11/29/30	0/2/2/2
27	OMC	B1	1832	27	-	0/9/27/28	0/2/2/2
27	OMG	B1	2562	27	-	0/5/27/28	0/3/3/3
27	OMG	B1	2391	27	-	3/5/27/28	0/3/3/3
1	4AC	A1	945	1	-	2/11/29/30	0/2/2/2
27	4AC	B1	1762	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	1190	1	-	2/7/25/26	0/2/2/2
27	4AC	B1	360	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	950	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	466	1	-	3/7/25/26	0/2/2/2
1	5MC	A1	681	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	786	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2888	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1639	27	-	2/11/29/30	0/2/2/2
27	OMG	B1	1904	27	-	1/5/27/28	0/3/3/3
27	5MC	B1	932	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	1885	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	200	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	1533	27	-	0/5/27/28	0/3/3/3
27	OMG	B1	2365	27	-	2/5/27/28	0/3/3/3
27	OMU	B1	2554	27	-	0/9/27/28	0/2/2/2
1	4AC	A1	1227	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	162	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	609	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	467	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	485	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1150	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	933	27	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	130	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1649	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	896	27	-	0/11/29/30	0/2/2/2
1	OMU	A1	488	1	-	0/9/27/28	0/2/2/2
27	OMU	B1	926	27	-	4/9/27/28	0/2/2/2
1	LV2	A1	927	1	-	0/9/29/30	0/2/2/2
27	OMC	B1	2735	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	2083	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1757	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2792	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	1484	1	-	0/7/25/26	0/2/2/2
27	5MC	B1	2047	27	-	0/7/25/26	0/2/2/2
27	OMG	B1	887	27	-	2/5/27/28	0/3/3/3
27	OMG	B1	675	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	2020	27	-	0/11/29/30	0/2/2/2
1	OMC	A1	1194	1	-	2/9/27/28	0/2/2/2
1	4AC	A1	367	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	2492	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	47	27	-	3/9/27/28	0/2/2/2
1	A2M	A1	361	1	-	1/5/27/28	0/3/3/3
1	4AC	A1	1221	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	1467	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	921	27	-	1/5/27/28	0/3/3/3
1	5MC	A1	605	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	827	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	920	27	-	1/5/27/28	0/3/3/3
28	4AC	B2	90	28	-	0/11/29/30	0/2/2/2
27	4AC	B1	337	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2059	27	-	0/9/27/28	0/2/2/2
1	4SU	A1	756	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	2876	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	1383	27	-	2/11/29/30	0/2/2/2
1	5MC	A1	951	1	-	0/7/25/26	0/2/2/2
1	4AC	A1	739	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1478	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	827	1	-	0/11/29/30	0/2/2/2
1	OMG	A1	504	1	-	3/5/27/28	0/3/3/3
27	4AC	B1	2602	27	-	0/11/29/30	0/2/2/2
1	OMC	A1	761	1	-	1/9/27/28	0/2/2/2
27	4AC	B1	2429	27	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	A1	231	1	-	0/11/29/30	0/2/2/2
1	A2M	A1	819	1	-	0/5/27/28	0/3/3/3
1	4AC	A1	5	1	-	1/11/29/30	0/2/2/2
27	5MC	B1	1973	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	732	27	-	0/11/29/30	0/2/2/2
1	OMC	A1	1028	1	-	0/9/27/28	0/2/2/2
1	4AC	A1	856	1	-	0/11/29/30	0/2/2/2
27	OMC	B1	2607	27	-	2/9/27/28	0/2/2/2
1	OMU	A1	425	1	-	4/9/27/28	0/2/2/2
27	OMC	B1	2557	27	-	1/9/27/28	0/2/2/2
27	OMG	B1	2180	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	98	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1314	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	142	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	499	1	-	2/11/29/30	0/2/2/2
27	OMC	B1	1099	27	-	0/9/27/28	0/2/2/2
1	4AC	A1	706	1	-	0/11/29/30	0/2/2/2
1	OMG	A1	329	1	-	3/5/27/28	0/3/3/3
27	4AC	B1	1128	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	2087	27	-	0/7/25/26	0/2/2/2
27	5MC	B1	1966	27	-	0/7/25/26	0/2/2/2
1	OMC	A1	1371	1	-	0/9/27/28	0/2/2/2
1	OMG	A1	1420	1	-	3/5/27/28	0/3/3/3
1	OMG	A1	541	1	-	0/5/27/28	0/3/3/3
1	OMG	A1	833	1	-	0/5/27/28	0/3/3/3
27	4AC	B1	116	27	-	0/11/29/30	0/2/2/2
1	MA6	A1	1457	1	-	1/7/29/30	0/3/3/3
1	5MC	A1	17	1	-	2/7/25/26	0/2/2/2
27	4AC	B1	2379	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1439	27	-	0/11/29/30	0/2/2/2
1	OMC	A1	117	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	721	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1178	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	624	1	-	0/11/29/30	0/2/2/2
1	4AC	A1	291	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	243	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	1965	27	-	0/5/27/28	0/3/3/3
1	5MC	A1	273	1	-	0/7/25/26	0/2/2/2
1	5MU	A1	926	1	-	1/7/25/26	0/2/2/2
27	4AC	B1	1290	27	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	A1	1110	1	-	0/9/27/28	0/2/2/2
1	5MC	A1	230	1	-	0/7/25/26	0/2/2/2
1	2MG	A1	1004	1	-	0/5/27/28	0/3/3/3
27	4AC	B1	1664	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2850	27	-	0/11/29/30	0/2/2/2
27	4SU	B1	2565	27	-	0/7/25/26	0/2/2/2
1	OMG	A1	901	1	-	0/5/27/28	0/3/3/3
1	7MG	A1	481	1	-	0/7/37/38	0/3/3/3
27	4AC	B1	1286	27	-	0/11/29/30	0/2/2/2
28	4AC	B2	120	28	-	0/11/29/30	0/2/2/2
1	4AC	A1	614	1	-	0/11/29/30	0/2/2/2
1	OMC	A1	426	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	2454	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	464	1	-	1/5/27/28	0/3/3/3
27	5MC	B1	2453	27	-	0/7/25/26	0/2/2/2
1	4AC	A1	546	1	-	0/11/29/30	0/2/2/2
27	OMU	B1	2401	27	-	1/9/27/28	0/2/2/2
1	OMG	A1	668	1	-	1/5/27/28	0/3/3/3
1	4AC	A1	307	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1818	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	271	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1822	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1743	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	382	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1608	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1706	27	-	0/11/29/30	0/2/2/2
27	A2M	B1	880	27	-	2/5/27/28	0/3/3/3
27	4AC	B1	1769	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	2067	27	-	0/7/25/26	0/2/2/2
27	5MC	B1	97	27	-	0/7/25/26	0/2/2/2
1	5MC	A1	1366	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	1345	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	534	1	-	0/11/29/30	0/2/2/2
1	OMG	A1	763	1	-	0/5/27/28	0/3/3/3
1	4AC	A1	1181	1	-	0/11/29/30	0/2/2/2
1	5MC	A1	687	1	-	0/7/25/26	0/2/2/2
27	LHH	B1	2968	27	-	2/13/31/32	0/2/2/2
27	4AC	B1	1435	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	2808	27	-	1/9/27/28	0/2/2/2
27	4AC	B1	2821	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	578	1	-	0/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LHH	A1	238	1	-	6/13/31/32	0/2/2/2
