



wwPDB EM Validation Summary Report ⓘ

Sep 29, 2026 – 03:09 pm BST

PDB ID : 9SUL / pdb_00009sul
EMDB ID : EMD-55224
Title : CRYO-EM STRUCTURE OF TRYPANOSOMA BRUCEI BLOODSTREAM
FORM 80S RIBOSOME
Authors : Rajan, K.S.; Yonath, A.
Deposited on : 2025-09-29
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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) : 2.51

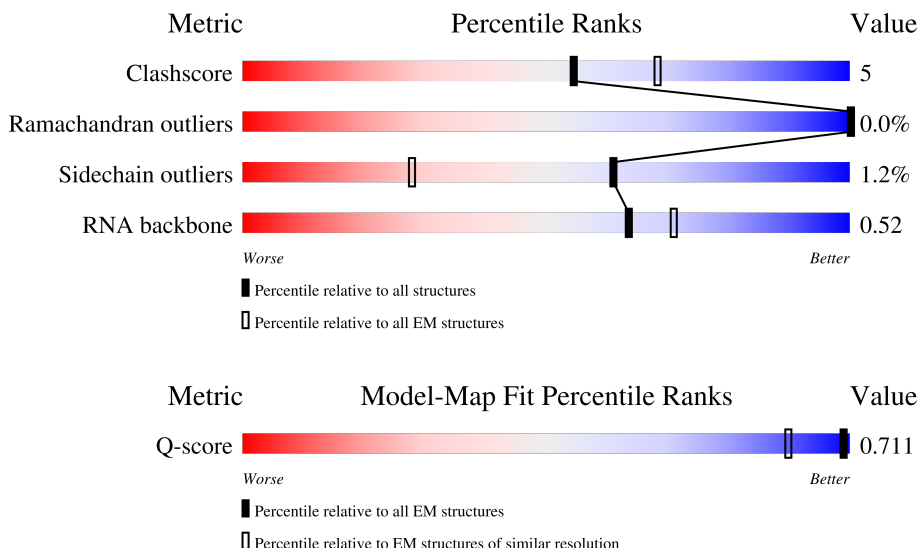
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.10 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.



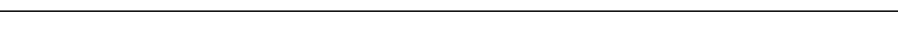
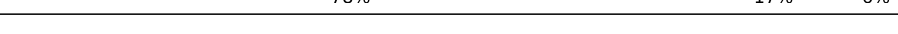
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2317 (1.60 - 2.60)

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

Mol	Chain	Length	Quality of chain
1	Et	95	
2	A0	256	
3	A1	273	

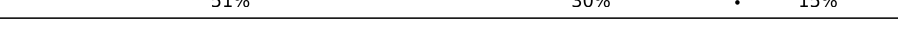
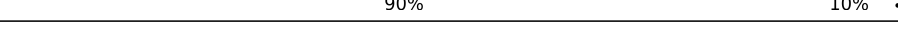
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Mol	Chain	Length	Quality of chain
4	A2	190	 81% 15% .
5	A3	250	 79% 16% 5%
6	A4	202	 82% 16% .
7	A5	220	 83% 5% 13%
8	A6	190	 83% 13% 5%
9	A7	318	 74% 22% . .
10	A8	57	 84% 14% .
11	A9	153	 39% 7% 54%
12	AA	2280	 45% 32% 5% 18%
13	AC	277	 60% 16% 25%
14	AD	172	 51% 7% 42%
15	AE	174	 84% . . 12%
16	AF	144	 10% 60% 22% 18%
17	AG	151	 85% 13% .
18	AH	144	 78% 17% 6%
19	AI	152	 64% 15% 20%
20	AJ	130	 90% 9% .
21	AK	149	 83% 11% . 5%
22	AL	142	 77% 9% . 13%
23	AM	153	 70% 12% . 18%
24	AO	167	 79% 13% 8%
25	AP	266	 71% 10% 18%
26	AQ	117	 61% 21% . 15%
27	AR	194	 39% 7% 54%
28	AS	143	 85% 12% . .

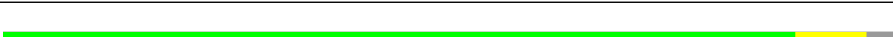
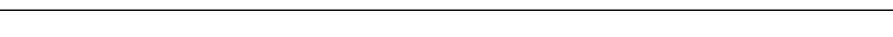
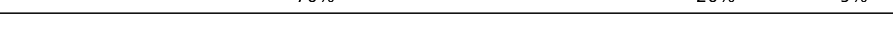
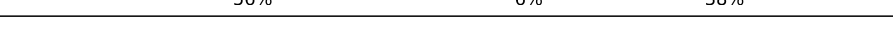
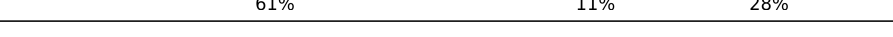
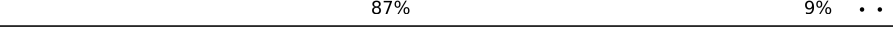
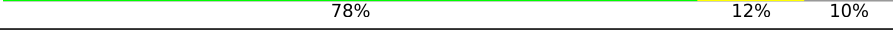
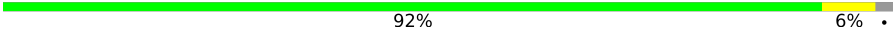
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Mol	Chain	Length	Quality of chain
29	AT	137	
30	AU	113	
31	AV	111	
32	AW	86	
33	AX	214	
34	AY	66	
35	AZ	103	
36	Az	279	
37	BA	1866	
38	BB	1544	
39	BC	209	
40	BD	120	
41	BE	217	
42	BF	78	
43	BG	183	
44	BH	136	
45	BI	193	
46	BK	213	
47	BL	194	
48	BN	218	
49	BO	222	
50	BP	189	
51	BQ	221	
52	BR	166	
53	BS	179	

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Mol	Chain	Length	Quality of chain
54	BT	260	
55	BU	159	
56	BV	130	
57	BW	139	
58	BX	164	
59	BY	125	
60	BZ	143	
61	Ba	133	
62	Bb	145	
63	Bc	146	
64	Bd	71	
65	Be	260	
66	Bf	429	
67	Bg	105	
68	Bh	188	
69	Bi	132	
70	Bj	170	
71	Bk	127	
72	Bl	149	
73	Bm	109	
74	Bn	84	
75	Bo	93	
76	Bp	82	
77	Bq	51	
78	Br	374	

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Mol	Chain	Length	Quality of chain
79	Bs	128	
80	Bt	106	
81	Bu	308	
82	Bv	192	
83	Bw	257	
84	Bx	276	
85	By	189	
86	Bz	34	

2 Entry composition

There are 95 unique types of molecules in this entry. The entry contains 211479 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 E-SITE TRNA.

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

- Molecule 2 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A0	223	Total	C	N	O	S	0	0
			1814	1143	341	322	8		

- Molecule 3 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A1	262	Total	C	N	O	S	0	0
			2062	1306	388	359	9		

- Molecule 4 is a protein called 40S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A2	183	Total	C	N	O	S	0	0
			1458	912	279	262	5		

- Molecule 5 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A3	238	Total	C	N	O	S	0	0
			1899	1179	393	323	4		

- Molecule 6 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A4	198	Total	C	N	O	S	0	0
			1642	1044	317	276	5		

- Molecule 7 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A5	192	Total	C	N	O	S	0	0
			1536	967	308	259	2		

- Molecule 8 is a protein called Probable 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A6	181	Total	C	N	O	S	0	0
			1495	941	301	245	8		

- Molecule 9 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A7	309	Total	C	N	O	S	0	0
			2374	1485	421	457	11		

- Molecule 10 is a protein called Putative ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A8	56	Total	C	N	O	S	0	0
			461	284	97	75	5		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A8	5	HIS	ASP	conflict	UNP G0UD55
A8	19	SER	ALA	conflict	UNP G0UD55
A8	50	ASN	HIS	conflict	UNP G0UD55

- Molecule 11 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A9	70	Total	C	N	O	S	0	1
			567	361	109	92	5		

- Molecule 12 is a RNA chain called SSU rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AA	1880	Total	C	N	O	P	1	0
			40169	17963	7203	13122	1881		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AC	208	Total	C	N	O	S	0	0
			1648	1049	297	291	11		

- Molecule 14 is a protein called 40S ribosomal protein S10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AD	99	Total	C	N	O	S	0	0
			814	531	140	139	4		

- Molecule 15 is a protein called 40S ribosomal proteins S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AE	153	Total	C	N	O	S	0	0
			1251	783	253	210	5		

- Molecule 16 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AF	118	Total	C	N	O	S	0	0
			922	565	167	182	8		

- Molecule 17 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AG	149	Total	C	N	O	S	0	0
			1193	749	235	202	7		

- Molecule 18 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AH	136	Total	C	N	O	S	0	0
			1015	623	195	188	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AH	131	IAS	ASP	conflict	UNP P19800

- Molecule 19 is a protein called 40S ribosomal protein S15, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AI	121	Total	C	N	O	S	0	0
			967	614	189	161	3		

- Molecule 20 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AJ	129	Total	C	N	O	S	0	0
			1018	645	191	174	8		

- Molecule 21 is a protein called 40S ribosomal protein S16, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AK	142	Total	C	N	O	S	0	0
			1144	731	215	195	3		

- Molecule 22 is a protein called 40S ribosomal protein S17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AL	124	Total	C	N	O	S	0	0
			967	614	188	160	5		

- Molecule 23 is a protein called 40S ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AM	126	Total	C	N	O	S	0	0
			1027	647	197	179	4		

- Molecule 24 is a protein called Ribosomal protein S19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AO	154	Total	C	N	O	S	0	0
			1220	770	242	199	9		

- Molecule 25 is a protein called 40S ribosomal protein S2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AP	218	Total	C	N	O	S	0	0
			1688	1078	298	303	9		

- Molecule 26 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AQ	100	Total	C	N	O	S	0	0
			800	501	152	144	3		

- Molecule 27 is a protein called 40S ribosomal protein S21, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AR	89	Total	C	N	O	S	0	0
			668	415	120	130	3		

- Molecule 28 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AS	140	Total	C	N	O	S	1	0
			1107	702	216	187	2		

- Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AT	129	Total	C	N	O	S	0	0
			1034	659	202	170	3		

- Molecule 30 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AU	73	Total	C	N	O	S	0	0
			569	362	102	100	5		

- Molecule 31 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AV	103	Total	C	N	O	S	0	0
			830	512	175	135	8		

- Molecule 32 is a protein called 40S ribosomal protein S27, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	AW	85	Total	C	N	O	S	0	0
			660	411	124	116	9		

- Molecule 33 is a protein called 40S ribosomal protein S3, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	AX	208	Total	C	N	O	S	0	0
			1652	1036	310	294	12		

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	AY	58	Total	C	N	O	S	0	0
			466	293	96	76	1		

- Molecule 35 is a protein called 40S ribosomal protein S33, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AZ	59	Total	C	N	O	S	0	0
			457	277	95	81	4		

- Molecule 36 is a protein called RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Az	174	Total	C	N	O	S	0	0
			1366	862	258	245	1		

- Molecule 37 is a RNA chain called LSUa rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BA	1541	Total	C	N	O	P	0	0
			33019	14754	6007	10717	1541		

- Molecule 38 is a RNA chain called LSUb rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BB	1123	Total	C	N	O	P	0	0
			23998	10736	4295	7844	1123		

- Molecule 39 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BC	160	Total	C	N	O	P	0	0
			3411	1529	610	1113	159		

- Molecule 40 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BD	120	Total	C	N	O	P	0	0
			2553	1140	452	842	119		

- Molecule 41 is a RNA chain called SrRNA-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BE	183	Total	C	N	O	P	0	0
			3879	1734	675	1287	183		

- Molecule 42 is a RNA chain called SrRNA-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BF	76	Total	C	N	O	P	0	0
			1587	710	258	543	76		

- Molecule 43 is a RNA chain called SrRNA-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BG	183	Total	C	N	O	P	0	0
			3919	1746	708	1282	183		

- Molecule 44 is a RNA chain called SrRNA-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BH	115	Total	C	N	O	P	0	0
			2458	1095	442	806	115		

- Molecule 45 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BI	192	Total	C	N	O	S	0	0
			1526	956	315	247	8		

- Molecule 46 is a protein called 60S ribosomal protein L10, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BK	194	Total	C	N	O	S	0	0
			1588	1002	314	260	12		

- Molecule 47 is a protein called 60S ribosomal protein L11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BL	174	Total	C	N	O	S	0	0
			1385	873	259	246	7		

- Molecule 48 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BN	215	Total	C	N	O	S	0	0
			1762	1097	365	294	6		

- Molecule 49 is a protein called 60S ribosomal protein L13a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BO	221	Total	C	N	O	S	0	0
			1802	1141	364	290	7		

- Molecule 50 is a protein called 40S ribosomal protein L14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BP	177	Total	C	N	O	S	0	0
			1411	889	278	240	4		

- Molecule 51 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BQ	203	Total	C	N	O	S	0	0
			1717	1077	370	265	5		

- Molecule 52 is a protein called 60S ribosomal protein L17, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BR	154	Total	C	N	O	S	0	0
			1244	782	246	208	8		

- Molecule 53 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BS	177	Total	C	N	O	S	0	0
			1462	921	290	244	7		

- Molecule 54 is a protein called 60S ribosomal protein L19, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BT	200	Total	C	N	O	S	0	0
			1644	1010	361	265	8		

- Molecule 55 is a protein called 60S ribosomal protein L21E, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BU	158	Total	C	N	O	S	0	0
			1261	802	247	206	6		

- Molecule 56 is a protein called 60S ribosomal protein L22, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BV	115	Total	C	N	O	S	0	0
			940	604	173	160	3		

- Molecule 57 is a protein called 60S ribosomal protein L23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BW	132	Total	C	N	O	S	0	0
			999	634	189	171	5		

- Molecule 58 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BX	118	Total	C	N	O	S	0	0
			966	614	182	168	2		

- Molecule 59 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BY	63	Total	C	N	O	S	0	0
			542	353	107	78	4		

- Molecule 60 is a protein called 60S ribosomal protein L26, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BZ	122	Total	C	N	O	S	1	0
			1002	619	213	165	5		

- Molecule 61 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	Ba	133	Total	C	N	O	S	0	0
			1099	696	223	176	4		

- Molecule 62 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	Bb	144	Total	C	N	O	S	0	0
			1137	717	228	186	6		

- Molecule 63 is a protein called 60S ribosomal protein L28, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Bc	144	Total	C	N	O	S	0	0
			1162	723	234	197	8		

- Molecule 64 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	Bd	69	Total	C	N	O	S	0	0
			561	343	126	91	1		

- Molecule 65 is a protein called 60S ribosomal protein L2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Be	254	Total	C	N	O	S	2	0
			1939	1205	399	322	13		

- Molecule 66 is a protein called Ribosomal protein L3, mitochondrial, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Bf	400	Total	C	N	O	S	0	0
			3212	2024	633	542	13		

- Molecule 67 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Bg	96	Total	C	N	O	S	0	0
			736	459	132	140	5		

- Molecule 68 is a protein called 60S ribosomal subunit protein L31, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Bh	117	Total	C	N	O	S	0	0
			953	609	190	151	3		

- Molecule 69 is a protein called 60S ribosomal protein L32, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bi	131	Total	C	N	O	S	0	0
			1075	678	217	176	4		

- Molecule 70 is a protein called 60S ribosomal protein L34, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bj	122	Total	C	N	O	S	0	0
			1006	620	227	155	4		

- Molecule 71 is a protein called 60S ribosomal protein L35, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bk	123	Total	C	N	O	S	0	0
			1014	636	217	158	3		

- Molecule 72 is a protein called 60S ribosomal protein L35A, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Bl	144	Total	C	N	O	S	0	0
			1163	728	239	193	3		

- Molecule 73 is a protein called Ribosomal protein L36, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bm	98	Total	C	N	O	S	0	0
			786	493	164	127	2		

- Molecule 74 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bn	82	Total	C	N	O	S	0	0
			693	422	160	105	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bo	89	Total	C	N	O	S	0	0
			699	434	144	115	6		

- Molecule 76 is a protein called 60S ribosomal protein L38, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bp	77	Total	C	N	O	S	0	0
			622	390	124	104	4		

- Molecule 77 is a protein called 60S ribosomal protein L39, putative.

Mol	Chain	Residues	Atoms				AltConf	Trace
77	Bq	50	Total	C	N	O	0	0
			457	297	98	62		

- Molecule 78 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Br	332	Total	C	N	O	S	0	0
			2607	1634	513	445	15		

- Molecule 79 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bs	50	Total	C	N	O	S	0	0
			392	247	80	60	5		

- Molecule 80 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bt	97	Total	C	N	O	S	0	0
			801	507	159	130	5		

- Molecule 81 is a protein called 60S ribosomal protein L5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bu	303	Total	C	N	O	S	0	0
			2395	1510	456	423	6		

- Molecule 82 is a protein called 60S ribosomal protein L6, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Bv	144	Total	C	N	O	S	0	0
			1106	701	203	199	3		

- Molecule 83 is a protein called 60S ribosomal protein L7, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Bw	227	Total	C	N	O	S	0	0
			1844	1172	355	309	8		

- Molecule 84 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bx	235	Total	C	N	O	S	0	0
			1875	1178	369	322	6		

- Molecule 85 is a protein called 60S ribosomal protein L9, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	By	186	Total	C	N	O	S	0	0
			1515	961	281	269	4		

- Molecule 86 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Bz	33	Total	C	N	O	S	0	0
			289	175	75	37	2		

- Molecule 87 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

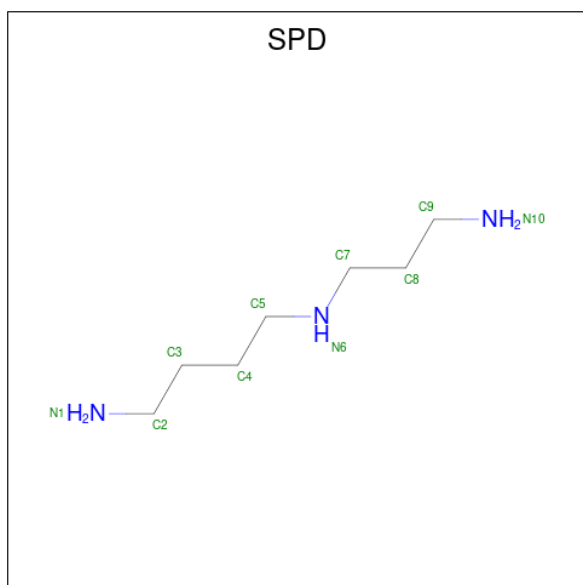
Mol	Chain	Residues	Atoms		AltConf
87	A3	1	Total	Mg	0
			1	1	
87	AA	40	Total	Mg	0
			40	40	
87	AO	1	Total	Mg	0
			1	1	
87	AV	1	Total	Mg	0
			1	1	
87	BA	92	Total	Mg	0
			92	92	
87	BB	66	Total	Mg	0
			66	66	

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Mol	Chain	Residues	Atoms		AltConf
87	BC	4	Total 4	Mg 4	0
87	BD	1	Total 1	Mg 1	0
87	BE	1	Total 1	Mg 1	0
87	BF	2	Total 2	Mg 2	0
87	BG	8	Total 8	Mg 8	0
87	BK	1	Total 1	Mg 1	0
87	BQ	2	Total 2	Mg 2	0
87	BR	1	Total 1	Mg 1	0
87	BU	1	Total 1	Mg 1	0
87	BW	1	Total 1	Mg 1	0
87	Bi	1	Total 1	Mg 1	0

- Molecule 88 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
88	A6	1	Total	C	N	0
			10	7	3	
88	AA	1	Total	C	N	0
			10	7	3	
88	AA	1	Total	C	N	0
			10	7	3	
88	AA	1	Total	C	N	0
			10	7	3	
88	AA	1	Total	C	N	0
			10	7	3	
88	AA	1	Total	C	N	0
			10	7	3	
88	AA	1	Total	C	N	0
			10	7	3	
88	AA	1	Total	C	N	0
			10	7	3	
88	AA	1	Total	C	N	0
			10	7	3	
88	AA	1	Total	C	N	0
			10	7	3	
88	AA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	

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Mol	Chain	Residues	Atoms			AltConf
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	

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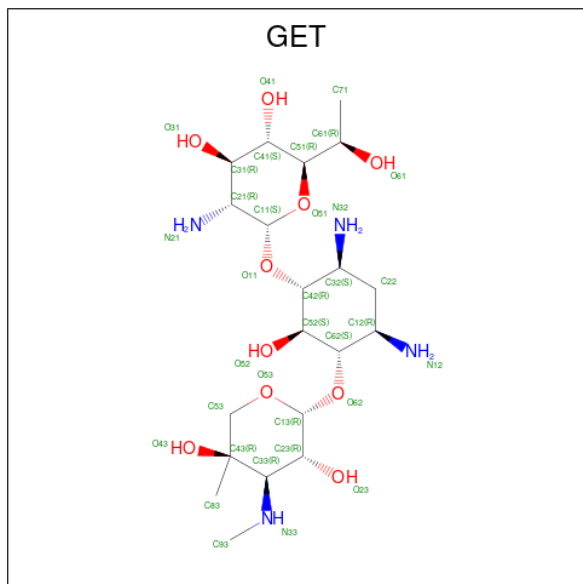
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Mol	Chain	Residues	Atoms			AltConf
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BA	1	Total	C	N	0
			10	7	3	
88	BB	1	Total	C	N	0
			10	7	3	
88	BB	1	Total	C	N	0
			10	7	3	
88	BB	1	Total	C	N	0
			10	7	3	
88	BB	1	Total	C	N	0
			10	7	3	
88	BB	1	Total	C	N	0
			10	7	3	
88	BB	1	Total	C	N	0
			10	7	3	
88	BB	1	Total	C	N	0
			10	7	3	
88	BC	1	Total	C	N	0
			10	7	3	
88	BC	1	Total	C	N	0
			10	7	3	
88	BC	1	Total	C	N	0
			10	7	3	
88	BE	1	Total	C	N	0
			10	7	3	
88	BG	1	Total	C	N	0
			10	7	3	
88	BG	1	Total	C	N	0
			10	7	3	
88	BQ	1	Total	C	N	0
			10	7	3	
88	Bd	1	Total	C	N	0
			10	7	3	

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

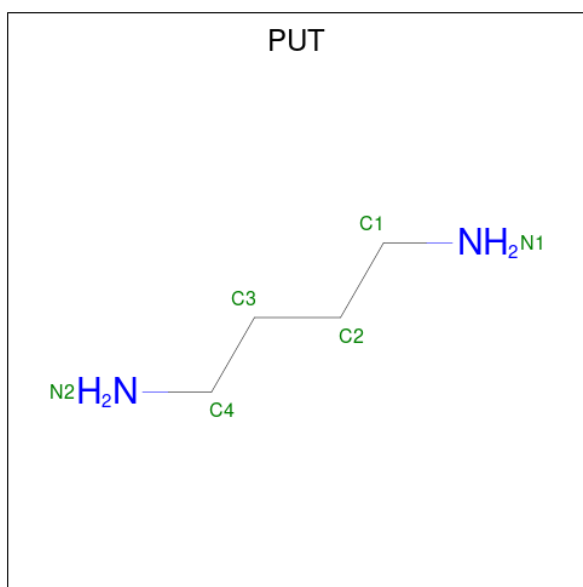
Mol	Chain	Residues	Atoms		AltConf
89	A9	1	Total	Zn	0
			1	1	
89	AV	1	Total	Zn	0
			1	1	
89	Bn	1	Total	Zn	0
			1	1	
89	Bo	1	Total	Zn	0
			1	1	
89	Bs	1	Total	Zn	0
			1	1	
89	Bt	1	Total	Zn	0
			1	1	

- Molecule 90 is GENETICIN (CCD ID: GET) (formula: $C_{20}H_{40}N_4O_{10}$).



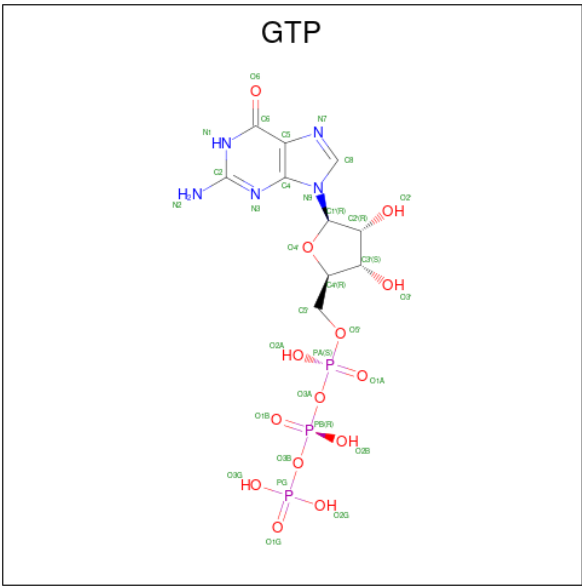
Mol	Chain	Residues	Atoms				AltConf
90	AA	1	Total	C	N	O	0
			34	20	4	10	
90	AA	1	Total	C	N	O	0
			34	20	4	10	
90	AA	1	Total	C	N	O	0
			34	20	4	10	

- Molecule 91 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
91	AA	1	Total	C	N	0
			6	4	2	
91	AA	1	Total	C	N	0
			6	4	2	
91	AA	1	Total	C	N	0
			6	4	2	
91	AA	1	Total	C	N	0
			6	4	2	
91	BA	1	Total	C	N	0
			6	4	2	
91	BA	1	Total	C	N	0
			6	4	2	
91	BA	1	Total	C	N	0
			6	4	2	
91	BA	1	Total	C	N	0
			6	4	2	
91	BA	1	Total	C	N	0
			6	4	2	
91	BB	1	Total	C	N	0
			6	4	2	
91	BB	1	Total	C	N	0
			6	4	2	
91	BB	1	Total	C	N	0
			6	4	2	
91	BB	1	Total	C	N	0
			6	4	2	

- Molecule 92 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
92	AA	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 93 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
93	AA	11	Total	K	0
			11	11	
93	BA	18	Total	K	0
			18	18	
93	BB	23	Total	K	0
			23	23	
93	BC	2	Total	K	0
			2	2	
93	BE	3	Total	K	0
			3	3	
93	BF	1	Total	K	0
			1	1	
93	BG	3	Total	K	0
			3	3	
93	BH	2	Total	K	0
			2	2	
93	BK	1	Total	K	0
			1	1	
93	BN	1	Total	K	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
93	BQ	1	Total K 1 1	0
93	Bb	1	Total K 1 1	0
93	Be	1	Total K 1 1	0
93	Bi	1	Total K 1 1	0

- Molecule 94 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	AltConf
94	AA	5	Total Na 5 5	0
94	BA	1	Total Na 1 1	0
94	BB	10	Total Na 10 10	0
94	Be	1	Total Na 1 1	0

- Molecule 95 is water.

