



## wwPDB EM Validation Summary Report ⓘ

Jun 21, 2026 – 01:59 am BST

PDB ID : 8B2L / pdb\_00008b2l  
EMDB ID : EMD-15806  
Title : Cryo-EM structure of the plant 80S ribosome  
Authors : Smirnova, J.; Loerke, J.; Kleinau, G.; Schmidt, A.; Buerger, J.; Meyer, E.H.; Mielke, T.; Scheerer, P.; Bock, R.; Spahn, C.M.T.; Zoschke, R.  
Deposited on : 2022-09-14  
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

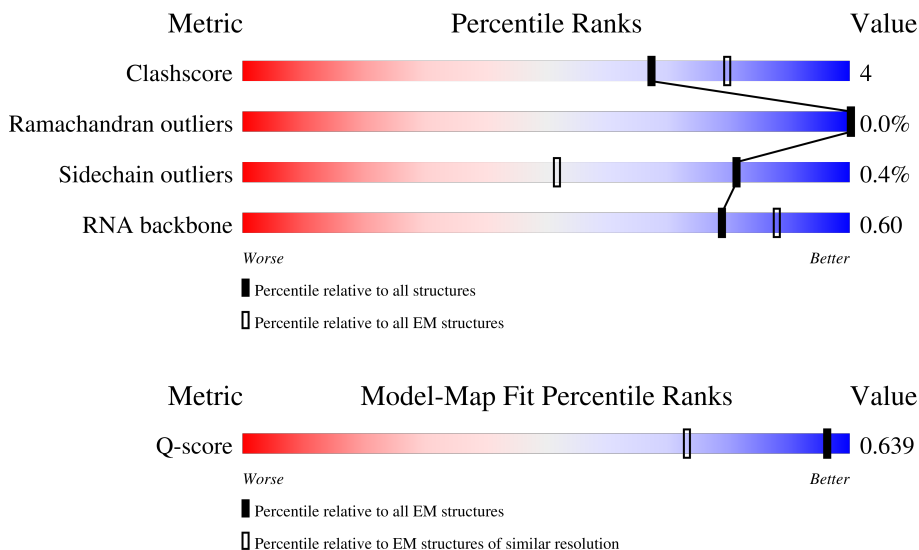
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.20 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.




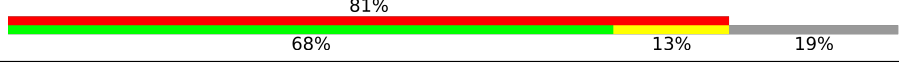
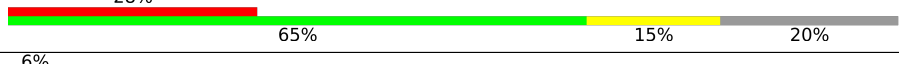


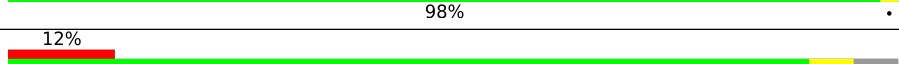
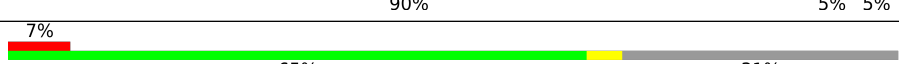
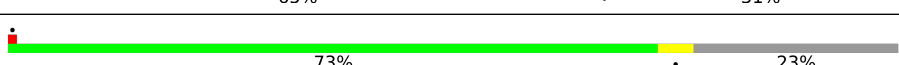
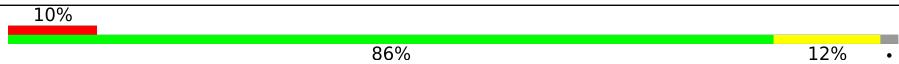



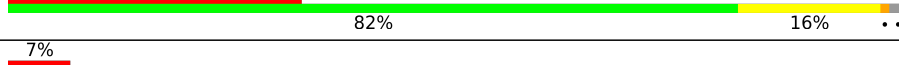

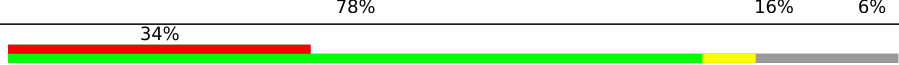

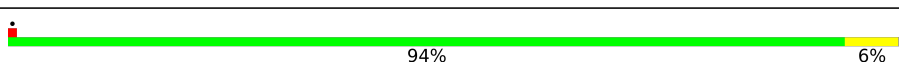

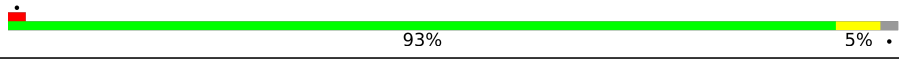

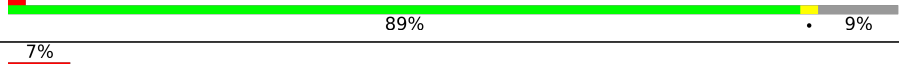




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3184 ( 1.71 - 2.70 )

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

Mol	Chain	Length	Quality of chain
1	A1	264	
2	k1	249	
3	h1	1808	

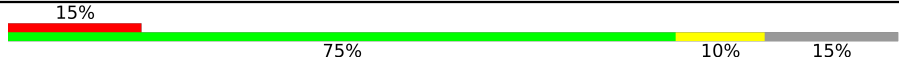







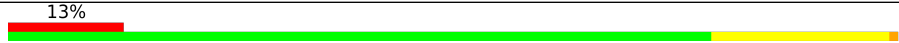

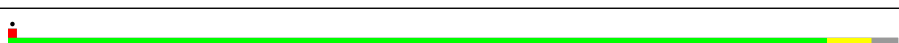

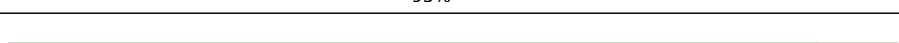
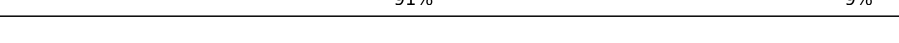
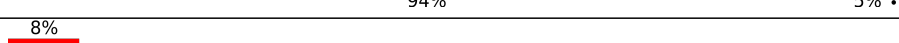
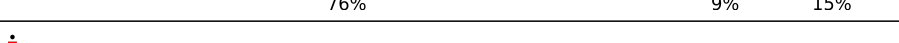
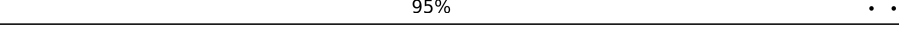
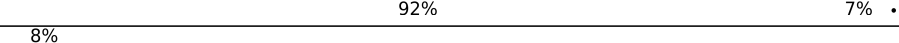
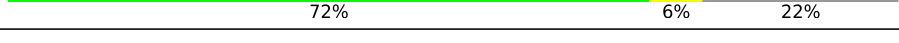

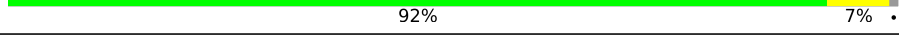
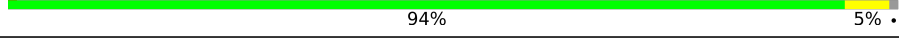



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Mol	Chain	Length	Quality of chain
4	I1	208	
5	C1	144	
6	D1	149	
7	E1	143	
8	F1	261	
9	G1	83	
10	H1	133	
11	I1	107	
12	J1	127	
13	K1	86	
14	L1	65	
15	M1	62	
16	N1	156	
17	O1	191	
18	P1	224	
19	Q1	328	
20	R1	122	
21	S1	150	
22	T1	142	
23	U1	152	
24	V1	56	
25	W1	151	
26	X1	159	
27	Y1	152	
28	Z1	336	