27	OMC	B1	2428	27	-	1/9/27/28	0/2/2/2
27	4AC	B1	19	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	904	27	-	0/9/27/28	0/2/2/2
27	4AC	B1	1551	27	-	0/11/29/30	0/2/2/2
28	4AC	B2	32	28	-	0/11/29/30	0/2/2/2
27	4AC	B1	688	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1264	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2028	27	-	0/5/27/28	0/3/3/3
1	OMU	A1	1165	1	-	0/9/27/28	0/2/2/2
28	4AC	B2	108	28	-	0/11/29/30	0/2/2/2
1	OMG	A1	132	1	-	2/5/27/28	0/3/3/3
27	A2M	B1	506	27	-	1/5/27/28	0/3/3/3
27	OMG	B1	2022	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	2469	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	719	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1052	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1322	27	-	1/11/29/30	0/2/2/2
1	OMG	A1	153	1	-	1/5/27/28	0/3/3/3
27	4AC	B1	344	27	-	0/11/29/30	0/2/2/2
27	OMU	B1	2668	27	-	1/9/27/28	0/2/2/2
27	4AC	B1	1100	27	-	0/11/29/30	0/2/2/2
27	OMC	B1	1914	27	-	1/9/27/28	0/2/2/2
27	4AC	B1	1067	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1911	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	1016	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	2113	27	-	0/11/29/30	0/2/2/2
1	OMU	A1	8	1	-	5/9/27/28	0/2/2/2
1	OMG	A1	507	1	-	0/5/27/28	0/3/3/3
27	5MC	B1	1983	27	-	0/7/25/26	0/2/2/2
27	LHH	B1	276	27	-	2/13/31/32	0/2/2/2
1	4AC	A1	1288	1	-	0/11/29/30	0/2/2/2
27	OMU	B1	1981	27	-	0/9/27/28	0/2/2/2
27	OMG	B1	2740	27	-	0/5/27/28	0/3/3/3
27	LHH	B1	527	27	-	2/13/31/32	0/2/2/2
27	4AC	B1	434	27	-	0/11/29/30	0/2/2/2
1	MA6	A1	1476	1	-	2/7/29/30	0/3/3/3
1	OMC	A1	1364	1	-	0/9/27/28	0/2/2/2
1	4AC	A1	141	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	2171	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
27	4AC	B1	48	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	2540	27	-	0/5/27/28	0/3/3/3
27	OMG	B1	2684	27	-	0/5/27/28	0/3/3/3
1	OMG	A1	227	1	-	0/5/27/28	0/3/3/3
1	4AC	A1	816	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	866	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2133	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	1003	1	-	1/5/27/28	0/3/3/3
1	OMU	A1	775	1	-	6/9/27/28	0/2/2/2
1	4AC	A1	41	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	2984	27	-	2/5/27/28	0/3/3/3
27	OMC	B1	2007	27	-	0/9/27/28	0/2/2/2
1	4AC	A1	216	1	-	0/11/29/30	0/2/2/2
27	5MC	B1	2901	27	-	0/7/25/26	0/2/2/2
27	4AC	B1	378	27	-	0/11/29/30	0/2/2/2
27	A2M	B1	940	27	-	1/5/27/28	0/3/3/3
27	4AC	B1	807	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	839	1	-	1/11/29/30	0/2/2/2
27	4AC	B1	2902	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	3023	27	-	0/11/29/30	0/2/2/2
1	4AC	A1	540	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1846	27	-	3/11/29/30	0/2/2/2
27	4AC	B1	1751	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	3020	27	-	0/11/29/30	0/2/2/2
1	OMC	A1	834	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	1967	27	-	1/11/29/30	0/2/2/2
27	4AC	B1	715	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	1313	27	-	1/11/29/30	0/2/2/2
27	4AC	B1	1301	27	-	2/11/29/30	0/2/2/2
27	4AC	B1	23	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	336	27	-	0/7/25/26	0/2/2/2
27	OMC	B1	2046	27	-	0/9/27/28	0/2/2/2
1	MA6	A1	1475	1	-	0/7/29/30	0/3/3/3
27	5MC	B1	1648	27	-	3/7/25/26	0/2/2/2
27	OMU	B1	1488	27	-	0/9/27/28	0/2/2/2
1	5MC	A1	777	1	-	0/7/25/26	0/2/2/2
27	OMC	B1	1489	27	-	2/9/27/28	0/2/2/2
27	4AC	B1	1501	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	1362	1	-	2/7/25/26	0/2/2/2
27	5MC	B1	2617	27	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	1064	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	3037	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	2875	27	-	0/7/25/26	0/2/2/2
1	5MC	A1	473	1	-	1/7/25/26	0/2/2/2
1	4AC	A1	1135	1	-	0/11/29/30	0/2/2/2
27	OMC	B1	501	27	-	1/9/27/28	0/2/2/2
27	5MU	B1	883	27	-	2/7/25/26	0/2/2/2
27	OMG	B1	55	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	599	27	-	0/11/29/30	0/2/2/2
1	OMG	A1	152	1	-	1/5/27/28	0/3/3/3
1	5MC	A1	815	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	1546	27	-	0/11/29/30	0/2/2/2
27	UR3	B1	2700	27	-	2/7/25/26	0/2/2/2
1	4AC	A1	1254	1	-	0/11/29/30	0/2/2/2
27	OMG	B1	2108	27	-	0/5/27/28	0/3/3/3
1	OMG	A1	228	1	-	1/5/27/28	0/3/3/3
1	5MC	A1	863	1	-	0/7/25/26	0/2/2/2
27	4AC	B1	1374	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	419	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	1123	1	-	0/7/25/26	0/2/2/2
27	5MC	B1	2082	27	-	0/7/25/26	0/2/2/2
1	5MC	A1	1012	1	-	0/7/25/26	0/2/2/2
27	5MU	B1	888	27	-	5/7/25/26	0/2/2/2
27	OMG	B1	214	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	580	27	-	0/11/29/30	0/2/2/2
1	5MC	A1	1486	1	-	6/7/25/26	0/2/2/2
1	OMG	A1	459	1	-	0/5/27/28	0/3/3/3
1	4AC	A1	444	1	-	0/11/29/30	0/2/2/2
1	OMU	A1	762	1	-	1/9/27/28	0/2/2/2
1	5MC	A1	523	1	-	0/7/25/26	0/2/2/2
27	5MC	B1	877	27	-	0/7/25/26	0/2/2/2
27	OMG	B1	530	27	-	2/5/27/28	0/3/3/3
27	4AC	B1	2749	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	641	27	-	1/11/29/30	0/2/2/2
27	OMG	B1	2659	27	-	0/5/27/28	0/3/3/3
27	A2M	B1	857	27	-	2/5/27/28	0/3/3/3
27	LHH	B1	1946	27	-	2/13/31/32	0/2/2/2
27	A2M	B1	2506	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	80	27	-	2/11/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	4AC	B1	2809	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	106	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	953	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	2844	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	813	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	3006	27	-	0/11/29/30	0/2/2/2
28	4AC	B2	117	28	-	0/11/29/30	0/2/2/2
27	4AC	B1	2432	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	979	27	-	1/11/29/30	0/2/2/2
1	OMG	A1	861	1	-	1/5/27/28	0/3/3/3
1	LHH	A1	1029	1	-	3/13/31/32	0/2/2/2
27	LHH	B1	502	27	-	3/13/31/32	0/2/2/2
27	4AC	B1	1579	27	-	0/11/29/30	0/2/2/2
27	OMG	B1	808	27	-	0/5/27/28	0/3/3/3
27	4AC	B1	1061	27	-	0/11/29/30	0/2/2/2
27	OMU	B1	454	27	-	3/9/27/28	0/2/2/2
1	4AC	A1	87	1	-	0/11/29/30	0/2/2/2
1	OMG	A1	455	1	-	1/5/27/28	0/3/3/3
1	OMC	A1	1226	1	-	0/9/27/28	0/2/2/2
27	4AC	B1	652	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	2526	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	227	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	1107	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	1344	27	-	0/7/25/26	0/2/2/2
27	OMG	B1	550	27	-	0/5/27/28	0/3/3/3
1	OMU	A1	1368	1	-	0/9/27/28	0/2/2/2
1	4AC	A1	1067	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	2008	27	-	0/11/29/30	0/2/2/2
27	5MC	B1	252	27	-	0/7/25/26	0/2/2/2
27	OMG	B1	2757	27	-	0/5/27/28	0/3/3/3
1	5MC	A1	1013	1	-	0/7/25/26	0/2/2/2
27	5MC	B1	1977	27	-	0/7/25/26	0/2/2/2
1	OMG	A1	645	1	-	1/5/27/28	0/3/3/3
1	4AC	A1	636	1	-	0/11/29/30	0/2/2/2
27	4AC	B1	1293	27	-	0/11/29/30	0/2/2/2
27	4AC	B1	3011	27	-	0/11/29/30	0/2/2/2