Mol	Chain	Residues	Atoms	AltConf
95	Et	5	Total O 5 5	0
95	A0	2	Total O 2 2	0
95	A5	3	Total O 3 3	0
95	AA	160	Total O 160 160	0
95	AE	1	Total O 1 1	0
95	AG	2	Total O 2 2	0
95	AJ	1	Total O 1 1	0
95	AV	1	Total O 1 1	0
95	AW	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
95	BA	1050	Total 1050	O 1050	0
95	BB	889	Total 889	O 889	0
95	BC	38	Total 38	O 38	0
95	BD	6	Total 6	O 6	0
95	BE	16	Total 16	O 16	0
95	BF	7	Total 7	O 7	0
95	BG	151	Total 151	O 151	0
95	BH	30	Total 30	O 30	0
95	BI	10	Total 10	O 10	0
95	BK	2	Total 2	O 2	0
95	BN	14	Total 14	O 14	0
95	BO	18	Total 18	O 18	0
95	BQ	43	Total 43	O 43	0
95	BR	12	Total 12	O 12	0
95	BT	15	Total 15	O 15	0
95	BU	6	Total 6	O 6	0
95	BW	12	Total 12	O 12	0
95	BX	1	Total 1	O 1	0
95	BY	2	Total 2	O 2	0
95	BZ	2	Total 2	O 2	0
95	Bb	20	Total 20	O 20	0

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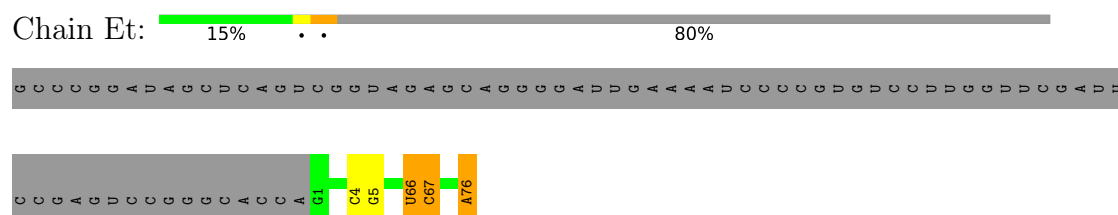
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Mol	Chain	Residues	Atoms		AltConf
95	Bd	5	Total 5	O 5	0
95	Be	49	Total 49	O 49	0
95	Bf	45	Total 45	O 45	0
95	Bh	6	Total 6	O 6	0
95	Bi	18	Total 18	O 18	0
95	Bj	15	Total 15	O 15	0
95	Bl	11	Total 11	O 11	0
95	Bn	17	Total 17	O 17	0
95	Bo	7	Total 7	O 7	0
95	Bq	3	Total 3	O 3	0
95	Br	30	Total 30	O 30	0
95	Bt	6	Total 6	O 6	0
95	Bu	1	Total 1	O 1	0
95	Bv	1	Total 1	O 1	0
95	Bw	11	Total 11	O 11	0
95	Bx	3	Total 3	O 3	0

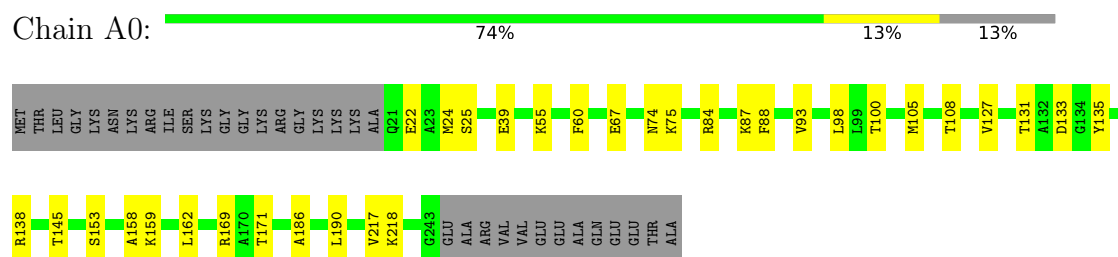
3 Residue-property plots [i](#)

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.

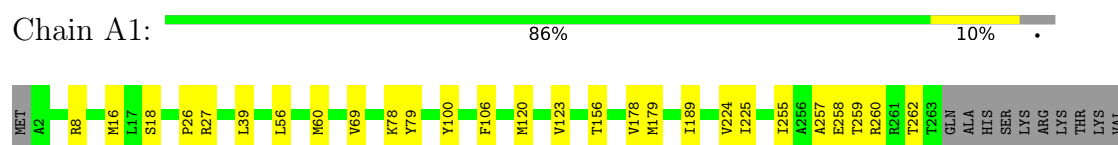
- Molecule 1: E-SITE tRNA



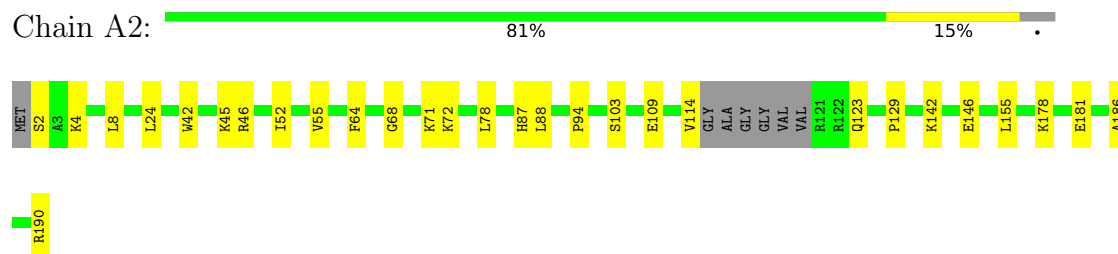
- Molecule 2: 40S ribosomal protein S3a



- Molecule 3: 40S ribosomal protein S4

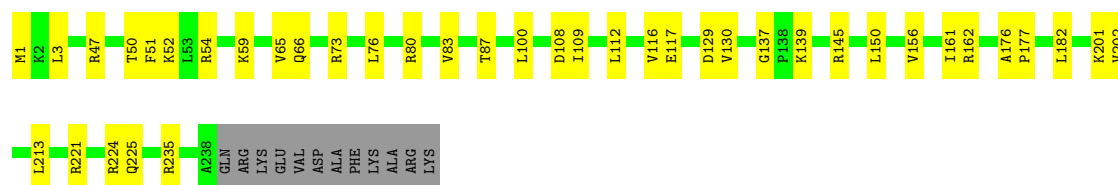


- Molecule 4: 40S ribosomal protein S5, putative



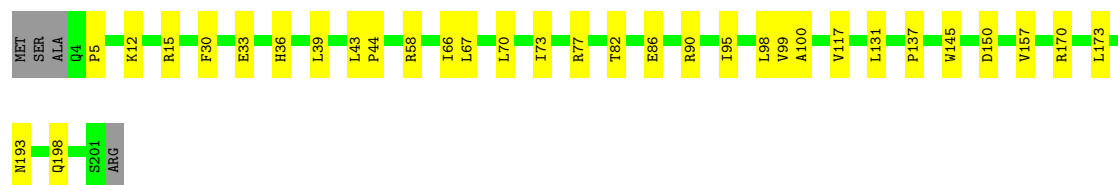
- Molecule 5: 40S ribosomal protein S6

Chain A3:  79% 16% 5%



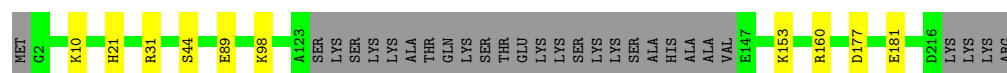
- Molecule 6: 40S ribosomal protein S7

Chain A4:  82% 16% .



- Molecule 7: 40S ribosomal protein S8

Chain A5:  83% 5% 13%



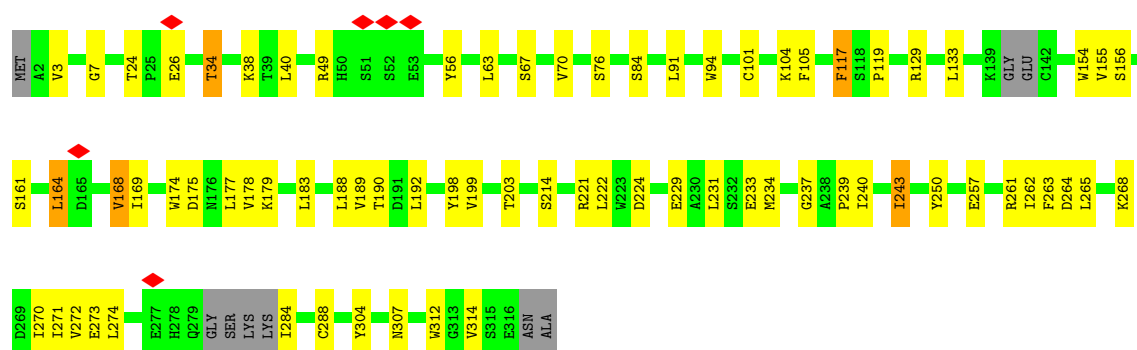
- Molecule 8: Probable 40S ribosomal protein S9

Chain A6:  83% 13% 5%



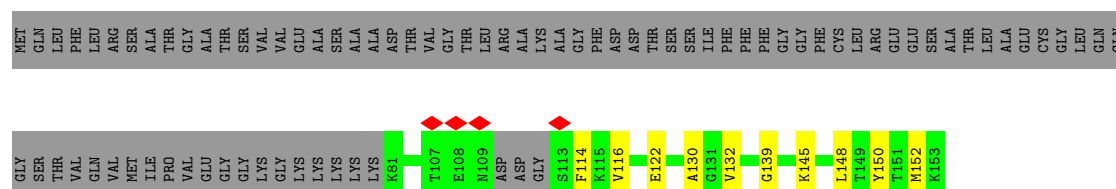
- Molecule 9: Small ribosomal subunit protein RACK1

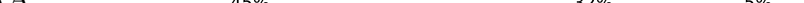
Chain A7:  74% 22% . .

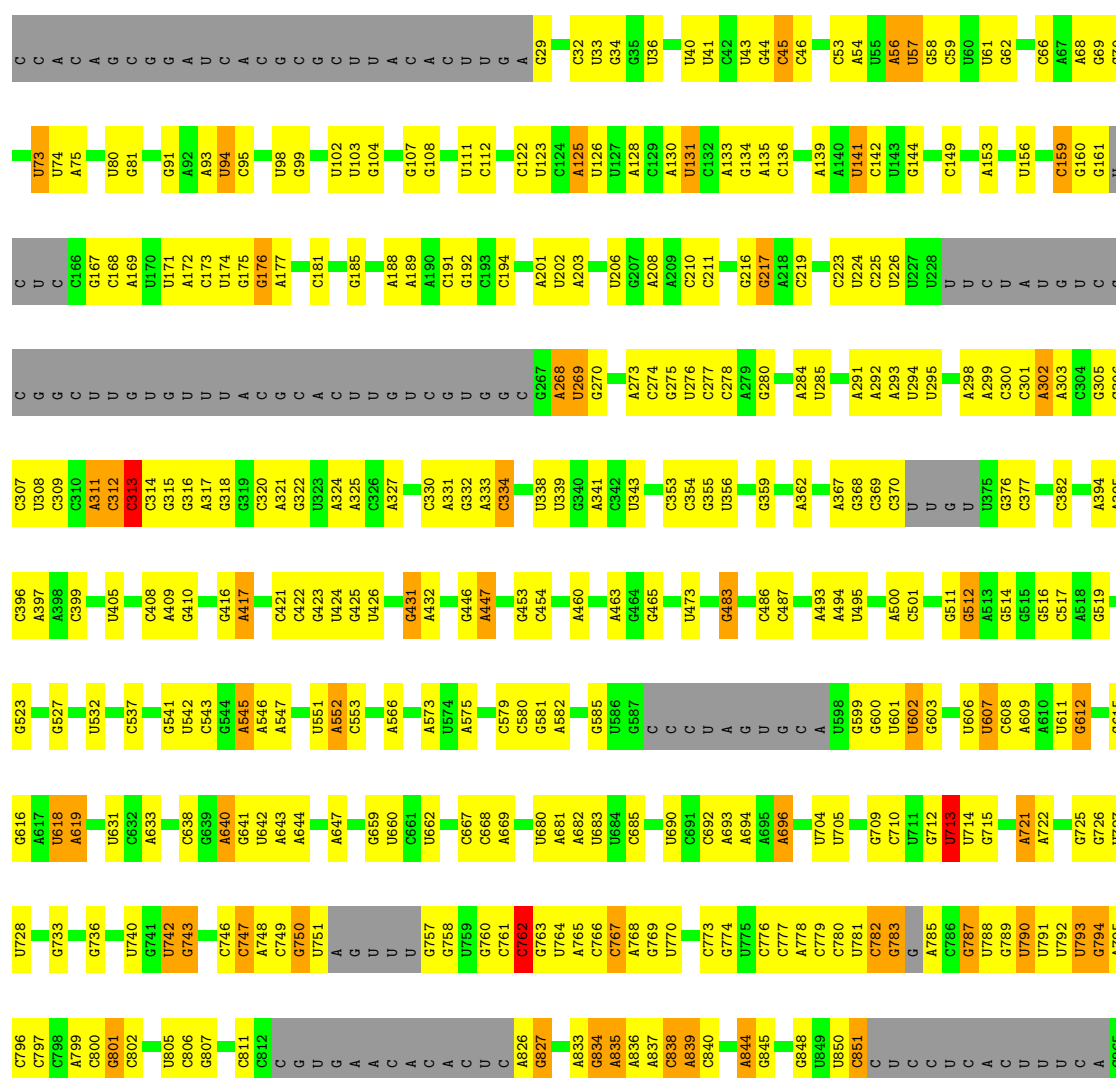


- Molecule 10: Putative ribosomal protein S29

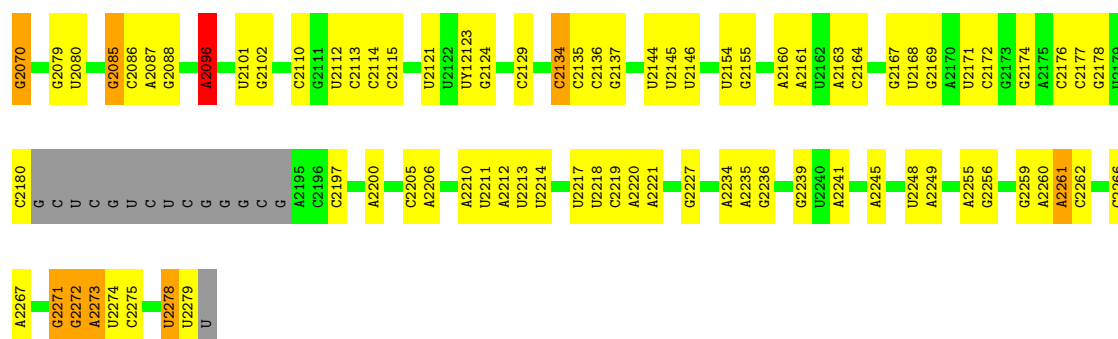
- Chain A9:



- Chain AA: 

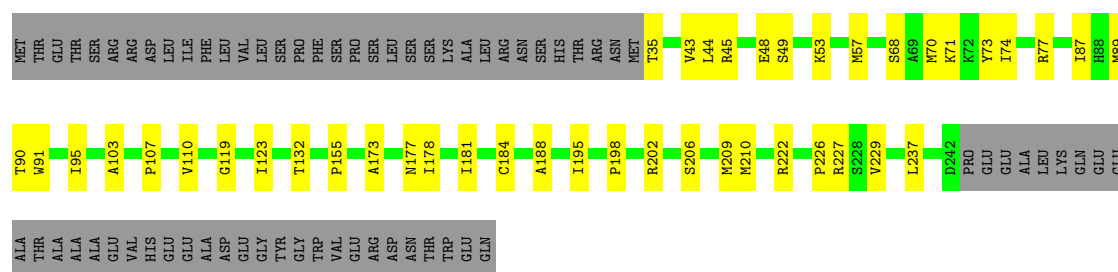


C1886	C1917	C1834	G1873	A1599	U1501	U	C1301	U185	A	G	G979	G866
G1987	C1918	A1835	U1674	C1600	U1502	G	A1302	U189	C	U	G980	C867
C1988	C1923	G1875	G1676	A1601	A1503	A	A1303	U190	A	C	G981	A868
G1991	G1924	C1602	C1504	C1603	C1504	G	C1305	G1191	U	G	A885	C872
A1992	A1925	C1604	A1505	G1605	A1505	U	U1308	A1192	C	U	A873	A873
U1993	C1926	G1606	U1509	G1606	U1509	U	G1309	A1200	A	U	U874	U874
C1994	A1927	G1607	G1512	A1607	G1512	C	A1310	G1201	U	U	C875	C875
A1998	G1931	C1608	G1513	A1608	G1513	C	C1311	G1202	C	C	G884	G884
A2008	C1932	U1609	G1517	U1610	G1517	C	A1316	A1210	G	G	G885	G885
A2009	A1936	U1611	A1518	U1612	A1518	A	U1317	A1211	A	U	C	C888
C2010	C1937	U1613	U1519	A1613	U1519	G	G1318	A1212	C	G	G993	G889
C2011	A1938	U1614	U1520	C1614	U1520	G	A1319	U1216	C	U	U998	U890
A2012	U1939	U1615	G1523	U1619	G1523	U	U1320	A1217	C	U	U999	C891
C2013	G1941	U1616	U1524	U1706	U1524	U	U1321	G1224	G	U	G1000	C892
C2014	U1942	U1617	G1531	G1622	G1531	U	G1322	A1221	G	U	U1004	U894
C2015	C1943	U1618	A1532	A1626	A1532	C	U1323	U1222	C	U	U1005	G895
A2016	A1944	U1619	U1533	G1627	U1533	G	G1324	U1223	C	U	U1006	A896
A2017	G1947	U1620	A1536	U1630	A1536	U	C1329	C1224	U	U	U1007	A
U2018	A1948	U1621	A1543	G1631	A1543	G	A	A1229	C1130	U	U1008	U898
C2019	G1949	U1622	A1547	U1633	A1547	G	U	U1235	A1131	U	U1009	U899
U2023	A1950	A1623	A1548	G1634	A1548	A	C	C1236	G1132	U	G1010	U900
A2024	A1951	U1624	U1549	A1635	U1549	U	A	U1237	G1133	G	G1011	G907
G2025	C1952	U1625	U1550	A1636	U1550	U	U	U1238	A1134	C	G1013	A911
C2028	A1953	U1626	A1552	C1640	A1552	A	G	C1239	U1135	C	U1014	A911
C2029	G1955	U1627	G1555	U1643	G1555	U	G	U1243	G1137	C	C1015	G917
A2030	A1956	U1628	C1563	G1644	C1563	C	U	A1243	U1138	C	U1017	G921
C2031	G1957	U1629	U1564	G1645	U1564	U	C	A1247	A1139	C	U1018	G921
G2034	U	U1630	C1565	U1646	C1565	U	C	U1250	G1144	A	G1020	U934
G2035	C	U1631	U1566	G1647	U1566	C	C	A1251	G1145	U	A1022	G935
G2036	A	U1632	U1567	U1648	U1567	U	G	A1255	U1146	C	G1023	C936
C2038	G	U1633	U1568	G1649	U1568	A	U	U1257	A1147	U	A1024	C937
C2039	C	U1634	U1569	U1650	U1569	U	G	G1257	G1148	C	U1025	G938
G2042	G	U1635	G1570	U1651	G1570	C	G	A1265	U1149	C	U1026	A939
U2043	C	U1636	C1571	U1652	C1571	C	C	U1265	G1153	U	A1027	C940
A2044	A	U1637	G1572	U1653	G1572	C	C	A1270	G1156	C	U1028	U941
U2045	U	U1638	U1575	U1654	U1575	C	C	U1276	A1150	U	G1029	U942
A2050	C	U1639	U1576	U1655	U1576	C	C	U1277	G1157	C	G1032	A944
U2051	U	U1640	G1577	U1656	G1577	U	G	U1278	A1158	U	C	U947
U2052	C	U1641	U1585	U1657	U1585	C	C	G1279	G1159	C	G	A948
A2053	A	U1642	U1586	U1658	U1586	U	U	A1281	U1163	A	C	C949
U2054	U	U1643	U1587	U1659	U1587	C	U	G1282	C1165	C	U	A950
U2058	G	U1644	G1578	U1660	G1578	C	G	A1282	U1169	U	G	A951
C2059	C	U1645	U1579	U1661	U1579	C	C	C1294	A1175	C	C	C971
G2060	U	U1646	U1580	U1662	U1580	C	U	A1295	G1178	U	U	A973
C2061	U	U1647	U1581	U1663	U1581	C	U	C1298	G1179	U	G	G974
G2062	G	U1648	U1582	U1664	U1582	C	G			U	U	C975
C2063	C	U1649	U1583	U1665	U1583	C	C			C	C	
A2064	A	U1650	U1584	U1666	U1584	C	C			U	U	
U2065	U	U1651	U1585	U1667	U1585	C	C			U	U	
U2068	C	U1652	U1586	U1668	U1586	C	C			U	U	
C2069	C	U1653	U1587	U1669	U1587	C	C			U	U	
G2070	U	U1654	U1588	U1670	U1588	C	C			U	U	
U2071	U	U1655	U1589	U1671	U1589	C	C			U	U	
U2072	C	U1656	U1590	U1672	U1590	C	C			U	U	
U2073	C	U1657	U1591	U1673	U1591	C	C			U	U	
U2074	C	U1658	U1592	U1674	U1592	C	C			U	U	
U2075	C	U1659	U1593	U1675	U1593	C	C			U	U	
U2076	C	U1660	U1594	U1676	U1594	C	C			U	U	
U2077	C	U1661	U1595	U1677	U1595	C	C			U	U	
U2078	C	U1662	U1596	U1678	U1596	C	C			U	U	
U2079	C	U1663	U1597	U1679	U1597	C	C			U	U	
U2080	C	U1664	U1598	U1680	U1598	C	C			U	U	
U2081	C	U1665	U1599	U1681	U1599	C	C			U	U	
U2082	C	U1666	U1600	U1682	U1600	C	C			U	U	
U2083	C	U1667	U1601	U1683	U1601	C	C			U	U	
U2084	C	U1668	U1602	U1684	U1602	C	C			U	U	
U2085	C	U1669	U1603	U1685	U1603	C	C			U	U	
U2086	C	U1670	U1604	U1686	U1604	C	C			U	U	
U2087	C	U1671	U1605	U1687	U1605	C	C			U	U	
U2088	C	U1672	U1606	U1688	U1606	C	C			U	U	
U2089	C	U1673	U1607	U1689	U1607	C	C			U	U	
U2090	C	U1674	U1608	U1690	U1608	C	C			U	U	
U2091	C	U1675	U1609	U1691	U1609	C	C			U	U	
U2092	C	U1676	U1610	U1692	U1610	C	C			U	U	
U2093	C	U1677	U1611	U1693	U1611	C	C			U	U	
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U2095	C	U1679	U1613	U1695	U1613	C	C			U	U	
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U2097	C	U1681	U1615	U1697	U1615	C	C			U	U	
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U2099	C	U1683	U1617	U1699	U1617	C	C			U	U	
U2100	C	U1684	U1618	U1700	U1618	C	C			U	U	
U2101	C	U1685	U1619	U1701	U1619	C	C			U	U	
U2102	C	U1686	U1620	U1702	U1620	C	C			U	U	
U2103	C	U1687	U1621	U1703	U1621	C	C			U	U	
U2104	C	U1688	U1622	U1704	U1622	C	C			U	U	
U2105	C	U1689	U1623	U1705	U1623	C	C			U	U	
U2106	C	U1690	U1624	U1706	U1624	C	C			U	U	
U2107	C	U1691	U1625	U1707	U1625	C	C			U	U	
U2108	C	U1692	U1626	U1708	U1626	C	C			U	U	
U2109	C	U1693	U1627	U1709	U1627	C	C			U	U	
U2110	C	U1694	U1628	U1710	U1628	C	C			U	U	
U2111	C	U1695	U1629	U1711	U1629	C	C			U	U	
U2112	C	U1696	U1630	U1712	U1630	C	C			U	U	
U2113	C	U1697	U1631	U1713	U1631	C	C			U	U	
U2114	C	U1698	U1632	U1714	U1632	C	C			U	U	
U2115	C	U1699	U1633	U1715	U1633	C	C			U	U	
U2116	C	U1700	U1634	U1716	U1634	C	C			U	U	
U2117	C	U1701	U1635	U1717	U1635	C	C			U	U	
U2118	C	U1702	U1636	U1718	U1636	C	C			U	U	
U2119	C	U1703	U1637	U1719	U1637	C	C			U	U	
U2120	C	U1704	U1638	U1720	U1638	C	C			U	U	
U2121	C	U1705	U1639	U1721	U1639	C	C			U	U	
U2122	C	U1706	U1640	U1722	U1640	C	C			U	U	
U2123	C	U1707	U1641	U1723	U1641	C	C			U	U	
U2124	C	U1708	U1642	U1724	U1642	C	C			U	U	
U2125	C	U1709	U1643	U1725	U1643	C	C			U	U	
U2126	C	U1710	U1644	U1726	U1644	C	C			U	U	
U2127	C	U1711	U1645	U1727	U1645	C	C			U	U	
U2128	C	U1712	U1646	U1728	U1646	C	C			U	U	
U2129	C	U1713	U1647	U1729	U1647	C	C			U	U	
U2130	C	U1714	U1648	U1730	U1648	C	C			U	U	
U2131	C	U1715	U1649	U1731	U1649	C	C			U	U	
U2132	C	U1716	U1650	U1732	U1650	C	C			U	U	
U2133	C	U1717	U1651	U1733	U1651	C	C			U	U	
U2134	C	U1718	U1652	U1734	U1652	C	C			U	U	
U2135	C	U1719	U1653	U1735	U1653	C	C			U	U	
U2136	C	U1720	U1654	U1736	U1654	C	C			U	U	
U2137	C	U1721	U1655	U1737	U1655	C	C			U	U	
U2138	C	U1722	U1656	U1738	U1656	C	C			U	U	
U2139	C	U1723	U1657	U1739	U1657	C	C			U	U	
U2140	C	U1724	U1658	U1740	U1658	C	C			U	U	
U2141	C	U1725	U1659	U1741	U1659	C	C			U	U	
U2142	C	U1726	U1660									



