



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 09:49 AM EDT

PDB ID : 7UQB / pdb_00007uqb
EMDB ID : EMD-26686
Title : Nucleoplasmic pre-60S intermediate of the Nog2 containing pre-rotation state from a SPB1-D52A strain with AIF4
Authors : Sekulski, K.; Cruz, V.E.; Weirich, C.S.; Erzberger, J.P.
Deposited on : 2022-04-19
Resolution : 2.43 Å(reported)
Based on initial model : 3JCT

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

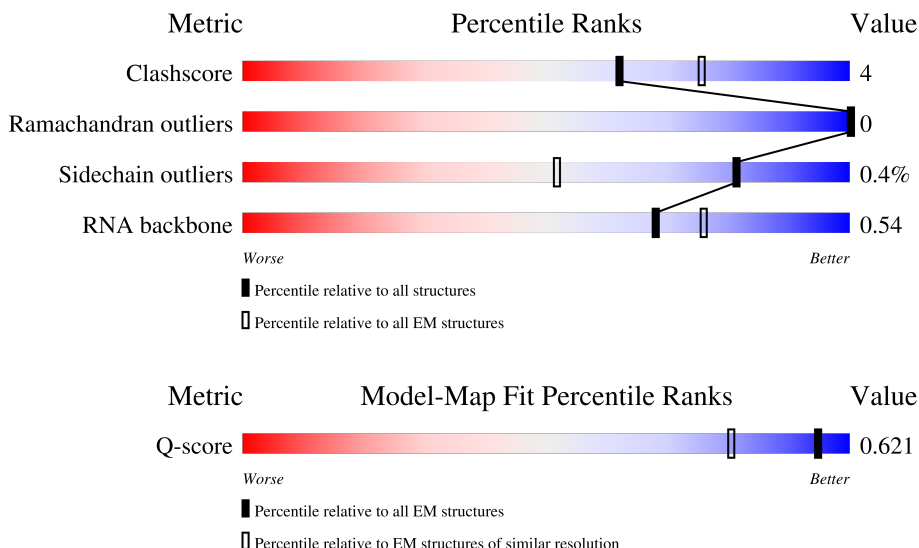
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.43 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5787 (1.94 - 2.93)

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

Mol	Chain	Length	Quality of chain
1	A	254	
2	1	3396	
3	2	158	

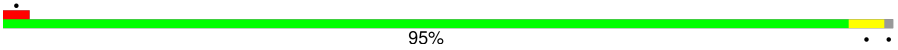
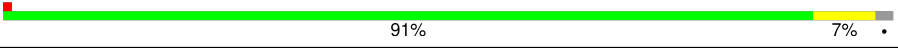
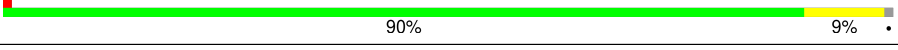
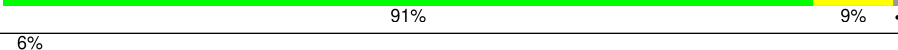
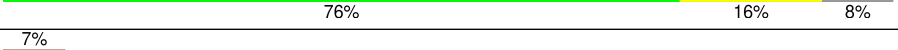
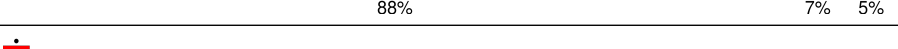
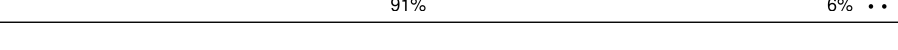
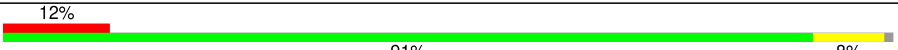
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Mol	Chain	Length	Quality of chain
4	3	121	
5	5	120	
6	6	74	
7	8	165	
8	9	175	
9	B	387	
10	C	362	
11	D	297	
12	E	176	
13	F	244	
14	G	256	
15	H	191	
16	I	166	
17	J	174	
18	K	376	
19	L	199	
20	M	138	
21	N	204	
22	O	199	
23	P	184	
24	Q	186	
25	R	189	
26	S	172	
27	T	160	
28	U	121	

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Mol	Chain	Length	Quality of chain
29	V	137	
30	W	236	
31	X	142	
32	Y	127	
33	Z	136	
34	a	149	
35	b	647	
36	c	105	
37	d	113	
38	e	130	
39	f	107	
40	g	121	
41	h	120	
42	i	100	
43	j	88	
44	k	78	
45	l	51	
46	m	486	
47	n	605	
48	o	220	
49	p	92	
50	q	455	
51	r	261	
52	s	77	
53	t	322	

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Mol	Chain	Length	Quality of chain
54	u	199	
55	v	344	
56	w	201	
57	x	514	
58	y	245	
59	z	106	
60	4	593	

2 Entry composition

There are 67 unique types of molecules in this entry. The entry contains 157949 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	213	Total	C	N	O	S	0	0
			1634	1023	326	284	1		

- Molecule 2 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	2991	Total	C	N	O	P	0	0
			64042	28618	11563	20870	2991		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 5 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	73	Total	C	N	O	S	0	0
			645	395	133	114	3		

- Molecule 6 is a RNA chain called ITS2 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	58	Total	C	N	O	P	0	0
			1227	550	210	409	58		

- Molecule 7 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	158	Total	C	N	O	S	0	0
			1196	750	216	228	2		

- Molecule 8 is a protein called Ribosome biogenesis protein ALB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	118	Total	C	N	O		0	0
			937	590	181	166			

- Molecule 9 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 10 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 11 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	270	Total	C	N	O	S	0	0
			2180	1379	382	417	2		

- Molecule 12 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	155	Total	C	N	O	S	0	0
			1230	795	221	213	1		

- Molecule 13 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	219	Total	C	N	O	S	0	0
			1761	1138	320	302	1		

- Molecule 14 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	224	Total	C	N	O	S	0	0
			1753	1122	314	314	3		

- Molecule 15 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 16 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	131	Total	C	N	O	S	0	0
			1059	662	195	198	4		

- Molecule 17 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	171	Total	C	N	O	S	0	0
			1368	856	256	252	4		

- Molecule 18 is a protein called Proteasome-interacting protein CIC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	268	Total	C	N	O	S	0	0
			2155	1387	355	409	4		

- Molecule 19 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	180	Total	C	N	O	S	0	0
			1438	892	296	250			

- Molecule 20 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 21 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	189	Total	C	N	O	S	0	0
			1620	1016	342	261	1		

- Molecule 22 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	175	Total	C	N	O		0	0
			1388	862	277	249			

- Molecule 24 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	147	Total	C	N	O	S	0	0
			1136	718	219	198	1		

- Molecule 25 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	156	Total	C	N	O		0	0
			1258	781	265	212			

- Molecule 26 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 27 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	114	Total	C	N	O	S	0	0
			905	568	175	159	3		

- Molecule 28 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	106	Total	C	N	O	0	0
			844	545	138	161		

- Molecule 29 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 30 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	234	Total	C	N	O	S	0	0
			1888	1194	323	365	6		

- Molecule 31 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	139	Total	C	N	O	S	0	0
			1088	697	194	195	2		

- Molecule 32 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 33 is a protein called 60S ribosomal protein L27-A.

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

- Molecule 34 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	92	Total	C	N	O	S	0	0
			731	477	129	124	1		

- Molecule 35 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	642	Total	C	N	O	S	0	0
			5185	3251	938	970	26		

- Molecule 36 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 37 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	107	Total	C	N	O	S	0	0
			873	553	165	154	1		

- Molecule 38 is a protein called 60S ribosomal protein L32.

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

- Molecule 39 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 40 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	112	Total	C	N	O	S	0	0
			881	546	179	152	4		

- Molecule 41 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 42 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 43 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 44 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	77	Total	C	N	O	S	0	0
			612	391	115	106			

- Molecule 45 is a protein called 60S ribosomal protein L39.

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

- Molecule 46 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	466	Total	C	N	O	S	0	0
			3754	2372	681	691	10		

- Molecule 47 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	369	Total	C	N	O	S	0	0
			3014	1954	521	530	9		

- Molecule 48 is a protein called Ribosome biogenesis protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	133	Total	C	N	O	S	0	0
			1107	716	198	189	4		

- Molecule 49 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 50 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	156	Total	C	N	O	S	0	0
			1298	821	233	243	1		

- Molecule 51 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	230	Total	C	N	O	S	0	0
			1860	1177	352	324	7		

- Molecule 52 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	72	Total	C	N	O	S	0	0
			602	377	118	104	3		

- Molecule 53 is a protein called Ribosome biogenesis protein RLP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	287	Total	C	N	O	S	0	0
			2306	1459	427	417	3		

- Molecule 54 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	150	Total	C	N	O	S	0	0
			1265	793	253	210	9		

- Molecule 55 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	v	293	Total	C	N	O	S	0	0
			2366	1512	415	422	17		

- Molecule 56 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	w	194	Total	C	N	O	S	0	0
			1541	965	277	294	5		

- Molecule 57 is a protein called RSA4 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	x	504	Total	C	N	O	S	0	0
			3927	2468	695	743	21		

- Molecule 58 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	y	244	Total	C	N	O	S	0	0
			1849	1146	319	377	7		

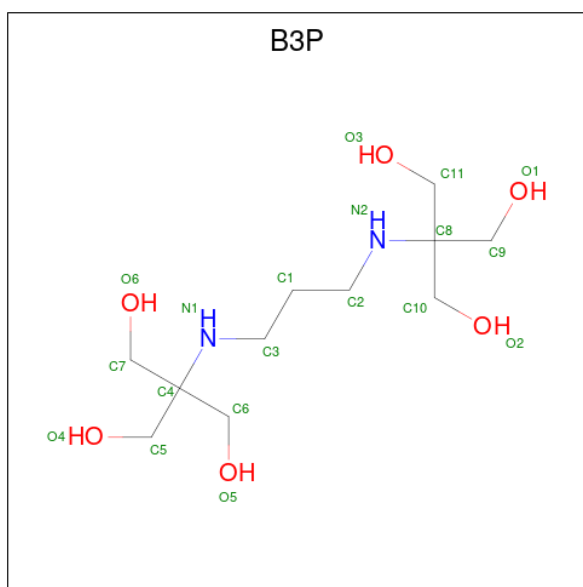
- Molecule 59 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	z	87	Total	C	N	O	S	0	0
			714	444	142	127	1		

- Molecule 60 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	4	538	Total	C	N	O	S	0	0
			4166	2633	718	800	15		

- Molecule 61 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: B3P) (formula: C₁₁H₂₆N₂O₆).



Mol	Chain	Residues	Atoms				AltConf
61	1	1	Total	C	N	O	0
			19	11	2	6	
61	1	1	Total	C	N	O	0
			19	11	2	6	
61	1	1	Total	C	N	O	0
			19	11	2	6	

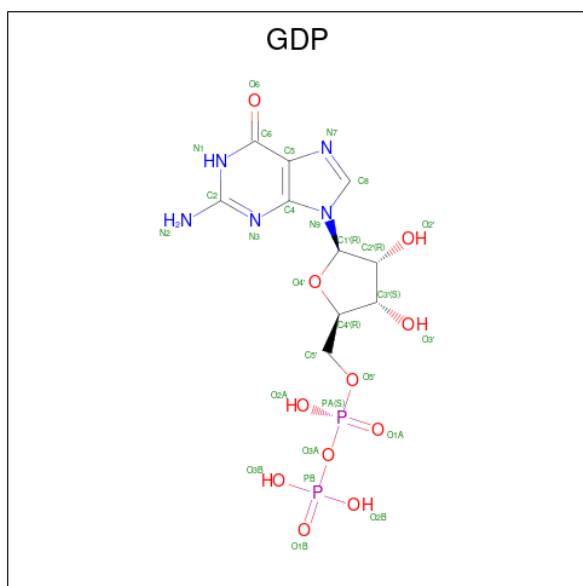
- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	1	76	Total	Mg	0
			76	76	
62	2	1	Total	Mg	0
			1	1	
62	R	1	Total	Mg	0
			1	1	
62	V	1	Total	Mg	0
			1	1	
62	b	1	Total	Mg	0
			1	1	
62	m	1	Total	Mg	0
			1	1	

- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn).

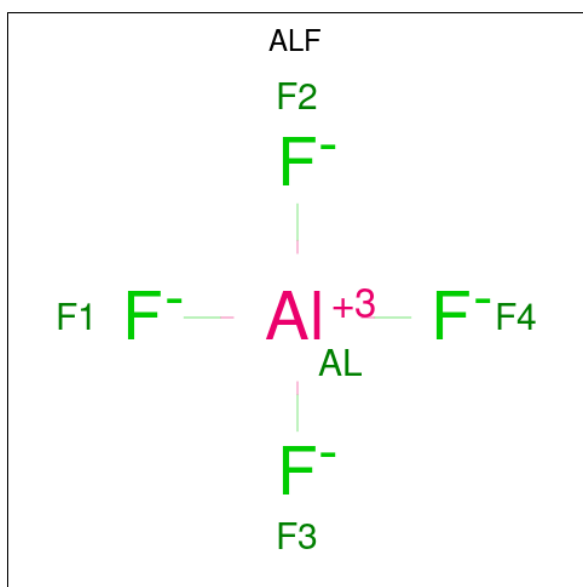
Mol	Chain	Residues	Atoms		AltConf
63	I	1	Total	Zn	0
			1	1	
63	g	1	Total	Zn	0
			1	1	
63	j	1	Total	Zn	0
			1	1	
63	p	1	Total	Zn	0
			1	1	
63	u	1	Total	Zn	0
			1	1	

- Molecule 64 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
64	b	1	Total	C	N	O	P	0
			28	10	5	11	2	
64	m	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 65 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
65	m	1	Total	Al	F	0
			5	1	4	

- Molecule 66 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
66	m	1	Total	K	0
			1	1	

- Molecule 67 is water.

Mol	Chain	Residues	Atoms		AltConf
67	A	2	Total	O	0
			2	2	
67	1	340	Total	O	0
			340	340	
67	2	7	Total	O	0
			7	7	
67	B	2	Total	O	0
			2	2	
67	C	1	Total	O	0
			1	1	
67	F	3	Total	O	0
			3	3	
67	N	2	Total	O	0
			2	2	

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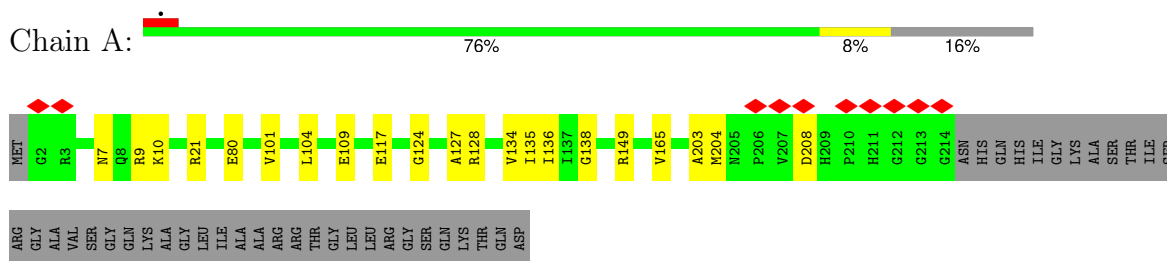
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Mol	Chain	Residues	Atoms		AltConf
67	O	1	Total 1	O 1	0
67	R	1	Total 1	O 1	0
67	V	3	Total 3	O 3	0
67	X	1	Total 1	O 1	0
67	b	3	Total 3	O 3	0
67	d	1	Total 1	O 1	0
67	j	4	Total 4	O 4	0
67	m	3	Total 3	O 3	0

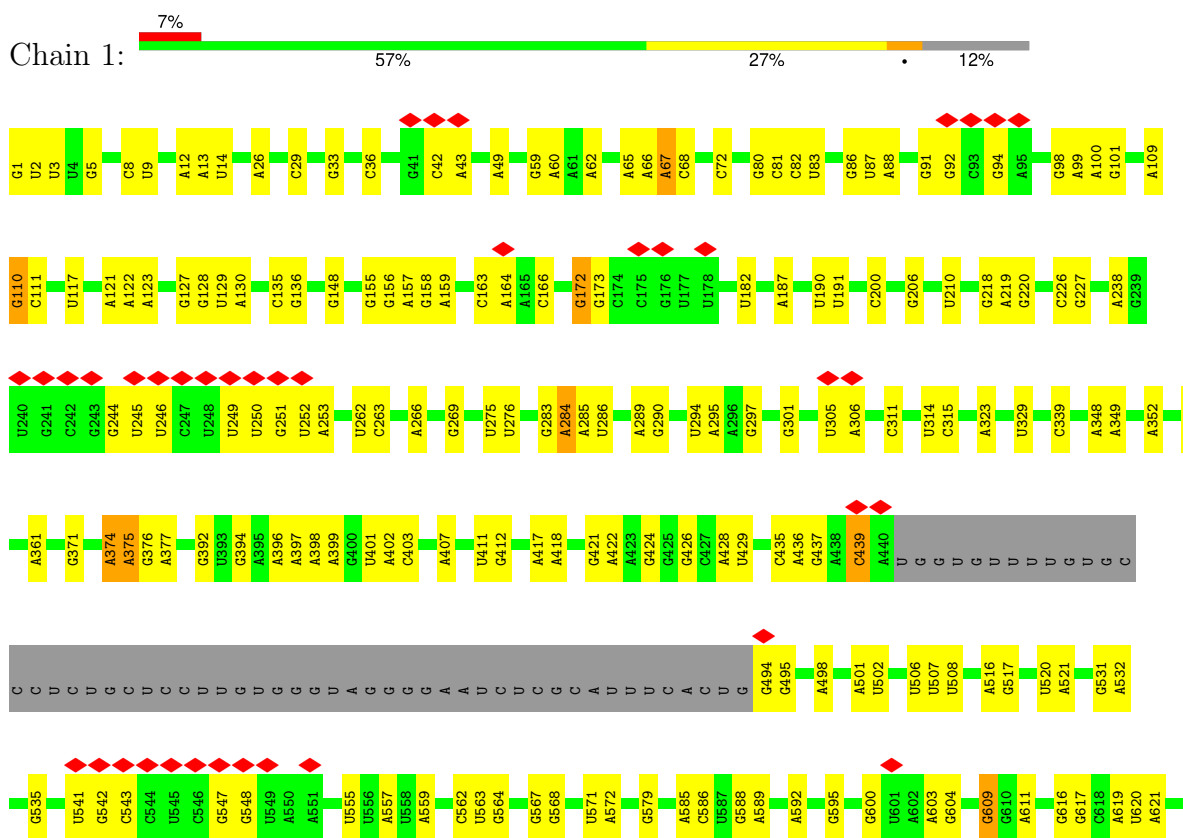
3 Residue-property plots [i](#)

