



## Full wwPDB EM Validation Report ⓘ

Oct 22, 2024 – 05:35 AM JST

PDB ID : 8K2D  
EMDB ID : EMD-36839  
Title : Cryo-EM structure of the yeast 80S ribosome with tigecycline, eEF2, Stm1 and eIF5A  
Authors : Buschauer, R.; Beckmann, R.; Cheng, J.  
Deposited on : 2023-07-12  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

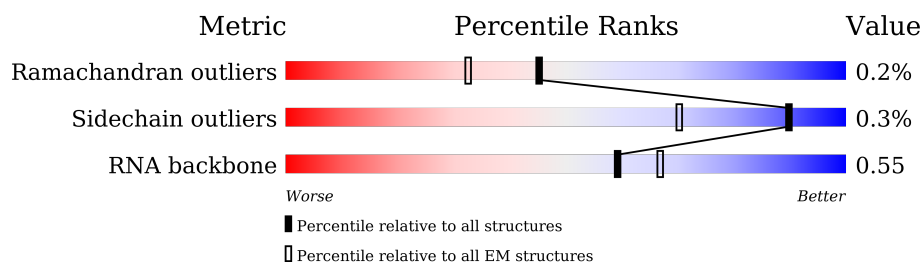
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 3.20 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.



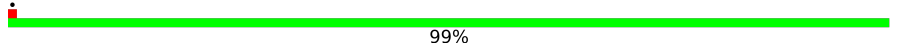
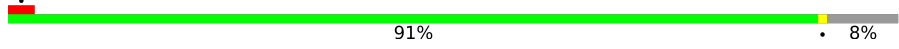
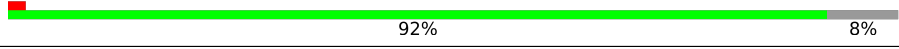
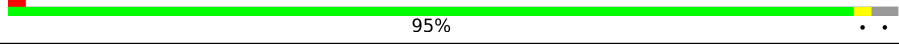
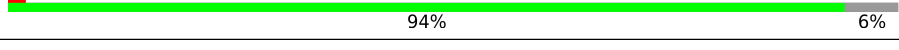
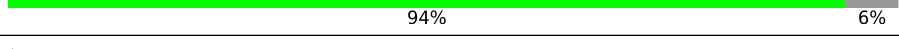
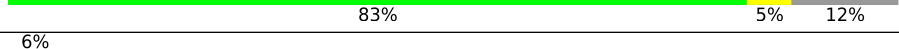
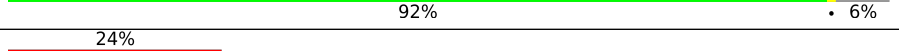
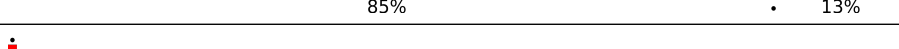
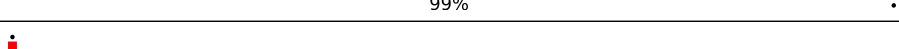
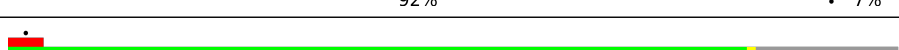

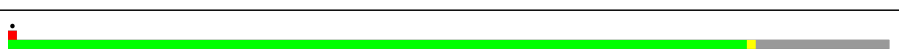
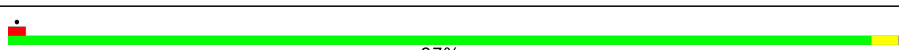
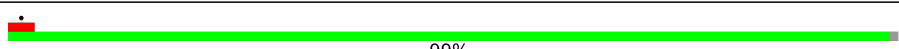

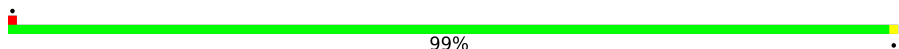
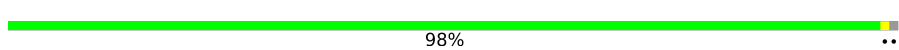
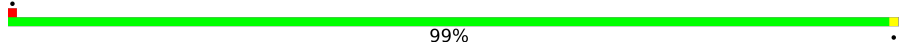
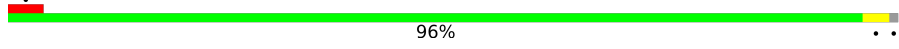
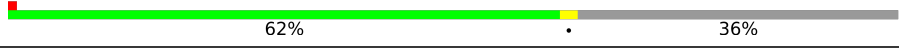
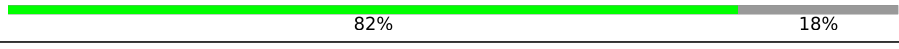
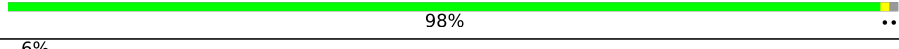


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	C2	1800	71% 21% • 6%
2	C1	3396	75% 18% • 6%
3	C4	121	83% 17%
4	C3	158	82% 16% ••
5	SA	252	81% • 18%
6	SB	255	84% • 15%
7	SC	254	84% • 15%
8	SD	240	91% • 7%

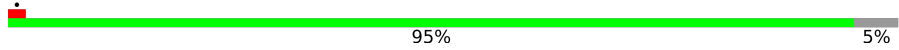

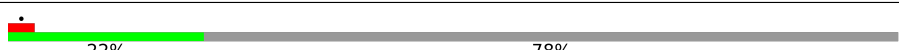
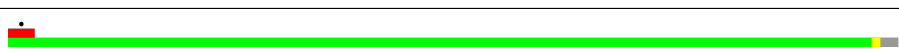
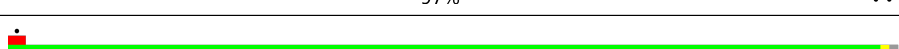
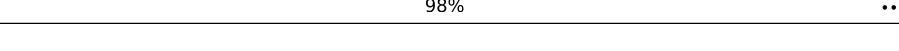
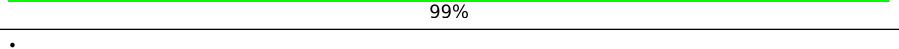
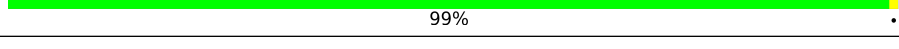
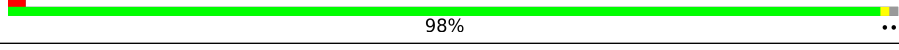

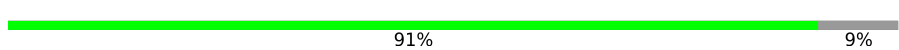

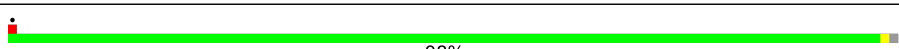

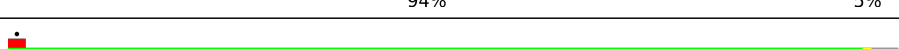
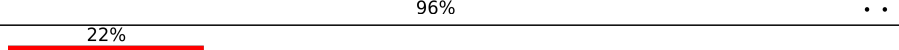
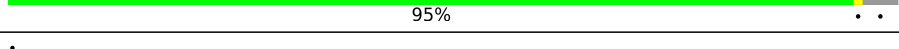
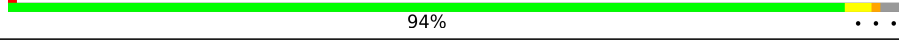
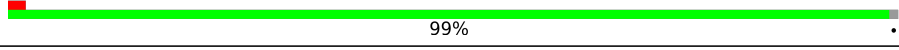
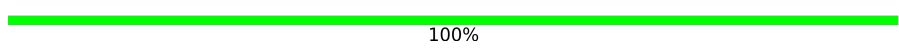
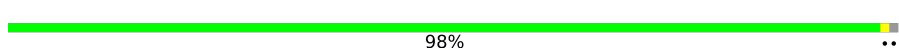
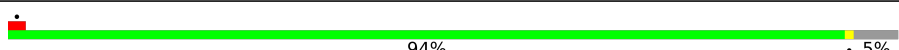

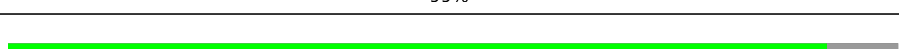
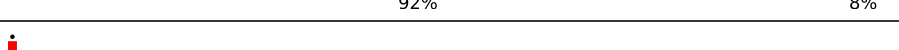
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Mol	Chain	Length	Quality of chain
9	SE	261	
10	SF	225	
11	SG	236	
12	SH	190	
13	SI	200	
14	SJ	197	
15	SK	105	
16	SL	156	
17	SM	143	
18	SN	151	
19	SO	137	
20	SP	142	
21	SQ	143	
22	SR	136	
23	SS	146	
24	ST	144	
25	SU	121	
26	SV	87	
27	SW	130	
28	SX	145	
29	SY	135	
30	SZ	108	
31	Sa	119	
32	Sb	82	
33	Sc	67	

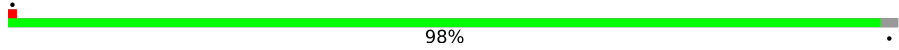


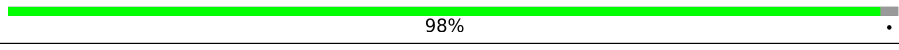
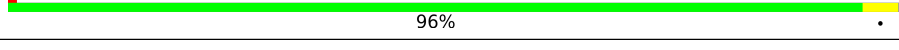
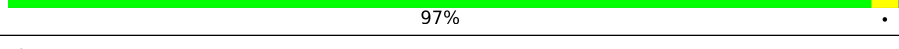
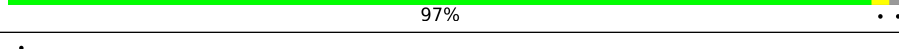
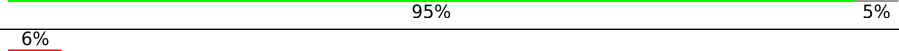
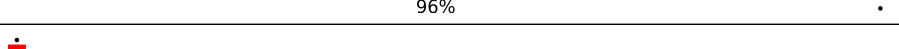
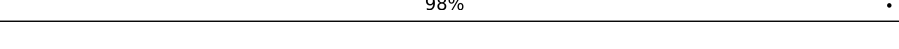
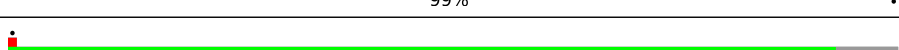
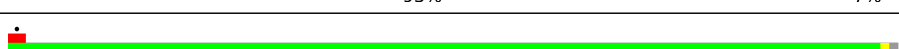
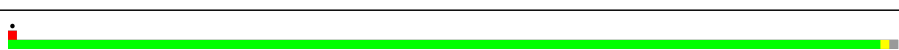
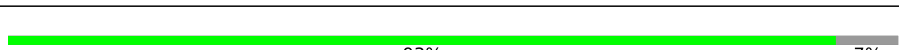
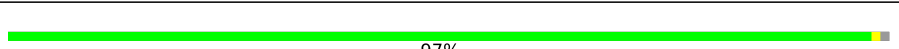
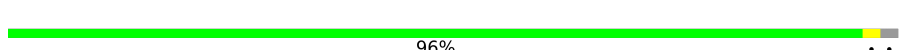

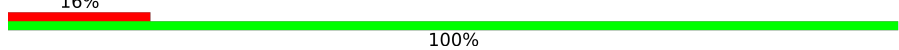
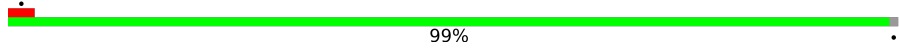
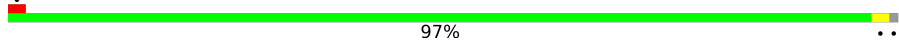
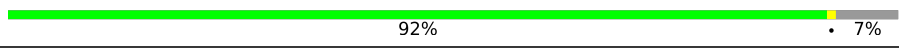
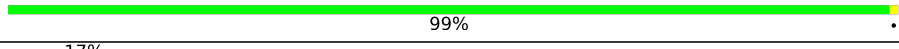

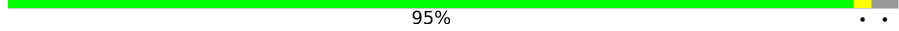

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Mol	Chain	Length	Quality of chain
34	Sd	56	
35	Se	63	
36	Sf	152	
37	Sg	319	
38	LA	254	
39	LB	387	
40	LC	362	
41	LD	297	
42	LE	176	
43	LF	244	
44	LG	256	
45	LH	191	
46	LI	221	
47	LJ	174	
48	LK	165	
49	LL	199	
50	LM	138	
51	LN	204	
52	LO	199	
53	LP	184	
54	LQ	186	
55	LR	189	
56	LS	172	
57	LT	160	
58	LU	121	

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Mol	Chain	Length	Quality of chain
59	LV	137	
60	LW	155	
61	LX	142	
62	LY	127	
63	LZ	136	
64	La	149	
65	Lb	59	
66	Lc	105	
67	Ld	113	
68	Le	130	
69	Lf	107	
70	Lg	121	
71	Lh	120	
72	Li	100	
73	Lj	88	
74	Lk	78	
75	Ll	51	
76	Lm	128	
77	Ln	25	
78	Lo	106	
79	Lp	92	
80	CE	157	
81	L1	217	
82	P0	312	
83	CD	842	

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Mol	Chain	Length	Quality of chain
84	CS	273	<div><div></div><div>44%</div><div></div><div>55%</div></div>

## 2 Entry composition

There are 88 unique types of molecules in this entry. The entry contains 210169 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 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C2	1700	Total	C	N	O	P	0	0
			36234	16201	6426	11907	1700		

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C1	3188	Total	C	N	O	P	0	0
			68200	30463	12307	22242	3188		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C4	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 4 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C3	157	Total	C	N	O	P	0	0
			3333	1491	584	1101	157		

- Molecule 5 is a protein called Small ribosomal subunit protein uS2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SA	206	Total	C	N	O	S	0	0
			1583	1017	281	283	2		

- Molecule 6 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	SB	216	Total	C	N	O	S	0	0
			1722	1091	312	315	4		

- Molecule 7 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SC	217	Total	C	N	O	S	0	0
			1635	1047	289	297	2		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 9 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SE	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 11 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SG	218	Total	C	N	O	S	0	0
			1755	1102	337	313	3		

- Molecule 12 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	SH	185	Total	C	N	O	0	0
			1486	954	266	266		

- Molecule 13 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 14 is a protein called 40S ribosomal protein S9-A.



Mol	Chain	Residues	Atoms					AltConf	Trace
14	SJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 15 is a protein called Small ribosomal subunit protein eS10A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SK	92	Total	C	N	O	S	0	0
			741	478	121	140	2		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	SL	146	Total	C	N	O	S	0	0
			1168	747	221	197	3		

- Molecule 17 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SM	124	Total	C	N	O	S	0	0
			890	560	156	172	2		

- Molecule 18 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 19 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	SO	128	Total	C	N	O	S	0	0
			949	582	188	176	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	SP	119	Total	C	N	O	S	0	0
			939	595	176	161	7		

- Molecule 21 is a protein called Small ribosomal subunit protein uS9A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	SQ	141	Total	C	N	O		
			1105	708	203	194	0	0

- Molecule 22 is a protein called Small ribosomal subunit protein eS17A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	SR	115	Total	C	N	O	S		
			896	557	172	165	2	0	0

- Molecule 23 is a protein called Small ribosomal subunit protein uS13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	SS	145	Total	C	N	O	S		
			1192	743	237	210	2	0	0

- Molecule 24 is a protein called Small ribosomal subunit protein eS19A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	ST	143	Total	C	N	O	S		
			1112	694	208	208	2	0	0

- Molecule 25 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SU	101	Total	C	N	O	S		
			805	512	145	147	1	0	0

- Molecule 26 is a protein called Small ribosomal subunit protein eS21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SV	87	Total	C	N	O	S		
			684	420	125	137	2	0	0

- Molecule 27 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SW	129	Total	C	N	O	S		
			1021	650	188	180	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SY	134	Total	C	N	O		0	0
			1073	676	208	189			

- Molecule 30 is a protein called Small ribosomal subunit protein eS25A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	SZ	69	Total	C	N	O		0	0
			558	357	103	98			

- Molecule 31 is a protein called Small ribosomal subunit protein eS26B.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Sa	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Sb	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 33 is a protein called Small ribosomal subunit protein eS28A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 34 is a protein called Small ribosomal subunit protein uS14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Sd	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 35 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Se	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 36 is a protein called Ubiquitin-ribosomal protein eS31 fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Sf	33	Total	C	N	O	S	0	0
			248	153	46	45	4		

- Molecule 37 is a protein called Small ribosomal subunit protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Sg	313	Total	C	N	O	S	0	0
			2403	1521	411	463	8		

- Molecule 38 is a protein called Large ribosomal subunit protein uL2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LA	252	Total	C	N	O	S	0	0
			1912	1190	388	333	1		

- Molecule 39 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LB	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 40 is a protein called Large ribosomal subunit protein uL4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LD	294	Total	C	N	O	S	0	0
			2359	1489	412	456	2		

- Molecule 42 is a protein called Large ribosomal subunit protein eL6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LE	157	Total	C	N	O	S	0	0
			1248	806	224	217	1		

- Molecule 43 is a protein called Large ribosomal subunit protein uL30A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	LF	223	Total	C	N	O	S	0	0
			1791	1155	325	310	1		

- Molecule 44 is a protein called Large ribosomal subunit protein eL8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LG	231	Total	C	N	O	S	0	0
			1763	1130	316	314	3		

- Molecule 45 is a protein called Large ribosomal subunit protein uL6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	LH	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 46 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	LI	209	Total	C	N	O	S	0	0
			1696	1077	321	293	5		

- Molecule 47 is a protein called Large ribosomal subunit protein uL5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	LJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 48 is a protein called Large ribosomal subunit protein uL11A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	LK	158	Total	C	N	O	S	0	0
			1196	750	216	228	2		

- Molecule 49 is a protein called Large ribosomal subunit protein eL13A.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	LL	194	Total	C	N	O	0	0
			1548	965	316	267		

- Molecule 50 is a protein called Large ribosomal subunit protein eL14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	LM	137	Total	C	N	O	S	0	0
			1059	678	200	179	2		

- Molecule 51 is a protein called Large ribosomal subunit protein eL15A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	LN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 52 is a protein called Large ribosomal subunit protein uL13A.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	LO	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 53 is a protein called Large ribosomal subunit protein uL22A.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	LP	175	Total	C	N	O	0	0
			1378	856	273	249		

- Molecule 54 is a protein called Large ribosomal subunit protein eL18A.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	LQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 55 is a protein called Large ribosomal subunit protein eL19A.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	LR	174	Total	C	N	O	0	0
			1365	843	286	236		

- Molecule 56 is a protein called Large ribosomal subunit protein eL20A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	LS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 57 is a protein called Large ribosomal subunit protein eL21A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	LT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 58 is a protein called Large ribosomal subunit protein eL22A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	LU	98	Total	C	N	O		0	0
			778	505	127	146			

- Molecule 59 is a protein called Large ribosomal subunit protein uL14A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	LV	134	Total	C	N	O	S	0	0
			993	623	187	176	7		

- Molecule 60 is a protein called Large ribosomal subunit protein eL24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	LW	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 61 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	LX	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 62 is a protein called Large ribosomal subunit protein uL24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LY	124	Total	C	N	O		0	0
			976	614	190	172			

- Molecule 63 is a protein called Large ribosomal subunit protein eL27A.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	LZ	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 64 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	La	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 65 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms				AltConf	Trace
65	Lb	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 66 is a protein called Large ribosomal subunit protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Lc	100	Total	C	N	O	S	0	0
			767	492	128	146	1		

- Molecule 67 is a protein called Large ribosomal subunit protein eL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ld	109	Total	C	N	O	S	0	0
			883	559	167	156	1		

- Molecule 68 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Le	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 69 is a protein called Large ribosomal subunit protein eL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Lf	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 70 is a protein called Large ribosomal subunit protein eL34A.



Mol	Chain	Residues	Atoms					AltConf	Trace
70	Lg	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 71 is a protein called Large ribosomal subunit protein uL29A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Lh	119	Total	C	N	O	S	0	0
			965	612	185	167	1		

- Molecule 72 is a protein called Large ribosomal subunit protein eL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Li	99	Total	C	N	O	S	0	0
			770	481	156	131	2		

- Molecule 73 is a protein called Large ribosomal subunit protein eL37A.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Lj	82	Total	C	N	O	S	0	0
			650	396	142	107	5		

- Molecule 74 is a protein called Large ribosomal subunit protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Lk	77	Total	C	N	O		0	0
			608	388	114	106			

- Molecule 75 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Ll	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 76 is a protein called Ubiquitin-ribosomal protein eL40A fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Lm	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 77 is a protein called Large ribosomal subunit protein eL41A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ln	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 78 is a protein called Large ribosomal subunit protein eL42A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Lo	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 79 is a protein called Large ribosomal subunit protein eL43A.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Lp	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 80 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	CE	146	Total	C	N	O	S	0	0
			1097	686	184	218	9		

- Molecule 81 is a protein called Large ribosomal subunit protein uL1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	L1	217	Total	C	N	O	S	0	0
			1718	1097	299	312	10		

- Molecule 82 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	P0	203	Total	C	N	O	S	0	0
			1571	1006	272	289	4		

- Molecule 83 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	CD	816	Total	C	N	O	S	0	0
			6348	4042	1079	1197	30		

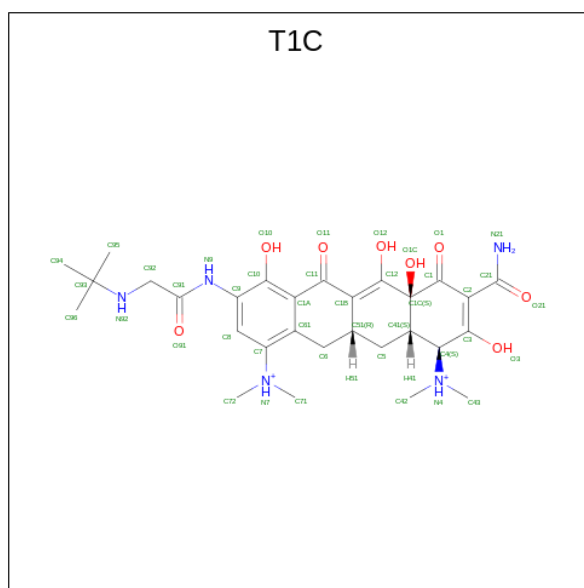
- Molecule 84 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
84	CS	122	Total	C	N	O	0	0
			919	541	184	194		

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
85	C2	1	Total	Zn	0
			1	1	
85	SM	1	Total	Zn	0
			1	1	
85	Sa	1	Total	Zn	0
			1	1	
85	Sb	1	Total	Zn	0
			1	1	
85	Lg	1	Total	Zn	0
			1	1	
85	Lj	1	Total	Zn	0
			1	1	
85	Lm	1	Total	Zn	0
			1	1	
85	Lo	1	Total	Zn	0
			1	1	
85	Lp	1	Total	Zn	0
			1	1	

- Molecule 86 is TIGECYCLINE (three-letter code: T1C) (formula: C<sub>29</sub>H<sub>41</sub>N<sub>5</sub>O<sub>8</sub>).