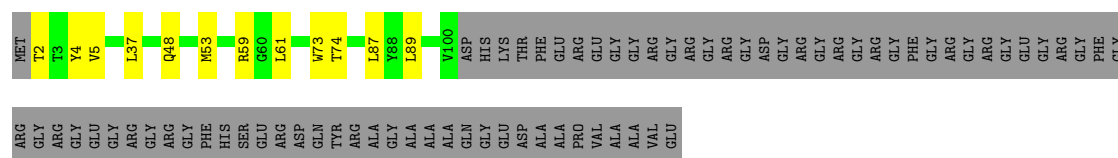
- Molecule 13: 40S ribosomal protein SA

Chain AC: 60% 16% 25%



- Molecule 14: 40S ribosomal protein S10, putative

Chain AD: 51% 7% 42%



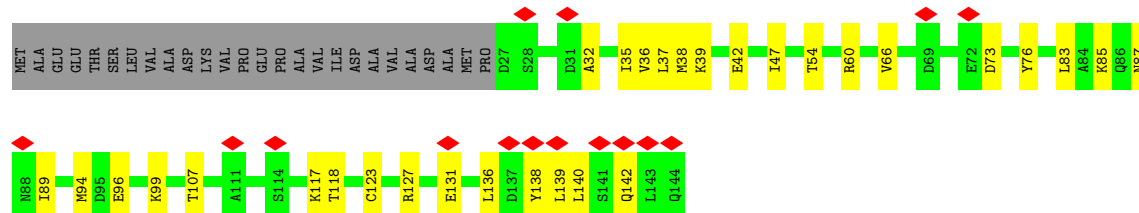
- Molecule 15: 40S ribosomal proteins S11, putative

Chain AE: 84% 12%



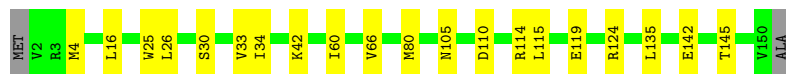
- Molecule 16: Small ribosomal subunit protein eS12

Chain AF: 10% 60% 22% 18%



- Molecule 17: 40S ribosomal protein S13, putative

Chain AG:  85% 13%



- Molecule 18: Small ribosomal subunit protein uS11

Chain AH:  78% 17% 6%



- Molecule 19: 40S ribosomal protein S15, putative

Chain AI:  64% 15% 20%



- Molecule 20: 40S ribosomal protein S15a, putative

Chain AJ:  90% 9%



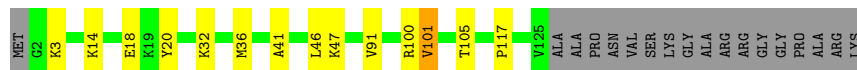
- Molecule 21: 40S ribosomal protein S16, putative

Chain AK:  83% 11% 5%



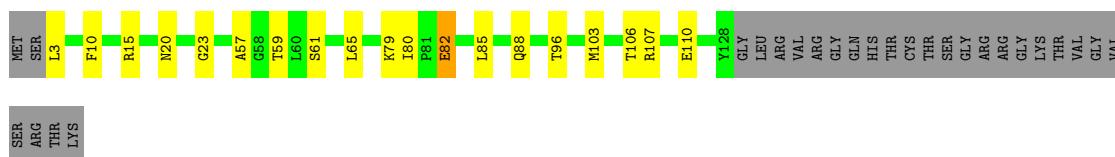
- Molecule 22: 40S ribosomal protein S17, putative

Chain AL:  77% 9% 13%



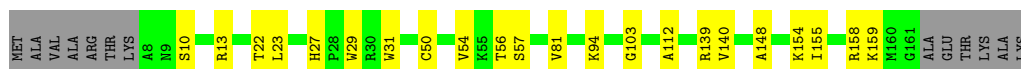
- Molecule 23: 40S ribosomal protein S18, putative

Chain AM:  70% 12% 18%



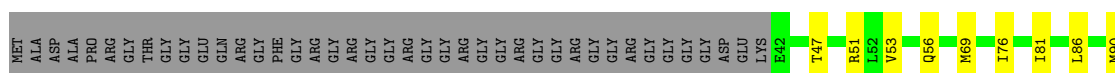
- Molecule 24: Ribosomal protein S19, putative

Chain AO: 79% 13% 8%



- Molecule 25: 40S ribosomal protein S2, putative

Chain AP: 71% 10% 18%



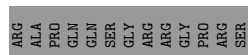
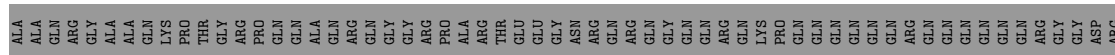
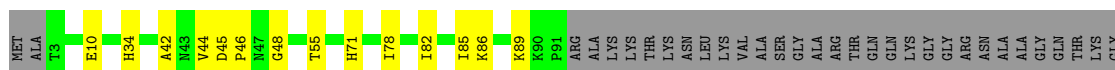
- Molecule 26: Small ribosomal subunit protein uS10

Chain AQ: 61% 21% 15%



- Molecule 27: 40S ribosomal protein S21, putative

Chain AR: 39% 7% 54%

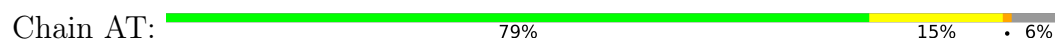


- Molecule 28: 40S ribosomal protein S23, putative

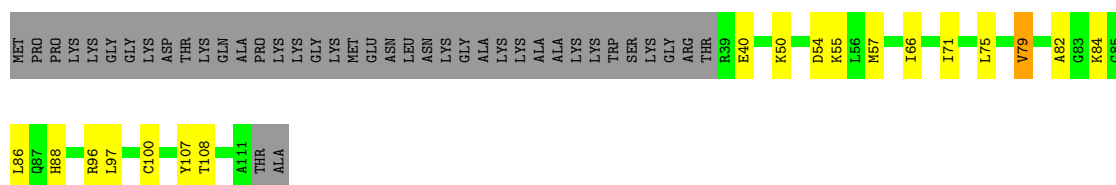
Chain AS: 85% 12% 2%



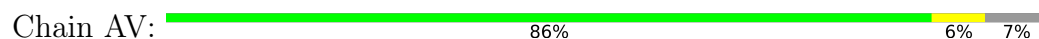
- Molecule 29: 40S ribosomal protein S24



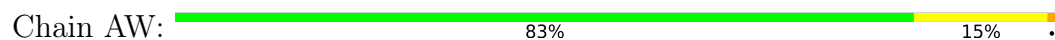
- Molecule 30: 40S ribosomal protein S25



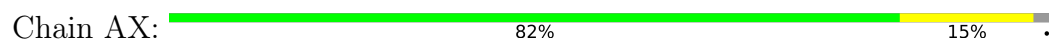
- Molecule 31: 40S ribosomal protein S26



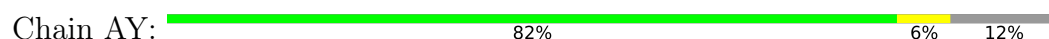
- Molecule 32: 40S ribosomal protein S27, putative

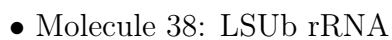


- Molecule 33: 40S ribosomal protein S3, putative



- Molecule 34: 40S ribosomal protein S30

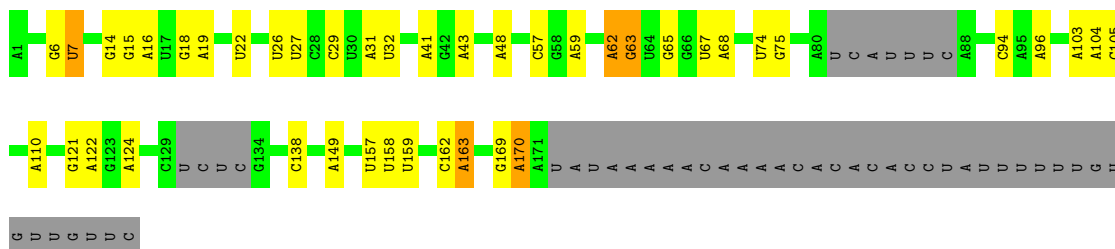




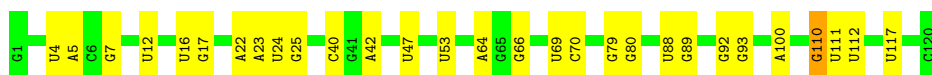
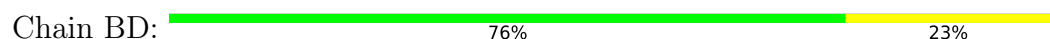
27%



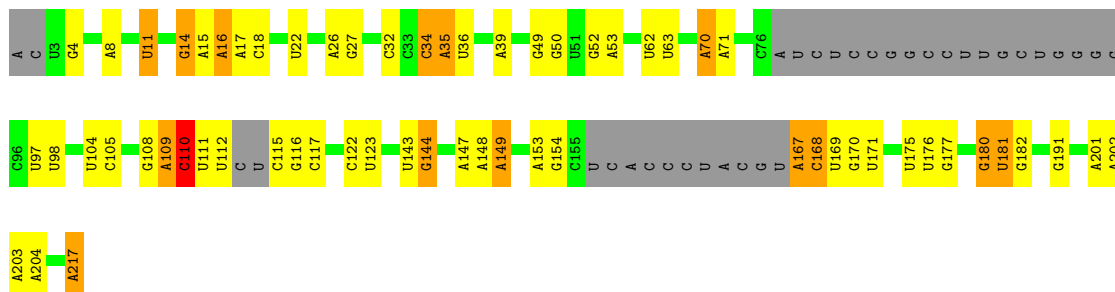
- Molecule 39: 5.8S rRNA



- Molecule 40: 5S rRNA



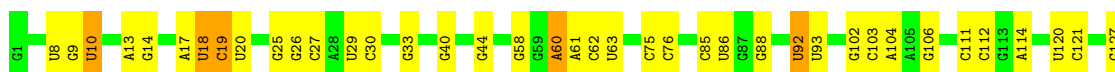
- Molecule 41: SrRNA-1



- Molecule 42: SrRNA-6



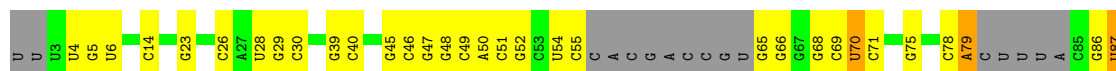
- Molecule 43: SrRNA-2





- Molecule 44: SrRNA-4

Chain BH: 51% 30% 15%



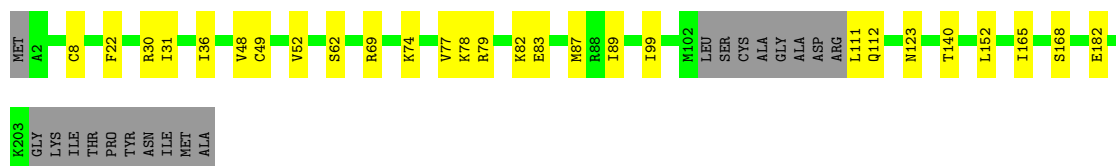
- Molecule 45: 60S ribosomal protein L18

Chain BI: 90% 10%



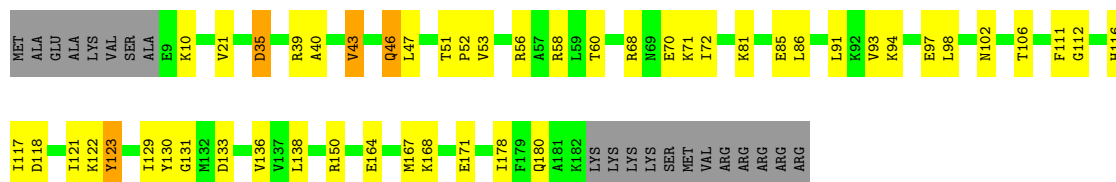
- Molecule 46: 60S ribosomal protein L10, putative

Chain BK: 78% 13% 9%



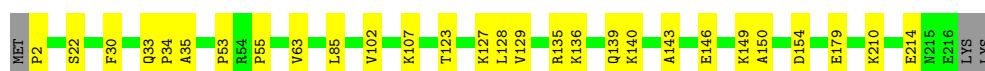
- Molecule 47: 60S ribosomal protein L11, putative

Chain BL: 64% 23% 10%



- Molecule 48: 60S ribosomal protein L13

Chain BN: 86% 13%



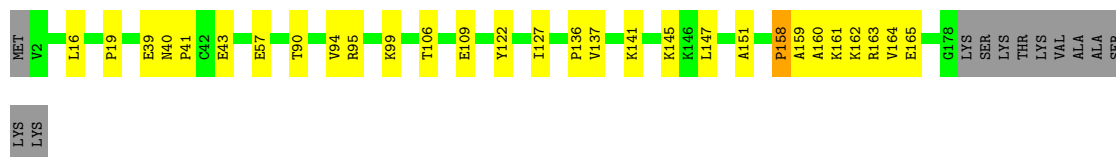
- Molecule 49: 60S ribosomal protein L13a, putative

Chain BO: 91% 8%



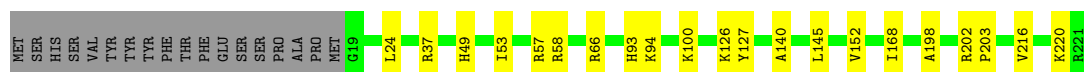
- Molecule 50: 40S ribosomal protein L14, putative

Chain BP: 78% 15% 6%



- Molecule 51: Ribosomal protein L15

Chain BQ: 82% 10% 8%



- Molecule 52: 60S ribosomal protein L17, putative

Chain BR: 87% 6% 7%



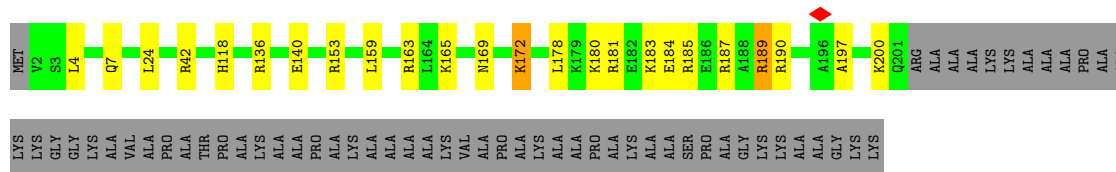
- Molecule 53: 60S ribosomal protein L18a

Chain BS: 89% 9% ..



- Molecule 54: 60S ribosomal protein L19, putative

Chain BT: 68% 8% 23%



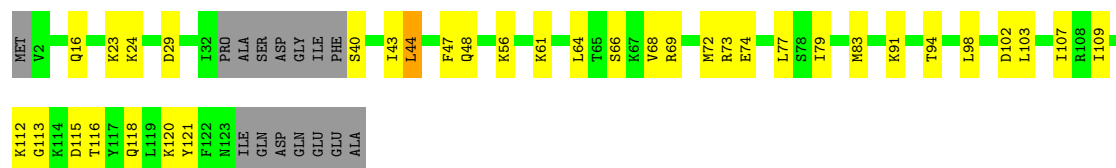
- Molecule 55: 60S ribosomal protein L21E, putative

Chain BU: 84% 14% ..



- Molecule 56: 60S ribosomal protein L22, putative

Chain BV: 



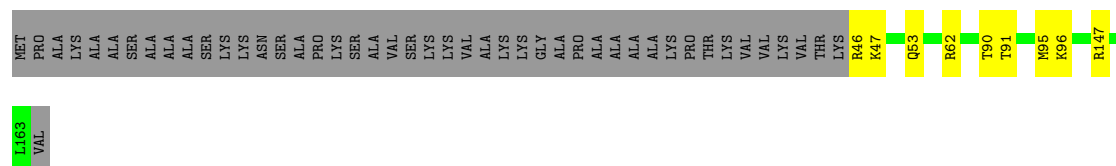
- Molecule 57: 60S ribosomal protein L23, putative

Chain BW: 

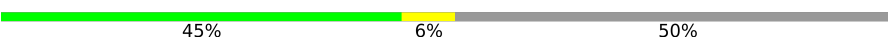


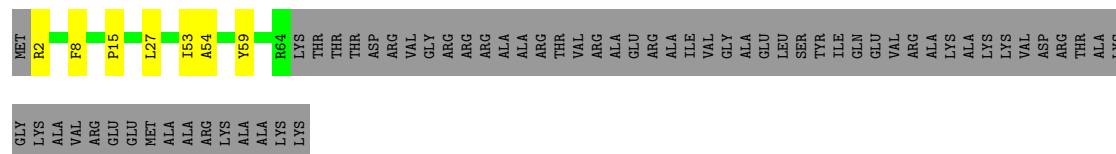
- Molecule 58: 60S ribosomal protein L23a

Chain BX: 



- Molecule 59: Ribosomal protein L24

Chain BY: 



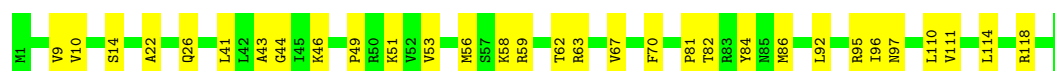
- Molecule 60: 60S ribosomal protein L26, putative

Chain BZ: 



- Molecule 61: 60S ribosomal protein L27

Chain Ba: 



- Molecule 62: 60S ribosomal protein L27a

Chain Bb:  89% 10%



- Molecule 63: 60S ribosomal protein L28, putative

Chain Bc:  82% 17%



- Molecule 64: 60S ribosomal protein L29

Chain Bd:  89% 8%



- Molecule 65: 60S ribosomal protein L2, putative

Chain Be:  90% 8%



- Molecule 66: Ribosomal protein L3, mitochondrial, putative

Chain Bf:  82% 11% 7%



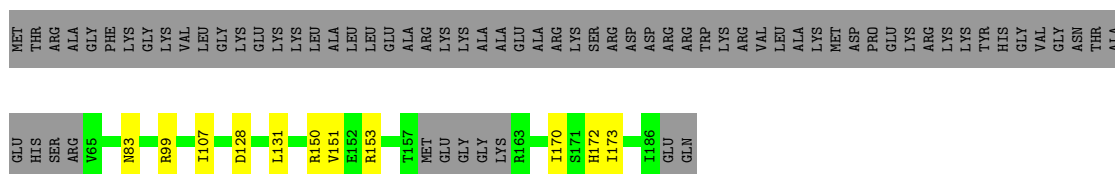
- Molecule 67: 60S ribosomal protein L30

Chain Bg:  70% 20% 9%



- Molecule 68: 60S ribosomal subunit protein L31, putative

Chain Bh:  56% 6% 38%



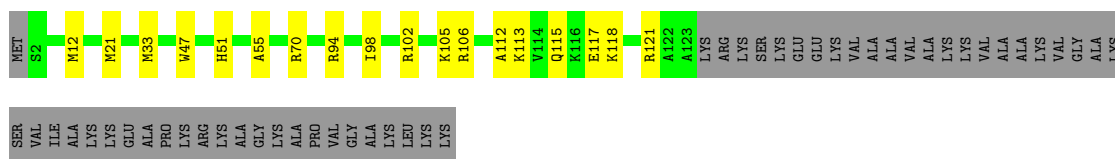
- Molecule 69: 60S ribosomal protein L32, putative

Chain Bi: 88% 11% ..



- Molecule 70: 60S ribosomal protein L34, putative

Chain Bj: 61% 11% 28%



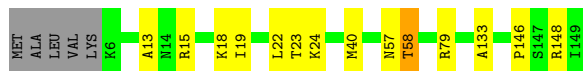
- Molecule 71: 60S ribosomal protein L35, putative

Chain Bk: 85% 12% .



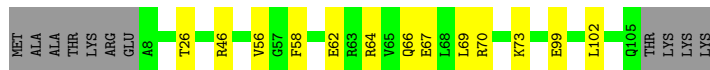
- Molecule 72: 60S ribosomal protein L35A, putative

Chain Bl: 87% 9% . .



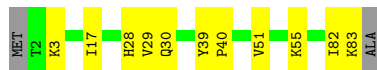
- Molecule 73: Ribosomal protein L36, putative

Chain Bm: 78% 12% 10%



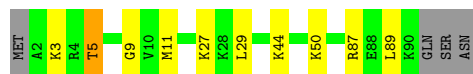
- Molecule 74: Ribosomal protein L37

Chain Bn: 85% 13% .



- Molecule 75: 60S ribosomal protein L37a, putative

Chain Bo:  85% 10% . .

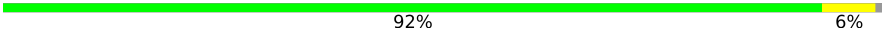


- Molecule 76: 60S ribosomal protein L38, putative

Chain Bp:  84% 10% 6%



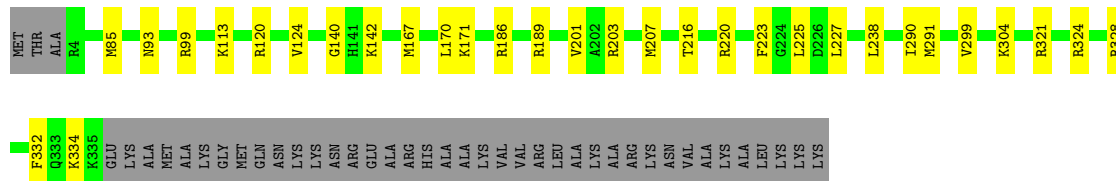
- Molecule 77: 60S ribosomal protein L39, putative

Chain Bq:  92% 6% .