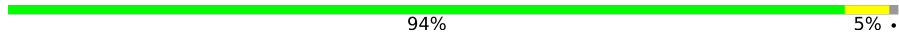







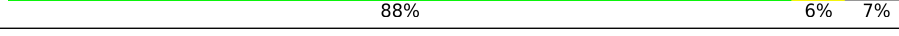


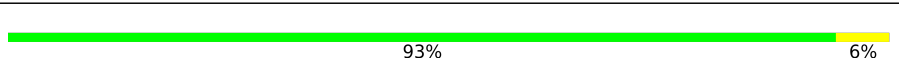






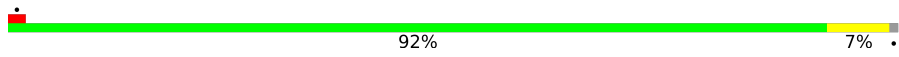
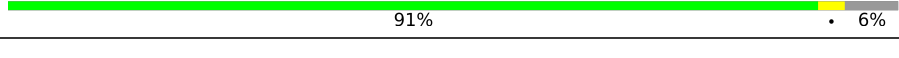
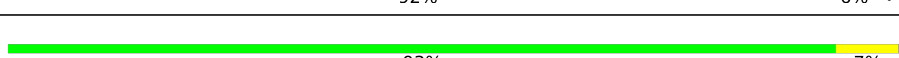
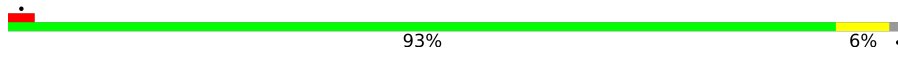



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Mol	Chain	Length	Quality of chain
29	a1	248	
30	b1	197	
31	c1	280	
32	d1	210	
33	e1	130	
34	f1	147	
35	B1	12	
36	W2	76	
36	i2	76	
37	C3	119	
38	D3	206	
39	E3	134	
40	F3	204	
41	G3	187	
42	H3	214	
43	I3	178	
44	J3	164	
45	K3	127	
46	L3	164	
47	M3	135	
48	N3	143	
49	O3	61	
50	P3	113	
51	Q3	120	
52	R3	133	

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Mol	Chain	Length	Quality of chain
53	S3	112	 94% 5%
54	T3	120	 5% 89% 6% 5%
55	U3	110	 87% 11%
56	V3	95	 87% 9%
57	W3	69	 84% 13%
58	X3	51	 90% 8%
59	Y3	128	 38% 60%
60	p3	25	 84% 16%
61	Z3	105	 88% 6% 7%
62	a3	92	 87% 12%
63	b3	230	 7% 85% 5% 10%
64	c3	258	 5% 86% 5% 10%
65	d3	206	 93% 6%
66	e3	140	 85% 9% 6%
67	f3	148	 91% 9%
68	g3	221	 91% 5%
69	h3	301	 89% 7%
70	j3	175	 81% 7% 12%
71	k3	154	 73% 24%
72	m3	146	 79% 6% 14%
73	n3	123	 92% 7%
74	o3	260	 91% 6%
75	q3	242	 92% 6%
76	r3	389	 93% 7%
77	s3	405	 93% 6%

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Mol	Chain	Length	Quality of chain
78	t3	181	
79	u3	194	
80	l3	24	
81	A3	3390	
82	B3	163	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	SPD	A3	3450	-	-	X	-

## 2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 361205 atoms, of which 151371 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 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A1	259	Total	C	H	N	O	S	0	0
			4254	1323	2180	387	357	7		

- Molecule 2 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	k1	230	Total	C	H	N	O	S	0	0
			3816	1156	1965	361	326	8		

- Molecule 3 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
3	h1	1626	Total	C	H	N	O	P	0	0
			52270	15549	17529	6195	11371	1626		

- Molecule 4 is a protein called 40S ribosomal protein S10-1-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	l1	91	Total	C	H	N	O	S	0	0
			1549	508	776	125	136	4		

- Molecule 5 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	C1	117	Total	C	H	N	O	S	0	0
			1778	553	900	153	165	7		

- Molecule 6 is a protein called 40S ribosomal protein S17-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	D1	119	Total	C	H	N	O	S	0	0
			1989	604	1026	178	177	4		

- Molecule 7 is a protein called 40S ribosomal protein S19-3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	E1	136	2172	676	1091	211	190	4	0	0

- Molecule 8 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	F1	216	3578	1118	1818	314	320	8	0	0

- Molecule 9 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	G1	83	1295	404	643	120	125	3	0	0

- Molecule 10 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	H1	127	2145	657	1111	200	174	3	0	0

- Molecule 11 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	I1	74	1204	365	621	109	106	3	0	0

- Molecule 12 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	J1	98	1610	491	818	161	132	8	0	0

- Molecule 13 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	K1	84	1307	404	656	122	118	7	0	0

- Molecule 14 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O	S		
14	L1	61	1018	303	525	102	86	2	0	0

- Molecule 15 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O	S		
15	M1	52	851	249	442	94	65	1	0	0

- Molecule 16 is a protein called ubiquitin-40S ribosomal protein S27a-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O	S		
16	N1	69	1143	360	581	103	94	5	0	0

- Molecule 17 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O	S		
17	O1	188	3125	972	1591	281	279	2	0	0

- Molecule 18 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O	S		
18	P1	186	3081	944	1570	300	263	4	0	0

- Molecule 19 is a protein called guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O	S		
19	Q1	309	4756	1512	2362	414	456	12	0	0

- Molecule 20 is a protein called 40S ribosomal protein S20-2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O	S		
20	R1	102	1668	505	864	151	145	3	0	0

- Molecule 21 is a protein called 40S ribosomal protein S14-2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
21	S1	132	Total	C	H	N	O	S	0	0
			2026	611	1028	197	185	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
22	T1	141	Total	C	H	N	O	S	0	0
			2264	695	1164	215	187	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	U1	142	Total	C	H	N	O	S	0	0
			2337	718	1184	227	202	6		

- Molecule 24 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	V1	55	Total	C	H	N	O	S	0	0
			871	274	430	90	71	6		

- Molecule 25 is a protein called 30S ribosomal protein S15, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
25	W1	149	Total	C	H	N	O	S	0	0
			2467	762	1278	223	202	2		

- Molecule 26 is a protein called 40S ribosomal protein S11-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
26	X1	145	Total	C	H	N	O	S	0	0
			2362	734	1207	222	194	5		

- Molecule 27 is a protein called 40S ribosomal protein S15-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	Y1	131	Total	C	H	N	O	S	0	0
			2193	681	1132	199	176	5		

- Molecule 28 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
28	Z1	202	3233	1023	1623	289	288	10	0	0

- Molecule 29 is a protein called 40S ribosomal protein S3-2-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	a1	211	3413	1052	1752	306	295	8	0	0

- Molecule 30 is a protein called 40S ribosomal protein S9-2-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
30	b1	183	3118	964	1595	301	253	5	0	0

- Molecule 31 is a protein called 40S ribosomal protein S2-3-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
31	c1	217	3472	1089	1786	300	289	8	0	0

- Molecule 32 is a protein called 40S ribosomal protein S5-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
32	d1	194	3103	953	1572	290	280	8	0	0

- Molecule 33 is a protein called 40S ribosomal protein S15a-1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
33	e1	129	2100	659	1068	188	180	5	0	0

- Molecule 34 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
34	f1	141	2332	722	1197	221	188	4	0	0

- Molecule 35 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
35	B1	12	360	108	120	24	96	12	0	0

- Molecule 36 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
36	i2	76	2452	726	822	298	530	76	0	0
36	W2	76	2451	726	822	298	529	76	0	0

- Molecule 37 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
37	C3	119	3823	1133	1285	457	829	119	0	0

- Molecule 38 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
38	D3	200	3296	1007	1691	324	270	4	0	0

- Molecule 39 is a protein called 60S ribosomal protein L14-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
39	E3	130	2206	678	1150	196	179	3	0	0

- Molecule 40 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
40	F3	203	3469	1071	1768	350	277	3	0	0