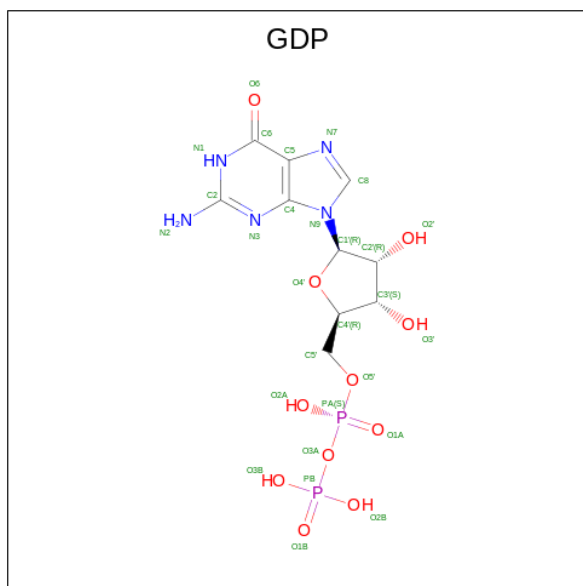


Mol	Chain	Residues	Atoms				AltConf
86	C1	1	Total	C	N	O	0
			42	29	5	8	
86	C1	1	Total	C	N	O	0
			42	29	5	8	
86	C1	1	Total	C	N	O	0
			42	29	5	8	
86	C1	1	Total	C	N	O	0
			42	29	5	8	
86	C1	1	Total	C	N	O	0
			42	29	5	8	

- Molecule 87 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
87	C1	2	Total	Mg	0
			2	2	
87	C3	1	Total	Mg	0
			1	1	
87	CD	1	Total	Mg	0
			1	1	

- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



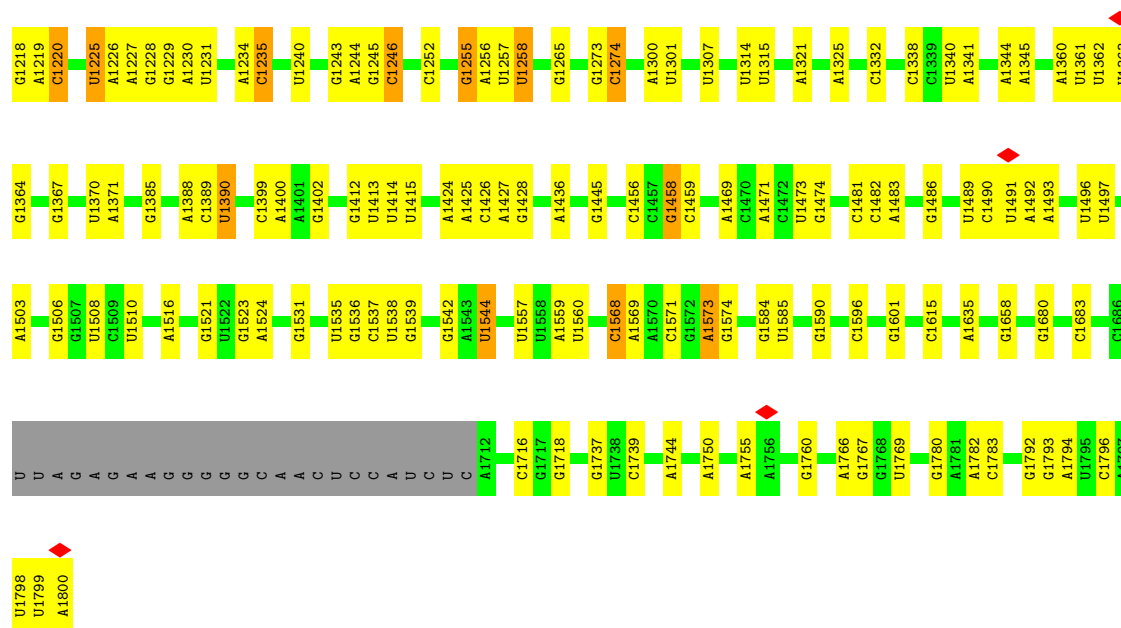
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
88	CD	1	28	10	5	11	2	0

### 3 Residue-property plots

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

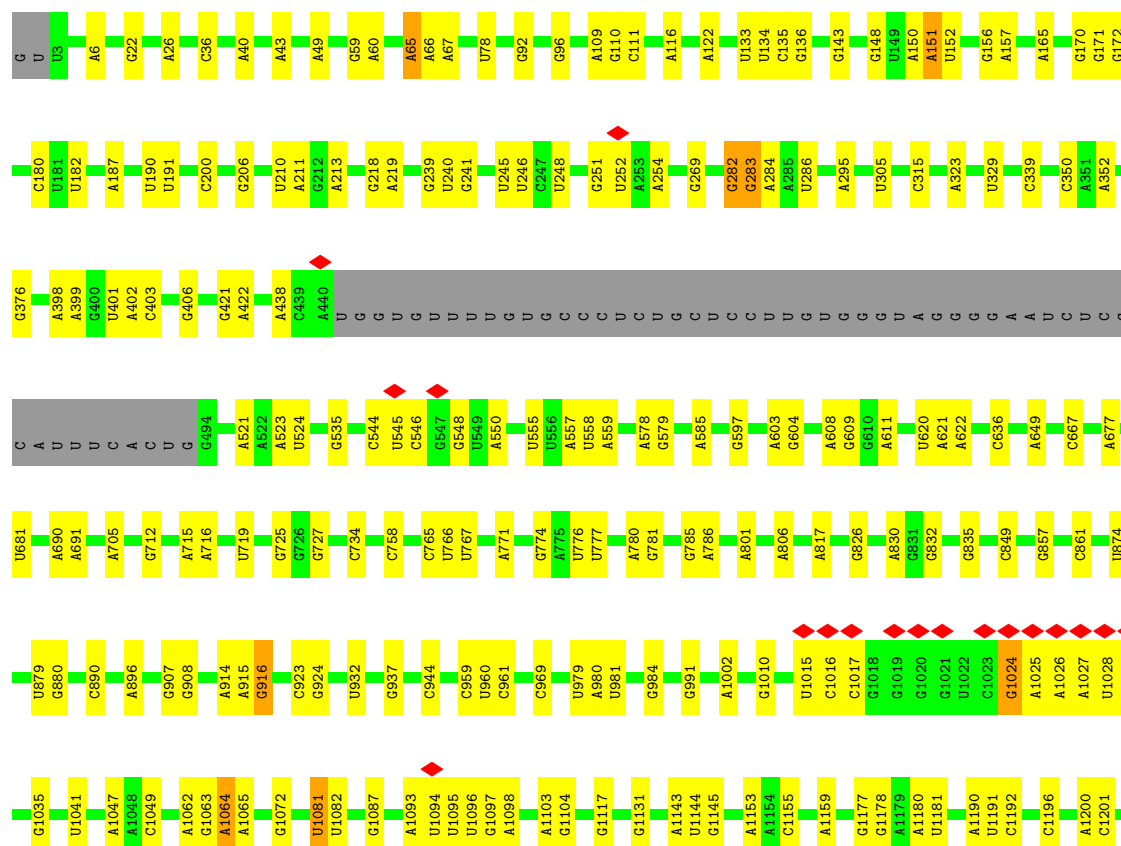
#### • Molecule 1: 18S rRNA





• Molecule 2: 23S rRNA

Chain C1:









• Molecule 3: 5S rRNA

Chain C4: 83% 17%



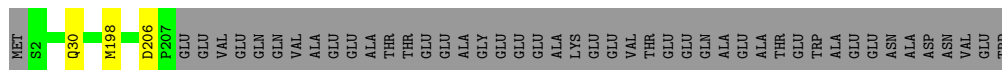
• Molecule 4: 5.8S rRNA

Chain C3: 82% 16% ..



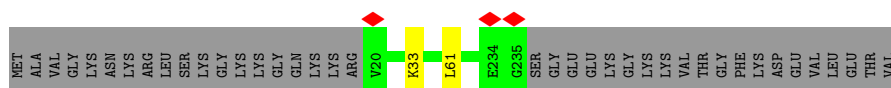
• Molecule 5: Small ribosomal subunit protein uS2A

Chain SA: 81% 18%



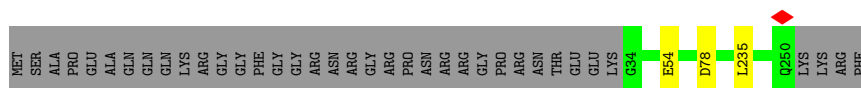
• Molecule 6: 40S ribosomal protein S1-A

Chain SB: 84% 15%



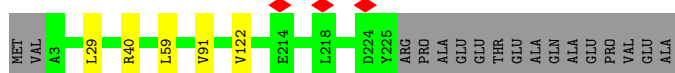
• Molecule 7: 40S ribosomal protein S2

Chain SC: 84% 15%



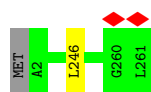
• Molecule 8: Small ribosomal subunit protein uS3

Chain SD: 91% 7%



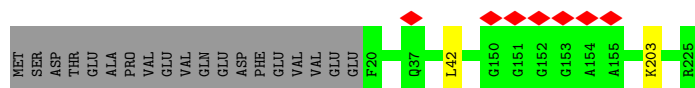
• Molecule 9: 40S ribosomal protein S4-A

Chain SE:  99%



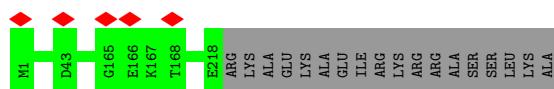
- Molecule 10: Small ribosomal subunit protein uS7

Chain SF:  91% 8%



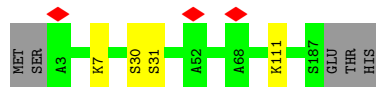
- Molecule 11: 40S ribosomal protein S6-A

Chain SG:  92% 8%



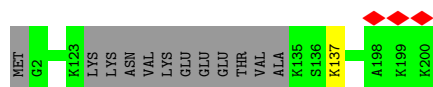
- Molecule 12: 40S ribosomal protein S7-A

Chain SH:  95% ..



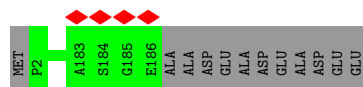
- Molecule 13: 40S ribosomal protein S8-A

Chain SI:  94% 6%




- Molecule 14: 40S ribosomal protein S9-A

Chain SJ:  94% 6%

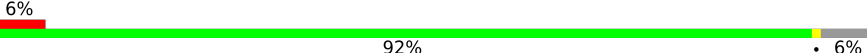


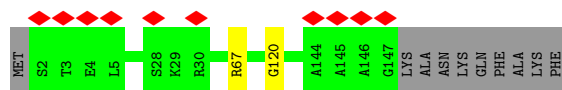
- Molecule 15: Small ribosomal subunit protein eS10A

Chain SK:  83% 5% 12%




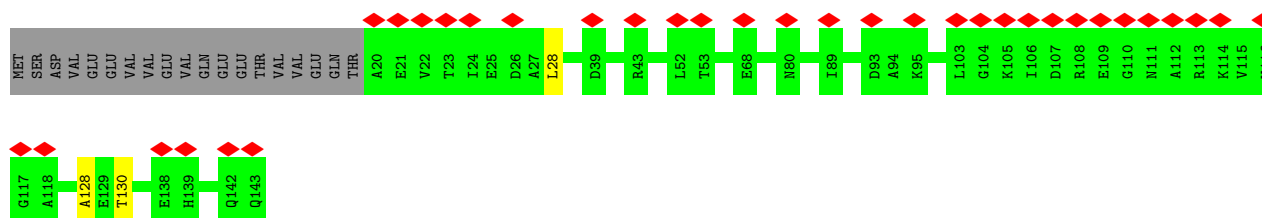
- Molecule 16: Small ribosomal subunit protein uS17A

Chain SL:  6% 92% 6%



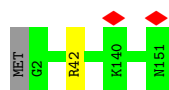
- Molecule 17: Small ribosomal subunit protein eS12

Chain SM:  24% 85% 13%



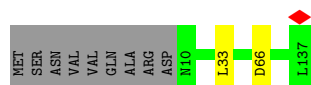
- Molecule 18: 40S ribosomal protein S13

Chain SN:  99% ..




- Molecule 19: 40S ribosomal protein S14-A

Chain SO:  92% 7%



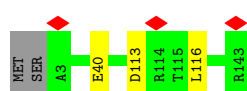
- Molecule 20: Small ribosomal subunit protein uS19

Chain SP:  83% 16%

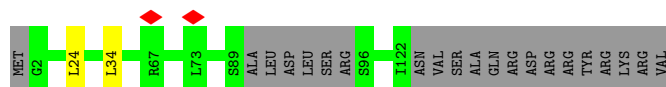
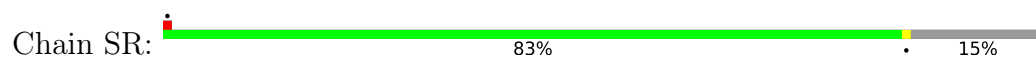


- Molecule 21: Small ribosomal subunit protein uS9A

Chain SQ:  97% ..



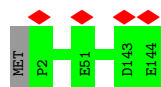
- Molecule 22: Small ribosomal subunit protein eS17A



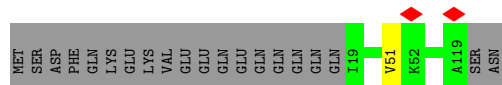
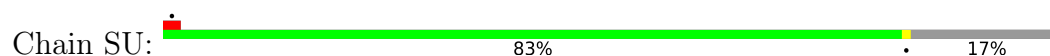
- Molecule 23: Small ribosomal subunit protein uS13A



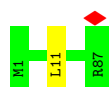
- Molecule 24: Small ribosomal subunit protein eS19A



- Molecule 25: Small ribosomal subunit protein uS10



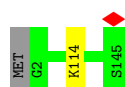
- Molecule 26: Small ribosomal subunit protein eS21A



- Molecule 27: 40S ribosomal protein S22-A



- Molecule 28: 40S ribosomal protein S23-A



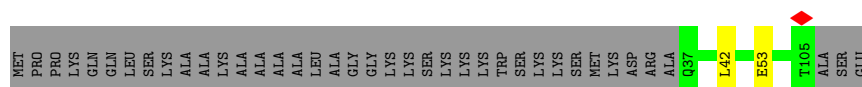
- Molecule 29: 40S ribosomal protein S24-A

Chain SY:  96%




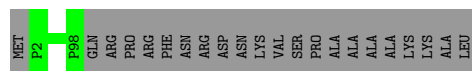
- Molecule 30: Small ribosomal subunit protein eS25A

Chain SZ:  62% 36%



- Molecule 31: Small ribosomal subunit protein eS26B

Chain Sa:  82% 18%

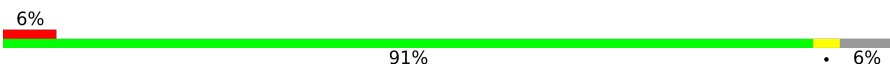


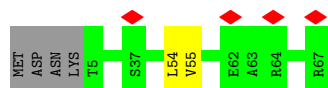
- Molecule 32: 40S ribosomal protein S27-A

Chain Sb:  98%



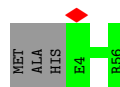
- Molecule 33: Small ribosomal subunit protein eS28A

Chain Sc:  6% 91% 6%



- Molecule 34: Small ribosomal subunit protein uS14A

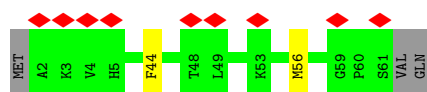
Chain Sd:  95% 5%



- Molecule 35: 40S ribosomal protein S30-A

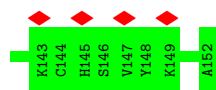
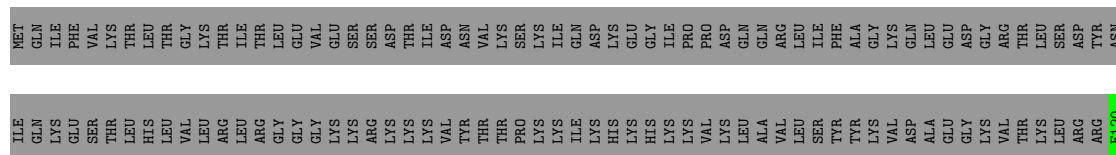
Chain Se:  14% 92% 5%





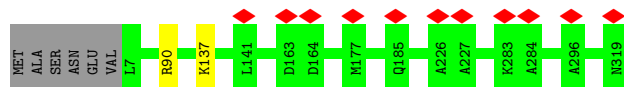
- Molecule 36: Ubiquitin-ribosomal protein eS31 fusion protein

Chain Sf: 22% 78%



- Molecule 37: Small ribosomal subunit protein RACK1

Chain Sg: 97% ..



- Molecule 38: Large ribosomal subunit protein uL2A

Chain LA: 98% ..



- Molecule 39: Large ribosomal subunit protein uL3

Chain LB: 99%



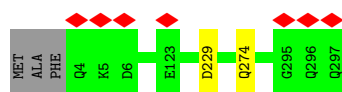
- Molecule 40: Large ribosomal subunit protein uL4A

Chain LC: 99% .

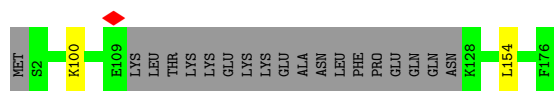
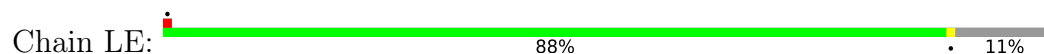


- Molecule 41: Large ribosomal subunit protein uL18

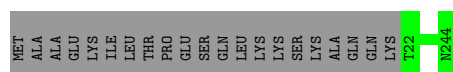
Chain LD: 98% ..



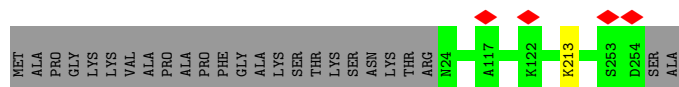
- Molecule 42: Large ribosomal subunit protein eL6A



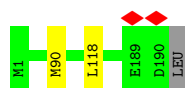
- Molecule 43: Large ribosomal subunit protein uL30A



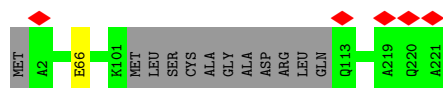
- Molecule 44: Large ribosomal subunit protein eL8A



- Molecule 45: Large ribosomal subunit protein uL6A



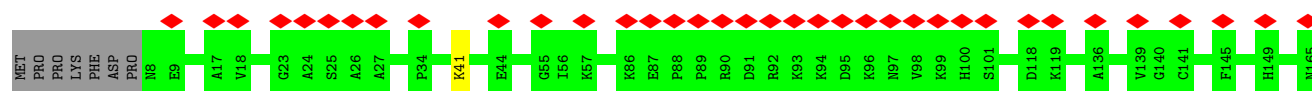
- Molecule 46: Large ribosomal subunit protein uL16



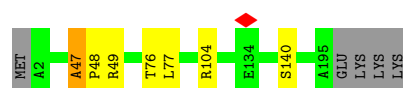
- Molecule 47: Large ribosomal subunit protein uL5A



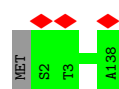
- Molecule 48: Large ribosomal subunit protein uL11A



- Molecule 49: Large ribosomal subunit protein eL13A



- Molecule 50: Large ribosomal subunit protein eL14A



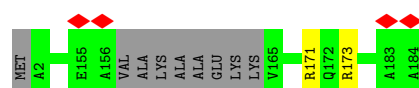
- Molecule 51: Large ribosomal subunit protein eL15A



- Molecule 52: Large ribosomal subunit protein uL13A



- Molecule 53: Large ribosomal subunit protein uL22A



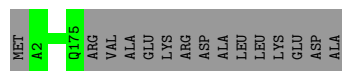
- Molecule 54: Large ribosomal subunit protein eL18A





- Molecule 55: Large ribosomal subunit protein eL19A

Chain LR:  92% 8%



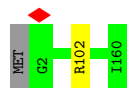
- Molecule 56: Large ribosomal subunit protein eL20A

Chain LS:  100%




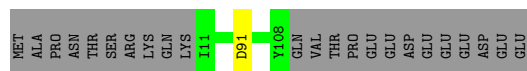
- Molecule 57: Large ribosomal subunit protein eL21A

Chain LT:  99%



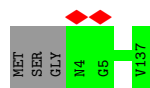
- Molecule 58: Large ribosomal subunit protein eL22A

Chain LU:  80% 19%



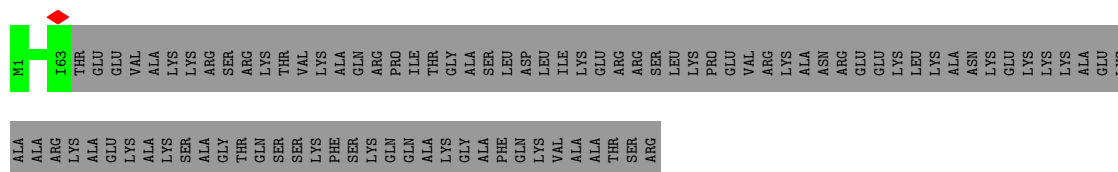
- Molecule 59: Large ribosomal subunit protein uL14A

Chain LV:  98%



- Molecule 60: Large ribosomal subunit protein eL24A

Chain LW:  41% 59%

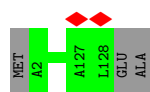


- Molecule 61: Large ribosomal subunit protein uL23

Chain LX:  85% 15%



Chain Le:  98%



- Molecule 69: Large ribosomal subunit protein eL33A

Chain Lf:  99%



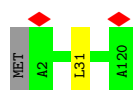
- Molecule 70: Large ribosomal subunit protein eL34A

Chain Lg:  93% 7%



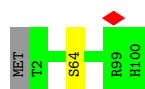
- Molecule 71: Large ribosomal subunit protein uL29A

Chain Lh:  98% ..



- Molecule 72: Large ribosomal subunit protein eL36A

Chain Li:  98% ..



- Molecule 73: Large ribosomal subunit protein eL37A

Chain Lj:  93% 7%



- Molecule 74: Large ribosomal subunit protein eL38

Chain Lk:  97% ..