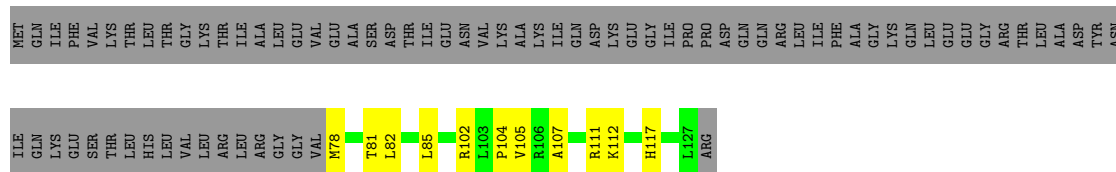
- Molecule 78: 60S ribosomal protein L4

Chain Br:  80% 8% 11%



- Molecule 79: Ubiquitin-60S ribosomal protein L40

Chain Bs:  30% 9% 61%

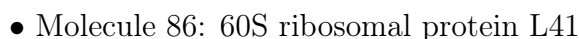
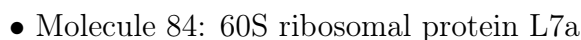


- Molecule 80: 60S ribosomal protein L44

Chain Bt:  83% 8% 8%



- Molecule 81: 60S ribosomal protein L5, putative





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	570752	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 ($e^-/\text{\AA}^2$)	1.05	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.260	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	395.76, 395.76, 395.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8245, 0.8245, 0.8245	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GET, PSU, A2M, SNC, K, PUT, OMG, UY1, NA, 5MC, HY3, IAS, 1MA, OMC, OMU, HIC, 7MG, B8N, MG, MA6, GTP, ZN, SPD

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	Et	0.45	0/450	0.84	0/698
2	A0	0.17	0/1841	0.38	0/2477
3	A1	0.16	0/2096	0.37	0/2819
4	A2	0.15	0/1480	0.34	0/1990
5	A3	0.16	0/1921	0.35	0/2563
6	A4	0.17	0/1656	0.36	0/2229
7	A5	0.16	0/1560	0.38	0/2086
8	A6	0.16	0/1525	0.36	0/2045
9	A7	0.15	0/2422	0.39	0/3301
10	A8	0.19	0/468	0.35	0/619
11	A9	0.11	0/580	0.31	0/771
12	AA	0.37	1/43870 (0.0%)	0.79	26/68332 (0.0%)
13	AC	0.15	0/1682	0.37	0/2275
14	AD	0.13	0/837	0.32	0/1129
15	AE	0.15	0/1276	0.34	0/1717
16	AF	0.16	0/918	0.43	0/1230
17	AG	0.17	0/1215	0.32	0/1629
18	AH	0.20	0/1021	0.42	0/1368
19	AI	0.14	0/988	0.31	0/1327
20	AJ	0.16	0/1035	0.34	0/1386
21	AK	0.15	0/1155	0.34	0/1550
22	AL	0.15	0/979	0.33	0/1312
23	AM	0.16	0/1044	0.36	0/1399
24	AO	0.13	0/1245	0.31	0/1665
25	AP	0.16	0/1723	0.37	0/2328
26	AQ	0.14	0/809	0.41	0/1091
27	AR	0.15	0/669	0.33	0/908
28	AS	0.15	0/1119	0.37	0/1495
29	AT	0.16	0/1050	0.37	0/1395
30	AU	0.23	0/575	0.51	0/769
31	AV	0.15	0/846	0.36	0/1132

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	AW	0.16	0/674	0.39	0/904
33	AX	0.13	0/1674	0.32	0/2236
34	AY	0.17	0/472	0.42	0/623
35	AZ	0.19	0/456	0.42	0/606
36	Az	0.17	0/1389	0.49	0/1870
37	BA	0.42	3/36024 (0.0%)	0.81	19/56130 (0.0%)
38	BB	0.44	3/25539 (0.0%)	0.85	20/39799 (0.1%)
39	BC	0.42	1/3662 (0.0%)	0.72	0/5700
40	BD	0.34	0/2852	0.71	0/4444
41	BE	0.37	0/4328	0.80	4/6731 (0.1%)
42	BF	0.34	0/1764	0.91	2/2740 (0.1%)
43	BG	0.43	0/4383	0.82	3/6835 (0.0%)
44	BH	0.39	0/2744	0.81	0/4270
45	BI	0.17	0/1552	0.37	0/2070
46	BK	0.16	0/1620	0.39	0/2171
47	BL	0.17	0/1406	0.44	2/1878 (0.1%)
48	BN	0.18	0/1793	0.42	0/2391
49	BO	0.17	0/1823	0.37	0/2431
50	BP	0.18	0/1431	0.38	1/1917 (0.1%)
51	BQ	0.18	0/1746	0.38	0/2331
52	BR	0.18	0/1269	0.35	0/1703
53	BS	0.17	0/1479	0.39	0/1986
54	BT	0.18	0/1661	0.40	0/2198
55	BU	0.17	0/1282	0.39	0/1722
56	BV	0.19	0/953	0.48	0/1268
57	BW	0.21	0/1016	0.42	0/1368
58	BX	0.15	0/983	0.35	0/1322
59	BY	0.19	0/562	0.42	0/756
60	BZ	0.15	0/1015	0.35	0/1353
61	Ba	0.18	0/1119	0.38	0/1489
62	Bb	0.18	0/1165	0.41	0/1554
63	Bc	0.16	0/1179	0.31	0/1573
64	Bd	0.18	0/572	0.37	0/766
65	Be	0.18	0/1972	0.42	0/2649
66	Bf	0.19	0/3269	0.38	0/4391
67	Bg	0.19	0/746	0.37	0/1008
68	Bh	0.17	0/970	0.38	0/1295
69	Bi	0.16	0/1097	0.34	0/1468
70	Bj	0.16	0/1024	0.37	0/1365
71	Bk	0.17	0/1022	0.42	0/1351
72	Bl	0.17	0/1187	0.41	0/1592
73	Bm	0.15	0/796	0.35	0/1057
74	Bn	0.20	0/707	0.45	0/942

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	Bo	0.26	0/711	0.48	0/946
76	Bp	0.18	0/631	0.44	0/840
77	Bq	0.19	0/471	0.35	0/626
78	Br	0.16	0/2660	0.36	0/3580
79	Bs	0.13	0/398	0.32	0/529
80	Bt	0.19	0/815	0.43	0/1077
81	Bu	0.17	0/2437	0.39	1/3271 (0.0%)
82	Bv	0.18	0/1115	0.36	0/1501
83	Bw	0.19	0/1879	0.41	0/2520
84	Bx	0.16	0/1892	0.36	0/2542
85	By	0.16	0/1536	0.37	0/2065
86	Bz	0.16	0/293	0.29	0/381
All	All	0.32	8/219270 (0.0%)	0.67	78/321166 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
56	BV	0	1
57	BW	0	1
60	BZ	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	BA	743	A2M	O3'-P	5.69	1.61	1.56
38	BB	545	A2M	O3'-P	5.25	1.61	1.56
38	BB	1388	A2M	O3'-P	5.25	1.61	1.56
39	BC	43	A2M	O3'-P	5.10	1.61	1.56
37	BA	746	A2M	O3'-P	5.10	1.61	1.56

The worst 5 of 78 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	BA	477	G	O4'-C1'-N9	7.84	114.47	108.20
37	BA	1671	G	O4'-C1'-N9	7.27	114.02	108.20
38	BB	1079	C	C2-N1-C1'	7.21	126.73	118.80
38	BB	1170	C	C6-N1-C2	-7.14	117.44	120.30
38	BB	990	C	N1-C2-O2	7.10	123.16	118.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
56	BV	102	ASP	Peptide
57	BW	82	ARG	Sidechain
60	BZ	57[A]	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Et	404	0	211	3	0
2	A0	1814	0	1883	20	0
3	A1	2062	0	2181	17	0
4	A2	1458	0	1513	18	0
5	A3	1899	0	2027	30	0
6	A4	1642	0	1723	23	0
7	A5	1536	0	1623	11	0
8	A6	1495	0	1562	19	0
9	A7	2374	0	2277	45	0
10	A8	461	0	467	4	0
11	A9	567	0	578	8	0
12	AA	40169	0	20309	411	0
13	AC	1648	0	1687	32	0
14	AD	814	0	819	7	0
15	AE	1251	0	1301	8	0
16	AF	922	0	939	24	0
17	AG	1193	0	1262	14	0
18	AH	1015	0	1025	17	0
19	AI	967	0	993	14	0
20	AJ	1018	0	1050	9	0
21	AK	1144	0	1202	12	0
22	AL	967	0	1026	10	0
23	AM	1027	0	1072	15	0
24	AO	1220	0	1286	13	0
25	AP	1688	0	1734	17	0
26	AQ	800	0	856	23	0
27	AR	668	0	668	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	AS	1107	0	1152	10	0
29	AT	1034	0	1117	12	0
30	AU	569	0	611	13	0
31	AV	830	0	864	6	0
32	AW	660	0	666	13	0
33	AX	1652	0	1721	22	0
34	AY	466	0	517	3	0
35	AZ	457	0	494	7	0
36	Az	1366	0	1394	40	0
37	BA	33019	0	16678	232	0
38	BB	23998	0	12137	195	0
39	BC	3411	0	1736	20	0
40	BD	2553	0	1293	14	0
41	BE	3879	0	1968	29	0
42	BF	1587	0	814	14	0
43	BG	3919	0	1975	24	0
44	BH	2458	0	1244	18	0
45	BI	1526	0	1646	15	0
46	BK	1588	0	1651	20	0
47	BL	1385	0	1423	39	0
48	BN	1762	0	1864	21	0
49	BO	1802	0	1947	18	0
50	BP	1411	0	1505	22	0
51	BQ	1717	0	1790	15	0
52	BR	1244	0	1301	6	0
53	BS	1462	0	1487	12	0
54	BT	1644	0	1754	20	0
55	BU	1261	0	1313	17	0
56	BV	940	0	979	22	0
57	BW	999	0	1062	13	0
58	BX	966	0	1030	11	0
59	BY	542	0	546	5	0
60	BZ	1002	0	1079	15	0
61	Ba	1099	0	1174	20	0
62	Bb	1137	0	1174	9	0
63	Bc	1162	0	1246	14	0
64	Bd	561	0	583	5	0
65	Be	1939	0	2000	14	0
66	Bf	3212	0	3337	33	0
67	Bg	736	0	758	11	0
68	Bh	953	0	1040	5	0
69	Bi	1075	0	1135	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
70	Bj	1006	0	1080	14	0
71	Bk	1014	0	1130	12	0
72	Bl	1163	0	1221	11	0
73	Bm	786	0	865	10	0
74	Bn	693	0	709	6	0
75	Bo	699	0	726	6	0
76	Bp	622	0	674	5	0
77	Bq	457	0	495	3	0
78	Br	2607	0	2695	23	0
79	Bs	392	0	412	6	0
80	Bt	801	0	861	6	0
81	Bu	2395	0	2462	26	0
82	Bv	1106	0	1156	17	0
83	Bw	1844	0	1929	13	0
84	Bx	1875	0	2003	20	0
85	By	1515	0	1589	19	0
86	Bz	289	0	325	3	0
87	A3	1	0	0	0	0
87	AA	40	0	0	0	0
87	AO	1	0	0	0	0
87	AV	1	0	0	0	0
87	BA	92	0	0	0	0
87	BB	66	0	0	0	0
87	BC	4	0	0	0	0
87	BD	1	0	0	0	0
87	BE	1	0	0	0	0
87	BF	2	0	0	0	0
87	BG	8	0	0	0	0
87	BK	1	0	0	0	0
87	BQ	2	0	0	0	0
87	BR	1	0	0	0	0
87	BU	1	0	0	0	0
87	BW	1	0	0	0	0
87	Bi	1	0	0	0	0
88	A6	10	0	19	1	0
88	AA	120	0	228	9	0
88	BA	330	0	627	13	0
88	BB	80	0	152	3	0
88	BC	30	0	57	1	0
88	BE	10	0	19	0	0
88	BG	20	0	38	1	0
88	BQ	10	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	Bd	10	0	19	1	0
89	A9	1	0	0	0	0
89	AV	1	0	0	0	0
89	Bn	1	0	0	0	0
89	Bo	1	0	0	0	0
89	Bs	1	0	0	0	0
89	Bt	1	0	0	0	0
90	AA	102	0	120	1	0
91	AA	24	0	48	1	0
91	BA	30	0	60	1	0
91	BB	30	0	60	2	0
92	AA	32	0	12	3	0
93	AA	11	0	0	0	0
93	BA	18	0	0	0	0
93	BB	23	0	0	0	0
93	BC	2	0	0	0	0
93	BE	3	0	0	0	0
93	BF	1	0	0	0	0
93	BG	3	0	0	0	0
93	BH	2	0	0	0	0
93	BK	1	0	0	0	0
93	BN	1	0	0	0	0
93	BQ	1	0	0	0	0
93	Bb	1	0	0	0	0
93	Be	1	0	0	0	0
93	Bi	1	0	0	0	0
94	AA	5	0	0	0	0
94	BA	1	0	0	0	0
94	BB	10	0	0	0	0
94	Be	1	0	0	0	0
95	A0	2	0	0	0	0
95	A5	3	0	0	0	0
95	AA	160	0	0	0	0
95	AE	1	0	0	0	0
95	AG	2	0	0	0	0
95	AJ	1	0	0	0	0
95	AV	1	0	0	0	0
95	AW	1	0	0	0	0
95	BA	1050	0	0	1	0
95	BB	889	0	0	2	0
95	BC	38	0	0	0	0
95	BD	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
95	BE	16	0	0	0	0
95	BF	7	0	0	0	0
95	BG	151	0	0	0	0
95	BH	30	0	0	0	0
95	BI	10	0	0	0	0
95	BK	2	0	0	0	0
95	BN	14	0	0	0	0
95	BO	18	0	0	1	0
95	BQ	43	0	0	0	0
95	BR	12	0	0	0	0
95	BT	15	0	0	0	0
95	BU	6	0	0	0	0
95	BW	12	0	0	0	0
95	BX	1	0	0	0	0
95	BY	2	0	0	0	0
95	BZ	2	0	0	0	0
95	Bb	20	0	0	0	0
95	Bd	5	0	0	0	0
95	Be	49	0	0	0	0
95	Bf	45	0	0	0	0
95	Bh	6	0	0	0	0
95	Bi	18	0	0	0	0
95	Bj	15	0	0	0	0
95	Bl	11	0	0	0	0
95	Bn	17	0	0	0	0
95	Bo	7	0	0	0	0
95	Bq	3	0	0	0	0
95	Br	30	0	0	0	0
95	Bt	6	0	0	0	0
95	Bu	1	0	0	0	0
95	Bv	1	0	0	0	0
95	Bw	11	0	0	1	0
95	Bx	3	0	0	0	0
95	Et	5	0	0	0	0
All	All	211479	0	156289	1865	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 1865 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)
37:BA:545:G:H1	37:BA:601:U:H3	1.01	0.91
33:AX:55:ARG:HE	33:AX:55:ARG:H	1.18	0.91
12:AA:2036:G:H5'	24:AO:103:GLY:HA2	1.50	0.91
12:AA:465:G:HO2'	12:AA:713:U:H5	1.14	0.90
47:BL:117:ILE:HD11	47:BL:123:TYR:HB2	1.56	0.85

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	A0	221/256 (86%)	217 (98%)	4 (2%)	0	100	100
3	A1	260/273 (95%)	252 (97%)	8 (3%)	0	100	100
4	A2	179/190 (94%)	176 (98%)	3 (2%)	0	100	100
5	A3	236/250 (94%)	232 (98%)	4 (2%)	0	100	100
6	A4	194/202 (96%)	187 (96%)	7 (4%)	0	100	100
7	A5	188/220 (86%)	187 (100%)	1 (0%)	0	100	100
8	A6	179/190 (94%)	174 (97%)	5 (3%)	0	100	100
9	A7	302/318 (95%)	289 (96%)	13 (4%)	0	100	100
10	A8	54/57 (95%)	54 (100%)	0	0	100	100
11	A9	66/153 (43%)	61 (92%)	5 (8%)	0	100	100
13	AC	206/277 (74%)	199 (97%)	7 (3%)	0	100	100
14	AD	97/172 (56%)	96 (99%)	1 (1%)	0	100	100
15	AE	151/174 (87%)	144 (95%)	7 (5%)	0	100	100
16	AF	115/144 (80%)	114 (99%)	1 (1%)	0	100	100
17	AG	147/151 (97%)	147 (100%)	0	0	100	100
18	AH	132/144 (92%)	126 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AI	119/152 (78%)	115 (97%)	4 (3%)	0	100	100
20	AJ	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
21	AK	139/149 (93%)	130 (94%)	9 (6%)	0	100	100
22	AL	122/142 (86%)	119 (98%)	3 (2%)	0	100	100
23	AM	124/153 (81%)	121 (98%)	3 (2%)	0	100	100
24	AO	152/167 (91%)	150 (99%)	2 (1%)	0	100	100
25	AP	216/266 (81%)	213 (99%)	3 (1%)	0	100	100
26	AQ	98/117 (84%)	95 (97%)	3 (3%)	0	100	100
27	AR	86/194 (44%)	85 (99%)	1 (1%)	0	100	100
28	AS	138/143 (96%)	135 (98%)	3 (2%)	0	100	100
29	AT	127/137 (93%)	120 (94%)	7 (6%)	0	100	100
30	AU	71/113 (63%)	68 (96%)	2 (3%)	1 (1%)	9	5
31	AV	101/111 (91%)	94 (93%)	7 (7%)	0	100	100
32	AW	83/86 (96%)	78 (94%)	5 (6%)	0	100	100
33	AX	206/214 (96%)	196 (95%)	10 (5%)	0	100	100
34	AY	56/66 (85%)	51 (91%)	5 (9%)	0	100	100
35	AZ	55/103 (53%)	53 (96%)	2 (4%)	0	100	100
36	Az	172/279 (62%)	160 (93%)	12 (7%)	0	100	100
45	BI	190/193 (98%)	186 (98%)	4 (2%)	0	100	100
46	BK	190/213 (89%)	184 (97%)	6 (3%)	0	100	100
47	BL	172/194 (89%)	169 (98%)	3 (2%)	0	100	100
48	BN	213/218 (98%)	205 (96%)	8 (4%)	0	100	100
49	BO	218/222 (98%)	215 (99%)	3 (1%)	0	100	100
50	BP	175/189 (93%)	171 (98%)	4 (2%)	0	100	100
51	BQ	200/221 (90%)	195 (98%)	5 (2%)	0	100	100
52	BR	152/166 (92%)	150 (99%)	2 (1%)	0	100	100
53	BS	173/179 (97%)	170 (98%)	3 (2%)	0	100	100
54	BT	198/260 (76%)	194 (98%)	4 (2%)	0	100	100
55	BU	155/159 (98%)	150 (97%)	5 (3%)	0	100	100
56	BV	111/130 (85%)	104 (94%)	7 (6%)	0	100	100
57	BW	130/139 (94%)	129 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
58	BX	116/164 (71%)	115 (99%)	1 (1%)	0	100	100
59	BY	61/125 (49%)	60 (98%)	1 (2%)	0	100	100
60	BZ	121/143 (85%)	118 (98%)	3 (2%)	0	100	100
61	Ba	131/133 (98%)	130 (99%)	1 (1%)	0	100	100
62	Bb	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
63	Bc	142/146 (97%)	141 (99%)	1 (1%)	0	100	100
64	Bd	67/71 (94%)	65 (97%)	2 (3%)	0	100	100
65	Be	253/260 (97%)	246 (97%)	7 (3%)	0	100	100
66	Bf	397/429 (92%)	388 (98%)	9 (2%)	0	100	100
67	Bg	94/105 (90%)	92 (98%)	2 (2%)	0	100	100
68	Bh	113/188 (60%)	111 (98%)	2 (2%)	0	100	100
69	Bi	129/132 (98%)	127 (98%)	2 (2%)	0	100	100
70	Bj	120/170 (71%)	117 (98%)	3 (2%)	0	100	100
71	Bk	121/127 (95%)	114 (94%)	7 (6%)	0	100	100
72	Bl	142/149 (95%)	138 (97%)	4 (3%)	0	100	100
73	Bm	96/109 (88%)	95 (99%)	1 (1%)	0	100	100
74	Bn	80/84 (95%)	78 (98%)	2 (2%)	0	100	100
75	Bo	87/93 (94%)	81 (93%)	6 (7%)	0	100	100
76	Bp	75/82 (92%)	73 (97%)	2 (3%)	0	100	100
77	Bq	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	5	2
78	Br	330/374 (88%)	317 (96%)	13 (4%)	0	100	100
79	Bs	48/128 (38%)	47 (98%)	1 (2%)	0	100	100
80	Bt	95/106 (90%)	89 (94%)	6 (6%)	0	100	100
81	Bu	299/308 (97%)	294 (98%)	5 (2%)	0	100	100
82	Bv	139/192 (72%)	134 (96%)	5 (4%)	0	100	100
83	Bw	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
84	Bx	230/276 (83%)	221 (96%)	9 (4%)	0	100	100
85	By	184/189 (97%)	179 (97%)	5 (3%)	0	100	100
86	Bz	31/34 (91%)	31 (100%)	0	0	100	100
All	All	11312/13146 (86%)	10988 (97%)	322 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	AU	40	GLU
77	Bq	50	HIS

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	A0	193/218 (88%)	190 (98%)	3 (2%)	55	64
3	A1	221/231 (96%)	220 (100%)	1 (0%)	81	88
4	A2	156/160 (98%)	155 (99%)	1 (1%)	78	86
5	A3	197/207 (95%)	195 (99%)	2 (1%)	68	76
6	A4	180/185 (97%)	179 (99%)	1 (1%)	78	86
7	A5	155/180 (86%)	154 (99%)	1 (1%)	78	86
8	A6	161/166 (97%)	159 (99%)	2 (1%)	63	72
9	A7	258/266 (97%)	248 (96%)	10 (4%)	28	31
10	A8	49/50 (98%)	46 (94%)	3 (6%)	17	15
11	A9	60/126 (48%)	60 (100%)	0	100	100
13	AC	183/243 (75%)	182 (100%)	1 (0%)	81	88
14	AD	87/131 (66%)	86 (99%)	1 (1%)	65	74
15	AE	138/156 (88%)	137 (99%)	1 (1%)	76	83
16	AF	99/119 (83%)	98 (99%)	1 (1%)	68	76
17	AG	128/131 (98%)	128 (100%)	0	100	100
18	AH	103/111 (93%)	102 (99%)	1 (1%)	68	76
19	AI	98/128 (77%)	96 (98%)	2 (2%)	48	56
20	AJ	108/109 (99%)	108 (100%)	0	100	100
21	AK	117/123 (95%)	116 (99%)	1 (1%)	70	78
22	AL	100/122 (82%)	99 (99%)	1 (1%)	68	76
23	AM	111/133 (84%)	109 (98%)	2 (2%)	51	60
24	AO	127/137 (93%)	126 (99%)	1 (1%)	73	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	AP	181/204 (89%)	180 (99%)	1 (1%)	78	86
26	AQ	90/104 (86%)	85 (94%)	5 (6%)	19	18
27	AR	72/149 (48%)	70 (97%)	2 (3%)	38	43
28	AS	115/117 (98%)	112 (97%)	3 (3%)	40	46
29	AT	108/116 (93%)	105 (97%)	3 (3%)	38	43
30	AU	63/94 (67%)	62 (98%)	1 (2%)	55	64
31	AV	90/97 (93%)	89 (99%)	1 (1%)	65	74
32	AW	74/75 (99%)	73 (99%)	1 (1%)	59	67
33	AX	176/180 (98%)	174 (99%)	2 (1%)	65	74
34	AY	48/53 (91%)	48 (100%)	0	100	100
35	AZ	50/84 (60%)	50 (100%)	0	100	100
36	Az	140/216 (65%)	139 (99%)	1 (1%)	76	83
45	BI	164/165 (99%)	164 (100%)	0	100	100
46	BK	169/185 (91%)	169 (100%)	0	100	100
47	BL	147/167 (88%)	140 (95%)	7 (5%)	23	23
48	BN	185/188 (98%)	183 (99%)	2 (1%)	65	74
49	BO	193/194 (100%)	191 (99%)	2 (1%)	68	76
50	BP	146/158 (92%)	146 (100%)	0	100	100
51	BQ	175/192 (91%)	174 (99%)	1 (1%)	78	86
52	BR	132/144 (92%)	132 (100%)	0	100	100
53	BS	156/158 (99%)	153 (98%)	3 (2%)	50	58
54	BT	162/198 (82%)	160 (99%)	2 (1%)	63	72
55	BU	132/133 (99%)	128 (97%)	4 (3%)	36	41
56	BV	98/116 (84%)	97 (99%)	1 (1%)	68	76
57	BW	103/108 (95%)	102 (99%)	1 (1%)	68	76
58	BX	105/136 (77%)	104 (99%)	1 (1%)	68	76
59	BY	56/102 (55%)	55 (98%)	1 (2%)	51	60
60	BZ	109/125 (87%)	107 (98%)	2 (2%)	51	60
61	Ba	117/117 (100%)	115 (98%)	2 (2%)	53	62
62	Bb	115/116 (99%)	115 (100%)	0	100	100
63	Bc	128/130 (98%)	127 (99%)	1 (1%)	73	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
64	Bd	57/59 (97%)	57 (100%)	0	100	100
65	Be	197/203 (97%)	196 (100%)	1 (0%)	81	88
66	Bf	340/359 (95%)	339 (100%)	1 (0%)	86	91
67	Bg	85/92 (92%)	83 (98%)	2 (2%)	43	49
68	Bh	106/162 (65%)	105 (99%)	1 (1%)	70	78
69	Bi	116/117 (99%)	115 (99%)	1 (1%)	70	78
70	Bj	103/137 (75%)	103 (100%)	0	100	100
71	Bk	105/114 (92%)	105 (100%)	0	100	100
72	Bl	122/126 (97%)	120 (98%)	2 (2%)	55	64
73	Bm	81/90 (90%)	78 (96%)	3 (4%)	30	33
74	Bn	70/71 (99%)	70 (100%)	0	100	100
75	Bo	72/76 (95%)	69 (96%)	3 (4%)	26	28
76	Bp	71/77 (92%)	69 (97%)	2 (3%)	38	43
77	Bq	46/47 (98%)	46 (100%)	0	100	100
78	Br	278/310 (90%)	278 (100%)	0	100	100
79	Bs	39/111 (35%)	36 (92%)	3 (8%)	12	9
80	Bt	87/95 (92%)	86 (99%)	1 (1%)	65	74
81	Bu	242/247 (98%)	240 (99%)	2 (1%)	73	81
82	Bv	118/159 (74%)	116 (98%)	2 (2%)	53	62
83	Bw	190/213 (89%)	190 (100%)	0	100	100
84	Bx	198/228 (87%)	196 (99%)	2 (1%)	68	76
85	By	169/172 (98%)	164 (97%)	5 (3%)	36	41
86	Bz	29/31 (94%)	29 (100%)	0	100	100
All	All	9749/11049 (88%)	9632 (99%)	117 (1%)	61	72

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BL	43	VAL
84	Bx	49	ILE
54	BT	172	LYS
82	Bv	164	LYS
75	Bo	89	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
56	BV	16	GLN
66	Bf	109	HIS
57	BW	26	ASN
62	Bb	104	ASN
68	Bh	132	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Et	17/95 (17%)	3 (17%)	0
12	AA	1860/2280 (81%)	414 (22%)	8 (0%)
37	BA	1519/1866 (81%)	244 (16%)	6 (0%)
38	BB	1117/1544 (72%)	199 (17%)	9 (0%)
39	BC	157/209 (75%)	19 (12%)	0
40	BD	119/120 (99%)	10 (8%)	0
41	BE	180/217 (82%)	33 (18%)	2 (1%)
42	BF	75/78 (96%)	17 (22%)	2 (2%)
43	BG	182/183 (99%)	25 (13%)	1 (0%)
44	BH	111/136 (81%)	21 (18%)	1 (0%)
All	All	5337/6728 (79%)	985 (18%)	29 (0%)

5 of 985 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	Et	66	U
1	Et	67	C
1	Et	76	A
12	AA	32	C
12	AA	45	C

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	BB	379	U
43	BG	18	U
38	BB	817	C
41	BE	180	G
38	BB	636	A