- Molecule 41 is a protein called 60S ribosomal protein L18-2-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
41	G3	186	3042	931	1580	283	245	3	0	0

- Molecule 42 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
42	H3	182	3181	946	1652	327	247	9	0	0

- Molecule 43 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
43	I3	177	3061	969	1556	277	251	8	0	0

- Molecule 44 is a protein called 60S ribosomal protein L21-1-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
44	J3	163	2672	823	1366	255	224	4	0	0

- Molecule 45 is a protein called 60S ribosomal protein L22-2-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
45	K3	99	1653	515	845	141	150	2	0	0

- Molecule 46 is a protein called 60S ribosomal protein L24-like.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
46	L3	62	1079	341	553	101	81	3	0	0

- Molecule 47 is a protein called eL27 (60S ribosomal protein L27).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
47	M3	134	2283	708	1184	206	183	2	0	0

- Molecule 48 is a protein called eL28 (60S ribosomal protein L28).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
48	N3	142	2298	701	1187	207	201	2	0	0

- Molecule 49 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
49	O3	49	831	250	419	95	66	1	0	0

- Molecule 50 is a protein called 60S ribosomal protein L30-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
50	P3	97	1526	475	781	130	135	5	0	0

- Molecule 51 is a protein called eL31 (60S ribosomal protein L31).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
51	Q3	108	1809	549	934	168	156	2	0	0

- Molecule 52 is a protein called 60S ribosomal protein L32-1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
52	R3	126	2151	655	1115	207	169	5	0	0

- Molecule 53 is a protein called eL33 (60S ribosomal protein L35a).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
53	S3	111	1832	571	932	171	153	5	0	0

- Molecule 54 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
54	T3	114	1939	579	1013	193	153	1	0	0

- Molecule 55 is a protein called eL36 (60S ribosomal protein L36).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
55	U3	98	1650	489	868	162	129	2	0	0

- Molecule 56 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
56	V3	86	1427	429	726	155	112	5	0	0

- Molecule 57 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
57	W3	68	1160	358	602	99	98	3	0	0

- Molecule 58 is a protein called 60S ribosomal protein L39-3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
58	X3	50	928	286	480	96	64	2	0	0

- Molecule 59 is a protein called ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
59	Y3	51	881	262	460	88	65	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
60	p3	25	527	145	289	62	28	3	0	0

- Molecule 61 is a protein called 60S ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
61	Z3	98	1629	494	842	157	131	5	0	0

- Molecule 62 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
62	a3	91	1453	443	745	136	124	5	0	0

- Molecule 63 is a protein called eL6 (60S ribosomal protein L6).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
63	b3	208	3360	1046	1749	290	271	4	0	0

- Molecule 64 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
64	c3	233	3907	1206	2028	347	319	7	0	0

- Molecule 65 is a protein called uL13 (60S ribosomal protein L13a).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
65	d3	205	3414	1046	1774	318	268	8	0	0

- Molecule 66 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
66	e3	131	2029	623	1044	183	170	9	0	0

- Molecule 67 is a protein called uL15 (60S ribosomal protein L27a).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
67	f3	147	2361	740	1200	228	190	3	0	0

- Molecule 68 is a protein called uL16 (60S ribosomal protein L10).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
68	g3	209	3397	1058	1726	329	273	11	0	0

- Molecule 69 is a protein called 60S ribosomal protein L5-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
69	h3	288	4715	1481	2374	426	429	5	0	0

- Molecule 70 is a protein called 50S ribosomal protein L22, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
70	j3	154	2515	775	1270	246	219	5	0	0

- Molecule 71 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
71	k3	117	1980	609	1030	170	169	2	0	0

- Molecule 72 is a protein called uL24 (60S ribosomal protein L26).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
72	m3	126	2124	634	1103	209	175	3	0	0

- Molecule 73 is a protein called 60S ribosomal protein L35-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
73	n3	122	2140	642	1141	191	165	1	0	0

- Molecule 74 is a protein called uL2 (60S ribosomal protein L8).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
74	o3	245	3791	1174	1911	381	315	10	0	0

- Molecule 75 is a protein called 60S ribosomal protein L7-4-like.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
75	q3	238	4016	1256	2058	359	339	4	0	0

- Molecule 76 is a protein called uL3 (60S ribosomal protein L3).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
76	r3	386	6327	1981	3223	578	530	15	0	0

- Molecule 77 is a protein called uL4 (60S ribosomal protein L4).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
77	s3	398	6324	1956	3227	583	548	10	0	0

- Molecule 78 is a protein called uL5 (60S ribosomal protein L11).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
78	t3	172	2836	882	1444	259	244	7	0	0

- Molecule 79 is a protein called uL6 (60S ribosomal protein L9).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
79	u3	191	3124	963	1604	276	276	5	0	0

- Molecule 80 is a protein called nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
80	l3	24	169	72	49	24	24	0	0

- Molecule 81 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
81	A3	3196	103169	30602	34651	12456	22264	3196	0	0

- Molecule 82 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
82	B3	163	5243	1555	1763	627	1135	163	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B3	85	U	C	conflict	GB 1782605526

- Molecule 83 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
83	h1	73	Total Mg 73 73	0
83	S1	1	Total Mg 1 1	0
83	U1	1	Total Mg 1 1	0
83	B1	1	Total Mg 1 1	0
83	C3	4	Total Mg 4 4	0
83	V3	1	Total Mg 1 1	0
83	e3	1	Total Mg 1 1	0
83	j3	1	Total Mg 1 1	0
83	q3	1	Total Mg 1 1	0
83	r3	2	Total Mg 2 2	0
83	A3	49	Total Mg 49 49	0

- Molecule 84 is POTASSIUM ION (CCD ID: K) (formula: K).

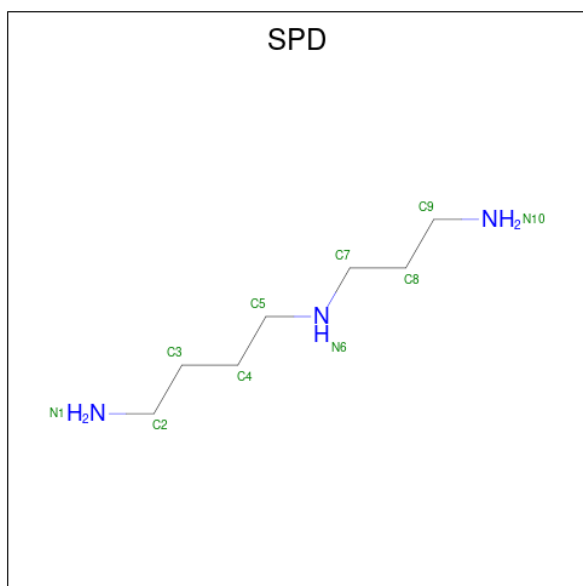
Mol	Chain	Residues	Atoms	AltConf
84	h1	42	Total K 42 42	0
84	S1	1	Total K 1 1	0
84	T1	1	Total K 1 1	0
84	U1	1	Total K 1 1	0
84	V1	1	Total K 1 1	0
84	W1	1	Total K 1 1	0
84	D3	1	Total K 1 1	0
84	R3	1	Total K 1 1	0
84	T3	1	Total K 1 1	0

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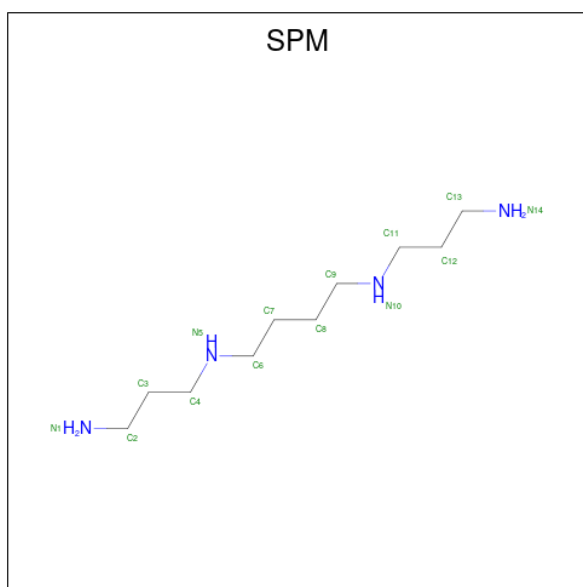
Mol	Chain	Residues	Atoms	AltConf
84	Z3	1	Total K 1 1	0
84	f3	2	Total K 2 2	0
84	g3	1	Total K 1 1	0
84	o3	2	Total K 2 2	0
84	r3	1	Total K 1 1	0
84	A3	83	Total K 83 83	0
84	B3	1	Total K 1 1	0

- Molecule 85 is SPERMIDINE (CCD ID: SPD) (formula:  $C_7H_{19}N_3$ ).



