



## wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:27 AM UTC

PDB ID : 8A98 / pdb\_00008a98  
EMDB ID : EMD-15272  
Title : CRYO-EM STRUCTURE OF LEISHMANIA MAJOR 80S RIBOSOME :  
snoRNA MUTANT  
Authors : Rajan, K.S.; Yonath, A.; Bashan, A.  
Deposited on : 2022-06-28  
Resolution : 2.46 Å (reported)  
Based on initial models : 6AZ1, 5T2A, 6AZ3

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:

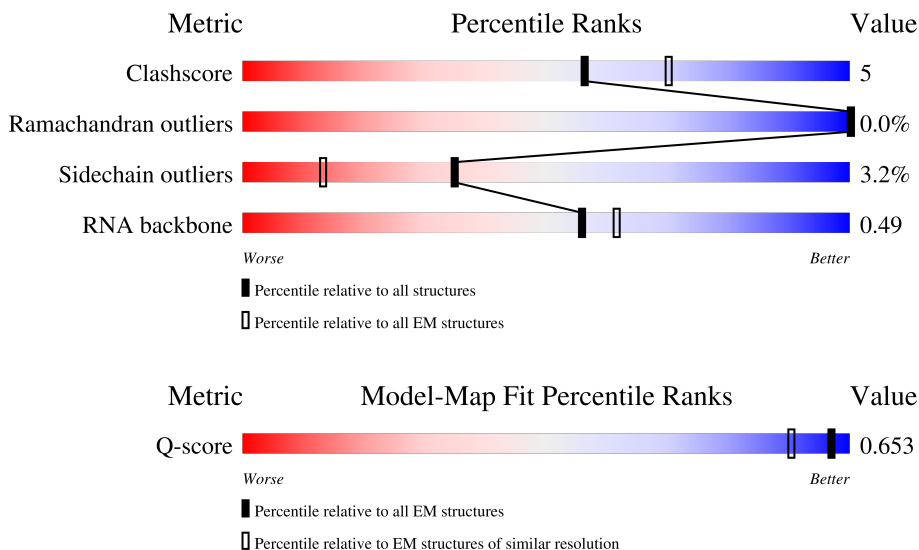
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.46 Å.

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
















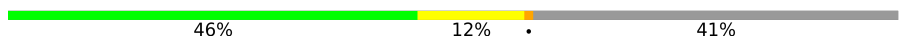






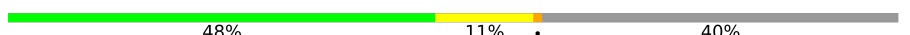




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6014 ( 1.96 - 2.96 )

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	SW	152	
2	SZ	137	
3	SY	164	









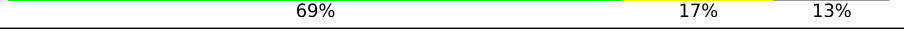

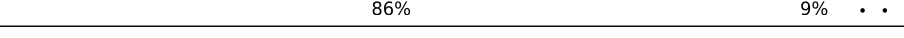
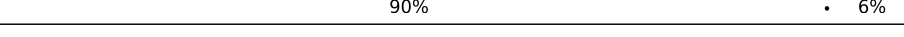

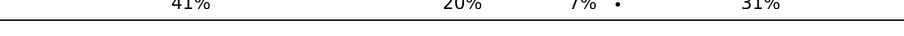


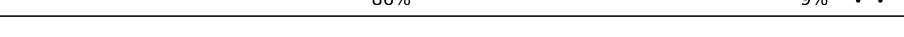

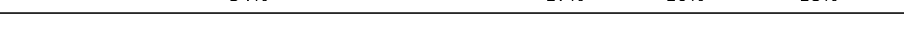






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Mol	Chain	Length	Quality of chain
4	SX	161	 80% 7% 14%
5	SV	143	 66% 13% 21%
6	SU	173	 77% 9% 14%
7	ST	151	 89% 7%
8	SS	57	 81% 14%
9	SR	153	 72% 5% 22%
10	SB	246	 66% 18% 15%
11	SC	219	 82% 15%
12	SD	190	 84% 12%
13	SE	273	 85% 10% 5%
14	SK	220	 74% 8% 18%
15	S4	19	 58% 32% 11%
16	Sg	312	 79% 17%
17	Sa	120	 46% 12% 41%
18	Sc	86	 80% 17%
19	Se	66	 68% 11% 21%
20	S1	2204	 49% 22% 7% 22%
21	SQ	141	 18% 80%
22	SP	143	 90% 10%
23	SO	144	 84% 9% 6%
24	SN	168	 48% 11% 40%
25	Sd	87	 64% 8% 25%
26	SM	116	 78% 9% 12%
27	SL	149	 91% 5%
28	SJ	130	 94% 5%

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Mol	Chain	Length	Quality of chain
29	SI	200	 90% 10%
30	SH	190	 85% 12%
31	SG	249	 83% 11% 6%
32	SF	265	 73% 10% 17%
33	SA	264	 74% 11% 15%
34	Sb	112	 83% 6% 11%
35	Sh	235	 32% 7% 60%
36	f	133	 90% 8%
37	d	104	 69% 17% 13%
38	c	252	 81% 8% 10%
39	a	127	 86% 9%
40	b	70	 90% 6%
41	1	1782	 58% 23% 7% 11%
42	2	1526	 41% 20% 7% 31%
43	4	183	 66% 30%
44	7	171	 67% 21% 6%
45	B	419	 86% 9%
46	8	123	 66% 26%
47	5	135	 54% 17% 10% 18%
48	A	260	 89% 8%
49	O	305	 70% 12% 17%
50	G	264	 81% 6% 12%
51	H	222	 95% 5%
52	M	204	 94% 6%
53	I	220	 82% 10% 7%



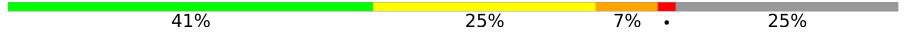


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Mol	Chain	Length	Quality of chain
54	P	198	88% 11% ..
55	Q	254	69% 6% 26%
56	R	179	85% 13% ..
57	E	190	71% 25% . .
58	6	73	47% 38% 12% .
59	T	166	85% 7% 8%
60	S	159	86% 9% .
61	K	175	75% 11% . 13%
62	D	188	66% 17% . 15%
63	L	145	94% 6% .
64	Y	134	84% 15% .
65	Z	147	81% 13% . 5%
66	F	195	66% 7% 27%
67	h	168	64% 10% . 25%
68	g	144	83% 11% . .
69	J	139	88% 5% 7%
70	V	145	75% 6% 19%
71	W	143	69% 13% 17%
72	U	129	64% 22% 13%
73	i	105	76% 14% 10%
74	p	106	82% 8% . 9%
75	o	92	80% 15% . .
76	X	124	44% 8% 48%
77	k	83	75% 11% . 12%
78	l	51	90% 8% .

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Mol	Chain	Length	Quality of chain
79	n	34	 74% 21% . .
80	C	373	 90% 8% . .
81	3	216	 41% 25% 7% . 25%
82	e	188	 77% 14% . . 8%
83	j	83	 87% 10% .

## 2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 197779 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Putative 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	SW	105	787	506	152	125	4	0	0

- Molecule 2 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SZ	122	967	620	184	160	3	1	0

- Molecule 3 is a protein called Putative 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SY	83	604	371	110	119	4	0	0

- Molecule 4 is a protein called 40S ribosomal protein S19-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SX	139	1071	682	204	181	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SX	37	SER	THR	conflict	UNP E9AEE8

- Molecule 5 is a protein called Putative 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SV	113	843	535	159	145	4	0	0

- Molecule 6 is a protein called Putative 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SU	148	1170	739	235	191	5	0	0

- Molecule 7 is a protein called Putative 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	ST	141	1145	723	228	186	8	0	0

- Molecule 8 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SS	55	428	265	87	72	4	0	0

- Molecule 9 is a protein called Putative 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SR	119	892	567	167	154	4	0	0

- Molecule 10 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SB	209	1643	1046	297	288	12	2	0

- Molecule 11 is a protein called Putative 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SC	212	1619	1028	296	282	13	2	0

- Molecule 12 is a protein called Putative 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SD	182	1513	951	308	246	8	1	0

- Molecule 13 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SE	260	2056	1304	396	347	9	2	0

- Molecule 14 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	SK	180	1424	895	300	227	2	0	0

- Molecule 15 is a RNA chain called E-site\_tRNA\_chain\_S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
15	S4	19	404	181	76	129	18	0	0

- Molecule 16 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Sg	300	2251	1415	399	424	13	0	0

- Molecule 17 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Sa	71	541	345	93	100	3	0	0

- Molecule 18 is a protein called Putative 40S ribosomal protein S27-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	Sc	84	638	396	123	111	8	0	0

- Molecule 19 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Se	52	404	253	87	63	1	0	0

- Molecule 20 is a RNA chain called SSU\_rRNA\_chain\_S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
20	S1	1727	36928	16523	6655	12024	1726	0	0

- Molecule 21 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	SQ	28	179	111	33	33	2	0	0

- Molecule 22 is a protein called Putative 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	SP	142	1115	704	222	186	3	3	0

- Molecule 23 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	SO	136	1012	625	197	182	8	1	0

- Molecule 24 is a protein called Putative 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	SN	101	813	521	143	142	7	0	0

- Molecule 25 is a protein called Putative 40S ribosomal protein S33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Sd	65	466	286	94	82	4	0	0

- Molecule 26 is a protein called Putative ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	SM	102	811	506	149	154	2	1	0

- Molecule 27 is a protein called Putative 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	SL	143	1130	727	209	191	3	0	0

- Molecule 28 is a protein called Putative 40S ribosomal protein S15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	SJ	129	1014	643	188	175	8	0	0

- Molecule 29 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	SI	200	1613	1026	307	272	8	0	0

- Molecule 30 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	SH	184	1437	894	277	259	7	0	0

- Molecule 31 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	SG	233	1809	1131	370	305	3	1	0

- Molecule 32 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	SF	220	1656	1063	299	284	10	0	0

- Molecule 33 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	SA	225	1834	1148	353	322	11	2	0

- Molecule 34 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sb	100	Total	C	N	O	S	0	0
			779	484	162	126	7		

- Molecule 35 is a protein called Putative RNA binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sh	94	Total	C	N	O	S	0	0
			657	406	125	124	2		

- Molecule 36 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	122	Total	C	N	O	S	0	0
			988	621	196	167	4		

- Molecule 37 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	90	Total	C	N	O	S	0	0
			625	388	114	118	5		

- Molecule 38 is a protein called Putative 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	c	227	Total	C	N	O	S	0	0
			1779	1134	340	294	11		

- Molecule 39 is a protein called Putative 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	a	123	Total	C	N	O	S	0	0
			955	597	199	157	2		

- Molecule 40 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	b	66	Total	C	N	O	0	0
			520	318	120	82		

- Molecule 41 is a RNA chain called LSUa\_rRNA\_chain\_1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
41	1	1579	33802	15099	6193	10932	1578	0	0

- Molecule 42 is a RNA chain called LSub\_rRNA\_chain\_2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
42	2	1047	22358	10009	4022	7280	1047	0	0

- Molecule 43 is a RNA chain called SR2\_chain\_4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
43	4	183	3906	1742	706	1275	183	0	0

- Molecule 44 is a RNA chain called 5.8S\_rRNA\_chain\_7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
44	7	160	3399	1520	599	1121	159	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	87	U	A	conflict	GB 1207899567

- Molecule 45 is a protein called Putative ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	B	402	3200	2019	636	532	13	7	0

- Molecule 46 is a RNA chain called 5S\_rRNA\_chain\_8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
46	8	118	2511	1123	448	822	118	0	0

- Molecule 47 is a RNA chain called SR4\_chain\_5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
47	5	111	2373	1058	431	773	111	0	0

- Molecule 48 is a protein called Putative 60S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	A	255	1973	1229	407	326	11	5	0

- Molecule 49 is a protein called Putative 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	O	252	1970	1259	373	333	5	3	0

- Molecule 50 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	G	233	1850	1160	370	313	7	2	0

- Molecule 51 is a protein called Putative 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	H	221	1771	1121	352	291	7	1	0

- Molecule 52 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	M	203	1714	1080	362	264	8	0	0

- Molecule 53 is a protein called eL13\_chain\_I.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	I	205	1593	993	318	274	8	0	0

- Molecule 54 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	P	197	1539	968	307	258	6	0	0

- Molecule 55 is a protein called Putative 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Q	189	1482	916	319	241	6	0	0

- Molecule 56 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	R	178	1447	921	277	244	5	0	0

- Molecule 57 is a protein called Putative 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	E	186	1439	911	267	255	6	0	0

- Molecule 58 is a RNA chain called SR6\_chain\_6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
58	6	71	1484	663	267	483	71	0	0

- Molecule 59 is a protein called Putative 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	T	153	1233	770	244	208	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	S	152	1203	764	236	200	3	0	0

- Molecule 61 is a protein called Putative 40S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	K	153	1193	746	234	206	7	0	0

- Molecule 62 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	D	159	1140	723	212	197	8	0	0

- Molecule 63 is a protein called Putative 60S ribosomal protein L27A/L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	L	144	1124	707	226	185	6	0	0

- Molecule 64 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	Y	132	1046	667	211	165	3	1	0

- Molecule 65 is a protein called Putative 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	Z	139	1052	642	221	184	5	0	0

- Molecule 66 is a protein called Putative 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	F	142	1045	665	194	184	2	0	0

- Molecule 67 is a protein called Putative 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	h	126	1016	626	222	162	6	1	0

- Molecule 68 is a protein called Putative ribosomal protein l35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	g	138	1101	684	233	179	5	0	0

- Molecule 69 is a protein called Putative 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	J	129	968	614	183	165	6	0	0

- Molecule 70 is a protein called Putative 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	V	118	939	595	176	165	3	0	0

- Molecule 71 is a protein called Putative 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	W	118	948	591	197	156	4	0	0

- Molecule 72 is a protein called Putative 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	U	112	879	572	154	151	2	0	0

- Molecule 73 is a protein called Putative 60S Ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	i	95	738	467	148	121	2	0	0

- Molecule 74 is a protein called Putative 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	p	96	722	460	144	116	2	0	0

- Molecule 75 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o	90	Total	C	N	O	S	0	0
			696	432	144	114	6		

- Molecule 76 is a protein called Putative ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	X	65	Total	C	N	O	S	0	0
			553	362	106	81	4		

- Molecule 77 is a protein called Putative ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	k	73	Total	C	N	O	S	0	0
			546	342	104	97	3		

- Molecule 78 is a protein called Putative 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	l	50	Total	C	N	O	S	0	0
			440	285	91	63	1		

- Molecule 79 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	n	33	Total	C	N	O	S	0	0
			259	161	60	37	1		

- Molecule 80 is a protein called Putative ribosomal protein L1a.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	C	366	Total	C	N	O	S	0	0
			2797	1745	554	483	15		

- Molecule 81 is a RNA chain called SR1\_chain\_3.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	3	161	Total	C	N	O	P	0	0
			3419	1529	596	1133	161		

- Molecule 82 is a protein called Putative 60S ribosomal subunit protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	e	173	Total	C	N	O	S	0	0
			1298	821	254	220	3		

- Molecule 83 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	j	80	Total	C	N	O	S	0	0
			662	403	151	102	6		

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
84	SS	1	Total	Mg	0
			1	1	
84	S1	23	Total	Mg	0
			23	23	
84	SL	1	Total	Mg	0
			1	1	
84	1	61	Total	Mg	0
			61	61	
84	2	31	Total	Mg	0
			31	31	
84	4	3	Total	Mg	0
			3	3	
84	7	4	Total	Mg	0
			4	4	
84	8	1	Total	Mg	0
			1	1	
84	5	1	Total	Mg	0
			1	1	
84	6	1	Total	Mg	0
			1	1	
84	T	1	Total	Mg	0
			1	1	
84	J	1	Total	Mg	0
			1	1	
84	3	1	Total	Mg	0
			1	1	

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
85	Sc	1	Total Zn 1 1	0
85	Sb	1	Total Zn 1 1	0
85	o	1	Total Zn 1 1	0
85	j	1	Total Zn 1 1	0

- Molecule 86 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
86	1	5	Total Na 5 5	0
86	2	3	Total Na 3 3	0

- Molecule 87 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
87	1	2	Total K 2 2	0

- Molecule 88 is water.