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

158 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$
38	PSU	BB	522	38	18,21,22	4.49	7 (38%)	22,30,33	1.74	5 (22%)
38	OMG	BB	1269	38	23,26,27	2.30	9 (39%)	33,38,41	2.22	12 (36%)
9	SNC	A7	157	9	4,7,8	0.70	0	1,7,9	0.86	0
38	PSU	BB	611	38	18,21,22	4.38	7 (38%)	22,30,33	1.63	4 (18%)
66	HIC	Bf	248	66	10,11,12	0.44	0	8,14,16	0.35	0
38	PSU	BB	629	38	18,21,22	4.50	7 (38%)	22,30,33	1.47	3 (13%)
12	OMG	AA	1700	12	23,26,27	2.37	9 (39%)	33,38,41	2.31	12 (36%)
12	OMC	AA	1844	12	19,22,23	3.01	8 (42%)	26,31,34	0.68	0
38	OMG	BB	71	38	23,26,27	2.38	8 (34%)	33,38,41	2.19	11 (33%)
37	OMC	BA	760	87,37	19,22,23	3.01	8 (42%)	26,31,34	0.67	0
38	PSU	BB	1160	38	18,21,22	4.46	7 (38%)	22,30,33	1.74	4 (18%)
55	SNC	BU	139	55	4,7,8	0.69	0	1,7,9	1.13	0
12	OMU	AA	714	12	19,22,23	2.99	8 (42%)	26,31,34	1.74	5 (19%)
16	SNC	AF	48	16	4,7,8	0.70	0	1,7,9	1.16	0
38	OMG	BB	1062	38	23,26,27	2.36	9 (39%)	33,38,41	2.35	12 (36%)
12	OMU	AA	36	12	19,22,23	2.94	8 (42%)	26,31,34	1.76	5 (19%)
38	5MC	BB	1324	87,93,38	18,22,23	3.51	7 (38%)	26,32,35	1.11	1 (3%)
12	PSU	AA	1612	12	18,21,22	4.49	7 (38%)	22,30,33	1.84	5 (22%)
37	A2M	BA	996	37	22,25,26	3.40	10 (45%)	31,36,39	2.31	9 (29%)
12	OMC	AA	2134	12	19,22,23	3.01	8 (42%)	26,31,34	0.71	0
38	A2M	BB	1388	38	22,25,26	3.40	10 (45%)	31,36,39	2.30	8 (25%)
12	OMG	AA	1517	12	23,26,27	2.38	9 (39%)	33,38,41	2.37	10 (30%)
12	MA6	AA	2260	12	23,26,27	1.35	3 (13%)	34,38,41	3.61	11 (32%)
37	A2M	BA	1665	37,38	22,25,26	3.37	10 (45%)	31,36,39	2.37	10 (32%)
38	OMU	BB	685	38	19,22,23	2.97	8 (42%)	26,31,34	1.58	5 (19%)
38	UY1	BB	578	87,93,38	19,22,23	0.61	1 (5%)	22,31,34	0.54	1 (4%)
37	OMC	BA	1006	37	19,22,23	2.89	8 (42%)	26,31,34	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MA6	AA	2261	12	23,26,27	1.34	3 (13%)	34,38,41	3.70	11 (32%)
38	A2M	BB	622	37,38	22,25,26	3.42	10 (45%)	31,36,39	2.34	11 (35%)
37	PSU	BA	1614	37,38	18,21,22	4.49	8 (44%)	22,30,33	1.67	4 (18%)
38	OMC	BB	601	38	19,22,23	2.91	8 (42%)	26,31,34	0.74	0
84	HY3	Bx	172	84	6,8,9	0.93	0	5,10,12	2.00	2 (40%)
39	A2M	BC	163	39,37	22,25,26	3.46	10 (45%)	31,36,39	2.32	10 (32%)
12	OMG	AA	1676	12	23,26,27	2.31	9 (39%)	33,38,41	2.34	12 (36%)
12	OMU	AA	57	12	19,22,23	2.99	8 (42%)	26,31,34	1.66	5 (19%)
39	OMG	BC	75	39	23,26,27	2.33	9 (39%)	33,38,41	2.27	13 (39%)
37	PSU	BA	737	87,37	18,21,22	4.48	8 (44%)	22,30,33	1.50	3 (13%)
37	PSU	BA	452	37	18,21,22	4.49	7 (38%)	22,30,33	1.81	5 (22%)
65	SNC	Be	195	65	4,7,8	0.65	0	1,7,9	1.19	0
39	A2M	BC	41	39	22,25,26	3.39	9 (40%)	31,36,39	2.38	10 (32%)
12	OMG	AA	2227	12	23,26,27	2.32	9 (39%)	33,38,41	2.37	13 (39%)
12	7MG	AA	2070	12	22,26,27	4.24	10 (45%)	29,39,42	1.97	9 (31%)
12	OMU	AA	1652	12	19,22,23	2.98	8 (42%)	26,31,34	1.55	5 (19%)
37	PSU	BA	1009	37	18,21,22	4.49	7 (38%)	22,30,33	1.60	4 (18%)
12	OMG	AA	1931	12	23,26,27	2.39	9 (39%)	33,38,41	2.37	11 (33%)
38	OMC	BB	377	38	19,22,23	3.03	8 (42%)	26,31,34	0.68	0
39	A2M	BC	43	39	22,25,26	3.38	10 (45%)	31,36,39	2.35	10 (32%)
12	B8N	AA	1596	12	24,29,30	3.11	8 (33%)	29,42,45	1.77	6 (20%)
6	SNC	A4	138	6	4,7,8	0.69	0	1,7,9	1.09	0
38	OMC	BB	1264	38	19,22,23	2.99	8 (42%)	26,31,34	0.83	0
12	OMG	AA	1603	12	23,26,27	2.38	9 (39%)	33,38,41	2.33	12 (36%)
38	A2M	BB	1201	38	22,25,26	3.38	10 (45%)	31,36,39	2.48	13 (41%)
38	PSU	BB	528	38	18,21,22	4.47	7 (38%)	22,30,33	1.72	5 (22%)
38	PSU	BB	1409	38	18,21,22	4.52	7 (38%)	22,30,33	1.74	5 (22%)
12	OMG	AA	1531	12	23,26,27	2.26	9 (39%)	33,38,41	2.21	13 (39%)
12	PSU	AA	2045	12	18,21,22	4.49	7 (38%)	22,30,33	1.64	4 (18%)
27	SNC	AR	58	27	4,7,8	0.67	0	1,7,9	0.52	0
53	SNC	BS	100	53	4,7,8	0.75	0	1,7,9	1.10	0
38	PSU	BB	680	87,38	18,21,22	4.40	7 (38%)	22,30,33	1.58	4 (18%)
38	A2M	BB	400	38	22,25,26	3.37	9 (40%)	31,36,39	2.37	9 (29%)
38	PSU	BB	1429	93,38	18,21,22	4.50	7 (38%)	22,30,33	1.65	4 (18%)
38	A2M	BB	545	38	22,25,26	3.32	10 (45%)	31,36,39	2.57	12 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	PSU	AA	1619	12	18,21,22	4.53	7 (38%)	22,30,33	1.75	5 (22%)
38	PSU	BB	644	38	18,21,22	4.47	7 (38%)	22,30,33	1.56	4 (18%)
12	OMC	AA	66	12	19,22,23	3.00	8 (42%)	26,31,34	0.84	0
38	OMG	BB	1245	38	23,26,27	2.36	9 (39%)	33,38,41	2.25	12 (36%)
38	PSU	BB	1319	38	18,21,22	4.52	7 (38%)	22,30,33	1.73	5 (22%)
12	OMC	AA	46	12	19,22,23	2.96	8 (42%)	26,31,34	0.66	0
37	PSU	BA	1129	37,93	18,21,22	4.49	7 (38%)	22,30,33	1.79	5 (22%)
38	PSU	BB	1210	38	18,21,22	4.51	7 (38%)	22,30,33	1.79	5 (22%)
37	A2M	BA	927	37	22,25,26	3.35	10 (45%)	31,36,39	2.43	11 (35%)
37	OMG	BA	1267	87,37	23,26,27	2.32	9 (39%)	33,38,41	2.22	15 (45%)
12	PSU	AA	61	12	18,21,22	4.55	7 (38%)	22,30,33	1.84	5 (22%)
12	PSU	AA	2121	12	18,21,22	4.48	7 (38%)	22,30,33	1.81	5 (22%)
12	A2M	AA	125	87,12	22,25,26	3.42	9 (40%)	31,36,39	2.36	9 (29%)
38	PSU	BB	1076	38	18,21,22	4.49	7 (38%)	22,30,33	1.94	5 (22%)
38	A2M	BB	1400	87,38	22,25,26	3.37	9 (40%)	31,36,39	2.50	11 (35%)
38	OMC	BB	1175	38	19,22,23	2.98	8 (42%)	26,31,34	0.83	0
37	OMG	BA	1028	37	23,26,27	2.33	9 (39%)	33,38,41	2.12	11 (33%)
37	PSU	BA	1609	37	18,21,22	4.49	7 (38%)	22,30,33	1.65	4 (18%)
38	PSU	BB	1434	38	18,21,22	4.25	8 (44%)	22,30,33	1.61	3 (13%)
37	PSU	BA	1169	37	18,21,22	4.52	7 (38%)	22,30,33	1.82	5 (22%)
38	OMG	BB	1094	38	23,26,27	2.31	9 (39%)	33,38,41	2.25	15 (45%)
18	IAS	AH	131	18	6,7,8	0.93	0	6,8,10	1.25	1 (16%)
37	PSU	BA	1086	37,93	18,21,22	4.51	7 (38%)	22,30,33	1.71	4 (18%)
12	OMG	AA	1895	87,12	23,26,27	2.33	9 (39%)	33,38,41	2.32	14 (42%)
37	OMU	BA	1742	37	19,22,23	2.99	8 (42%)	26,31,34	1.66	4 (15%)
38	PSU	BB	1419	38	18,21,22	4.49	7 (38%)	22,30,33	1.80	6 (27%)
38	OMG	BB	1247	38	23,26,27	2.35	9 (39%)	33,38,41	2.31	13 (39%)
37	OMC	BA	1608	37	19,22,23	3.04	8 (42%)	26,31,34	0.88	1 (3%)
37	OMU	BA	916	37	19,22,23	2.96	8 (42%)	26,31,34	1.56	5 (19%)
51	HY3	BQ	203	51	6,8,9	0.85	0	5,10,12	1.13	1 (20%)
12	OMU	AA	2054	12	19,22,23	3.01	8 (42%)	26,31,34	1.73	5 (19%)
39	OMU	BC	7	39,37	19,22,23	2.98	8 (42%)	26,31,34	1.65	5 (19%)
12	PSU	AA	1710	12	18,21,22	4.47	7 (38%)	22,30,33	1.74	3 (13%)
37	PSU	BA	1080	37,38	18,21,22	4.54	7 (38%)	22,30,33	1.75	4 (18%)
38	OMU	BB	73	38	19,22,23	2.90	7 (36%)	26,31,34	1.49	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	PSU	BA	258	37	18,21,22	4.49	7 (38%)	22,30,33	1.63	4 (18%)
37	OMU	BA	46	37	19,22,23	2.97	8 (42%)	26,31,34	1.85	6 (23%)
37	OMG	BA	1605	37	23,26,27	2.40	9 (39%)	33,38,41	2.28	15 (45%)
12	PSU	AA	2278	12	18,21,22	4.45	7 (38%)	22,30,33	1.66	5 (22%)
21	HY3	AK	47	21	6,8,9	0.89	0	5,10,12	1.46	1 (20%)
39	PSU	BC	74	39	18,21,22	4.51	7 (38%)	22,30,33	1.78	5 (22%)
37	A2M	BA	762	37	22,25,26	3.41	10 (45%)	31,36,39	2.35	10 (32%)
38	PSU	BB	1403	87,38	18,21,22	4.24	8 (44%)	22,30,33	1.64	5 (22%)
49	HY3	BO	88	49	6,8,9	0.89	0	5,10,12	1.31	1 (20%)
37	OMG	BA	1621	87,37,38	23,26,27	2.29	9 (39%)	33,38,41	2.24	13 (39%)
28	HY3	AS	62	28	6,8,9	0.88	0	5,10,12	1.15	1 (20%)
38	OMC	BB	1413	38	19,22,23	3.01	8 (42%)	26,31,34	0.75	0
38	OMU	BB	1093	38	19,22,23	2.96	8 (42%)	26,31,34	1.63	5 (19%)
38	OMG	BB	72	37,38	23,26,27	2.33	8 (34%)	33,38,41	2.14	10 (30%)
38	OMG	BB	673	38	23,26,27	2.32	9 (39%)	33,38,41	2.31	13 (39%)
12	PSU	AA	1592	12	18,21,22	4.53	7 (38%)	22,30,33	1.75	5 (22%)
38	PSU	BB	490	38	18,21,22	4.52	7 (38%)	22,30,33	1.67	4 (18%)
12	OMU	AA	1674	12	19,22,23	3.00	8 (42%)	26,31,34	1.70	5 (19%)
12	OMC	AA	1932	12	19,22,23	2.99	8 (42%)	26,31,34	0.78	0
38	PSU	BB	455	93,38	18,21,22	4.52	8 (44%)	22,30,33	1.90	5 (22%)
12	A2M	AA	56	12	22,25,26	3.43	10 (45%)	31,36,39	2.31	10 (32%)
38	A2M	BB	590	38	22,25,26	3.36	9 (40%)	31,36,39	2.45	11 (35%)
12	PSU	AA	131	12	18,21,22	4.45	8 (44%)	22,30,33	1.80	4 (18%)
38	OMG	BB	552	38	23,26,27	2.37	9 (39%)	33,38,41	2.33	12 (36%)
37	OMG	BA	1709	37	23,26,27	2.32	9 (39%)	33,38,41	2.33	12 (36%)
37	1MA	BA	742	87,37	21,25,26	0.34	0	31,37,40	0.47	0
37	OMU	BA	1181	37	19,22,23	2.99	8 (42%)	26,31,34	1.75	5 (19%)
12	A2M	AA	2096	12	22,25,26	3.40	9 (40%)	31,36,39	2.40	11 (35%)
38	A2M	BB	588	37,93,38	22,25,26	3.35	10 (45%)	31,36,39	2.44	10 (32%)
38	A2M	BB	646	38	22,25,26	3.37	9 (40%)	31,36,39	2.27	9 (29%)
38	OMG	BB	659	87,38	23,26,27	2.31	9 (39%)	33,38,41	2.23	13 (39%)
53	SNC	BS	10	53	4,7,8	0.75	0	1,7,9	0.46	0
6	HY3	A4	137	6	6,8,9	0.87	0	5,10,12	1.25	1 (20%)
12	PSU	AA	1276	12	18,21,22	4.54	7 (38%)	22,30,33	1.61	3 (13%)
38	PSU	BB	615	38	18,21,22	4.50	7 (38%)	22,30,33	1.61	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	OMU	BB	1435	38	19,22,23	2.96	7 (36%)	26,31,34	1.50	4 (15%)
37	OMG	BA	925	37	23,26,27	2.31	9 (39%)	33,38,41	2.30	13 (39%)
38	PSU	BB	1280	38	18,21,22	4.48	7 (38%)	22,30,33	1.75	6 (27%)
38	5MC	BB	542	87,38	18,22,23	3.48	7 (38%)	26,32,35	1.04	2 (7%)
12	UY1	AA	2123	12	19,22,23	0.41	0	22,31,34	0.99	3 (13%)
37	A2M	BA	746	37	22,25,26	3.40	9 (40%)	31,36,39	2.38	10 (32%)
37	OMU	BA	1448	37	19,22,23	3.07	8 (42%)	26,31,34	1.71	4 (15%)
82	HY3	Bv	65	82	6,8,9	0.88	0	5,10,12	1.19	1 (20%)
38	PSU	BB	1398	87,38	18,21,22	4.37	7 (38%)	22,30,33	1.82	6 (27%)
37	A2M	BA	743	37,38	22,25,26	3.37	9 (40%)	31,36,39	2.34	10 (32%)
12	PSU	AA	1907	12	18,21,22	4.53	7 (38%)	22,30,33	1.74	5 (22%)
12	OMU	AA	1899	12	19,22,23	3.01	8 (42%)	26,31,34	1.77	5 (19%)
12	PSU	AA	2146	12	18,21,22	4.53	8 (44%)	22,30,33	1.66	3 (13%)
37	OMU	BA	1330	37	19,22,23	3.03	8 (42%)	26,31,34	1.71	4 (15%)
37	A2M	BA	1620	87,37,38	22,25,26	3.35	9 (40%)	31,36,39	2.37	11 (35%)
38	A2M	BB	95	38	22,25,26	3.47	9 (40%)	31,36,39	2.41	11 (35%)
37	A2M	BA	254	37	22,25,26	3.41	9 (40%)	31,36,39	2.37	10 (32%)
12	PSU	AA	662	12	18,21,22	4.49	7 (38%)	22,30,33	1.65	5 (22%)
37	PSU	BA	1166	37	18,21,22	4.52	8 (44%)	22,30,33	1.66	4 (18%)
12	PSU	AA	1610	12	18,21,22	4.49	8 (44%)	22,30,33	1.63	4 (18%)
37	A2M	BA	1024	37	22,25,26	3.39	10 (45%)	31,36,39	2.33	11 (35%)
37	PSU	BA	1258	37	18,21,22	4.56	7 (38%)	22,30,33	1.80	5 (22%)
38	PSU	BB	1334	38	18,21,22	4.31	8 (44%)	22,30,33	1.79	5 (22%)
12	A2M	AA	721	87,12	22,25,26	3.37	10 (45%)	31,36,39	2.48	12 (38%)
38	A2M	BB	609	38	22,25,26	3.40	10 (45%)	31,36,39	2.35	8 (25%)
37	PSU	BA	1248	37,93	18,21,22	4.51	7 (38%)	22,30,33	1.73	5 (22%)

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
38	PSU	BB	522	38	-	2/7/25/26	0/2/2/2
38	OMG	BB	1269	38	-	0/9/27/28	0/3/3/3
9	SNC	A7	157	9	-	0/0/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	PSU	BB	611	38	-	0/7/25/26	0/2/2/2
66	HIC	Bf	248	66	-	0/5/6/8	0/1/1/1
38	PSU	BB	629	38	-	0/7/25/26	0/2/2/2
12	OMG	AA	1700	12	-	0/9/27/28	0/3/3/3
12	OMC	AA	1844	12	-	0/9/27/28	0/2/2/2
38	OMG	BB	71	38	-	0/9/27/28	0/3/3/3
37	OMC	BA	760	87,37	-	1/9/27/28	0/2/2/2
38	PSU	BB	1160	38	-	0/7/25/26	0/2/2/2
55	SNC	BU	139	55	-	0/0/6/8	-
12	OMU	AA	714	12	-	0/9/27/28	0/2/2/2
16	SNC	AF	48	16	-	0/0/6/8	-
38	OMG	BB	1062	38	-	3/9/27/28	0/3/3/3
12	OMU	AA	36	12	-	5/9/27/28	0/2/2/2
38	5MC	BB	1324	87,93,38	-	4/7/25/26	0/2/2/2
12	PSU	AA	1612	12	-	0/7/25/26	0/2/2/2
37	A2M	BA	996	37	-	0/9/27/28	0/3/3/3
12	OMC	AA	2134	12	-	0/9/27/28	0/2/2/2
38	A2M	BB	1388	38	-	0/9/27/28	0/3/3/3
12	OMG	AA	1517	12	-	0/9/27/28	0/3/3/3
12	MA6	AA	2260	12	-	0/11/29/30	0/3/3/3
37	A2M	BA	1665	37,38	-	1/9/27/28	0/3/3/3
38	OMU	BB	685	38	-	0/9/27/28	0/2/2/2
38	UY1	BB	578	87,93,38	-	4/9/27/28	0/2/2/2
37	OMC	BA	1006	37	-	0/9/27/28	0/2/2/2
12	MA6	AA	2261	12	-	2/11/29/30	0/3/3/3
38	A2M	BB	622	37,38	-	0/9/27/28	0/3/3/3
37	PSU	BA	1614	37,38	-	0/7/25/26	0/2/2/2
38	OMC	BB	601	38	-	0/9/27/28	0/2/2/2
84	HY3	Bx	172	84	-	1/1/12/14	0/1/1/1
39	A2M	BC	163	39,37	-	0/9/27/28	0/3/3/3
12	OMG	AA	1676	12	-	0/9/27/28	0/3/3/3
12	OMU	AA	57	12	-	1/9/27/28	0/2/2/2
39	OMG	BC	75	39	-	0/9/27/28	0/3/3/3
37	PSU	BA	737	87,37	-	0/7/25/26	0/2/2/2
37	PSU	BA	452	37	-	0/7/25/26	0/2/2/2
65	SNC	Be	195	65	-	0/0/6/8	-
39	A2M	BC	41	39	-	0/9/27/28	0/3/3/3
12	OMG	AA	2227	12	-	0/9/27/28	0/3/3/3
12	7MG	AA	2070	12	-	0/7/37/38	0/3/3/3
12	OMU	AA	1652	12	-	1/9/27/28	0/2/2/2
37	PSU	BA	1009	37	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	OMG	AA	1931	12	-	0/9/27/28	0/3/3/3
38	OMC	BB	377	38	-	0/9/27/28	0/2/2/2
39	A2M	BC	43	39	-	0/9/27/28	0/3/3/3
12	B8N	AA	1596	12	-	1/16/34/35	0/2/2/2
6	SNC	A4	138	6	-	0/0/6/8	-
38	OMC	BB	1264	38	-	1/9/27/28	0/2/2/2
12	OMG	AA	1603	12	-	1/9/27/28	0/3/3/3
38	A2M	BB	1201	38	-	0/9/27/28	0/3/3/3
38	PSU	BB	528	38	-	0/7/25/26	0/2/2/2
38	PSU	BB	1409	38	-	2/7/25/26	0/2/2/2
12	OMG	AA	1531	12	-	1/9/27/28	0/3/3/3
12	PSU	AA	2045	12	-	0/7/25/26	0/2/2/2
27	SNC	AR	58	27	-	0/0/6/8	-
53	SNC	BS	100	53	-	0/0/6/8	-
38	PSU	BB	680	87,38	-	0/7/25/26	0/2/2/2
38	A2M	BB	400	38	-	1/9/27/28	0/3/3/3
38	PSU	BB	1429	93,38	-	0/7/25/26	0/2/2/2
38	A2M	BB	545	38	-	2/9/27/28	0/3/3/3
12	PSU	AA	1619	12	-	2/7/25/26	0/2/2/2
38	PSU	BB	644	38	-	0/7/25/26	0/2/2/2
12	OMC	AA	66	12	-	0/9/27/28	0/2/2/2
38	OMG	BB	1245	38	-	0/9/27/28	0/3/3/3
38	PSU	BB	1319	38	-	0/7/25/26	0/2/2/2
12	OMC	AA	46	12	-	0/9/27/28	0/2/2/2
37	PSU	BA	1129	37,93	-	0/7/25/26	0/2/2/2
38	PSU	BB	1210	38	-	0/7/25/26	0/2/2/2
37	A2M	BA	927	37	-	0/9/27/28	0/3/3/3
37	OMG	BA	1267	87,37	-	0/9/27/28	0/3/3/3
12	PSU	AA	61	12	-	0/7/25/26	0/2/2/2
12	PSU	AA	2121	12	-	0/7/25/26	0/2/2/2
12	A2M	AA	125	87,12	-	0/9/27/28	0/3/3/3
38	PSU	BB	1076	38	-	0/7/25/26	0/2/2/2
38	A2M	BB	1400	87,38	-	0/9/27/28	0/3/3/3
38	OMC	BB	1175	38	-	0/9/27/28	0/2/2/2
37	OMG	BA	1028	37	-	1/9/27/28	0/3/3/3
37	PSU	BA	1609	37	-	0/7/25/26	0/2/2/2
38	PSU	BB	1434	38	-	0/7/25/26	0/2/2/2
37	PSU	BA	1169	37	-	0/7/25/26	0/2/2/2
38	OMG	BB	1094	38	-	1/9/27/28	0/3/3/3
18	IAS	AH	131	18	-	1/7/7/8	-
37	PSU	BA	1086	37,93	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	OMG	AA	1895	87,12	-	3/9/27/28	0/3/3/3
37	OMU	BA	1742	37	-	0/9/27/28	0/2/2/2
38	PSU	BB	1419	38	-	0/7/25/26	0/2/2/2
38	OMG	BB	1247	38	-	0/9/27/28	0/3/3/3
37	OMC	BA	1608	37	-	3/9/27/28	0/2/2/2
37	OMU	BA	916	37	-	0/9/27/28	0/2/2/2
51	HY3	BQ	203	51	-	1/1/12/14	0/1/1/1
12	OMU	AA	2054	12	-	2/9/27/28	0/2/2/2
39	OMU	BC	7	39,37	-	1/9/27/28	0/2/2/2
12	PSU	AA	1710	12	-	2/7/25/26	0/2/2/2
37	PSU	BA	1080	37,38	-	2/7/25/26	0/2/2/2
38	OMU	BB	73	38	-	0/9/27/28	0/2/2/2
37	PSU	BA	258	37	-	0/7/25/26	0/2/2/2
37	OMU	BA	46	37	-	0/9/27/28	0/2/2/2
37	OMG	BA	1605	37	-	0/9/27/28	0/3/3/3
12	PSU	AA	2278	12	-	1/7/25/26	0/2/2/2
21	HY3	AK	47	21	-	0/1/12/14	0/1/1/1
39	PSU	BC	74	39	-	0/7/25/26	0/2/2/2
37	A2M	BA	762	37	-	0/9/27/28	0/3/3/3
38	PSU	BB	1403	87,38	-	0/7/25/26	0/2/2/2
49	HY3	BO	88	49	-	0/1/12/14	0/1/1/1
37	OMG	BA	1621	87,37,38	-	1/9/27/28	0/3/3/3
28	HY3	AS	62	28	-	0/1/12/14	0/1/1/1
38	OMC	BB	1413	38	-	0/9/27/28	0/2/2/2
38	OMU	BB	1093	38	-	0/9/27/28	0/2/2/2
38	OMG	BB	72	37,38	-	0/9/27/28	0/3/3/3
38	OMG	BB	673	38	-	0/9/27/28	0/3/3/3
12	PSU	AA	1592	12	-	0/7/25/26	0/2/2/2
38	PSU	BB	490	38	-	0/7/25/26	0/2/2/2
12	OMU	AA	1674	12	-	0/9/27/28	0/2/2/2
12	OMC	AA	1932	12	-	0/9/27/28	0/2/2/2
38	PSU	BB	455	93,38	-	0/7/25/26	0/2/2/2
12	A2M	AA	56	12	-	1/9/27/28	0/3/3/3
38	A2M	BB	590	38	-	0/9/27/28	0/3/3/3
12	PSU	AA	131	12	-	2/7/25/26	0/2/2/2
38	OMG	BB	552	38	-	2/9/27/28	0/3/3/3
37	OMG	BA	1709	37	-	0/9/27/28	0/3/3/3
37	1MA	BA	742	87,37	-	2/7/25/26	0/3/3/3
37	OMU	BA	1181	37	-	0/9/27/28	0/2/2/2
12	A2M	AA	2096	12	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	A2M	BB	588	37,93,38	-	3/9/27/28	0/3/3/3
38	A2M	BB	646	38	-	0/9/27/28	0/3/3/3
38	OMG	BB	659	87,38	-	0/9/27/28	0/3/3/3
53	SNC	BS	10	53	-	0/0/6/8	-
6	HY3	A4	137	6	-	1/1/12/14	0/1/1/1
12	PSU	AA	1276	12	-	0/7/25/26	0/2/2/2
38	PSU	BB	615	38	-	0/7/25/26	0/2/2/2
38	OMU	BB	1435	38	-	0/9/27/28	0/2/2/2
37	OMG	BA	925	37	-	0/9/27/28	0/3/3/3
38	PSU	BB	1280	38	-	0/7/25/26	0/2/2/2
38	5MC	BB	542	87,38	-	0/7/25/26	0/2/2/2
12	UY1	AA	2123	12	-	1/9/27/28	0/2/2/2
37	A2M	BA	746	37	-	1/9/27/28	0/3/3/3
37	OMU	BA	1448	37	-	2/9/27/28	0/2/2/2
82	HY3	Bv	65	82	-	1/1/12/14	0/1/1/1
38	PSU	BB	1398	87,38	-	0/7/25/26	0/2/2/2
37	A2M	BA	743	37,38	-	3/9/27/28	0/3/3/3
12	PSU	AA	1907	12	-	2/7/25/26	0/2/2/2
12	OMU	AA	1899	12	-	2/9/27/28	0/2/2/2
12	PSU	AA	2146	12	-	0/7/25/26	0/2/2/2
37	OMU	BA	1330	37	-	2/9/27/28	0/2/2/2
37	A2M	BA	1620	87,37,38	-	0/9/27/28	0/3/3/3
38	A2M	BB	95	38	-	0/9/27/28	0/3/3/3
37	A2M	BA	254	37	-	0/9/27/28	0/3/3/3
12	PSU	AA	662	12	-	0/7/25/26	0/2/2/2
37	PSU	BA	1166	37	-	2/7/25/26	0/2/2/2
12	PSU	AA	1610	12	-	3/7/25/26	0/2/2/2
37	A2M	BA	1024	37	-	0/9/27/28	0/3/3/3
37	PSU	BA	1258	37	-	0/7/25/26	0/2/2/2
38	PSU	BB	1334	38	-	0/7/25/26	0/2/2/2
12	A2M	AA	721	87,12	-	4/9/27/28	0/3/3/3
38	A2M	BB	609	38	-	1/9/27/28	0/3/3/3
37	PSU	BA	1248	37,93	-	1/7/25/26	0/2/2/2