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

- Molecule 1: 60S ribosomal protein L2-A

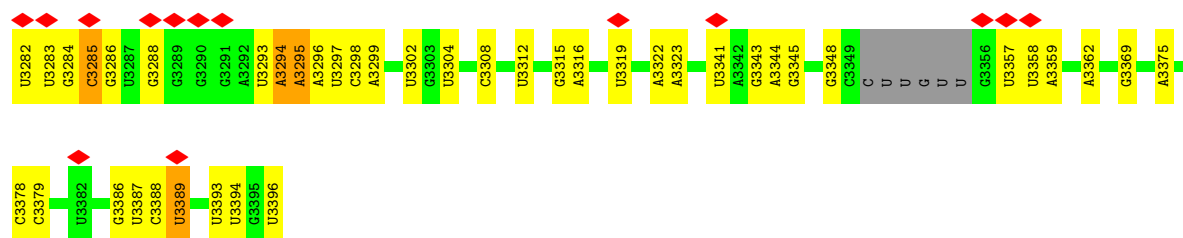


- Molecule 2: 25S rRNA

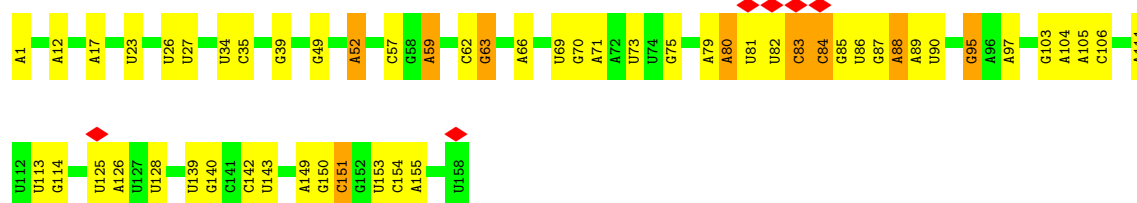




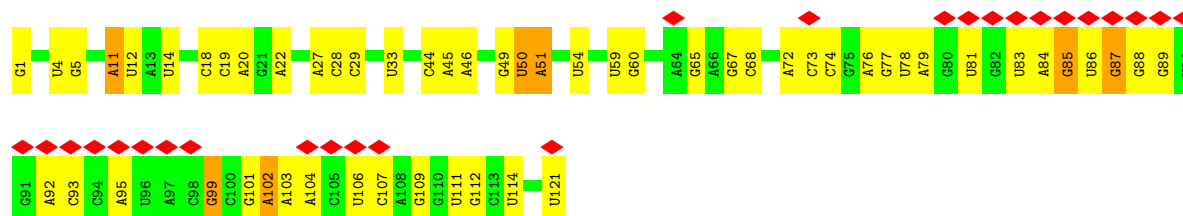
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A3172	A3086	U2978	U2883	A2802	U2547	G2412	G	G2240	U2140
G3173	A3175	U2979	C2884	A2803	C2548	A2413	A	U2241	A2141
G3174	C3089	U2980	A2887	A2804	C2549	G2414	C	A2242	A2142
G3176	A3091	U2981	C2889	C2810	U2550	C2415	C	A2243	C2146
U3179	C3092	A2982	G2898	A2811	U2551	U2416	G	A2244	A2158
A3180	C3093	C2983	C2899	A2812	C2552	U2417	C	C2245	U2159
C3181	C3096	U2986	G2900	A2813	G2555	A2419	U	C2248	G2160
A3187	C3097	A2987	G2901	G2814	G2556	A2421	G	G2249	G2161
U3192	G3098	U2990	A2919	G2815	A2561	U2422	A	G2250	A2167
C3193	U3100	G2990	G2730	G2816	U2565	C2426	U2314	G2253	A2168
C3194	G3101	A2994	U2921	U2818	C2568	U2427	G2315	U2254	G2169
U3195	G3102	A2995	G2922	A2819	A2569	U2428	U2317	A	G2177
U3196	A3103	U2996	U2923	A2820	U2570	G2429	U2318	A	U2191
G3199	U3104	G2997	U2924	C2821	U2571	A2430	U2334	C	U2192
U3207	G3112	A3001	C2925	U2822	C2572	U2433	G2335	U	U2193
A3209	G3112	A3006	A2926	G2824	G2573	U2434	U2336	U	U2194
A3210	G3120	U3007	C2927	A2825	G2576	G2435	U2340	G	C2197
C3217	U3121	A3012	U2928	G2826	G2576	A2438	A2262	A2263	A2198
A3218	A3122	U3013	C2929	G2830	G2585	A2439	U2344	U2264	G2199
G3219	A3127	U3014	G2930	G2831	G2586	G2440	A2345	C2265	U2200
G3224	G3128	G3015	U2935	G2832	A2589	A2441	U2347	U2266	G2201
U3231	A3129	A3021	C2936	G2833	A2593	G2442	A2348	C2267	C2202
C3232	U3130	G3022	G2937	G2834	C2594	A2443	U2349	U2269	U2203
A3244	A3131	U3023	U2938	U2842	A2617	C2444	C2350	A2270	C2204
A3245	U3132	A3024	U2939	U2843	G2603	A2445	U2351	A2271	U2205
G3246	G3133	G3025	U2940	A2674	G2606	U	A2357	G2272	G2206
G3247	A3134	G3026	U2941	C2675	G2607	A	A2358	G2273	A2207
U3252	U3135	U3032	U2942	A2676	U2608	G	A2367	U2274	A2208
U3259	U3136	A3033	G2943	A2677	A2609	A	A2368	G2275	U2209
G3263	U3137	G3045	U2944	A2678	U2610	G	G2371	C2276	G2210
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A3268	U3152	U3055	G2946	A2680	G2612	G	A2373	A	C2212
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C3276	C3154	U3057	G2948	U2682	U2617	A	G2375	G	G2218
U3280	U3155	U3058	U2949	C2683	G2618	A	U2388	C	A2219
U3281	U3156	U3066	U2950	U2684	G2619	U	G2393	U	A2220
A3286	U3157	C3067	G2951	A2685	G2620	A	G2396	C	A2221
A3274	C3161	U3070	U2952	A2686	G2623	A	A2397	G	A2222
U3275	A3163	C3072	U2953	A2687	C2624	G	A2398	A	A2223
C3276	C3164	A3073	U2954	C2625	A2626	G	A2401	U	A2224
U3280	C3165	U3078	G2955	C2627	C2628	G	A2402	C	U2225
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U3281	A3167	U3079	G2957	A2629	U2630	G	A2404	A	C2227
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U3281	U3169	U3079	U2959	A2632	U2632	G	U2408	A	A2229
U3281	U3170	U3079	U2960	A2633	A2635	G	U2408	A	C2230
U3281	U3171	U3079	U2961	A2634	A2636	G	U2408	A	C2231
U3281	U3172	U3079	U2962	A2635	A2637	G	U2408	A	C2232
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U3281	U3175	U3079	U2965	A2638	A2640	G	U2408	A	C2235
U3281	U3176	U3079	U2966	A2639	A2641	G	U2408	A	C2236
U3281	U3177	U3079	U2967	A2640	A2642	G	U2408	A	C2237
U3281	U3178	U3079	U2968	A2641	A2643	G	U2408	A	C2238
U3281	U3179	U3079	U2969	A2642	A2644	G	U2408	A	C2239
U3281	U3180	U3079	U2970	A2643	A2645	G	U2408	A	C2240
U3281	U3181	U3079	U2971	A2644	A2646	G	U2408	A	C2241
U3281	U3182	U3079	U2972	A2645	A2647	G	U2408	A	C2242
U3281	U3183	U3079	U2973	A2646	A2648	G	U2408	A	C2243
U3281	U3184	U3079	U2974	A2647	A2649	G	U2408	A	C2244
U3281	U3185	U3079	U2975	A2648	A2650	G	U2408	A	C2245
U3281	U3186	U3079	U2976	A2649	A2651	G	U2408	A	C2246
U3281	U3187	U3079	U2977	A2650	A2652	G	U2408	A	C2247
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U3281	U3189	U3079	U2979	A2652	A2654	G	U2408	A	C2249
U3281	U3190	U3079	U2980	A2653	A2655	G	U2408	A	C2250
U3281	U3191	U3079	U2981	A2654	A2656	G	U2408	A	C2251
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U3281	U3193	U3079	U2983	A2656	A2658	G	U2408	A	C2253
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U3281	U3195	U3079	U2985	A2658	A2660	G	U2408	A	C2255
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U3281	U3199	U3079	U2989	A2662	A2664	G	U2408	A	C2259
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U3281	U3202	U3079	U2992	A2665	A2667	G	U2408	A	C2262
U3281	U3203	U3079	U2993	A2666	A2668	G	U2408	A	C2263
U3281	U3204	U3079	U2994	A2667	A2669	G	U2408	A	C2264
U3281	U3205	U3079	U2995	A2668	A2670	G	U2408	A	C2265
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U3281	U3207	U3079	U2997	A2670	A2672	G	U2408	A	C2267
U3281	U3208	U3079	U2998	A2671	A2673	G	U2408	A	C2268
U3281	U3209	U3079	U2999	A2672	A2674	G	U2408	A	C2269
U3281	U3210	U3079	U3000	A2673	A2675	G	U2408	A	C2270
U3281	U3211	U3079	U3001	A2674	A2676	G	U2408	A	C2271
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U3281	U3213	U3079	U3003	A2676	A2678	G	U2408	A	C2273
U3281	U3214	U3079	U3004	A2677	A2679	G	U2408	A	C2274
U3281	U3215	U3079	U3005	A2678	A2680	G	U2408	A	C2275
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U3281	U3217	U3079	U3007	A2680	A2682	G	U2408	A	C2277
U3281	U3218	U3079	U3008	A2681	A2683	G	U2408	A	C2278
U3281	U3219	U3079	U3009	A2682	A2684	G	U2408	A	C2279
U3281	U3220	U3079	U3010	A2683	A2685	G	U2408	A	C2280
U3281	U3221	U3079	U3011	A2684	A2686	G	U2408	A	C2281
U3281	U3222	U3079	U3012	A2685	A2687	G	U2408	A	C2282
U3281	U3223	U3079	U3013	A2686	A2688	G	U2408	A	C2283
U3281	U3224	U3079	U3014	A2687	A2689	G	U2408	A	C2284
U3281	U3225	U3079	U3015	A2688	A2690	G	U2408	A	C2285
U3281	U3226	U3079	U3016	A2689	A2691	G	U2408	A	C2286
U3281	U3227	U3079	U3017	A2690	A2692	G	U2408	A	C2287
U3281	U3228	U3079	U3018	A2691	A2693	G	U2408	A	C2288
U3281	U3229	U3079	U3019	A2692	A2694	G	U2408	A	C2289
U3281	U3230	U3079	U3020	A2693	A2695	G	U2408	A	C2290
U3281	U3231	U3079	U3021	A2694	A2696	G	U2408	A	C2291
U3281	U3232	U3079	U3022	A2695	A2697	G	U2408	A	C2292
U3281	U3233	U3079	U3023	A2696	A2698	G	U2408	A	C2293
U3281	U3234	U3079	U3024	A2697	A2699	G	U2408	A	C2294
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U3281	U3238	U3079	U3028	A2701	A2703	G	U2408	A	C2298
U3281	U3239	U3079	U3029	A2702	A2704	G	U2408	A	C2299
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U3281	U3243	U3079	U3033	A2706	A2708	G	U2408	A	C2303
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U3281	U3245	U3079	U3035	A2708	A2710	G	U2408	A	C2305
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U3281	U3247	U3079	U3037	A2710	A2712	G	U2408	A	C2307
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U3281	U3249	U3079	U3039	A2712	A2714	G	U2408	A	C2309
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U3281	U3252	U3079	U3042	A2715	A2717	G	U2408	A	C2312
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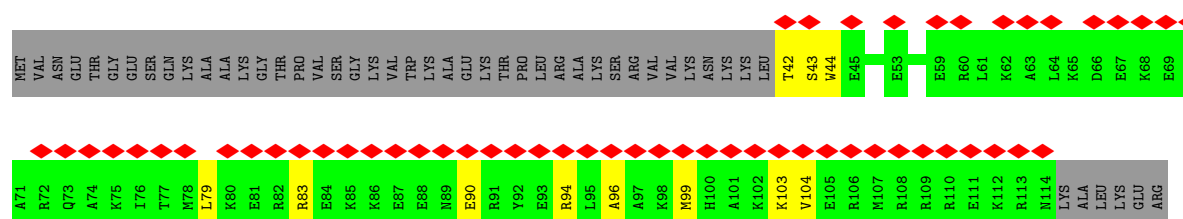
• Molecule 3: 5.8S rRNA



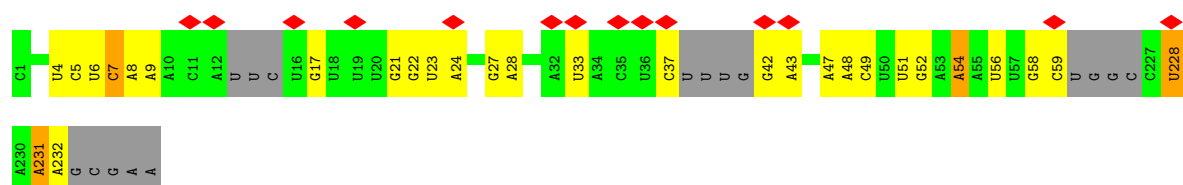
• Molecule 4: 5S rRNA



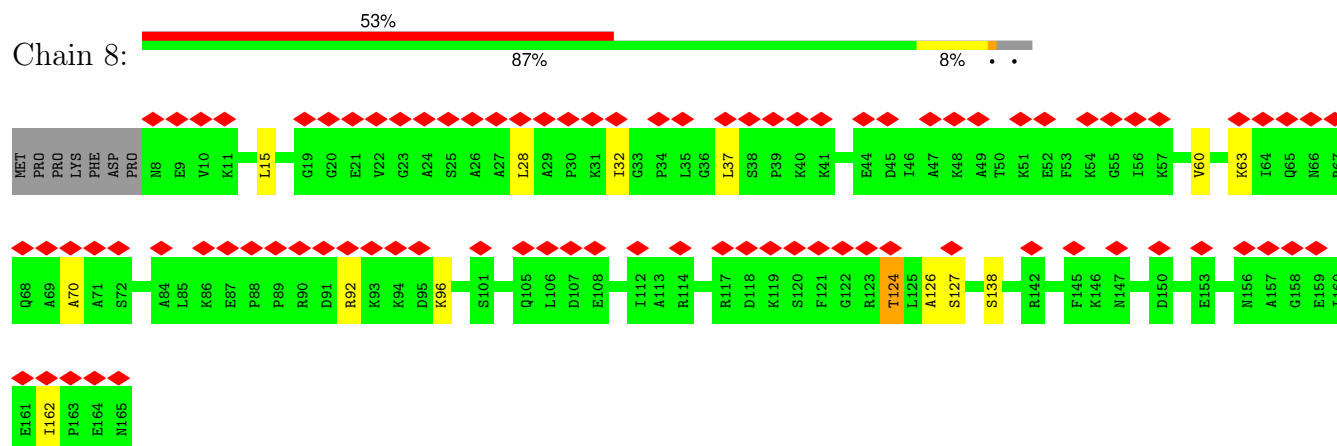
• Molecule 5: rRNA-processing protein



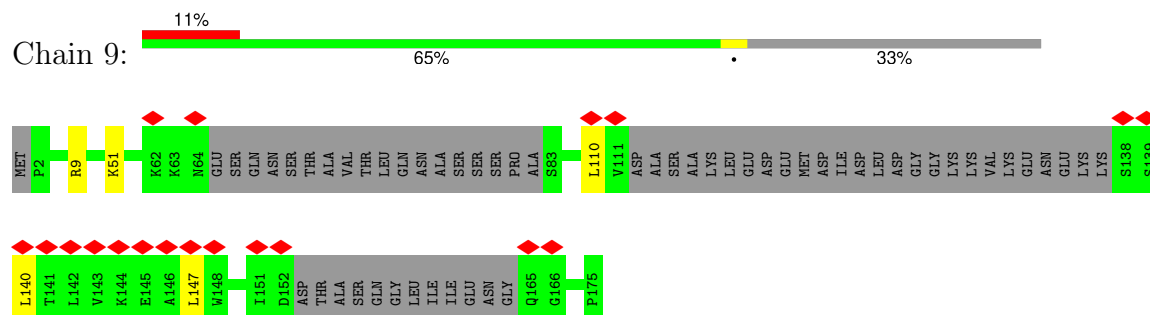
• Molecule 6: ITS2 rRNA



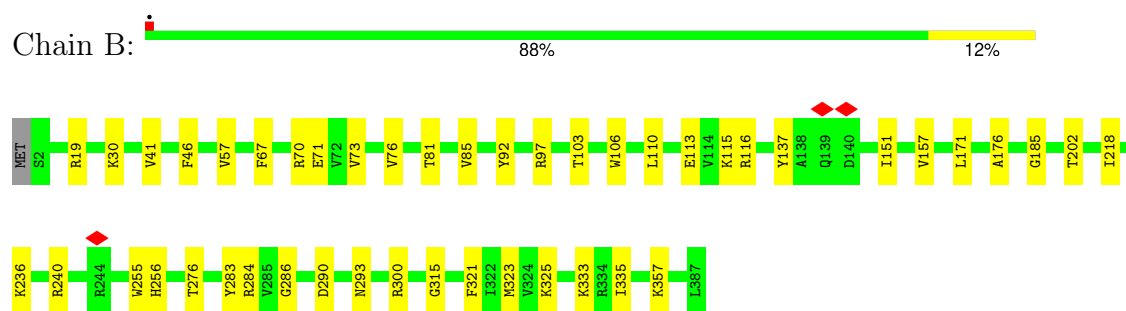
Chain 8:



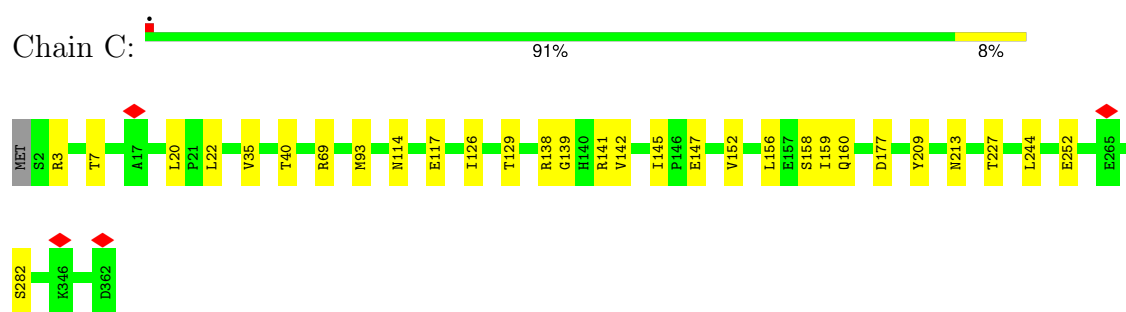
Chain 9:

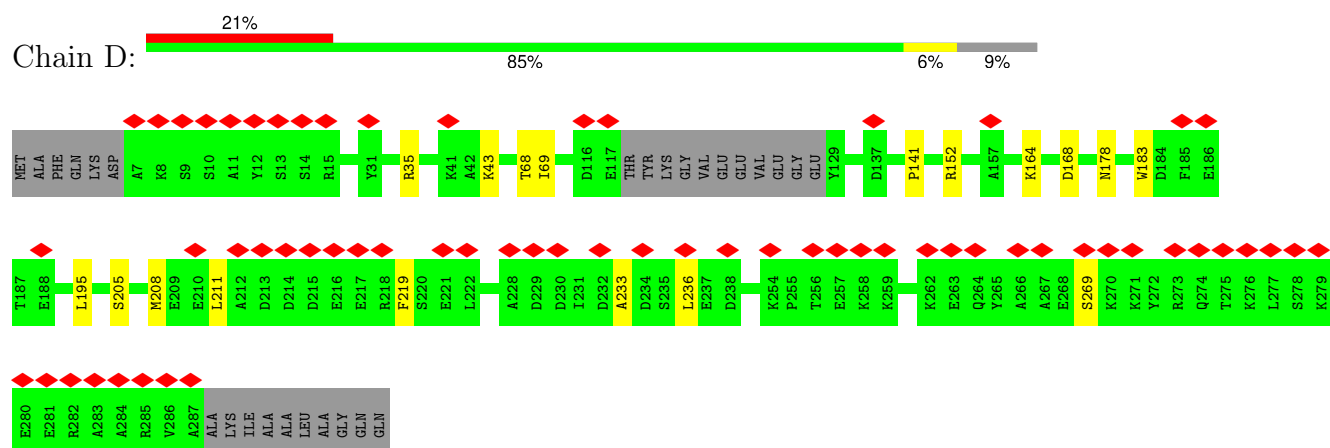


Chain B:

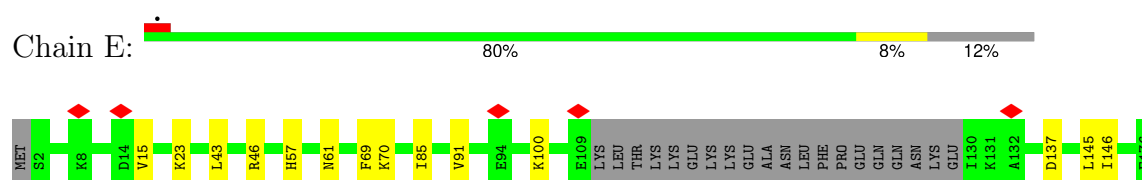


Chain C:

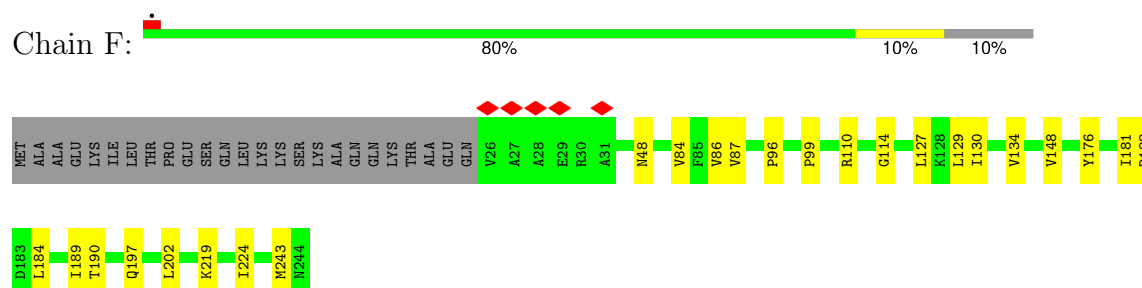




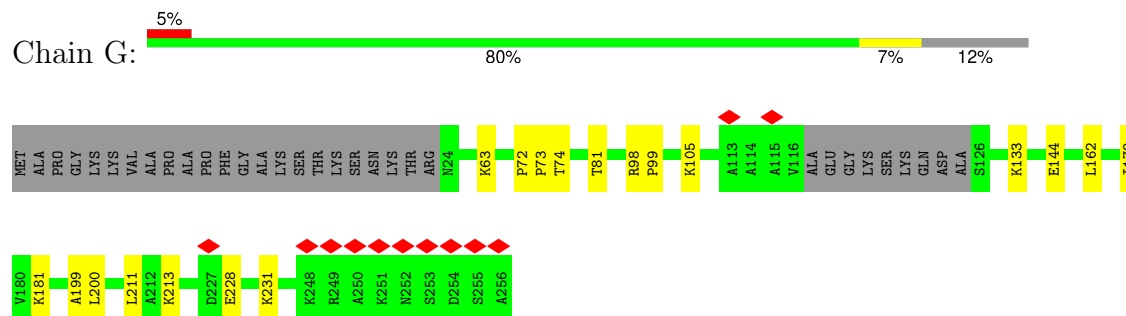
- Molecule 12: 60S ribosomal protein L6-A