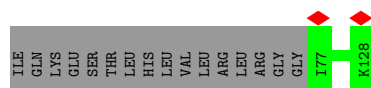
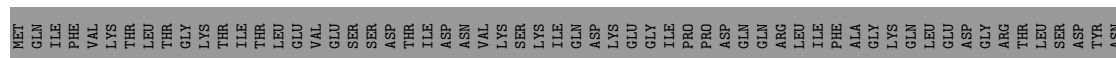
- Molecule 75: Large ribosomal subunit protein eL39

Chain Ll:  96%



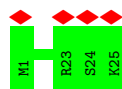
- Molecule 76: Ubiquitin-ribosomal protein eL40A fusion protein

Chain Lm:  41% 59%



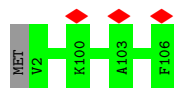
- Molecule 77: Large ribosomal subunit protein eL41A

Chain Ln:  16% 100%



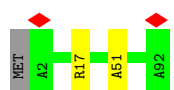
- Molecule 78: Large ribosomal subunit protein eL42A

Chain Lo:  99%



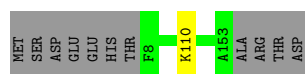
- Molecule 79: Large ribosomal subunit protein eL43A

Chain Lp:  97%



- Molecule 80: Eukaryotic translation initiation factor 5A-1

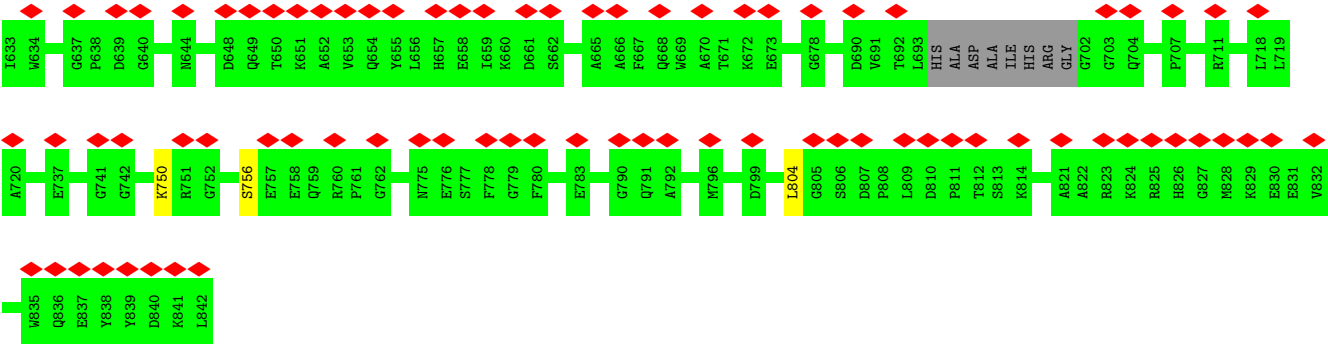
Chain CE:  92% 7%



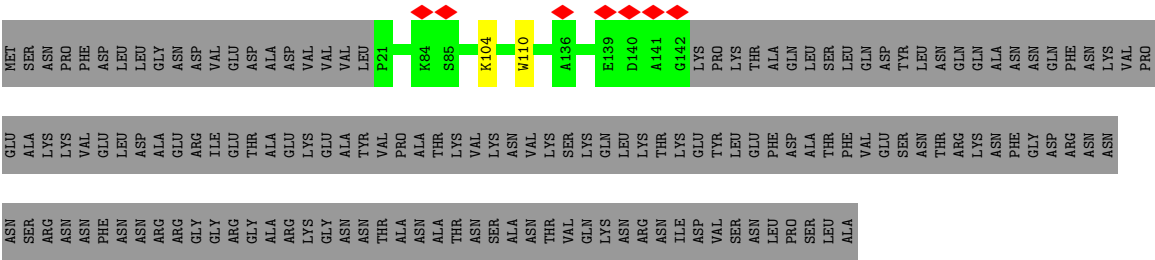
- Molecule 81: Large ribosomal subunit protein uL1A

Chain L1:  99%





• Molecule 84: Suppressor protein STM1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105095	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.447	Depositor
Minimum map value	-0.053	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	406.56, 406.56, 406.56	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.847, 0.847, 0.847	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: T1C, GDP, 5CT, MG, ZN

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	C2	0.49	0/40528	0.96	94/63141 (0.1%)
2	C1	0.70	0/76341	0.93	113/119019 (0.1%)
3	C4	0.55	0/2883	0.90	3/4491 (0.1%)
4	C3	0.66	0/3724	0.90	6/5798 (0.1%)
5	SA	0.36	0/1623	0.71	1/2222 (0.0%)
6	SB	0.39	0/1748	0.69	2/2352 (0.1%)
7	SC	0.43	1/1665 (0.1%)	0.70	2/2263 (0.1%)
8	SD	0.39	0/1759	0.77	3/2368 (0.1%)
9	SE	0.37	0/2109	0.71	1/2839 (0.0%)
10	SF	0.33	0/1629	0.66	0/2202
11	SG	0.30	0/1779	0.62	0/2379
12	SH	0.33	0/1511	0.69	0/2036
13	SI	0.36	0/1514	0.68	0/2021
14	SJ	0.38	0/1519	0.68	0/2035
15	SK	0.44	0/757	0.75	0/1022
16	SL	0.36	0/1194	0.58	0/1610
17	SM	0.36	0/898	0.80	1/1220 (0.1%)
18	SN	0.39	0/1215	0.67	0/1638
19	SO	0.34	0/960	0.72	2/1290 (0.2%)
20	SP	0.35	0/959	0.75	0/1288
21	SQ	0.36	0/1125	0.71	0/1510
22	SR	0.37	0/904	0.77	2/1210 (0.2%)
23	SS	0.39	0/1211	0.80	1/1628 (0.1%)
24	ST	0.32	0/1130	0.60	0/1517
25	SU	0.34	0/815	0.72	0/1102
26	SV	0.40	0/693	0.77	1/935 (0.1%)
27	SW	0.35	0/1038	0.65	1/1395 (0.1%)
28	SX	0.36	0/1139	0.66	0/1518
29	SY	0.36	0/1087	0.78	1/1449 (0.1%)
30	SZ	0.40	1/566 (0.2%)	0.74	1/761 (0.1%)
31	Sa	0.36	0/782	0.66	0/1047
32	Sb	0.29	0/620	0.69	0/838



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Sc	0.33	0/499	0.86	2/670 (0.3%)
34	Sd	0.34	0/452	0.70	0/600
35	Se	0.43	0/483	0.82	1/643 (0.2%)
36	Sf	0.31	0/253	0.65	0/340
37	Sg	0.32	0/2456	0.70	0/3343
38	LA	0.43	0/1946	0.72	0/2614
39	LB	0.41	0/3146	0.63	0/4228
40	LC	0.40	0/2800	0.65	0/3790
41	LD	0.36	0/2408	0.62	1/3248 (0.0%)
42	LE	0.36	0/1269	0.65	1/1705 (0.1%)
43	LF	0.38	0/1828	0.61	0/2461
44	LG	0.38	0/1795	0.66	0/2429
45	LH	0.42	0/1531	0.71	2/2062 (0.1%)
46	LI	0.39	0/1732	0.65	1/2323 (0.0%)
47	LJ	0.34	0/1374	0.71	0/1842
48	LK	0.32	0/1210	0.58	0/1627
49	LL	0.40	0/1573	0.73	1/2113 (0.0%)
50	LM	0.36	0/1074	0.65	0/1446
51	LN	0.48	0/1757	0.68	0/2354
52	LO	0.47	2/1585 (0.1%)	0.65	0/2128
53	LP	0.38	0/1400	0.61	0/1882
54	LQ	0.34	0/1465	0.63	0/1965
55	LR	0.37	0/1382	0.62	0/1849
56	LS	0.44	0/1481	0.67	0/1990
57	LT	0.40	0/1300	0.64	0/1743
58	LU	0.36	0/794	0.66	1/1076 (0.1%)
59	LV	0.39	0/1008	0.65	0/1356
60	LW	0.43	0/533	0.67	0/707
61	LX	0.41	0/974	0.69	0/1314
62	LY	0.32	0/987	0.63	0/1318
63	LZ	0.39	0/1118	0.68	1/1497 (0.1%)
64	La	0.38	0/1204	0.67	1/1612 (0.1%)
65	Lb	0.33	0/473	0.62	0/629
66	Lc	0.33	0/775	0.56	0/1040
67	Ld	0.37	0/897	0.64	0/1205
68	Le	0.43	0/1041	0.67	0/1394
69	Lf	0.44	0/868	0.64	0/1168
70	Lg	0.38	0/890	0.65	0/1189
71	Lh	0.39	0/974	0.66	2/1297 (0.2%)
72	Li	0.33	0/777	0.64	0/1033
73	Lj	0.45	0/665	0.62	0/882
74	Lk	0.32	0/614	0.71	0/822
75	Ll	0.41	0/443	0.71	0/588

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
76	Lm	0.35	0/423	0.64	0/562
77	Ln	0.32	0/234	0.75	0/300
78	Lo	0.37	0/860	0.61	0/1136
79	Lp	0.41	0/701	0.70	0/934
80	CE	0.37	0/1097	0.69	0/1476
81	L1	0.40	0/1745	0.67	1/2342 (0.0%)
82	P0	0.30	0/1598	0.60	0/2161
83	CD	0.37	1/6469 (0.0%)	0.73	12/8760 (0.1%)
84	CS	0.40	1/929 (0.1%)	0.66	0/1245
All	All	0.53	6/224715 (0.0%)	0.84	262/328582 (0.1%)

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
5	SA	0	1
10	SF	0	1
12	SH	0	3
16	SL	0	1
17	SM	0	1
21	SQ	0	2
23	SS	0	2
25	SU	0	1
29	SY	0	1
32	Sb	0	1
35	Se	0	1
37	Sg	0	1
38	LA	0	1
40	LC	0	1
47	LJ	0	1
49	LL	0	2
57	LT	0	1
64	La	0	1
65	Lb	0	1
72	Li	0	1
79	Lp	0	1
83	CD	0	2
All	All	0	28

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	SC	54	GLU	CD-OE2	-7.58	1.17	1.25
52	LO	4	GLU	CD-OE2	-6.18	1.18	1.25
84	CS	110	TRP	CB-CG	-6.13	1.39	1.50
30	SZ	53	GLU	CD-OE1	-5.33	1.19	1.25
83	CD	610	ASP	CB-CG	5.29	1.62	1.51
52	LO	4	GLU	CB-CG	-5.15	1.42	1.52

All (262) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C2	190	C	N3-C4-C5	9.40	125.66	121.90
58	LU	91	ASP	CB-CG-OD1	9.25	126.63	118.30
35	Se	56	MET	CG-SD-CE	-9.24	85.41	100.20
1	C2	1246	C	N1-C2-O2	9.16	124.40	118.90
83	CD	542	LEU	CB-CG-CD2	-9.07	95.59	111.00
2	C1	2741	C	C6-N1-C2	-8.98	116.71	120.30
1	C2	1389	C	C2-N1-C1'	8.84	128.52	118.80
7	SC	78	ASP	CB-CG-OD1	8.24	125.72	118.30
1	C2	1458	G	N3-C4-C5	-8.11	124.55	128.60
1	C2	1246	C	C2-N1-C1'	7.92	127.52	118.80
2	C1	406	G	O4'-C1'-N9	7.92	114.54	108.20
2	C1	2568	C	N3-C2-O2	-7.88	116.38	121.90
1	C2	190	C	N1-C2-O2	7.72	123.53	118.90
1	C2	144	U	C2-N1-C1'	7.68	126.92	117.70
83	CD	240	MET	CG-SD-CE	7.64	112.42	100.20
83	CD	615	ARG	NE-CZ-NH2	-7.53	116.53	120.30
3	C4	39	C	N1-C2-O2	7.46	123.38	118.90
1	C2	1246	C	N3-C2-O2	-7.43	116.70	121.90
8	SD	59	LEU	CA-CB-CG	7.24	131.96	115.30
1	C2	1560	U	C2-N1-C1'	7.24	126.39	117.70
2	C1	2537	U	C2-N1-C1'	7.18	126.32	117.70
1	C2	1458	G	C2-N3-C4	7.09	115.45	111.90
1	C2	697	C	N1-C2-O2	7.08	123.15	118.90
1	C2	1258	U	N1-C2-O2	7.04	127.73	122.80
1	C2	191	C	O4'-C1'-N1	7.04	113.83	108.20
1	C2	229	U	C2-N1-C1'	7.01	126.11	117.70
1	C2	1220	C	C2-N1-C1'	6.97	126.47	118.80
1	C2	1258	U	N3-C2-O2	-6.96	117.33	122.20
42	LE	154	LEU	CA-CB-CG	6.94	131.26	115.30
2	C1	3058	U	C2-N1-C1'	6.87	125.94	117.70
1	C2	1225	U	C2-N1-C1'	6.86	125.93	117.70
2	C1	2537	U	C5-C6-N1	6.84	126.12	122.70
2	C1	2772	C	P-O3'-C3'	6.83	127.90	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C1	1283	C	N1-C2-O2	6.82	122.99	118.90
1	C2	190	C	C6-N1-C2	6.81	123.03	120.30
1	C2	1573	A	OP2-P-O3'	6.80	120.15	105.20
29	SY	53	ASP	CB-CG-OD1	6.78	124.40	118.30
2	C1	2843	U	N1-C2-O2	6.76	127.53	122.80
2	C1	2550	U	C2-N1-C1'	6.74	125.79	117.70
19	SO	66	ASP	CB-CG-OD1	6.73	124.36	118.30
2	C1	2836	C	C2-N1-C1'	6.69	126.16	118.80
5	SA	198	MET	CA-CB-CG	6.68	124.65	113.30
2	C1	1815	U	P-O3'-C3'	6.67	127.70	119.70
64	La	47	LYS	C-N-CA	6.63	138.27	121.70
2	C1	835	G	O4'-C1'-N9	6.59	113.48	108.20
1	C2	1458	G	N3-C4-N9	6.59	129.95	126.00
2	C1	2741	C	N3-C2-O2	-6.58	117.29	121.90
83	CD	610	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	C2	1274	C	N3-C2-O2	-6.56	117.31	121.90
2	C1	1604	G	C4-N9-C1'	6.54	135.00	126.50
1	C2	1225	U	N1-C2-O2	6.51	127.36	122.80
1	C2	1560	U	N3-C2-O2	-6.51	117.64	122.20
3	C4	39	C	C2-N1-C1'	6.50	125.95	118.80
2	C1	1307	G	P-O3'-C3'	6.46	127.45	119.70
2	C1	2550	U	N1-C2-O2	6.45	127.31	122.80
2	C1	1817	G	O4'-C1'-N9	6.45	113.36	108.20
63	LZ	103	GLN	CA-CB-CG	6.43	127.55	113.40
1	C2	965	U	C2-N1-C1'	6.40	125.38	117.70
1	C2	697	C	C2-N1-C1'	6.36	125.80	118.80
2	C1	3058	U	N1-C2-O2	6.35	127.25	122.80
2	C1	2567	C	N1-C2-O2	6.35	122.71	118.90
1	C2	1390	U	C2-N1-C1'	6.34	125.31	117.70
1	C2	1390	U	N1-C2-O2	6.34	127.24	122.80
8	SD	122	VAL	CG1-CB-CG2	-6.33	100.77	110.90
2	C1	1081	U	P-O3'-C3'	6.33	127.29	119.70
83	CD	312	LYS	CA-CB-CG	6.30	127.26	113.40
27	SW	93	LEU	CA-CB-CG	6.29	129.78	115.30
1	C2	1560	U	N1-C2-O2	6.28	127.19	122.80
1	C2	1390	U	N3-C2-O2	-6.27	117.81	122.20
1	C2	1573	A	P-O3'-C3'	6.25	127.20	119.70
2	C1	2132	C	N3-C2-O2	-6.25	117.53	121.90
1	C2	453	U	N1-C2-O2	6.24	127.17	122.80
1	C2	1258	U	C2-N1-C1'	6.23	125.18	117.70
2	C1	1283	C	N3-C2-O2	-6.22	117.55	121.90
1	C2	185	U	C2-N1-C1'	6.21	125.15	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C1	2537	U	N1-C2-O2	6.21	127.14	122.80
1	C2	1389	C	C6-N1-C2	-6.20	117.82	120.30
2	C1	2112	U	P-O3'-C3'	6.19	127.13	119.70
71	Lh	31	LEU	CB-CG-CD1	6.19	121.52	111.00
23	SS	38	VAL	CG1-CB-CG2	-6.18	101.02	110.90
1	C2	272	U	P-O3'-C3'	6.17	127.10	119.70
2	C1	2550	U	N3-C2-O2	-6.17	117.88	122.20
1	C2	453	U	C2-N1-C1'	6.16	125.09	117.70
2	C1	3317	U	P-O3'-C3'	6.15	127.08	119.70
1	C2	1458	G	C4-N9-C1'	6.14	134.49	126.50
2	C1	2843	U	N3-C2-O2	-6.14	117.90	122.20
1	C2	1058	U	P-O3'-C3'	6.13	127.06	119.70
2	C1	2478	C	N1-C2-O2	6.13	122.58	118.90
1	C2	852	C	C2-N1-C1'	6.12	125.54	118.80
1	C2	1596	C	C2-N1-C1'	6.12	125.53	118.80
3	C4	39	C	N3-C2-O2	-6.08	117.64	121.90
2	C1	2726	C	C2-N1-C1'	6.08	125.48	118.80
1	C2	190	C	N3-C2-O2	-6.07	117.65	121.90
1	C2	144	U	C6-N1-C1'	-6.07	112.71	121.20
2	C1	2836	C	N1-C2-O2	6.06	122.54	118.90
8	SD	29	LEU	CA-CB-CG	6.04	129.19	115.30
2	C1	3058	U	N3-C2-O2	-6.03	117.98	122.20
26	SV	11	LEU	CA-CB-CG	6.03	129.16	115.30
2	C1	2652	U	N3-C2-O2	-6.02	117.98	122.20
2	C1	1716	U	P-O3'-C3'	5.98	126.88	119.70
1	C2	1225	U	N3-C2-O2	-5.97	118.02	122.20
1	C2	1389	C	C6-N1-C1'	-5.96	113.65	120.80
4	C3	100	U	C2-N1-C1'	5.96	124.85	117.70
83	CD	119	LEU	CA-CB-CG	-5.95	101.61	115.30
2	C1	2552	C	N1-C2-O2	5.93	122.46	118.90
2	C1	2843	U	C2-N1-C1'	5.93	124.82	117.70
2	C1	1024	G	O4'-C1'-N9	5.92	112.94	108.20
2	C1	3034	C	N1-C2-O2	5.91	122.44	118.90
2	C1	3228	C	P-O3'-C3'	5.91	126.79	119.70
1	C2	1274	C	N1-C2-O2	5.89	122.43	118.90
6	SB	33	LYS	C-N-CA	5.86	136.34	121.70
1	C2	184	C	C2-N1-C1'	5.84	125.22	118.80
22	SR	34	LEU	CA-CB-CG	5.83	128.72	115.30
2	C1	283	G	C4-N9-C1'	5.83	134.08	126.50
1	C2	185	U	N1-C2-O2	5.82	126.87	122.80
2	C1	1448	U	N3-C2-O2	-5.81	118.13	122.20
1	C2	1220	C	C5-C6-N1	5.81	123.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C3	156	U	N1-C2-O2	5.80	126.86	122.80
83	CD	615	ARG	CB-CG-CD	-5.80	96.53	111.60
1	C2	270	C	C2-N1-C1'	5.75	125.12	118.80
1	C2	697	C	N3-C2-O2	-5.75	117.88	121.90
1	C2	361	C	C5-C6-N1	5.74	123.87	121.00
1	C2	1255	G	OP1-P-O3'	5.73	117.80	105.20
81	L1	159	LEU	CB-CG-CD2	5.72	120.73	111.00
49	LL	140	SER	C-N-CA	5.71	135.97	121.70
2	C1	3363	U	N3-C2-O2	-5.71	118.21	122.20
2	C1	524	U	N1-C2-O2	5.71	126.79	122.80
1	C2	758	U	N3-C2-O2	-5.70	118.21	122.20
1	C2	697	C	C6-N1-C2	-5.70	118.02	120.30
4	C3	76	C	C5-C6-N1	5.69	123.84	121.00
2	C1	65	A	P-O3'-C3'	5.69	126.53	119.70
2	C1	36	C	N1-C2-O2	5.68	122.31	118.90
2	C1	758	C	C2-N1-C1'	5.68	125.05	118.80
1	C2	116	U	N3-C2-O2	-5.67	118.23	122.20
4	C3	156	U	C2-N1-C1'	5.66	124.50	117.70
1	C2	1544	U	N1-C2-O2	5.66	126.76	122.80
1	C2	1389	C	C5-C6-N1	5.66	123.83	121.00
2	C1	2405	C	C6-N1-C2	-5.65	118.04	120.30
2	C1	1878	G	C4-N9-C1'	5.64	133.83	126.50
1	C2	1389	C	N1-C2-O2	5.64	122.28	118.90
2	C1	1257	C	C6-N1-C2	-5.61	118.05	120.30
1	C2	1246	C	C6-N1-C1'	-5.61	114.07	120.80
2	C1	1604	G	C8-N9-C1'	-5.60	119.72	127.00
1	C2	453	U	N3-C2-O2	-5.58	118.30	122.20
41	LD	229	ASP	CB-CG-OD1	5.57	123.31	118.30
2	C1	1763	U	N1-C2-O2	5.57	126.69	122.80
45	LH	118	LEU	CB-CG-CD2	-5.57	101.54	111.00
1	C2	1214	U	N1-C2-O2	5.54	126.68	122.80
33	Sc	55	VAL	CG1-CB-CG2	5.53	119.75	110.90
1	C2	795	U	C2-N1-C1'	5.53	124.34	117.70
1	C2	1220	C	N1-C2-O2	5.51	122.21	118.90
2	C1	2137	U	C2-N1-C1'	5.51	124.32	117.70
2	C1	3034	C	C6-N1-C2	-5.50	118.10	120.30
1	C2	558	U	P-O3'-C3'	5.49	126.29	119.70
83	CD	340	LEU	CA-CB-CG	5.48	127.91	115.30
19	SO	33	LEU	CA-CB-CG	5.48	127.90	115.30
1	C2	103	A	P-O3'-C3'	5.48	126.27	119.70
2	C1	283	G	N3-C4-N9	5.47	129.28	126.00
2	C1	1239	C	C2-N1-C1'	5.47	124.81	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C1	315	C	C2-N1-C1'	5.46	124.81	118.80
83	CD	284	LEU	CA-CB-CG	5.46	127.86	115.30
2	C1	2366	C	C2-N1-C1'	5.46	124.81	118.80
83	CD	542	LEU	CB-CG-CD1	5.46	120.28	111.00
2	C1	2726	C	N3-C2-O2	-5.46	118.08	121.90
2	C1	2336	U	N1-C2-O2	5.44	126.61	122.80
2	C1	2726	C	C6-N1-C2	-5.44	118.12	120.30
2	C1	2531	C	N1-C2-O2	5.42	122.15	118.90
1	C2	1196	A	P-O3'-C3'	5.41	126.19	119.70
1	C2	1332	C	C2-N1-C1'	5.40	124.74	118.80
2	C1	969	C	C6-N1-C2	-5.40	118.14	120.30
2	C1	2274	U	N1-C2-O2	5.39	126.58	122.80
30	SZ	42	LEU	CA-CB-CG	5.39	127.70	115.30
2	C1	78	U	N3-C2-O2	-5.38	118.43	122.20
2	C1	2585	G	N3-C4-N9	5.38	129.23	126.00
4	C3	80	A	P-O3'-C3'	5.38	126.15	119.70
1	C2	758	U	N1-C2-O2	5.36	126.55	122.80
2	C1	916	G	OP1-P-O3'	5.33	116.94	105.20
9	SE	246	LEU	CA-CB-CG	5.33	127.57	115.30
1	C2	417	A	P-O3'-C3'	5.33	126.10	119.70
1	C2	583	C	C5-C6-N1	5.33	123.67	121.00
1	C2	1021	C	C2-N1-C1'	5.33	124.66	118.80
1	C2	1214	U	C2-N1-C1'	5.33	124.10	117.70
1	C2	698	U	N1-C2-O2	5.33	126.53	122.80
2	C1	2568	C	O4'-C1'-N1	5.32	112.46	108.20
2	C1	2585	G	N3-C4-C5	-5.32	125.94	128.60
2	C1	3048	A	O4'-C1'-N9	5.32	112.46	108.20
2	C1	1190	A	C4-N9-C1'	5.31	135.86	126.30
45	LH	90	MET	CG-SD-CE	-5.30	91.72	100.20
1	C2	1568	C	P-O3'-C3'	5.29	126.05	119.70
2	C1	1277	C	N1-C2-O2	5.29	122.07	118.90
2	C1	2585	G	C4-N9-C1'	5.28	133.36	126.50
1	C2	1456	C	C2-N1-C1'	5.27	124.60	118.80
2	C1	2954	U	N1-C2-O2	5.27	126.49	122.80
2	C1	3214	U	C2-N1-C1'	5.26	124.02	117.70
2	C1	1235	U	N3-C4-O4	5.26	123.08	119.40
2	C1	2652	U	N1-C2-O2	5.26	126.48	122.80
7	SC	54	GLU	OE1-CD-OE2	-5.26	116.99	123.30
2	C1	3131	U	C2-N1-C1'	5.26	124.01	117.70
2	C1	916	G	P-O3'-C3'	5.25	126.00	119.70
1	C2	185	U	N3-C2-O2	-5.25	118.52	122.20
71	Lh	31	LEU	CB-CG-CD2	-5.24	102.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C2	698	U	N3-C2-O2	-5.24	118.53	122.20
1	C2	1458	G	C8-N9-C4	-5.24	104.31	106.40
4	C3	64	U	N3-C2-O2	-5.24	118.53	122.20
2	C1	3269	U	P-O3'-C3'	5.24	125.98	119.70
83	CD	804	LEU	CA-CB-CG	5.24	127.34	115.30
2	C1	734	C	N1-C2-O2	5.23	122.04	118.90
22	SR	24	LEU	CA-CB-CG	5.23	127.34	115.30
2	C1	3356	G	P-O3'-C3'	5.23	125.97	119.70
1	C2	4	C	C2-N1-C1'	5.22	124.55	118.80
2	C1	3034	C	N3-C2-O2	-5.21	118.25	121.90
1	C2	1214	U	N3-C2-O2	-5.21	118.55	122.20
1	C2	1097	U	N1-C2-O2	5.21	126.44	122.80
1	C2	1535	U	N3-C2-O2	-5.20	118.56	122.20
1	C2	1255	G	P-O3'-C3'	5.19	125.93	119.70
2	C1	151	A	P-O3'-C3'	5.19	125.93	119.70
33	Sc	54	LEU	CA-CB-CG	5.19	127.24	115.30
6	SB	61	LEU	CA-CB-CG	5.19	127.24	115.30
2	C1	524	U	N3-C2-O2	-5.18	118.58	122.20
2	C1	3104	U	N3-C2-O2	-5.16	118.59	122.20
2	C1	2552	C	C2-N1-C1'	5.15	124.46	118.80
2	C1	1095	U	N1-C2-O2	5.14	126.40	122.80
1	C2	120	U	N3-C2-O2	-5.14	118.61	122.20
2	C1	2821	C	N1-C2-O2	5.13	121.98	118.90
2	C1	1604	G	N3-C4-N9	5.13	129.08	126.00
1	C2	1097	U	P-O3'-C3'	5.13	125.85	119.70
2	C1	3158	G	P-O3'-C3'	5.13	125.85	119.70
2	C1	2266	U	N1-C2-O2	5.11	126.38	122.80
2	C1	1878	G	N3-C4-C5	-5.10	126.05	128.60
1	C2	1544	U	N3-C2-O2	-5.10	118.63	122.20
2	C1	3117	C	N1-C2-O2	5.10	121.96	118.90
2	C1	282	G	P-O3'-C3'	5.10	125.82	119.70
2	C1	2606	G	N3-C4-C5	-5.10	126.05	128.60
2	C1	2954	U	C2-N1-C1'	5.10	123.82	117.70
2	C1	2545	C	C2-N1-C1'	5.09	124.40	118.80
2	C1	283	G	C8-N9-C1'	-5.09	120.38	127.00
2	C1	2899	C	C2-N1-C1'	5.09	124.40	118.80
2	C1	2366	C	C6-N1-C2	-5.09	118.27	120.30
2	C1	2366	C	C5-C6-N1	5.08	123.54	121.00
2	C1	2741	C	C5-C6-N1	5.08	123.54	121.00
1	C2	609	U	N3-C2-O2	-5.08	118.64	122.20
2	C1	1762	C	N1-C2-O2	5.08	121.95	118.90
1	C2	1235	C	N1-C2-O2	5.07	121.94	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C2	190	C	C2-N3-C4	-5.06	117.37	119.90
1	C2	422	G	P-O3'-C3'	5.06	125.77	119.70
1	C2	691	C	C2-N1-C1'	5.05	124.36	118.80
2	C1	1064	A	P-O3'-C3'	5.05	125.77	119.70
2	C1	1763	U	C2-N1-C1'	5.05	123.77	117.70
2	C1	2683	U	C2-N1-C1'	5.05	123.77	117.70
17	SM	28	LEU	CA-CB-CG	5.05	126.92	115.30
2	C1	1604	G	N3-C4-C5	-5.05	126.08	128.60
1	C2	120	U	N1-C2-O2	5.04	126.33	122.80
2	C1	2132	C	N1-C2-O2	5.04	121.92	118.90
1	C2	1497	U	N1-C2-O2	5.04	126.33	122.80
2	C1	2763	U	N1-C2-O2	5.03	126.32	122.80
46	LI	66	GLU	CA-CB-CG	5.02	124.45	113.40
1	C2	1683	C	C2-N1-C1'	5.02	124.33	118.80
2	C1	2336	U	N3-C2-O2	-5.02	118.69	122.20
83	CD	538	LEU	CA-CB-CG	5.01	126.83	115.30
2	C1	734	C	C2-N1-C1'	5.00	124.30	118.80
2	C1	2336	U	C2-N1-C1'	5.00	123.70	117.70
2	C1	2716	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
83	CD	750	LYS	Peptide
83	CD	756	SER	Peptide
38	LA	13	GLY	Peptide
40	LC	144	LYS	Peptide
47	LJ	94	ARG	Peptide
49	LL	47	ALA	Peptide
49	LL	49	ARG	Peptide
57	LT	102	ARG	Sidechain
64	La	17	ALA	Peptide
65	Lb	21	ILE	Peptide
72	Li	64	SER	Peptide
79	Lp	51	ALA	Peptide
5	SA	206	ASP	Peptide
10	SF	42	LEU	Peptide
12	SH	111	LYS	Peptide
12	SH	30	SER	Peptide
12	SH	31	SER	Peptide
16	SL	120	GLY	Peptide