The worst 5 of 1119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	BA	1080	PSU	C6-C5	11.97	1.49	1.35
12	AA	1276	PSU	C6-C5	11.92	1.49	1.35
37	BA	1086	PSU	C6-C5	11.92	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	AA	2146	PSU	C6-C5	11.91	1.49	1.35
37	BA	1258	PSU	C6-C5	11.89	1.49	1.35

The worst 5 of 947 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	AA	2261	MA6	N1-C6-N6	-15.57	100.06	117.08
12	AA	2260	MA6	N1-C6-N6	-14.78	100.92	117.08
12	AA	2261	MA6	C5-C6-N6	8.50	140.10	125.30
12	AA	2260	MA6	C5-C6-N6	7.97	139.18	125.30
12	AA	1517	OMG	C1'-N9-C8	-7.01	106.73	126.70

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A4	137	HY3	O-C-CA-C3
12	AA	56	A2M	C1'-C2'-O2'-CM'
12	AA	57	OMU	C1'-C2'-O2'-CM2
12	AA	131	PSU	C3'-C4'-C5'-O5'
12	AA	131	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

42 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
66	Bf	248	HIC	1	0
37	BA	760	OMC	1	0
38	BB	1062	OMG	1	0
37	BA	996	A2M	1	0
12	AA	2134	OMC	2	0
38	BB	1388	A2M	1	0
37	BA	1665	A2M	2	0
38	BB	622	A2M	2	0
37	BA	1614	PSU	1	0
38	BB	601	OMC	1	0
84	Bx	172	HY3	1	0
39	BC	163	A2M	1	0
12	AA	57	OMU	2	0
12	AA	1652	OMU	1	0
38	BB	1201	A2M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	AA	2045	PSU	2	0
38	BB	400	A2M	2	0
38	BB	1429	PSU	1	0
38	BB	545	A2M	1	0
38	BB	644	PSU	1	0
12	AA	125	A2M	1	0
37	BA	1609	PSU	1	0
37	BA	1086	PSU	1	0
12	AA	1895	OMG	1	0
37	BA	1608	OMC	1	0
37	BA	916	OMU	1	0
39	BC	7	OMU	2	0
21	AK	47	HY3	1	0
37	BA	762	A2M	2	0
49	BO	88	HY3	1	0
12	AA	56	A2M	1	0
37	BA	1181	OMU	1	0
12	AA	2096	A2M	1	0
38	BB	588	A2M	2	0
38	BB	646	A2M	2	0
82	Bv	65	HY3	1	0
37	BA	743	A2M	1	0
37	BA	254	A2M	2	0
37	BA	1166	PSU	1	0
37	BA	1024	A2M	1	0
38	BB	1334	PSU	1	0
38	BB	609	A2M	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 396 ligands modelled in this entry, 316 are monoatomic - leaving 80 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
88	SPD	BA	1922	-	9,9,9	0.43	0	8,8,8	0.36	0
88	SPD	BE	305	-	9,9,9	0.44	0	8,8,8	0.27	0
91	PUT	BB	1610	-	5,5,5	0.23	0	4,4,4	0.14	0
88	SPD	BA	1908	-	9,9,9	0.44	0	8,8,8	0.18	0
88	SPD	AA	2373	-	9,9,9	0.43	0	8,8,8	0.24	0
88	SPD	AA	2376	-	9,9,9	0.43	0	8,8,8	0.27	0
88	SPD	AA	2311	-	9,9,9	0.43	0	8,8,8	0.32	0
88	SPD	BB	1609	-	9,9,9	0.43	0	8,8,8	0.37	0
88	SPD	BA	1919	-	9,9,9	0.42	0	8,8,8	0.41	0
88	SPD	BB	1605	-	9,9,9	0.42	0	8,8,8	0.39	0
88	SPD	BA	1911	-	9,9,9	0.43	0	8,8,8	0.41	0
88	SPD	BA	2040	-	9,9,9	0.42	0	8,8,8	0.34	0
88	SPD	BG	201	-	9,9,9	0.43	0	8,8,8	0.19	0
88	SPD	BG	202	-	9,9,9	0.44	0	8,8,8	0.33	0
88	SPD	BA	1901	-	9,9,9	0.40	0	8,8,8	0.36	0
88	SPD	A6	201	-	9,9,9	0.42	0	8,8,8	0.35	0
88	SPD	BA	1910	-	9,9,9	0.42	0	8,8,8	0.22	0
88	SPD	BB	1606	-	9,9,9	0.44	0	8,8,8	0.47	0
88	SPD	BA	2048	-	9,9,9	0.43	0	8,8,8	0.23	0
91	PUT	BA	1907	-	5,5,5	0.24	0	4,4,4	0.15	0
88	SPD	BA	1913	-	9,9,9	0.42	0	8,8,8	0.24	0
88	SPD	BA	1921	-	9,9,9	0.42	0	8,8,8	0.45	0
88	SPD	BA	1916	-	9,9,9	0.42	0	8,8,8	0.26	0
88	SPD	BC	309	-	9,9,9	0.45	0	8,8,8	0.35	0
91	PUT	BB	1601	-	5,5,5	0.23	0	4,4,4	0.21	0
88	SPD	BA	1926	-	9,9,9	0.45	0	8,8,8	0.23	0
88	SPD	BB	1604	-	9,9,9	0.41	0	8,8,8	0.46	0
88	SPD	AA	2302	-	9,9,9	0.42	0	8,8,8	0.46	0
88	SPD	BA	1904	-	9,9,9	0.43	0	8,8,8	0.28	0
88	SPD	BA	1915	-	9,9,9	0.43	0	8,8,8	0.58	0
88	SPD	BA	2039	-	9,9,9	0.42	0	8,8,8	0.26	0
88	SPD	BA	2042	-	9,9,9	0.42	0	8,8,8	0.28	0
88	SPD	Bd	101	-	9,9,9	0.44	0	8,8,8	0.29	0
88	SPD	BQ	304	-	9,9,9	0.43	0	8,8,8	0.29	0
88	SPD	BA	2049	-	9,9,9	0.43	0	8,8,8	0.37	0
88	SPD	AA	2375	-	9,9,9	0.42	0	8,8,8	0.40	0
91	PUT	BB	1603	-	5,5,5	0.23	0	4,4,4	0.08	0
91	PUT	BA	1918	-	5,5,5	0.24	0	4,4,4	0.20	0
91	PUT	AA	2308	-	5,5,5	0.23	0	4,4,4	0.18	0
91	PUT	BA	1920	-	5,5,5	0.25	0	4,4,4	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
88	SPD	BA	1903	-	9,9,9	0.47	0	8,8,8	0.24	0
88	SPD	BA	1924	-	9,9,9	0.44	0	8,8,8	0.23	0
91	PUT	BA	2038	-	5,5,5	0.23	0	4,4,4	0.22	0
88	SPD	BA	1925	-	9,9,9	0.44	0	8,8,8	0.34	0
88	SPD	BA	1923	-	9,9,9	0.43	0	8,8,8	0.23	0
88	SPD	BB	1712	-	9,9,9	0.43	0	8,8,8	0.27	0
91	PUT	AA	2312	-	5,5,5	0.23	0	4,4,4	0.19	0
88	SPD	BC	307	-	9,9,9	0.43	0	8,8,8	0.38	0
91	PUT	BB	1607	-	5,5,5	0.23	0	4,4,4	0.19	0
91	PUT	BB	1608	-	5,5,5	0.24	0	4,4,4	0.15	0
90	GET	AA	2304	-	33,36,36	0.48	0	43,55,55	0.54	0
91	PUT	BA	1902	-	5,5,5	0.23	0	4,4,4	0.15	0
88	SPD	BA	1905	-	9,9,9	0.44	0	8,8,8	0.28	0
88	SPD	BA	1906	-	9,9,9	0.43	0	8,8,8	0.31	0
88	SPD	BA	2043	-	9,9,9	0.43	0	8,8,8	0.34	0
90	GET	AA	2370	-	33,36,36	0.48	0	43,55,55	0.62	0
88	SPD	AA	2374	-	9,9,9	0.43	0	8,8,8	0.19	0
88	SPD	AA	2301	-	9,9,9	0.44	0	8,8,8	0.34	0
92	GTP	AA	2309	87	30,34,34	0.84	0	46,54,54	1.60	10 (21%)
88	SPD	BA	1909	-	9,9,9	0.43	0	8,8,8	0.36	0
88	SPD	BC	308	-	9,9,9	0.43	0	8,8,8	0.47	0
88	SPD	BA	1917	-	9,9,9	0.43	0	8,8,8	0.31	0
91	PUT	AA	2310	-	5,5,5	0.23	0	4,4,4	0.30	0
88	SPD	BB	1602	-	9,9,9	0.43	0	8,8,8	0.55	0
88	SPD	BA	1912	-	9,9,9	0.46	0	8,8,8	0.23	0
88	SPD	BA	2047	-	9,9,9	0.42	0	8,8,8	0.31	0
88	SPD	AA	2303	-	9,9,9	0.44	0	8,8,8	0.16	0
88	SPD	AA	2306	-	9,9,9	0.42	0	8,8,8	0.35	0
88	SPD	BB	1711	-	9,9,9	0.41	0	8,8,8	0.18	0
88	SPD	BA	2045	-	9,9,9	0.43	0	8,8,8	0.30	0
88	SPD	AA	2305	-	9,9,9	0.43	0	8,8,8	0.32	0
88	SPD	BA	2046	-	9,9,9	0.41	0	8,8,8	0.32	0
88	SPD	AA	2371	-	9,9,9	0.42	0	8,8,8	0.34	0
88	SPD	BA	1914	-	9,9,9	0.43	0	8,8,8	0.35	0
90	GET	AA	2372	-	33,36,36	0.42	0	43,55,55	0.59	1 (2%)
88	SPD	AA	2307	-	9,9,9	0.44	0	8,8,8	0.22	0
88	SPD	BA	2041	-	9,9,9	0.43	0	8,8,8	0.31	0
88	SPD	BA	2044	-	9,9,9	0.43	0	8,8,8	0.29	0
91	PUT	AA	2313	-	5,5,5	0.23	0	4,4,4	0.16	0
88	SPD	BB	1611	-	9,9,9	0.43	0	8,8,8	0.24	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
88	SPD	BA	1922	-	-	1/7/7/7	-
88	SPD	BE	305	-	-	1/7/7/7	-
91	PUT	BB	1610	-	-	0/3/3/3	-
88	SPD	BA	1908	-	-	1/7/7/7	-
88	SPD	AA	2373	-	-	1/7/7/7	-
88	SPD	AA	2376	-	-	0/7/7/7	-
88	SPD	AA	2311	-	-	0/7/7/7	-
88	SPD	BB	1609	-	-	1/7/7/7	-
88	SPD	BA	1919	-	-	0/7/7/7	-
88	SPD	BB	1605	-	-	0/7/7/7	-
88	SPD	BA	1911	-	-	1/7/7/7	-
88	SPD	BA	2040	-	-	0/7/7/7	-
88	SPD	BG	201	-	-	1/7/7/7	-
88	SPD	BG	202	-	-	0/7/7/7	-
88	SPD	BA	1901	-	-	0/7/7/7	-
88	SPD	A6	201	-	-	0/7/7/7	-
88	SPD	BA	1910	-	-	1/7/7/7	-
88	SPD	BB	1606	-	-	0/7/7/7	-
88	SPD	BA	2048	-	-	0/7/7/7	-
91	PUT	BA	1907	-	-	0/3/3/3	-
88	SPD	BA	1913	-	-	2/7/7/7	-
88	SPD	BA	1921	-	-	0/7/7/7	-
88	SPD	BA	1916	-	-	3/7/7/7	-
88	SPD	BC	309	-	-	0/7/7/7	-
91	PUT	BB	1601	-	-	0/3/3/3	-
88	SPD	BA	1926	-	-	1/7/7/7	-
88	SPD	BB	1604	-	-	3/7/7/7	-
88	SPD	AA	2302	-	-	2/7/7/7	-
88	SPD	BA	1904	-	-	2/7/7/7	-
88	SPD	BA	1915	-	-	0/7/7/7	-
88	SPD	BA	2039	-	-	0/7/7/7	-
88	SPD	BA	2042	-	-	0/7/7/7	-
88	SPD	Bd	101	-	-	1/7/7/7	-
88	SPD	BQ	304	-	-	0/7/7/7	-
88	SPD	BA	2049	-	-	1/7/7/7	-
88	SPD	AA	2375	-	-	0/7/7/7	-
91	PUT	BB	1603	-	-	1/3/3/3	-
91	PUT	BA	1918	-	-	0/3/3/3	-
91	PUT	AA	2308	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
91	PUT	BA	1920	-	-	2/3/3/3	-
88	SPD	BA	1903	-	-	3/7/7/7	-
88	SPD	BA	1924	-	-	0/7/7/7	-
91	PUT	BA	2038	-	-	1/3/3/3	-
88	SPD	BA	1925	-	-	2/7/7/7	-
88	SPD	BA	1923	-	-	1/7/7/7	-
88	SPD	BB	1712	-	-	1/7/7/7	-
91	PUT	AA	2312	-	-	0/3/3/3	-
88	SPD	BC	307	-	-	0/7/7/7	-
91	PUT	BB	1607	-	-	0/3/3/3	-
91	PUT	BB	1608	-	-	1/3/3/3	-
90	GET	AA	2304	-	-	4/13/74/74	2/3/3/3
91	PUT	BA	1902	-	-	0/3/3/3	-
88	SPD	BA	1905	-	-	1/7/7/7	-
88	SPD	BA	1906	-	-	3/7/7/7	-
88	SPD	BA	2043	-	-	0/7/7/7	-
90	GET	AA	2370	-	-	1/13/74/74	0/3/3/3
88	SPD	AA	2374	-	-	1/7/7/7	-
88	SPD	AA	2301	-	-	0/7/7/7	-
92	GTP	AA	2309	87	-	1/22/38/38	0/3/3/3
88	SPD	BA	1909	-	-	0/7/7/7	-
88	SPD	BC	308	-	-	0/7/7/7	-
88	SPD	BA	1917	-	-	1/7/7/7	-
91	PUT	AA	2310	-	-	0/3/3/3	-
88	SPD	BB	1602	-	-	1/7/7/7	-
88	SPD	BA	1912	-	-	0/7/7/7	-
88	SPD	BA	2047	-	-	1/7/7/7	-
88	SPD	AA	2303	-	-	2/7/7/7	-
88	SPD	AA	2306	-	-	1/7/7/7	-
88	SPD	BB	1711	-	-	0/7/7/7	-
88	SPD	BA	2045	-	-	1/7/7/7	-
88	SPD	AA	2305	-	-	2/7/7/7	-
88	SPD	BA	2046	-	-	0/7/7/7	-
88	SPD	AA	2371	-	-	0/7/7/7	-
88	SPD	BA	1914	-	-	1/7/7/7	-
90	GET	AA	2372	-	-	1/13/74/74	0/3/3/3
88	SPD	AA	2307	-	-	0/7/7/7	-
88	SPD	BA	2041	-	-	0/7/7/7	-
88	SPD	BA	2044	-	-	1/7/7/7	-
91	PUT	AA	2313	-	-	0/3/3/3	-
88	SPD	BB	1611	-	-	1/7/7/7	-

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
92	AA	2309	GTP	C5-C4-N3	-4.40	121.32	128.46
92	AA	2309	GTP	C2-N3-C4	4.35	120.05	112.30
92	AA	2309	GTP	PB-O3B-PG	-2.79	123.27	132.83
92	AA	2309	GTP	N9-C4-N3	2.68	131.33	125.94
92	AA	2309	GTP	N9-C8-N7	-2.68	108.34	113.39

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	AA	2304	GET	C12-C62-O62-C13
90	AA	2304	GET	C23-C33-N33-C93
90	AA	2370	GET	C23-C33-N33-C93
90	AA	2372	GET	C23-C33-N33-C93
88	AA	2302	SPD	C3-C4-C5-N6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	AA	2304	GET	C12-C22-C32-C42-C52-C62
90	AA	2304	GET	C11-C21-C31-C41-C51-O51

28 monomers are involved in 38 short contacts:

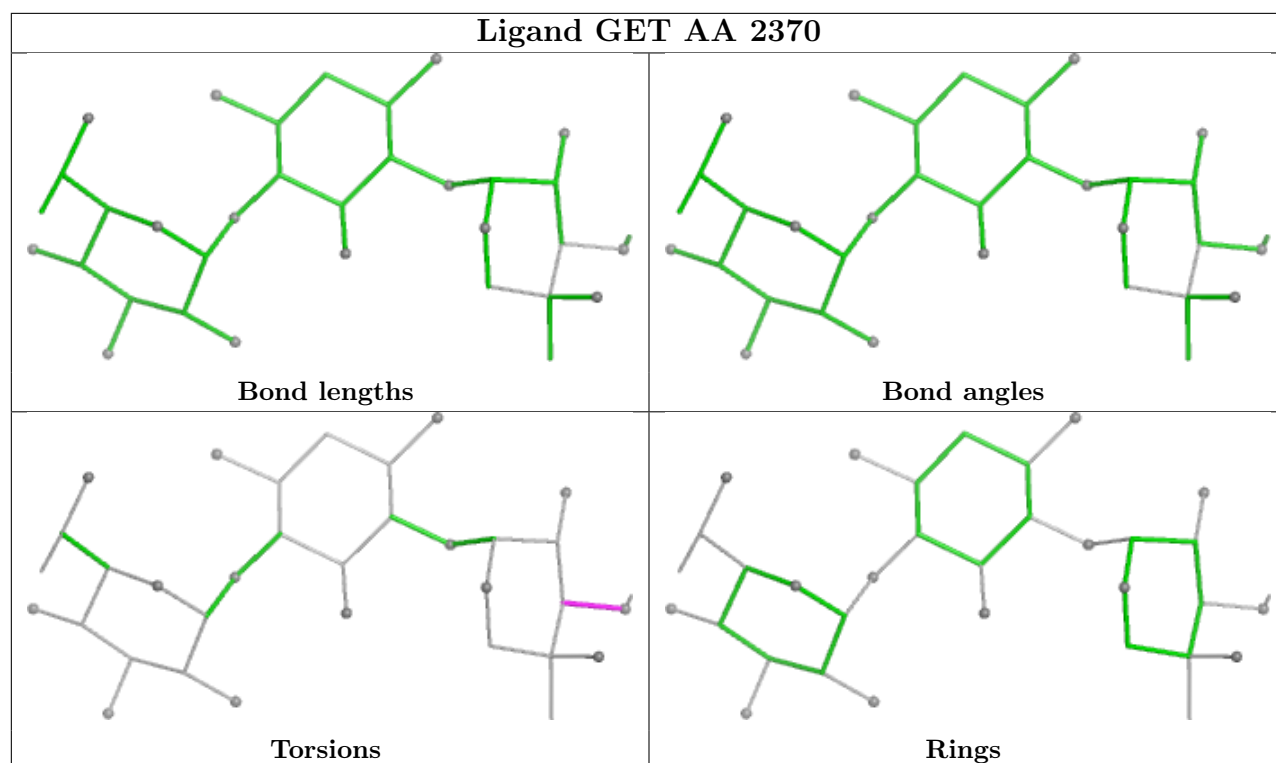
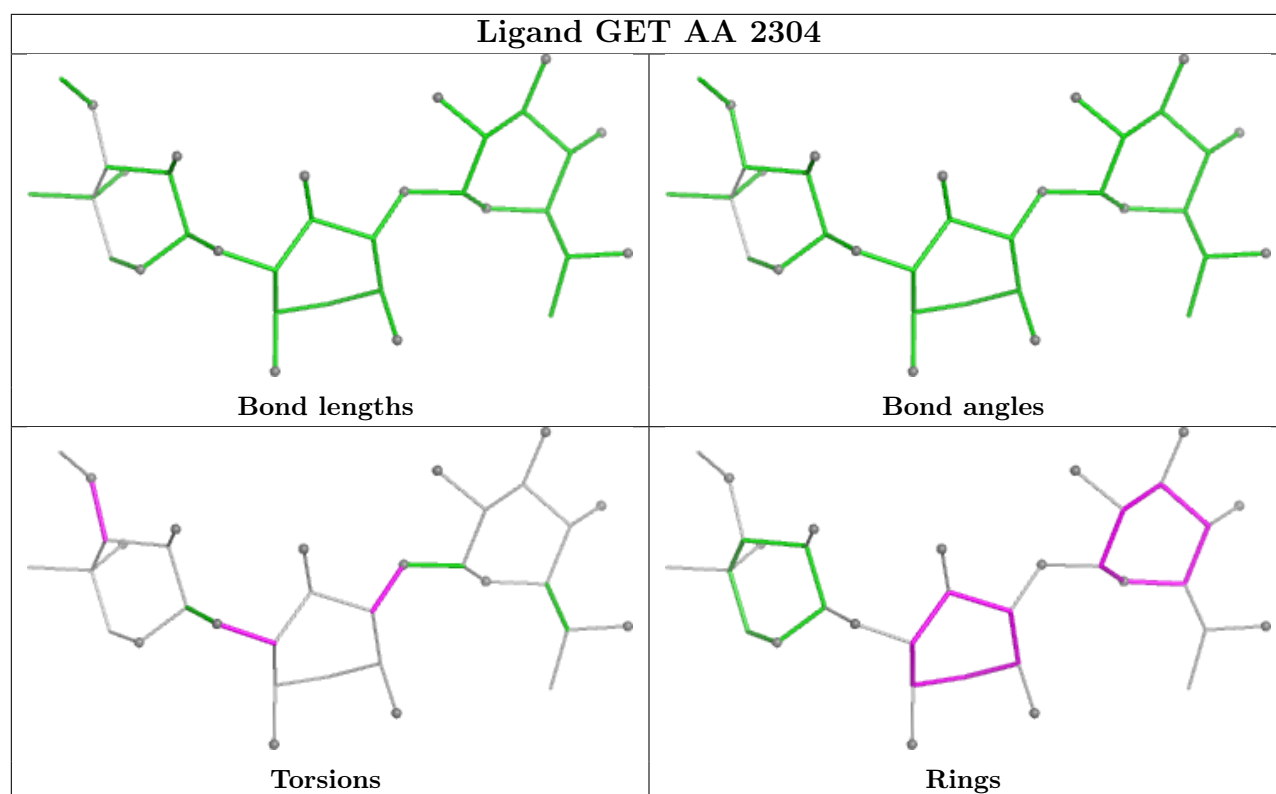
Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	BA	1908	SPD	1	0
88	AA	2311	SPD	1	0
88	BB	1605	SPD	2	0
88	BG	202	SPD	1	0
88	A6	201	SPD	1	0
88	BB	1606	SPD	1	0
88	BA	2048	SPD	1	0
88	BA	1916	SPD	1	0
91	BB	1601	PUT	2	0
88	BA	1915	SPD	2	0
88	BA	2039	SPD	1	0
88	BA	2042	SPD	1	0
88	Bd	101	SPD	1	0
88	BQ	304	SPD	1	0