The worst 5 of 2607 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B1	940	A2M	O4'-C1'	15.34	1.62	1.41
1	A1	819	A2M	O4'-C1'	15.32	1.62	1.41
27	B1	880	A2M	O4'-C1'	15.32	1.62	1.41
27	B1	506	A2M	O4'-C1'	15.27	1.62	1.41
1	A1	361	A2M	O4'-C1'	15.17	1.62	1.41

The worst 5 of 997 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	1475	MA6	N1-C6-N6	-14.02	102.31	117.06
1	A1	1476	MA6	N1-C6-N6	-13.82	102.51	117.06
1	A1	1457	MA6	C1'-N9-C4	13.77	150.84	126.64
1	A1	1457	MA6	N1-C6-N6	-13.30	103.06	117.06
1	A1	1475	MA6	C1'-N9-C4	13.22	149.88	126.64

There are no chirality outliers.

5 of 163 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A1	132	OMG	O4'-C4'-C5'-O5'
1	A1	152	OMG	C1'-C2'-O2'-CM2
1	A1	153	OMG	C1'-C2'-O2'-CM2
1	A1	238	LHH	C5-C4-N4-C7
1	A1	238	LHH	N3-C4-N4-C7

There are no ring outliers.

149 monomers are involved in 191 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	2562	OMG	1	0
27	B1	2391	OMG	2	0
1	A1	945	4AC	6	0
27	B1	1762	4AC	1	0
1	A1	1190	5MC	1	0
27	B1	360	4AC	1	0
27	B1	950	4AC	1	0
1	A1	466	5MC	1	0
27	B1	2888	4AC	1	0
27	B1	1639	4AC	1	0
27	B1	1904	OMG	2	0
27	B1	932	5MC	1	0
27	B1	1885	4AC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	2554	OMU	1	0
27	B1	485	4AC	2	0
27	B1	1150	4AC	2	0
27	B1	933	4AC	1	0
27	B1	130	4AC	1	0
27	B1	896	4AC	1	0
1	A1	488	OMU	1	0
27	B1	926	OMU	2	0
27	B1	2735	OMC	1	0
27	B1	2047	5MC	1	0
27	B1	887	OMG	2	0
27	B1	675	OMG	2	0
27	B1	2492	4AC	1	0
27	B1	47	OMC	1	0
1	A1	361	A2M	2	0
1	A1	1221	4AC	1	0
1	A1	1467	4AC	1	0
27	B1	827	4AC	1	0
28	B2	90	4AC	1	0
27	B1	337	4AC	2	0
1	A1	427	4AC	1	0
1	A1	739	4AC	1	0
27	B1	1478	4AC	1	0
1	A1	827	4AC	1	0
1	A1	819	A2M	1	0
27	B1	732	4AC	1	0
1	A1	856	4AC	3	0
27	B1	98	4AC	1	0
27	B1	142	4AC	1	0
27	B1	1099	OMC	1	0
1	A1	706	4AC	1	0
1	A1	329	OMG	2	0
1	A1	1371	OMC	2	0
1	A1	541	OMG	1	0
27	B1	116	4AC	2	0
27	B1	2379	4AC	2	0
1	A1	117	OMC	1	0
27	B1	721	4AC	2	0
1	A1	1110	OMU	1	0
27	B1	2850	4AC	1	0
1	A1	901	OMG	1	0
27	B1	1286	4AC	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A1	614	4AC	1	0
1	A1	220	4AC	1	0
1	A1	464	OMG	1	0
1	A1	668	OMG	2	0
1	A1	307	4AC	1	0
27	B1	1818	4AC	1	0
27	B1	1743	4AC	1	0
1	A1	382	4AC	1	0
27	B1	1608	4AC	1	0
27	B1	1706	4AC	1	0
27	B1	1769	4AC	1	0
27	B1	97	5MC	1	0
1	A1	1366	5MC	1	0
1	A1	534	4AC	1	0
1	A1	763	OMG	1	0
27	B1	1435	4AC	1	0
27	B1	2808	OMC	1	0
27	B1	2821	4AC	1	0
27	B1	2428	OMC	1	0
27	B1	19	4AC	1	0
27	B1	1551	4AC	1	0
28	B2	32	4AC	1	0
27	B1	1264	4AC	1	0
27	B1	2028	OMG	1	0
1	A1	1165	OMU	1	0
28	B2	108	4AC	1	0
1	A1	132	OMG	1	0
27	B1	506	A2M	6	0
1	A1	719	4AC	1	0
27	B1	1322	4AC	1	0
1	A1	153	OMG	1	0
27	B1	1914	OMC	1	0
27	B1	2113	4AC	3	0
1	A1	507	OMG	2	0
27	B1	1983	5MC	1	0
1	A1	1288	4AC	2	0
27	B1	1981	OMU	1	0
1	A1	1476	MA6	1	0
1	A1	1364	OMC	2	0
27	B1	2213	4AC	1	0
27	B1	2684	OMG	1	0
1	A1	227	OMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A1	41	4AC	1	0
27	B1	940	A2M	1	0
1	A1	839	4AC	1	0
27	B1	3020	4AC	1	0
1	A1	834	OMC	1	0
27	B1	336	5MC	2	0
1	A1	1475	MA6	2	0
27	B1	1648	5MC	2	0
27	B1	1488	OMU	1	0
27	B1	1489	OMC	1	0
27	B1	1501	4AC	1	0
27	B1	1064	4AC	1	0
27	B1	3037	4AC	1	0
1	A1	473	5MC	2	0
1	A1	1135	4AC	1	0
27	B1	55	OMG	1	0
27	B1	599	4AC	1	0
1	A1	152	OMG	2	0
1	A1	1254	4AC	1	0
1	A1	228	OMG	1	0
27	B1	1374	4AC	2	0
27	B1	419	4AC	1	0
27	B1	580	4AC	1	0
1	A1	459	OMG	1	0
1	A1	444	4AC	2	0
1	A1	762	OMU	2	0
27	B1	877	5MC	1	0
27	B1	530	OMG	1	0
27	B1	2749	4AC	2	0
27	B1	641	4AC	1	0
27	B1	106	4AC	3	0
27	B1	953	4AC	1	0
1	A1	405	4AC	1	0
27	B1	2844	4AC	1	0
27	B1	813	4AC	2	0
27	B1	3006	4AC	1	0
27	B1	2432	4AC	1	0
27	B1	979	4AC	2	0
1	A1	861	OMG	3	0
27	B1	1579	4AC	1	0
27	B1	808	OMG	2	0
27	B1	1061	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B1	454	OMU	1	0
1	A1	87	4AC	2	0
1	A1	1226	OMC	1	0
27	B1	1107	4AC	1	0
27	B1	550	OMG	2	0
1	A1	1368	OMU	1	0
1	A1	1013	5MC	1	0
27	B1	1977	5MC	2	0
1	A1	636	4AC	1	0
27	B1	3011	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 [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