Mol	Chain	Residues	Atoms	AltConf
88	SZ	1	Total O 1 1	0
88	SY	1	Total O 1 1	0
88	SX	7	Total O 7 7	0
88	ST	5	Total O 5 5	0
88	SS	1	Total O 1 1	0
88	SR	2	Total O 2 2	0
88	SB	3	Total O 3 3	0
88	SC	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
88	SD	1	Total 1	O 1	0
88	SE	1	Total 1	O 1	0
88	SK	1	Total 1	O 1	0
88	S4	1	Total 1	O 1	0
88	Sg	3	Total 3	O 3	0
88	Sa	1	Total 1	O 1	0
88	Sc	2	Total 2	O 2	0
88	S1	237	Total 237	O 237	0
88	SP	3	Total 3	O 3	0
88	SO	2	Total 2	O 2	0
88	SN	3	Total 3	O 3	0
88	Sd	1	Total 1	O 1	0
88	SH	4	Total 4	O 4	0
88	SF	2	Total 2	O 2	0
88	Sb	2	Total 2	O 2	0
88	f	16	Total 16	O 16	0
88	d	3	Total 3	O 3	0
88	c	4	Total 4	O 4	0
88	a	3	Total 3	O 3	0
88	1	918	Total 918	O 918	0
88	2	536	Total 536	O 536	0

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Mol	Chain	Residues	Atoms		AltConf
88	4	73	Total 73	O 73	0
88	7	85	Total 85	O 85	0
88	B	29	Total 29	O 29	0
88	8	17	Total 17	O 17	0
88	5	37	Total 37	O 37	0
88	A	30	Total 30	O 30	0
88	G	4	Total 4	O 4	0
88	H	9	Total 9	O 9	0
88	M	28	Total 28	O 28	0
88	I	21	Total 21	O 21	0
88	P	12	Total 12	O 12	0
88	Q	6	Total 6	O 6	0
88	R	1	Total 1	O 1	0
88	E	1	Total 1	O 1	0
88	6	3	Total 3	O 3	0
88	T	14	Total 14	O 14	0
88	S	4	Total 4	O 4	0
88	K	1	Total 1	O 1	0
88	L	17	Total 17	O 17	0
88	h	12	Total 12	O 12	0
88	g	9	Total 9	O 9	0

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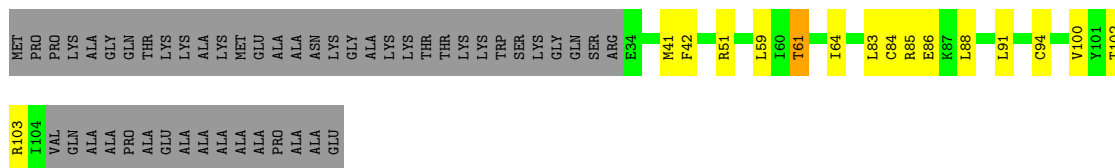
Mol	Chain	Residues	Atoms		AltConf
88	J	1	Total 1	O 1	0
88	V	6	Total 6	O 6	0
88	W	2	Total 2	O 2	0
88	i	1	Total 1	O 1	0
88	p	13	Total 13	O 13	0
88	o	2	Total 2	O 2	0
88	X	2	Total 2	O 2	0
88	k	2	Total 2	O 2	0
88	l	6	Total 6	O 6	0
88	C	21	Total 21	O 21	0
88	3	31	Total 31	O 31	0
88	e	9	Total 9	O 9	0
88	j	13	Total 13	O 13	0



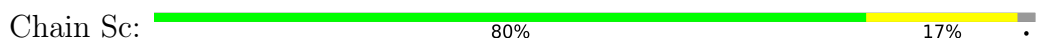




• Molecule 17: 40S ribosomal protein S25



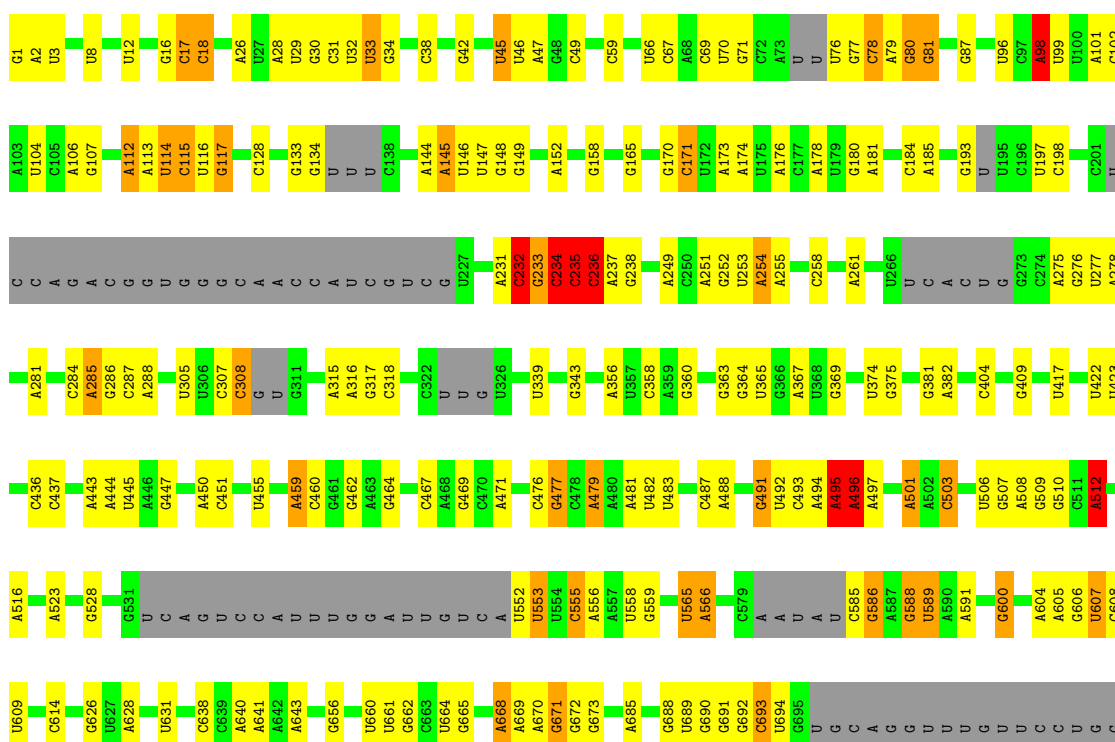
• Molecule 18: Putative 40S ribosomal protein S27-1



• Molecule 19: 40S ribosomal protein S30



• Molecule 20: SSU\_rRNA\_chain\_S1

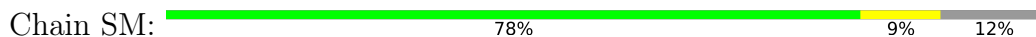




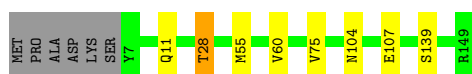




- Molecule 26: Putative ribosomal protein S20



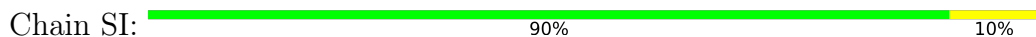
- Molecule 27: Putative 40S ribosomal protein S16



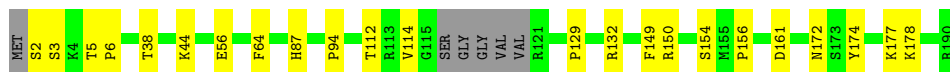
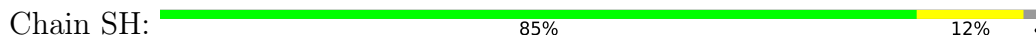
- Molecule 28: Putative 40S ribosomal protein S15A



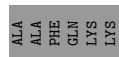
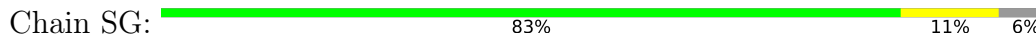
- Molecule 29: 40S ribosomal protein S7



- Molecule 30: 40S ribosomal protein S5



- Molecule 31: 40S ribosomal protein S6

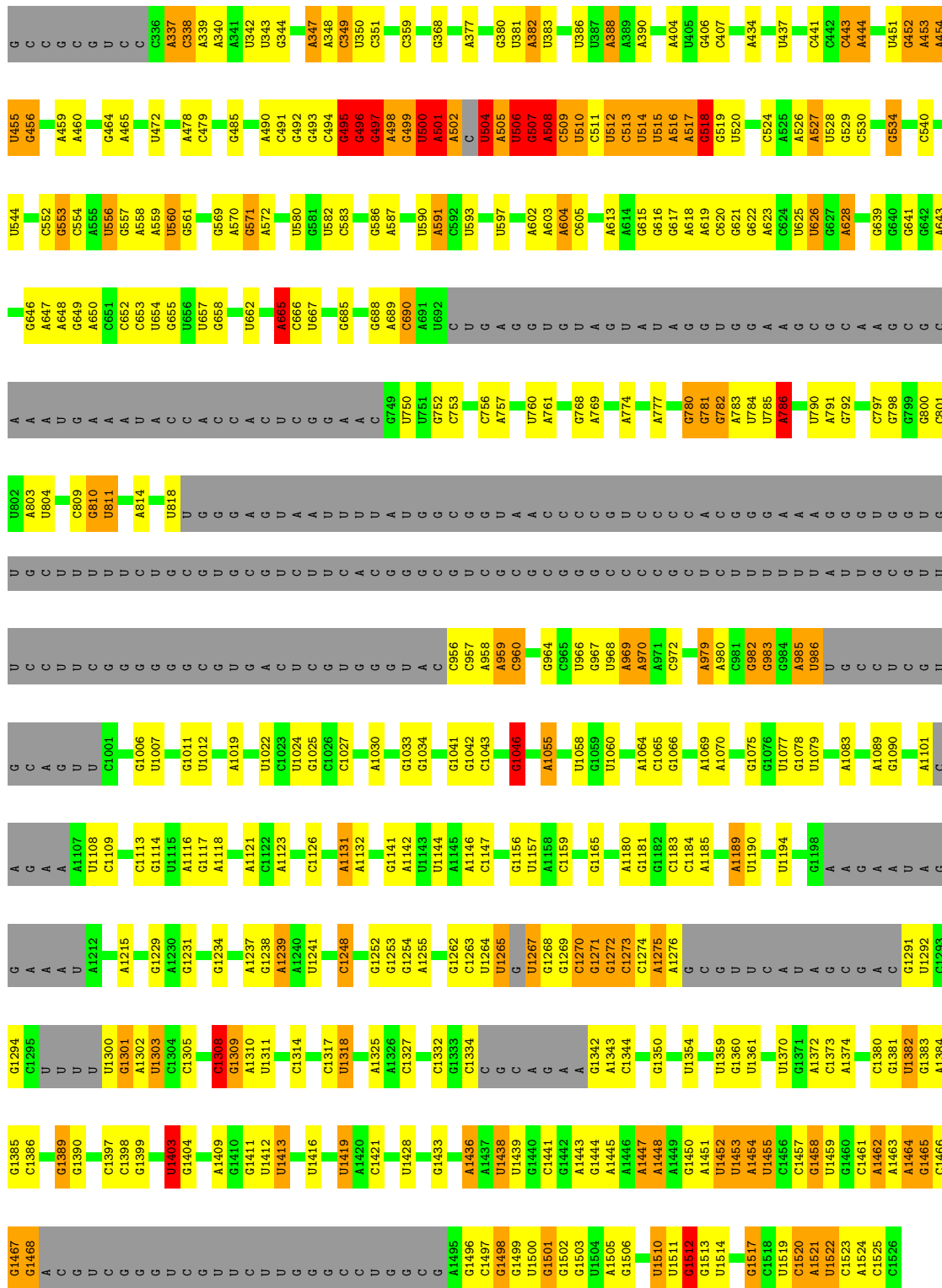


- Molecule 32: 40S ribosomal protein S2



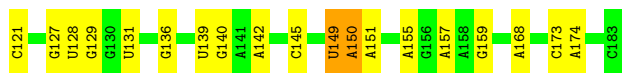




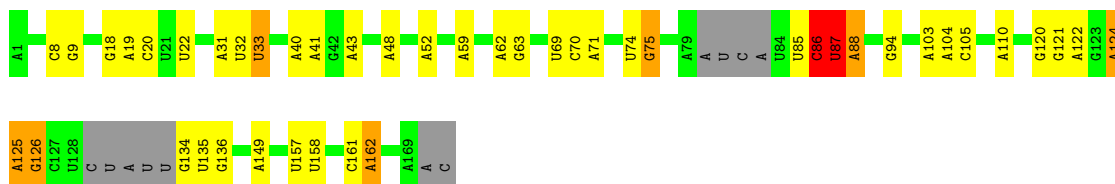


• Molecule 43: SR2\_chain\_4

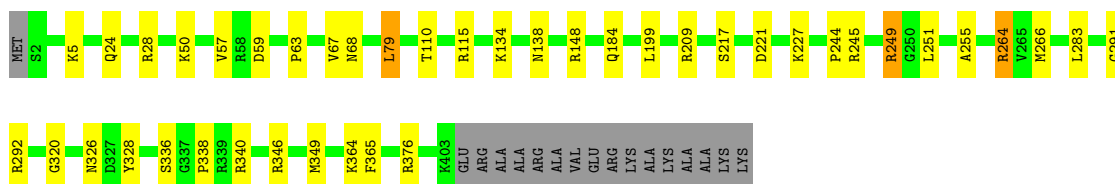
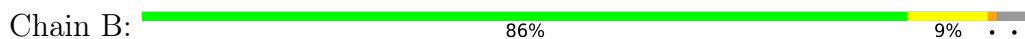




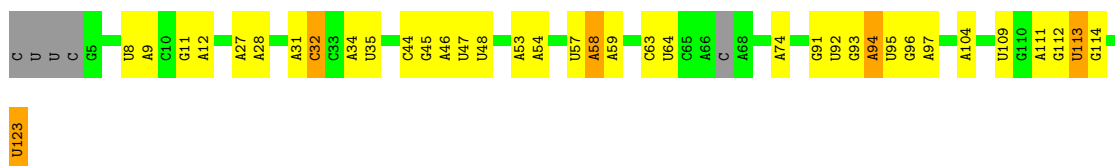
• Molecule 44: 5.8S\_rRNA\_chain\_7



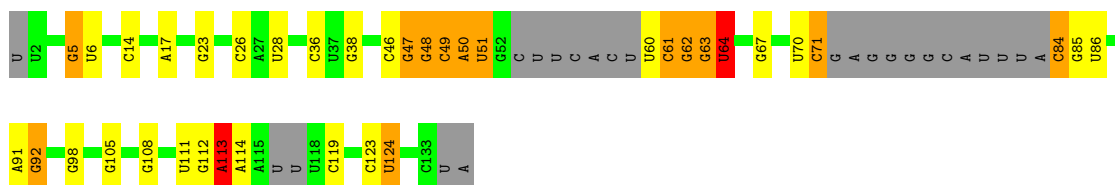
• Molecule 45: Putative ribosomal protein L3



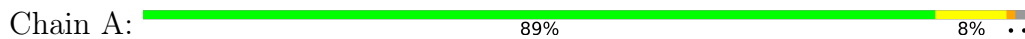
• Molecule 46: 5S\_rRNA\_chain\_8



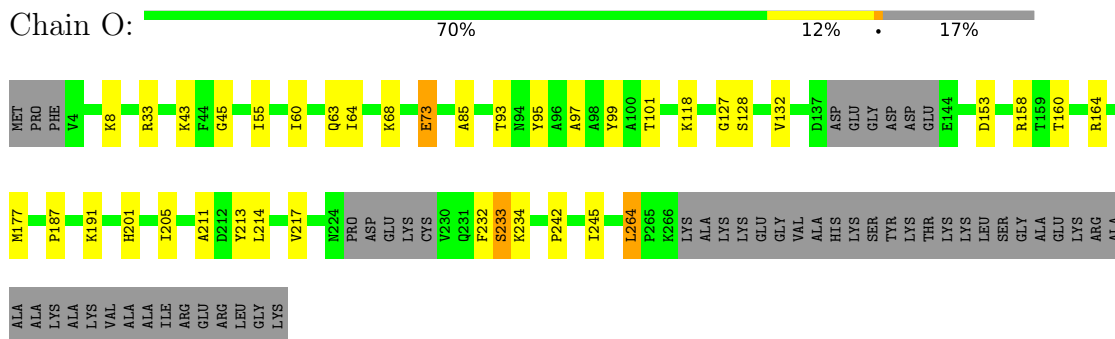
• Molecule 47: SR4\_chain\_5



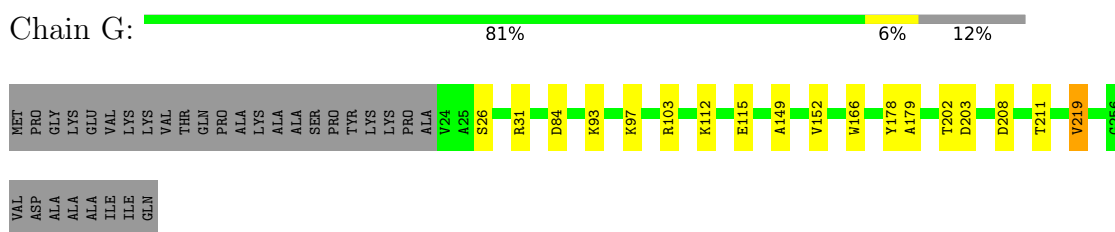
• Molecule 48: Putative 60S ribosomal protein L2



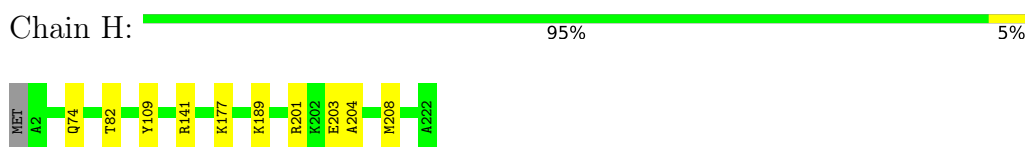
- Molecule 49: Putative 60S ribosomal protein L5



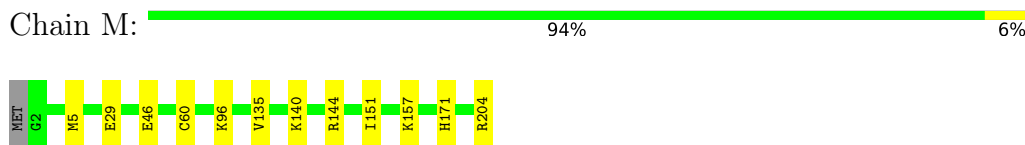
- Molecule 50: 60S ribosomal protein L7a



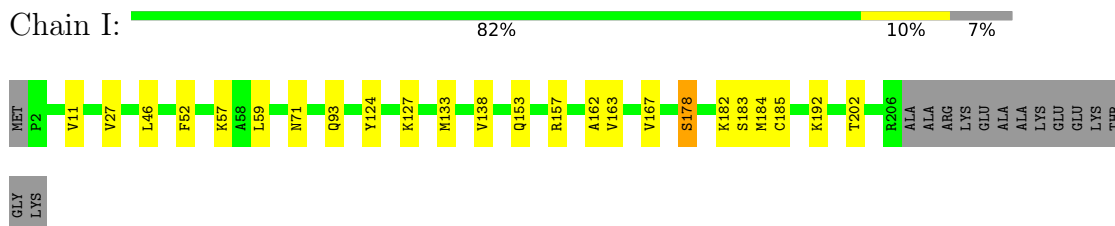
- Molecule 51: Putative 60S ribosomal protein L13a