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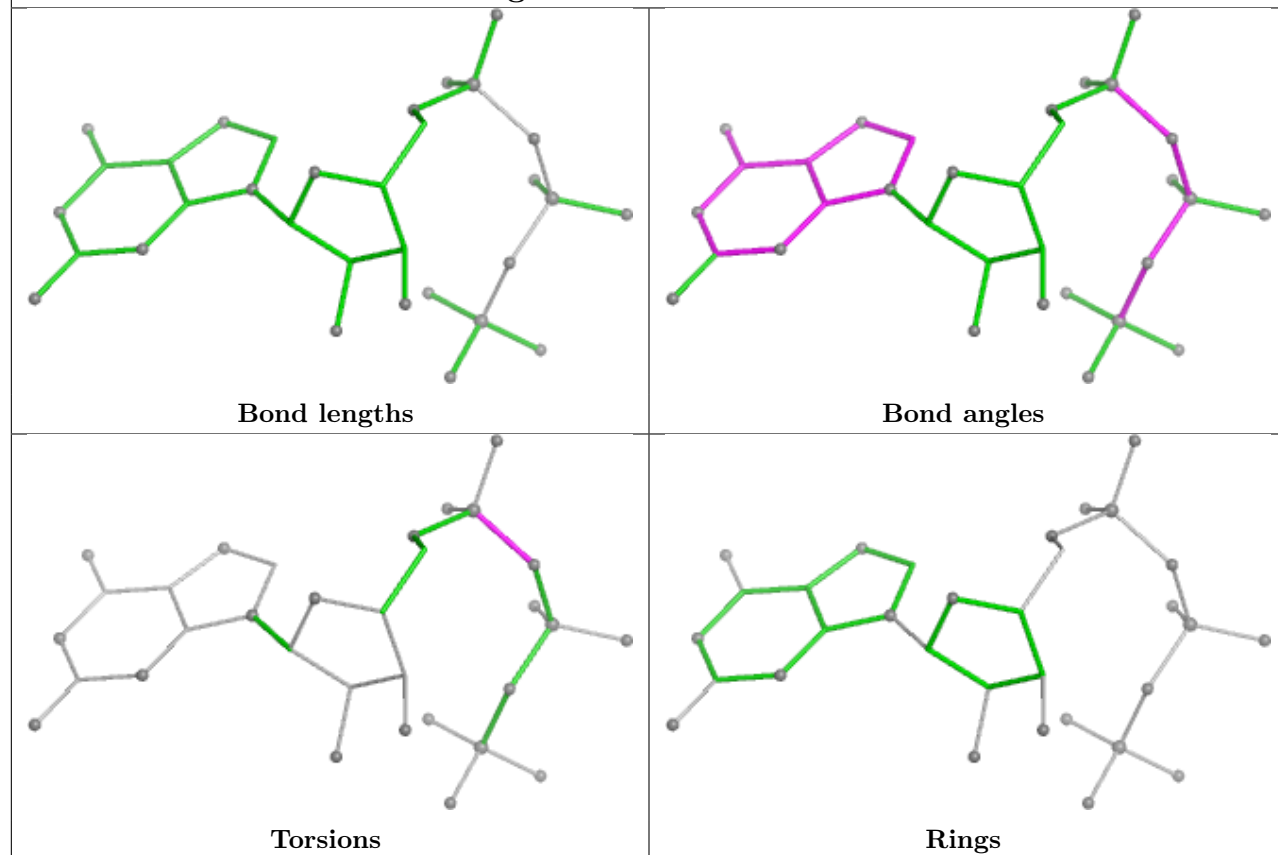
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	AA	2375	SPD	4	0
91	BA	1920	PUT	1	0
88	BC	307	SPD	1	0
90	AA	2304	GET	1	0
88	BA	2043	SPD	1	0
88	AA	2374	SPD	2	0
92	AA	2309	GTP	3	0
91	AA	2310	PUT	1	0
88	BA	1912	SPD	2	0
88	BA	2047	SPD	1	0
88	AA	2303	SPD	1	0
88	AA	2306	SPD	1	0
88	BA	2046	SPD	1	0
88	BA	2044	SPD	1	0

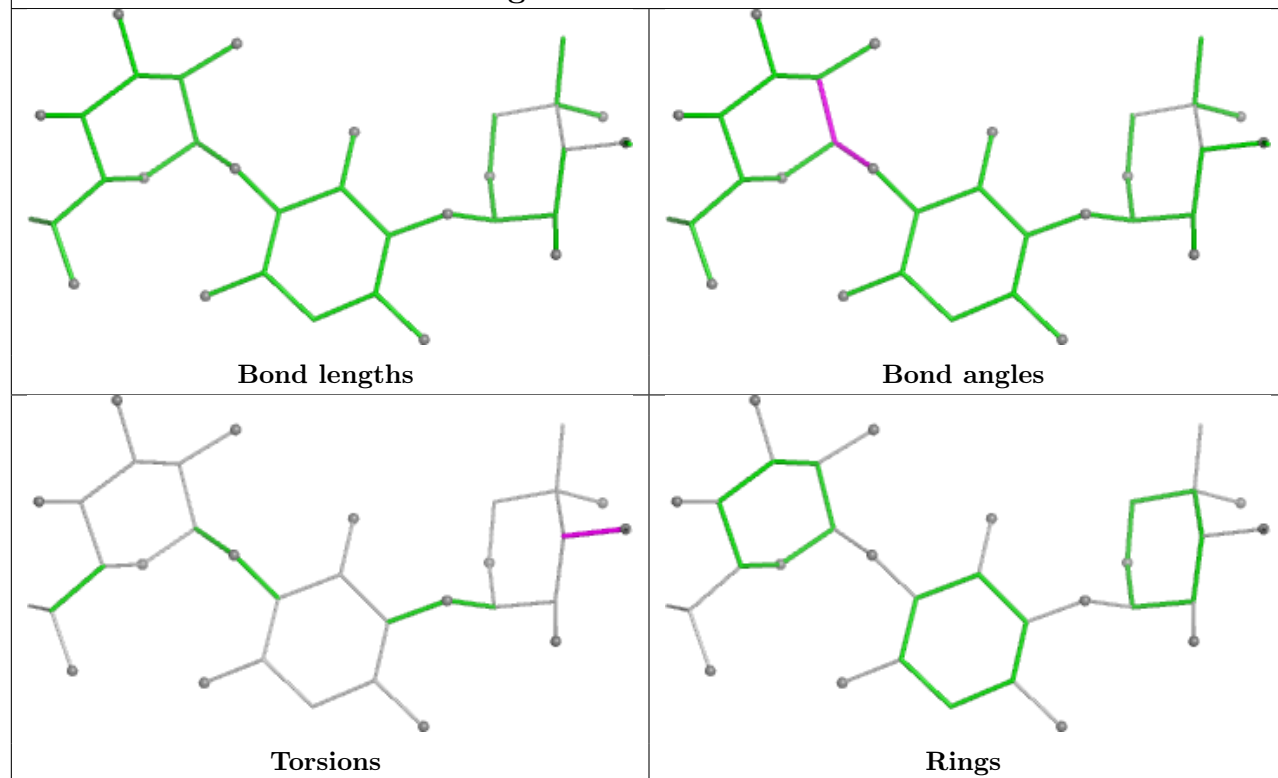
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand GTP AA 2309



Ligand GET AA 2372



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
1	Et	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Et	7:A	O3'	65:G	P	18.05

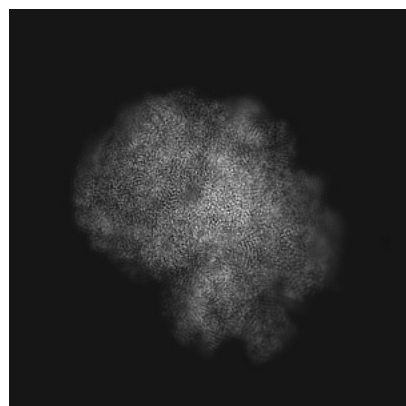
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55224. These allow visual inspection of the internal detail of the map and identification of artifacts.

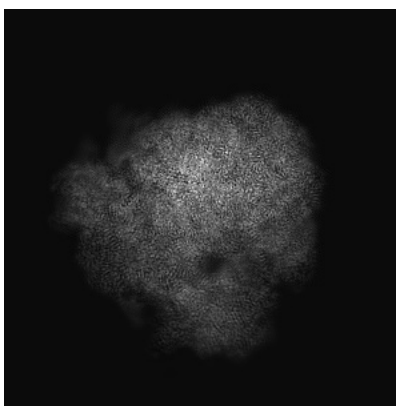
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

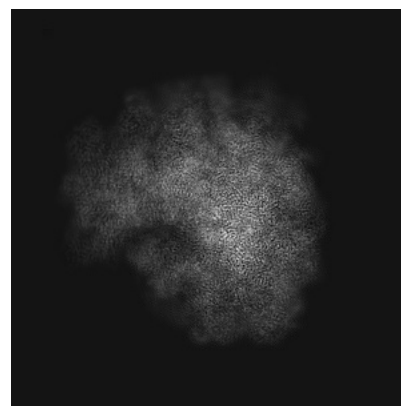
6.1.1 Primary map



X

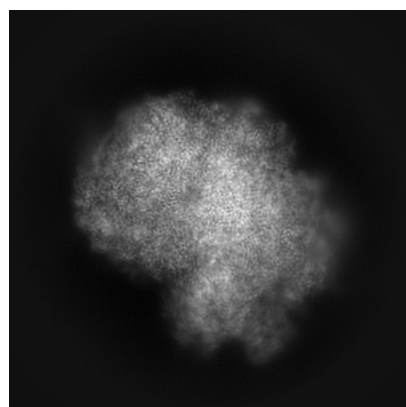


Y

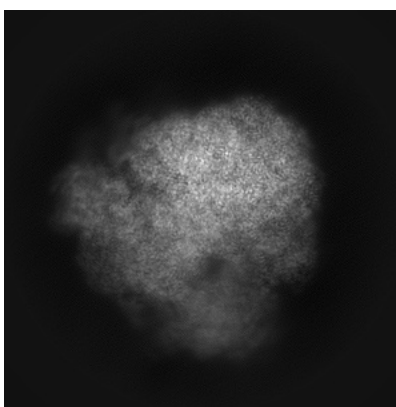


Z

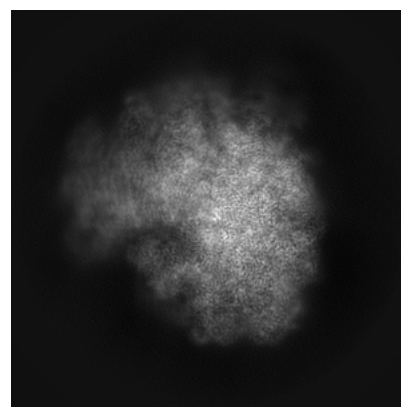
6.1.2 Raw map



X



Y

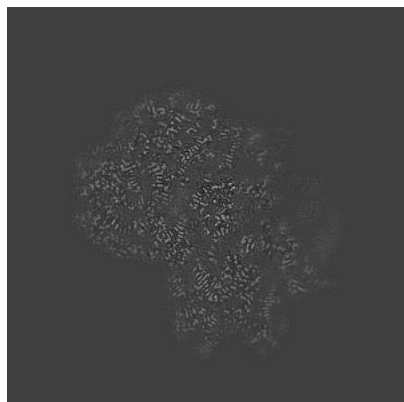


Z

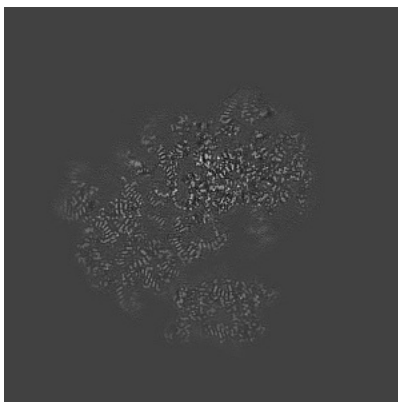
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

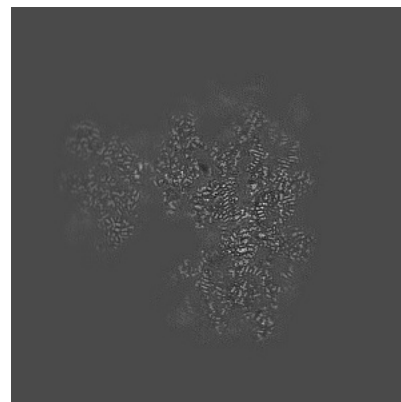
6.2.1 Primary map



X Index: 240

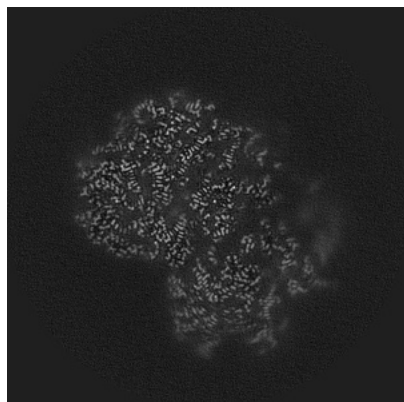


Y Index: 240

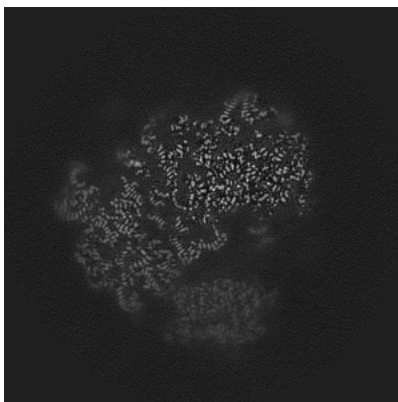


Z Index: 240

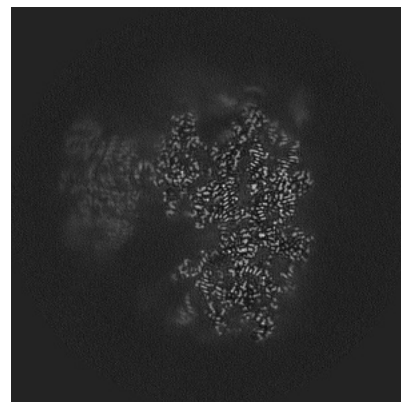
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

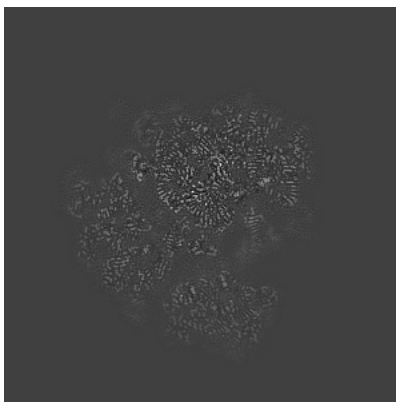
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

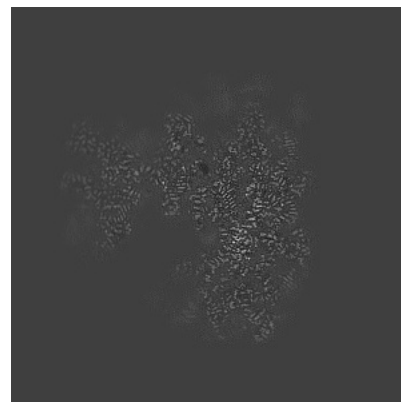
6.3.1 Primary map



X Index: 273

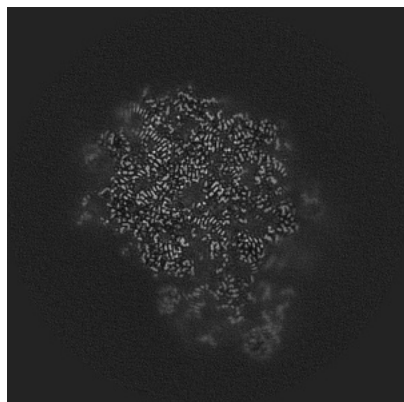


Y Index: 252

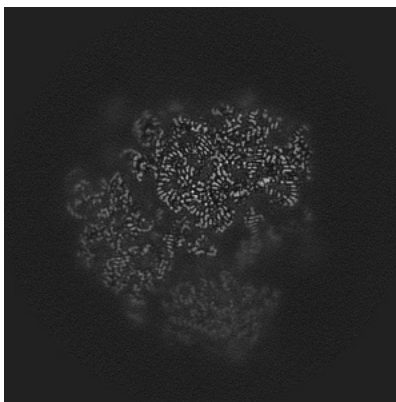


Z Index: 236

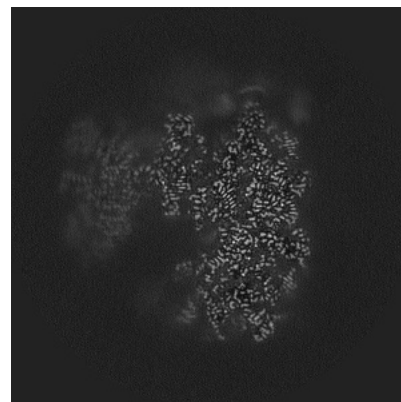
6.3.2 Raw map



X Index: 273



Y Index: 252

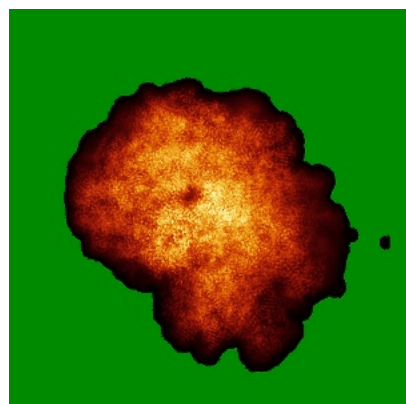


Z Index: 236

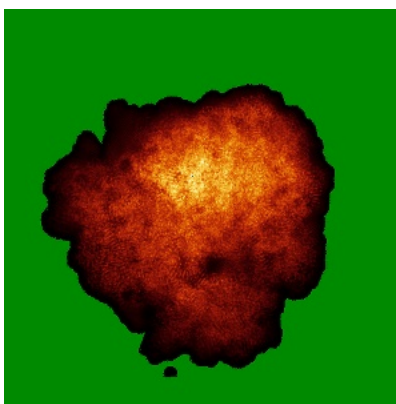
The images above show the largest variance slices of the map in three orthogonal directions.

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

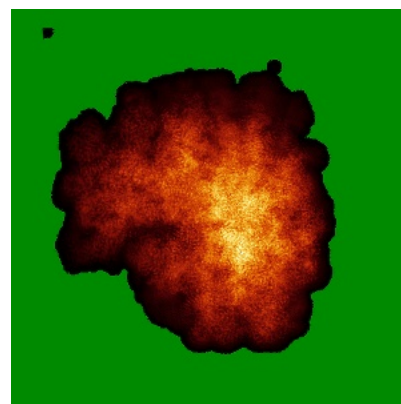
6.4.1 Primary map



X

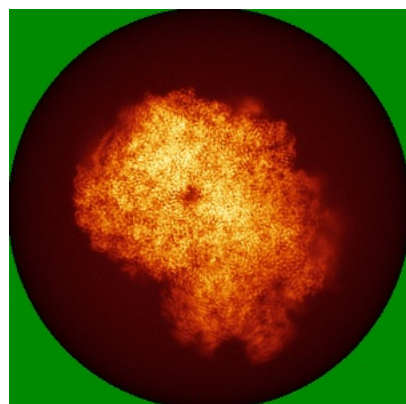


Y

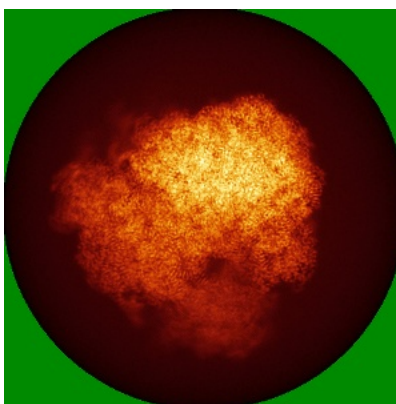


Z

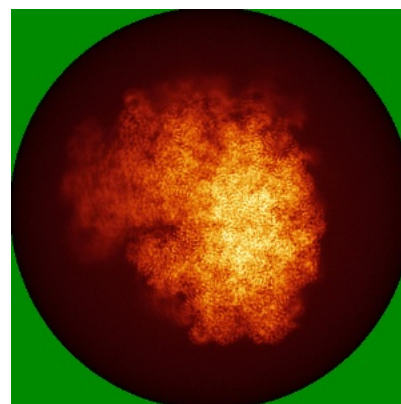
6.4.2 Raw map



X



Y

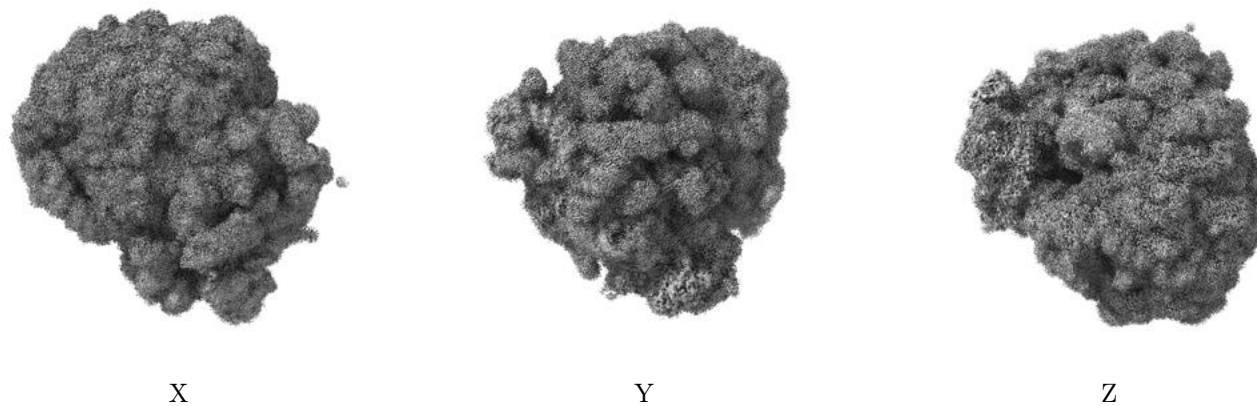


Z

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.