Mol	Chain	Residues	Atoms	AltConf
85	h1	1	Total C N 10 7 3	0
85	A3	1	Total C N 10 7 3	0

- Molecule 86 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	N	
86	h1	1	40	10	26	4	0
86	h1	1	40	10	26	4	0
86	h1	1	40	10	26	4	0
86	A3	1	40	10	26	4	0
86	A3	1	40	10	26	4	0

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
87	J1	1	1	1	0
87	N1	1	1	1	0
87	V1	1	1	1	0
87	V3	1	1	1	0
87	Y3	1	1	1	0
87	Z3	1	1	1	0
87	a3	1	1	1	0

- Molecule 88 is water.

Mol	Chain	Residues	Atoms		AltConf
88	A1	7	Total 7	O 7	0
88	k1	5	Total 5	O 5	0
88	h1	2039	Total 2039	O 2039	0
88	E1	12	Total 12	O 12	0
88	F1	13	Total 13	O 13	0
88	I1	1	Total 1	O 1	0
88	J1	25	Total 25	O 25	0
88	K1	6	Total 6	O 6	0
88	M1	1	Total 1	O 1	0
88	O1	1	Total 1	O 1	0
88	P1	20	Total 20	O 20	0
88	R1	12	Total 12	O 12	0
88	S1	32	Total 32	O 32	0
88	T1	43	Total 43	O 43	0
88	U1	7	Total 7	O 7	0
88	V1	4	Total 4	O 4	0
88	W1	20	Total 20	O 20	0
88	X1	21	Total 21	O 21	0
88	Y1	6	Total 6	O 6	0
88	Z1	1	Total 1	O 1	0
88	b1	11	Total 11	O 11	0

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Mol	Chain	Residues	Atoms		AltConf
88	c1	12	Total 12	O 12	0
88	d1	12	Total 12	O 12	0
88	e1	16	Total 16	O 16	0
88	f1	10	Total 10	O 10	0
88	B1	17	Total 17	O 17	0
88	i2	7	Total 7	O 7	0
88	W2	13	Total 13	O 13	0
88	C3	91	Total 91	O 91	0
88	D3	43	Total 43	O 43	0
88	F3	105	Total 105	O 105	0
88	G3	52	Total 52	O 52	0
88	H3	10	Total 10	O 10	0
88	I3	14	Total 14	O 14	0
88	J3	27	Total 27	O 27	0
88	M3	2	Total 2	O 2	0
88	N3	10	Total 10	O 10	0
88	O3	27	Total 27	O 27	0
88	Q3	3	Total 3	O 3	0
88	R3	42	Total 42	O 42	0
88	S3	6	Total 6	O 6	0
88	T3	14	Total 14	O 14	0

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Mol	Chain	Residues	Atoms		AltConf
88	U3	4	Total 4	O 4	0
88	V3	29	Total 29	O 29	0
88	X3	7	Total 7	O 7	0
88	Y3	2	Total 2	O 2	0
88	p3	9	Total 9	O 9	0
88	Z3	21	Total 21	O 21	0
88	a3	6	Total 6	O 6	0
88	b3	1	Total 1	O 1	0
88	c3	10	Total 10	O 10	0
88	d3	13	Total 13	O 13	0
88	e3	12	Total 12	O 12	0
88	f3	48	Total 48	O 48	0
88	g3	16	Total 16	O 16	0
88	h3	15	Total 15	O 15	0
88	j3	16	Total 16	O 16	0
88	k3	14	Total 14	O 14	0
88	m3	9	Total 9	O 9	0
88	n3	15	Total 15	O 15	0
88	o3	56	Total 56	O 56	0
88	q3	29	Total 29	O 29	0
88	r3	27	Total 27	O 27	0

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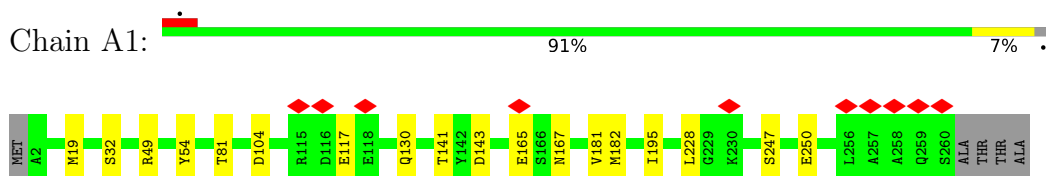
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Mol	Chain	Residues	Atoms		AltConf
88	s3	65	Total 65	O 65	0
88	t3	1	Total 1	O 1	0
88	u3	2	Total 2	O 2	0
88	A3	3383	Total 3383	O 3383	0
88	B3	162	Total 162	O 162	0

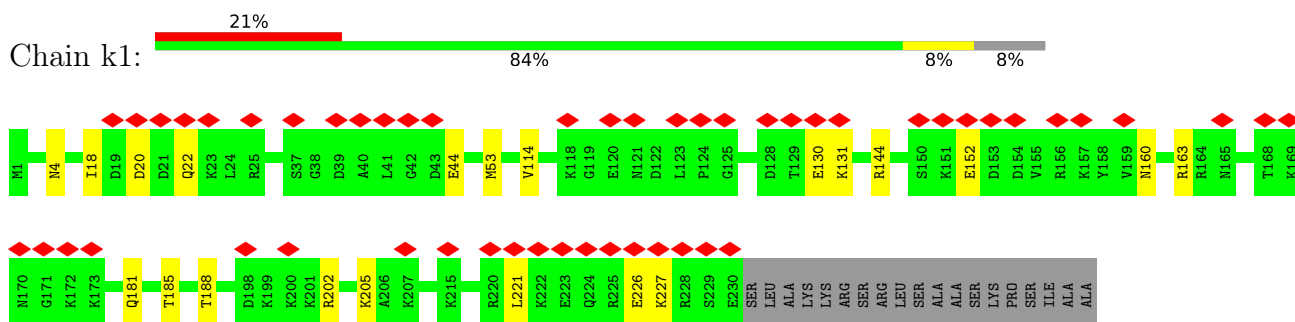
### 3 Residue-property plots [i](#)

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.