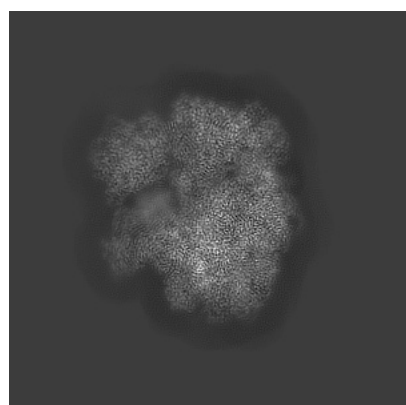
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53098. These allow visual inspection of the internal detail of the map and identification of artifacts.

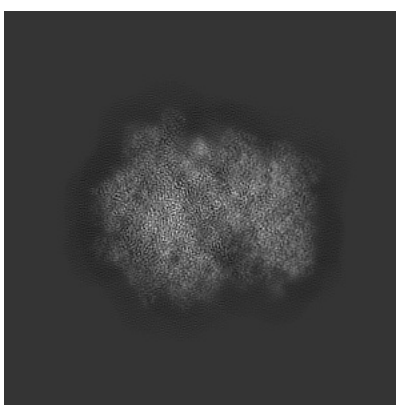
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

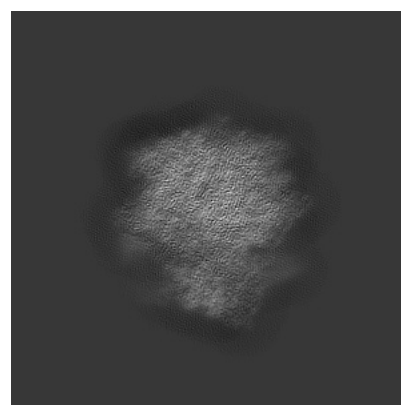
#### 6.1.1 Primary map



X



Y

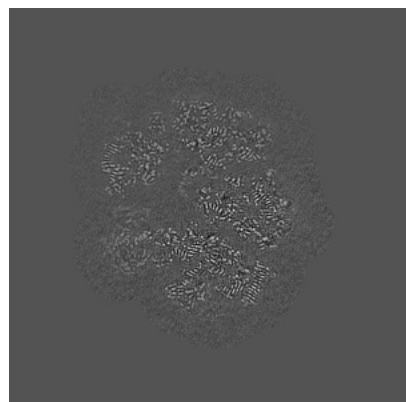


Z

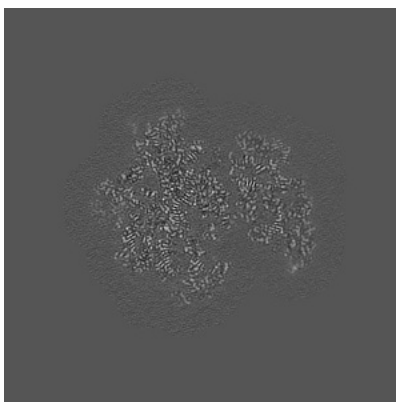
The images above show the map projected in three orthogonal directions.

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

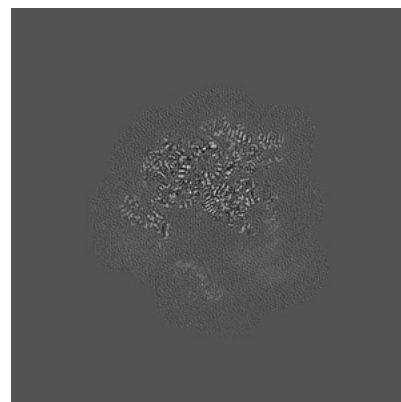
#### 6.2.1 Primary map



X Index: 224



Y Index: 224

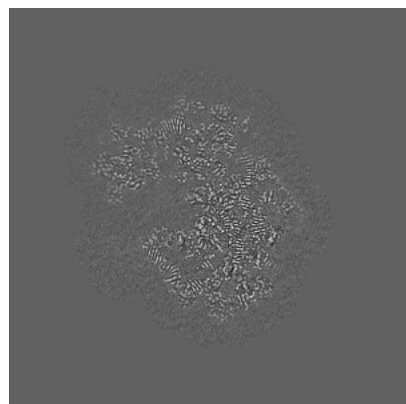


Z Index: 224

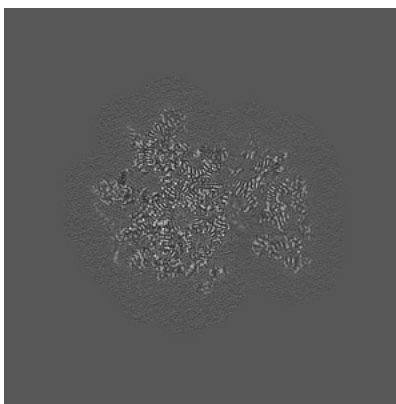
The images above show central slices of the map in three orthogonal directions.