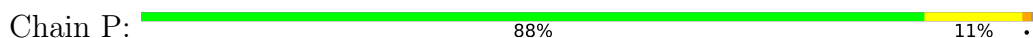
- Molecule 52: Ribosomal protein L15



- Molecule 53: eL13\_chain\_I



- Molecule 54: 60S ribosomal protein L18

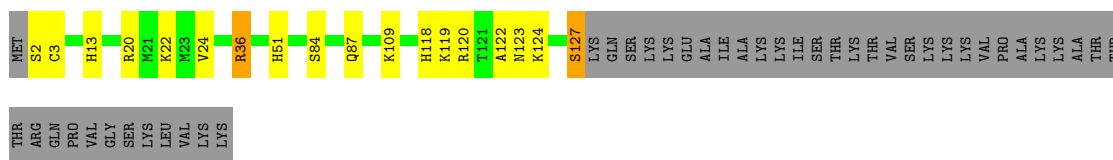







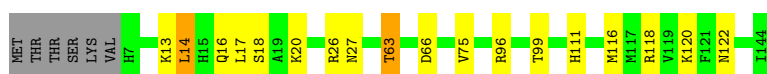
- Molecule 67: Putative 60S ribosomal protein L34

Chain h:  64% 10% 25%




- Molecule 68: Putative ribosomal protein l35a

Chain g:  83% 11%




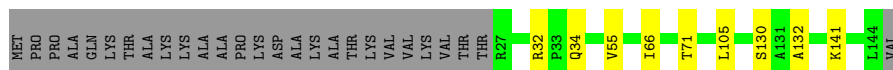
- Molecule 69: Putative 60S ribosomal protein L23

Chain J:  88% 5% 7%



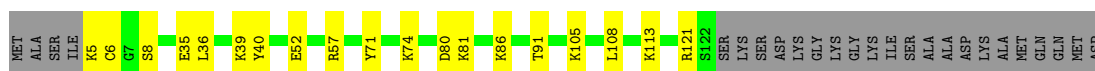
- Molecule 70: Putative 60S ribosomal protein L23a

Chain V:  75% 6% 19%



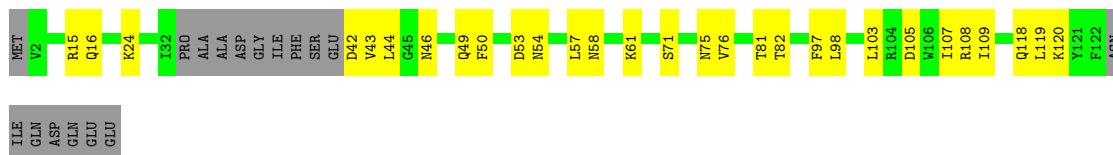
- Molecule 71: Putative 60S ribosomal protein L26

Chain W:  69% 13% 17%




- Molecule 72: Putative 60S ribosomal protein L22

Chain U:  64% 22% 13%

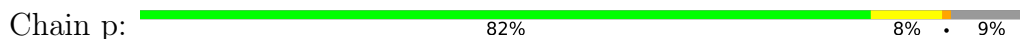


- Molecule 73: Putative 60S Ribosomal protein L36

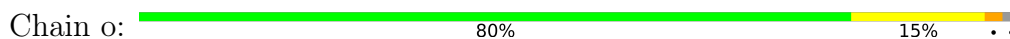
Chain i:  76% 14% 10%



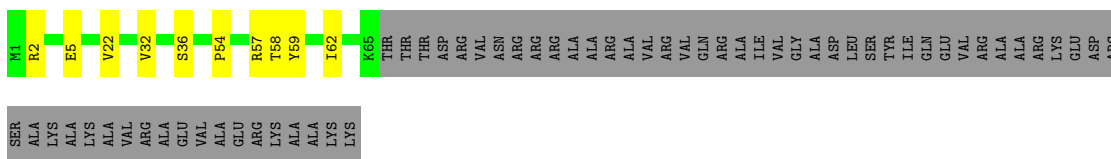
- Molecule 74: Putative 60S ribosomal protein L44



- Molecule 75: 60S ribosomal protein L37a



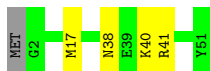
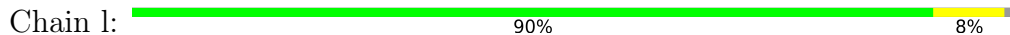
- Molecule 76: Putative ribosomal protein L24



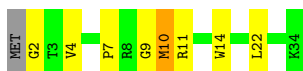
- Molecule 77: Putative ribosomal protein L38




- Molecule 78: Putative 60S ribosomal protein L39

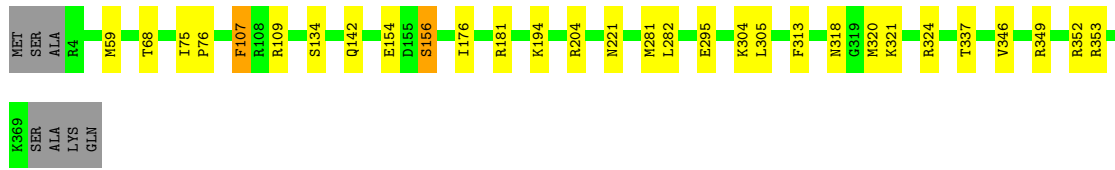


- Molecule 79: 60S ribosomal protein L41



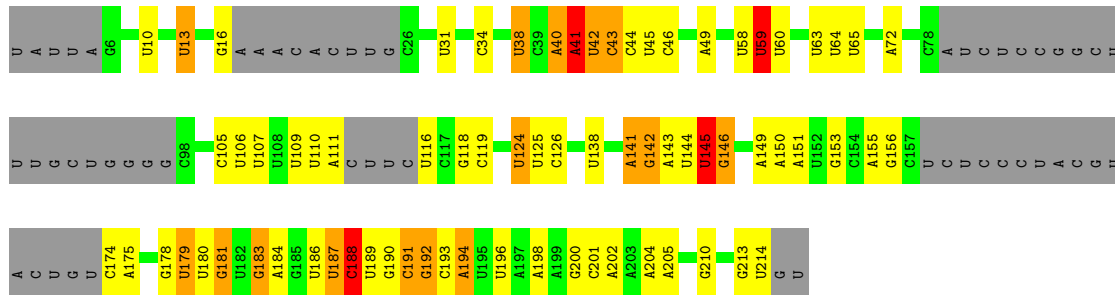
- Molecule 80: Putative ribosomal protein L1a

Chain C:  90% 8% ..




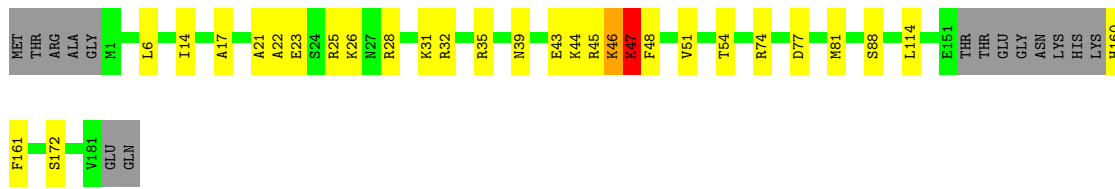
• Molecule 81: SR1\_chain\_3

Chain 3:  41% 25% 7% . 25%




• Molecule 82: Putative 60S ribosomal subunit protein L31

Chain e:  77% 14% .. 8%



• Molecule 83: Ribosomal protein L37

Chain j:  87% 10% .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	345376	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.367	Depositor
Minimum map value	-0.141	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	374.0, 374.0, 374.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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: 1MA, ZN, PSU, NA, MA6, OMU, K, G7M, OMG, OMC, 5MC, A2M, C4J, MG

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	SW	0.25	0/804	0.29	0/1090
2	SZ	0.15	0/988	0.29	0/1322
3	SY	0.12	0/610	0.35	0/829
4	SX	0.28	0/1100	0.38	0/1485
5	SV	0.20	0/850	0.31	0/1141
6	SU	0.18	0/1196	0.30	0/1613
7	ST	0.18	0/1168	0.35	0/1567
8	SS	0.28	0/433	0.40	0/578
9	SR	0.28	0/908	0.34	0/1232
10	SB	0.16	0/1679	0.30	0/2273
11	SC	0.21	0/1647	0.34	0/2208
12	SD	0.15	0/1541	0.32	0/2066
13	SE	0.16	0/2100	0.32	0/2830
14	SK	0.20	0/1445	0.33	0/1937
15	S4	0.28	0/450	0.41	0/698
16	Sg	0.29	0/2306	0.46	1/3144 (0.0%)
17	Sa	0.27	0/546	0.45	0/738
18	Sc	0.16	0/651	0.33	0/877
19	Se	0.15	0/410	0.35	0/544
20	S1	0.32	2/40111 (0.0%)	0.43	43/62469 (0.1%)
21	SQ	0.15	0/178	0.28	0/242
22	SP	0.25	0/1144	0.41	0/1533
23	SO	0.38	0/1027	0.55	0/1382
24	SN	0.24	0/836	0.39	0/1134
25	Sd	0.24	0/468	0.38	0/630
26	SM	0.22	0/821	0.32	0/1112
27	SL	0.27	0/1151	0.34	0/1547
28	SJ	0.17	0/1031	0.30	0/1382
29	SI	0.15	0/1643	0.29	0/2215
30	SH	0.27	0/1459	0.34	0/1958
31	SG	0.14	0/1833	0.26	0/2458
32	SF	0.18	0/1692	0.32	0/2294

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	SA	0.16	0/1862	0.30	0/2505
34	Sb	0.18	0/796	0.33	0/1070
35	Sh	0.14	0/664	0.38	0/904
36	f	0.35	0/1008	0.42	0/1351
37	d	0.29	0/635	0.36	0/871
38	c	0.31	0/1812	0.40	0/2440
39	a	0.28	0/965	0.34	0/1295
40	b	0.31	0/531	0.40	0/712
41	1	0.45	1/37000 (0.0%)	0.50	42/57678 (0.1%)
42	2	0.45	2/23546 (0.0%)	0.52	33/36681 (0.1%)
43	4	0.39	0/4341	0.42	0/6767
44	7	0.46	0/3669	0.48	5/5710 (0.1%)
45	B	0.34	0/3283	0.47	0/4421
46	8	0.28	0/2806	0.32	0/4367
47	5	0.47	0/2650	0.59	5/4123 (0.1%)
48	A	0.34	0/2029	0.47	0/2722
49	O	0.24	0/2007	0.37	0/2696
50	G	0.31	0/1883	0.44	0/2535
51	H	0.35	0/1810	0.48	1/2435 (0.0%)
52	M	0.36	0/1754	0.47	0/2342
53	I	0.30	0/1626	0.42	1/2186 (0.0%)
54	P	0.31	0/1564	0.40	0/2092
55	Q	0.32	0/1500	0.43	0/2000
56	R	0.35	0/1481	0.49	0/1997
57	E	0.27	0/1458	0.44	0/1971
58	6	0.33	0/1658	0.52	0/2580
59	T	0.34	0/1257	0.46	0/1683
60	S	0.29	0/1230	0.40	0/1658
61	K	0.24	0/1212	0.34	0/1634
62	D	0.26	0/1159	0.48	0/1565
63	L	0.33	0/1151	0.44	0/1538
64	Y	0.26	0/1070	0.39	0/1437
65	Z	0.26	0/1066	0.36	0/1431
66	F	0.27	0/1065	0.40	1/1451 (0.1%)
67	h	0.47	2/1035 (0.2%)	0.54	4/1378 (0.3%)
68	g	0.38	0/1124	0.48	0/1511
69	J	0.39	0/985	0.54	0/1329
70	V	0.30	0/954	0.41	0/1284
71	W	0.30	0/962	0.43	0/1284
72	U	0.24	0/892	0.37	0/1192
73	i	0.25	0/750	0.38	0/1003
74	p	0.31	0/733	0.44	0/977
75	o	0.37	0/708	0.54	0/944

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	X	0.29	0/574	0.42	0/774
77	k	0.26	0/554	0.41	0/751
78	l	0.35	0/453	0.42	0/606
79	n	0.60	0/263	0.87	1/348 (0.3%)
80	C	0.42	0/2847	0.61	1/3836 (0.0%)
81	3	0.47	0/3792	0.67	19/5895 (0.3%)
82	e	0.45	0/1314	0.70	0/1761
83	j	0.39	0/676	0.53	0/902
All	All	0.36	7/206390 (0.0%)	0.46	157/303151 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	36[A]	ARG	C-O	7.47	1.33	1.24
67	h	36[B]	ARG	C-O	7.47	1.33	1.24
20	S1	512	A2M	O3'-P	5.25	1.61	1.56
42	2	527	A2M	O3'-P	5.16	1.61	1.56
42	2	572	A2M	O3'-P	5.14	1.61	1.56

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	1	214	C	P-O3'-C3'	-10.62	104.27	120.20
42	2	508	A	P-O3'-C3'	-10.09	105.07	120.20
41	1	487	A	P-O3'-C3'	-9.04	106.65	120.20
20	S1	232	C	P-O3'-C3'	-9.03	106.66	120.20
42	2	497	G	P-O3'-C3'	-8.80	107.00	120.20

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	SW	787	0	772	5	0
2	SZ	967	0	1013	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	SY	604	0	589	11	0
4	SX	1071	0	1068	9	0
5	SV	843	0	861	10	0
6	SU	1170	0	1180	9	0
7	ST	1145	0	1211	6	0
8	SS	428	0	418	7	0
9	SR	892	0	871	8	0
10	SB	1643	0	1658	32	0
11	SC	1619	0	1671	18	0
12	SD	1513	0	1588	15	0
13	SE	2056	0	2155	17	0
14	SK	1424	0	1501	10	0
15	S4	404	0	211	4	0
16	Sg	2251	0	2116	30	0
17	Sa	541	0	561	8	0
18	Sc	638	0	624	7	0
19	Se	404	0	434	4	0
20	S1	36928	0	18662	318	0
21	SQ	179	0	160	2	0
22	SP	1115	0	1162	9	0
23	SO	1012	0	1023	11	0
24	SN	813	0	787	17	0
25	Sd	466	0	476	5	0
26	SM	811	0	854	5	0
27	SL	1130	0	1190	5	0
28	SJ	1014	0	1044	6	0
29	SI	1613	0	1669	11	0
30	SH	1437	0	1464	11	0
31	SG	1809	0	1889	18	0
32	SF	1656	0	1706	14	0
33	SA	1834	0	1920	20	0
34	Sb	779	0	793	7	0
35	Sh	657	0	615	14	0
36	f	988	0	1023	0	0
37	d	625	0	567	10	0
38	c	1779	0	1822	16	0
39	a	955	0	983	11	0
40	b	520	0	531	2	0
41	1	33802	0	17053	269	0
42	2	22358	0	11347	234	0
43	4	3906	0	1975	27	0
44	7	3399	0	1721	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B	3200	0	3297	28	0
46	8	2511	0	1272	24	0
47	5	2373	0	1205	25	0
48	A	1973	0	2040	20	0
49	O	1970	0	2011	24	0
50	G	1850	0	1956	10	0
51	H	1771	0	1854	7	0
52	M	1714	0	1793	7	0
53	I	1593	0	1614	12	0
54	P	1539	0	1648	20	0
55	Q	1482	0	1500	15	0
56	R	1447	0	1481	17	0
57	E	1439	0	1489	29	0
58	6	1484	0	758	15	0
59	T	1233	0	1278	8	0
60	S	1203	0	1240	9	0
61	K	1193	0	1219	13	0
62	D	1140	0	1071	22	0
63	L	1124	0	1151	5	0
64	Y	1046	0	1084	15	0
65	Z	1052	0	1072	16	0
66	F	1045	0	1052	6	0
67	h	1016	0	1070	15	0
68	g	1101	0	1138	12	0
69	J	968	0	1023	2	0
70	V	939	0	992	8	0
71	W	948	0	1019	12	0
72	U	879	0	896	17	0
73	i	738	0	785	12	0
74	p	722	0	732	5	0
75	o	696	0	716	10	0
76	X	553	0	555	4	0
77	k	546	0	537	5	0
78	l	440	0	461	4	0
79	n	259	0	269	7	0
80	C	2797	0	2875	20	0
81	3	3419	0	1733	41	0
82	e	1298	0	1360	24	0
83	j	662	0	669	6	0
84	1	61	0	0	0	0
84	2	31	0	0	0	0
84	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	4	3	0	0	0	0
84	5	1	0	0	0	0
84	6	1	0	0	0	0
84	7	4	0	0	0	0
84	8	1	0	0	0	0
84	J	1	0	0	0	0
84	S1	23	0	0	0	0
84	SL	1	0	0	0	0
84	SS	1	0	0	0	0
84	T	1	0	0	0	0
85	Sb	1	0	0	0	0
85	Sc	1	0	0	0	0
85	j	1	0	0	0	0
85	o	1	0	0	0	0
86	1	5	0	0	0	0
86	2	3	0	0	0	0
87	1	2	0	0	0	0
88	1	918	0	0	27	0
88	2	536	0	0	34	0
88	3	31	0	0	0	0
88	4	73	0	0	5	0
88	5	37	0	0	0	0
88	6	3	0	0	0	0
88	7	85	0	0	3	0
88	8	17	0	0	4	0
88	A	30	0	0	4	0
88	B	29	0	0	4	0
88	C	21	0	0	0	0
88	E	1	0	0	0	0
88	G	4	0	0	0	0
88	H	9	0	0	0	0
88	I	21	0	0	1	0
88	J	1	0	0	0	0
88	K	1	0	0	0	0
88	L	17	0	0	0	0
88	M	28	0	0	1	0
88	P	12	0	0	0	0
88	Q	6	0	0	0	0
88	R	1	0	0	0	0
88	S	4	0	0	0	0
88	S1	237	0	0	34	0
88	S4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	SB	3	0	0	1	0
88	SC	1	0	0	0	0
88	SD	1	0	0	0	0
88	SE	1	0	0	0	0
88	SF	2	0	0	0	0
88	SH	4	0	0	0	0
88	SK	1	0	0	0	0
88	SN	3	0	0	2	0
88	SO	2	0	0	1	0
88	SP	3	0	0	0	0
88	SR	2	0	0	1	0
88	SS	1	0	0	0	0
88	ST	5	0	0	0	0
88	SX	7	0	0	0	0
88	SY	1	0	0	0	0
88	SZ	1	0	0	0	0
88	Sa	1	0	0	1	0
88	Sb	2	0	0	0	0
88	Sc	2	0	0	0	0
88	Sd	1	0	0	0	0
88	Sg	3	0	0	1	0
88	T	14	0	0	0	0
88	V	6	0	0	0	0
88	W	2	0	0	1	0
88	X	2	0	0	0	0
88	a	3	0	0	1	0
88	c	4	0	0	0	0
88	d	3	0	0	0	0
88	e	9	0	0	1	0
88	f	16	0	0	0	0
88	g	9	0	0	1	0
88	h	12	0	0	0	0
88	i	1	0	0	0	0
88	j	13	0	0	0	0
88	k	2	0	0	0	0
88	l	6	0	0	1	0
88	o	2	0	0	0	0
88	p	13	0	0	0	0
All	All	197779	0	142853	1623	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 1623 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)
20:S1:955:A:N6	20:S1:980:G:H1	1.46	1.13
41:1:1776:G:H1	42:2:6:A:N6	1.49	1.09
20:S1:1574:G:H1	20:S1:1613:C:H5	1.10	0.97
81:3:156:G:H1	81:3:175:A:H2	1.12	0.95
47:5:64:U:H5	47:5:92:G:H1	1.06	0.95