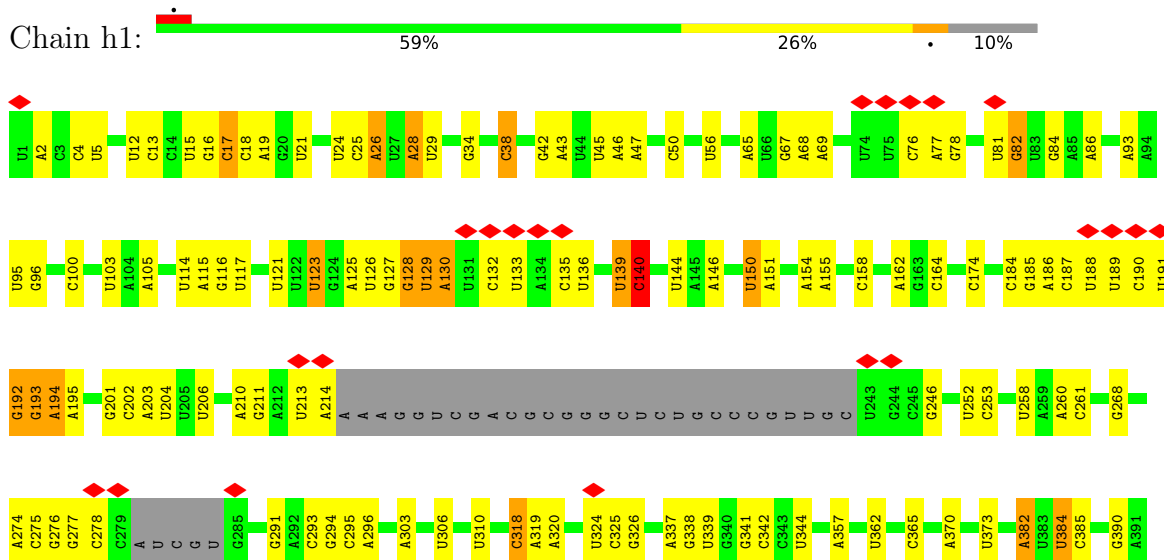
- Molecule 1: 40S ribosomal protein S4

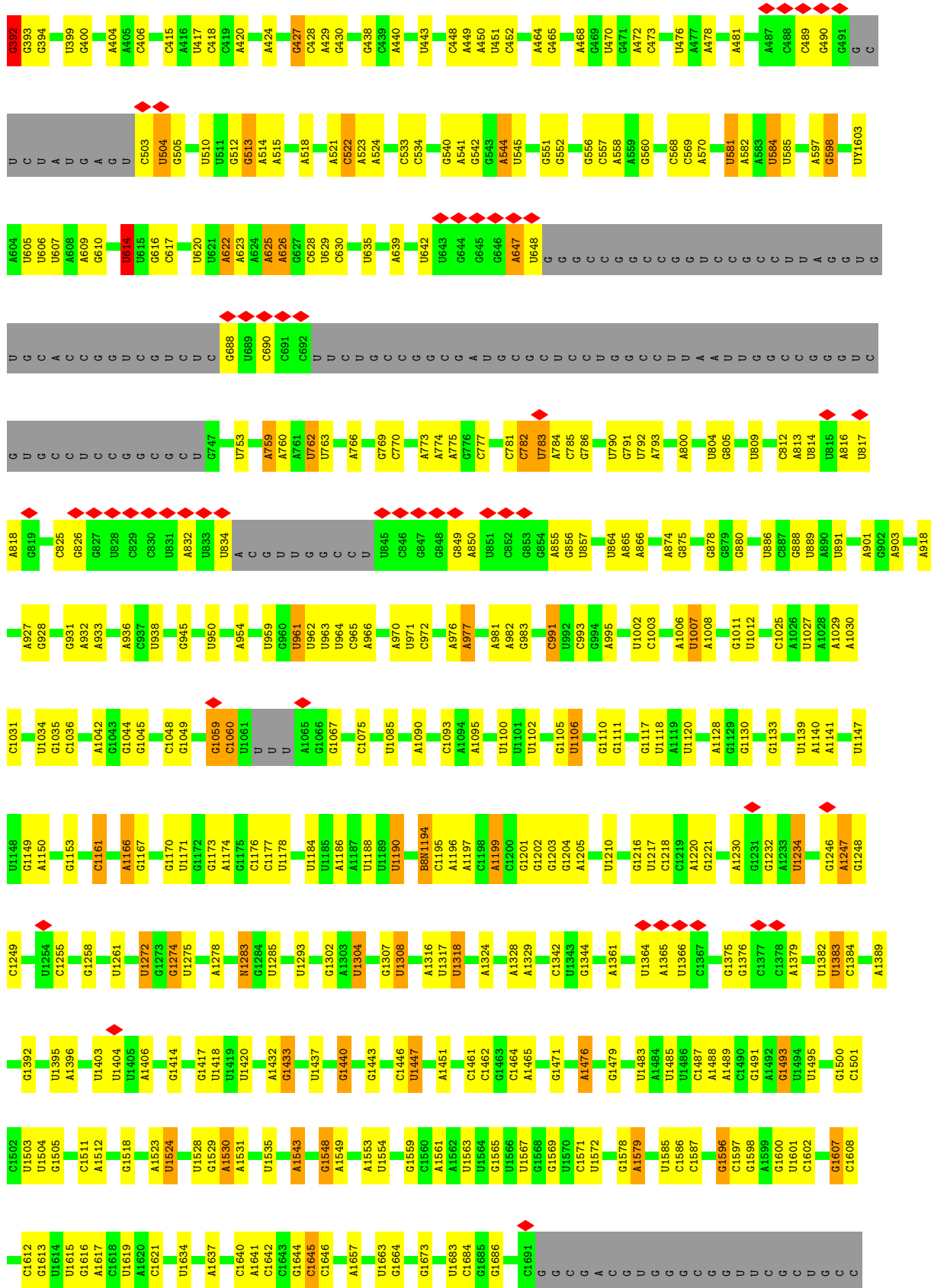


- Molecule 2: 40S ribosomal protein S6



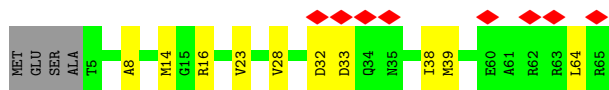
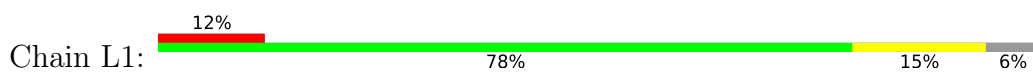
- Molecule 3: 18S rRNA



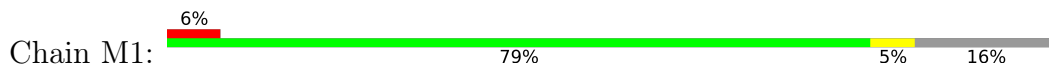




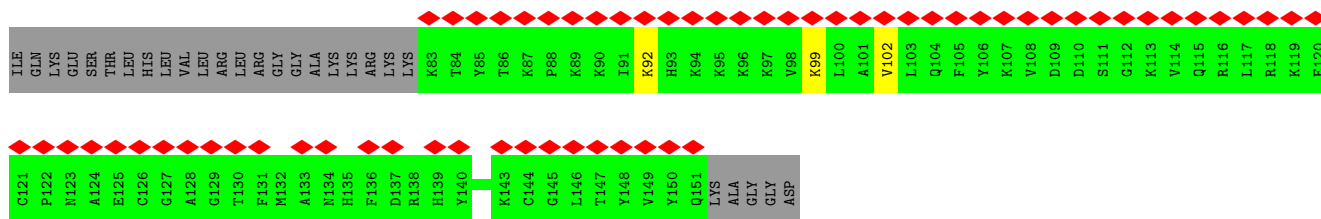
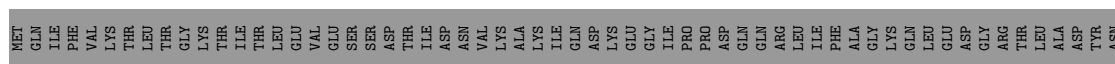
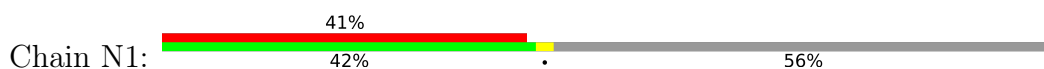