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

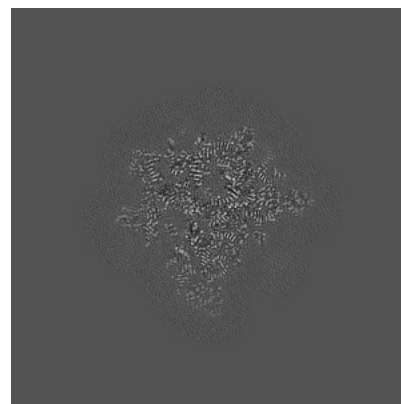
### 6.3.1 Primary map



X Index: 242



Y Index: 233

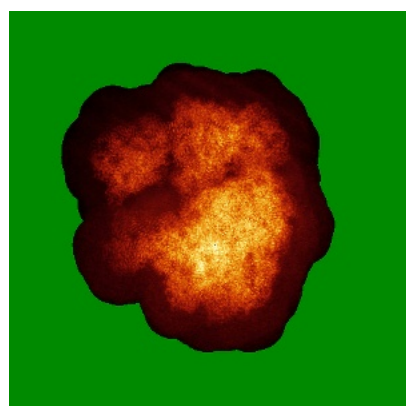


Z Index: 188

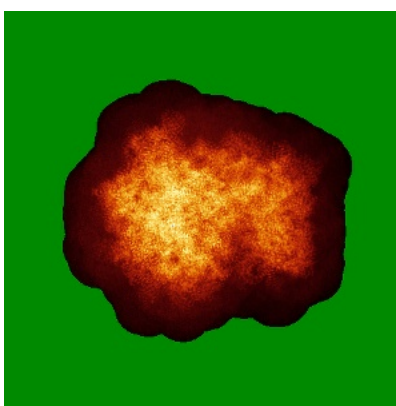
The images above show the largest variance slices of the map in three orthogonal directions.

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

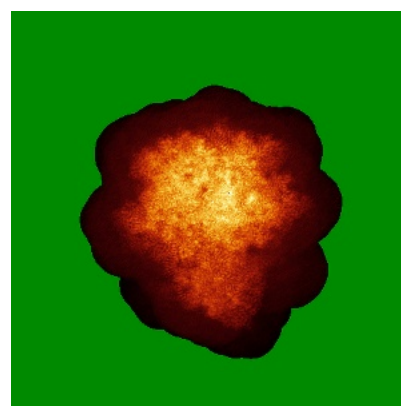
### 6.4.1 Primary map



X



Y

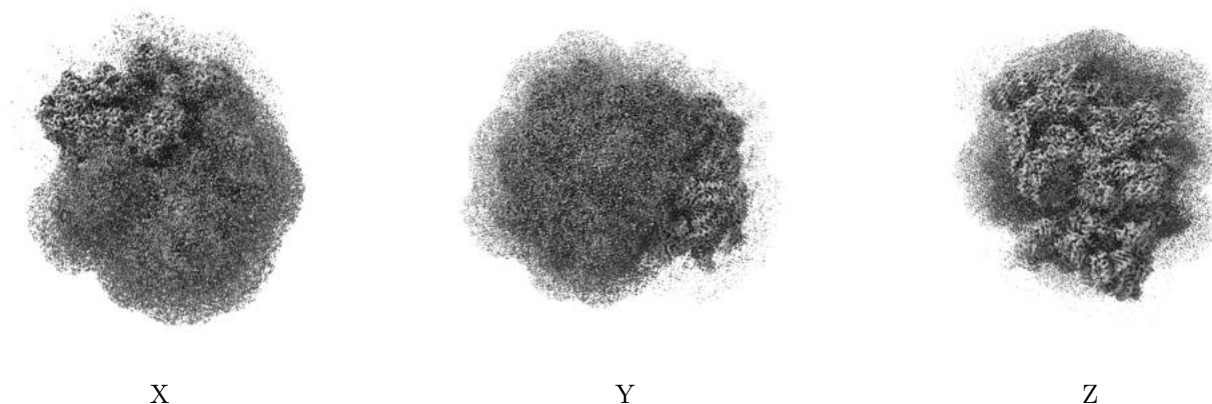


Z

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 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

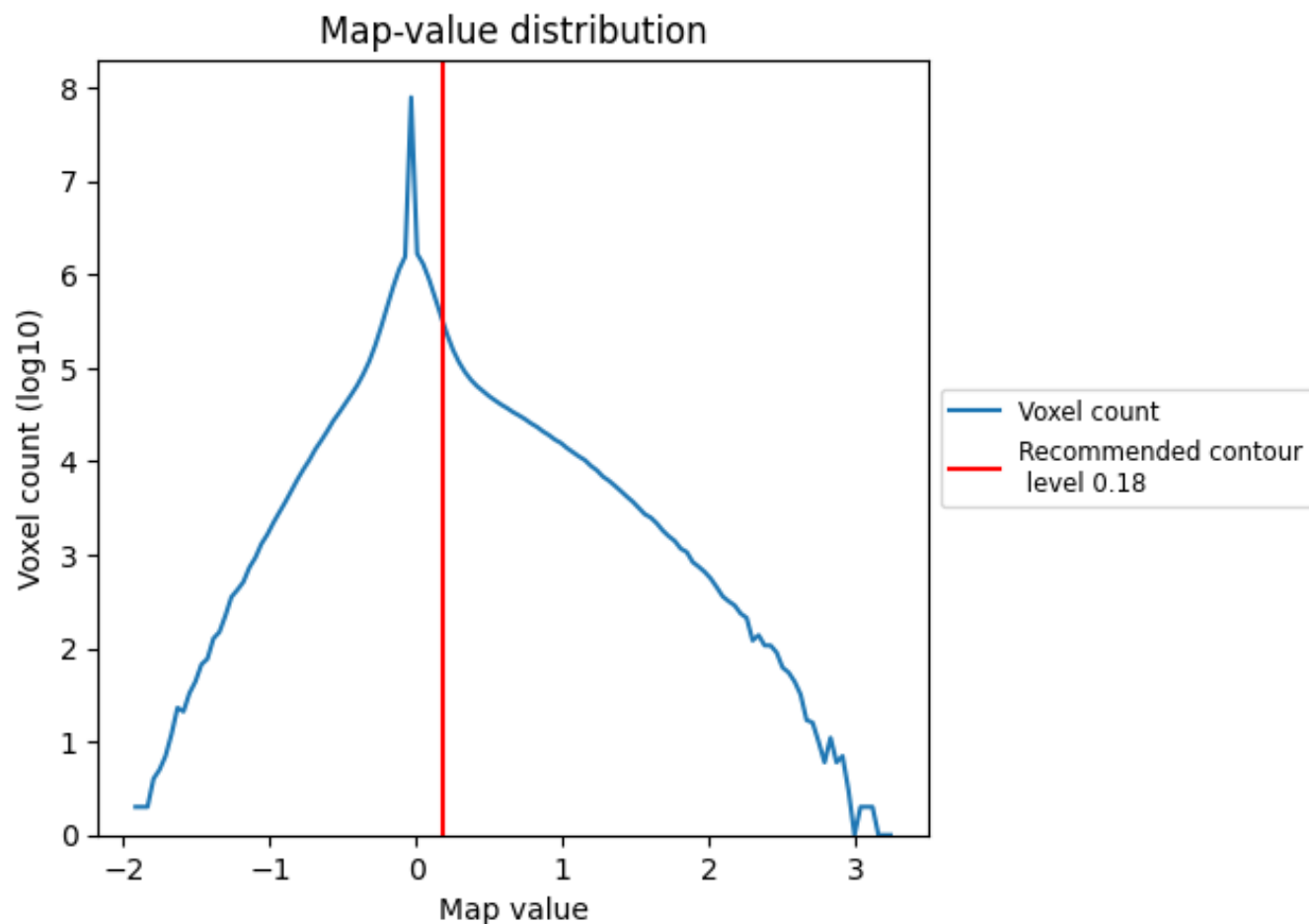
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