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	
1	SW	101/152 (66%)	97 (96%)	4 (4%)	0	100	100
2	SZ	121/137 (88%)	116 (96%)	5 (4%)	0	100	100
3	SY	81/164 (49%)	79 (98%)	2 (2%)	0	100	100
4	SX	137/161 (85%)	129 (94%)	8 (6%)	0	100	100
5	SV	109/143 (76%)	105 (96%)	4 (4%)	0	100	100
6	SU	146/173 (84%)	139 (95%)	7 (5%)	0	100	100
7	ST	139/151 (92%)	131 (94%)	8 (6%)	0	100	100
8	SS	53/57 (93%)	49 (92%)	4 (8%)	0	100	100
9	SR	117/153 (76%)	115 (98%)	2 (2%)	0	100	100
10	SB	207/246 (84%)	199 (96%)	8 (4%)	0	100	100
11	SC	212/219 (97%)	206 (97%)	6 (3%)	0	100	100
12	SD	181/190 (95%)	174 (96%)	7 (4%)	0	100	100
13	SE	260/273 (95%)	256 (98%)	4 (2%)	0	100	100
14	SK	176/220 (80%)	173 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Sg	294/312 (94%)	269 (92%)	25 (8%)	0	100	100
17	Sa	69/120 (58%)	65 (94%)	4 (6%)	0	100	100
18	Sc	82/86 (95%)	78 (95%)	4 (5%)	0	100	100
19	Se	48/66 (73%)	43 (90%)	5 (10%)	0	100	100
21	SQ	24/141 (17%)	24 (100%)	0	0	100	100
22	SP	143/143 (100%)	141 (99%)	2 (1%)	0	100	100
23	SO	135/144 (94%)	130 (96%)	5 (4%)	0	100	100
24	SN	99/168 (59%)	94 (95%)	5 (5%)	0	100	100
25	Sd	63/87 (72%)	57 (90%)	6 (10%)	0	100	100
26	SM	101/116 (87%)	99 (98%)	2 (2%)	0	100	100
27	SL	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
28	SJ	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
29	SI	198/200 (99%)	195 (98%)	3 (2%)	0	100	100
30	SH	180/190 (95%)	175 (97%)	5 (3%)	0	100	100
31	SG	232/249 (93%)	229 (99%)	3 (1%)	0	100	100
32	SF	218/265 (82%)	214 (98%)	4 (2%)	0	100	100
33	SA	225/264 (85%)	224 (100%)	1 (0%)	0	100	100
34	Sb	98/112 (88%)	94 (96%)	4 (4%)	0	100	100
35	Sh	92/235 (39%)	85 (92%)	7 (8%)	0	100	100
36	f	120/133 (90%)	116 (97%)	4 (3%)	0	100	100
37	d	88/104 (85%)	85 (97%)	3 (3%)	0	100	100
38	c	225/252 (89%)	218 (97%)	7 (3%)	0	100	100
39	a	121/127 (95%)	115 (95%)	6 (5%)	0	100	100
40	b	64/70 (91%)	63 (98%)	1 (2%)	0	100	100
45	B	407/419 (97%)	397 (98%)	10 (2%)	0	100	100
48	A	258/260 (99%)	252 (98%)	6 (2%)	0	100	100
49	O	249/305 (82%)	235 (94%)	14 (6%)	0	100	100
50	G	233/264 (88%)	225 (97%)	8 (3%)	0	100	100
51	H	220/222 (99%)	219 (100%)	1 (0%)	0	100	100
52	M	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
53	I	203/220 (92%)	192 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	P	195/198 (98%)	188 (96%)	7 (4%)	0	100	100
55	Q	187/254 (74%)	184 (98%)	3 (2%)	0	100	100
56	R	176/179 (98%)	174 (99%)	2 (1%)	0	100	100
57	E	184/190 (97%)	174 (95%)	10 (5%)	0	100	100
59	T	151/166 (91%)	148 (98%)	3 (2%)	0	100	100
60	S	150/159 (94%)	143 (95%)	7 (5%)	0	100	100
61	K	151/175 (86%)	145 (96%)	6 (4%)	0	100	100
62	D	155/188 (82%)	146 (94%)	9 (6%)	0	100	100
63	L	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
64	Y	131/134 (98%)	128 (98%)	3 (2%)	0	100	100
65	Z	137/147 (93%)	134 (98%)	3 (2%)	0	100	100
66	F	138/195 (71%)	135 (98%)	3 (2%)	0	100	100
67	h	125/168 (74%)	119 (95%)	6 (5%)	0	100	100
68	g	136/144 (94%)	131 (96%)	4 (3%)	1 (1%)	18	24
69	J	127/139 (91%)	125 (98%)	2 (2%)	0	100	100
70	V	116/145 (80%)	114 (98%)	2 (2%)	0	100	100
71	W	116/143 (81%)	113 (97%)	3 (3%)	0	100	100
72	U	108/129 (84%)	105 (97%)	3 (3%)	0	100	100
73	i	91/105 (87%)	88 (97%)	3 (3%)	0	100	100
74	p	94/106 (89%)	81 (86%)	13 (14%)	0	100	100
75	o	88/92 (96%)	78 (89%)	10 (11%)	0	100	100
76	X	63/124 (51%)	61 (97%)	2 (3%)	0	100	100
77	k	71/83 (86%)	69 (97%)	2 (3%)	0	100	100
78	l	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
79	n	31/34 (91%)	28 (90%)	3 (10%)	0	100	100
80	C	364/373 (98%)	354 (97%)	10 (3%)	0	100	100
82	e	169/188 (90%)	159 (94%)	9 (5%)	1 (1%)	21	27
83	j	78/83 (94%)	76 (97%)	2 (3%)	0	100	100
All	All	10720/12433 (86%)	10343 (96%)	375 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
82	e	47	LYS
68	g	20	LYS

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	SW	74/130 (57%)	74 (100%)	0	100	100
2	SZ	100/118 (85%)	97 (97%)	3 (3%)	36	51
3	SY	63/116 (54%)	62 (98%)	1 (2%)	55	69
4	SX	107/131 (82%)	106 (99%)	1 (1%)	70	81
5	SV	83/126 (66%)	80 (96%)	3 (4%)	31	45
6	SU	121/152 (80%)	117 (97%)	4 (3%)	33	48
7	ST	122/132 (92%)	121 (99%)	1 (1%)	73	83
8	SS	42/49 (86%)	40 (95%)	2 (5%)	23	34
9	SR	86/130 (66%)	82 (95%)	4 (5%)	23	35
10	SB	175/202 (87%)	169 (97%)	6 (3%)	32	47
11	SC	168/184 (91%)	161 (96%)	7 (4%)	26	39
12	SD	160/164 (98%)	156 (98%)	4 (2%)	42	56
13	SE	215/225 (96%)	214 (100%)	1 (0%)	81	87
14	SK	138/176 (78%)	136 (99%)	2 (1%)	59	72
16	Sg	235/265 (89%)	220 (94%)	15 (6%)	16	22
17	Sa	58/95 (61%)	54 (93%)	4 (7%)	14	19
18	Sc	68/76 (90%)	66 (97%)	2 (3%)	37	52
19	Se	40/54 (74%)	39 (98%)	1 (2%)	42	56
21	SQ	15/120 (12%)	15 (100%)	0	100	100
22	SP	114/117 (97%)	112 (98%)	2 (2%)	51	65
23	SO	101/113 (89%)	98 (97%)	3 (3%)	36	51
24	SN	85/128 (66%)	82 (96%)	3 (4%)	32	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	Sd	46/75 (61%)	43 (94%)	3 (6%)	15	21
26	SM	94/104 (90%)	90 (96%)	4 (4%)	26	38
27	SL	114/120 (95%)	112 (98%)	2 (2%)	51	65
28	SJ	108/111 (97%)	106 (98%)	2 (2%)	50	64
29	SI	174/186 (94%)	167 (96%)	7 (4%)	28	41
30	SH	150/159 (94%)	146 (97%)	4 (3%)	39	54
31	SG	180/208 (86%)	177 (98%)	3 (2%)	53	67
32	SF	170/208 (82%)	165 (97%)	5 (3%)	37	52
33	SA	198/222 (89%)	192 (97%)	6 (3%)	36	51
34	Sb	80/93 (86%)	80 (100%)	0	100	100
35	Sh	59/177 (33%)	54 (92%)	5 (8%)	10	11
36	f	104/115 (90%)	102 (98%)	2 (2%)	50	64
37	d	60/89 (67%)	58 (97%)	2 (3%)	33	48
38	c	174/209 (83%)	170 (98%)	4 (2%)	44	59
39	a	93/118 (79%)	90 (97%)	3 (3%)	34	49
40	b	52/58 (90%)	51 (98%)	1 (2%)	50	64
45	B	331/351 (94%)	322 (97%)	9 (3%)	39	54
48	A	202/204 (99%)	198 (98%)	4 (2%)	48	63
49	O	191/242 (79%)	184 (96%)	7 (4%)	30	44
50	G	192/221 (87%)	187 (97%)	5 (3%)	40	55
51	H	183/188 (97%)	182 (100%)	1 (0%)	81	87
52	M	179/180 (99%)	176 (98%)	3 (2%)	53	67
53	I	165/183 (90%)	158 (96%)	7 (4%)	26	39
54	P	163/164 (99%)	161 (99%)	2 (1%)	63	74
55	Q	138/198 (70%)	136 (99%)	2 (1%)	59	72
56	R	155/159 (98%)	147 (95%)	8 (5%)	21	30
57	E	157/172 (91%)	144 (92%)	13 (8%)	10	12
59	T	131/143 (92%)	129 (98%)	2 (2%)	57	70
60	S	125/134 (93%)	123 (98%)	2 (2%)	55	69
61	K	121/145 (83%)	115 (95%)	6 (5%)	22	32
62	D	104/162 (64%)	96 (92%)	8 (8%)	12	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
63	L	113/114 (99%)	110 (97%)	3 (3%)	39	54
64	Y	106/116 (91%)	105 (99%)	1 (1%)	70	81
65	Z	106/118 (90%)	103 (97%)	3 (3%)	38	54
66	F	103/153 (67%)	100 (97%)	3 (3%)	37	52
67	h	105/146 (72%)	102 (97%)	3 (3%)	37	52
68	g	112/121 (93%)	107 (96%)	5 (4%)	24	37
69	J	102/111 (92%)	98 (96%)	4 (4%)	28	42
70	V	100/124 (81%)	98 (98%)	2 (2%)	48	63
71	W	102/122 (84%)	99 (97%)	3 (3%)	37	52
72	U	88/114 (77%)	79 (90%)	9 (10%)	7	6
73	i	75/88 (85%)	73 (97%)	2 (3%)	39	54
74	p	66/92 (72%)	64 (97%)	2 (3%)	36	51
75	o	70/74 (95%)	65 (93%)	5 (7%)	13	18
76	X	58/104 (56%)	55 (95%)	3 (5%)	21	30
77	k	56/74 (76%)	50 (89%)	6 (11%)	6	6
78	l	44/47 (94%)	44 (100%)	0	100	100
79	n	24/32 (75%)	22 (92%)	2 (8%)	10	12
80	C	287/301 (95%)	278 (97%)	9 (3%)	35	50
82	e	128/158 (81%)	118 (92%)	10 (8%)	11	14
83	j	67/70 (96%)	66 (98%)	1 (2%)	57	70
All	All	8675/10380 (84%)	8398 (97%)	277 (3%)	35	49

5 of 277 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
72	U	75	ASN
73	i	51	VAL
80	C	142	GLN
32	SF	245	THR
32	SF	61	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 227 such sidechains are listed below:

Mol	Chain	Res	Type
48	A	140	ASN
82	e	39	ASN
54	P	132	GLN
80	C	183	ASN
70	V	140	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	S4	17/19 (89%)	6 (35%)	0
20	S1	1702/2204 (77%)	357 (20%)	15 (0%)
41	1	1564/1782 (87%)	318 (20%)	24 (1%)
42	2	1036/1526 (67%)	217 (20%)	17 (1%)
43	4	182/183 (99%)	35 (19%)	2 (1%)
44	7	157/171 (91%)	24 (15%)	0
46	8	116/123 (94%)	13 (11%)	1 (0%)
47	5	107/135 (79%)	26 (24%)	3 (2%)
58	6	70/73 (95%)	29 (41%)	5 (7%)
81	3	156/216 (72%)	33 (21%)	3 (1%)
All	All	5107/6432 (79%)	1058 (20%)	70 (1%)

5 of 1058 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	S4	2	C
15	S4	5	G
15	S4	7	A
15	S4	69	G
15	S4	70	C

5 of 70 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
43	4	149	U
47	5	48	G
58	6	51	A
41	1	581	G
41	1	485	A