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Mol	Chain	Res	Type	Group
17	SM	128	ALA	Peptide
21	SQ	113	ASP	Peptide
21	SQ	40	GLU	Peptide
23	SS	60	GLU	Peptide
23	SS	90	ASN	Peptide
25	SU	51	VAL	Peptide
29	SY	51	GLU	Peptide
32	Sb	75	GLU	Peptide
35	Se	44	PHE	Peptide
37	Sg	90	ARG	Sidechain

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	
5	SA	204/252 (81%)	175 (86%)	28 (14%)	1 (0%)	25	60
6	SB	214/255 (84%)	196 (92%)	18 (8%)	0	100	100
7	SC	215/254 (85%)	201 (94%)	13 (6%)	1 (0%)	25	60
8	SD	221/240 (92%)	195 (88%)	25 (11%)	1 (0%)	25	60
9	SE	258/261 (99%)	234 (91%)	24 (9%)	0	100	100
10	SF	204/225 (91%)	176 (86%)	28 (14%)	0	100	100
11	SG	216/236 (92%)	202 (94%)	14 (6%)	0	100	100
12	SH	183/190 (96%)	161 (88%)	22 (12%)	0	100	100
13	SI	184/200 (92%)	175 (95%)	9 (5%)	0	100	100
14	SJ	183/197 (93%)	168 (92%)	15 (8%)	0	100	100
15	SK	90/105 (86%)	76 (84%)	9 (10%)	5 (6%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	SL	144/156 (92%)	134 (93%)	10 (7%)	0	100	100
17	SM	122/143 (85%)	85 (70%)	36 (30%)	1 (1%)	16	51
18	SN	148/151 (98%)	138 (93%)	10 (7%)	0	100	100
19	SO	126/137 (92%)	106 (84%)	20 (16%)	0	100	100
20	SP	117/142 (82%)	105 (90%)	11 (9%)	1 (1%)	14	49
21	SQ	139/143 (97%)	123 (88%)	15 (11%)	1 (1%)	19	54
22	SR	111/136 (82%)	102 (92%)	9 (8%)	0	100	100
23	SS	143/146 (98%)	127 (89%)	15 (10%)	1 (1%)	19	54
24	ST	141/144 (98%)	132 (94%)	9 (6%)	0	100	100
25	SU	99/121 (82%)	94 (95%)	5 (5%)	0	100	100
26	SV	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
27	SW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
28	SX	142/145 (98%)	135 (95%)	7 (5%)	0	100	100
29	SY	132/135 (98%)	117 (89%)	13 (10%)	2 (2%)	8	38
30	SZ	67/108 (62%)	65 (97%)	2 (3%)	0	100	100
31	Sa	95/119 (80%)	81 (85%)	14 (15%)	0	100	100
32	Sb	79/82 (96%)	67 (85%)	12 (15%)	0	100	100
33	Sc	61/67 (91%)	54 (88%)	7 (12%)	0	100	100
34	Sd	51/56 (91%)	49 (96%)	2 (4%)	0	100	100
35	Se	58/63 (92%)	50 (86%)	8 (14%)	0	100	100
36	Sf	31/152 (20%)	27 (87%)	4 (13%)	0	100	100
37	Sg	311/319 (98%)	277 (89%)	34 (11%)	0	100	100
38	LA	250/254 (98%)	225 (90%)	25 (10%)	0	100	100
39	LB	384/387 (99%)	366 (95%)	18 (5%)	0	100	100
40	LC	359/362 (99%)	325 (90%)	33 (9%)	1 (0%)	37	69
41	LD	292/297 (98%)	277 (95%)	15 (5%)	0	100	100
42	LE	153/176 (87%)	140 (92%)	13 (8%)	0	100	100
43	LF	221/244 (91%)	218 (99%)	3 (1%)	0	100	100
44	LG	229/256 (90%)	206 (90%)	23 (10%)	0	100	100
45	LH	188/191 (98%)	182 (97%)	6 (3%)	0	100	100
46	LI	205/221 (93%)	196 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	LJ	167/174 (96%)	141 (84%)	25 (15%)	1 (1%)	22	57
48	LK	156/165 (94%)	152 (97%)	4 (3%)	0	100	100
49	LL	192/199 (96%)	171 (89%)	17 (9%)	4 (2%)	5	31
50	LM	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
51	LN	201/204 (98%)	193 (96%)	8 (4%)	0	100	100
52	LO	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
53	LP	171/184 (93%)	167 (98%)	4 (2%)	0	100	100
54	LQ	183/186 (98%)	177 (97%)	6 (3%)	0	100	100
55	LR	172/189 (91%)	169 (98%)	3 (2%)	0	100	100
56	LS	170/172 (99%)	167 (98%)	3 (2%)	0	100	100
57	LT	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
58	LU	96/121 (79%)	93 (97%)	3 (3%)	0	100	100
59	LV	132/137 (96%)	127 (96%)	5 (4%)	0	100	100
60	LW	61/155 (39%)	59 (97%)	2 (3%)	0	100	100
61	LX	118/142 (83%)	107 (91%)	11 (9%)	0	100	100
62	LY	122/127 (96%)	117 (96%)	5 (4%)	0	100	100
63	LZ	133/136 (98%)	118 (89%)	12 (9%)	3 (2%)	5	29
64	La	146/149 (98%)	124 (85%)	20 (14%)	2 (1%)	9	40
65	Lb	56/59 (95%)	46 (82%)	10 (18%)	0	100	100
66	Lc	98/105 (93%)	93 (95%)	5 (5%)	0	100	100
67	Ld	107/113 (95%)	101 (94%)	6 (6%)	0	100	100
68	Le	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
69	Lf	104/107 (97%)	97 (93%)	7 (7%)	0	100	100
70	Lg	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
71	Lh	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
72	Li	97/100 (97%)	92 (95%)	5 (5%)	0	100	100
73	Lj	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
74	Lk	75/78 (96%)	70 (93%)	4 (5%)	1 (1%)	10	41
75	Ll	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
76	Lm	50/128 (39%)	50 (100%)	0	0	100	100
77	Ln	23/25 (92%)	22 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
78	Lo	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
79	Lp	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
80	CE	143/157 (91%)	130 (91%)	12 (8%)	1 (1%)	19	54
81	L1	215/217 (99%)	190 (88%)	24 (11%)	1 (0%)	25	60
82	P0	201/312 (64%)	194 (96%)	7 (4%)	0	100	100
83	CD	810/842 (96%)	749 (92%)	58 (7%)	3 (0%)	30	64
84	CS	120/273 (44%)	113 (94%)	7 (6%)	0	100	100
All	All	12460/13846 (90%)	11502 (92%)	927 (7%)	31 (0%)	45	75

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	SK	81	ASN
29	SY	32	ARG
47	LJ	95	ASN
49	LL	48	PRO
80	CE	110	LYS
15	SK	88	PRO
20	SP	126	VAL
21	SQ	116	LEU
29	SY	52	LYS
40	LC	339	LEU
49	LL	76	THR
64	La	48	TYR
83	CD	483	PHE
15	SK	54	TYR
49	LL	77	LEU
63	LZ	101	PHE
83	CD	465	LYS
7	SC	235	LEU
49	LL	47	ALA
81	L1	59	PRO
8	SD	91	VAL
17	SM	130	THR
23	SS	91	ASP
74	Lk	17	ARG
5	SA	30	GLN
15	SK	3	MET
15	SK	30	ALA
63	LZ	102	GLU

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Mol	Chain	Res	Type
83	CD	481	MET
63	LZ	104	PRO
64	La	18	GLY

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	SA	165/210 (79%)	165 (100%)	0	100	100
6	SB	192/224 (86%)	192 (100%)	0	100	100
7	SC	176/205 (86%)	176 (100%)	0	100	100
8	SD	182/195 (93%)	181 (100%)	1 (0%)	86	93
9	SE	221/222 (100%)	221 (100%)	0	100	100
10	SF	173/191 (91%)	172 (99%)	1 (1%)	84	92
11	SG	187/201 (93%)	187 (100%)	0	100	100
12	SH	165/170 (97%)	164 (99%)	1 (1%)	84	92
13	SI	150/161 (93%)	149 (99%)	1 (1%)	81	92
14	SJ	158/166 (95%)	158 (100%)	0	100	100
15	SK	73/98 (74%)	73 (100%)	0	100	100
16	SL	129/137 (94%)	128 (99%)	1 (1%)	79	90
17	SM	88/119 (74%)	88 (100%)	0	100	100
18	SN	127/128 (99%)	126 (99%)	1 (1%)	79	90
19	SO	97/105 (92%)	97 (100%)	0	100	100
20	SP	98/118 (83%)	98 (100%)	0	100	100
21	SQ	117/119 (98%)	117 (100%)	0	100	100
22	SR	92/124 (74%)	92 (100%)	0	100	100
23	SS	128/129 (99%)	128 (100%)	0	100	100
24	ST	115/116 (99%)	115 (100%)	0	100	100
25	SU	94/114 (82%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	SV	74/74 (100%)	74 (100%)	0	100	100
27	SW	110/111 (99%)	110 (100%)	0	100	100
28	SX	119/120 (99%)	118 (99%)	1 (1%)	79	90
29	SY	112/113 (99%)	112 (100%)	0	100	100
30	SZ	61/89 (68%)	61 (100%)	0	100	100
31	Sa	83/100 (83%)	83 (100%)	0	100	100
32	Sb	70/71 (99%)	70 (100%)	0	100	100
33	Sc	56/60 (93%)	56 (100%)	0	100	100
34	Sd	47/49 (96%)	47 (100%)	0	100	100
35	Se	51/54 (94%)	51 (100%)	0	100	100
36	Sf	27/135 (20%)	27 (100%)	0	100	100
37	Sg	255/262 (97%)	254 (100%)	1 (0%)	89	94
38	LA	192/196 (98%)	191 (100%)	1 (0%)	86	93
39	LB	318/323 (98%)	317 (100%)	1 (0%)	91	96
40	LC	288/289 (100%)	287 (100%)	1 (0%)	91	96
41	LD	243/245 (99%)	242 (100%)	1 (0%)	89	94
42	LE	135/153 (88%)	134 (99%)	1 (1%)	81	92
43	LF	187/205 (91%)	187 (100%)	0	100	100
44	LG	177/208 (85%)	176 (99%)	1 (1%)	84	92
45	LH	170/171 (99%)	170 (100%)	0	100	100
46	LI	177/187 (95%)	177 (100%)	0	100	100
47	LJ	147/150 (98%)	147 (100%)	0	100	100
48	LK	129/136 (95%)	128 (99%)	1 (1%)	79	90
49	LL	154/159 (97%)	153 (99%)	1 (1%)	84	92
50	LM	108/109 (99%)	108 (100%)	0	100	100
51	LN	175/176 (99%)	175 (100%)	0	100	100
52	LO	160/162 (99%)	160 (100%)	0	100	100
53	LP	139/146 (95%)	137 (99%)	2 (1%)	62	82
54	LQ	150/151 (99%)	149 (99%)	1 (1%)	81	92
55	LR	133/154 (86%)	133 (100%)	0	100	100
56	LS	156/156 (100%)	156 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	LT	136/137 (99%)	136 (100%)	0	100	100
58	LU	85/107 (79%)	85 (100%)	0	100	100
59	LV	103/105 (98%)	103 (100%)	0	100	100
60	LW	55/129 (43%)	55 (100%)	0	100	100
61	LX	104/118 (88%)	104 (100%)	0	100	100
62	LY	107/110 (97%)	107 (100%)	0	100	100
63	LZ	115/116 (99%)	114 (99%)	1 (1%)	75	89
64	La	118/119 (99%)	118 (100%)	0	100	100
65	Lb	46/47 (98%)	46 (100%)	0	100	100
66	Lc	84/88 (96%)	84 (100%)	0	100	100
67	Ld	94/97 (97%)	94 (100%)	0	100	100
68	Le	109/111 (98%)	109 (100%)	0	100	100
69	Lf	90/91 (99%)	90 (100%)	0	100	100
70	Lg	95/103 (92%)	95 (100%)	0	100	100
71	Lh	103/105 (98%)	103 (100%)	0	100	100
72	Li	80/82 (98%)	80 (100%)	0	100	100
73	Lj	67/71 (94%)	67 (100%)	0	100	100
74	Lk	67/69 (97%)	67 (100%)	0	100	100
75	Ll	45/46 (98%)	44 (98%)	1 (2%)	47	73
76	Lm	47/116 (40%)	47 (100%)	0	100	100
77	Ln	23/23 (100%)	23 (100%)	0	100	100
78	Lo	90/91 (99%)	90 (100%)	0	100	100
79	Lp	71/72 (99%)	70 (99%)	1 (1%)	62	82
80	CE	116/132 (88%)	116 (100%)	0	100	100
81	L1	198/198 (100%)	198 (100%)	0	100	100
82	P0	171/254 (67%)	169 (99%)	2 (1%)	67	85
83	CD	695/715 (97%)	691 (99%)	4 (1%)	84	92
84	CS	97/228 (42%)	96 (99%)	1 (1%)	73	87
All	All	10541/11646 (90%)	10512 (100%)	29 (0%)	90	96

All (29) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
8	SD	40	ARG
10	SF	203	LYS
12	SH	7	LYS
13	SI	137	LYS
16	SL	67	ARG
18	SN	42	ARG
28	SX	114	LYS
37	Sg	137	LYS
38	LA	247	ARG
39	LB	332	ARG
40	LC	197	ARG
41	LD	274	GLN
42	LE	100	LYS
44	LG	213	LYS
48	LK	41	LYS
49	LL	104	ARG
53	LP	171	ARG
53	LP	173	ARG
54	LQ	116	LYS
63	LZ	93	LYS
75	Ll	45	ARG
79	Lp	17	ARG
82	P0	7	LYS
82	P0	157	LYS
83	CD	32	LYS
83	CD	42	ARG
83	CD	253	LYS
83	CD	555	LYS
84	CS	104	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
5	SA	32	HIS
10	SF	127	GLN
24	ST	138	GLN
26	SV	74	GLN
29	SY	106	GLN
67	Ld	57	GLN
75	Ll	33	ASN
78	Lo	47	GLN

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C2	1693/1800 (94%)	389 (22%)	20 (1%)
2	C1	3182/3396 (93%)	605 (19%)	29 (0%)
3	C4	120/121 (99%)	19 (15%)	0
4	C3	156/158 (98%)	24 (15%)	1 (0%)
All	All	5151/5475 (94%)	1037 (20%)	50 (0%)

All (1037) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C2	4	C
1	C2	17	C
1	C2	25	C
1	C2	26	A
1	C2	27	U
1	C2	34	G
1	C2	42	G
1	C2	43	A
1	C2	45	U
1	C2	46	A
1	C2	47	A
1	C2	57	G
1	C2	60	U
1	C2	63	G
1	C2	66	U
1	C2	67	A
1	C2	68	A
1	C2	71	A
1	C2	72	A
1	C2	77	U
1	C2	78	A
1	C2	79	C
1	C2	104	A
1	C2	114	C
1	C2	115	G
1	C2	123	G
1	C2	127	G
1	C2	128	U
1	C2	132	U
1	C2	137	U
1	C2	140	A
1	C2	141	U

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Mol	Chain	Res	Type
1	C2	144	U
1	C2	153	G
1	C2	158	U
1	C2	166	C
1	C2	168	A
1	C2	178	U
1	C2	179	A
1	C2	185	U
1	C2	188	A
1	C2	189	C
1	C2	190	C
1	C2	191	C
1	C2	192	U
1	C2	193	U
1	C2	194	U
1	C2	195	G
1	C2	196	G
1	C2	197	A
1	C2	198	A
1	C2	220	A
1	C2	229	U
1	C2	230	C
1	C2	233	C
1	C2	235	G
1	C2	238	U
1	C2	239	C
1	C2	240	U
1	C2	241	U
1	C2	246	G
1	C2	250	C
1	C2	257	A
1	C2	265	A
1	C2	266	A
1	C2	271	A
1	C2	272	U
1	C2	273	G
1	C2	275	C
1	C2	276	C
1	C2	277	U
1	C2	278	U
1	C2	280	U
1	C2	287	G

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Mol	Chain	Res	Type
1	C2	299	A
1	C2	308	C
1	C2	309	C
1	C2	314	C
1	C2	316	A
1	C2	319	U
1	C2	322	G
1	C2	333	A
1	C2	337	G
1	C2	338	C
1	C2	352	A
1	C2	359	A
1	C2	360	A
1	C2	361	C
1	C2	369	A
1	C2	387	A
1	C2	390	G
1	C2	400	A
1	C2	402	C
1	C2	404	G
1	C2	416	A
1	C2	417	A
1	C2	418	G
1	C2	422	G
1	C2	423	G
1	C2	424	C
1	C2	425	A
1	C2	426	G
1	C2	431	C
1	C2	434	G
1	C2	439	U
1	C2	444	C
1	C2	448	C
1	C2	452	A
1	C2	454	U
1	C2	464	A
1	C2	469	C
1	C2	475	A
1	C2	477	A
1	C2	486	G
1	C2	488	G
1	C2	500	C

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Mol	Chain	Res	Type
1	C2	501	U
1	C2	506	A
1	C2	507	U
1	C2	510	G
1	C2	511	A
1	C2	512	A
1	C2	514	G
1	C2	515	A
1	C2	519	C
1	C2	527	A
1	C2	532	U
1	C2	533	U
1	C2	534	A
1	C2	538	A
1	C2	539	G
1	C2	540	G
1	C2	542	A
1	C2	548	G
1	C2	549	G
1	C2	551	G
1	C2	555	A
1	C2	556	A
1	C2	557	G
1	C2	558	U
1	C2	559	C
1	C2	561	G
1	C2	565	C
1	C2	574	G
1	C2	577	G
1	C2	578	U
1	C2	579	A
1	C2	580	A
1	C2	583	C
1	C2	594	A
1	C2	595	G
1	C2	606	A
1	C2	611	U
1	C2	619	A
1	C2	620	A
1	C2	623	A
1	C2	624	G
1	C2	629	U