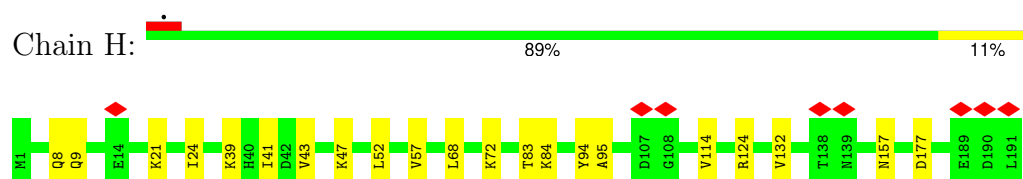
- Molecule 13: 60S ribosomal protein L7-A



- Molecule 14: 60S ribosomal protein L8-A

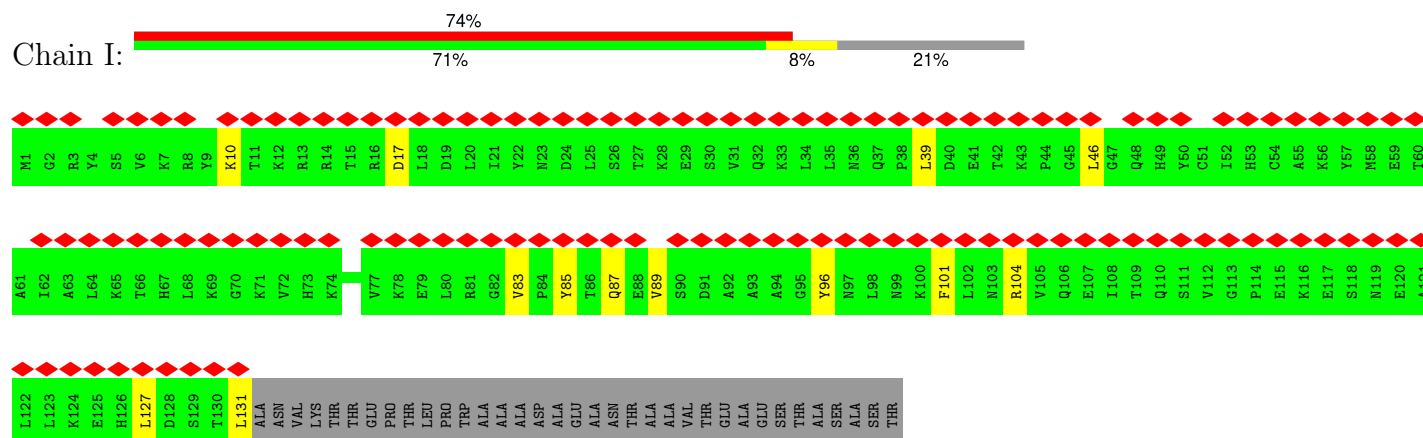


- Molecule 15: 60S ribosomal protein L9-A



- Molecule 16: Bud site selection protein 20

Chain I:



LYS
ARG
SER
SER
GLU
LEU
GLU
LYS
GLU
SER
SER
SER
SER
GLU
ALA
VAL
LYS
LYS
ALA
LYS
SER

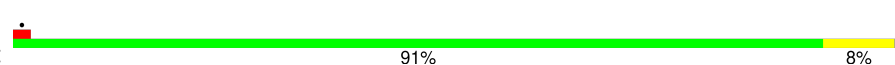
- Molecule 19: 60S ribosomal protein L13-A

Chain L: 

MET
ALA
ILE
SER
LYS
ASN
LEU
PRO
ILE
LYS
GLU
SER
ASN
HIS
PHE
R15
W18
Q19
E20
D27
K31
R36
I46
R73
A90
I95
Q106
N129
G130
K131
A132
P133
E134
T144
A151
T152
E164
G181
E184
K185
R186
A187
R188
E189
K190
A191

E192
A193
E194
ALA
GLU
LYS
LYS
LYS

- Molecule 20: 60S ribosomal protein L14-A

Chain M: 

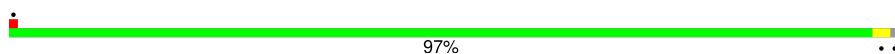
MET
S2
T3
D4
S5
I6
V7
K8
N11
K25
L32
G48
V53
Q62
W94
R106
K137
A138

- Molecule 21: 60S ribosomal protein L15-A

Chain N: 

MET
G2
A3
Y4
K5
Y6
L7
R12
V18
R65
R71
F76
LYS
GLY
ALA
THR
TYR
GLY
LYS
PRO
THR
ASN
GLN
GLY
VAL
ASN
E91
L116
N117
S126
Y129
V155
H158
A161
R162
T183
K184
A185
G186
R187
K204

- Molecule 22: 60S ribosomal protein L16-A

Chain O: 

MET
SER
Y3
K12
R49
L84
K171
Y199

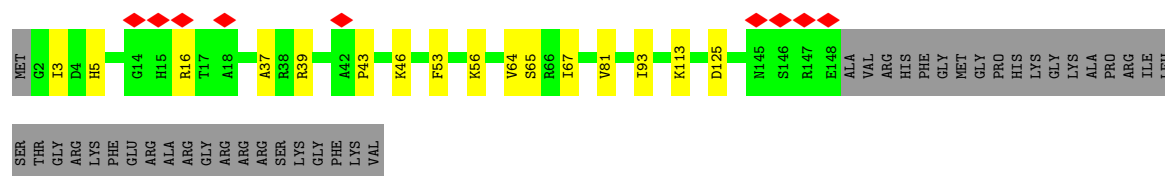
- Molecule 23: 60S ribosomal protein L17-A

Chain P: 

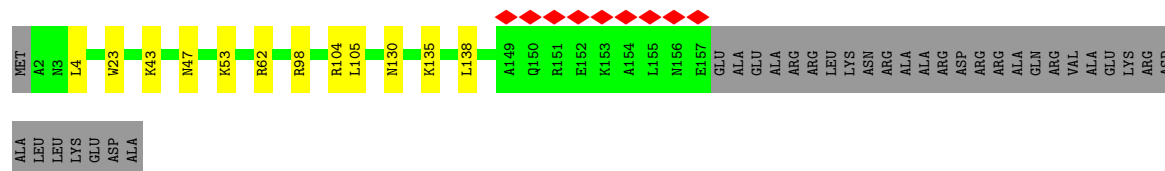
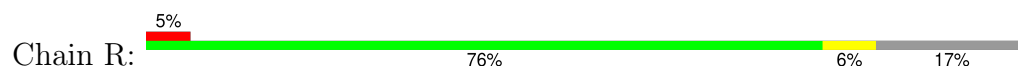
MET
A2
R3
L22
I36
E49
R56
I67
G68
R69
E75
Q92
L95
A98
L107
A122
P123
K124
Q125
R126
E140
S141
S142
P143
I146
E147
L148
E152
E155
ALA
VAL
ALA
LYS
ALA
ALA
GLU
LYS
K164
R167
A184

- Molecule 24: 60S ribosomal protein L18-A

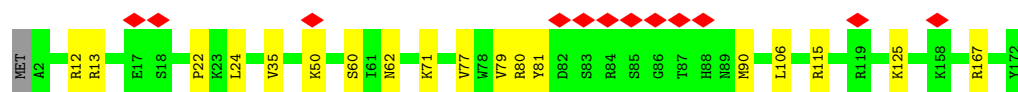
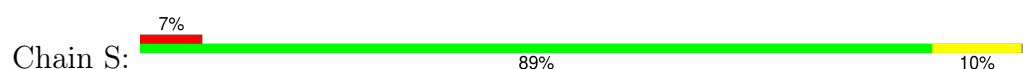
Chain Q: 



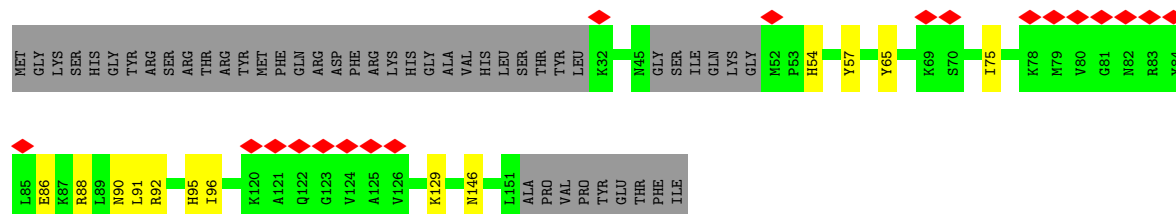
- Molecule 25: 60S ribosomal protein L19-A



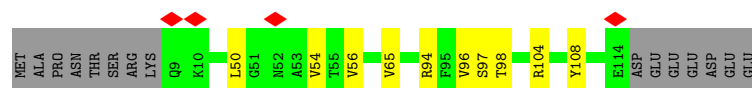
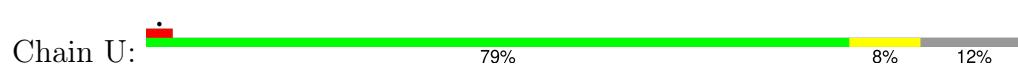
- Molecule 26: 60S ribosomal protein L20-A



- Molecule 27: 60S ribosomal protein L21-A



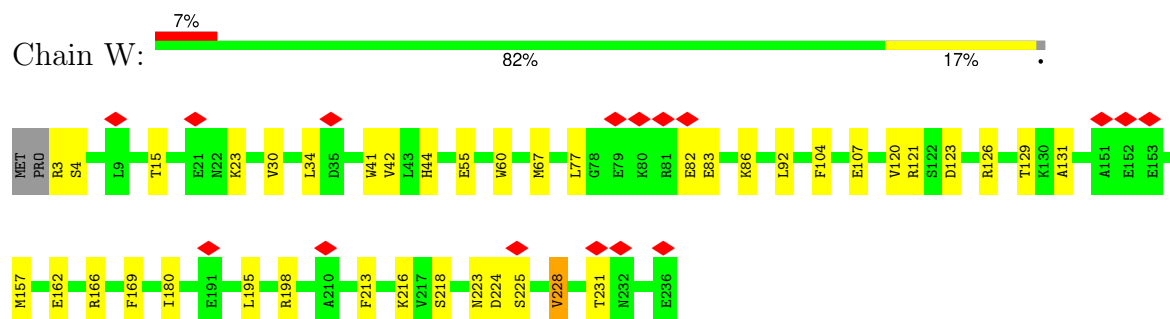
- Molecule 28: 60S ribosomal protein L22-A



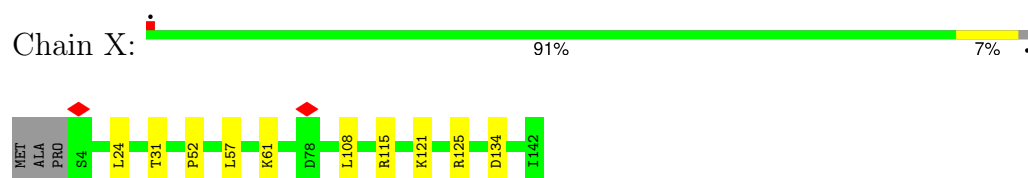
- Molecule 29: 60S ribosomal protein L23-A



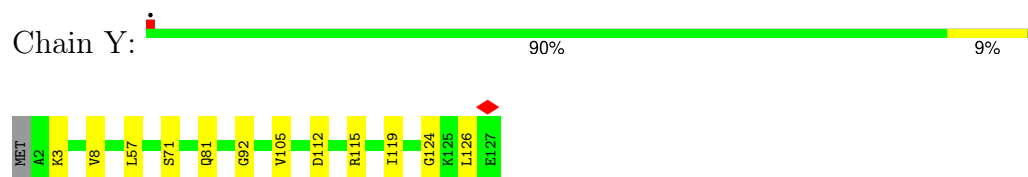
- Molecule 30: Ribosome assembly factor MRT4



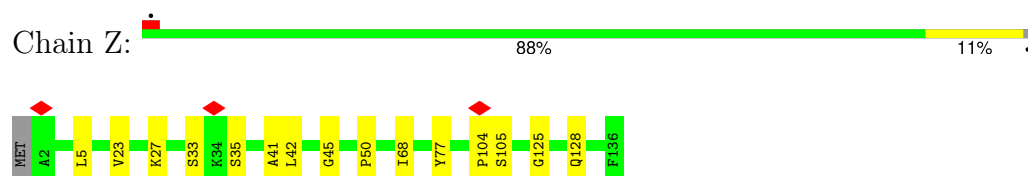
- Molecule 31: 60S ribosomal protein L25



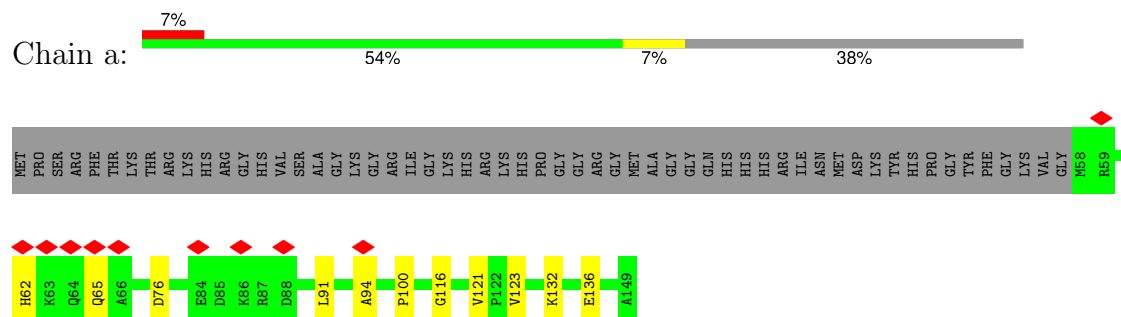
- Molecule 32: 60S ribosomal protein L26-A



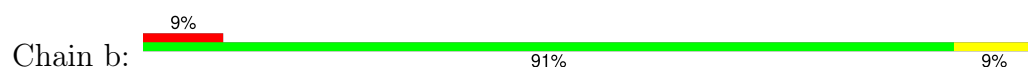
- Molecule 33: 60S ribosomal protein L27-A

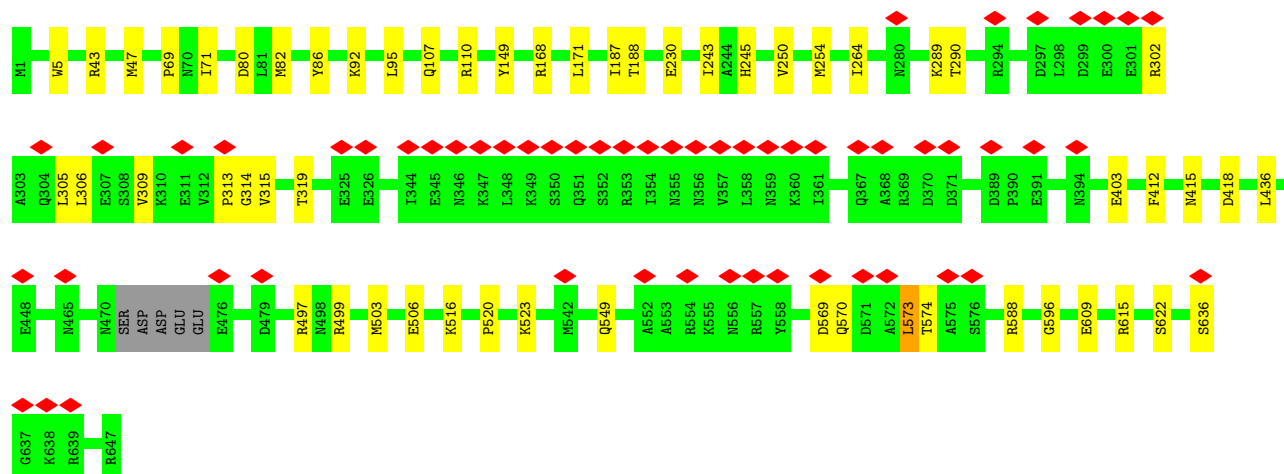


- Molecule 34: 60S ribosomal protein L28

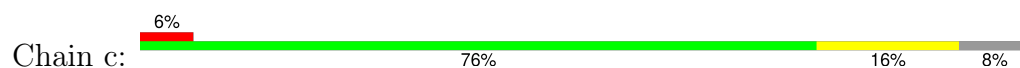


- Molecule 35: Nucleolar GTP-binding protein 1

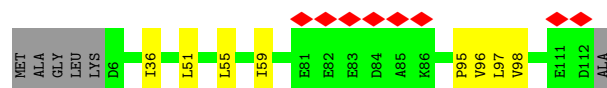
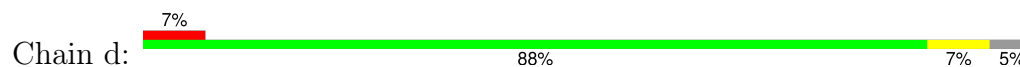




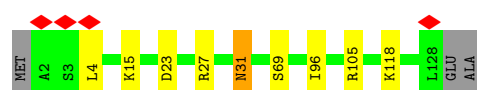
- Molecule 36: 60S ribosomal protein L30



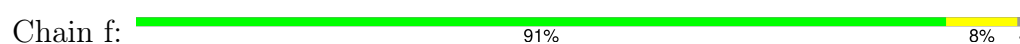
- Molecule 37: 60S ribosomal protein L31-A



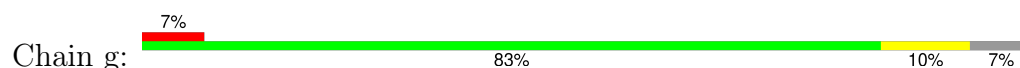
- Molecule 38: 60S ribosomal protein L32



- Molecule 39: 60S ribosomal protein L33-A

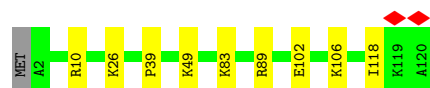


- Molecule 40: 60S ribosomal protein L34-A

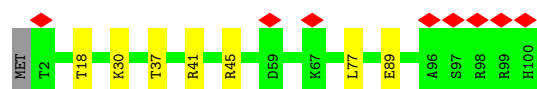




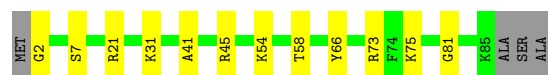
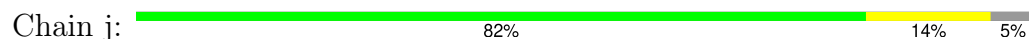
- Molecule 41: 60S ribosomal protein L35-A



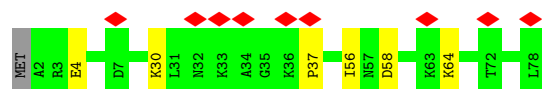
- Molecule 42: 60S ribosomal protein L36-A



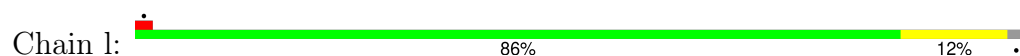
- Molecule 43: 60S ribosomal protein L37-A



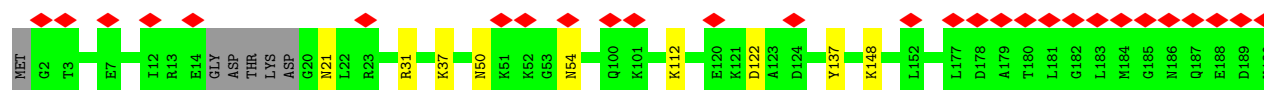
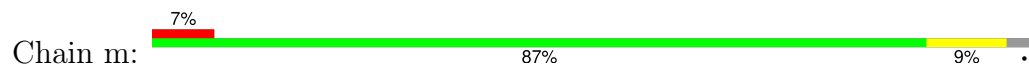
- Molecule 44: 60S ribosomal protein L38