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

152 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$
20	OMU	S1	2048	20	19,22,23	2.95	7 (36%)	25,31,34	1.90	5 (20%)
44	PSU	7	74	44	18,21,22	4.47	8 (44%)	21,30,33	2.00	5 (23%)
20	G7M	S1	1995	20	23,26,27	3.75	11 (47%)	34,39,42	1.73	7 (20%)
42	OMC	2	1159	42	19,22,23	2.81	7 (36%)	25,31,34	0.81	0
41	PSU	1	239	41	18,21,22	4.50	7 (38%)	21,30,33	1.86	5 (23%)
41	OMU	1	1371	41	19,22,23	2.97	8 (42%)	25,31,34	2.21	6 (24%)
42	PSU	2	1403	42	18,21,22	4.38	9 (50%)	21,30,33	1.84	4 (19%)
42	OMG	2	1078	42	23,26,27	2.30	8 (34%)	32,38,41	2.46	13 (40%)
20	OMG	S1	1647	20	23,26,27	2.36	9 (39%)	32,38,41	2.46	13 (40%)
41	A2M	1	437	41	22,25,26	3.27	10 (45%)	30,36,39	3.11	11 (36%)
20	OMU	S1	8	20	19,22,23	3.01	8 (42%)	25,31,34	1.86	5 (20%)
20	A2M	S1	2021	20	22,25,26	3.26	9 (40%)	30,36,39	3.05	12 (40%)
42	A2M	2	95	42	22,25,26	3.30	10 (45%)	30,36,39	2.94	12 (40%)
42	PSU	2	1265	42	18,21,22	4.62	7 (38%)	21,30,33	1.85	5 (23%)
20	PSU	S1	1156	20	18,21,22	4.65	7 (38%)	21,30,33	1.90	5 (23%)
20	PSU	S1	33	20	18,21,22	4.65	7 (38%)	21,30,33	1.95	5 (23%)
20	OMU	S1	661	20	19,22,23	2.99	8 (42%)	25,31,34	1.82	4 (16%)
20	OMU	S1	1621	20	19,22,23	2.99	8 (42%)	25,31,34	1.87	5 (20%)
41	PSU	1	1533	42,41	18,21,22	4.31	8 (44%)	21,30,33	2.23	6 (28%)
42	A2M	2	1384	42	22,25,26	3.25	10 (45%)	30,36,39	3.01	13 (43%)
20	OMC	S1	1866	20	19,22,23	2.81	8 (42%)	25,31,34	0.71	0
42	PSU	2	506	42	18,21,22	1.41	3 (16%)	21,30,33	2.27	5 (23%)
42	OMC	2	1397	42	19,22,23	2.73	8 (42%)	25,31,34	0.83	0
41	A2M	1	955	41	22,25,26	3.26	10 (45%)	30,36,39	2.97	12 (40%)
41	PSU	1	870	41,84	18,21,22	4.40	8 (44%)	21,30,33	1.98	5 (23%)
42	OMG	2	1046	42	23,26,27	2.39	9 (39%)	32,38,41	2.48	13 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	PSU	S1	607	20	18,21,22	4.69	7 (38%)	21,30,33	1.90	5 (23%)
42	OMG	2	1231	42	23,26,27	2.32	8 (34%)	32,38,41	2.41	13 (40%)
20	5MC	S1	2061	20	19,22,23	1.65	3 (15%)	26,32,35	1.21	2 (7%)
20	OMG	S1	1550	20	23,26,27	2.41	9 (39%)	32,38,41	2.52	12 (37%)
42	PSU	2	662	42,84	18,21,22	4.37	8 (44%)	21,30,33	1.95	5 (23%)
20	PSU	S1	1539	20	18,21,22	4.45	7 (38%)	21,30,33	1.89	4 (19%)
20	C4J	S1	1543	20	25,29,30	2.89	9 (36%)	28,42,45	1.58	5 (17%)
42	PSU	2	1058	42	18,21,22	4.48	8 (44%)	21,30,33	1.90	4 (19%)
20	5MC	S1	1544	20	19,22,23	3.64	8 (42%)	26,32,35	1.06	1 (3%)
41	OMC	1	695	41	19,22,23	2.73	8 (42%)	25,31,34	0.73	0
44	A2M	7	43	44	22,25,26	3.29	10 (45%)	30,36,39	3.07	11 (36%)
41	A2M	1	678	42,41	22,25,26	3.28	9 (40%)	30,36,39	3.04	13 (43%)
42	A2M	2	570	42,41	22,25,26	3.28	10 (45%)	30,36,39	3.17	14 (46%)
42	OMG	2	71	42	23,26,27	2.33	8 (34%)	32,38,41	2.30	14 (43%)
41	PSU	1	672	41,84	18,21,22	4.37	8 (44%)	21,30,33	2.07	5 (23%)
41	A2M	1	1539	42,41,87,84	22,25,26	3.24	10 (45%)	30,36,39	3.08	14 (46%)
42	5MC	2	524	42,84	19,22,23	3.46	8 (42%)	26,32,35	1.08	2 (7%)
20	OMC	S1	38	20	19,22,23	2.93	8 (42%)	25,31,34	0.76	0
20	A2M	S1	28	20	22,25,26	3.20	9 (40%)	30,36,39	3.06	11 (36%)
20	OMG	S1	1623	20	23,26,27	2.36	8 (34%)	32,38,41	2.58	10 (31%)
42	OMU	2	1419	42	19,22,23	2.92	8 (42%)	25,31,34	1.80	4 (16%)
20	PSU	S1	1657	20	18,21,22	4.44	7 (38%)	21,30,33	1.77	4 (19%)
42	OMG	2	1229	42	23,26,27	2.33	9 (39%)	32,38,41	2.44	13 (40%)
42	A2M	2	527	42	22,25,26	3.32	10 (45%)	30,36,39	3.39	14 (46%)
42	OMC	2	359	42	19,22,23	2.88	8 (42%)	25,31,34	0.66	0
20	OMG	S1	600	20	23,26,27	2.41	9 (39%)	32,38,41	2.55	10 (31%)
41	PSU	1	1171	41	18,21,22	4.29	9 (50%)	21,30,33	1.91	5 (23%)
20	PSU	S1	104	20	18,21,22	4.58	7 (38%)	21,30,33	1.92	5 (23%)
42	A2M	2	665	42	22,25,26	3.28	10 (45%)	30,36,39	2.96	12 (40%)
20	OMG	S1	2151	20	23,26,27	2.42	9 (39%)	32,38,41	2.63	11 (34%)
41	PSU	1	1664	41	18,21,22	4.35	8 (44%)	21,30,33	1.84	4 (19%)
42	A2M	2	628	42	22,25,26	3.31	11 (50%)	30,36,39	2.96	13 (43%)
41	OMG	1	1626	41	23,26,27	2.31	8 (34%)	32,38,41	2.38	14 (43%)
42	PSU	2	1354	42	18,21,22	4.44	7 (38%)	21,30,33	2.05	5 (23%)
42	PSU	2	510	42	18,21,22	1.42	3 (16%)	21,30,33	2.09	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	A2M	S1	479	20	22,25,26	3.23	10 (45%)	30,36,39	3.07	12 (40%)
20	OMG	S1	1478	20	23,26,27	2.38	8 (34%)	32,38,41	2.51	14 (43%)
42	A2M	2	1372	42	22,25,26	3.31	10 (45%)	30,36,39	3.09	11 (36%)
42	PSU	2	626	42	18,21,22	4.34	8 (44%)	21,30,33	1.89	4 (19%)
42	PSU	2	437	42	18,21,22	4.31	8 (44%)	21,30,33	2.03	5 (23%)
41	PSU	1	940	41	18,21,22	4.40	8 (44%)	21,30,33	1.95	5 (23%)
42	OMU	2	667	42	19,22,23	2.90	8 (42%)	25,31,34	1.91	5 (20%)
42	OMU	2	1077	42	19,22,23	2.94	8 (42%)	25,31,34	1.89	4 (16%)
20	MA6	S1	2185	20	23,26,27	1.53	5 (21%)	33,38,41	2.95	13 (39%)
42	OMC	2	1248	42	19,22,23	2.81	8 (42%)	25,31,34	0.93	1 (4%)
42	OMC	2	443	42	19,22,23	0.85	0	25,31,34	1.06	0
41	A2M	1	681	41	22,25,26	3.26	10 (45%)	30,36,39	3.06	12 (40%)
20	A2M	S1	668	20	22,25,26	3.22	9 (40%)	30,36,39	3.09	12 (40%)
42	OMC	2	1317	42	19,22,23	2.76	8 (42%)	25,31,34	0.89	1 (4%)
42	OMG	2	534	42	23,26,27	2.32	8 (34%)	32,38,41	2.46	10 (31%)
20	MA6	S1	2184	20	23,26,27	1.55	6 (26%)	33,38,41	2.93	12 (36%)
42	PSU	2	1318	42	18,21,22	4.38	8 (44%)	21,30,33	1.86	4 (19%)
42	OMU	2	560	42	19,22,23	2.93	7 (36%)	25,31,34	1.84	4 (16%)
44	A2M	7	162	44,41	22,25,26	3.26	10 (45%)	30,36,39	3.16	11 (36%)
42	PSU	2	1382	42	18,21,22	4.38	9 (50%)	21,30,33	1.93	6 (28%)
41	A2M	1	697	41	22,25,26	3.28	10 (45%)	30,36,39	3.08	11 (36%)
42	OMU	2	73	42	19,22,23	2.86	7 (36%)	25,31,34	1.80	5 (20%)
42	OMG	2	641	42	23,26,27	2.33	9 (39%)	32,38,41	2.38	15 (46%)
42	A2M	2	1185	42	22,25,26	3.23	9 (40%)	30,36,39	3.11	13 (43%)
20	PSU	S1	2202	20	18,21,22	4.59	7 (38%)	21,30,33	1.89	5 (23%)
41	OMU	1	847	41	19,22,23	2.82	7 (36%)	25,31,34	2.00	5 (20%)
42	A2M	2	572	42	22,25,26	3.29	10 (45%)	30,36,39	3.12	12 (40%)
81	OMU	3	13	81	19,22,23	2.92	7 (36%)	25,31,34	1.94	5 (20%)
42	PSU	2	472	42	18,21,22	4.49	7 (38%)	21,30,33	1.93	5 (23%)
42	PSU	2	500	42	18,21,22	1.42	3 (16%)	21,30,33	2.23	4 (19%)
20	A2M	S1	512	20	22,25,26	1.48	4 (18%)	30,36,39	2.25	11 (36%)
44	PSU	7	69	44	18,21,22	4.44	8 (44%)	21,30,33	1.92	4 (19%)
41	OMG	1	1190	41	23,26,27	2.36	9 (39%)	32,38,41	2.49	13 (40%)
42	PSU	2	1144	42	18,21,22	4.44	8 (44%)	21,30,33	2.09	4 (19%)
41	PSU	1	422	41	18,21,22	4.47	8 (44%)	21,30,33	2.05	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	PSU	S1	1533	20	18,21,22	4.45	7 (38%)	21,30,33	1.99	5 (23%)
41	PSU	1	1017	41	18,21,22	4.29	8 (44%)	21,30,33	1.88	5 (23%)
20	PSU	S1	2046	20	18,21,22	4.51	7 (38%)	21,30,33	2.08	5 (23%)
42	OMU	2	1359	42	19,22,23	2.93	8 (42%)	25,31,34	1.91	5 (20%)
41	PSU	1	1402	41	18,21,22	4.29	9 (50%)	21,30,33	2.02	4 (19%)
42	PSU	2	1060	42	18,21,22	4.47	8 (44%)	21,30,33	1.93	4 (19%)
41	OMG	1	856	41	23,26,27	2.31	9 (39%)	32,38,41	2.43	14 (43%)
42	OMG	2	655	42	23,26,27	2.31	8 (34%)	32,38,41	2.40	11 (34%)
41	1MA	1	677	41,84	21,25,26	0.65	0	30,37,40	0.74	1 (3%)
42	5MC	2	1308	42	19,22,23	3.71	8 (42%)	26,32,35	1.28	3 (11%)
20	A2M	S1	98	20	22,25,26	3.21	9 (40%)	30,36,39	3.01	13 (43%)
42	A2M	2	591	42	22,25,26	3.28	10 (45%)	30,36,39	3.00	12 (40%)
20	PSU	S1	12	20	18,21,22	4.49	7 (38%)	21,30,33	2.14	6 (28%)
42	PSU	2	1264	42	18,21,22	4.63	7 (38%)	21,30,33	1.99	5 (23%)
41	PSU	1	1528	41	18,21,22	4.41	8 (44%)	21,30,33	1.89	4 (19%)
42	OMG	2	1253	42	23,26,27	2.33	8 (34%)	32,38,41	2.37	12 (37%)
20	OMU	S1	1833	20	19,22,23	3.07	8 (42%)	25,31,34	1.86	5 (20%)
43	OMG	4	74	43	23,26,27	2.27	8 (34%)	32,38,41	2.36	14 (43%)
20	A2M	S1	897	20	22,25,26	3.27	9 (40%)	30,36,39	3.03	13 (43%)
41	PSU	1	1181	41	18,21,22	4.44	7 (38%)	21,30,33	1.92	5 (23%)
41	A2M	1	858	41	22,25,26	3.19	9 (40%)	30,36,39	3.07	12 (40%)
20	OMU	S1	1979	20	19,22,23	2.91	8 (42%)	25,31,34	1.89	5 (20%)
42	A2M	2	604	42,41	22,25,26	3.23	10 (45%)	30,36,39	3.07	11 (36%)
20	PSU	S1	1566	20	18,21,22	1.39	3 (16%)	21,30,33	2.15	5 (23%)
42	A2M	2	382	42	22,25,26	3.27	10 (45%)	30,36,39	2.97	12 (40%)
20	OMU	S1	29	20	19,22,23	3.05	8 (42%)	25,31,34	1.85	5 (20%)
20	PSU	S1	609	20	18,21,22	4.60	7 (38%)	21,30,33	1.97	5 (23%)
20	OMC	S1	18	20	19,22,23	2.90	8 (42%)	25,31,34	0.73	0
20	OMG	S1	1829	20	23,26,27	2.34	9 (39%)	32,38,41	2.48	11 (34%)
41	OMC	1	1527	41	19,22,23	2.70	7 (36%)	25,31,34	0.73	0
41	OMG	1	1540	42,41	23,26,27	2.31	9 (39%)	32,38,41	2.40	13 (40%)
20	PSU	S1	1841	20	18,21,22	4.53	7 (38%)	21,30,33	2.00	5 (23%)
41	OMG	1	1524	41	23,26,27	2.35	8 (34%)	32,38,41	2.57	12 (37%)
41	OMU	1	1659	41	19,22,23	2.84	7 (36%)	25,31,34	1.94	5 (20%)
20	OMU	S1	1777	20	19,22,23	3.00	8 (42%)	25,31,34	1.85	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
41	OMG	1	959	41	23,26,27	2.38	9 (39%)	32,38,41	2.67	9 (28%)
20	OMG	S1	1865	20	23,26,27	2.35	9 (39%)	32,38,41	2.51	12 (37%)
42	PSU	2	504	42	18,21,22	1.36	2 (11%)	21,30,33	2.29	5 (23%)
20	PSU	S1	1246	20	18,21,22	4.59	8 (44%)	21,30,33	1.84	4 (19%)
42	PSU	2	597	42	18,21,22	4.31	8 (44%)	21,30,33	2.07	4 (19%)
20	PSU	S1	455	20	18,21,22	4.63	7 (38%)	21,30,33	2.05	5 (23%)
42	PSU	2	1303	42	18,21,22	4.63	8 (44%)	21,30,33	2.07	6 (28%)
42	OMC	2	583	42	19,22,23	2.71	7 (36%)	25,31,34	0.79	1 (4%)
42	PSU	2	593	42	18,21,22	4.33	9 (50%)	21,30,33	2.13	5 (23%)
41	OMU	1	1107	41	19,22,23	2.84	8 (42%)	25,31,34	1.91	6 (24%)
42	PSU	2	1194	42	18,21,22	4.37	8 (44%)	21,30,33	2.15	5 (23%)
44	OMG	7	75	44	23,26,27	2.32	9 (39%)	32,38,41	2.42	13 (40%)
42	OMG	2	1360	42	23,26,27	2.35	9 (39%)	32,38,41	2.44	12 (37%)
42	PSU	2	1361	42	18,21,22	4.55	7 (38%)	21,30,33	2.09	5 (23%)
41	PSU	1	1011	42,41	18,21,22	4.58	7 (38%)	21,30,33	2.07	5 (23%)
41	OMU	1	845	41	19,22,23	2.86	7 (36%)	25,31,34	1.87	5 (20%)
20	PSU	S1	1192	20	18,21,22	4.53	7 (38%)	21,30,33	1.76	4 (19%)
42	PSU	2	78	42	18,21,22	4.40	9 (50%)	21,30,33	1.89	5 (23%)
42	PSU	2	1413	42	18,21,22	4.34	8 (44%)	21,30,33	1.91	4 (19%)
41	OMC	1	1552	41	19,22,23	2.82	8 (42%)	25,31,34	0.78	0
20	OMC	S1	2140	20	19,22,23	2.98	8 (42%)	25,31,34	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	OMU	S1	2048	20	-	0/9/27/28	0/2/2/2
44	PSU	7	74	44	-	0/7/25/26	0/2/2/2
20	G7M	S1	1995	20	-	0/7/25/26	0/3/3/3
42	OMC	2	1159	42	-	0/9/27/28	0/2/2/2
41	PSU	1	239	41	-	2/7/25/26	0/2/2/2
41	OMU	1	1371	41	-	4/9/27/28	0/2/2/2
42	PSU	2	1403	42	-	1/7/25/26	0/2/2/2
42	OMG	2	1078	42	-	0/9/27/28	0/3/3/3
20	OMG	S1	1647	20	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	A2M	1	437	41	-	1/9/27/28	0/3/3/3
20	OMU	S1	8	20	-	6/9/27/28	0/2/2/2
20	A2M	S1	2021	20	-	3/9/27/28	0/3/3/3
42	A2M	2	95	42	-	1/9/27/28	0/3/3/3
42	PSU	2	1265	42	-	2/7/25/26	0/2/2/2
20	PSU	S1	1156	20	-	0/7/25/26	0/2/2/2
20	PSU	S1	33	20	-	2/7/25/26	0/2/2/2
20	OMU	S1	661	20	-	0/9/27/28	0/2/2/2
20	OMU	S1	1621	20	-	0/9/27/28	0/2/2/2
41	PSU	1	1533	42,41	-	0/7/25/26	0/2/2/2
42	A2M	2	1384	42	-	1/9/27/28	0/3/3/3
20	OMC	S1	1866	20	-	0/9/27/28	0/2/2/2
42	PSU	2	506	42	-	1/7/25/26	0/2/2/2
42	OMC	2	1397	42	-	0/9/27/28	0/2/2/2
41	A2M	1	955	41	-	0/9/27/28	0/3/3/3
41	PSU	1	870	41,84	-	0/7/25/26	0/2/2/2
42	OMG	2	1046	42	-	2/9/27/28	0/3/3/3
20	PSU	S1	607	20	-	6/7/25/26	0/2/2/2
42	OMG	2	1231	42	-	0/9/27/28	0/3/3/3
20	5MC	S1	2061	20	-	0/7/25/26	0/2/2/2
20	OMG	S1	1550	20	-	2/9/27/28	0/3/3/3
42	PSU	2	662	42,84	-	0/7/25/26	0/2/2/2
20	PSU	S1	1539	20	-	1/7/25/26	0/2/2/2
20	C4J	S1	1543	20	-	3/16/34/35	0/2/2/2
42	PSU	2	1058	42	-	0/7/25/26	0/2/2/2
20	5MC	S1	1544	20	-	0/7/25/26	0/2/2/2
41	OMC	1	695	41	-	0/9/27/28	0/2/2/2
44	A2M	7	43	44	-	0/9/27/28	0/3/3/3
41	A2M	1	678	42,41	-	0/9/27/28	0/3/3/3
42	A2M	2	570	42,41	-	4/9/27/28	0/3/3/3
42	OMG	2	71	42	-	0/9/27/28	0/3/3/3
41	PSU	1	672	41,84	-	0/7/25/26	0/2/2/2
41	A2M	1	1539	42,41,87,84	-	0/9/27/28	0/3/3/3
42	5MC	2	524	42,84	-	0/7/25/26	0/2/2/2
20	OMC	S1	38	20	-	0/9/27/28	0/2/2/2
20	A2M	S1	28	20	-	0/9/27/28	0/3/3/3
20	OMG	S1	1623	20	-	0/9/27/28	0/3/3/3
42	OMU	2	1419	42	-	1/9/27/28	0/2/2/2
20	PSU	S1	1657	20	-	1/7/25/26	0/2/2/2
42	OMG	2	1229	42	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	A2M	2	527	42	-	2/9/27/28	0/3/3/3
42	OMC	2	359	42	-	0/9/27/28	0/2/2/2
20	OMG	S1	600	20	-	2/9/27/28	0/3/3/3
41	PSU	1	1171	41	-	2/7/25/26	0/2/2/2
20	PSU	S1	104	20	-	0/7/25/26	0/2/2/2
42	A2M	2	665	42	-	3/9/27/28	0/3/3/3
20	OMG	S1	2151	20	-	0/9/27/28	0/3/3/3
41	PSU	1	1664	41	-	0/7/25/26	0/2/2/2
42	A2M	2	628	42	-	2/9/27/28	0/3/3/3
41	OMG	1	1626	41	-	0/9/27/28	0/3/3/3
42	PSU	2	1354	42	-	0/7/25/26	0/2/2/2
42	PSU	2	510	42	-	0/7/25/26	0/2/2/2
20	A2M	S1	479	20	-	1/9/27/28	0/3/3/3
20	OMG	S1	1478	20	-	1/9/27/28	0/3/3/3
42	A2M	2	1372	42	-	0/9/27/28	0/3/3/3
42	PSU	2	626	42	-	0/7/25/26	0/2/2/2
42	PSU	2	437	42	-	0/7/25/26	0/2/2/2
41	PSU	1	940	41	-	0/7/25/26	0/2/2/2
42	OMU	2	667	42	-	0/9/27/28	0/2/2/2
42	OMU	2	1077	42	-	0/9/27/28	0/2/2/2
20	MA6	S1	2185	20	-	1/11/29/30	0/3/3/3
42	OMC	2	1248	42	-	1/9/27/28	0/2/2/2
42	OMC	2	443	42	-	4/9/27/28	0/2/2/2
41	A2M	1	681	41	-	3/9/27/28	0/3/3/3
20	A2M	S1	668	20	-	5/9/27/28	0/3/3/3
42	OMC	2	1317	42	-	0/9/27/28	0/2/2/2
42	OMG	2	534	42	-	2/9/27/28	0/3/3/3
20	MA6	S1	2184	20	-	0/11/29/30	0/3/3/3
42	PSU	2	1318	42	-	0/7/25/26	0/2/2/2
42	OMU	2	560	42	-	1/9/27/28	0/2/2/2
44	A2M	7	162	44,41	-	1/9/27/28	0/3/3/3
42	PSU	2	1382	42	-	0/7/25/26	0/2/2/2
41	A2M	1	697	41	-	1/9/27/28	0/3/3/3
42	OMU	2	73	42	-	0/9/27/28	0/2/2/2
42	OMG	2	641	42	-	0/9/27/28	0/3/3/3
42	A2M	2	1185	42	-	3/9/27/28	0/3/3/3
20	PSU	S1	2202	20	-	1/7/25/26	0/2/2/2
41	OMU	1	847	41	-	0/9/27/28	0/2/2/2
42	A2M	2	572	42	-	0/9/27/28	0/3/3/3
81	OMU	3	13	81	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	PSU	2	472	42	-	0/7/25/26	0/2/2/2
42	PSU	2	500	42	-	3/7/25/26	0/2/2/2
20	A2M	S1	512	20	-	3/9/27/28	0/3/3/3
44	PSU	7	69	44	-	2/7/25/26	0/2/2/2
41	OMG	1	1190	41	-	0/9/27/28	0/3/3/3
42	PSU	2	1144	42	-	0/7/25/26	0/2/2/2
41	PSU	1	422	41	-	0/7/25/26	0/2/2/2
20	PSU	S1	1533	20	-	2/7/25/26	0/2/2/2
41	PSU	1	1017	41	-	0/7/25/26	0/2/2/2
20	PSU	S1	2046	20	-	0/7/25/26	0/2/2/2
42	OMU	2	1359	42	-	1/9/27/28	0/2/2/2
41	PSU	1	1402	41	-	1/7/25/26	0/2/2/2
42	PSU	2	1060	42	-	1/7/25/26	0/2/2/2
41	OMG	1	856	41	-	0/9/27/28	0/3/3/3
42	OMG	2	655	42	-	1/9/27/28	0/3/3/3
41	1MA	1	677	41,84	-	0/7/25/26	0/3/3/3
42	5MC	2	1308	42	-	6/7/25/26	0/2/2/2
20	A2M	S1	98	20	-	1/9/27/28	0/3/3/3
42	A2M	2	591	42	-	0/9/27/28	0/3/3/3
20	PSU	S1	12	20	-	0/7/25/26	0/2/2/2
42	PSU	2	1264	42	-	0/7/25/26	0/2/2/2
41	PSU	1	1528	41	-	0/7/25/26	0/2/2/2
42	OMG	2	1253	42	-	0/9/27/28	0/3/3/3
20	OMU	S1	1833	20	-	3/9/27/28	0/2/2/2
43	OMG	4	74	43	-	0/9/27/28	0/3/3/3
20	A2M	S1	897	20	-	2/9/27/28	0/3/3/3
41	PSU	1	1181	41	-	3/7/25/26	0/2/2/2
41	A2M	1	858	41	-	0/9/27/28	0/3/3/3
20	OMU	S1	1979	20	-	3/9/27/28	0/2/2/2
42	A2M	2	604	42,41	-	1/9/27/28	0/3/3/3
20	PSU	S1	1566	20	-	0/7/25/26	0/2/2/2
42	A2M	2	382	42	-	1/9/27/28	0/3/3/3
20	OMU	S1	29	20	-	0/9/27/28	0/2/2/2
20	PSU	S1	609	20	-	0/7/25/26	0/2/2/2
20	OMC	S1	18	20	-	0/9/27/28	0/2/2/2
20	OMG	S1	1829	20	-	2/9/27/28	0/3/3/3
41	OMC	1	1527	41	-	0/9/27/28	0/2/2/2
41	OMG	1	1540	42,41	-	2/9/27/28	0/3/3/3
20	PSU	S1	1841	20	-	1/7/25/26	0/2/2/2
41	OMG	1	1524	41	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	OMU	1	1659	41	-	0/9/27/28	0/2/2/2
20	OMU	S1	1777	20	-	0/9/27/28	0/2/2/2
41	OMG	1	959	41	-	2/9/27/28	0/3/3/3
20	OMG	S1	1865	20	-	0/9/27/28	0/3/3/3
42	PSU	2	504	42	-	3/7/25/26	0/2/2/2
20	PSU	S1	1246	20	-	2/7/25/26	0/2/2/2
42	PSU	2	597	42	-	0/7/25/26	0/2/2/2
20	PSU	S1	455	20	-	0/7/25/26	0/2/2/2
42	PSU	2	1303	42	-	2/7/25/26	0/2/2/2
42	OMC	2	583	42	-	0/9/27/28	0/2/2/2
42	PSU	2	593	42	-	0/7/25/26	0/2/2/2
41	OMU	1	1107	41	-	0/9/27/28	0/2/2/2
42	PSU	2	1194	42	-	0/7/25/26	0/2/2/2
44	OMG	7	75	44	-	0/9/27/28	0/3/3/3
42	OMG	2	1360	42	-	0/9/27/28	0/3/3/3
42	PSU	2	1361	42	-	2/7/25/26	0/2/2/2
41	PSU	1	1011	42,41	-	1/7/25/26	0/2/2/2
41	OMU	1	845	41	-	0/9/27/28	0/2/2/2
20	PSU	S1	1192	20	-	2/7/25/26	0/2/2/2
42	PSU	2	78	42	-	2/7/25/26	0/2/2/2
42	PSU	2	1413	42	-	0/7/25/26	0/2/2/2
41	OMC	1	1552	41	-	0/9/27/28	0/2/2/2
20	OMC	S1	2140	20	-	2/9/27/28	0/2/2/2