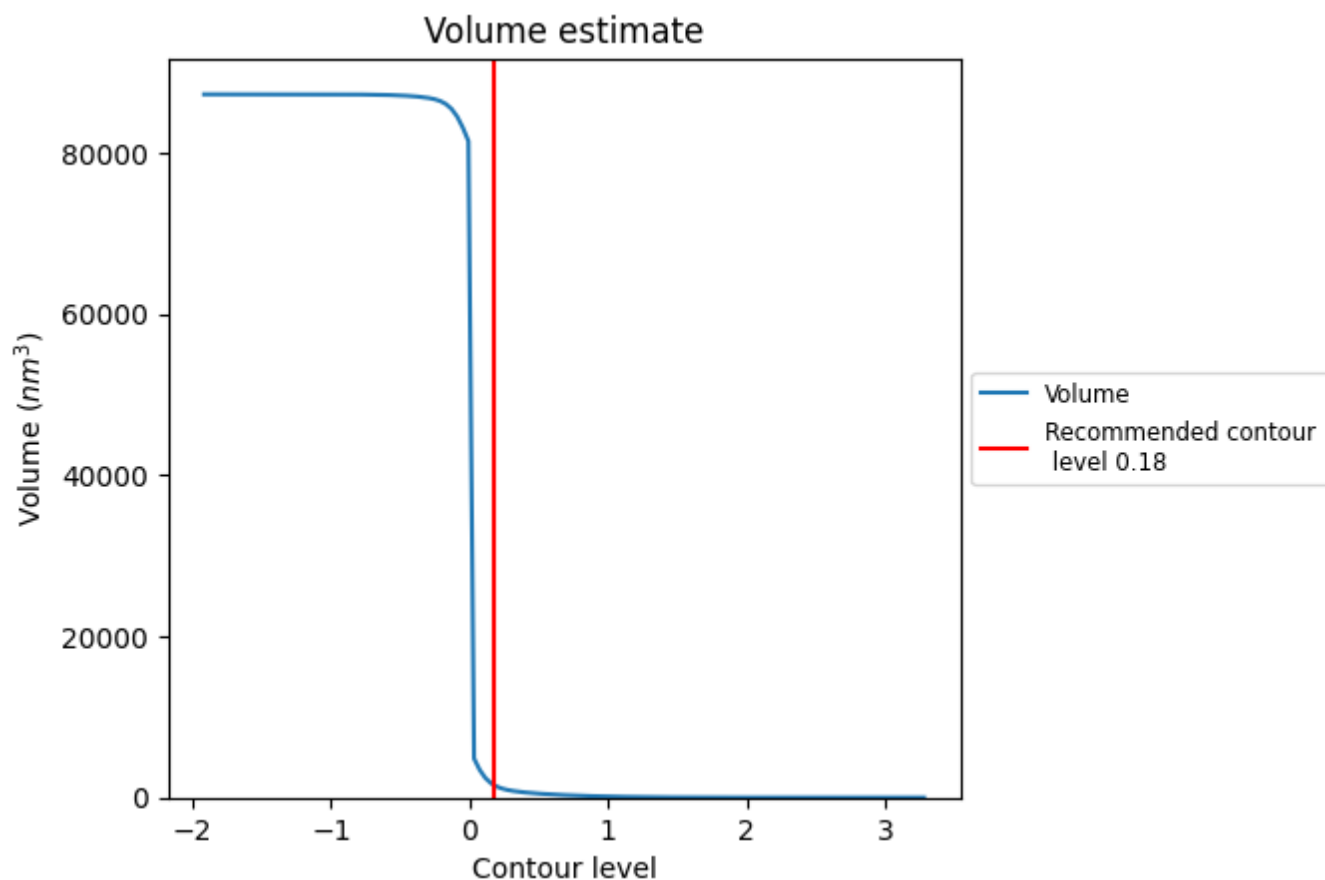
This section contains the results of statistical analysis of the map.