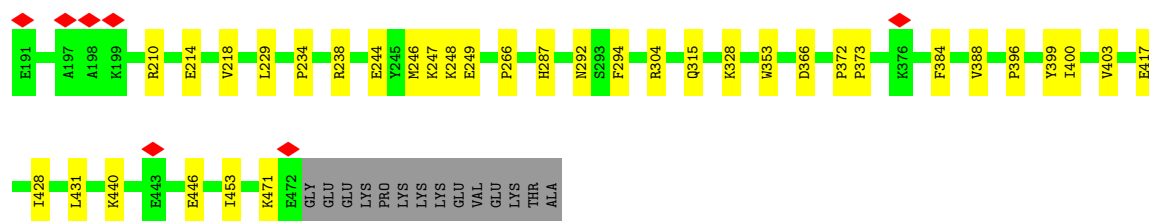


- Molecule 45: 60S ribosomal protein L39

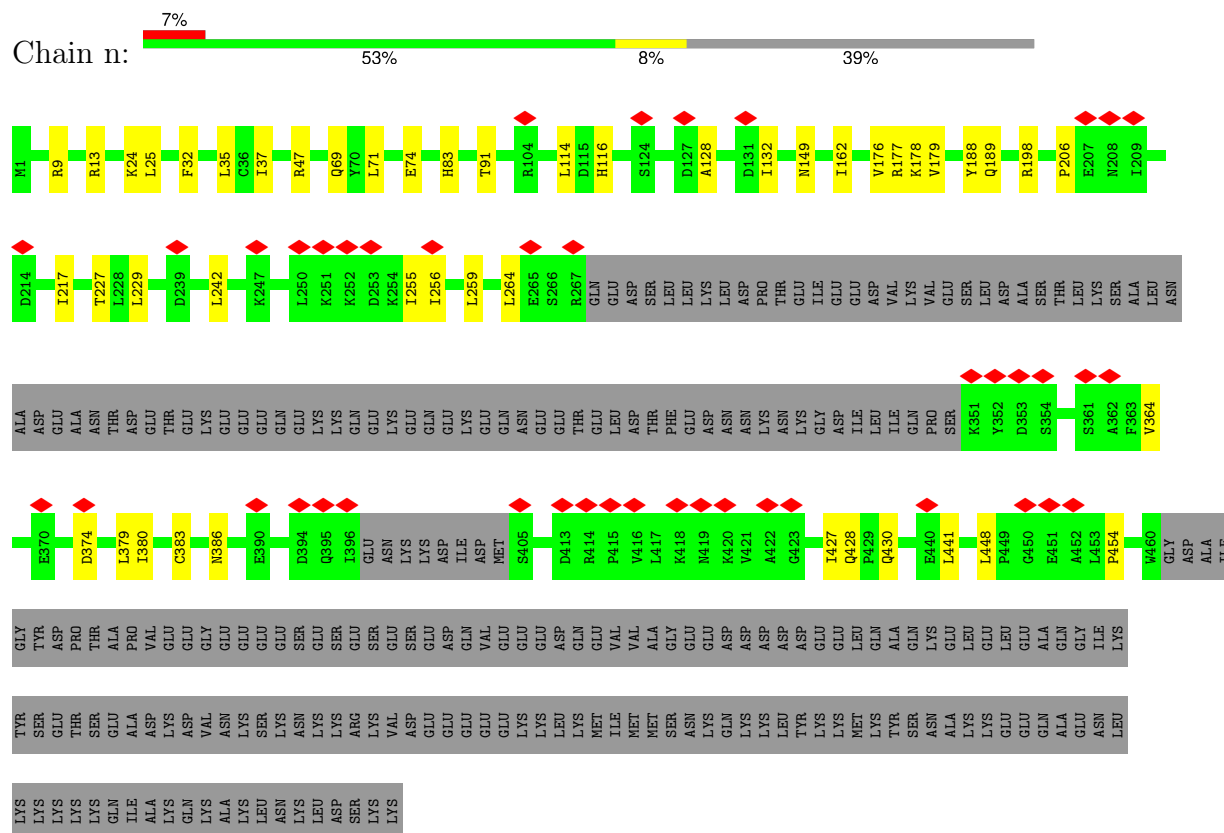


- Molecule 46: Nucleolar GTP-binding protein 2

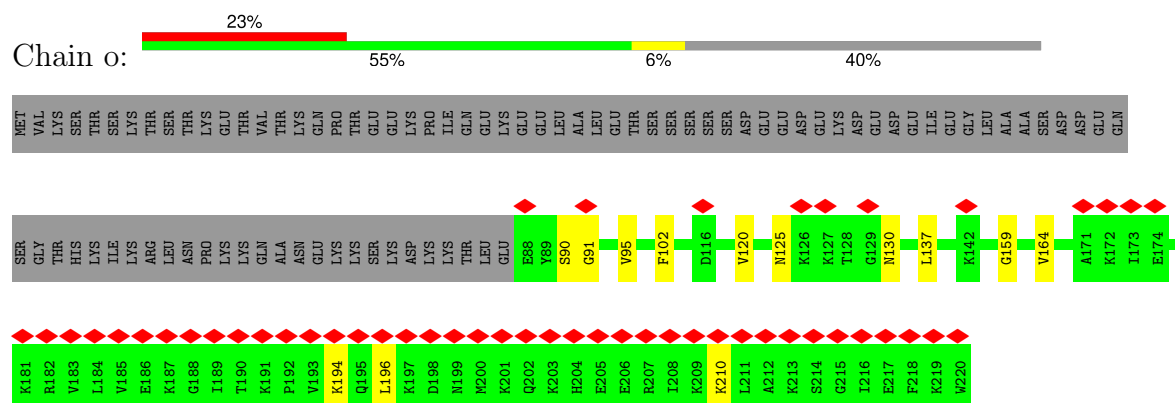




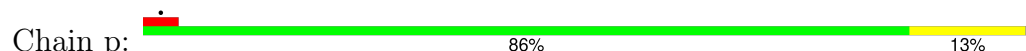
• Molecule 47: Pescadillo homolog



• Molecule 48: Ribosome biogenesis protein 15

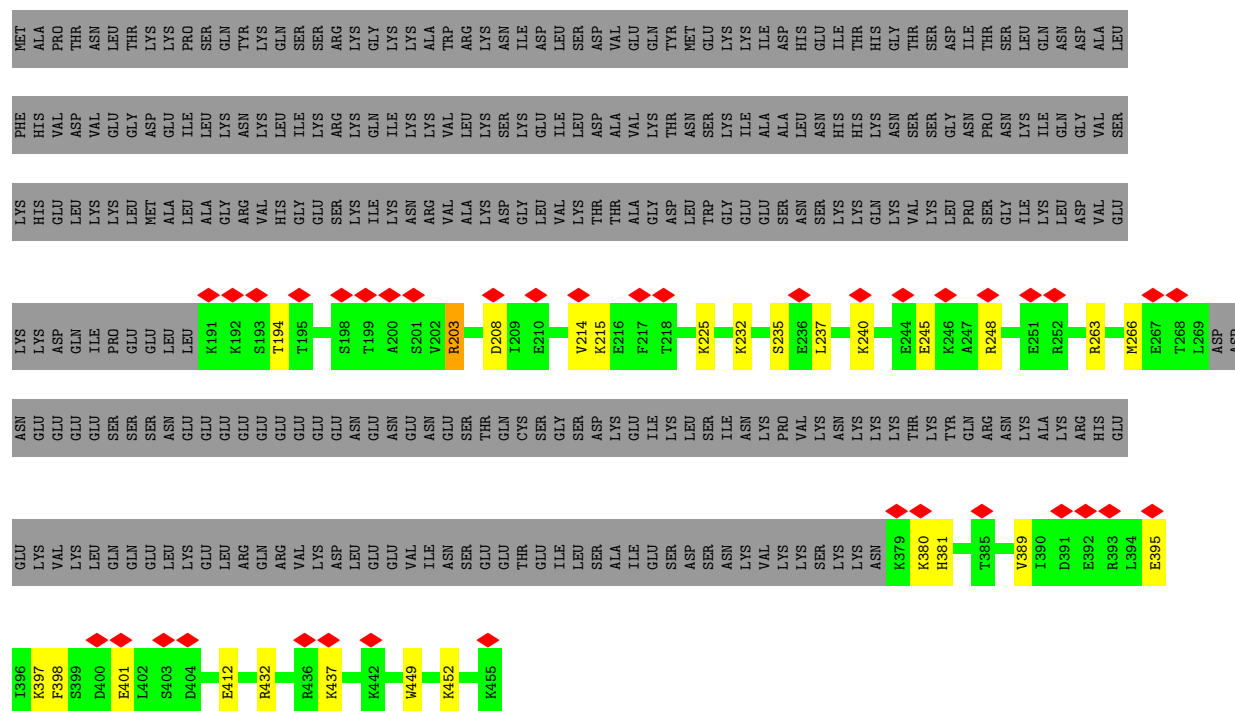


• Molecule 49: 60S ribosomal protein L43-A

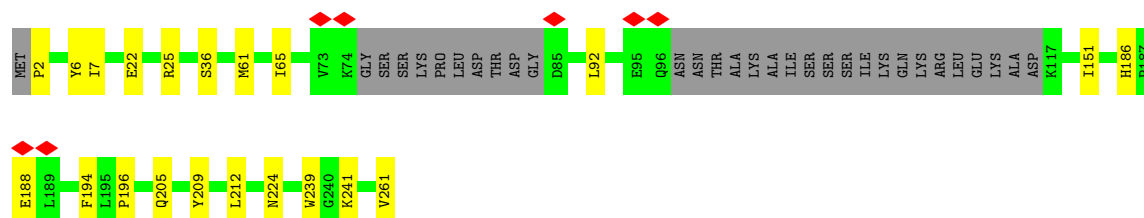
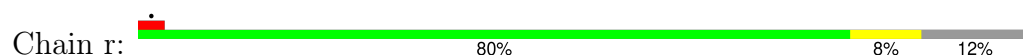




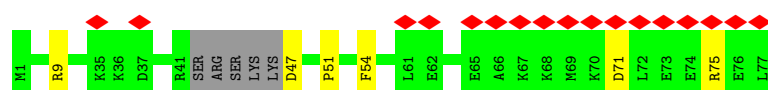
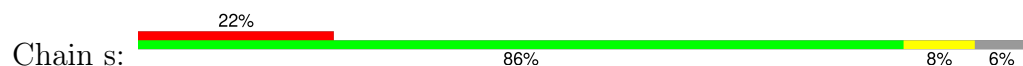
• Molecule 50: Ribosome biogenesis protein NOP53



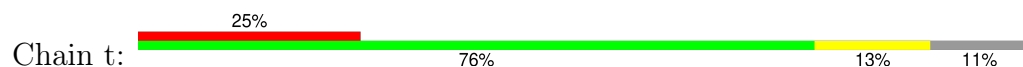
• Molecule 51: Ribosome biogenesis protein NSA2

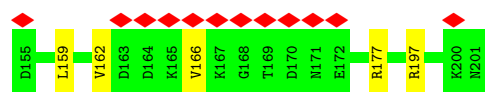


• Molecule 52: Nuclear GTP-binding protein NUG1

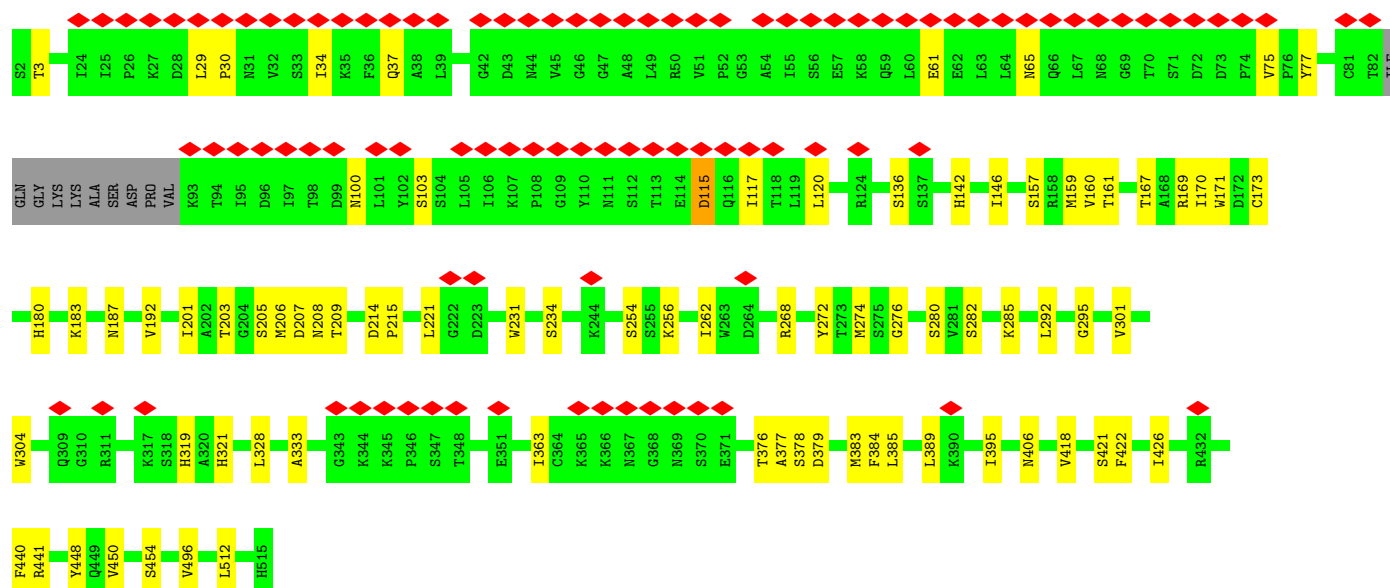
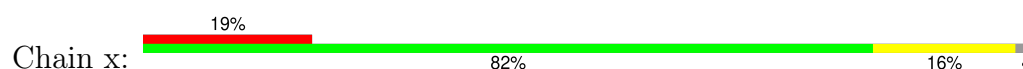


• Molecule 53: Ribosome biogenesis protein RLP7

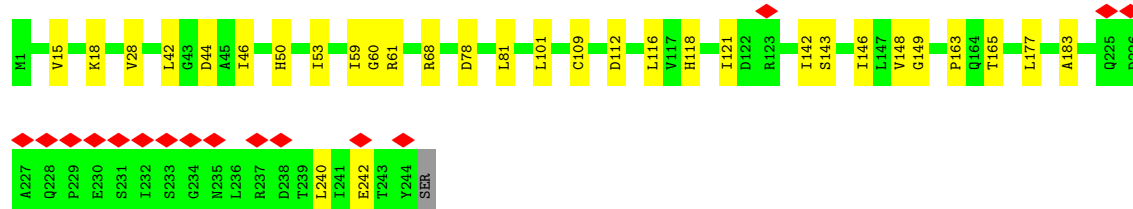
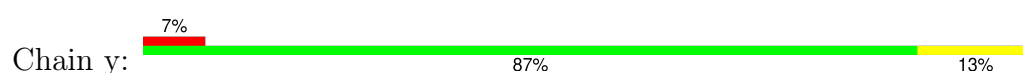




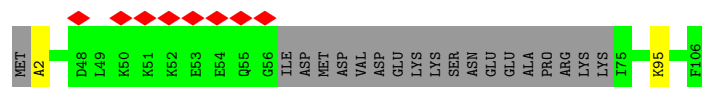
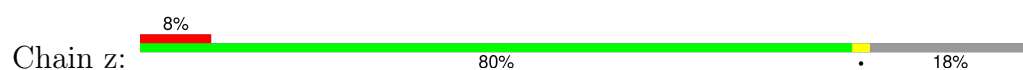
• Molecule 57: RSA4 isoform 1



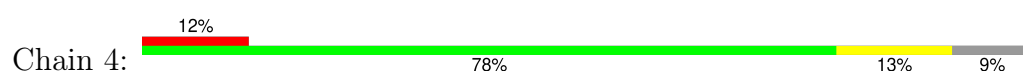
• Molecule 58: Eukaryotic translation initiation factor 6

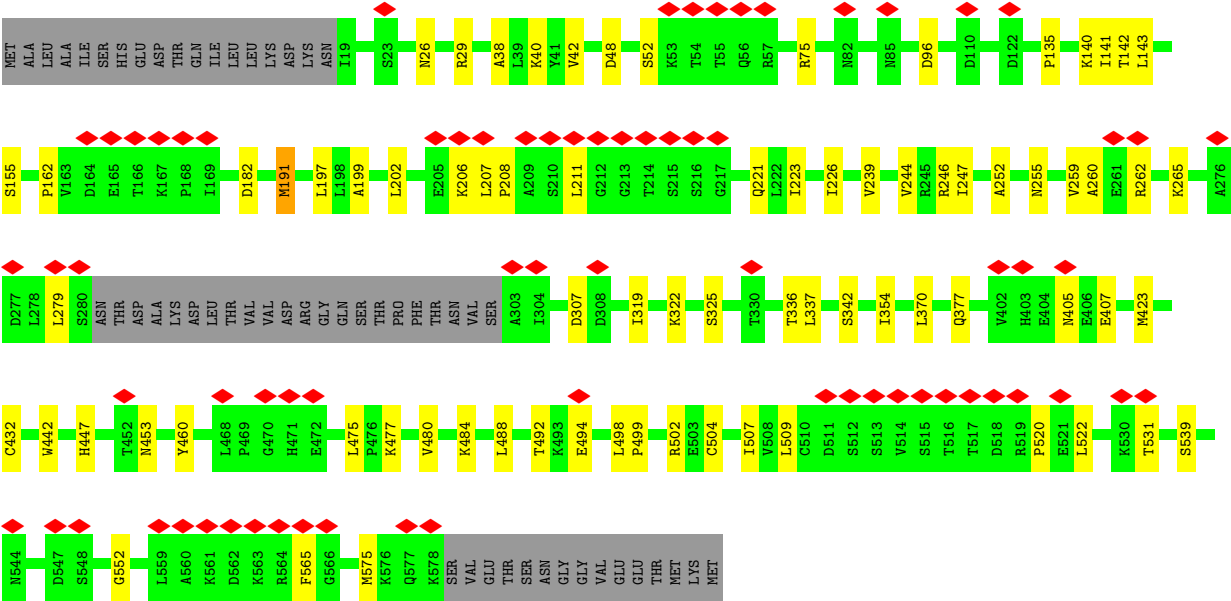


• Molecule 59: UPF0642 protein YBL028C



• Molecule 60: Probable metalloprotease ARX1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	414994	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.440	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.032	Depositor
Map size ($\text{\AA}$)	427.19998, 427.19998, 427.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ALF, MG, OMC, GDP, OMU, 1MA, 5MC, A2M, OMG, ZN, PSU, B3P, K

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	A	0.13	0/1666	0.36	0/2241
2	1	0.16	0/70382	0.31	0/109722
3	2	0.15	0/3724	0.30	0/5798
4	3	0.10	0/2861	0.22	0/4457
5	5	0.13	0/649	0.24	0/848
6	6	0.13	0/1367	0.28	0/2118
7	8	0.12	0/1210	0.29	0/1627
8	9	0.11	0/948	0.24	0/1264
9	B	0.14	0/3152	0.35	0/4239
10	C	0.13	0/2801	0.32	0/3792
11	D	0.11	0/2227	0.27	0/3004
12	E	0.13	0/1251	0.33	0/1682
13	F	0.14	0/1798	0.33	0/2420
14	G	0.14	0/1784	0.32	0/2408
15	H	0.13	0/1539	0.34	0/2073
16	I	0.12	0/1075	0.29	0/1443
17	J	0.11	0/1389	0.31	0/1860
18	K	0.11	0/2190	0.29	0/2955
19	L	0.12	0/1460	0.31	0/1960
20	M	0.14	0/1074	0.32	0/1446
21	N	0.14	0/1654	0.33	0/2213
22	O	0.17	0/1585	0.33	0/2128
23	P	0.14	0/1410	0.37	0/1893
24	Q	0.12	0/1153	0.28	0/1555
25	R	0.13	0/1275	0.28	0/1702
26	S	0.12	0/1473	0.29	0/1980
27	T	0.12	0/916	0.27	0/1226
28	U	0.13	0/861	0.37	0/1167
29	V	0.14	0/1018	0.35	0/1369
30	W	0.11	0/1920	0.29	0/2586
31	X	0.13	0/1103	0.34	0/1484
32	Y	0.12	0/1004	0.33	0/1341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Z	0.12	0/1118	0.29	0/1497
34	a	0.11	0/747	0.25	0/1008
35	b	0.14	0/5270	0.32	0/7080
36	c	0.13	0/751	0.29	0/1008
37	d	0.13	0/887	0.32	0/1191
38	e	0.12	0/1041	0.31	0/1394
39	f	0.15	0/868	0.35	0/1168
40	g	0.14	0/891	0.33	0/1191
41	h	0.14	0/978	0.29	0/1301
42	i	0.12	0/778	0.29	0/1034
43	j	0.15	0/680	0.35	0/901
44	k	0.12	0/618	0.29	0/826
45	l	0.14	0/443	0.33	0/588
46	m	0.13	0/3828	0.31	0/5154
47	n	0.13	0/3085	0.31	0/4166
48	o	0.11	0/1129	0.30	0/1502
49	p	0.15	0/701	0.35	0/934
50	q	0.14	0/1321	0.35	0/1766
51	r	0.13	0/1892	0.31	0/2528
52	s	0.13	0/608	0.26	0/798
53	t	0.13	0/2333	0.30	0/3128
54	u	0.14	0/1287	0.32	0/1711
55	v	0.12	0/2410	0.31	0/3220
56	w	0.12	0/1565	0.28	0/2108
57	x	0.12	0/4022	0.35	0/5460
58	y	0.13	0/1872	0.34	0/2548
59	z	0.13	0/721	0.26	0/948
60	4	0.12	0/4242	0.29	0/5758
All	All	0.14	0/166005	0.31	0/239917