The worst 5 of 1200 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S1	607	PSU	C6-C5	12.67	1.49	1.35
20	S1	33	PSU	C6-C5	12.30	1.48	1.35
20	S1	1156	PSU	C6-C5	12.28	1.48	1.35
20	S1	1246	PSU	C6-C5	12.25	1.48	1.35
41	1	1011	PSU	C6-C5	12.25	1.48	1.35

The worst 5 of 1070 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	2185	MA6	N1-C6-N6	-10.25	104.36	116.86
20	S1	2184	MA6	N1-C6-N6	-9.80	104.91	116.86
41	1	959	OMG	C1'-N9-C8	-7.91	104.27	126.73
20	S1	2151	OMG	C1'-N9-C8	-7.71	104.83	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	S1	1623	OMG	C1'-N9-C8	-7.70	104.85	126.73

There are no chirality outliers.

5 of 138 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	7	69	PSU	O4'-C1'-C5-C4
44	7	69	PSU	O4'-C1'-C5-C6
44	7	162	A2M	C1'-C2'-O2'-CM'
20	S1	33	PSU	C3'-C4'-C5'-O5'
20	S1	33	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

48 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	S1	2048	OMU	1	0
20	S1	1995	G7M	1	0
42	2	1403	PSU	2	0
41	1	437	A2M	1	0
42	2	95	A2M	1	0
20	S1	1621	OMU	1	0
42	2	506	PSU	2	0
42	2	1046	OMG	1	0
20	S1	2061	5MC	2	0
41	1	695	OMC	1	0
42	2	1419	OMU	1	0
20	S1	1657	PSU	2	0
42	2	665	A2M	2	0
42	2	628	A2M	1	0
42	2	510	PSU	2	0
20	S1	479	A2M	1	0
42	2	626	PSU	1	0
20	S1	2185	MA6	1	0
42	2	443	OMC	1	0
20	S1	2184	MA6	1	0
42	2	1318	PSU	1	0
42	2	560	OMU	1	0
44	7	162	A2M	1	0
42	2	1382	PSU	1	0
41	1	697	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	S1	2202	PSU	1	0
41	1	847	OMU	1	0
81	3	13	OMU	1	0
42	2	500	PSU	1	0
20	S1	512	A2M	1	0
42	2	1308	5MC	2	0
20	S1	98	A2M	1	0
42	2	591	A2M	2	0
20	S1	1833	OMU	1	0
42	2	604	A2M	1	0
20	S1	1566	PSU	1	0
42	2	382	A2M	3	0
20	S1	18	OMC	1	0
20	S1	1829	OMG	2	0
41	1	1659	OMU	1	0
41	1	959	OMG	2	0
42	2	504	PSU	2	0
20	S1	1246	PSU	1	0
44	7	75	OMG	1	0
41	1	1011	PSU	2	0
41	1	845	OMU	1	0
42	2	78	PSU	1	0
42	2	1413	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 144 ligands modelled in this entry, 144 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	1	2
15	S4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S4	7:A	O3'	65:G	P	19.26
1	1	1097:A	O3'	1100:C	P	10.20
1	1	552:G	O3'	554:A	P	4.04

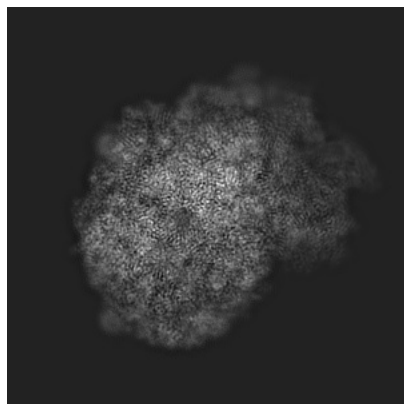
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15272. These allow visual inspection of the internal detail of the map and identification of artifacts.

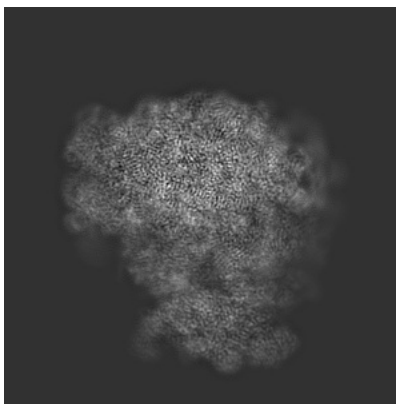
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

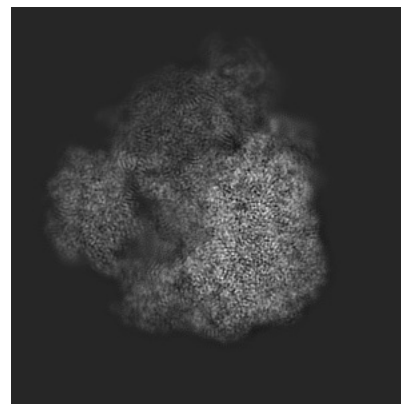
#### 6.1.1 Primary map



X

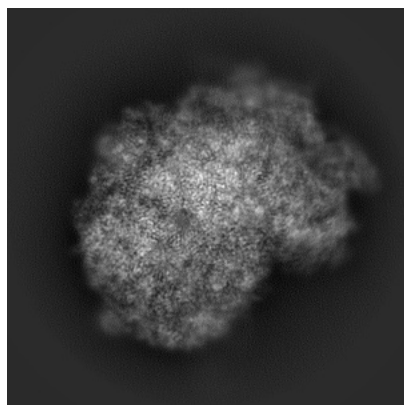


Y

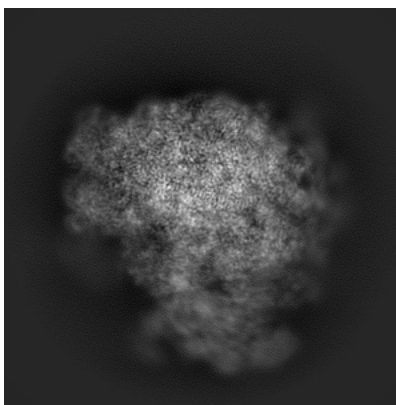


Z

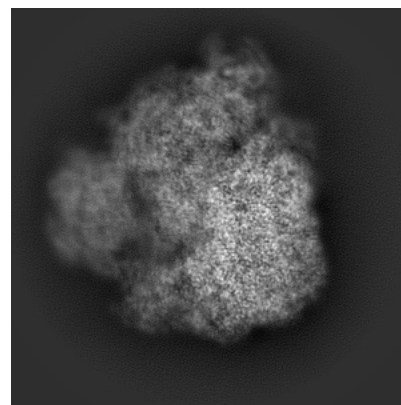
#### 6.1.2 Raw map



X



Y

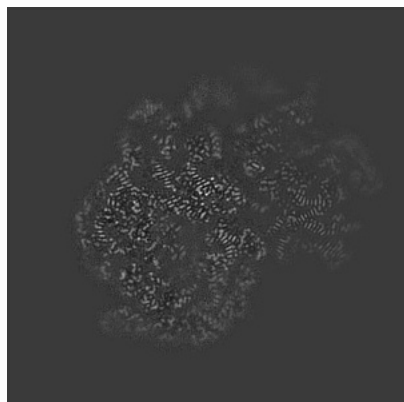


Z

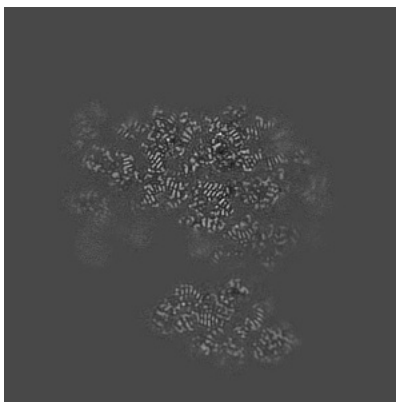
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

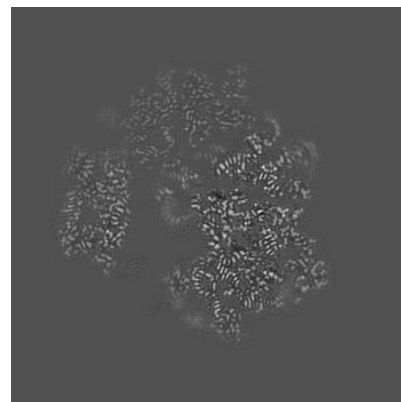
### 6.2.1 Primary map



X Index: 220

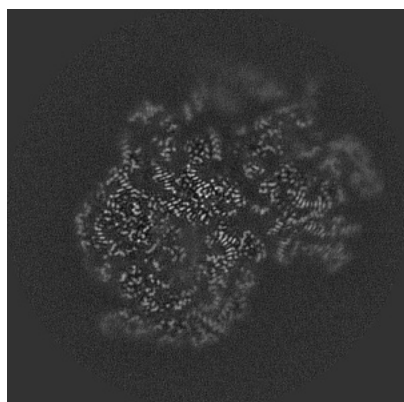


Y Index: 220

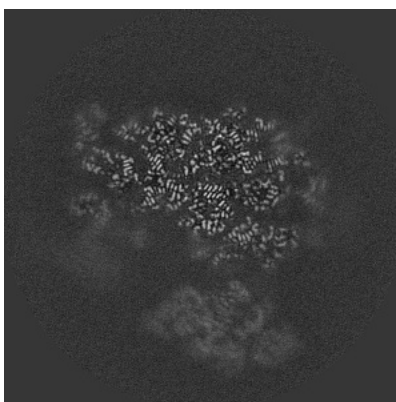


Z Index: 220

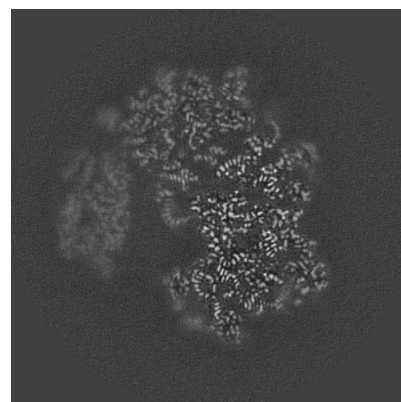
### 6.2.2 Raw map



X Index: 220



Y Index: 220

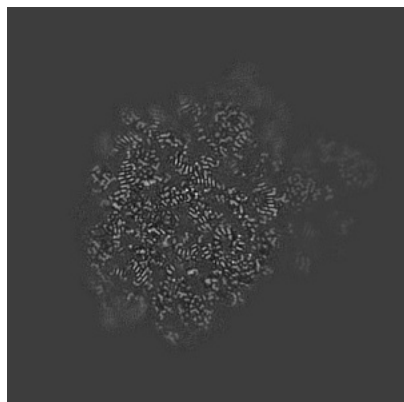


Z Index: 220

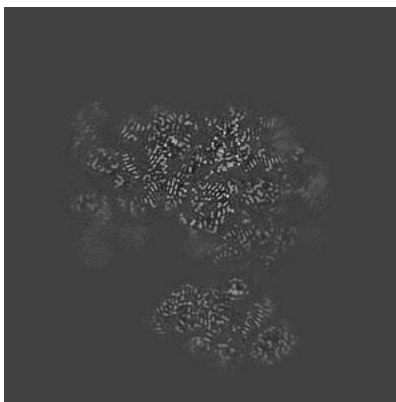
The images above show central slices of the map in three orthogonal directions.