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Mol	Chain	Res	Type
1	C2	634	G
1	C2	635	A
1	C2	639	U
1	C2	640	U
1	C2	648	G
1	C2	691	C
1	C2	696	C
1	C2	698	U
1	C2	738	G
1	C2	742	U
1	C2	743	U
1	C2	751	G
1	C2	754	A
1	C2	755	A
1	C2	756	A
1	C2	757	A
1	C2	765	G
1	C2	766	U
1	C2	774	A
1	C2	775	G
1	C2	779	U
1	C2	781	U
1	C2	782	U
1	C2	783	G
1	C2	788	A
1	C2	789	A
1	C2	793	A
1	C2	794	U
1	C2	795	U
1	C2	803	A
1	C2	811	A
1	C2	812	A
1	C2	813	U
1	C2	815	G
1	C2	816	G
1	C2	820	U
1	C2	826	U
1	C2	829	A
1	C2	830	U
1	C2	831	U
1	C2	833	U
1	C2	835	U

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Mol	Chain	Res	Type
1	C2	850	A
1	C2	851	U
1	C2	856	A
1	C2	863	A
1	C2	886	U
1	C2	898	A
1	C2	901	G
1	C2	913	G
1	C2	914	G
1	C2	932	U
1	C2	933	A
1	C2	934	C
1	C2	935	U
1	C2	942	G
1	C2	951	A
1	C2	959	U
1	C2	960	U
1	C2	964	U
1	C2	966	A
1	C2	969	C
1	C2	970	A
1	C2	992	A
1	C2	1009	U
1	C2	1021	C
1	C2	1023	A
1	C2	1026	A
1	C2	1028	C
1	C2	1030	A
1	C2	1031	U
1	C2	1039	A
1	C2	1040	G
1	C2	1052	U
1	C2	1053	G
1	C2	1057	U
1	C2	1058	U
1	C2	1059	U
1	C2	1060	U
1	C2	1062	A
1	C2	1076	A
1	C2	1082	C
1	C2	1086	A
1	C2	1092	A

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Mol	Chain	Res	Type
1	C2	1093	A
1	C2	1096	C
1	C2	1097	U
1	C2	1098	U
1	C2	1100	G
1	C2	1126	G
1	C2	1138	A
1	C2	1147	A
1	C2	1150	G
1	C2	1158	C
1	C2	1159	C
1	C2	1160	A
1	C2	1167	G
1	C2	1185	U
1	C2	1194	A
1	C2	1196	A
1	C2	1197	C
1	C2	1199	G
1	C2	1200	G
1	C2	1202	A
1	C2	1212	G
1	C2	1217	A
1	C2	1218	G
1	C2	1219	A
1	C2	1220	C
1	C2	1225	U
1	C2	1226	A
1	C2	1228	G
1	C2	1229	G
1	C2	1230	A
1	C2	1231	U
1	C2	1234	A
1	C2	1235	C
1	C2	1240	U
1	C2	1243	G
1	C2	1244	A
1	C2	1245	G
1	C2	1246	C
1	C2	1252	C
1	C2	1255	G
1	C2	1256	A
1	C2	1257	U

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Mol	Chain	Res	Type
1	C2	1258	U
1	C2	1265	G
1	C2	1273	G
1	C2	1274	C
1	C2	1300	A
1	C2	1301	U
1	C2	1307	U
1	C2	1314	U
1	C2	1315	U
1	C2	1321	A
1	C2	1325	A
1	C2	1338	C
1	C2	1340	U
1	C2	1341	A
1	C2	1344	A
1	C2	1345	A
1	C2	1360	A
1	C2	1361	U
1	C2	1362	U
1	C2	1363	U
1	C2	1364	G
1	C2	1367	G
1	C2	1370	U
1	C2	1371	A
1	C2	1385	G
1	C2	1388	A
1	C2	1390	U
1	C2	1399	C
1	C2	1400	A
1	C2	1402	G
1	C2	1412	G
1	C2	1413	U
1	C2	1414	U
1	C2	1415	U
1	C2	1424	A
1	C2	1425	A
1	C2	1426	C
1	C2	1427	A
1	C2	1428	G
1	C2	1436	A
1	C2	1445	G
1	C2	1459	C

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Mol	Chain	Res	Type
1	C2	1469	A
1	C2	1471	A
1	C2	1473	U
1	C2	1474	G
1	C2	1481	C
1	C2	1482	C
1	C2	1483	A
1	C2	1486	G
1	C2	1489	U
1	C2	1490	C
1	C2	1491	U
1	C2	1492	A
1	C2	1493	A
1	C2	1496	U
1	C2	1503	A
1	C2	1506	G
1	C2	1508	U
1	C2	1510	U
1	C2	1516	A
1	C2	1521	G
1	C2	1523	G
1	C2	1524	A
1	C2	1531	G
1	C2	1536	G
1	C2	1537	C
1	C2	1539	G
1	C2	1542	G
1	C2	1544	U
1	C2	1557	U
1	C2	1559	A
1	C2	1569	A
1	C2	1571	C
1	C2	1573	A
1	C2	1574	G
1	C2	1584	G
1	C2	1585	U
1	C2	1590	G
1	C2	1601	G
1	C2	1615	C
1	C2	1635	A
1	C2	1658	G
1	C2	1680	G

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Mol	Chain	Res	Type
1	C2	1716	C
1	C2	1718	G
1	C2	1737	G
1	C2	1739	C
1	C2	1744	A
1	C2	1750	A
1	C2	1755	A
1	C2	1760	G
1	C2	1766	A
1	C2	1767	G
1	C2	1769	U
1	C2	1780	G
1	C2	1782	A
1	C2	1783	C
1	C2	1792	G
1	C2	1793	G
1	C2	1794	A
1	C2	1796	C
1	C2	1798	U
1	C2	1799	U
1	C2	1800	A
2	C1	6	A
2	C1	22	G
2	C1	26	A
2	C1	40	A
2	C1	43	A
2	C1	49	A
2	C1	59	G
2	C1	60	A
2	C1	65	A
2	C1	66	A
2	C1	67	A
2	C1	92	G
2	C1	96	G
2	C1	109	A
2	C1	110	G
2	C1	111	C
2	C1	116	A
2	C1	122	A
2	C1	133	U
2	C1	134	U
2	C1	135	C

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Mol	Chain	Res	Type
2	C1	136	G
2	C1	143	G
2	C1	148	G
2	C1	150	A
2	C1	151	A
2	C1	152	U
2	C1	156	G
2	C1	157	A
2	C1	165	A
2	C1	171	G
2	C1	172	G
2	C1	180	C
2	C1	182	U
2	C1	187	A
2	C1	190	U
2	C1	191	U
2	C1	200	C
2	C1	206	G
2	C1	210	U
2	C1	211	A
2	C1	213	A
2	C1	218	G
2	C1	219	A
2	C1	239	G
2	C1	240	U
2	C1	241	G
2	C1	245	U
2	C1	246	U
2	C1	248	U
2	C1	251	G
2	C1	252	U
2	C1	254	A
2	C1	269	G
2	C1	283	G
2	C1	284	A
2	C1	286	U
2	C1	295	A
2	C1	305	U
2	C1	323	A
2	C1	329	U
2	C1	339	C
2	C1	350	C

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Mol	Chain	Res	Type
2	C1	352	A
2	C1	376	G
2	C1	398	A
2	C1	399	A
2	C1	401	U
2	C1	402	A
2	C1	403	C
2	C1	421	G
2	C1	422	A
2	C1	438	A
2	C1	521	A
2	C1	523	A
2	C1	535	G
2	C1	544	C
2	C1	545	U
2	C1	546	C
2	C1	548	G
2	C1	550	A
2	C1	555	U
2	C1	557	A
2	C1	558	U
2	C1	559	A
2	C1	578	A
2	C1	579	G
2	C1	585	A
2	C1	597	G
2	C1	603	A
2	C1	604	G
2	C1	608	A
2	C1	609	G
2	C1	611	A
2	C1	620	U
2	C1	621	A
2	C1	622	A
2	C1	636	C
2	C1	649	A
2	C1	667	C
2	C1	677	A
2	C1	681	U
2	C1	690	A
2	C1	691	A
2	C1	705	A

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Mol	Chain	Res	Type
2	C1	712	G
2	C1	715	A
2	C1	716	A
2	C1	719	U
2	C1	725	G
2	C1	727	G
2	C1	765	C
2	C1	766	U
2	C1	767	U
2	C1	771	A
2	C1	774	G
2	C1	776	U
2	C1	777	U
2	C1	780	A
2	C1	781	G
2	C1	785	G
2	C1	786	A
2	C1	801	A
2	C1	806	A
2	C1	817	A
2	C1	826	G
2	C1	830	A
2	C1	832	G
2	C1	849	C
2	C1	857	G
2	C1	861	C
2	C1	874	U
2	C1	879	U
2	C1	880	G
2	C1	890	C
2	C1	896	A
2	C1	907	G
2	C1	908	G
2	C1	914	A
2	C1	915	A
2	C1	916	G
2	C1	923	C
2	C1	924	G
2	C1	932	U
2	C1	937	G
2	C1	944	C
2	C1	959	C

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Mol	Chain	Res	Type
2	C1	960	U
2	C1	961	C
2	C1	979	U
2	C1	980	A
2	C1	981	U
2	C1	984	G
2	C1	991	G
2	C1	1002	A
2	C1	1010	G
2	C1	1015	U
2	C1	1016	C
2	C1	1017	C
2	C1	1024	G
2	C1	1025	A
2	C1	1026	A
2	C1	1027	A
2	C1	1028	U
2	C1	1029	G
2	C1	1030	A
2	C1	1032	C
2	C1	1035	G
2	C1	1041	U
2	C1	1047	A
2	C1	1049	C
2	C1	1063	G
2	C1	1064	A
2	C1	1065	A
2	C1	1072	G
2	C1	1081	U
2	C1	1082	U
2	C1	1087	G
2	C1	1093	A
2	C1	1094	U
2	C1	1096	U
2	C1	1097	G
2	C1	1098	A
2	C1	1103	A
2	C1	1104	G
2	C1	1117	G
2	C1	1131	G
2	C1	1143	A
2	C1	1144	U

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Mol	Chain	Res	Type
2	C1	1145	G
2	C1	1153	A
2	C1	1155	C
2	C1	1159	A
2	C1	1177	G
2	C1	1178	G
2	C1	1180	A
2	C1	1181	U
2	C1	1191	U
2	C1	1192	C
2	C1	1196	C
2	C1	1200	A
2	C1	1201	C
2	C1	1207	G
2	C1	1208	U
2	C1	1217	A
2	C1	1219	C
2	C1	1220	U
2	C1	1221	A
2	C1	1222	G
2	C1	1223	A
2	C1	1230	G
2	C1	1232	C
2	C1	1235	U
2	C1	1236	G
2	C1	1239	C
2	C1	1241	U
2	C1	1243	G
2	C1	1245	A
2	C1	1246	G
2	C1	1254	C
2	C1	1256	G
2	C1	1258	U
2	C1	1259	A
2	C1	1263	A
2	C1	1265	U
2	C1	1281	G
2	C1	1285	G
2	C1	1286	A
2	C1	1287	A
2	C1	1289	G
2	C1	1295	G

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Mol	Chain	Res	Type
2	C1	1301	A
2	C1	1305	U
2	C1	1307	G
2	C1	1308	A
2	C1	1309	U
2	C1	1313	G
2	C1	1330	A
2	C1	1345	G
2	C1	1348	U
2	C1	1354	G
2	C1	1357	G
2	C1	1380	G
2	C1	1386	A
2	C1	1392	G
2	C1	1399	A
2	C1	1400	G
2	C1	1417	G
2	C1	1418	A
2	C1	1419	A
2	C1	1434	G
2	C1	1437	C
2	C1	1446	A
2	C1	1450	G
2	C1	1455	U
2	C1	1469	C
2	C1	1482	A
2	C1	1483	G
2	C1	1484	U
2	C1	1487	G
2	C1	1488	G
2	C1	1508	C
2	C1	1522	U
2	C1	1523	U
2	C1	1536	G
2	C1	1539	A
2	C1	1546	A
2	C1	1554	U
2	C1	1555	U
2	C1	1560	G
2	C1	1574	C
2	C1	1575	A
2	C1	1576	G

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Mol	Chain	Res	Type
2	C1	1577	G
2	C1	1578	C
2	C1	1581	C
2	C1	1583	A
2	C1	1587	A
2	C1	1589	A
2	C1	1593	A
2	C1	1605	A
2	C1	1619	A
2	C1	1620	U
2	C1	1629	U
2	C1	1639	C
2	C1	1642	A
2	C1	1643	A
2	C1	1644	C
2	C1	1645	U
2	C1	1646	G
2	C1	1657	C
2	C1	1658	G
2	C1	1683	A
2	C1	1696	A
2	C1	1716	U
2	C1	1717	U
2	C1	1724	U
2	C1	1736	G
2	C1	1741	A
2	C1	1750	A
2	C1	1751	G
2	C1	1760	A
2	C1	1762	C
2	C1	1765	U
2	C1	1770	G
2	C1	1775	G
2	C1	1778	G
2	C1	1780	G
2	C1	1794	G
2	C1	1797	A
2	C1	1808	G
2	C1	1812	G
2	C1	1814	A
2	C1	1816	A
2	C1	1817	G

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Mol	Chain	Res	Type
2	C1	1818	U
2	C1	1821	U
2	C1	1839	A
2	C1	1841	A
2	C1	1842	A
2	C1	1846	C
2	C1	1849	C
2	C1	1858	A
2	C1	1866	C
2	C1	1867	A
2	C1	1878	G
2	C1	1879	A
2	C1	1880	U
2	C1	1886	A
2	C1	1893	A
2	C1	1906	G
2	C1	1907	C
2	C1	1925	U
2	C1	2101	C
2	C1	2102	U
2	C1	2110	G
2	C1	2111	G
2	C1	2113	A
2	C1	2114	C
2	C1	2121	G
2	C1	2122	G
2	C1	2131	A
2	C1	2140	U
2	C1	2144	A
2	C1	2158	A
2	C1	2169	G
2	C1	2171	G
2	C1	2175	U
2	C1	2176	U
2	C1	2205	U
2	C1	2206	G
2	C1	2208	A
2	C1	2209	U
2	C1	2223	A
2	C1	2225	U
2	C1	2229	A
2	C1	2232	A

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Mol	Chain	Res	Type
2	C1	2244	A
2	C1	2249	G
2	C1	2256	A
2	C1	2257	C
2	C1	2260	U
2	C1	2267	C
2	C1	2268	U
2	C1	2269	U
2	C1	2272	G
2	C1	2273	G
2	C1	2274	U
2	C1	2281	A
2	C1	2287	C
2	C1	2288	G
2	C1	2307	G
2	C1	2308	C
2	C1	2310	U
2	C1	2313	A
2	C1	2315	G
2	C1	2334	U
2	C1	2335	G
2	C1	2373	A
2	C1	2374	C
2	C1	2375	G
2	C1	2385	G
2	C1	2388	U
2	C1	2394	G
2	C1	2397	A
2	C1	2401	A
2	C1	2402	A
2	C1	2403	G
2	C1	2404	A
2	C1	2411	U
2	C1	2418	G
2	C1	2419	A
2	C1	2437	G
2	C1	2439	A
2	C1	2446	U
2	C1	2448	G
2	C1	2453	U
2	C1	2455	U
2	C1	2456	A

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Mol	Chain	Res	Type
2	C1	2458	A
2	C1	2460	U
2	C1	2463	G
2	C1	2468	A
2	C1	2469	G
2	C1	2473	C
2	C1	2485	A
2	C1	2488	A
2	C1	2490	C
2	C1	2498	U
2	C1	2502	A
2	C1	2511	A
2	C1	2514	U
2	C1	2515	A
2	C1	2522	G
2	C1	2523	A
2	C1	2524	A
2	C1	2526	C
2	C1	2536	A
2	C1	2538	U
2	C1	2539	C
2	C1	2540	A
2	C1	2541	U
2	C1	2542	U
2	C1	2543	U
2	C1	2544	U
2	C1	2547	A
2	C1	2549	G
2	C1	2552	C
2	C1	2554	A
2	C1	2568	C
2	C1	2569	A
2	C1	2570	U
2	C1	2571	U
2	C1	2572	C
2	C1	2573	G
2	C1	2585	G
2	C1	2593	A
2	C1	2594	C
2	C1	2606	G
2	C1	2607	G
2	C1	2614	G

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Mol	Chain	Res	Type
2	C1	2626	A
2	C1	2635	A
2	C1	2648	G
2	C1	2652	U
2	C1	2656	A
2	C1	2663	G
2	C1	2666	C
2	C1	2672	G
2	C1	2674	A
2	C1	2677	G
2	C1	2678	A
2	C1	2683	U
2	C1	2688	U
2	C1	2689	A
2	C1	2691	A
2	C1	2694	A
2	C1	2696	A
2	C1	2704	A
2	C1	2705	A
2	C1	2708	C
2	C1	2714	G
2	C1	2719	U
2	C1	2727	A
2	C1	2728	G
2	C1	2729	U
2	C1	2737	C
2	C1	2746	A
2	C1	2752	U
2	C1	2753	G
2	C1	2755	C
2	C1	2772	C
2	C1	2773	C
2	C1	2777	G
2	C1	2778	G
2	C1	2796	G
2	C1	2800	G
2	C1	2801	A
2	C1	2803	A
2	C1	2810	C
2	C1	2814	G
2	C1	2817	A
2	C1	2818	U

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Mol	Chain	Res	Type
2	C1	2844	C
2	C1	2845	A
2	C1	2849	C
2	C1	2853	A
2	C1	2861	U
2	C1	2867	C
2	C1	2871	G
2	C1	2872	A
2	C1	2875	U
2	C1	2887	A
2	C1	2888	U
2	C1	2889	C
2	C1	2898	G
2	C1	2899	C
2	C1	2911	A
2	C1	2923	U
2	C1	2933	A
2	C1	2935	U
2	C1	2936	A
2	C1	2938	G
2	C1	2941	A
2	C1	2942	C
2	C1	2947	G
2	C1	2948	C
2	C1	2954	U
2	C1	2983	C
2	C1	2990	G
2	C1	2996	U
2	C1	2997	G
2	C1	3011	A
2	C1	3012	A
2	C1	3021	A
2	C1	3022	G
2	C1	3048	A
2	C1	3056	U
2	C1	3059	G
2	C1	3078	U
2	C1	3079	U
2	C1	3086	A
2	C1	3092	C
2	C1	3109	G
2	C1	3117	C

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Mol	Chain	Res	Type
2	C1	3122	A
2	C1	3129	A
2	C1	3130	A
2	C1	3131	U
2	C1	3142	A
2	C1	3143	C
2	C1	3153	U
2	C1	3158	G
2	C1	3159	C
2	C1	3165	A
2	C1	3170	A
2	C1	3172	A
2	C1	3173	G
2	C1	3174	A
2	C1	3176	G
2	C1	3178	A
2	C1	3179	U
2	C1	3181	C
2	C1	3186	A
2	C1	3187	A
2	C1	3196	U
2	C1	3206	C
2	C1	3207	U
2	C1	3210	A
2	C1	3217	C
2	C1	3218	A
2	C1	3219	G
2	C1	3224	G
2	C1	3227	A
2	C1	3229	G
2	C1	3234	A
2	C1	3235	C
2	C1	3238	G
2	C1	3243	A
2	C1	3244	A
2	C1	3245	A
2	C1	3247	G
2	C1	3259	U
2	C1	3263	G
2	C1	3269	U
2	C1	3270	U
2	C1	3273	A

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Mol	Chain	Res	Type
2	C1	3275	U
2	C1	3276	G
2	C1	3279	A
2	C1	3280	U
2	C1	3281	U
2	C1	3283	U
2	C1	3287	U
2	C1	3288	G
2	C1	3289	G
2	C1	3290	G
2	C1	3294	A
2	C1	3303	G
2	C1	3304	U
2	C1	3313	U
2	C1	3316	A
2	C1	3317	U
2	C1	3318	G
2	C1	3319	U
2	C1	3320	A
2	C1	3335	A
2	C1	3341	U
2	C1	3342	A
2	C1	3345	G
2	C1	3351	U
2	C1	3352	U
2	C1	3355	U
2	C1	3356	G
2	C1	3357	U
2	C1	3358	U
2	C1	3362	A
2	C1	3363	U
2	C1	3368	U
2	C1	3369	G
2	C1	3375	A
2	C1	3378	C
2	C1	3386	G
2	C1	3389	U
2	C1	3396	U
3	C4	7	G
3	C4	11	A
3	C4	22	A
3	C4	29	C

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Mol	Chain	Res	Type
3	C4	33	U
3	C4	38	U
3	C4	52	G
3	C4	54	U
3	C4	55	A
3	C4	56	A
3	C4	65	G
3	C4	73	C
3	C4	74	C
3	C4	76	A
3	C4	91	G
3	C4	93	C
3	C4	102	A
3	C4	112	G
3	C4	121	U
4	C3	34	U
4	C3	35	C
4	C3	59	A
4	C3	62	C
4	C3	63	G
4	C3	75	G
4	C3	80	A
4	C3	81	U
4	C3	82	U
4	C3	83	C
4	C3	84	C
4	C3	86	U
4	C3	87	G
4	C3	95	G
4	C3	104	A
4	C3	106	C
4	C3	111	A
4	C3	113	U
4	C3	116	G
4	C3	125	U
4	C3	126	A
4	C3	138	A
4	C3	148	G
4	C3	156	U

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C2	103	A
1	C2	187	G
1	C2	272	U
1	C2	417	A
1	C2	422	G
1	C2	555	A
1	C2	558	U
1	C2	755	A
1	C2	1051	G
1	C2	1058	U
1	C2	1097	U
1	C2	1196	A
1	C2	1227	A
1	C2	1255	G
1	C2	1344	A
1	C2	1458	G
1	C2	1481	C
1	C2	1538	U
1	C2	1568	C
1	C2	1573	A
2	C1	65	A
2	C1	151	A
2	C1	170	G
2	C1	282	G
2	C1	715	A
2	C1	1062	A
2	C1	1064	A
2	C1	1081	U
2	C1	1216	C
2	C1	1307	G
2	C1	1493	G
2	C1	1645	U
2	C1	1716	U
2	C1	1815	U
2	C1	1816	A
2	C1	1841	A
2	C1	2101	C
2	C1	2112	U
2	C1	2662	G
2	C1	2772	C
2	C1	3078	U
2	C1	3121	U
2	C1	3158	G

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Mol	Chain	Res	Type
2	C1	3228	C
2	C1	3269	U
2	C1	3289	G
2	C1	3317	U
2	C1	3356	G
2	C1	3357	U
4	C3	80	A

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
80	5CT	CE	51	80	13,14,15	0.75	0	9,15,17	1.01	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
80	5CT	CE	51	80	-	7/13/14/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
80	CE	51	5CT	C1-C2-C3-C4
80	CE	51	5CT	O1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
80	CE	51	5CT	C-CA-CB-CG
80	CE	51	5CT	O-C-CA-CB
80	CE	51	5CT	CG-CD-CE-NZ
80	CE	51	5CT	CE-CD-CG-CB
80	CE	51	5CT	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 13 are monoatomic - leaving 7 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$
86	T1C	C1	3405	-	44,45,45	1.20	4 (9%)	53,72,72	1.50	6 (11%)
86	T1C	C1	3402	-	44,45,45	1.20	4 (9%)	53,72,72	1.17	3 (5%)
86	T1C	C1	3401	-	44,45,45	1.18	4 (9%)	53,72,72	1.44	8 (15%)
88	GDP	CD	902	87	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)
86	T1C	C1	3403	-	44,45,45	1.16	3 (6%)	53,72,72	0.93	1 (1%)
86	T1C	C1	3406	87	44,45,45	1.18	3 (6%)	53,72,72	1.14	4 (7%)
86	T1C	C1	3404	87	44,45,45	1.20	4 (9%)	53,72,72	1.09	5 (9%)