### 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](#)

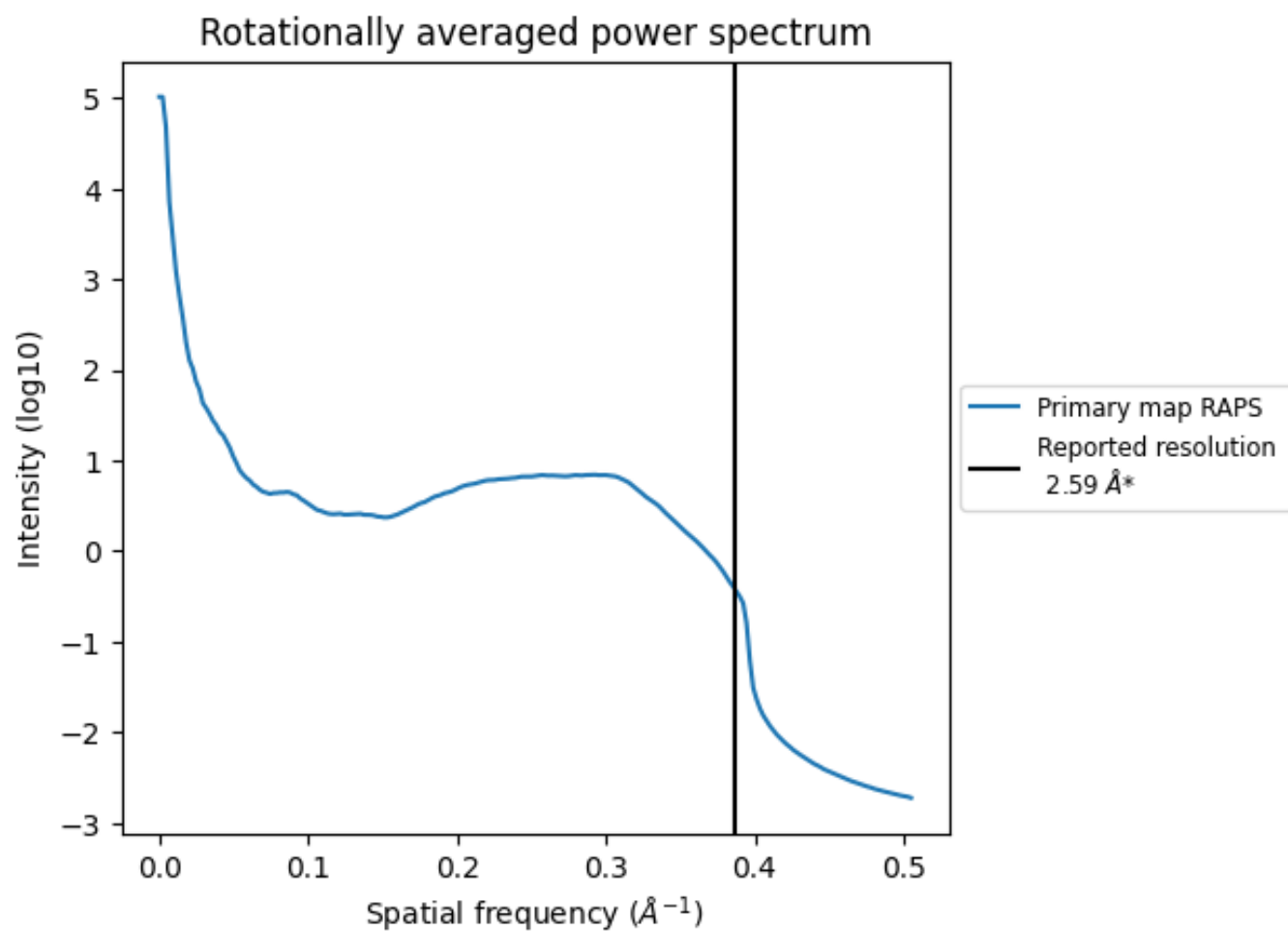


The volume at the recommended contour level is 1531  $\text{nm}^3$ ; this corresponds to an approximate mass of 1383 kDa.

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 0.386 Å<sup>-1</sup>

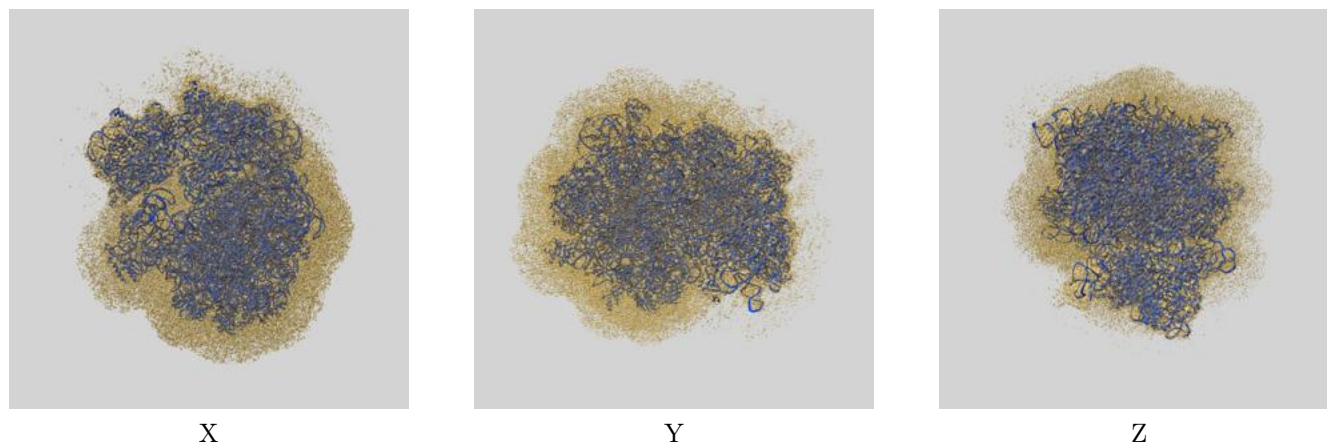
## 8 Fourier-Shell correlation

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

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

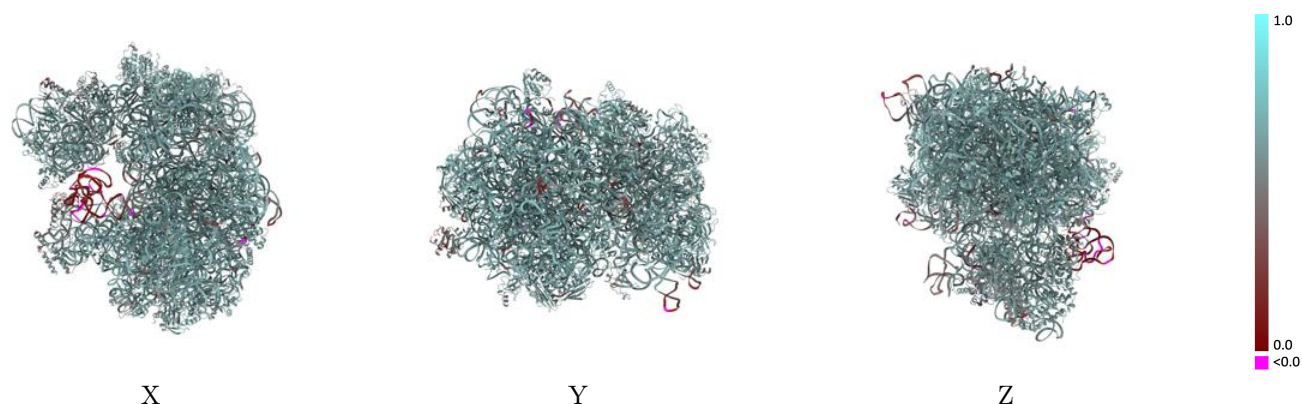
This section contains information regarding the fit between EMDB map EMD-53098 and PDB model 9QF4. Per-residue inclusion information can be found in section [3](#) on page [19](#).

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



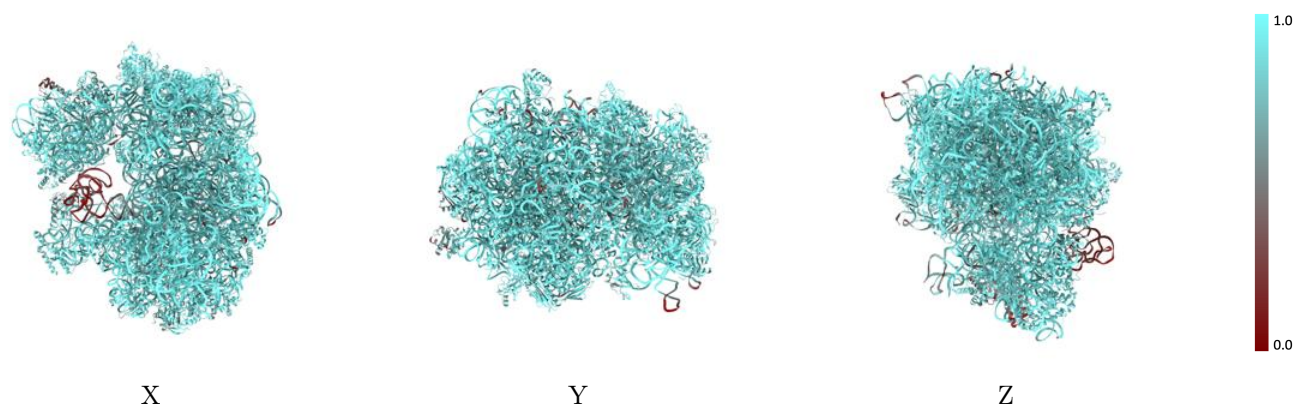
The images above show the 3D surface view of the map at the recommended contour level 0.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