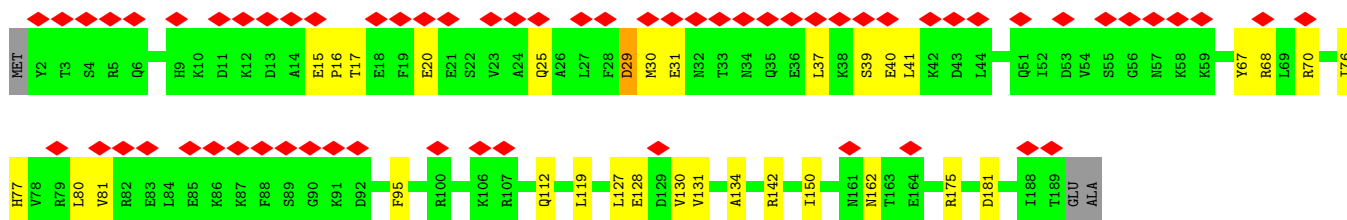
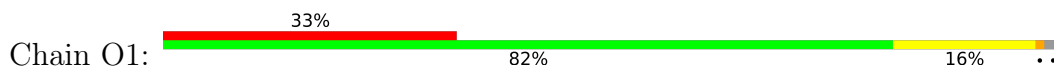
• Molecule 15: 40S ribosomal protein S30



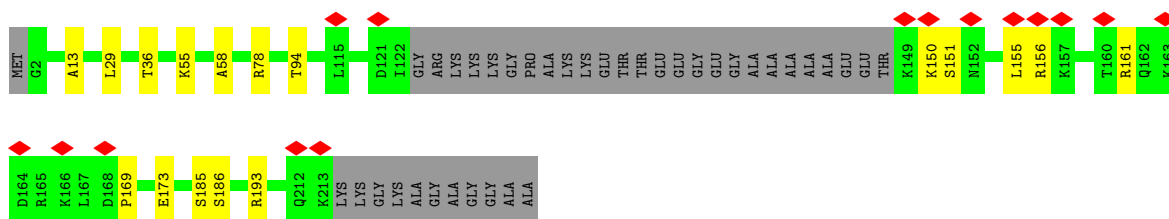
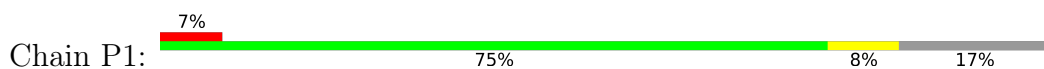
• Molecule 16: ubiquitin-40S ribosomal protein S27a-like



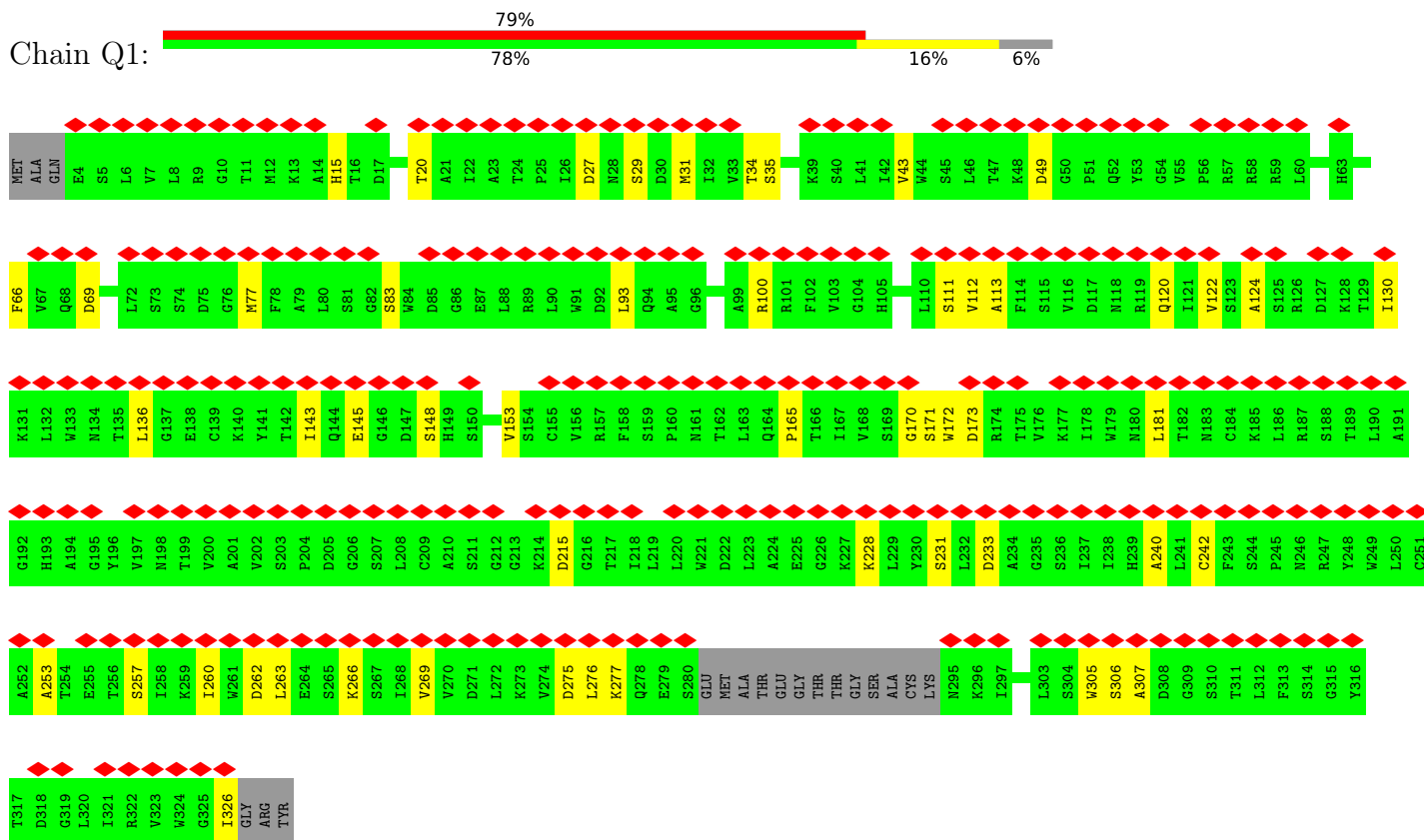
• Molecule 17: 40S ribosomal protein S7



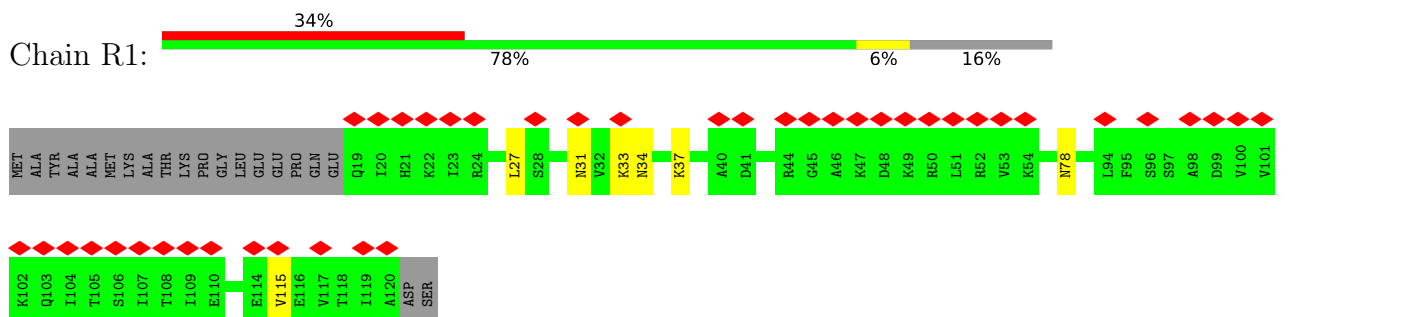
• Molecule 18: 40S ribosomal protein S8



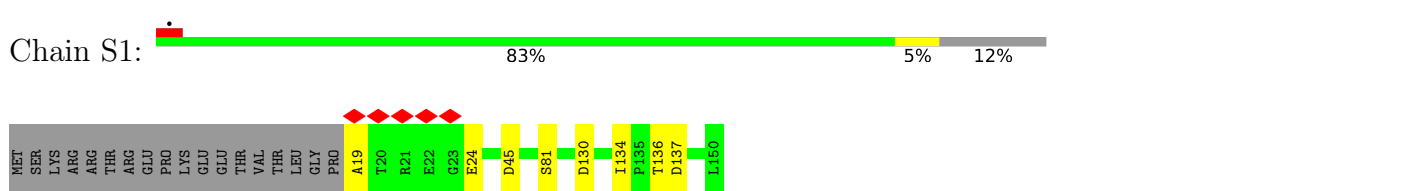
• Molecule 19: guanine nucleotide-binding protein subunit beta-like protein