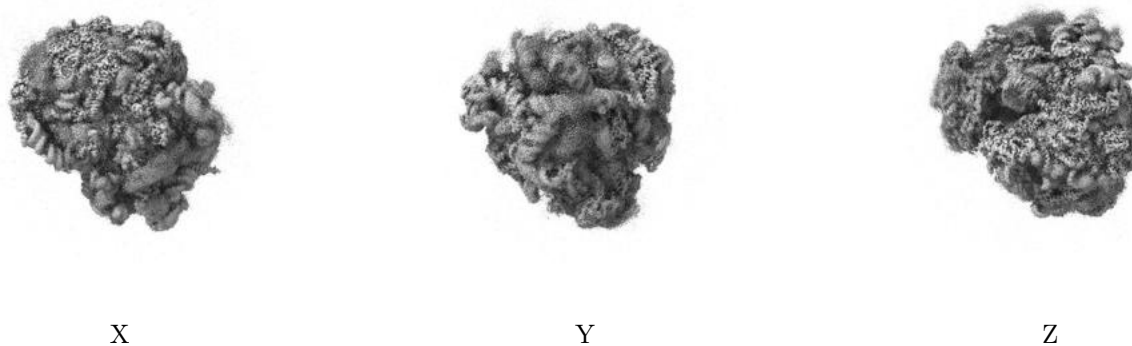
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

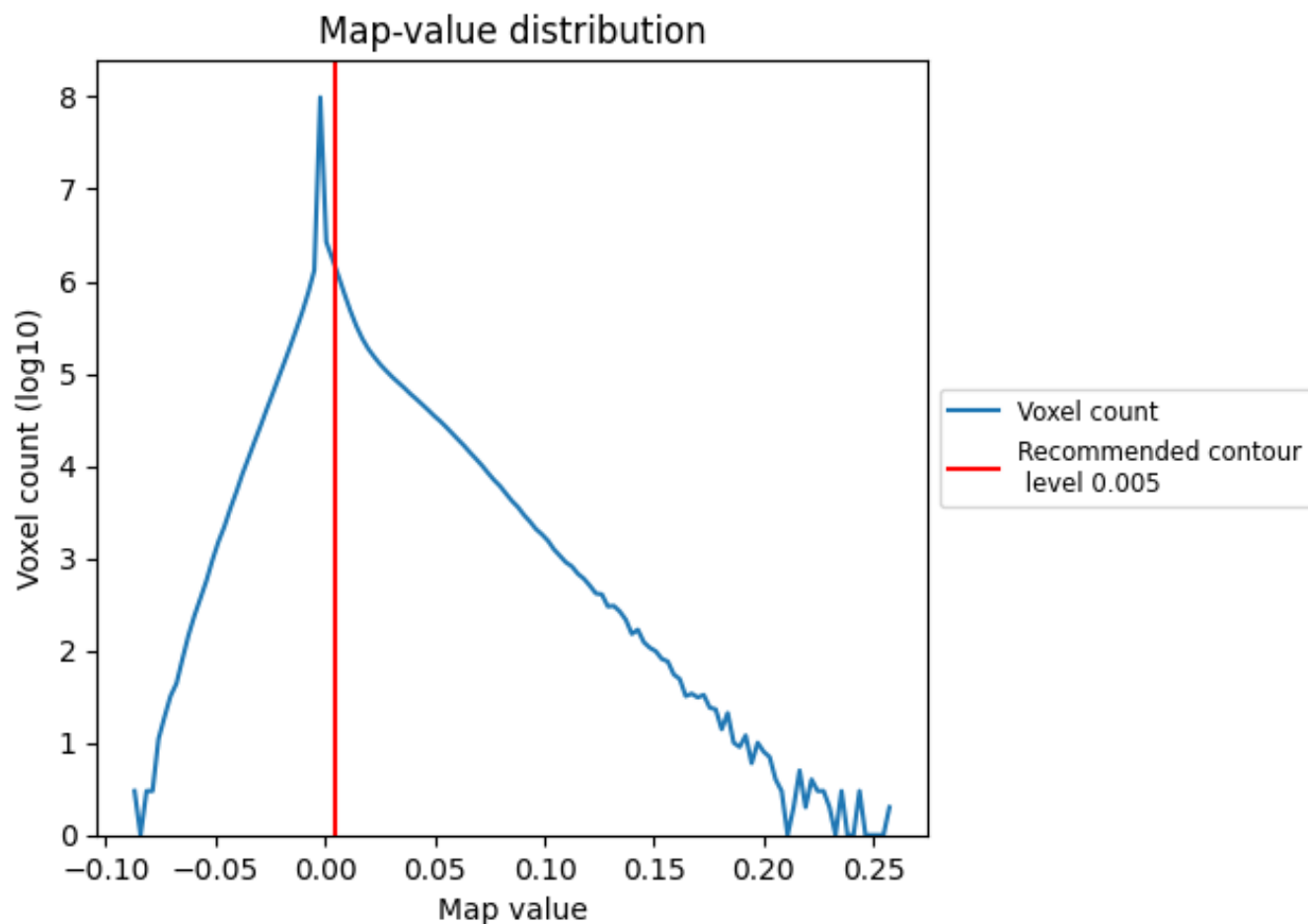
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

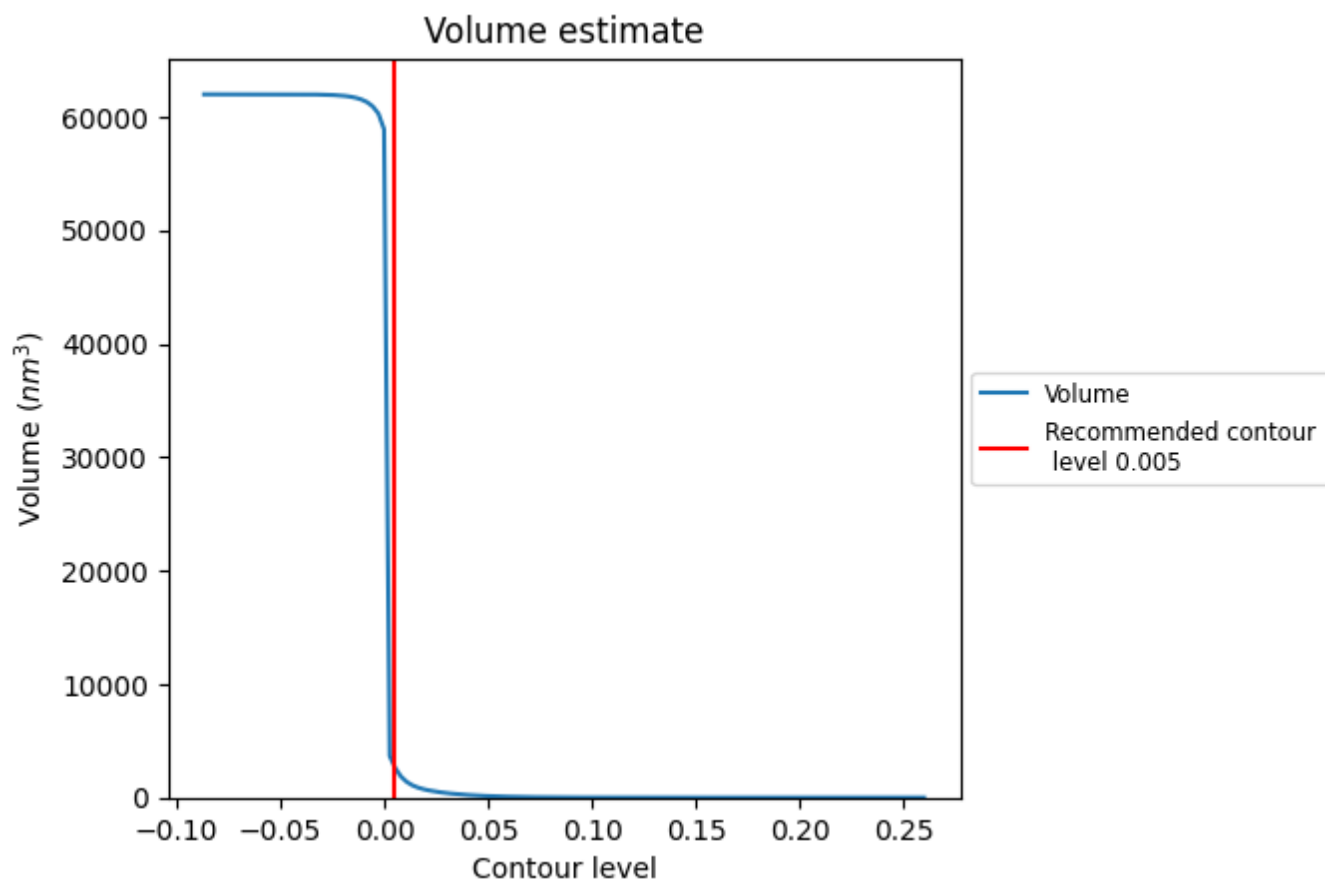
This section contains the results of statistical analysis of the map.

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.

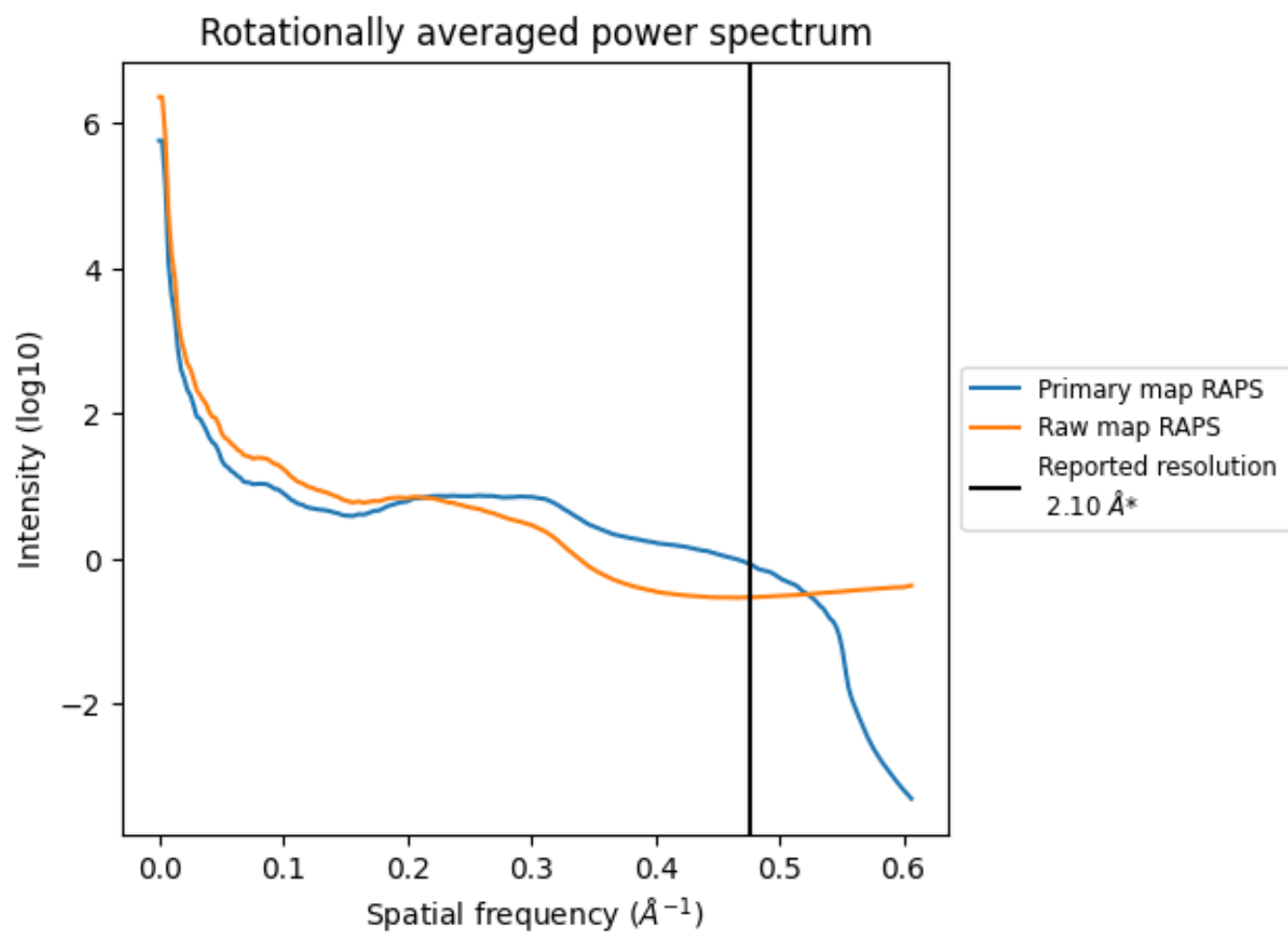
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2699 nm³; this corresponds to an approximate mass of 2438 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 ⓘ

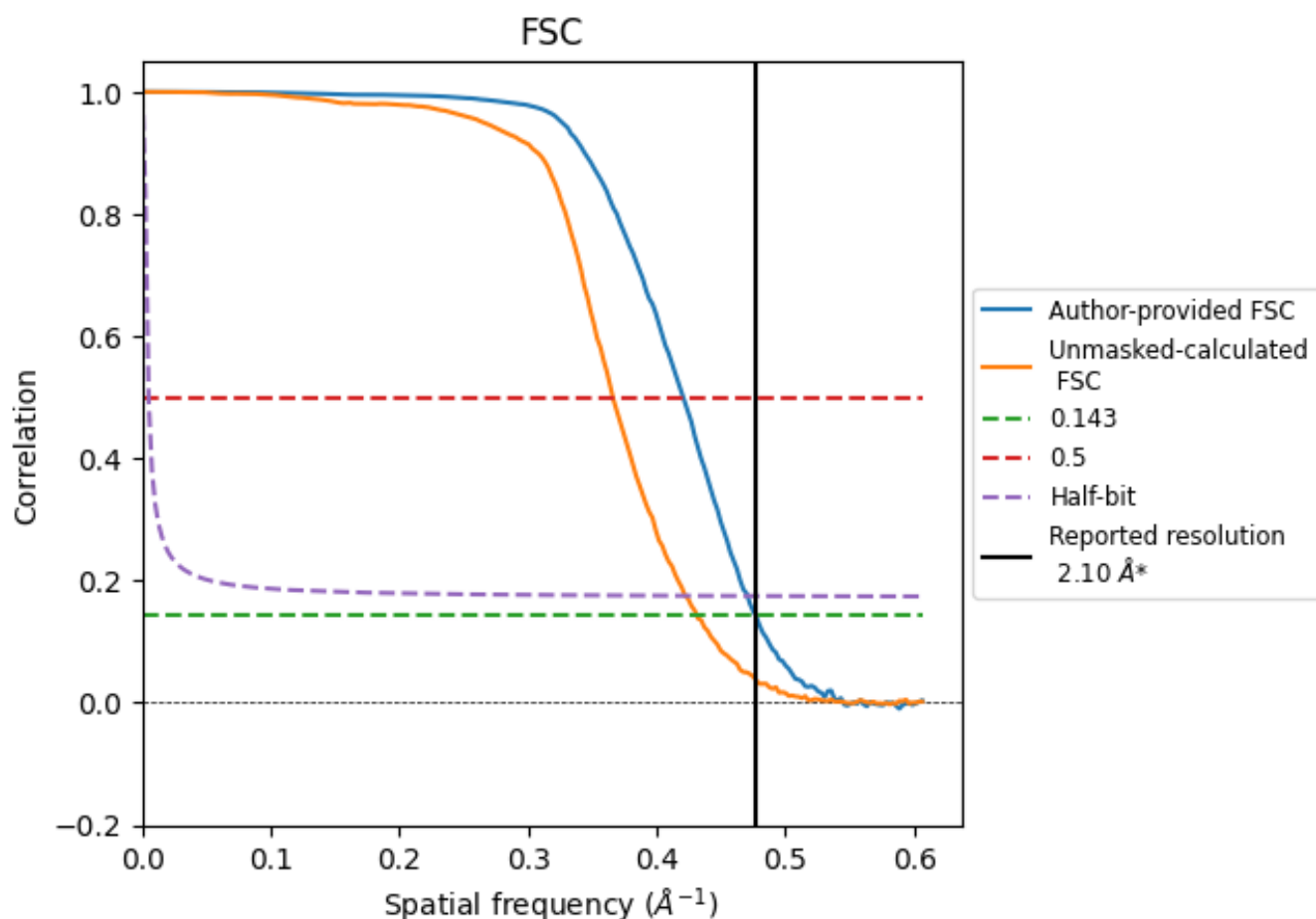


*Reported resolution corresponds to spatial frequency of 0.476 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

8.2 Resolution estimates [i](#)

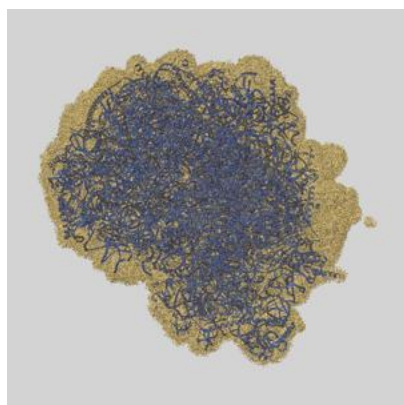
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.10	2.38	2.12
Unmasked-calculated*	2.32	2.73	2.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.32 differs from the reported value 2.1 by more than 10 %

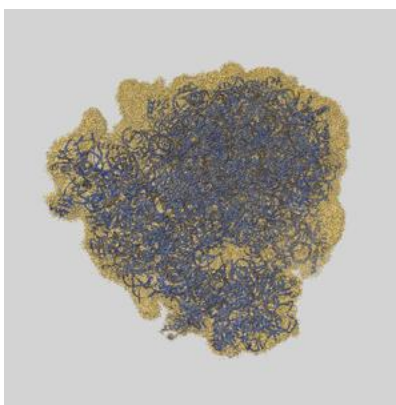
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55224 and PDB model 9SUL. Per-residue inclusion information can be found in section [3](#) on page [30](#).

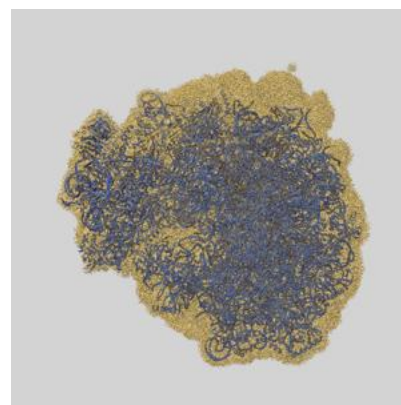
9.1 Map-model overlay [i](#)



X



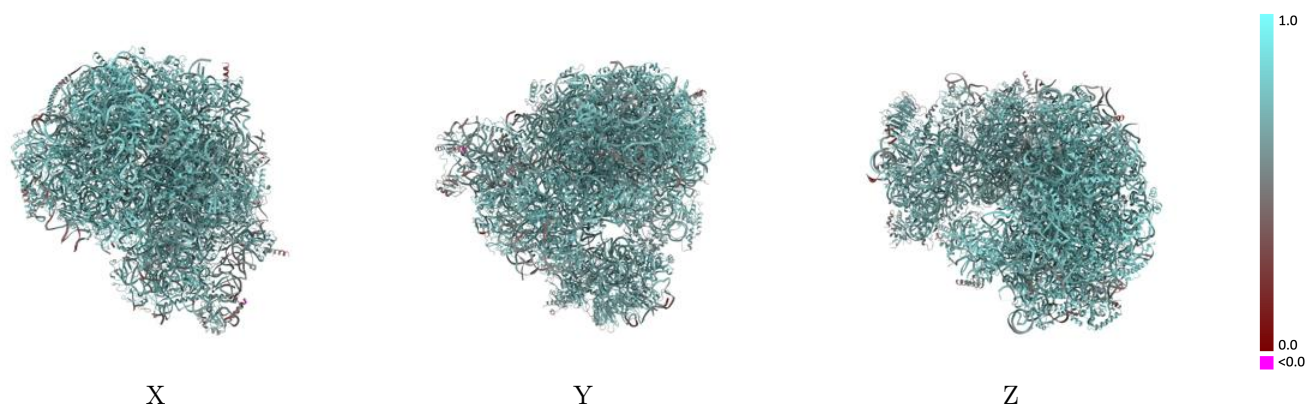
Y



Z

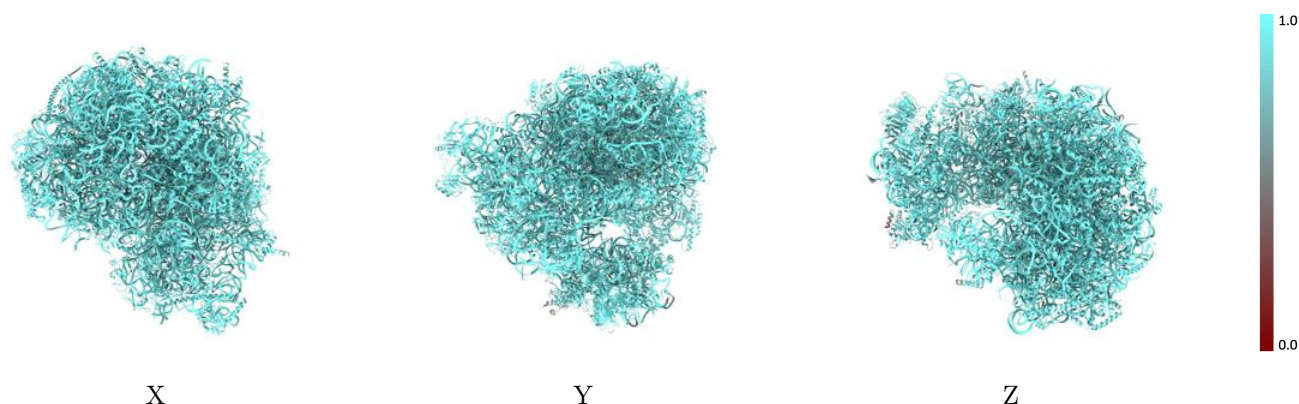
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



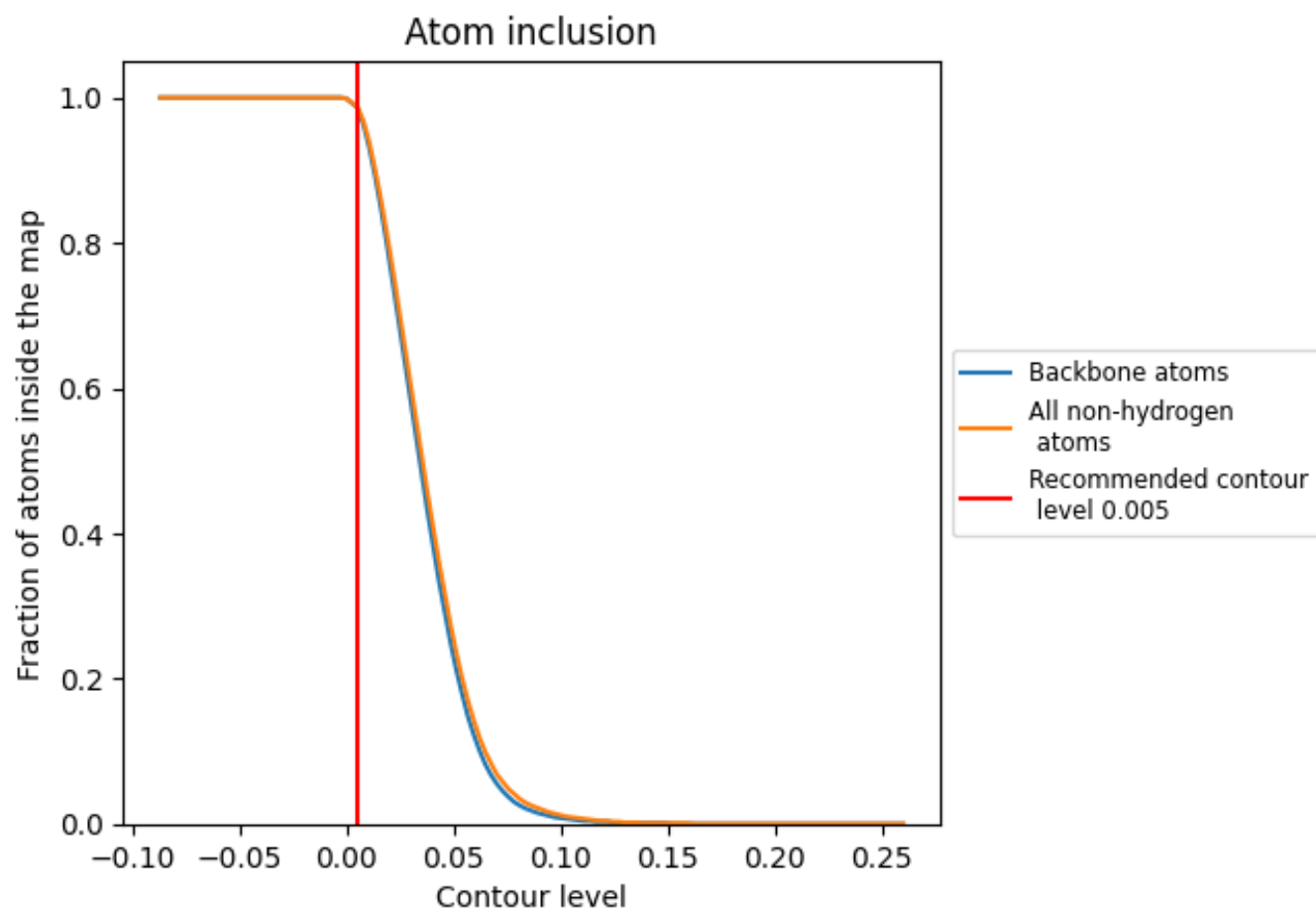
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.005).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9880	 0.7110
A0	 0.9900	 0.7110
A1	 0.9930	 0.7290
A2	 0.9930	 0.7010
A3	 0.9880	 0.6750
A4	 0.9890	 0.6950
A5	 0.9930	 0.7360
A6	 0.9870	 0.7160
A7	 0.9510	 0.6320
A8	 0.9980	 0.7130
A9	 0.8630	 0.5900
AA	 0.9890	 0.6770
AC	 0.9960	 0.6980
AD	 0.9750	 0.6730
AE	 0.9880	 0.7260
AF	 0.7330	 0.5400
AG	 0.9950	 0.7400
AH	 0.9850	 0.7020
AI	 0.9530	 0.6630
AJ	 0.9960	 0.7510
AK	 0.9900	 0.7030
AL	 0.9880	 0.6520
AM	 0.9680	 0.6780
AO	 0.9920	 0.6970
AP	 0.9840	 0.7140
AQ	 0.9260	 0.6420
AR	 0.9940	 0.7170
AS	 0.9910	 0.7310
AT	 0.9920	 0.7020
AU	 0.9700	 0.6770
AV	 0.9920	 0.7140
AW	 0.9810	 0.6800
AX	 0.9690	 0.6660
AY	 0.9580	 0.6570
AZ	 1.0000	 0.6440



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Chain	Atom inclusion	Q-score
Az	 0.9350	 0.5370
BA	 0.9960	 0.7360
BB	 0.9940	 0.7210
BC	 0.9970	 0.7320
BD	 0.9980	 0.7120
BE	 0.9930	 0.7000
BF	 0.9890	 0.6820
BG	 0.9980	 0.7290
BH	 0.9890	 0.6870
BI	 0.9950	 0.7710
BK	 0.9900	 0.7290
BL	 0.9730	 0.6180
BN	 0.9910	 0.7450
BO	 0.9980	 0.7760
BP	 0.9910	 0.7080
BQ	 1.0000	 0.7900
BR	 0.9980	 0.7870
BS	 0.9930	 0.7520
BT	 0.9760	 0.6990
BU	 0.9740	 0.7040
BV	 0.9740	 0.6040
BW	 0.9970	 0.7660
BX	 0.9970	 0.7460
BY	 1.0000	 0.7530
BZ	 0.9990	 0.7570
Ba	 0.9930	 0.7090
Bb	 0.9940	 0.7750
Bc	 0.9960	 0.7540
Bd	 0.9960	 0.7650
Be	 0.9990	 0.7850
Bf	 0.9940	 0.7640
Bg	 0.9920	 0.7300
Bh	 0.9960	 0.7560
Bi	 0.9950	 0.7760
Bj	 0.9800	 0.7180
Bk	 0.9900	 0.7070
Bl	 0.9980	 0.7750
Bm	 0.9990	 0.7440
Bn	 0.9990	 0.7910
Bo	 0.9960	 0.7690
Bp	 0.9850	 0.6820
Bq	 0.9980	 0.7650

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Chain	Atom inclusion	Q-score
Br	 0.9960	 0.7600
Bs	 0.9740	 0.6720
Bt	 0.9970	 0.7600
Bu	 0.9620	 0.6710
Bv	 0.9810	 0.7070
Bw	 0.9840	 0.7380
Bx	 0.9810	 0.7140
By	 0.9900	 0.6950
Bz	 0.9960	 0.7460
Et	 1.0000	 0.6250