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
54	u	0	1
56	w	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	u	75	ARG	Sidechain
56	w	46	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1634	0	1685	13	0
2	1	64042	0	32235	452	0
3	2	3353	0	1695	27	0
4	3	2579	0	1304	23	0
5	5	645	0	688	6	0
6	6	1227	0	622	18	0
7	8	1196	0	1257	11	0
8	9	937	0	1008	5	0
9	B	3081	0	3165	28	0
10	C	2749	0	2863	33	0
11	D	2180	0	2134	16	0
12	E	1230	0	1320	13	0
13	F	1761	0	1843	15	0
14	G	1753	0	1845	20	0
15	H	1518	0	1587	13	0
16	I	1059	0	1089	11	0
17	J	1368	0	1401	21	0
18	K	2155	0	2230	38	0
19	L	1438	0	1493	9	0
20	M	1059	0	1154	10	0
21	N	1620	0	1679	16	0
22	O	1555	0	1659	3	0
23	P	1388	0	1423	22	0
24	Q	1136	0	1214	21	0
25	R	1258	0	1342	9	0
26	S	1437	0	1475	14	0
27	T	905	0	957	19	0
28	U	844	0	855	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	V	1003	0	1048	4	0
30	W	1888	0	1917	23	0
31	X	1088	0	1175	6	0
32	Y	993	0	1081	8	0
33	Z	1092	0	1155	8	0
34	a	731	0	773	7	0
35	b	5185	0	5250	39	0
36	c	743	0	797	10	0
37	d	873	0	914	5	0
38	e	1020	0	1090	11	0
39	f	850	0	880	6	0
40	g	881	0	945	11	0
41	h	969	0	1078	7	0
42	i	771	0	849	5	0
43	j	665	0	668	8	0
44	k	612	0	682	4	0
45	l	436	0	475	7	0
46	m	3754	0	3823	32	0
47	n	3014	0	3094	35	0
48	o	1107	0	1159	9	0
49	p	694	0	734	8	0
50	q	1298	0	1343	24	0
51	r	1860	0	1965	17	0
52	s	602	0	661	4	0
53	t	2306	0	2454	36	0
54	u	1265	0	1314	14	0
55	v	2366	0	2452	43	0
56	w	1541	0	1597	21	0
57	x	3927	0	3893	49	0
58	y	1849	0	1836	19	0
59	z	714	0	760	2	0
60	4	4166	0	4248	50	0
61	1	57	0	78	5	0
62	1	76	0	0	0	0
62	2	1	0	0	0	0
62	R	1	0	0	0	0
62	V	1	0	0	0	0
62	b	1	0	0	0	0
62	m	1	0	0	0	0
63	I	1	0	0	0	0
63	g	1	0	0	0	0
63	j	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
63	p	1	0	0	0	0
63	u	1	0	0	0	0
64	b	28	0	12	1	0
64	m	28	0	12	0	0
65	m	5	0	0	1	0
66	m	1	0	0	0	0
67	1	340	0	0	2	0
67	2	7	0	0	0	0
67	A	2	0	0	0	0
67	B	2	0	0	0	0
67	C	1	0	0	0	0
67	F	3	0	0	0	0
67	N	2	0	0	0	0
67	O	1	0	0	0	0
67	R	1	0	0	0	0
67	V	3	0	0	0	0
67	X	1	0	0	0	0
67	b	3	0	0	0	0
67	d	1	0	0	0	0
67	j	4	0	0	0	0
67	m	3	0	0	0	0
All	All	157949	0	125434	1196	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 1196 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:142:VAL:CB	10:C:145:ILE:HD12	1.46	1.41
24:Q:3:ILE:HD11	24:Q:5:HIS:CE1	1.69	1.28
10:C:142:VAL:CB	10:C:145:ILE:CD1	2.23	1.16
55:v:132:THR:HG22	55:v:226:ILE:HG21	1.21	1.13
55:v:132:THR:HG22	55:v:226:ILE:CG2	1.82	1.08

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/254 (83%)	202 (96%)	9 (4%)	0	100	100
5	5	71/120 (59%)	71 (100%)	0	0	100	100
7	8	156/165 (94%)	150 (96%)	6 (4%)	0	100	100
8	9	110/175 (63%)	108 (98%)	2 (2%)	0	100	100
9	B	384/387 (99%)	379 (99%)	5 (1%)	0	100	100
10	C	359/362 (99%)	348 (97%)	11 (3%)	0	100	100
11	D	266/297 (90%)	261 (98%)	5 (2%)	0	100	100
12	E	151/176 (86%)	149 (99%)	2 (1%)	0	100	100
13	F	217/244 (89%)	211 (97%)	6 (3%)	0	100	100
14	G	220/256 (86%)	216 (98%)	4 (2%)	0	100	100
15	H	189/191 (99%)	184 (97%)	5 (3%)	0	100	100
16	I	129/166 (78%)	125 (97%)	4 (3%)	0	100	100
17	J	169/174 (97%)	166 (98%)	3 (2%)	0	100	100
18	K	262/376 (70%)	256 (98%)	6 (2%)	0	100	100
19	L	178/199 (89%)	174 (98%)	4 (2%)	0	100	100
20	M	135/138 (98%)	131 (97%)	4 (3%)	0	100	100
21	N	185/204 (91%)	178 (96%)	7 (4%)	0	100	100
22	O	195/199 (98%)	194 (100%)	1 (0%)	0	100	100
23	P	171/184 (93%)	164 (96%)	7 (4%)	0	100	100
24	Q	145/186 (78%)	144 (99%)	1 (1%)	0	100	100
25	R	154/189 (82%)	151 (98%)	3 (2%)	0	100	100
26	S	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
27	T	110/160 (69%)	107 (97%)	3 (3%)	0	100	100
28	U	104/121 (86%)	100 (96%)	4 (4%)	0	100	100
29	V	134/137 (98%)	131 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	W	232/236 (98%)	230 (99%)	2 (1%)	0	100	100
31	X	137/142 (96%)	133 (97%)	4 (3%)	0	100	100
32	Y	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
33	Z	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
34	a	90/149 (60%)	86 (96%)	4 (4%)	0	100	100
35	b	638/647 (99%)	617 (97%)	21 (3%)	0	100	100
36	c	95/105 (90%)	95 (100%)	0	0	100	100
37	d	105/113 (93%)	104 (99%)	1 (1%)	0	100	100
38	e	125/130 (96%)	124 (99%)	1 (1%)	0	100	100
39	f	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
40	g	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
41	h	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
42	i	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
43	j	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
44	k	75/78 (96%)	75 (100%)	0	0	100	100
45	l	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
46	m	462/486 (95%)	452 (98%)	10 (2%)	0	100	100
47	n	363/605 (60%)	353 (97%)	10 (3%)	0	100	100
48	o	131/220 (60%)	129 (98%)	2 (2%)	0	100	100
49	p	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
50	q	152/455 (33%)	144 (95%)	8 (5%)	0	100	100
51	r	224/261 (86%)	220 (98%)	4 (2%)	0	100	100
52	s	68/77 (88%)	67 (98%)	1 (2%)	0	100	100
53	t	283/322 (88%)	280 (99%)	3 (1%)	0	100	100
54	u	148/199 (74%)	146 (99%)	2 (1%)	0	100	100
55	v	291/344 (85%)	283 (97%)	8 (3%)	0	100	100
56	w	192/201 (96%)	190 (99%)	2 (1%)	0	100	100
57	x	500/514 (97%)	488 (98%)	12 (2%)	0	100	100
58	y	242/245 (99%)	232 (96%)	10 (4%)	0	100	100
59	z	83/106 (78%)	83 (100%)	0	0	100	100
60	4	534/593 (90%)	527 (99%)	7 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	10648/12402 (86%)	10401 (98%)	247 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/196 (85%)	166 (100%)	0	100	100
5	5	67/106 (63%)	67 (100%)	0	100	100
7	8	129/136 (95%)	128 (99%)	1 (1%)	73	81
8	9	106/153 (69%)	106 (100%)	0	100	100
9	B	322/323 (100%)	321 (100%)	1 (0%)	86	91
10	C	288/289 (100%)	286 (99%)	2 (1%)	76	83
11	D	226/245 (92%)	226 (100%)	0	100	100
12	E	133/153 (87%)	132 (99%)	1 (1%)	73	81
13	F	184/205 (90%)	184 (100%)	0	100	100
14	G	185/208 (89%)	185 (100%)	0	100	100
15	H	171/171 (100%)	169 (99%)	2 (1%)	63	74
16	I	117/141 (83%)	117 (100%)	0	100	100
17	J	148/150 (99%)	148 (100%)	0	100	100
18	K	247/346 (71%)	247 (100%)	0	100	100
19	L	142/159 (89%)	141 (99%)	1 (1%)	76	83
20	M	108/109 (99%)	108 (100%)	0	100	100
21	N	165/176 (94%)	165 (100%)	0	100	100
22	O	160/162 (99%)	159 (99%)	1 (1%)	78	85
23	P	141/146 (97%)	140 (99%)	1 (1%)	76	83
24	Q	121/151 (80%)	121 (100%)	0	100	100
25	R	129/154 (84%)	129 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	S	155/156 (99%)	155 (100%)	0	100	100
27	T	98/137 (72%)	98 (100%)	0	100	100
28	U	93/107 (87%)	93 (100%)	0	100	100
29	V	104/105 (99%)	104 (100%)	0	100	100
30	W	211/213 (99%)	210 (100%)	1 (0%)	81	87
31	X	116/118 (98%)	114 (98%)	2 (2%)	53	66
32	Y	109/110 (99%)	108 (99%)	1 (1%)	70	80
33	Z	115/116 (99%)	115 (100%)	0	100	100
34	a	76/119 (64%)	76 (100%)	0	100	100
35	b	568/573 (99%)	564 (99%)	4 (1%)	76	83
36	c	81/88 (92%)	81 (100%)	0	100	100
37	d	94/97 (97%)	94 (100%)	0	100	100
38	e	109/111 (98%)	108 (99%)	1 (1%)	70	80
39	f	90/91 (99%)	90 (100%)	0	100	100
40	g	95/103 (92%)	95 (100%)	0	100	100
41	h	104/105 (99%)	104 (100%)	0	100	100
42	i	81/82 (99%)	81 (100%)	0	100	100
43	j	69/71 (97%)	69 (100%)	0	100	100
44	k	68/69 (99%)	68 (100%)	0	100	100
45	l	45/46 (98%)	45 (100%)	0	100	100
46	m	411/428 (96%)	408 (99%)	3 (1%)	76	83
47	n	332/548 (61%)	332 (100%)	0	100	100
48	o	118/199 (59%)	117 (99%)	1 (1%)	73	81
49	p	71/72 (99%)	70 (99%)	1 (1%)	59	70
50	q	145/420 (34%)	144 (99%)	1 (1%)	76	83
51	r	203/229 (89%)	202 (100%)	1 (0%)	81	87
52	s	65/70 (93%)	65 (100%)	0	100	100
53	t	256/287 (89%)	255 (100%)	1 (0%)	84	89
54	u	133/180 (74%)	133 (100%)	0	100	100
55	v	264/309 (85%)	263 (100%)	1 (0%)	84	89
56	w	172/178 (97%)	171 (99%)	1 (1%)	78	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	x	442/450 (98%)	435 (98%)	7 (2%)	55	68
58	y	210/211 (100%)	210 (100%)	0	100	100
59	z	77/95 (81%)	77 (100%)	0	100	100
60	4	471/520 (91%)	467 (99%)	4 (1%)	73	81
All	All	9306/10692 (87%)	9266 (100%)	40 (0%)	81	89

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	w	166	VAL
57	x	450	VAL
57	x	75	VAL
57	x	159	MET
60	4	191	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
42	i	35	ASN
51	r	179	GLN
43	j	48	ASN
47	n	165	GLN
55	v	238	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	1	2976/3396 (87%)	512 (17%)	6 (0%)
3	2	157/158 (99%)	26 (16%)	0
4	3	120/121 (99%)	26 (21%)	0
6	6	54/74 (72%)	20 (37%)	0
All	All	3307/3749 (88%)	584 (17%)	6 (0%)

5 of 584 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	1	2	U
2	1	5	G

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Mol	Chain	Res	Type
2	1	14	U
2	1	26	A
2	1	42	C

5 of 6 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	1	1568	U
2	1	3121	U
2	1	3283	U
2	1	588	G
2	1	374	A

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

57 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	OMC	1	2197	2	19,22,23	0.48	0	25,31,34	0.66	0
2	OMG	1	867	2	23,26,27	1.11	4 (17%)	32,38,41	0.88	1 (3%)
2	OMG	1	1450	2,62	23,26,27	1.10	4 (17%)	32,38,41	0.81	0
2	PSU	1	2349	2,62	18,21,22	1.10	1 (5%)	21,30,33	1.49	6 (28%)
2	PSU	1	2880	2	18,21,22	1.19	1 (5%)	21,30,33	1.52	4 (19%)
2	PSU	1	2735	2	18,21,22	1.15	1 (5%)	21,30,33	1.57	4 (19%)
2	OMU	1	2421	2	19,22,23	0.83	1 (5%)	25,31,34	0.91	2 (8%)
2	PSU	1	2264	2	18,21,22	1.21	2 (11%)	21,30,33	1.56	4 (19%)
2	PSU	1	1124	2	18,21,22	1.18	1 (5%)	21,30,33	1.57	4 (19%)
2	PSU	1	2826	2,62	18,21,22	1.12	1 (5%)	21,30,33	1.64	4 (19%)
2	PSU	1	986	2	18,21,22	1.15	2 (11%)	21,30,33	1.46	4 (19%)
2	PSU	1	2865	2	18,21,22	1.21	2 (11%)	21,30,33	1.55	4 (19%)
2	OMU	1	2729	2	19,22,23	0.76	1 (5%)	25,31,34	0.93	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	1	2129	2	18,21,22	1.13	1 (5%)	21,30,33	1.52	4 (19%)
4	PSU	3	50	4	18,21,22	1.23	2 (11%)	21,30,33	1.60	4 (19%)
2	PSU	1	960	2	18,21,22	1.17	2 (11%)	21,30,33	1.49	4 (19%)
2	A2M	1	1133	2	22,25,26	1.37	2 (9%)	30,36,39	1.02	2 (6%)
2	OMU	1	2724	2	19,22,23	0.83	1 (5%)	25,31,34	0.85	1 (4%)
2	PSU	1	2351	2	18,21,22	1.16	1 (5%)	21,30,33	1.58	4 (19%)
2	PSU	1	1110	2	18,21,22	1.22	2 (11%)	21,30,33	1.54	5 (23%)
2	A2M	1	649	2	22,25,26	1.35	3 (13%)	30,36,39	0.99	2 (6%)
2	OMC	1	663	2	19,22,23	0.53	0	25,31,34	0.70	0
2	A2M	1	876	2	22,25,26	1.35	2 (9%)	30,36,39	0.92	1 (3%)
2	OMG	1	908	2	23,26,27	1.17	4 (17%)	32,38,41	0.89	1 (3%)
2	OMC	1	1437	2,62	19,22,23	0.57	0	25,31,34	1.01	1 (4%)
2	PSU	1	2266	2	18,21,22	1.20	2 (11%)	21,30,33	1.54	5 (23%)
2	PSU	1	2314	2	18,21,22	1.14	1 (5%)	21,30,33	1.54	4 (19%)
2	OMU	1	2417	2	19,22,23	0.81	1 (5%)	25,31,34	0.91	2 (8%)
2	OMG	1	2815	2	23,26,27	1.16	4 (17%)	32,38,41	0.88	1 (3%)
2	OMC	1	2959	2	19,22,23	0.54	0	25,31,34	0.81	1 (4%)
3	PSU	2	73	3	18,21,22	1.10	1 (5%)	21,30,33	1.56	4 (19%)
2	A2M	1	817	2,62	22,25,26	1.33	2 (9%)	30,36,39	0.97	2 (6%)
2	1MA	1	2142	2,62	21,25,26	0.50	0	30,37,40	0.81	1 (3%)
2	OMG	1	805	2	23,26,27	1.14	4 (17%)	32,38,41	0.93	1 (3%)
2	OMG	1	2793	2	23,26,27	1.21	4 (17%)	32,38,41	0.98	1 (3%)
2	OMU	1	2921	2	19,22,23	0.90	1 (5%)	25,31,34	0.93	2 (8%)
2	OMU	1	898	2	19,22,23	0.76	1 (5%)	25,31,34	0.93	2 (8%)
2	OMC	1	650	2	19,22,23	0.52	0	25,31,34	0.65	0
2	PSU	1	966	2	18,21,22	1.24	3 (16%)	21,30,33	1.57	4 (19%)
2	A2M	1	807	2	22,25,26	1.39	3 (13%)	30,36,39	0.96	2 (6%)
2	PSU	1	776	2	18,21,22	1.23	3 (16%)	21,30,33	1.58	4 (19%)
2	PSU	1	990	2	18,21,22	1.16	1 (5%)	21,30,33	1.51	4 (19%)
2	OMU	1	1888	2	19,22,23	1.17	1 (5%)	25,31,34	1.34	4 (16%)
2	PSU	1	2133	2	18,21,22	1.04	1 (5%)	21,30,33	1.62	4 (19%)
2	5MC	1	2278	2	19,22,23	1.66	3 (15%)	26,32,35	1.11	3 (11%)
2	PSU	1	2340	2	18,21,22	1.13	1 (5%)	21,30,33	1.57	4 (19%)
2	OMC	1	2948	2	19,22,23	0.52	0	25,31,34	0.88	1 (4%)
2	PSU	1	2416	2	18,21,22	1.18	1 (5%)	21,30,33	1.62	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OMG	1	2791	2	23,26,27	1.20	4 (17%)	32,38,41	0.89	1 (3%)
2	PSU	1	2191	2	18,21,22	1.15	1 (5%)	21,30,33	1.59	4 (19%)
2	OMU	1	2347	2	19,22,23	0.83	1 (5%)	25,31,34	0.82	1 (4%)
2	5MC	1	2870	2	19,22,23	1.57	3 (15%)	26,32,35	1.15	2 (7%)
2	PSU	1	2923	2	18,21,22	1.25	3 (16%)	21,30,33	1.30	5 (23%)
2	A2M	1	2220	2	22,25,26	1.50	4 (18%)	30,36,39	1.08	3 (10%)
2	PSU	1	2975	2	18,21,22	1.14	1 (5%)	21,30,33	1.67	4 (19%)
2	OMC	1	2337	2	19,22,23	0.50	0	25,31,34	0.69	0
2	A2M	1	1449	2,62	22,25,26	1.30	2 (9%)	30,36,39	0.94	2 (6%)

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
2	OMC	1	2197	2	-	2/9/27/28	0/2/2/2
2	OMG	1	867	2	-	0/9/27/28	0/3/3/3
2	OMG	1	1450	2,62	-	2/9/27/28	0/3/3/3
2	PSU	1	2349	2,62	-	0/7/25/26	0/2/2/2
2	PSU	1	2880	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2735	2	-	0/7/25/26	0/2/2/2
2	OMU	1	2421	2	-	2/9/27/28	0/2/2/2
2	PSU	1	2264	2	-	0/7/25/26	0/2/2/2
2	PSU	1	1124	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2826	2,62	-	1/7/25/26	0/2/2/2
2	PSU	1	986	2	-	1/7/25/26	0/2/2/2
2	PSU	1	2865	2	-	2/7/25/26	0/2/2/2
2	OMU	1	2729	2	-	0/9/27/28	0/2/2/2
2	PSU	1	2129	2	-	0/7/25/26	0/2/2/2
4	PSU	3	50	4	-	2/7/25/26	0/2/2/2
2	PSU	1	960	2	-	2/7/25/26	0/2/2/2
2	A2M	1	1133	2	-	0/9/27/28	0/3/3/3
2	OMU	1	2724	2	-	0/9/27/28	0/2/2/2
2	PSU	1	2351	2	-	0/7/25/26	0/2/2/2
2	PSU	1	1110	2	-	0/7/25/26	0/2/2/2
2	A2M	1	649	2	-	3/9/27/28	0/3/3/3
2	OMC	1	663	2	-	1/9/27/28	0/2/2/2
2	A2M	1	876	2	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMG	1	908	2	-	0/9/27/28	0/3/3/3
2	OMC	1	1437	2,62	-	4/9/27/28	0/2/2/2
2	PSU	1	2266	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2314	2	-	0/7/25/26	0/2/2/2
2	OMU	1	2417	2	-	2/9/27/28	0/2/2/2
2	OMG	1	2815	2	-	0/9/27/28	0/3/3/3
2	OMC	1	2959	2	-	0/9/27/28	0/2/2/2
3	PSU	2	73	3	-	0/7/25/26	0/2/2/2
2	A2M	1	817	2,62	-	2/9/27/28	0/3/3/3
2	1MA	1	2142	2,62	-	2/7/25/26	0/3/3/3
2	OMG	1	805	2	-	1/9/27/28	0/3/3/3
2	OMG	1	2793	2	-	0/9/27/28	0/3/3/3
2	OMU	1	2921	2	-	7/9/27/28	0/2/2/2
2	OMU	1	898	2	-	0/9/27/28	0/2/2/2
2	OMC	1	650	2	-	0/9/27/28	0/2/2/2
2	PSU	1	966	2	-	0/7/25/26	0/2/2/2
2	A2M	1	807	2	-	0/9/27/28	0/3/3/3
2	PSU	1	776	2	-	2/7/25/26	0/2/2/2
2	PSU	1	990	2	-	0/7/25/26	0/2/2/2
2	OMU	1	1888	2	-	2/9/27/28	0/2/2/2
2	PSU	1	2133	2	-	0/7/25/26	0/2/2/2
2	5MC	1	2278	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2340	2	-	3/7/25/26	0/2/2/2
2	OMC	1	2948	2	-	2/9/27/28	0/2/2/2
2	PSU	1	2416	2	-	3/7/25/26	0/2/2/2
2	OMG	1	2791	2	-	3/9/27/28	0/3/3/3
2	PSU	1	2191	2	-	0/7/25/26	0/2/2/2
2	OMU	1	2347	2	-	0/9/27/28	0/2/2/2
2	5MC	1	2870	2	-	0/7/25/26	0/2/2/2
2	PSU	1	2923	2	-	3/7/25/26	0/2/2/2
2	A2M	1	2220	2	-	2/9/27/28	0/3/3/3
2	PSU	1	2975	2	-	0/7/25/26	0/2/2/2
2	OMC	1	2337	2	-	0/9/27/28	0/2/2/2
2	A2M	1	1449	2,62	-	0/9/27/28	0/3/3/3

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2278	5MC	C5-C4	6.02	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2870	5MC	C5-C4	5.65	1.48	1.44
2	1	1888	OMU	C2-N1	4.53	1.45	1.38
2	1	876	A2M	O5'-C5'	-3.67	1.33	1.44
2	1	1449	A2M	O5'-C5'	-3.64	1.33	1.44

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	1	2975	PSU	C6-C5-C4	4.69	121.34	118.17
2	1	2865	PSU	C6-C5-C4	4.69	121.34	118.17
4	3	50	PSU	C6-C5-C4	4.62	121.29	118.17
2	1	2826	PSU	C6-C5-C4	4.56	121.25	118.17
2	1	2416	PSU	C6-C5-C4	4.52	121.23	118.17

There are no chirality outliers.