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
86	T1C	C1	3405	-	-	16/22/80/80	0/4/4/4
86	T1C	C1	3402	-	-	13/22/80/80	0/4/4/4
86	T1C	C1	3401	-	-	11/22/80/80	0/4/4/4
88	GDP	CD	902	87	-	3/12/32/32	0/3/3/3
86	T1C	C1	3403	-	-	9/22/80/80	0/4/4/4
86	T1C	C1	3406	87	-	13/22/80/80	0/4/4/4
86	T1C	C1	3404	87	-	13/22/80/80	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	C1	3402	T1C	C21-N21	5.50	1.48	1.33
86	C1	3401	T1C	C21-N21	5.49	1.48	1.33
86	C1	3405	T1C	C21-N21	5.45	1.47	1.33
86	C1	3403	T1C	C21-N21	5.44	1.47	1.33
86	C1	3406	T1C	C21-N21	5.42	1.47	1.33
86	C1	3404	T1C	C21-N21	5.42	1.47	1.33
88	CD	902	GDP	C6-N1	-2.44	1.34	1.37
86	C1	3405	T1C	C4-N4	2.43	1.52	1.47
86	C1	3404	T1C	C4-N4	2.36	1.52	1.47
86	C1	3402	T1C	C4-N4	2.34	1.52	1.47
86	C1	3406	T1C	O11-C11	2.23	1.28	1.23
86	C1	3401	T1C	O11-C11	2.23	1.28	1.23
86	C1	3402	T1C	O11-C11	2.22	1.27	1.23
86	C1	3405	T1C	O11-C11	2.21	1.27	1.23
86	C1	3403	T1C	C7-N7	2.20	1.48	1.42
86	C1	3404	T1C	O11-C11	2.20	1.27	1.23
86	C1	3401	T1C	C7-N7	2.16	1.48	1.42
86	C1	3403	T1C	O11-C11	2.15	1.27	1.23
86	C1	3404	T1C	C7-N7	2.12	1.48	1.42
86	C1	3402	T1C	C7-N7	2.12	1.48	1.42
86	C1	3406	T1C	C7-N7	2.07	1.48	1.42
86	C1	3405	T1C	C7-N7	2.02	1.47	1.42
86	C1	3401	T1C	C4-N4	2.01	1.51	1.47

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	C1	3405	T1C	C1-C1C-C12	4.92	115.64	109.88
86	C1	3401	T1C	C11-C1B-C12	4.63	122.47	118.80
86	C1	3402	T1C	C1C-C1-C2	4.41	122.75	115.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	C1	3401	T1C	C1C-C1-C2	4.21	122.43	115.75
86	C1	3405	T1C	C11-C1B-C12	4.12	122.06	118.80
86	C1	3401	T1C	C1C-C41-C4	3.87	116.93	111.64
88	CD	902	GDP	PA-O3A-PB	-3.80	119.80	132.83
86	C1	3403	T1C	C11-C1B-C12	3.66	121.70	118.80
86	C1	3406	T1C	C11-C1B-C12	3.47	121.55	118.80
86	C1	3405	T1C	C8-C7-N7	-3.40	116.35	120.91
86	C1	3405	T1C	C61-C7-N7	3.38	123.04	118.91
86	C1	3406	T1C	O1C-C1C-C12	-3.31	104.84	110.14
86	C1	3406	T1C	C1-C1C-C12	3.27	113.72	109.88
88	CD	902	GDP	C3'-C2'-C1'	3.20	105.80	100.98
86	C1	3405	T1C	O1C-C1C-C12	-3.13	105.14	110.14
86	C1	3402	T1C	C11-C1B-C12	3.01	121.18	118.80
86	C1	3404	T1C	C11-C1B-C12	2.95	121.13	118.80
86	C1	3405	T1C	C1C-C41-C4	2.94	115.65	111.64
86	C1	3406	T1C	C1C-C41-C4	2.70	115.33	111.64
86	C1	3401	T1C	O1C-C1C-C12	-2.67	105.87	110.14
86	C1	3404	T1C	C1C-C1-C2	2.64	119.95	115.75
86	C1	3401	T1C	C51-C5-C41	-2.59	105.93	110.49
86	C1	3404	T1C	O1C-C1C-C12	-2.58	106.01	110.14
86	C1	3401	T1C	C1-C1C-C12	2.56	112.89	109.88
86	C1	3404	T1C	C1-C1C-C12	2.46	112.76	109.88
88	CD	902	GDP	C5-C6-N1	2.45	118.29	113.95
86	C1	3404	T1C	C1C-C41-C4	2.41	114.94	111.64
86	C1	3401	T1C	O1C-C1C-C41	-2.39	107.16	110.09
86	C1	3402	T1C	O1C-C1C-C12	-2.36	106.37	110.14
88	CD	902	GDP	C8-N7-C5	2.28	107.33	102.99
86	C1	3401	T1C	C72-N7-C71	-2.03	109.58	116.12

There are no chirality outliers.

All (78) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	C1	3401	T1C	C94-C93-N92-C92
86	C1	3401	T1C	C95-C93-N92-C92
86	C1	3401	T1C	C96-C93-N92-C92
86	C1	3401	T1C	C41-C4-N4-C43
86	C1	3401	T1C	C1-C2-C21-O21
86	C1	3401	T1C	C1-C2-C21-N21
86	C1	3402	T1C	C92-C91-N9-C9
86	C1	3402	T1C	C1-C2-C21-O21
86	C1	3402	T1C	C1-C2-C21-N21

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Mol	Chain	Res	Type	Atoms
86	C1	3403	T1C	C92-C91-N9-C9
86	C1	3403	T1C	O91-C91-N9-C9
86	C1	3403	T1C	C1-C2-C21-O21
86	C1	3403	T1C	C1-C2-C21-N21
86	C1	3404	T1C	C91-C92-N92-C93
86	C1	3404	T1C	C92-C91-N9-C9
86	C1	3404	T1C	C1-C2-C21-O21
86	C1	3404	T1C	C1-C2-C21-N21
86	C1	3405	T1C	C94-C93-N92-C92
86	C1	3405	T1C	C95-C93-N92-C92
86	C1	3405	T1C	C92-C91-N9-C9
86	C1	3405	T1C	C3-C4-N4-C43
86	C1	3405	T1C	C1-C2-C21-O21
86	C1	3405	T1C	C1-C2-C21-N21
86	C1	3406	T1C	C92-C91-N9-C9
86	C1	3406	T1C	C41-C4-N4-C42
86	C1	3406	T1C	C1-C2-C21-O21
86	C1	3406	T1C	C1-C2-C21-N21
86	C1	3404	T1C	O91-C91-N9-C9
86	C1	3406	T1C	O91-C91-N9-C9
86	C1	3402	T1C	O91-C91-N9-C9
86	C1	3405	T1C	C96-C93-N92-C92
86	C1	3405	T1C	O91-C91-N9-C9
86	C1	3404	T1C	C10-C9-N9-C91
86	C1	3401	T1C	C10-C9-N9-C91
88	CD	902	GDP	C3'-C4'-C5'-O5'
86	C1	3406	T1C	N9-C91-C92-N92
86	C1	3404	T1C	O91-C91-C92-N92
86	C1	3406	T1C	O91-C91-C92-N92
86	C1	3404	T1C	C8-C9-N9-C91
86	C1	3401	T1C	C8-C9-N9-C91
86	C1	3404	T1C	N9-C91-C92-N92
86	C1	3402	T1C	O91-C91-C92-N92
86	C1	3402	T1C	N9-C91-C92-N92
88	CD	902	GDP	O4'-C4'-C5'-O5'
86	C1	3403	T1C	N9-C91-C92-N92
86	C1	3401	T1C	C91-C92-N92-C93
86	C1	3402	T1C	C91-C92-N92-C93
86	C1	3405	T1C	C91-C92-N92-C93
86	C1	3406	T1C	C91-C92-N92-C93
86	C1	3403	T1C	O91-C91-C92-N92
86	C1	3405	T1C	C41-C4-N4-C43

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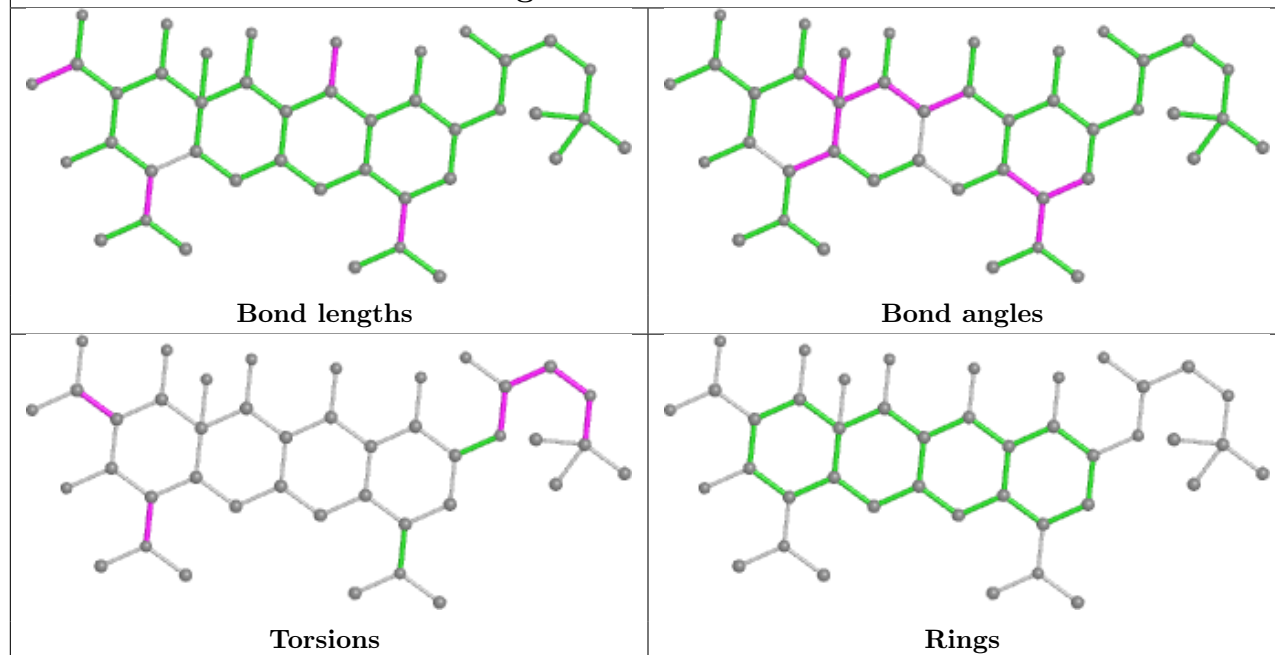
Mol	Chain	Res	Type	Atoms
86	C1	3405	T1C	C41-C4-N4-C42
86	C1	3405	T1C	C3-C4-N4-C42
86	C1	3406	T1C	C3-C4-N4-C43
86	C1	3401	T1C	C3-C2-C21-N21
86	C1	3404	T1C	C3-C2-C21-N21
86	C1	3406	T1C	C3-C2-C21-N21
86	C1	3405	T1C	O91-C91-C92-N92
86	C1	3401	T1C	C3-C2-C21-O21
86	C1	3402	T1C	C3-C2-C21-O21
86	C1	3404	T1C	C3-C2-C21-O21
86	C1	3406	T1C	C3-C2-C21-O21
86	C1	3405	T1C	N9-C91-C92-N92
86	C1	3402	T1C	C95-C93-N92-C92
86	C1	3406	T1C	C61-C7-N7-C72
86	C1	3403	T1C	C91-C92-N92-C93
86	C1	3406	T1C	C61-C7-N7-C71
88	CD	902	GDP	C5'-O5'-PA-O3A
86	C1	3402	T1C	C96-C93-N92-C92
86	C1	3402	T1C	C61-C7-N7-C71
86	C1	3402	T1C	C61-C7-N7-C72
86	C1	3404	T1C	C41-C4-N4-C43
86	C1	3404	T1C	C41-C4-N4-C42
86	C1	3402	T1C	C3-C2-C21-N21
86	C1	3403	T1C	C3-C2-C21-N21
86	C1	3405	T1C	C3-C2-C21-N21
86	C1	3403	T1C	C3-C2-C21-O21
86	C1	3405	T1C	C3-C2-C21-O21

There are no ring outliers.

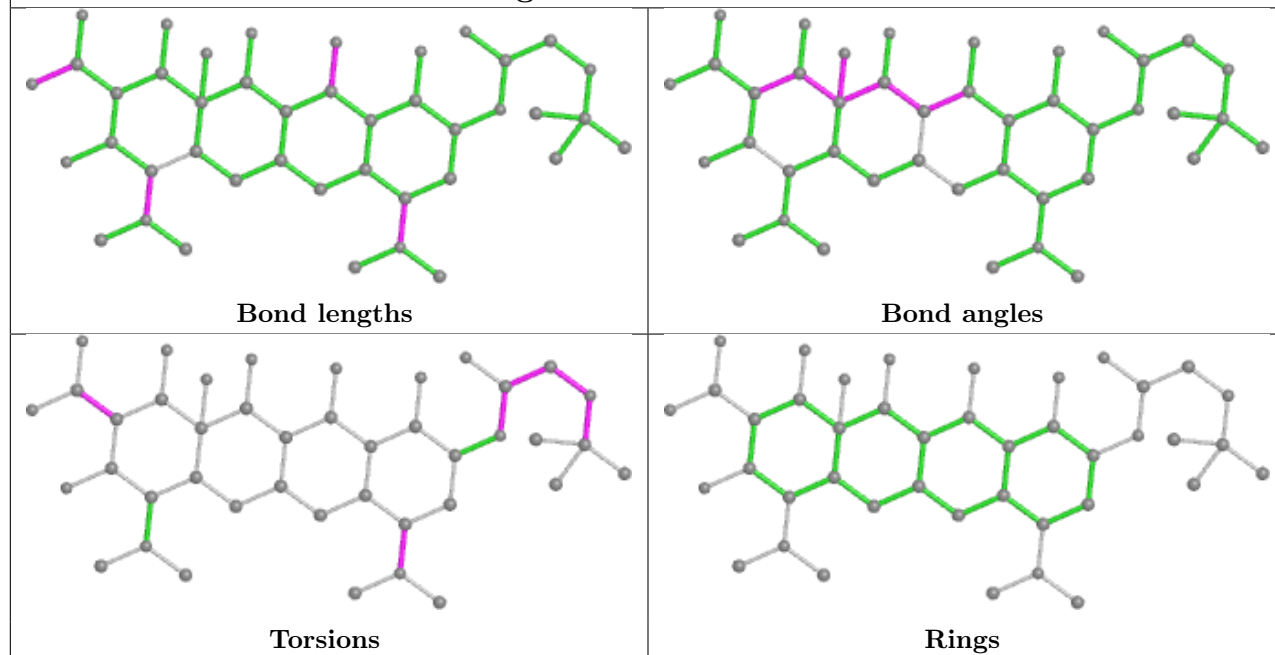
No monomer is involved in short contacts.

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.