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

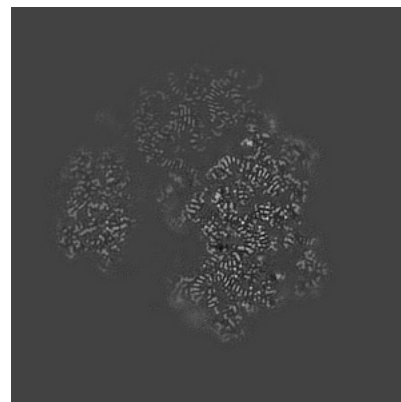
### 6.3.1 Primary map



X Index: 265

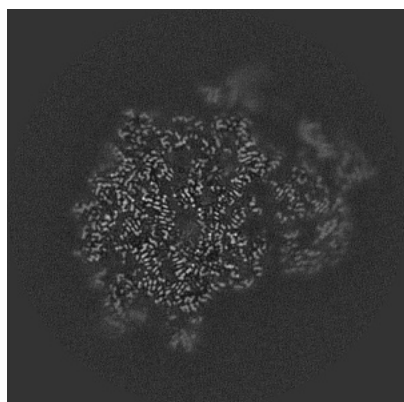


Y Index: 222

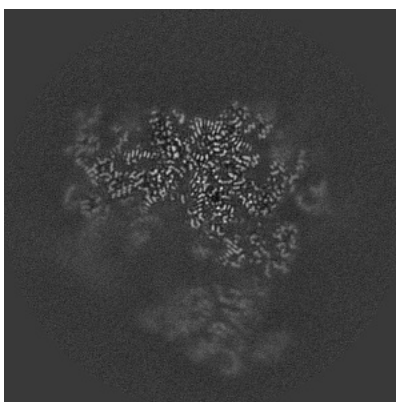


Z Index: 226

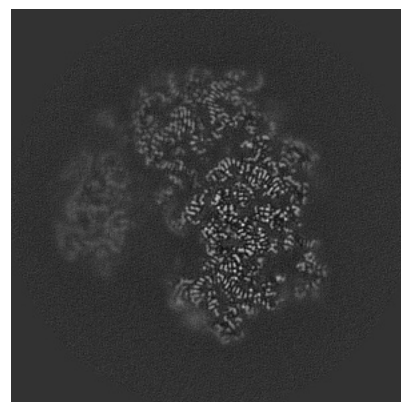
### 6.3.2 Raw map



X Index: 249



Y Index: 212

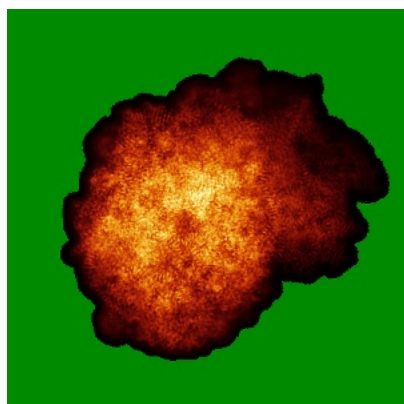


Z Index: 226

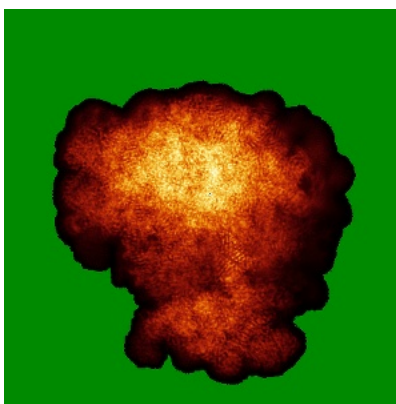
The images above show the largest variance slices of the map in three orthogonal directions.

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

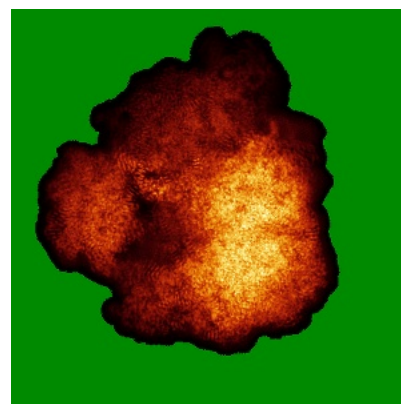
### 6.4.1 Primary map



X

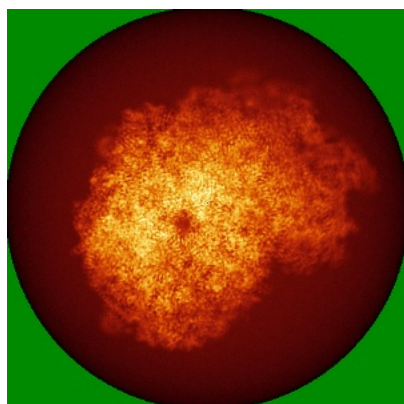


Y

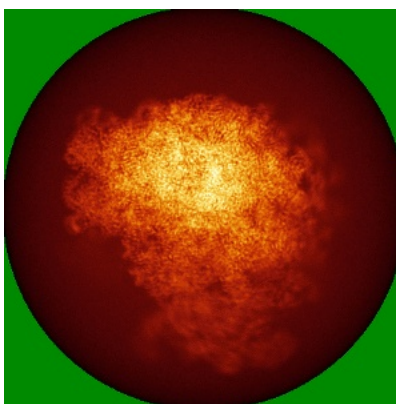


Z

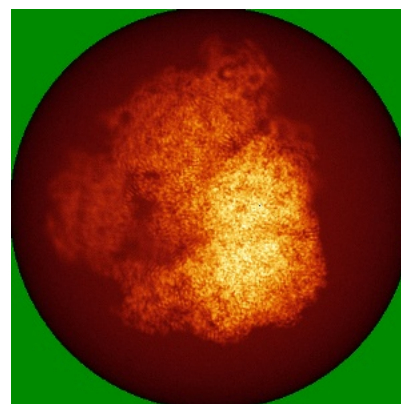
### 6.4.2 Raw map



X



Y

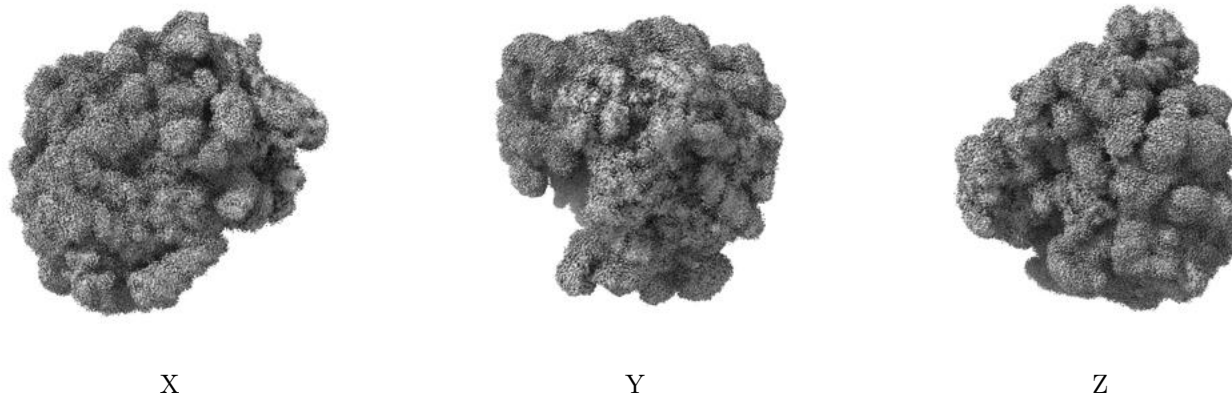


Z

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

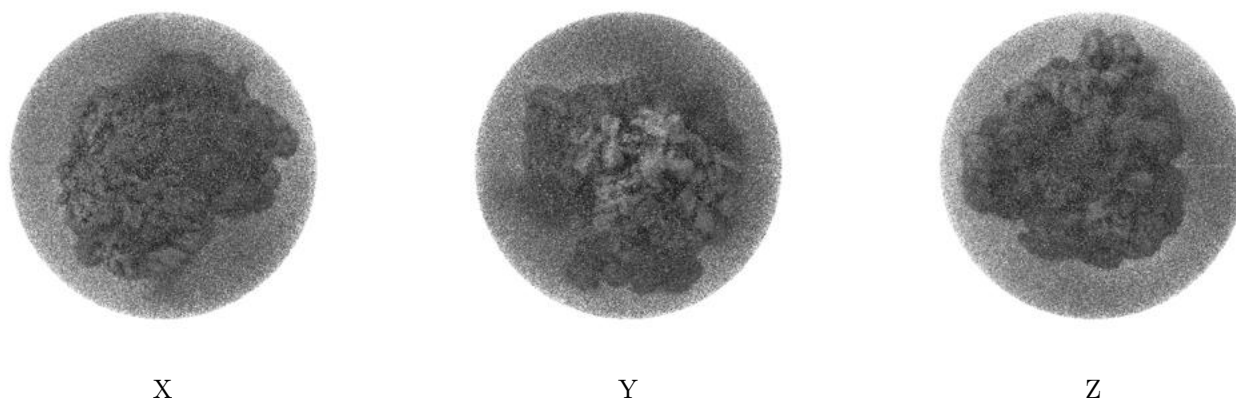
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

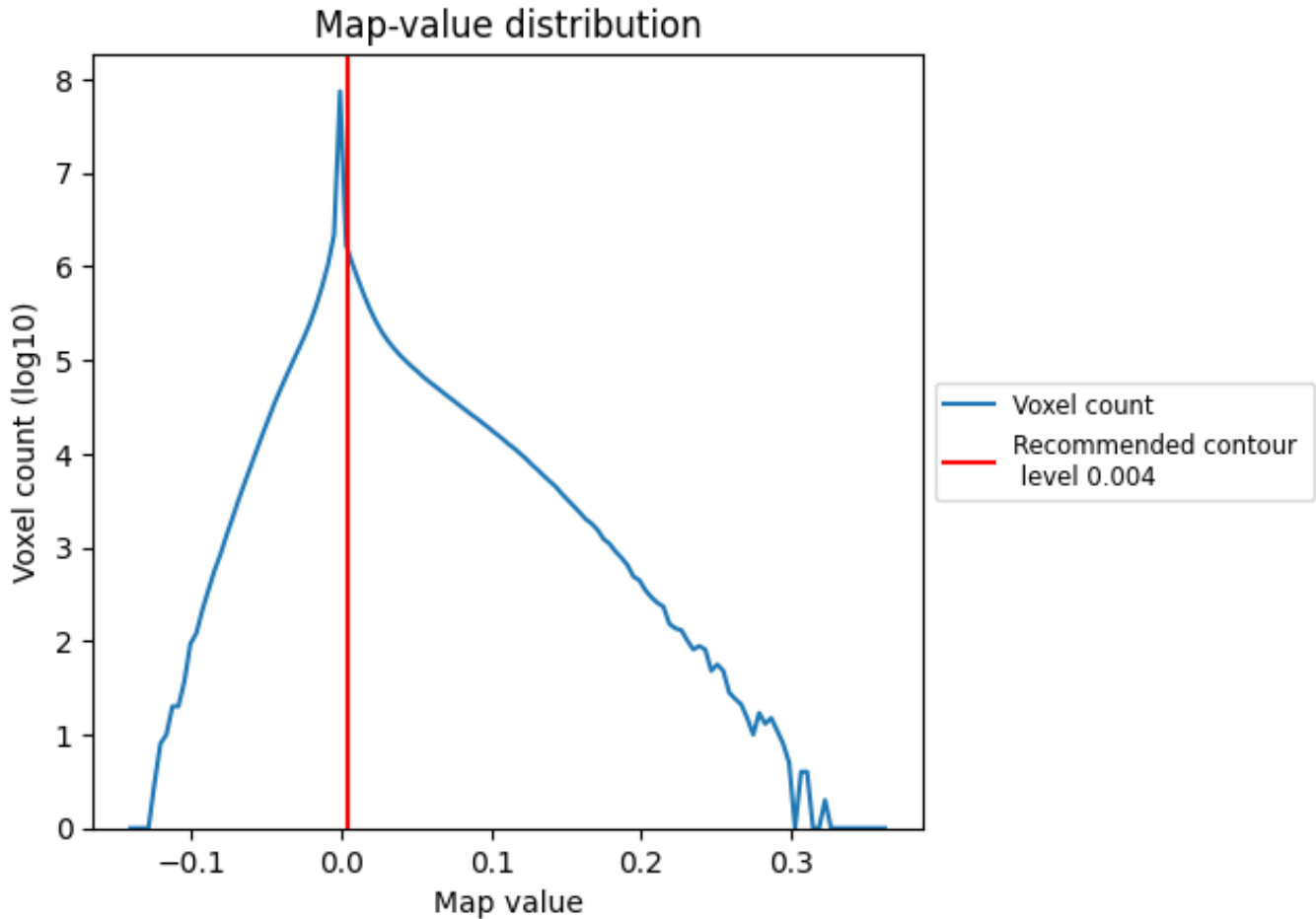
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

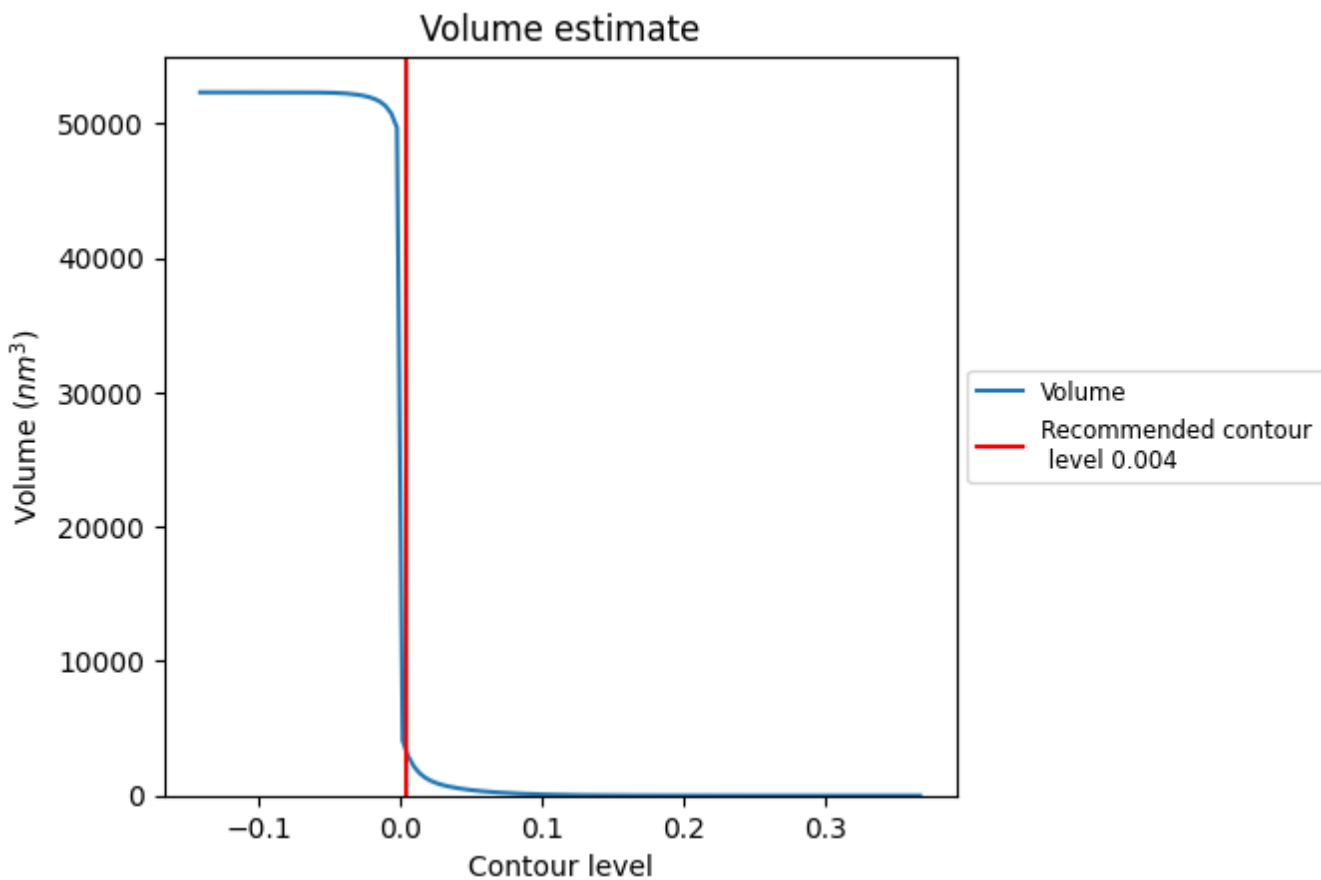
This section contains the results of statistical analysis of the map.