5 of 56 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1	776	PSU	C3'-C4'-C5'-O5'
2	1	776	PSU	O4'-C4'-C5'-O5'
2	1	960	PSU	O4'-C4'-C5'-O5'
2	1	1437	OMC	C1'-C2'-O2'-CM2
2	1	1450	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

19 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	1450	OMG	1	0
2	1	2880	PSU	1	0
2	1	986	PSU	1	0
2	1	1133	A2M	1	0
2	1	2724	OMU	2	0
2	1	663	OMC	2	0
2	1	876	A2M	1	0
2	1	908	OMG	1	0
2	1	1437	OMC	2	0
2	1	2314	PSU	1	0
2	1	2417	OMU	1	0
2	1	2959	OMC	2	0
2	1	2793	OMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1	898	OMU	2	0
2	1	807	A2M	1	0
2	1	2191	PSU	1	0
2	1	2347	OMU	1	0
2	1	2220	A2M	2	0
2	1	1449	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 93 ligands modelled in this entry, 87 are monoatomic - leaving 6 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
61	B3P	1	3403	-	18,18,18	1.58	2 (11%)	23,23,23	1.88	6 (26%)
61	B3P	1	3401	62	18,18,18	1.50	2 (11%)	23,23,23	1.87	6 (26%)
61	B3P	1	3402	-	18,18,18	1.52	2 (11%)	23,23,23	1.92	6 (26%)
64	GDP	m	801	66,62,65	29,30,30	1.17	3 (10%)	45,47,47	1.73	6 (13%)
65	ALF	m	802	67,64	4,4,4	1.45	0	-		
64	GDP	b	801	62	29,30,30	1.15	3 (10%)	45,47,47	1.74	6 (13%)

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
61	B3P	1	3403	-	-	8/28/28/28	-
61	B3P	1	3401	62	-	4/28/28/28	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	B3P	1	3402	-	-	11/28/28/28	-
64	GDP	m	801	66,62,65	-	3/16/32/32	0/3/3/3
64	GDP	b	801	62	-	3/16/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	1	3403	B3P	C6-C4	5.36	1.59	1.53
61	1	3402	B3P	C6-C4	5.04	1.59	1.53
61	1	3401	B3P	C6-C4	5.02	1.59	1.53
64	b	801	GDP	C5-C4	3.07	1.47	1.38
64	m	801	GDP	C5-C4	3.05	1.47	1.38

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
64	b	801	GDP	C5-C4-N3	-6.00	118.84	128.39
64	m	801	GDP	C5-C4-N3	-5.83	119.10	128.39
61	1	3403	B3P	O5-C6-C4	5.06	121.98	111.68
61	1	3402	B3P	O5-C6-C4	5.02	121.88	111.68
64	b	801	GDP	C2-N3-C4	4.97	120.86	112.30

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

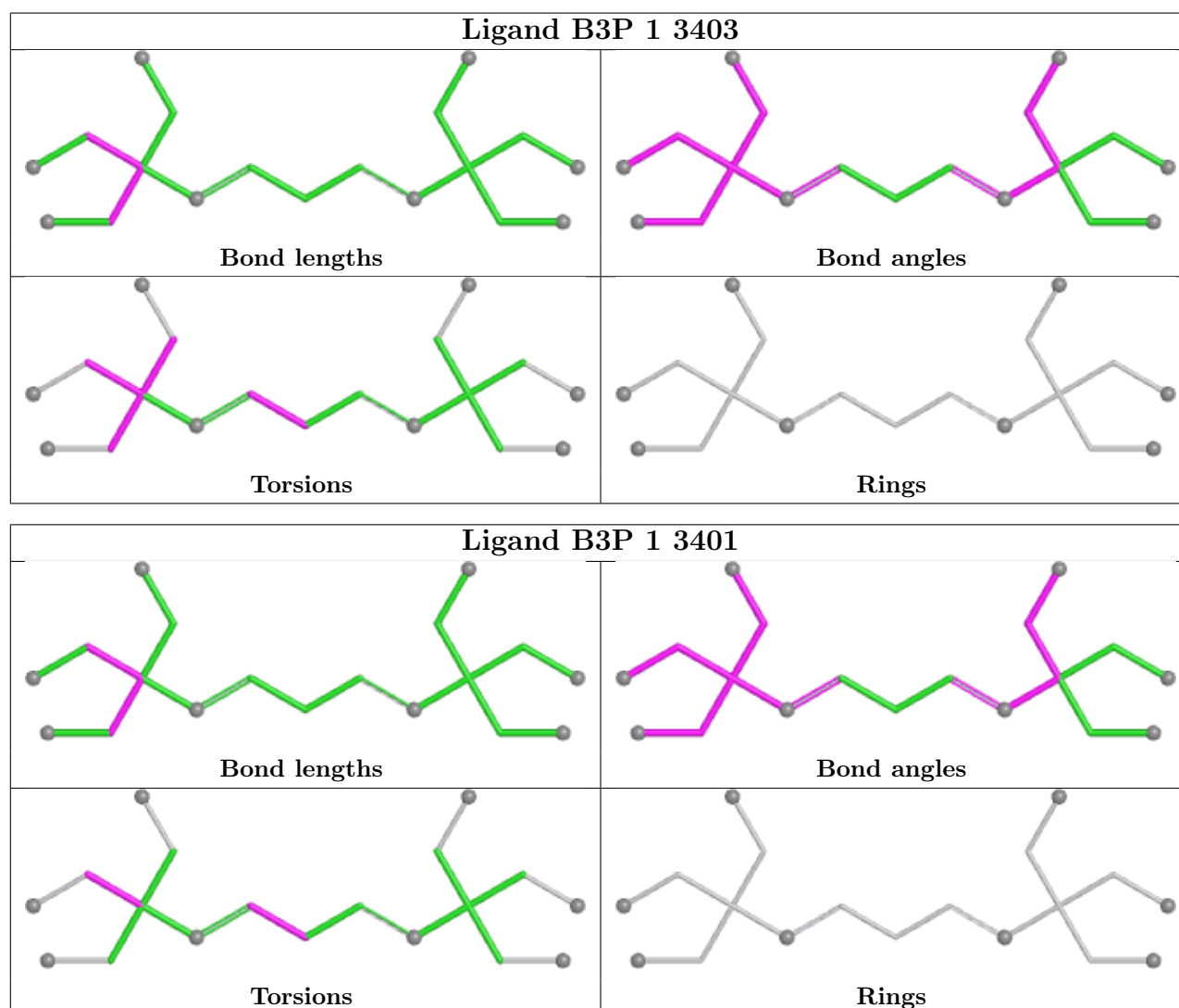
Mol	Chain	Res	Type	Atoms
61	1	3401	B3P	N1-C4-C6-O5
61	1	3401	B3P	C5-C4-C6-O5
61	1	3401	B3P	C7-C4-C6-O5
61	1	3402	B3P	N1-C4-C5-O4
61	1	3402	B3P	C6-C4-C5-O4

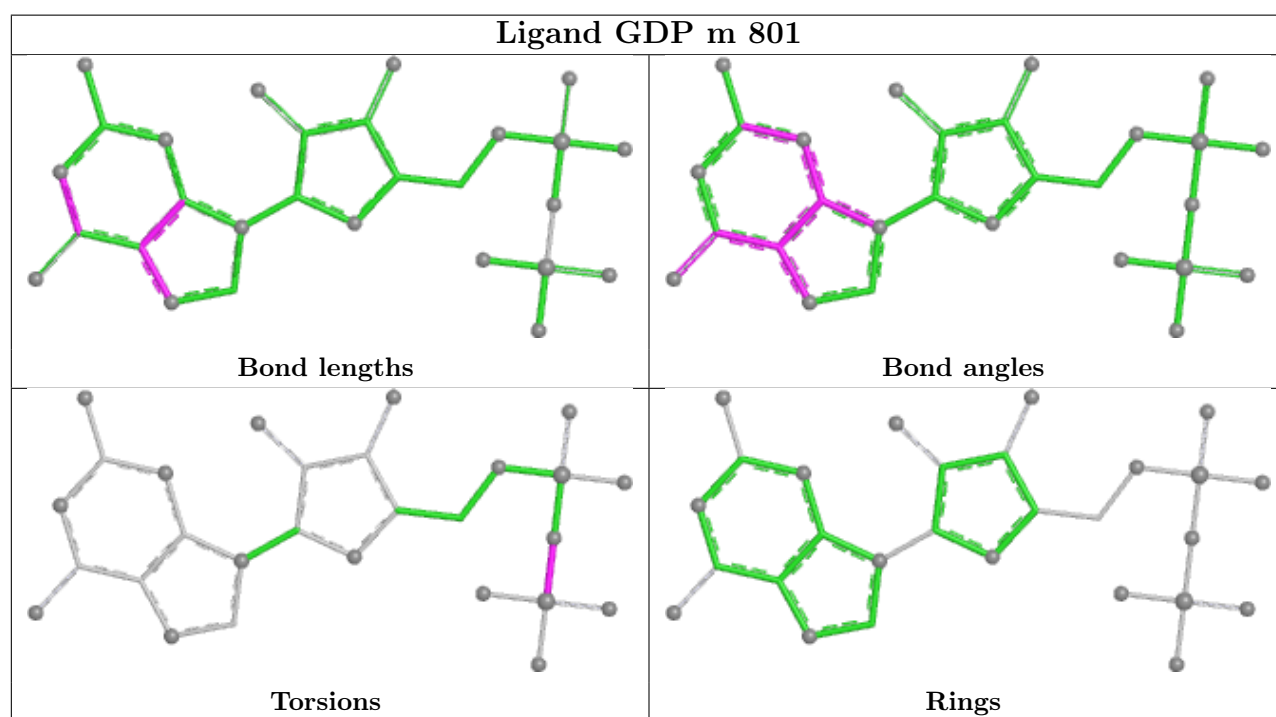
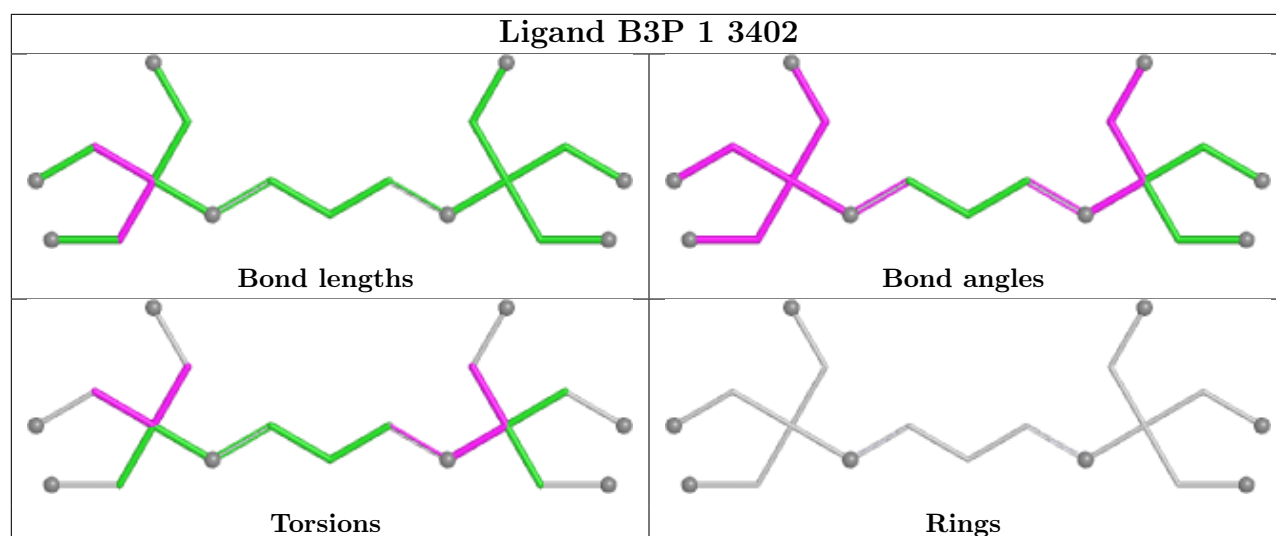
There are no ring outliers.

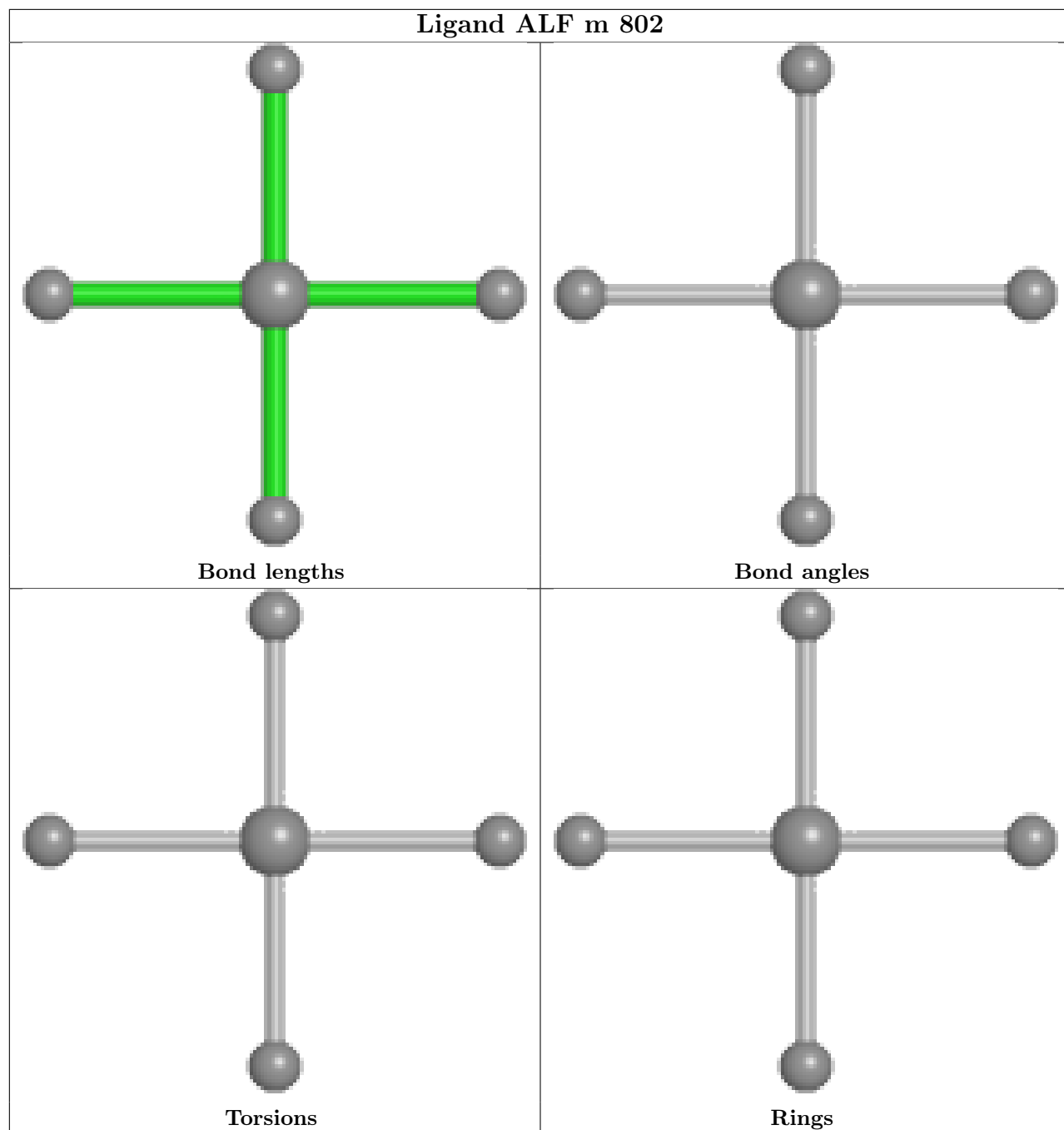
4 monomers are involved in 7 short contacts:

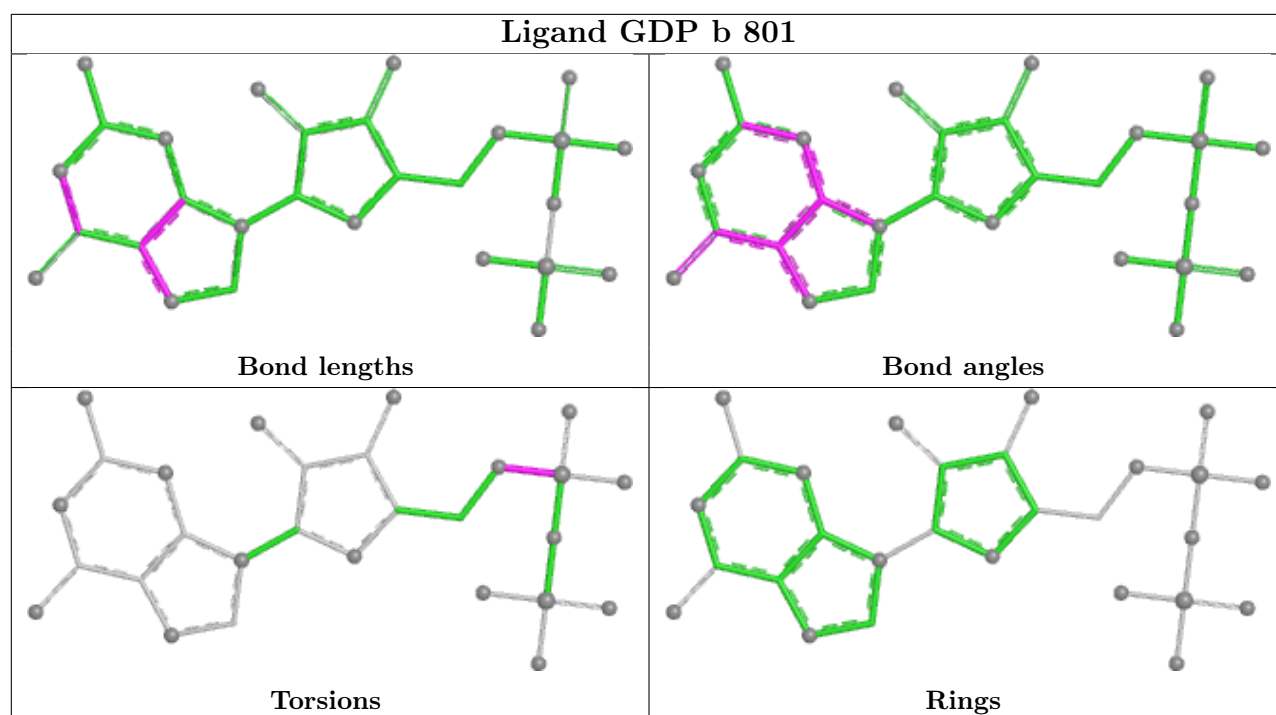
Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	1	3403	B3P	2	0
61	1	3401	B3P	3	0
65	m	802	ALF	1	0
64	b	801	GDP	1	0

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









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.

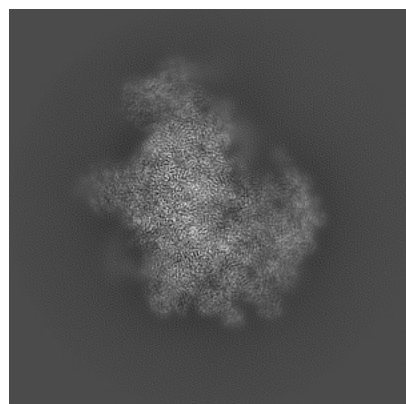
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26686. These allow visual inspection of the internal detail of the map and identification of artifacts.