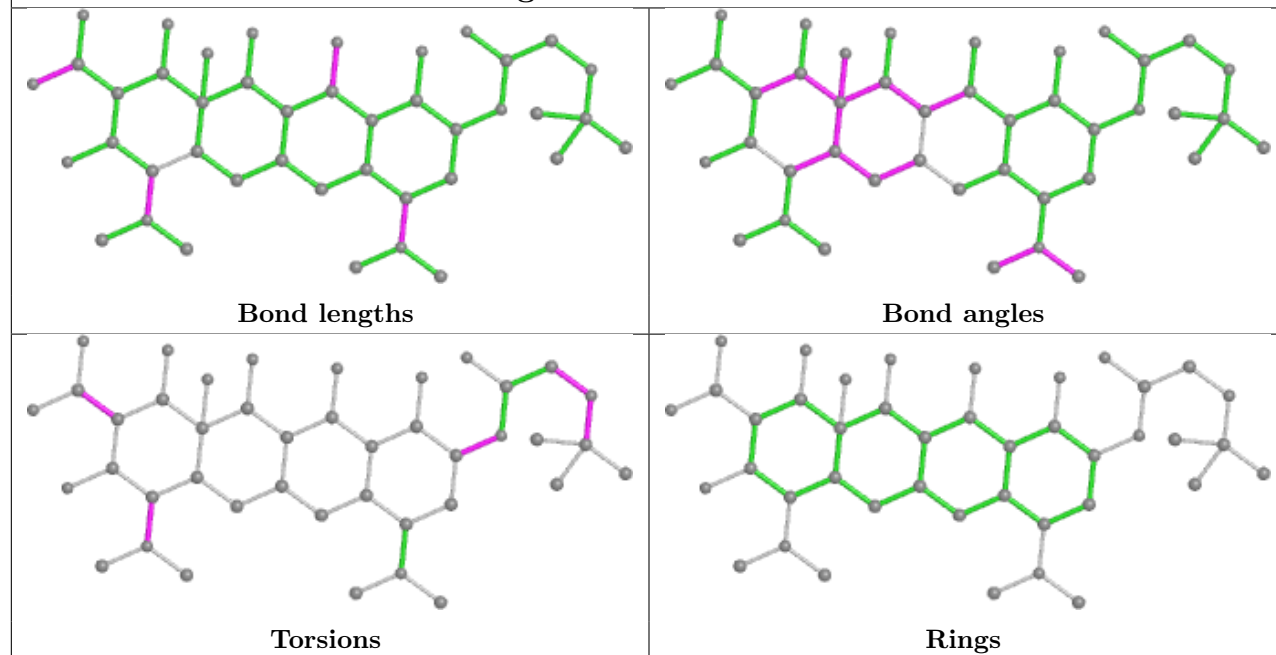
## Ligand T1C C1 3405



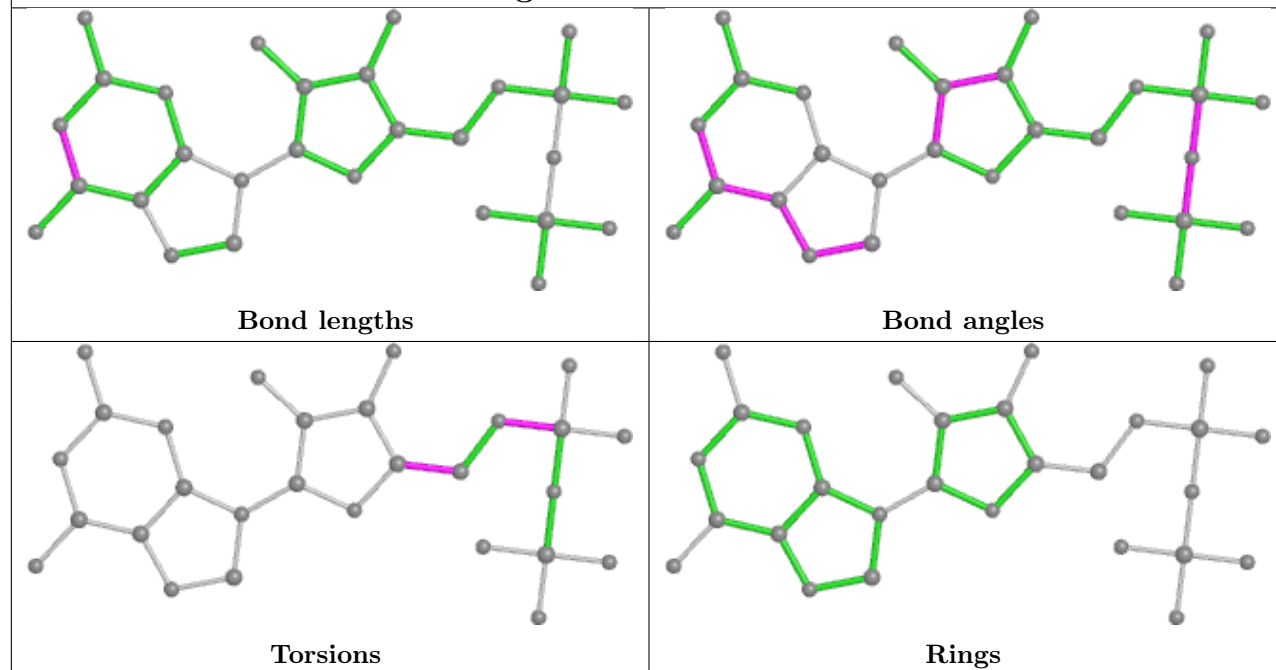
## Ligand T1C C1 3402



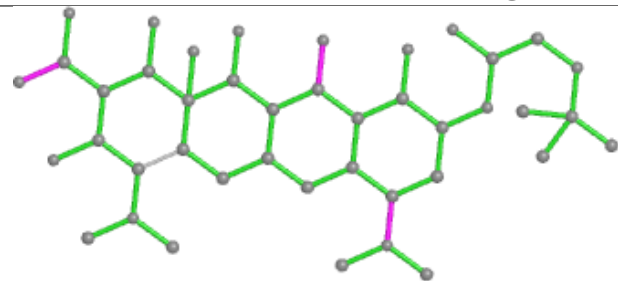
## Ligand T1C C1 3401



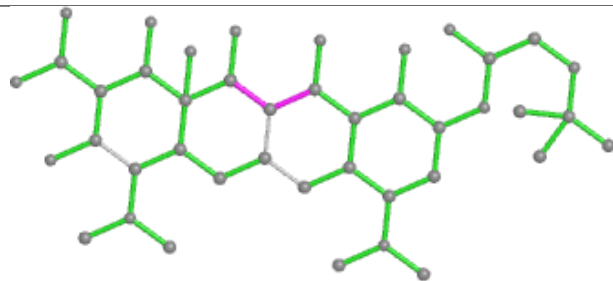
## Ligand GDP CD 902



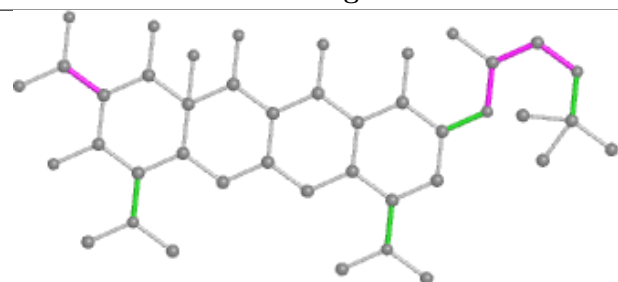
## Ligand T1C C1 3403



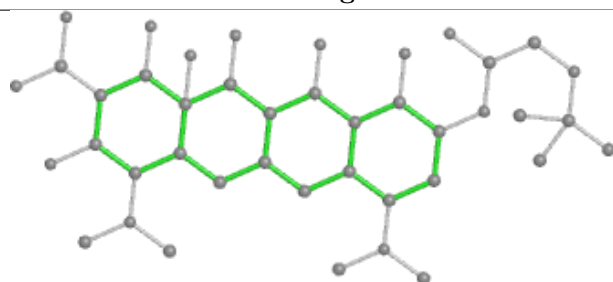
Bond lengths



Bond angles

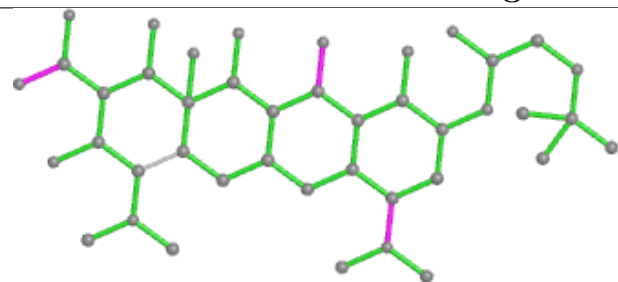


Torsions

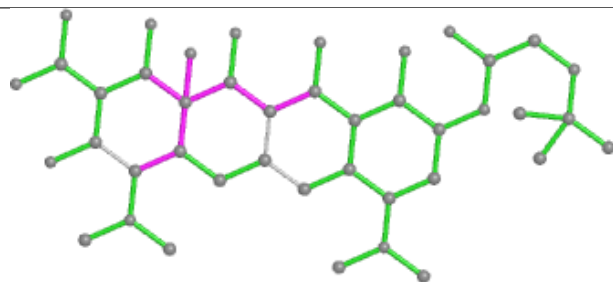


Rings

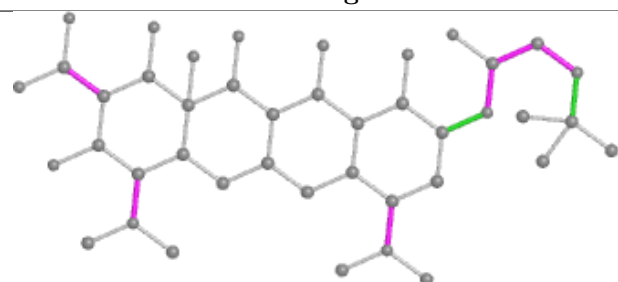
## Ligand T1C C1 3406



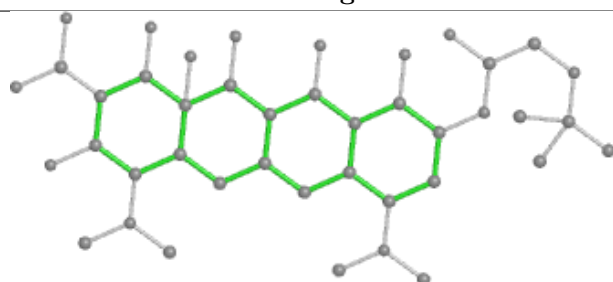
Bond lengths



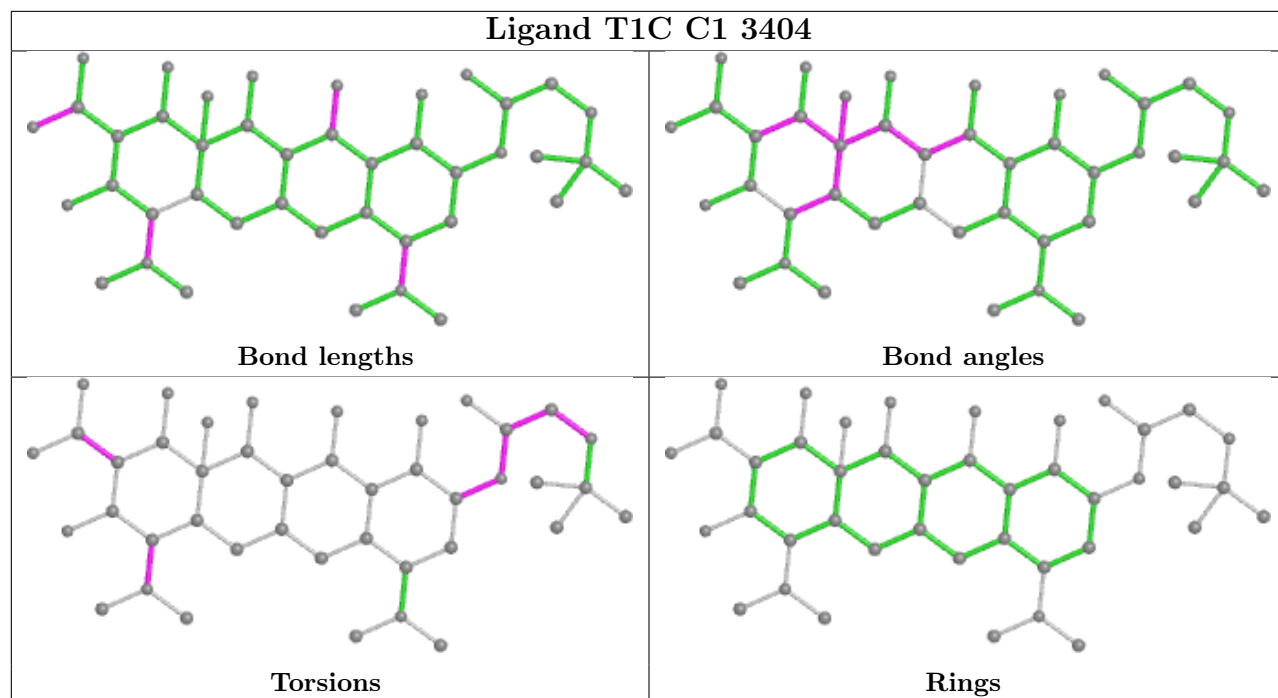
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

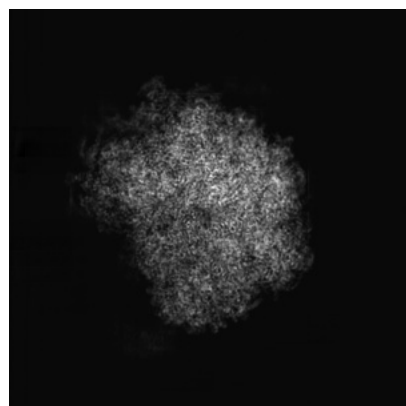
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36839. These allow visual inspection of the internal detail of the map and identification of artifacts.

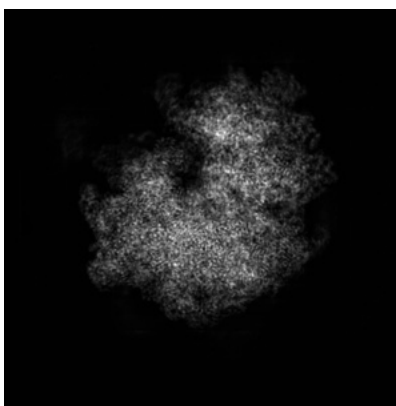
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

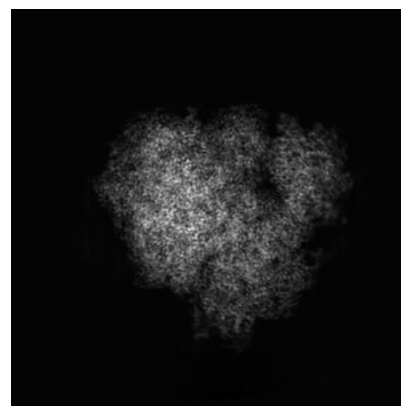
#### 6.1.1 Primary map



X

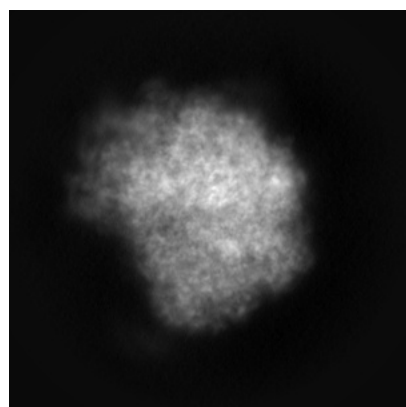


Y

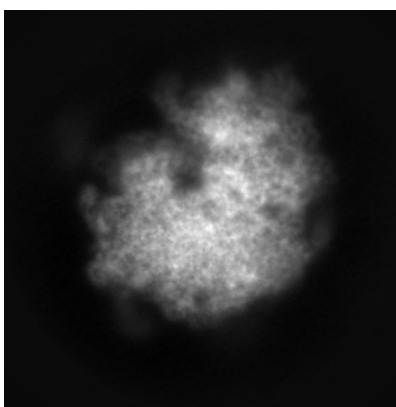


Z

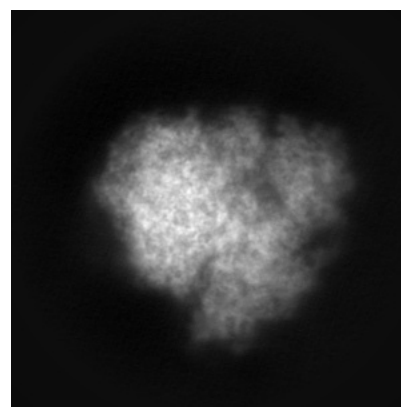
#### 6.1.2 Raw map



X



Y

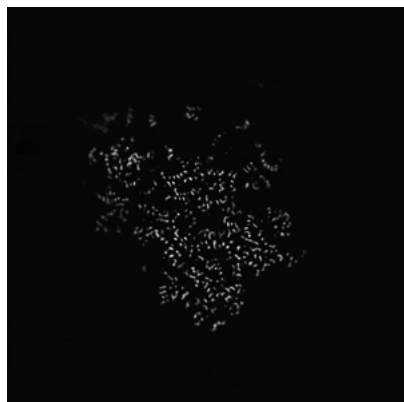


Z

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

## 6.2 Central slices [i](#)

### 6.2.1 Primary map



X Index: 240

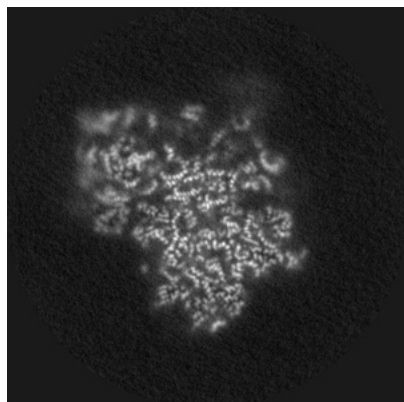


Y Index: 240

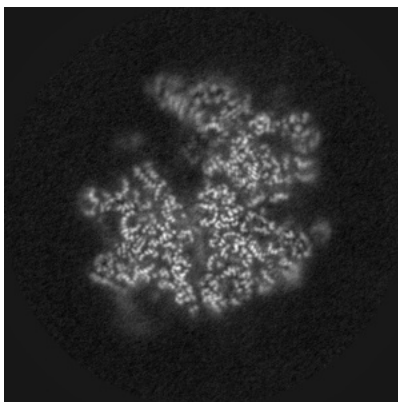


Z Index: 240

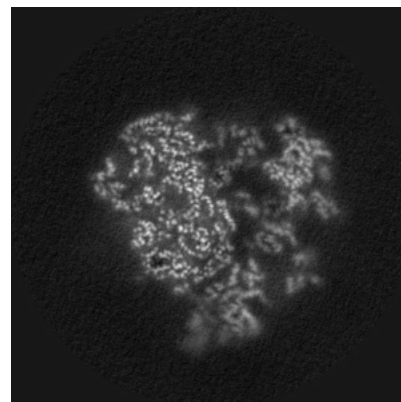
### 6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

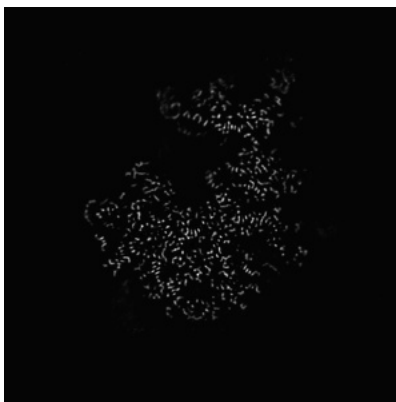
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 215

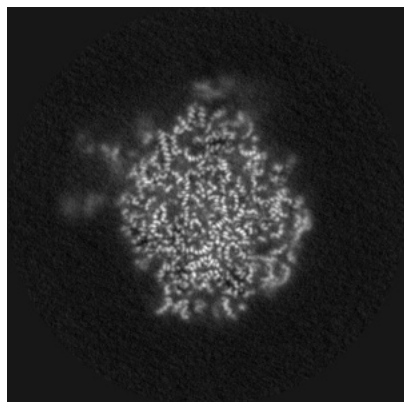


Y Index: 257

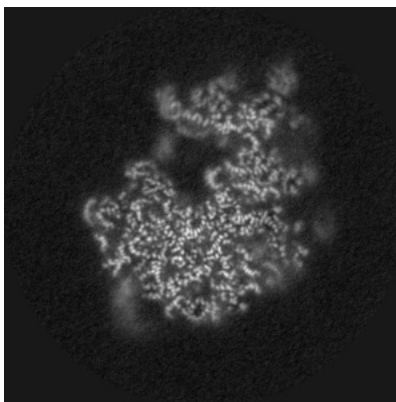


Z Index: 273

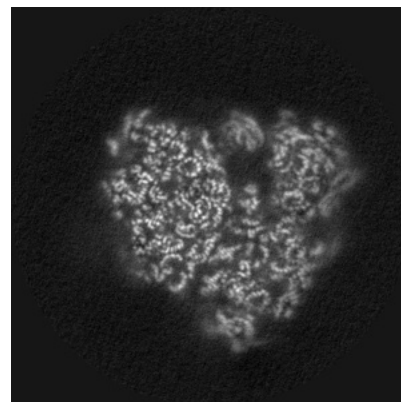
### 6.3.2 Raw map



X Index: 214



Y Index: 257



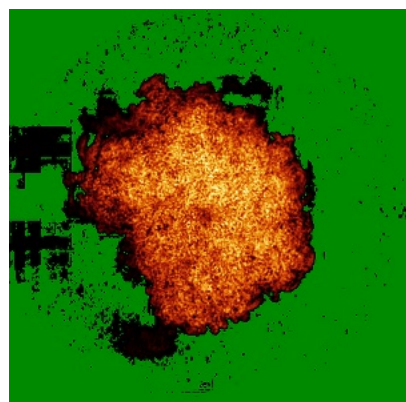
Z Index: 268

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

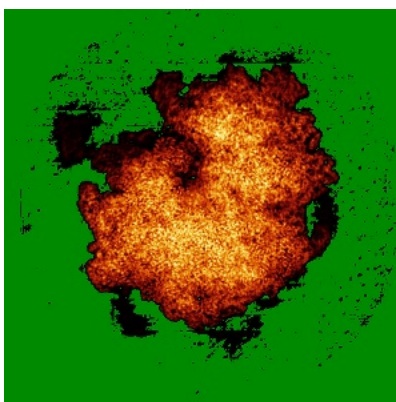


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

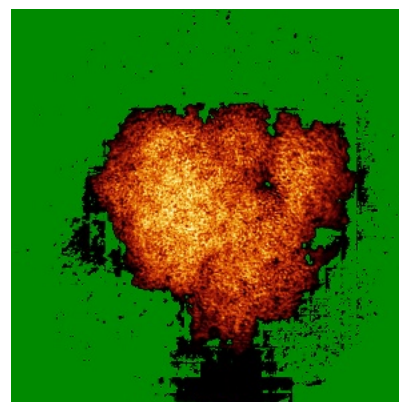
### 6.4.1 Primary map



X

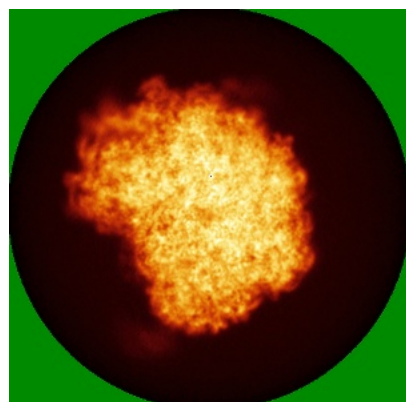


Y

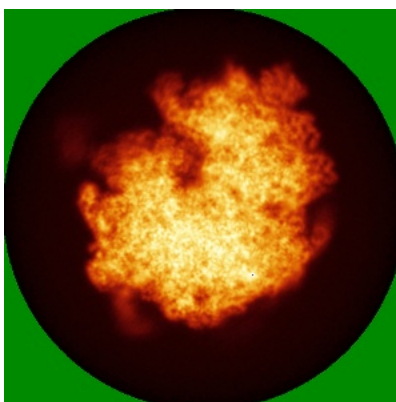


Z

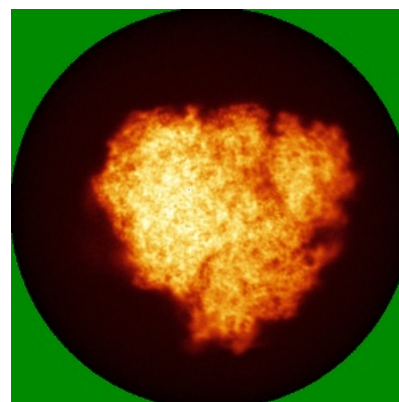
### 6.4.2 Raw map



X



Y

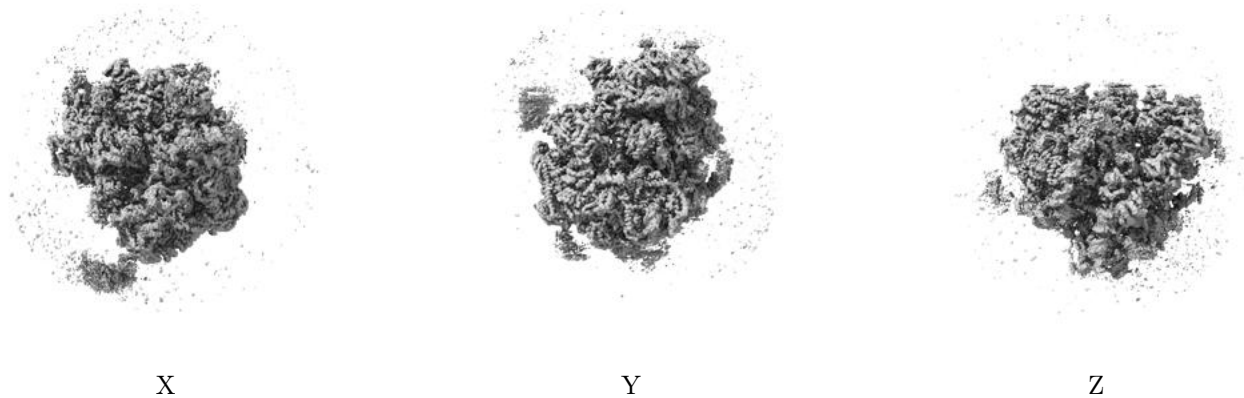


Z

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.

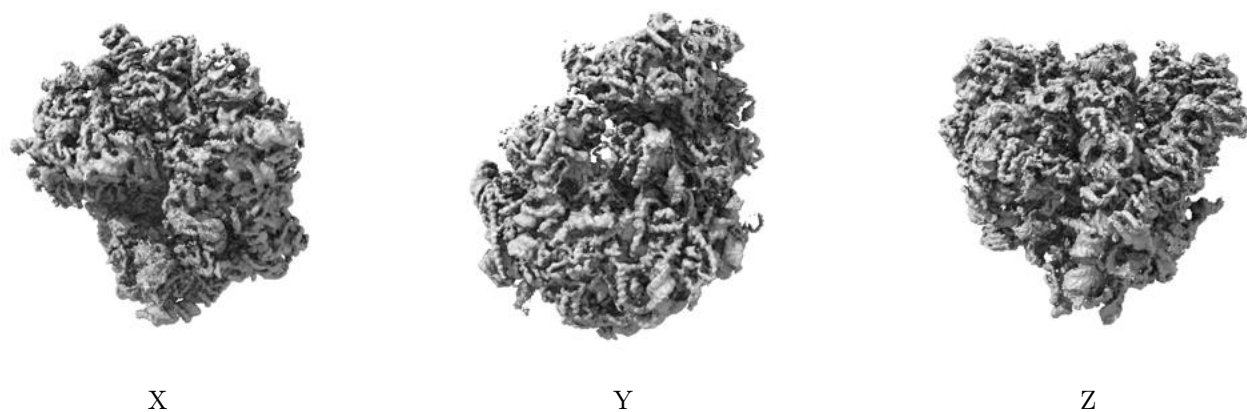
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

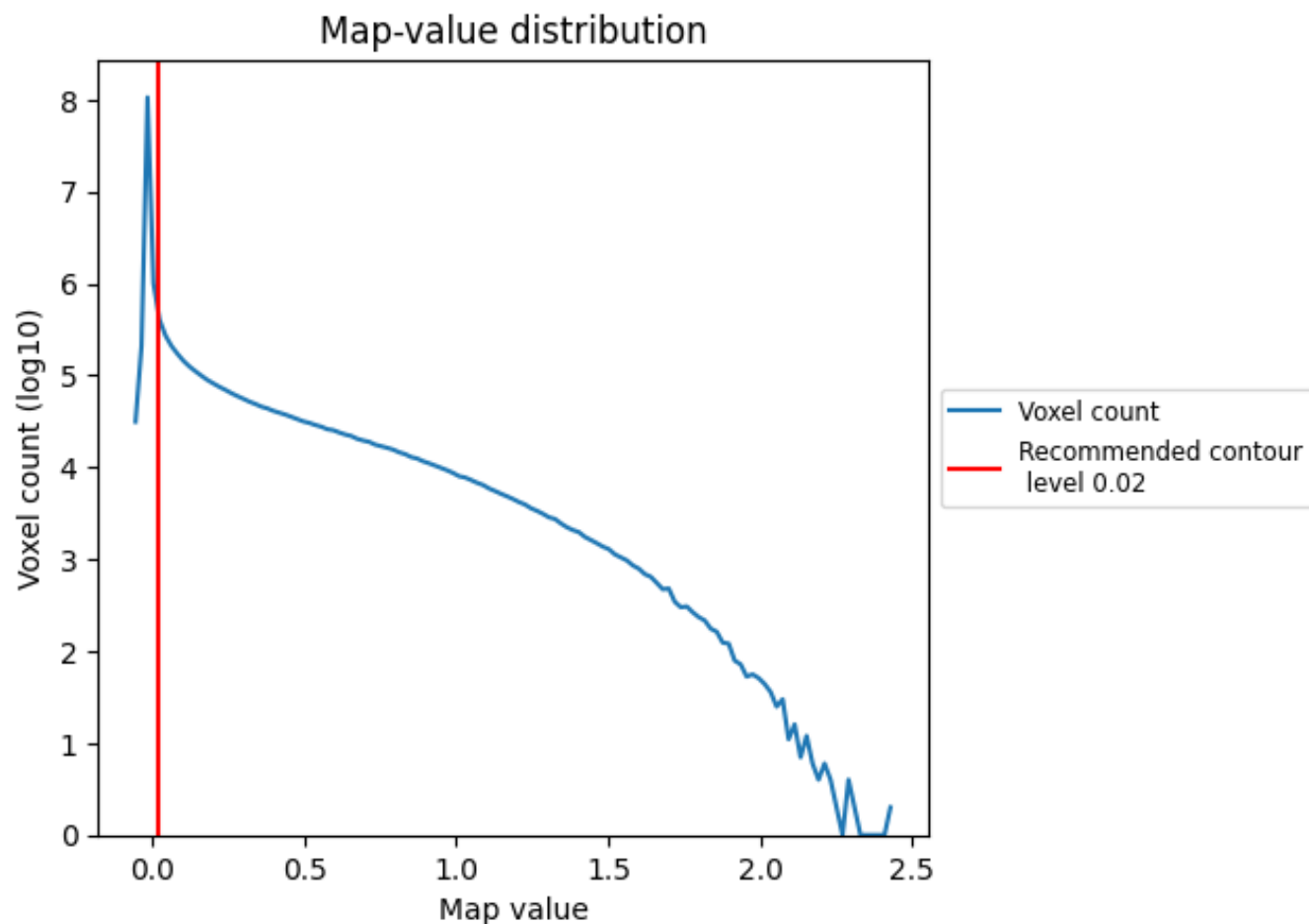
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

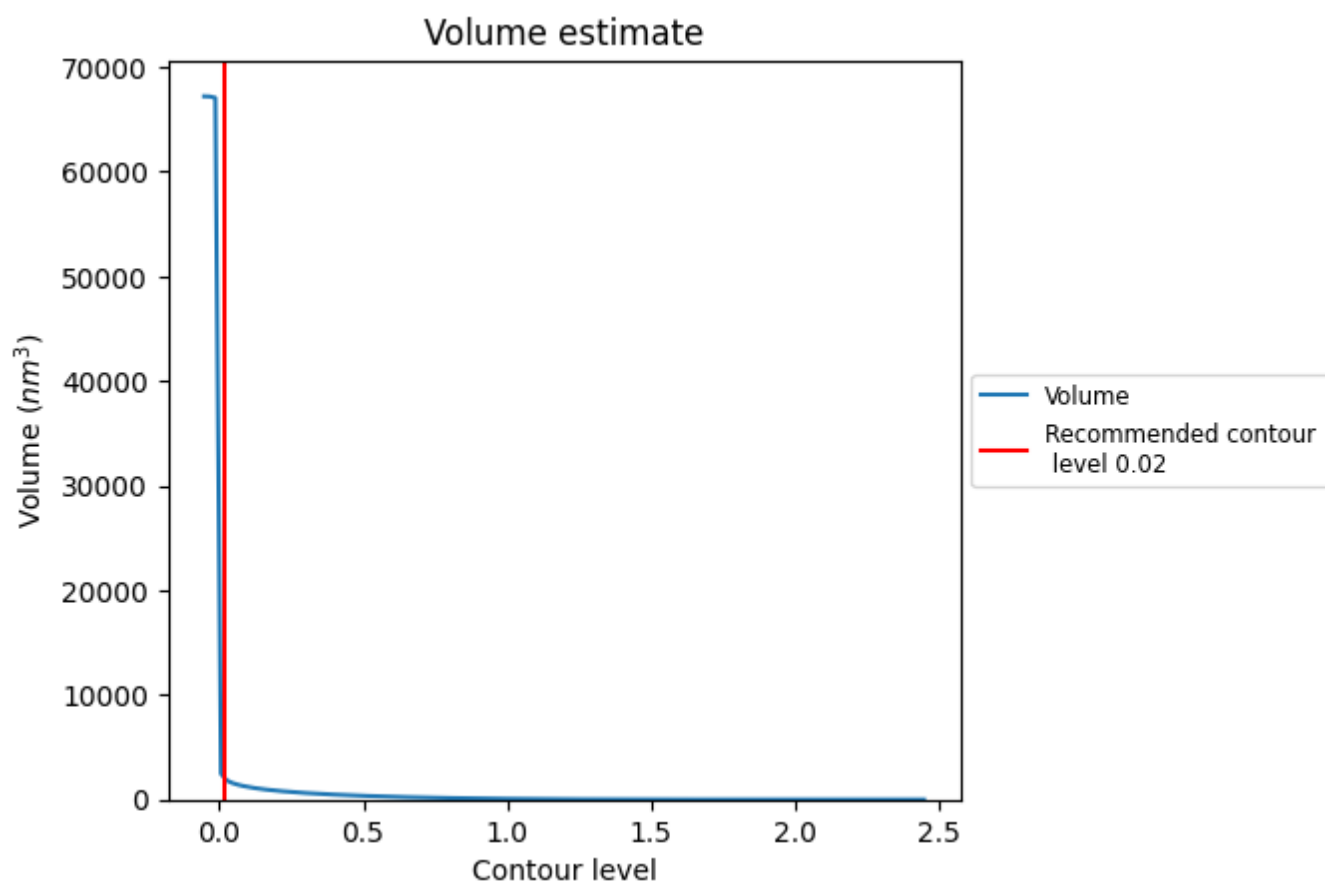
This section contains the results of statistical analysis of the map.