• Molecule 20: 40S ribosomal protein S20-2



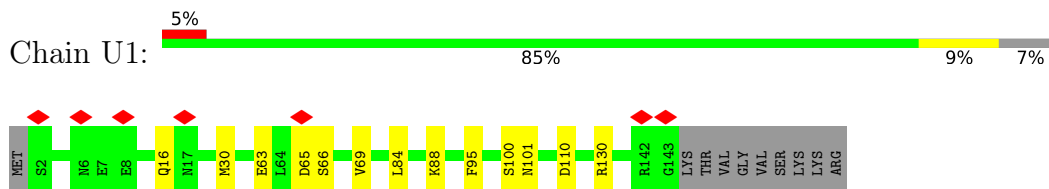
• Molecule 21: 40S ribosomal protein S14-2



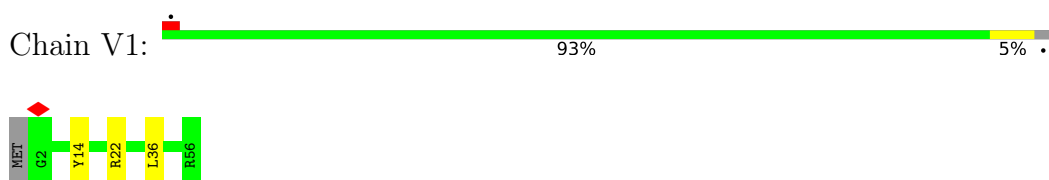
• Molecule 22: 40S ribosomal protein S23



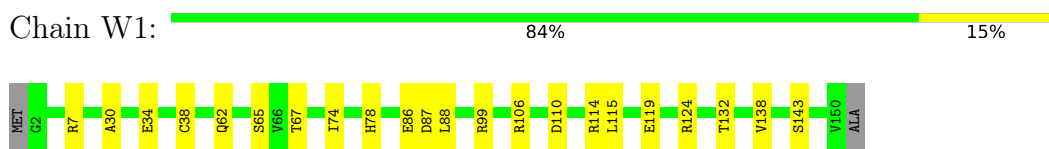
• Molecule 23: 40S ribosomal protein S18



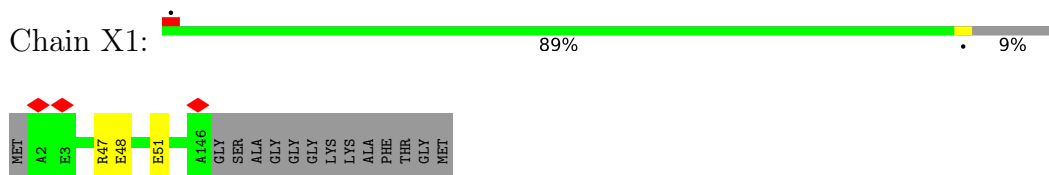
• Molecule 24: 40S ribosomal protein S29



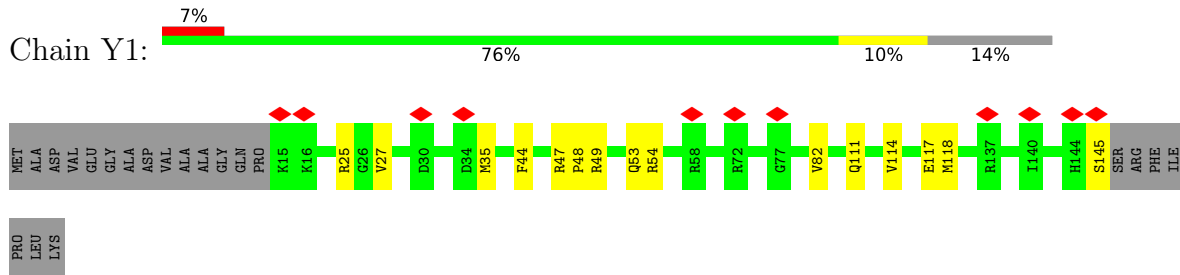
• Molecule 25: 30S ribosomal protein S15, chloroplastic



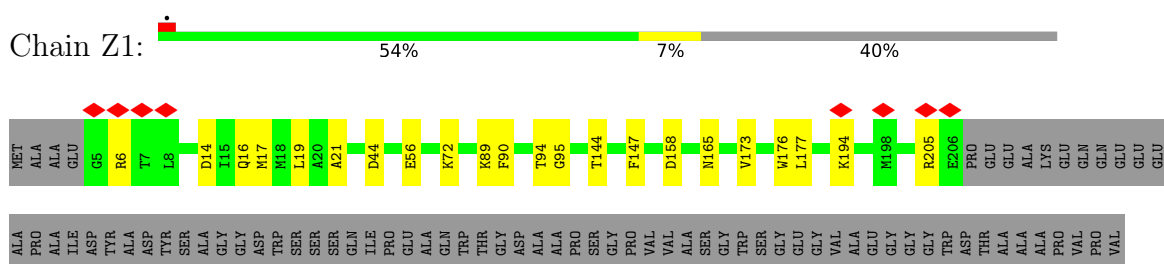
• Molecule 26: 40S ribosomal protein S11-like



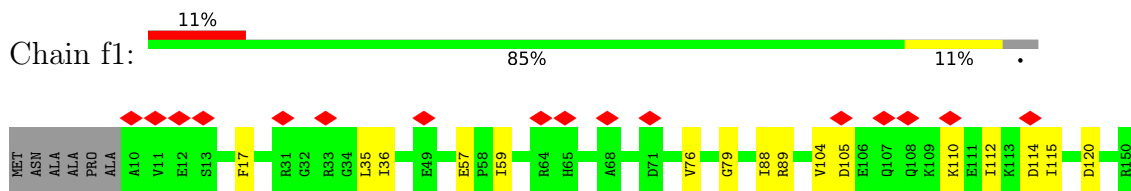
• Molecule 27: 40S ribosomal protein S15-like