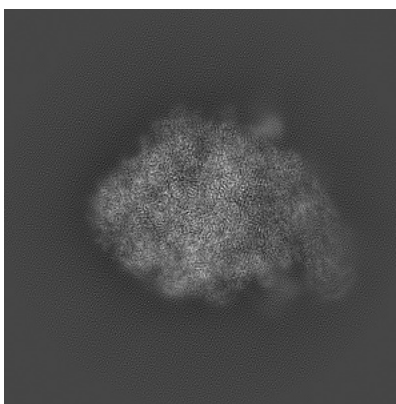
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

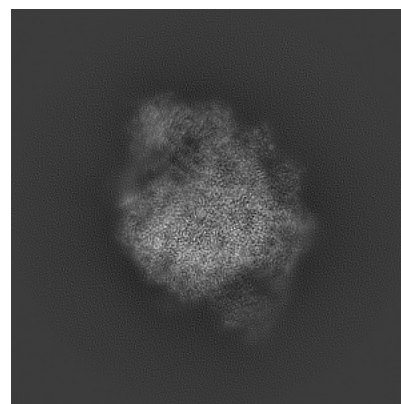
6.1.1 Primary map



X

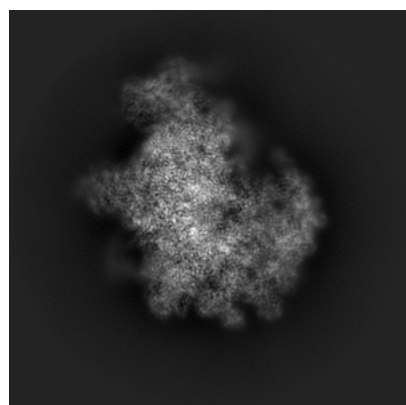


Y

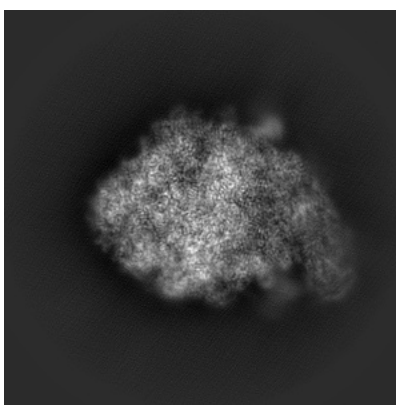


Z

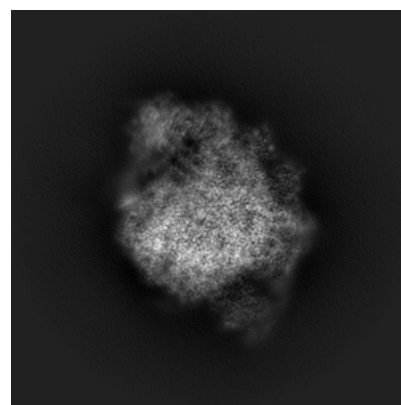
6.1.2 Raw map



X



Y

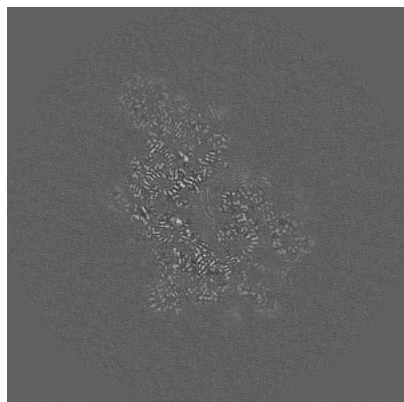


Z

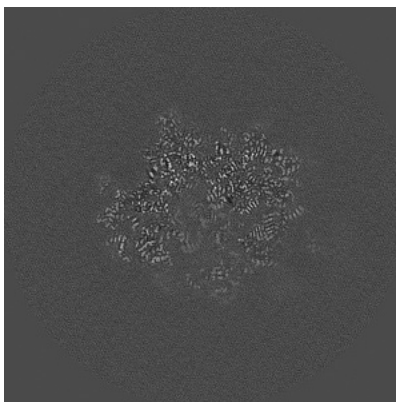
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

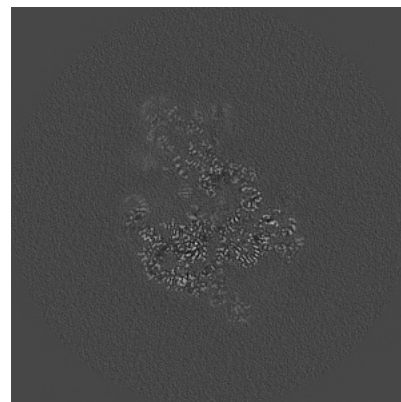
6.2.1 Primary map



X Index: 200

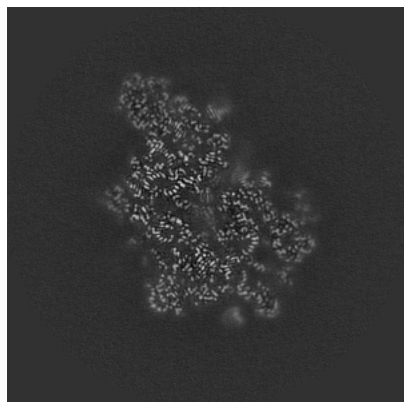


Y Index: 200

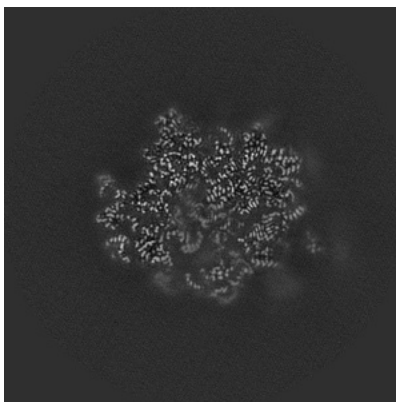


Z Index: 200

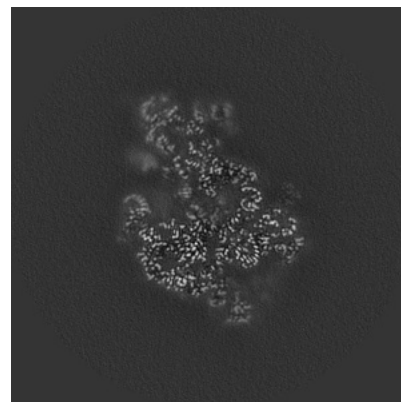
6.2.2 Raw map



X Index: 200



Y Index: 200

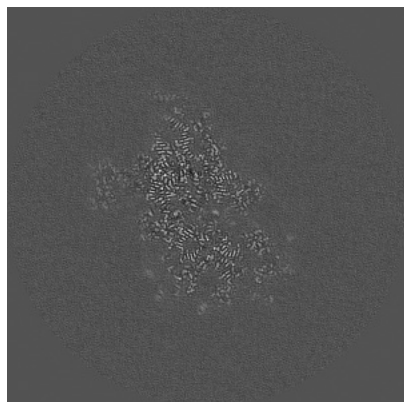


Z Index: 200

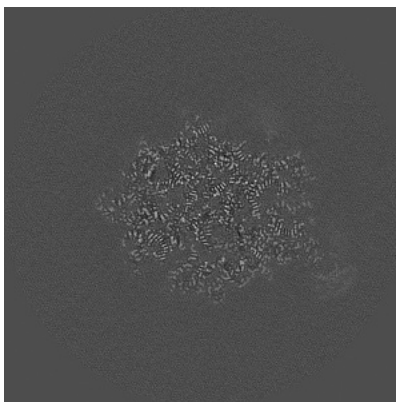
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

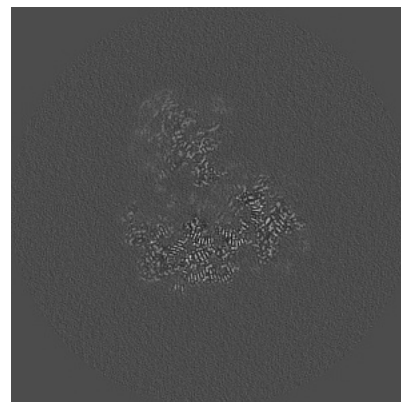
6.3.1 Primary map



X Index: 224

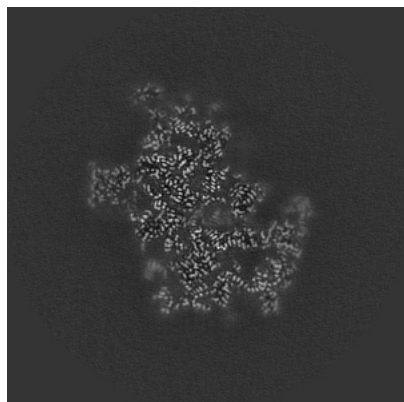


Y Index: 174

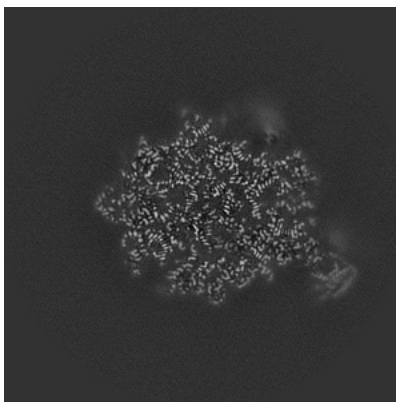


Z Index: 189

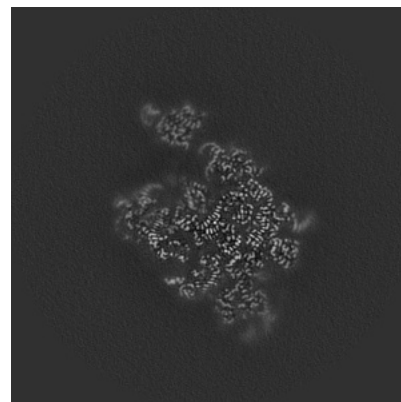
6.3.2 Raw map



X Index: 216



Y Index: 174

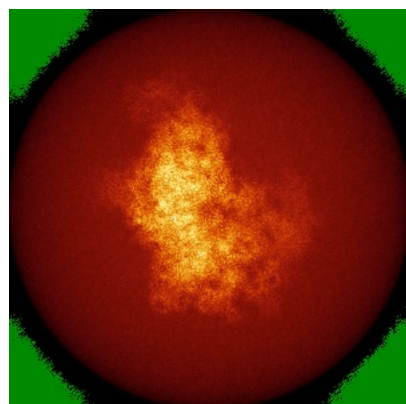


Z Index: 221

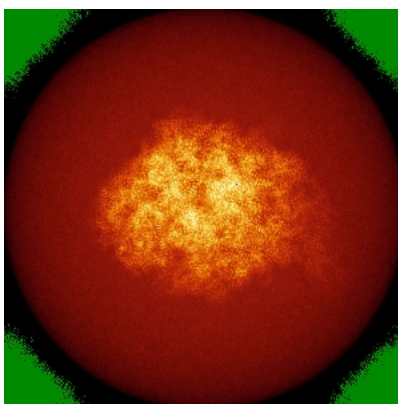
The images above show the largest variance slices of the map in three orthogonal directions.

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

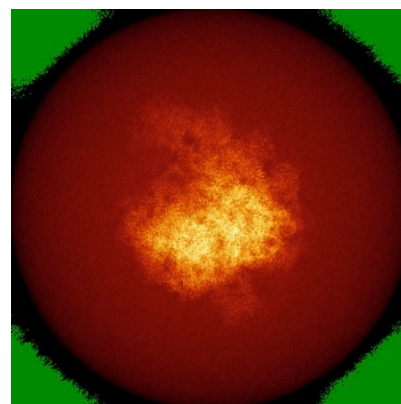
6.4.1 Primary map



X

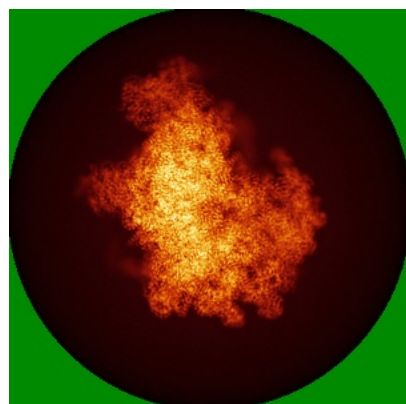


Y



Z

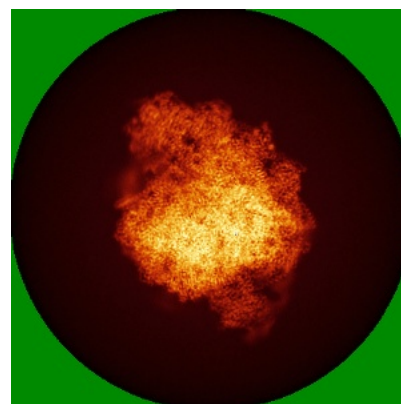
6.4.2 Raw map



X



Y

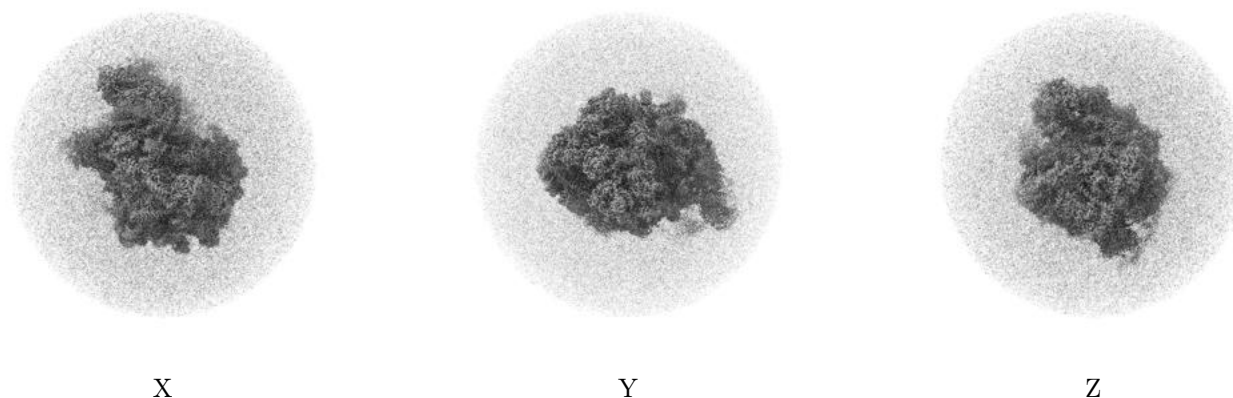


Z

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.

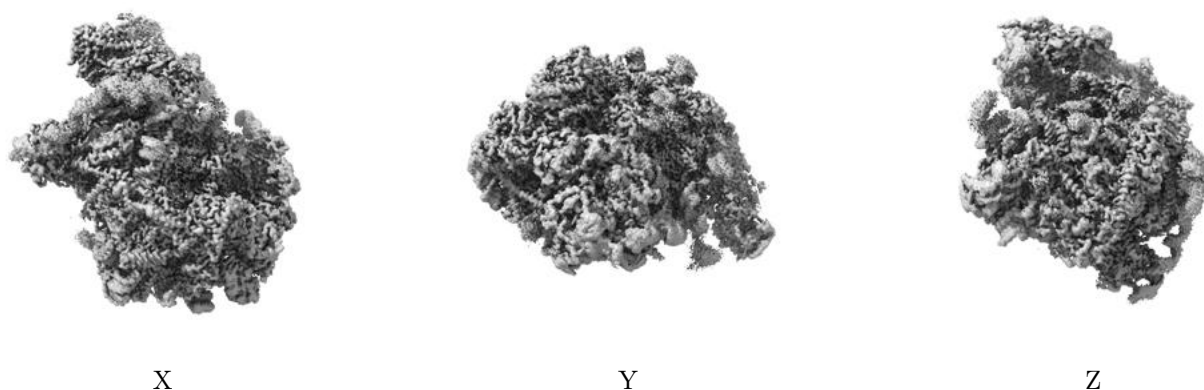
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. 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.

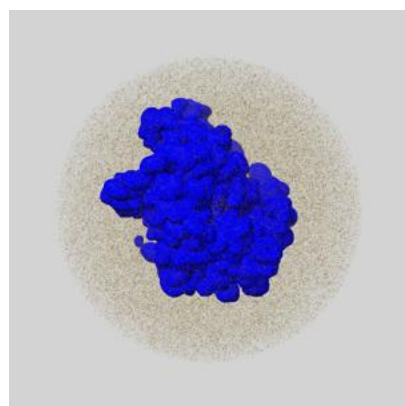
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

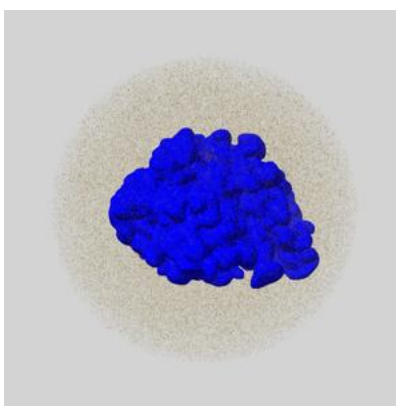
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

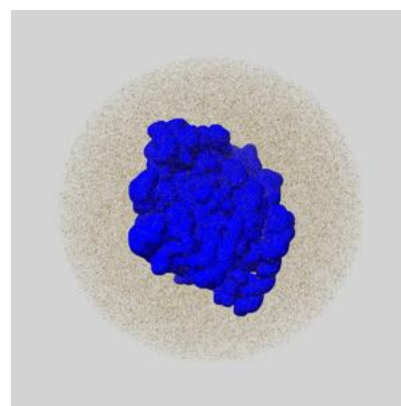
6.6.1 emd_26686_msk_1.map [i](#)



X



Y

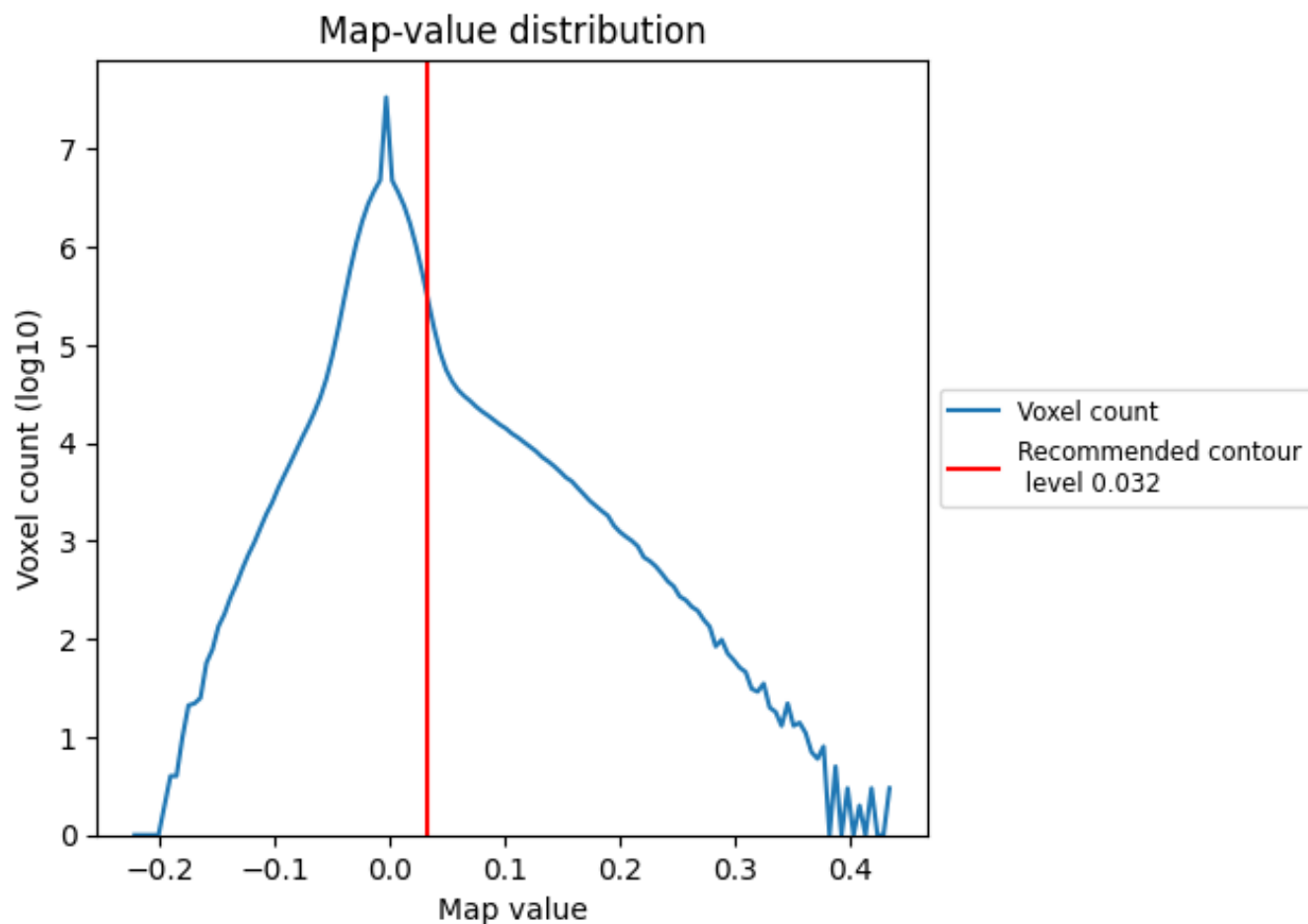


Z

7 Map analysis [i](#)

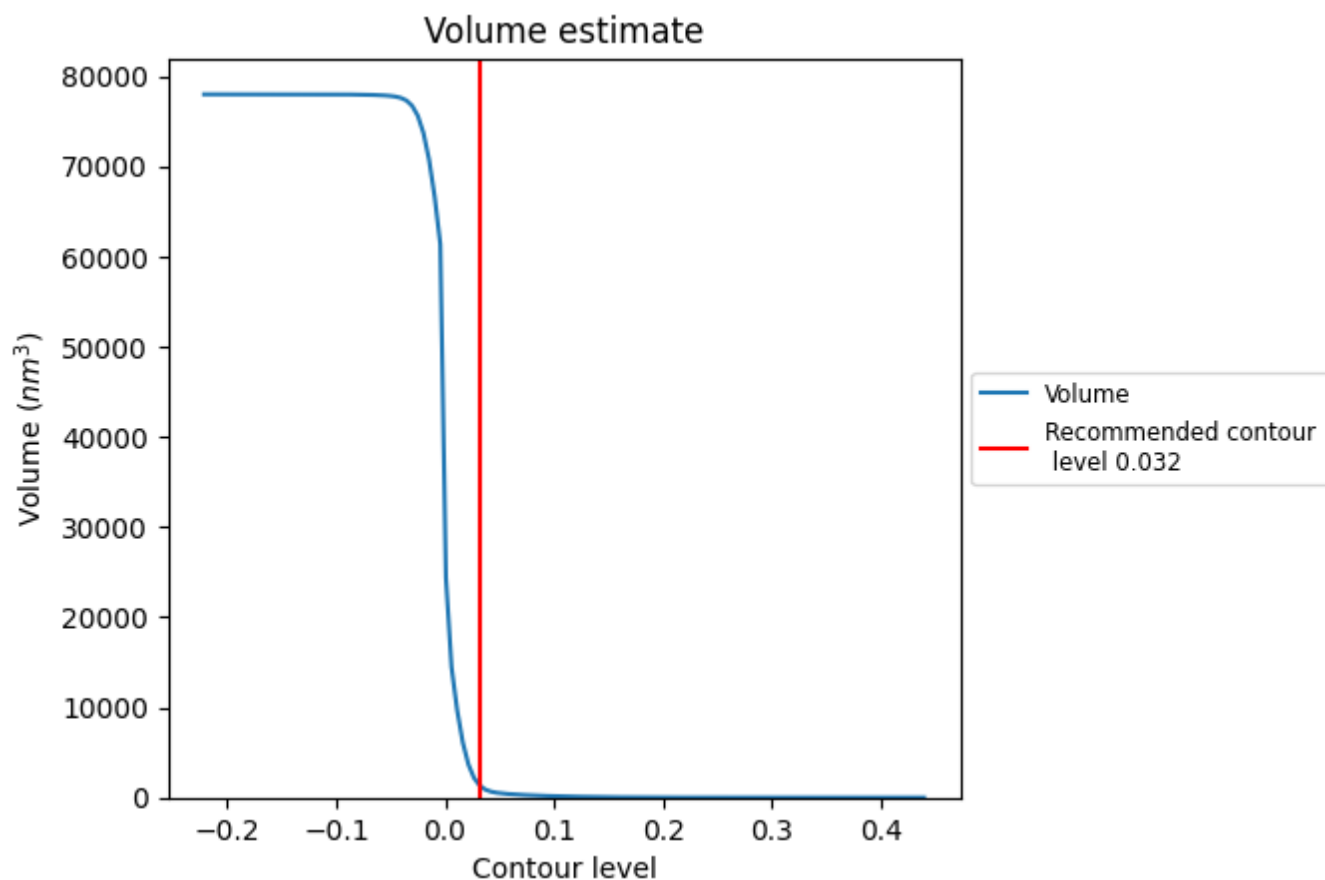
This section contains the results of statistical analysis of the map.