### 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.

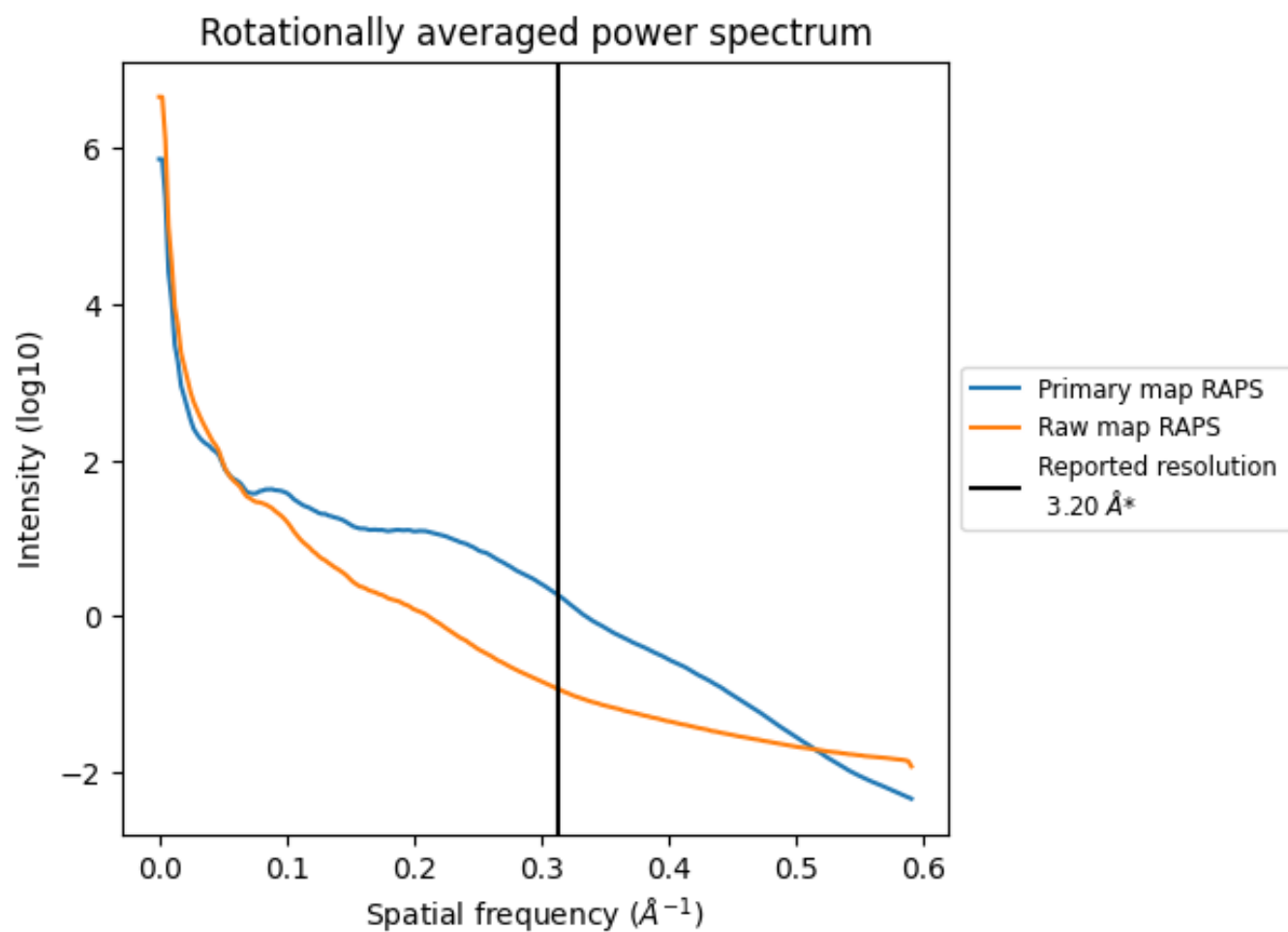
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2009 nm<sup>3</sup>; this corresponds to an approximate mass of 1814 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 ⓘ

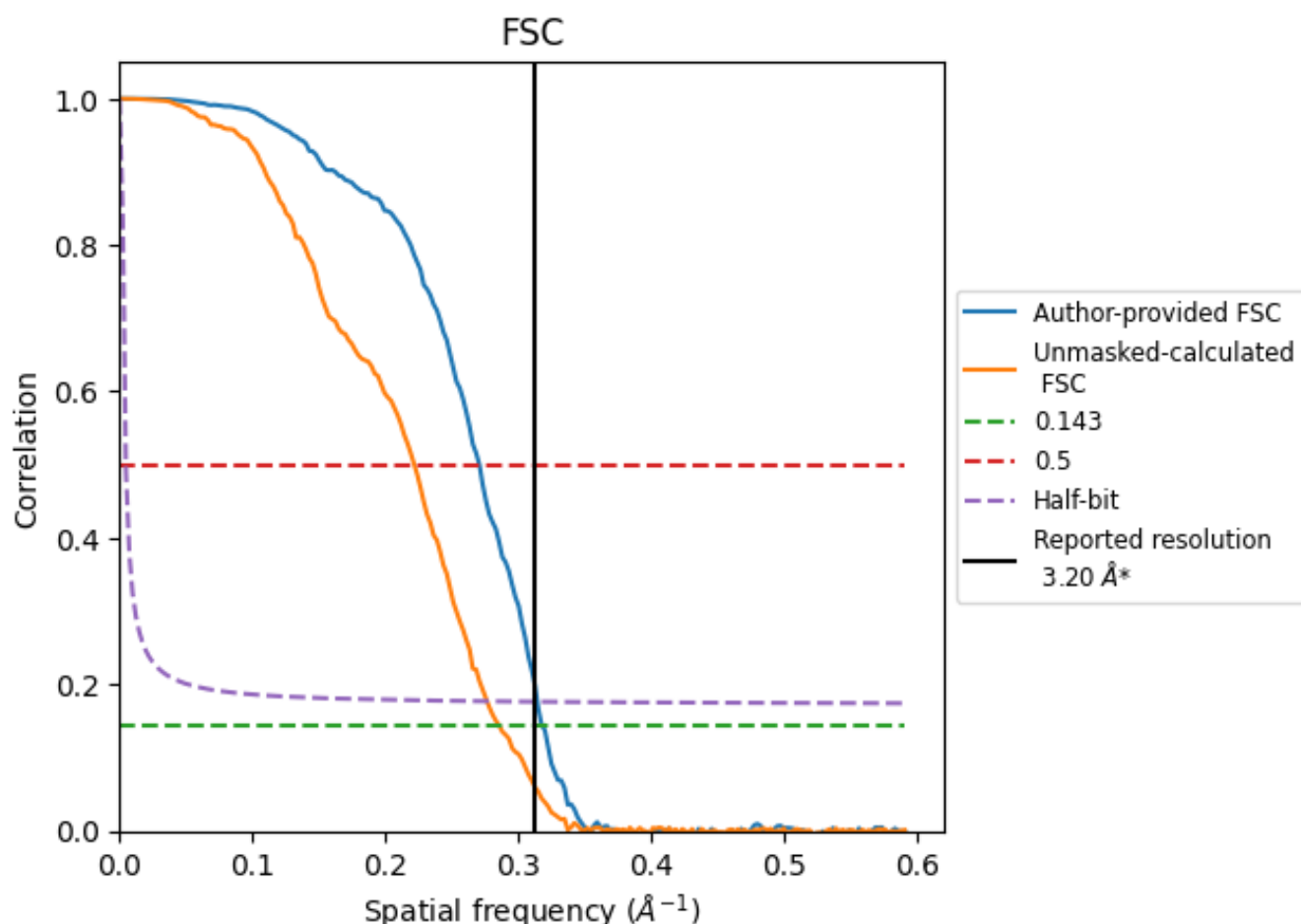


\*Reported resolution corresponds to spatial frequency of  $0.312 \text{ \AA}^{-1}$

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

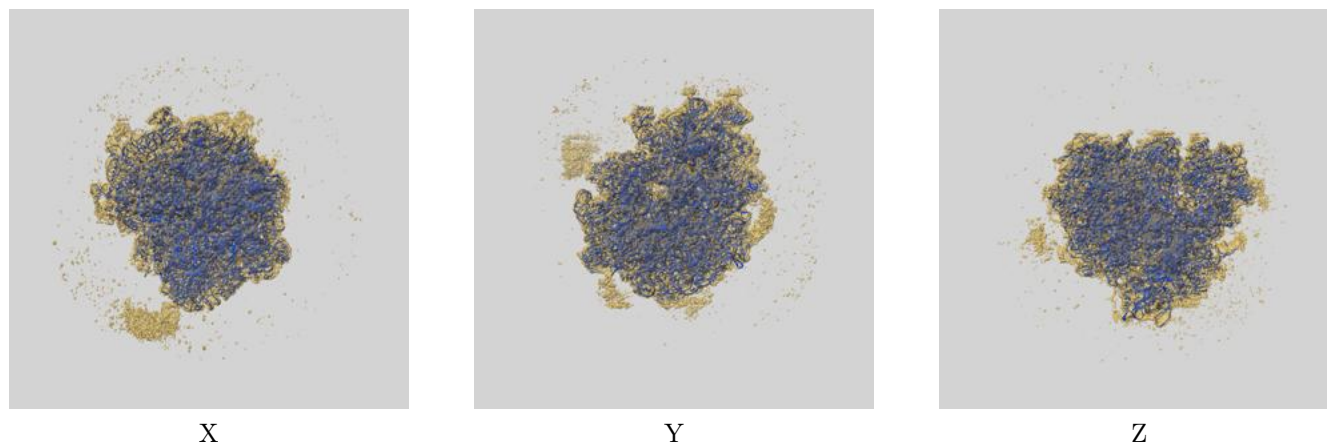
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.70	3.18
Unmasked-calculated*	3.50	4.51	3.62

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

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

This section contains information regarding the fit between EMDB map EMD-36839 and PDB model 8K2D. Per-residue inclusion information can be found in [section 3](#) on [page 22](#).

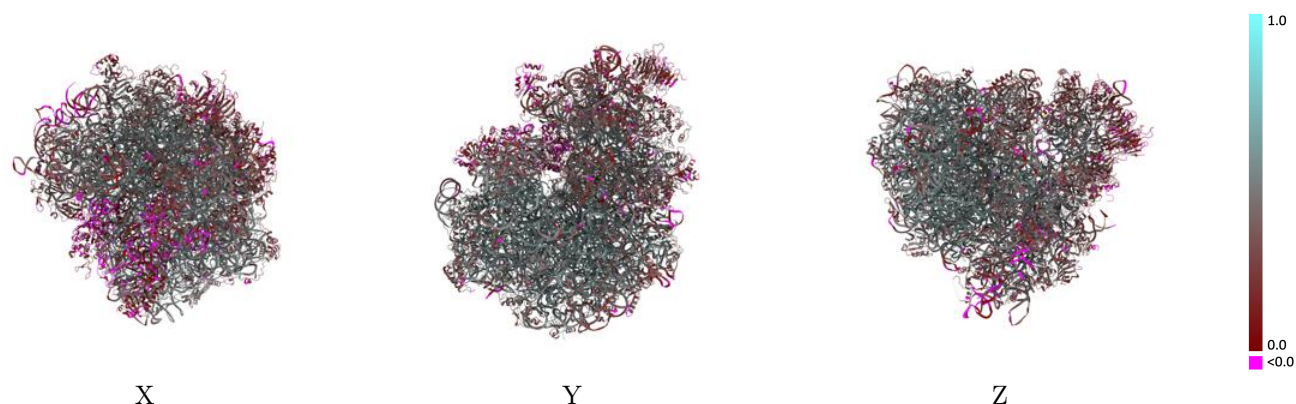
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

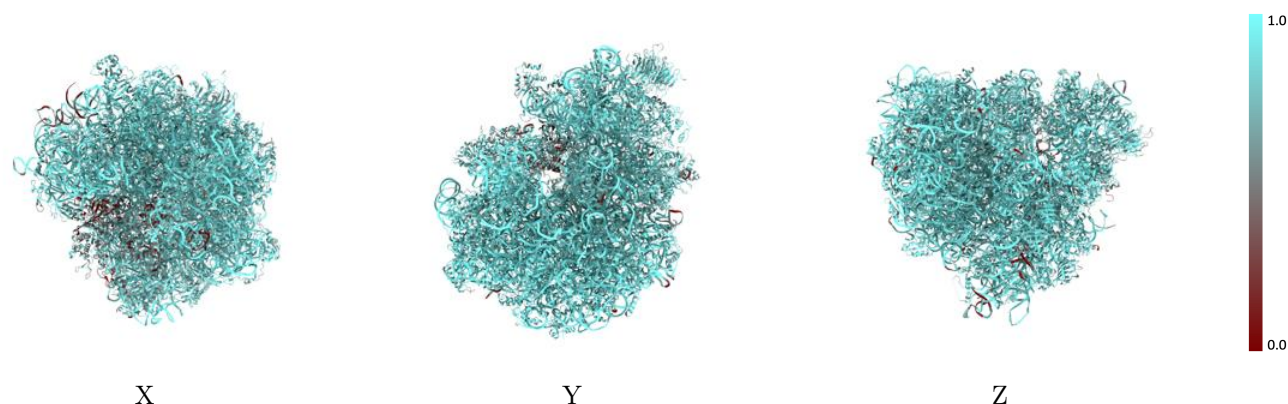


## 9.2 Q-score mapped to coordinate model [i](#)



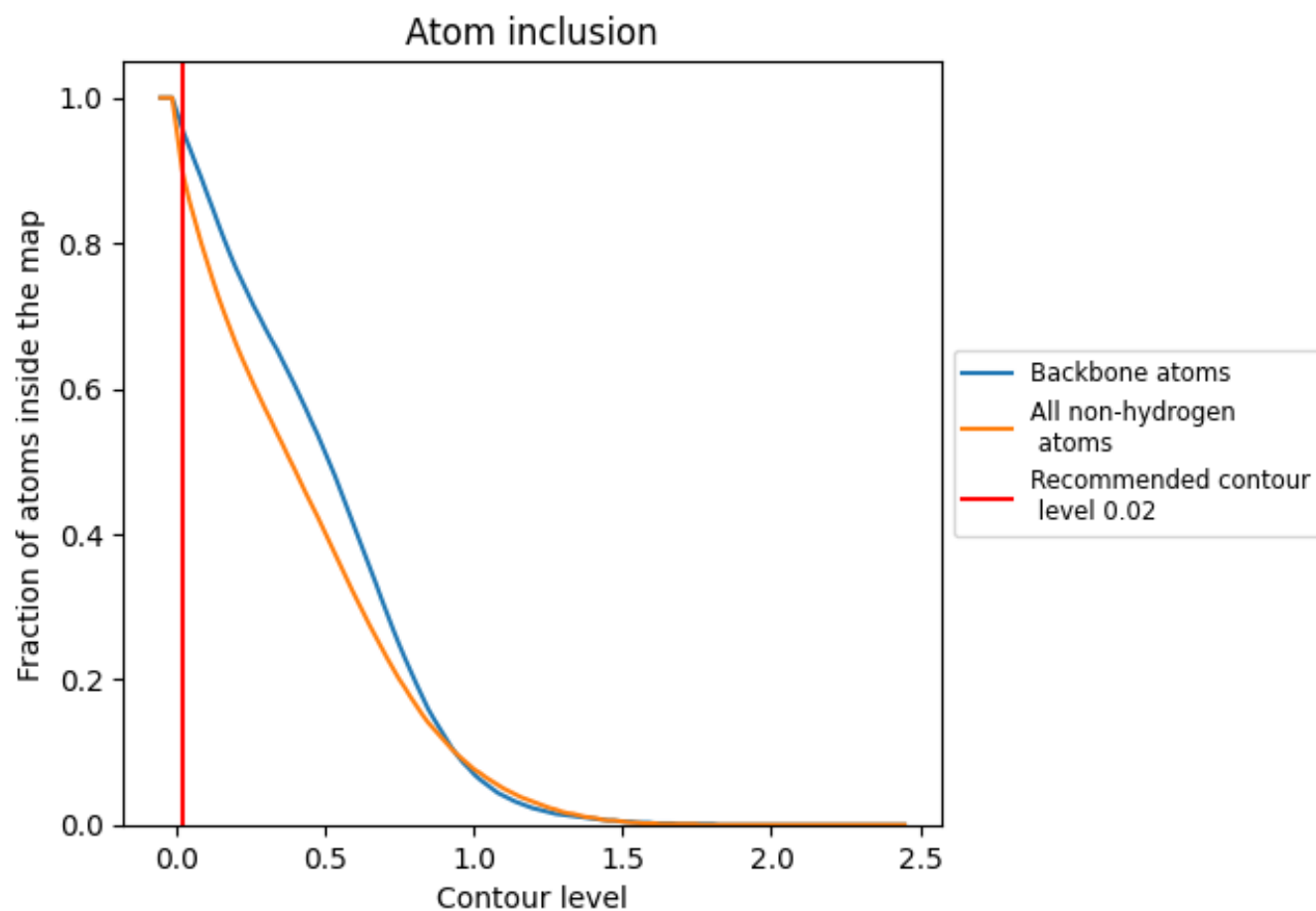
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9000	 0.4230
C1	 0.9620	 0.5020
C2	 0.9420	 0.4350
C3	 0.9710	 0.5150
C4	 0.9860	 0.5090
CD	 0.4440	 0.0840
CE	 0.8360	 0.3830
CS	 0.7520	 0.2870
L1	 0.8120	 0.3130
LA	 0.9230	 0.4870
LB	 0.9210	 0.4770
LC	 0.9180	 0.4430
LD	 0.8600	 0.3730
LE	 0.8800	 0.4040
LF	 0.9230	 0.4680
LG	 0.8900	 0.3810
LH	 0.8950	 0.4250
LI	 0.8790	 0.4210
LJ	 0.8710	 0.3800
LK	 0.5530	 0.0950
LL	 0.8960	 0.4120
LM	 0.9060	 0.4350
LN	 0.9420	 0.5080
LO	 0.9290	 0.4850
LP	 0.9130	 0.4790
LQ	 0.9180	 0.4610
LR	 0.9230	 0.4750
LS	 0.9190	 0.4660
LT	 0.9040	 0.4640
LU	 0.8670	 0.3870
LV	 0.9040	 0.4670
LW	 0.9010	 0.4500
LX	 0.8910	 0.4410
LY	 0.8850	 0.4330
LZ	 0.8970	 0.4020



















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Chain	Atom inclusion	Q-score
La	 0.9290	 0.4640
Lb	 0.8580	 0.4070
Lc	 0.8600	 0.4080
Ld	 0.8540	 0.4350
Le	 0.9000	 0.4730
Lf	 0.9430	 0.5020
Lg	 0.9100	 0.4730
Lh	 0.8680	 0.4160
Li	 0.8590	 0.3880
Lj	 0.9540	 0.5330
Lk	 0.8590	 0.3490
Ll	 0.9160	 0.4700
Lm	 0.8810	 0.4510
Ln	 0.6840	 0.3370
Lo	 0.8720	 0.4510
Lp	 0.9060	 0.4630
P0	 0.5980	 0.1070
SA	 0.9010	 0.3580
SB	 0.8390	 0.3260
SC	 0.8940	 0.4070
SD	 0.8300	 0.3090
SE	 0.8760	 0.3740
SF	 0.8050	 0.2530
SG	 0.7980	 0.2840
SH	 0.8310	 0.2840
SI	 0.8710	 0.3860
SJ	 0.8450	 0.3470
SK	 0.8350	 0.2590
SL	 0.8710	 0.4210
SM	 0.6440	 0.0520
SN	 0.8800	 0.3890
SO	 0.8720	 0.3790
SP	 0.8410	 0.2920
SQ	 0.8480	 0.2960
SR	 0.8280	 0.2760
SS	 0.8530	 0.2990
ST	 0.8320	 0.2860
SU	 0.8430	 0.2770
SV	 0.8780	 0.3650
SW	 0.9220	 0.4620
SX	 0.8850	 0.4200
SY	 0.8000	 0.3060

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Chain	Atom inclusion	Q-score
SZ	 0.8080	 0.2260
Sa	 0.9040	 0.4240
Sb	 0.8990	 0.3820
Sc	 0.7900	 0.2750
Sd	 0.9050	 0.4130
Se	 0.7230	 0.2750
Sf	 0.6430	 0.0470
Sg	 0.8050	 0.1970