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



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

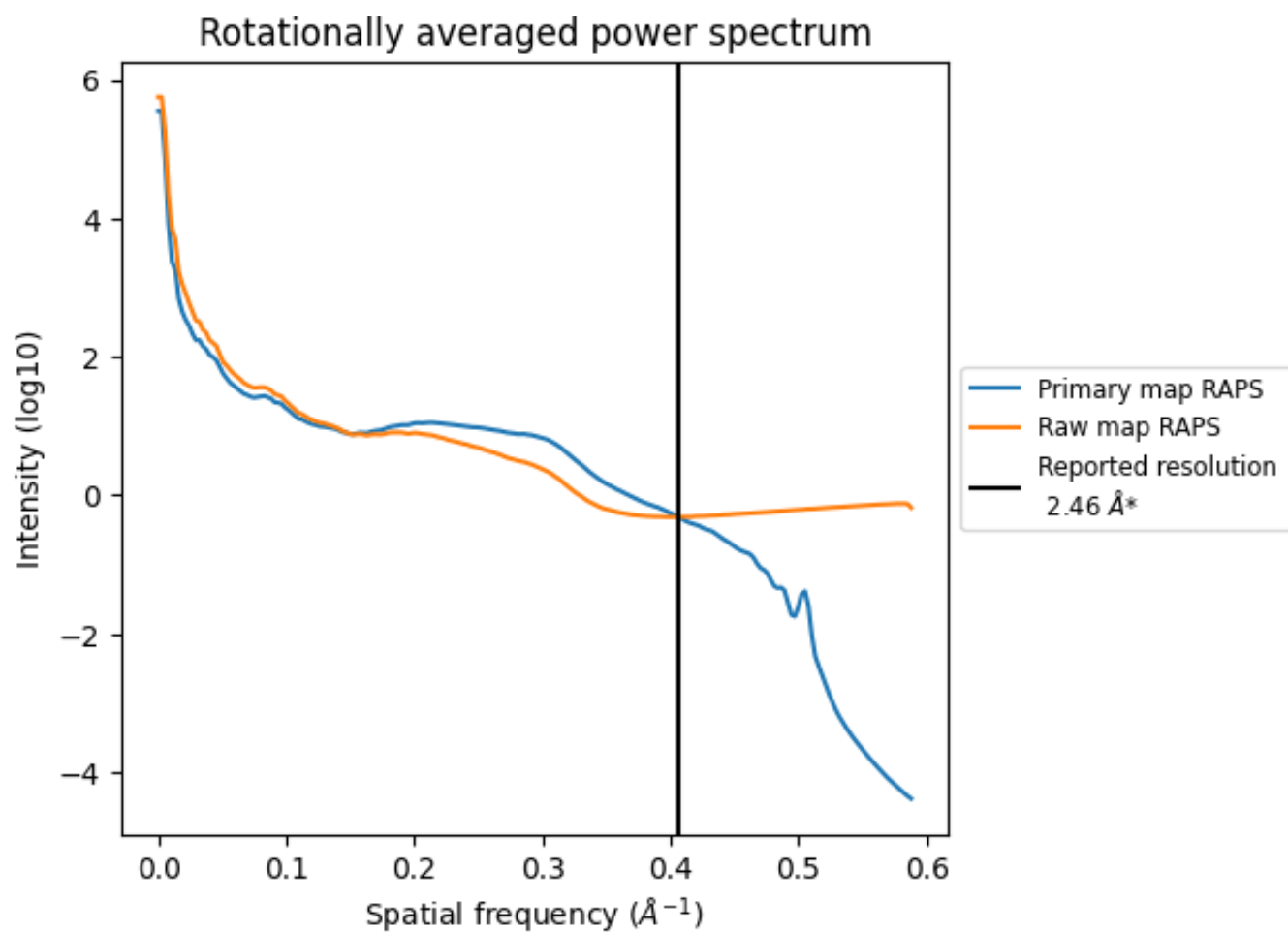
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3475  $\text{nm}^3$ ; this corresponds to an approximate mass of 3139 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

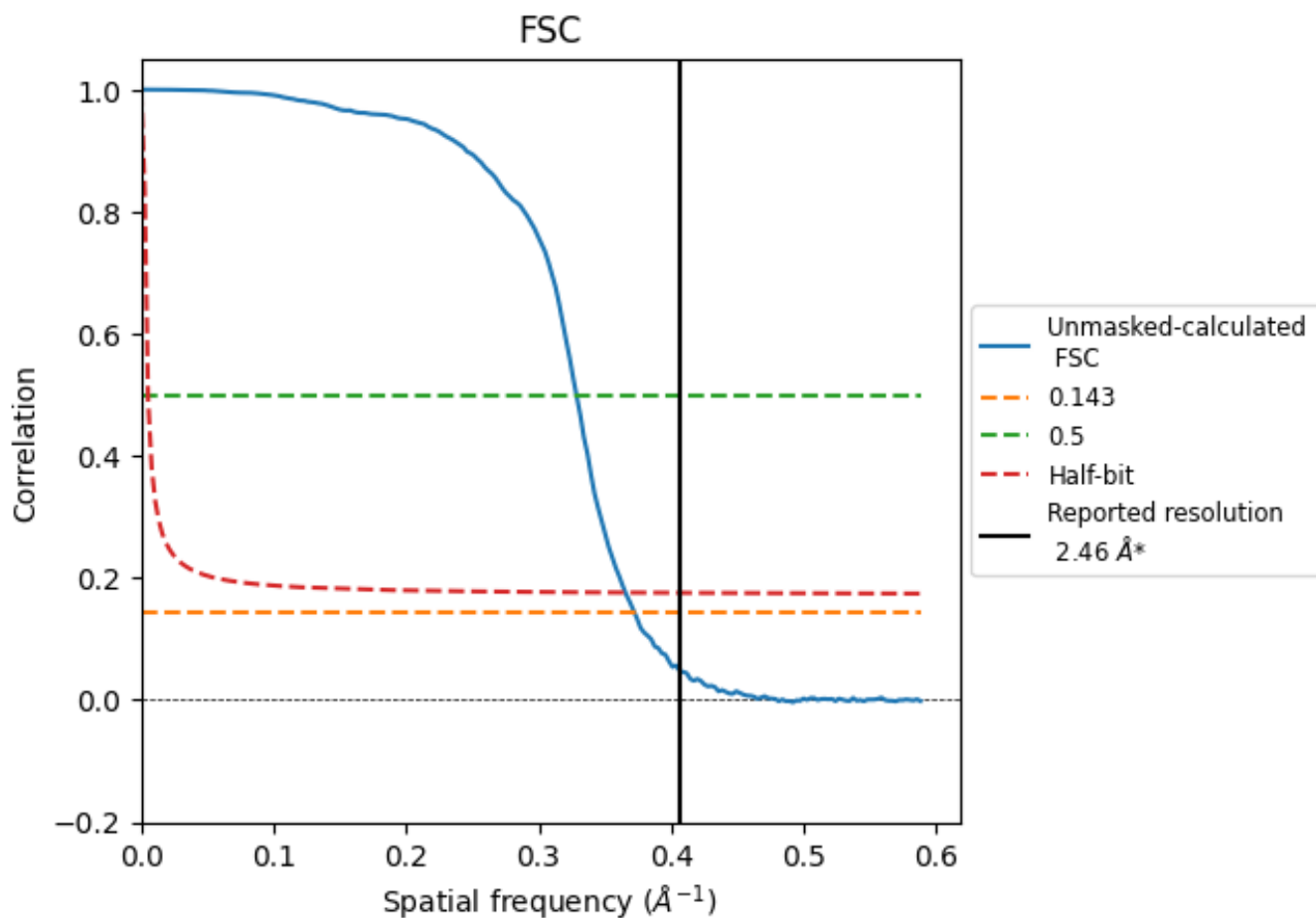


\*Reported resolution corresponds to spatial frequency of 0.407 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.407 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

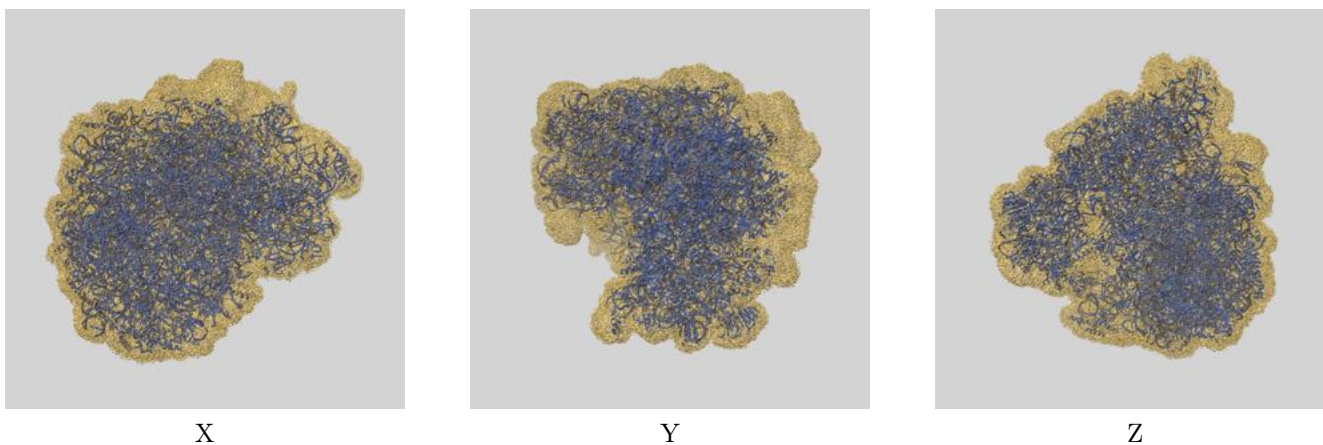
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.69	3.04	2.74

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

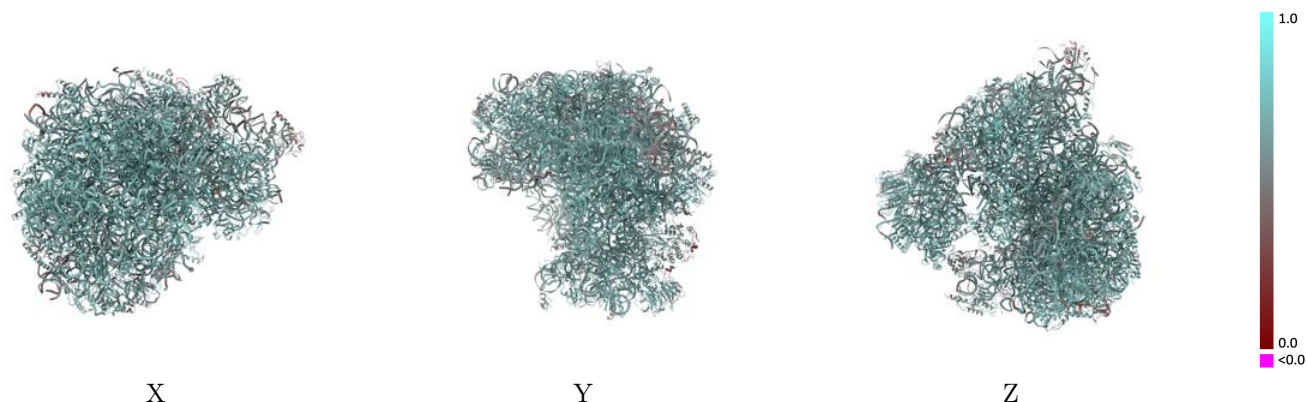
This section contains information regarding the fit between EMDB map EMD-15272 and PDB model 8A98. Per-residue inclusion information can be found in section 3 on page 24.

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



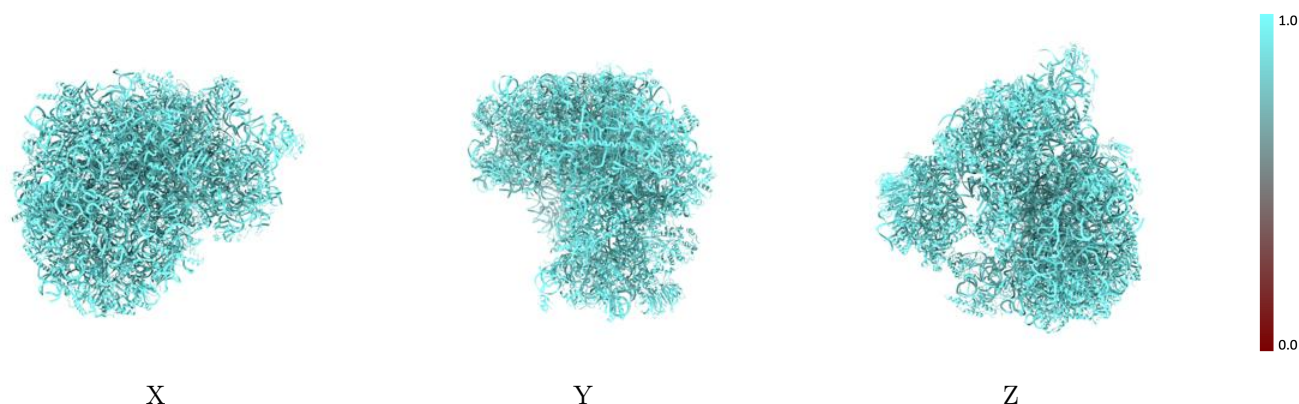
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



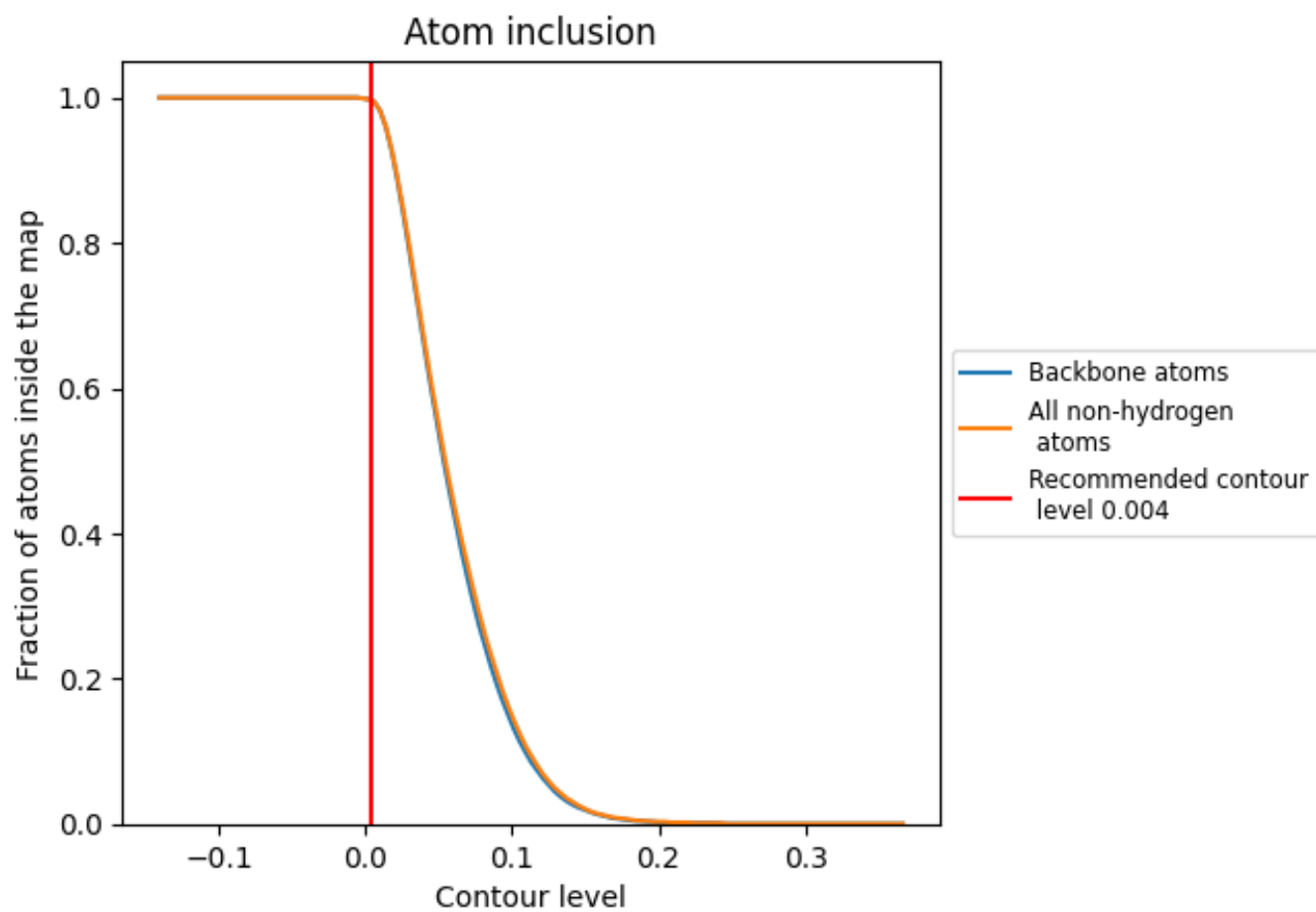
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9970	 0.6530
1	 0.9990	 0.6610
2	 0.9980	 0.6570
3	 0.9960	 0.6410
4	 0.9980	 0.6440
5	 0.9990	 0.6550
6	 0.9980	 0.6150
7	 1.0000	 0.6800
8	 0.9990	 0.6120
A	 1.0000	 0.7100
B	 0.9990	 0.6990
C	 0.9990	 0.6740
D	 0.9980	 0.5280
E	 0.9990	 0.5910
F	 0.9980	 0.6430
G	 0.9970	 0.6500
H	 0.9990	 0.6910
I	 0.9980	 0.6740
J	 0.9990	 0.6930
K	 0.9990	 0.6320
L	 0.9990	 0.7010
M	 0.9990	 0.7190
O	 1.0000	 0.6070
P	 0.9990	 0.6960
Q	 0.9980	 0.6590
R	 0.9970	 0.6680
S	 1.0000	 0.6660
S1	 0.9960	 0.6450
S4	 0.9950	 0.5650
SA	 0.9950	 0.6520
SB	 0.9890	 0.5470
SC	 1.0000	 0.6260
SD	 0.9850	 0.6420
SE	 0.9940	 0.6700
SF	 0.9910	 0.6410

















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Chain	Atom inclusion	Q-score
SG	 0.9940	 0.6410
SH	 0.9980	 0.6630
SI	 0.9920	 0.6410
SJ	 0.9980	 0.6960
SK	 0.9940	 0.6700
SL	 0.9980	 0.6680
SM	 0.9970	 0.6400
SN	 0.9990	 0.6230
SO	 0.9930	 0.6650
SP	 0.9910	 0.6780
SQ	 0.9940	 0.5380
SR	 0.9990	 0.6660
SS	 0.9950	 0.6510
ST	 0.9930	 0.6780
SU	 0.9970	 0.6860
SV	 0.9640	 0.5630
SW	 1.0000	 0.6660
SX	 0.9990	 0.6700
SY	 0.9730	 0.5840
SZ	 0.9950	 0.6460
Sa	 0.9920	 0.6290
Sb	 1.0000	 0.6550
Sc	 0.9790	 0.5890
Sd	 0.9960	 0.6170
Se	 0.9800	 0.6070
Sg	 0.9950	 0.6100
Sh	 0.9560	 0.4460
T	 0.9990	 0.7110
U	 1.0000	 0.5860
V	 0.9980	 0.6810
W	 0.9990	 0.6710
X	 1.0000	 0.6860
Y	 0.9980	 0.6370
Z	 0.9990	 0.6500
a	 1.0000	 0.6700
b	 1.0000	 0.6880
c	 1.0000	 0.6850
d	 1.0000	 0.6370
e	 0.9940	 0.6450
f	 0.9990	 0.7060
g	 0.9990	 0.6780
h	 0.9990	 0.6630

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Chain	Atom inclusion	Q-score
i	 0.9970	 0.6380
j	 0.9980	 0.7250
k	 0.9960	 0.6300
l	 1.0000	 0.7140
n	 0.9880	 0.6180
o	 0.9960	 0.6780
p	 0.9960	 0.6280