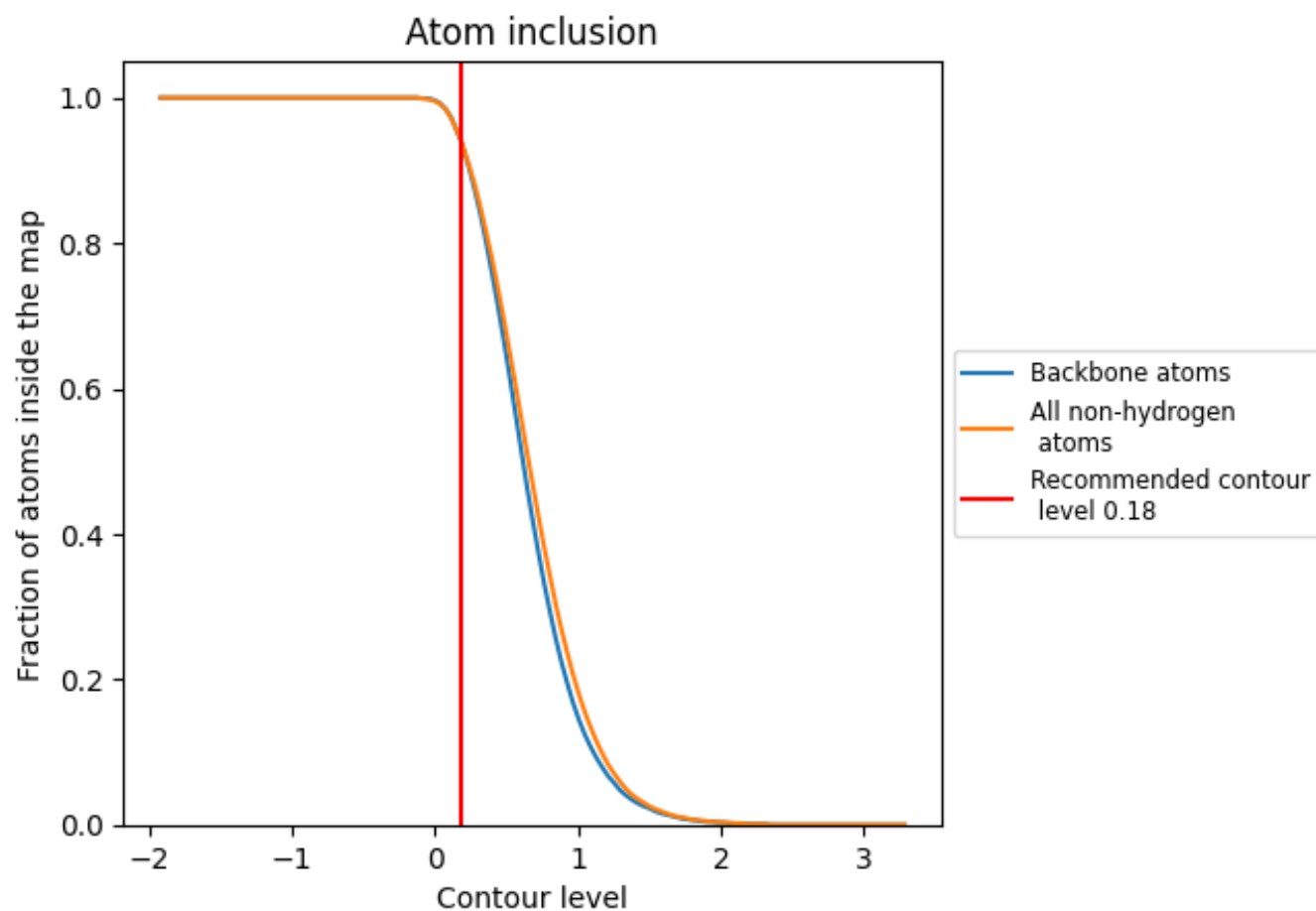
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9430	 0.6110
A1	 0.9560	 0.6030
Aa	 0.9180	 0.6000
Ab	 0.7910	 0.5500
Ac	 0.9140	 0.6010
Ad	 0.9420	 0.6200
Ae	 0.9560	 0.6300
Af	 0.9410	 0.6240
Ag	 0.8370	 0.5520
Ah	 0.8950	 0.5950
Ai	 0.9740	 0.6430
Aj	 0.9540	 0.6310
Ak	 0.9430	 0.6200
Al	 0.6910	 0.5180
Am	 0.9280	 0.6030
An	 0.9410	 0.6250
Ao	 0.9130	 0.5950
Ap	 0.8860	 0.5690
Aq	 0.9500	 0.6280
Ar	 0.9710	 0.6430
As	 0.8500	 0.5520
At	 0.9010	 0.5920
Au	 0.9480	 0.6170
Av	 0.9220	 0.6050
Aw	 0.9260	 0.6040
Ax	 0.8250	 0.5600
Ay	 0.9440	 0.6180
B1	 0.9470	 0.6100
B2	 0.9570	 0.5840
BA	 0.9850	 0.6660
BB	 0.9650	 0.6500
BC	 0.9790	 0.6540
BD	 0.7970	 0.4940
BE	 0.9450	 0.6180
BF	 0.9370	 0.6170



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Chain	Atom inclusion	Q-score
BG	 0.7330	 0.4760
BH	 0.9760	 0.6450
BI	 0.9770	 0.6530
BJ	 0.9780	 0.6540
BK	 0.9160	 0.5800
BL	 0.9460	 0.6210
BM	 0.9120	 0.5910
BN	 0.9960	 0.6780
BO	 0.9030	 0.5760
BP	 0.9830	 0.6490
BQ	 0.9750	 0.6410
BR	 0.9780	 0.6600
BS	 0.9900	 0.6610
BT	 0.9600	 0.6420
BU	 0.9680	 0.6370
BV	 0.9840	 0.6520
BW	 0.9030	 0.6000
BX	 0.9740	 0.6480
BY	 0.9310	 0.6070
BZ	 0.9550	 0.6280
Ba	 0.9790	 0.6560
Bb	 0.9840	 0.6590
Bc	 0.9710	 0.6470
Bd	 0.9920	 0.6690
Be	 0.9760	 0.6580
Bf	 0.9860	 0.6630
Bg	 0.9810	 0.6370
Bh	 0.9570	 0.6380
Bi	 0.9700	 0.6540
Bj	 0.9250	 0.5950
Bk	 0.9670	 0.6410
Bl	 0.7120	 0.5210