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.

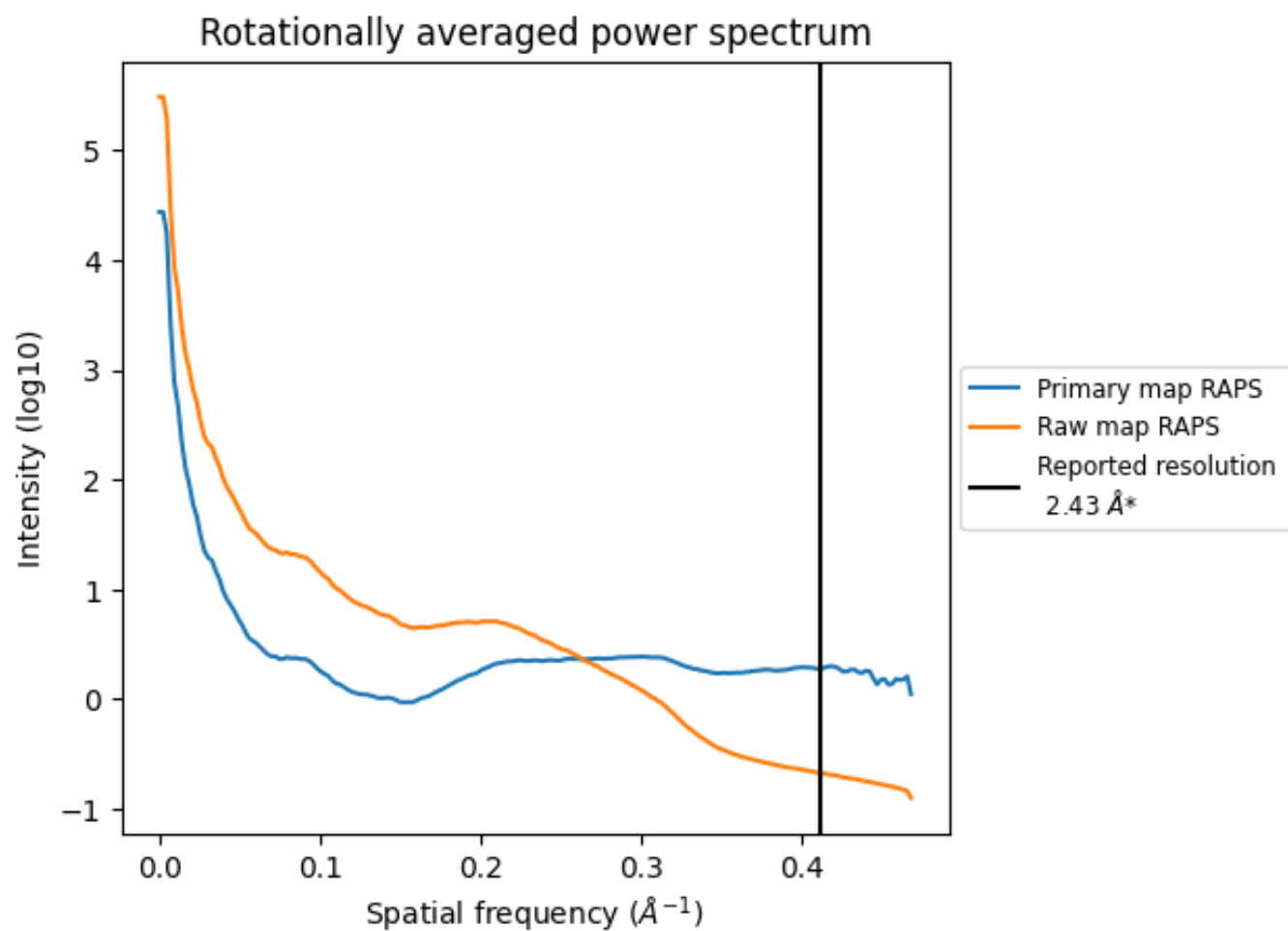
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1308 nm^3 ; this corresponds to an approximate mass of 1181 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 ⓘ

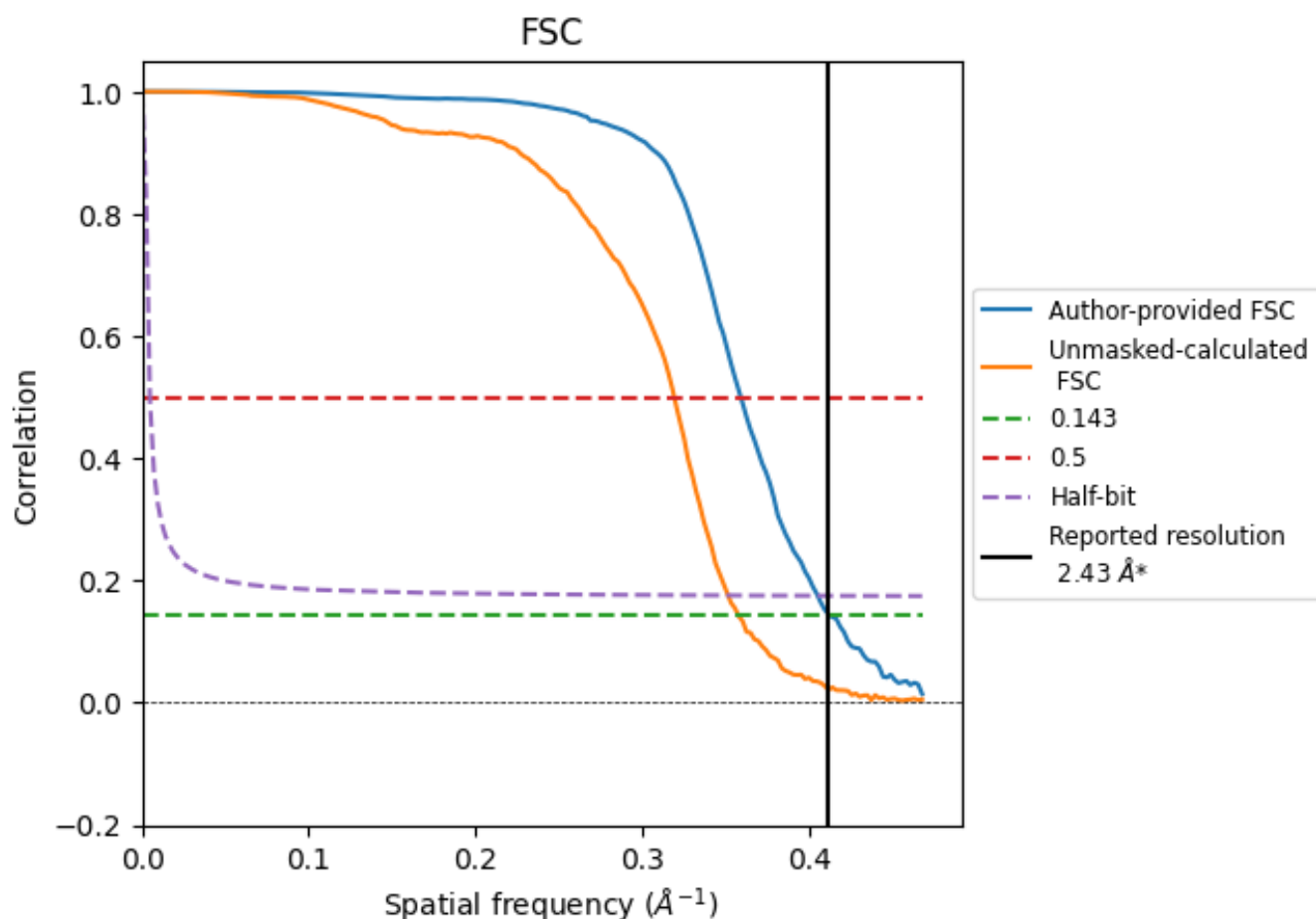


*Reported resolution corresponds to spatial frequency of 0.412 Å⁻¹

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 0.412 Å⁻¹

8.2 Resolution estimates [i](#)

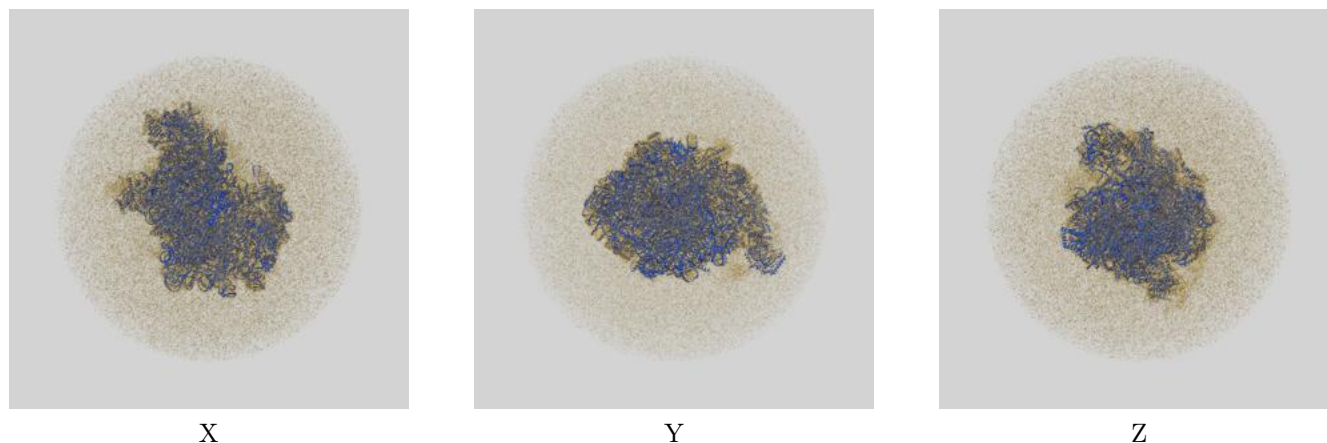
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.43	-	-
Author-provided FSC curve	2.42	2.78	2.47
Unmasked-calculated*	2.79	3.13	2.84

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.79 differs from the reported value 2.43 by more than 10 %

9 Map-model fit [i](#)

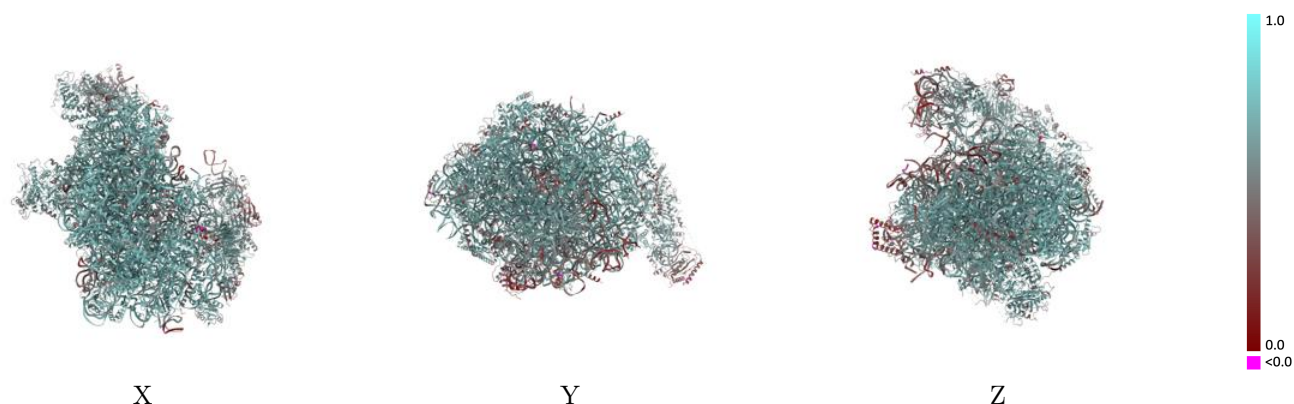
This section contains information regarding the fit between EMDB map EMD-26686 and PDB model 7UQB. Per-residue inclusion information can be found in section [3](#) on page [19](#).

9.1 Map-model overlay [i](#)



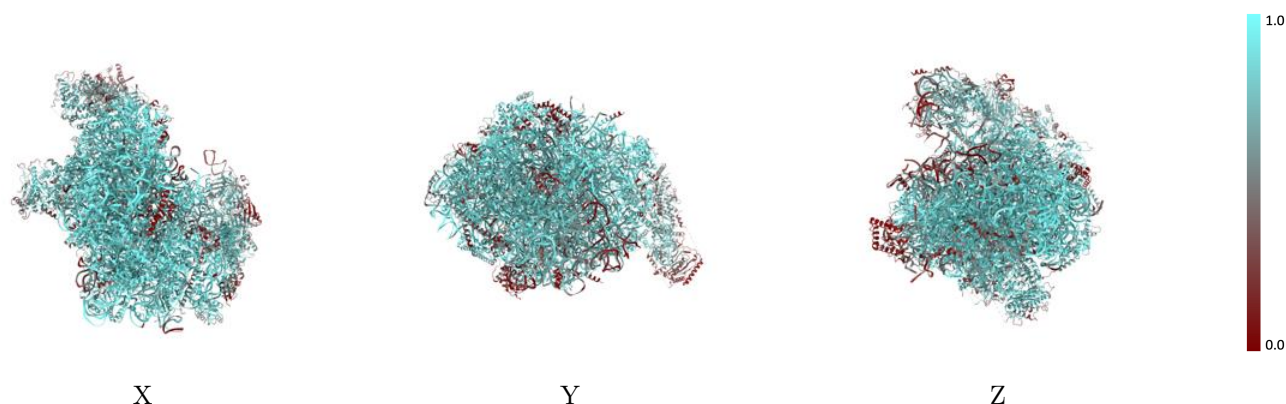
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



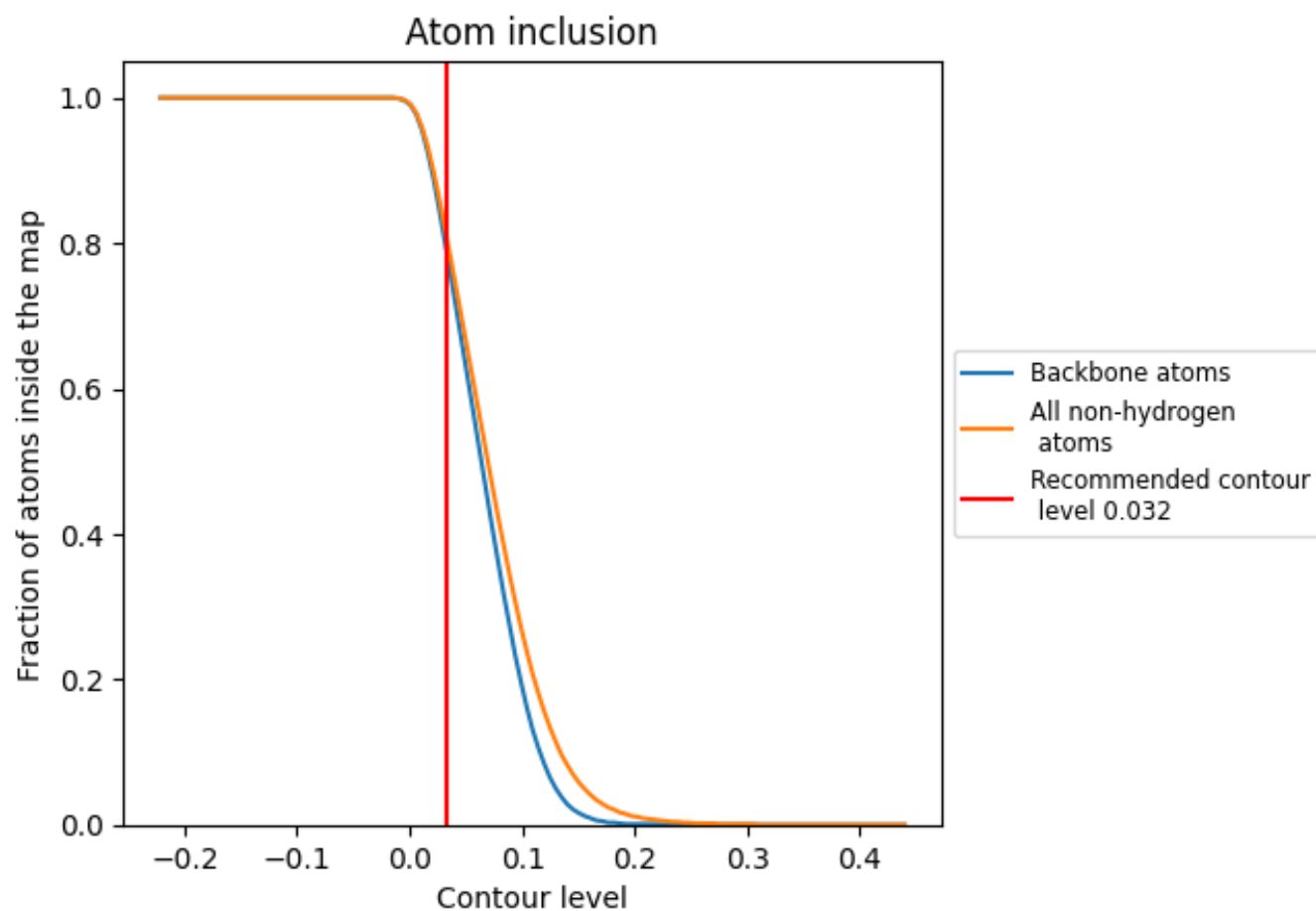
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 82% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8160	 0.6210
1	 0.8720	 0.6290
2	 0.9540	 0.6800
3	 0.5990	 0.4310
4	 0.7440	 0.6080
5	 0.2570	 0.3740
6	 0.6030	 0.4860
8	 0.3960	 0.4670
9	 0.7670	 0.6320
A	 0.9180	 0.7000
B	 0.9610	 0.7140
C	 0.9270	 0.6900
D	 0.6470	 0.5310
E	 0.8630	 0.6550
F	 0.9240	 0.6830
G	 0.8640	 0.6470
H	 0.8800	 0.6620
I	 0.1450	 0.4980
J	 0.2870	 0.3590
K	 0.3370	 0.4190
L	 0.8160	 0.6290
M	 0.9150	 0.6790
N	 0.9480	 0.6940
O	 0.9500	 0.7090
P	 0.9310	 0.6970
Q	 0.8540	 0.6410
R	 0.8990	 0.6770
S	 0.8510	 0.6460
T	 0.6730	 0.5630
U	 0.8470	 0.6440
V	 0.9210	 0.6900
W	 0.7370	 0.5850
X	 0.9310	 0.6890
Y	 0.9110	 0.6810
Z	 0.8690	 0.6480



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Chain	Atom inclusion	Q-score
a	 0.8140	 0.6220
b	 0.8150	 0.6310
c	 0.8540	 0.6340
d	 0.8830	 0.6770
e	 0.9280	 0.6980
f	 0.9700	 0.7170
g	 0.8910	 0.6720
h	 0.9110	 0.6830
i	 0.7560	 0.5950
j	 0.9750	 0.7210
k	 0.7530	 0.6110
l	 0.9780	 0.7270
m	 0.8290	 0.6430
n	 0.7380	 0.6000
o	 0.5210	 0.4940
p	 0.9000	 0.6800
q	 0.6300	 0.5600
r	 0.8970	 0.6810
s	 0.6630	 0.5620
t	 0.5740	 0.5400
u	 0.8720	 0.6640
v	 0.6990	 0.5710
w	 0.6670	 0.5720
x	 0.7100	 0.5680
y	 0.8790	 0.6620
z	 0.8250	 0.6400