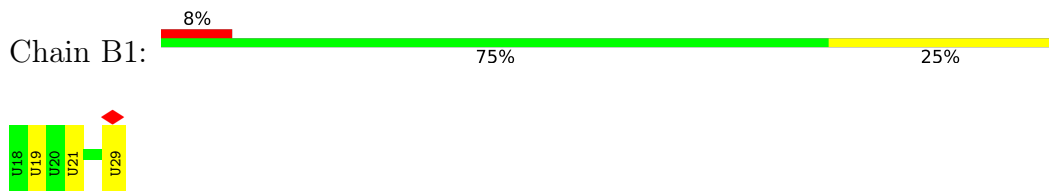
• Molecule 28: 40S ribosomal protein SA



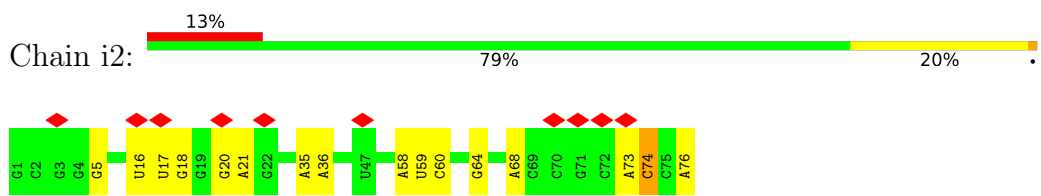




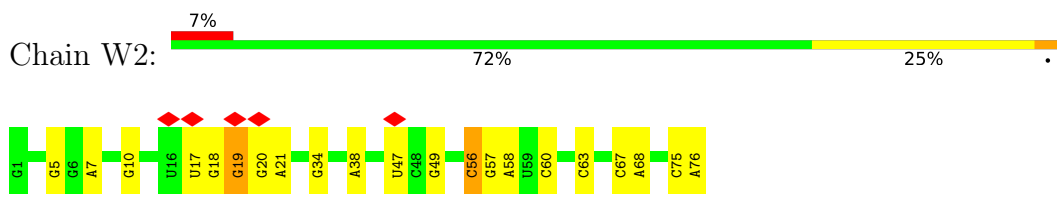
• Molecule 35: mRNA



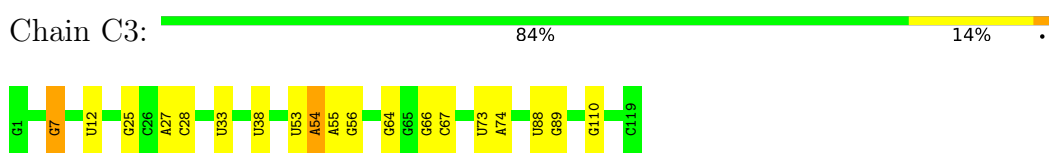
• Molecule 36: tRNA



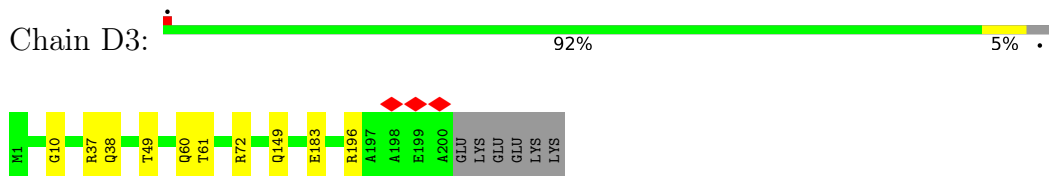
• Molecule 36: tRNA



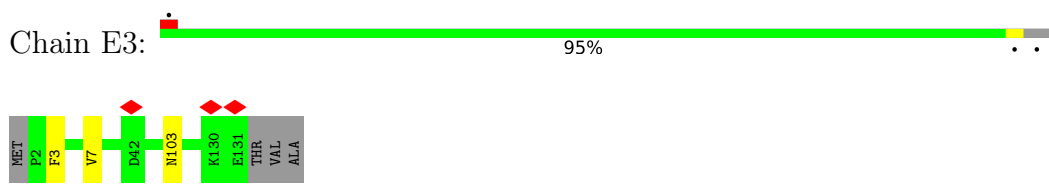
• Molecule 37: 5S rRNA



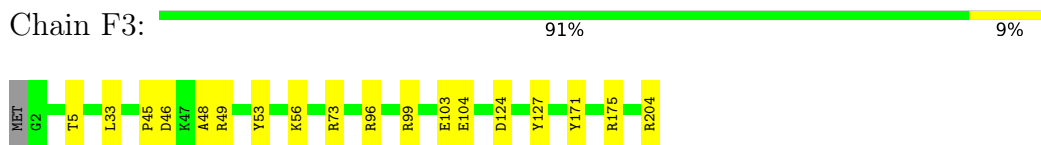
• Molecule 38: 60S ribosomal protein L13



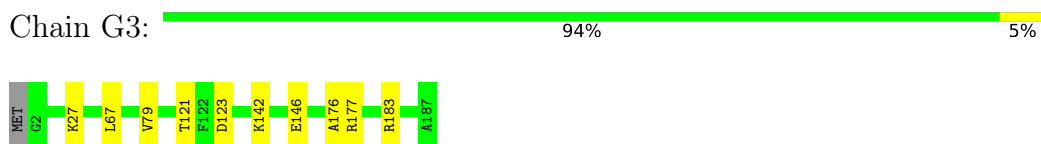
• Molecule 39: 60S ribosomal protein L14-1



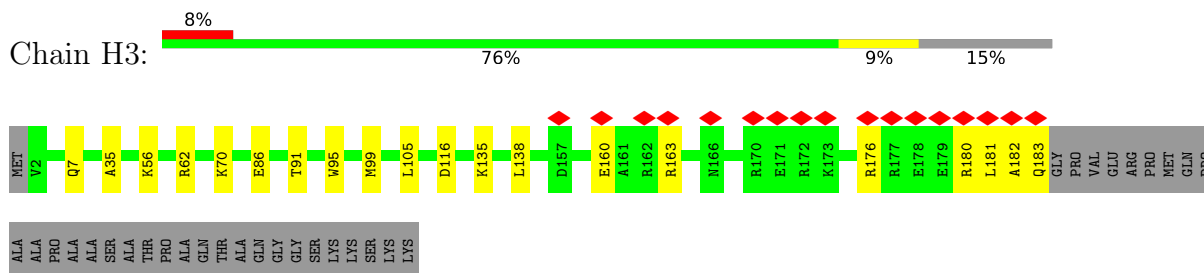
- Molecule 40: Ribosomal protein L15



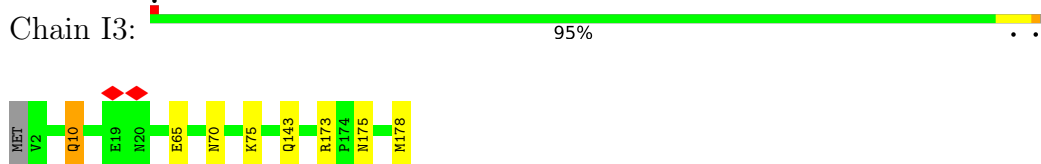
- Molecule 41: 60S ribosomal protein L18-2-like



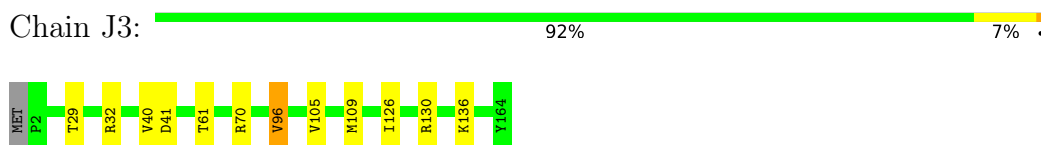
- Molecule 42: Ribosomal protein L19



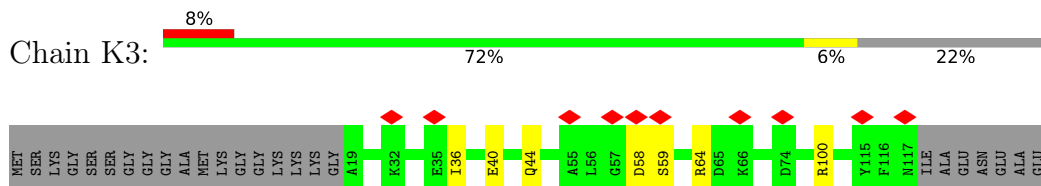
- Molecule 43: 60S ribosomal protein L18a



- Molecule 44: 60S ribosomal protein L21-1-like



- Molecule 45: 60S ribosomal protein L22-2-like



- Molecule 46: 60S ribosomal protein L24-like



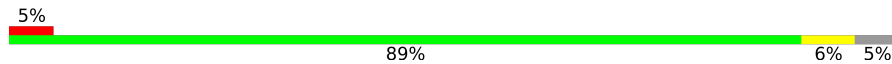


- Molecule 53: eL33 (60S ribosomal protein L35a)

Chain S3:  94% 5%




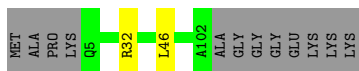
- Molecule 54: 60S ribosomal protein L34

Chain T3:  5% 89% 6% 5%




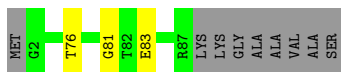
- Molecule 55: eL36 (60S ribosomal protein L36)

Chain U3:  87% 11%




- Molecule 56: Ribosomal protein L37

Chain V3:  87% 9%



- Molecule 57: 60S ribosomal protein L38

Chain W3:  84% 13%



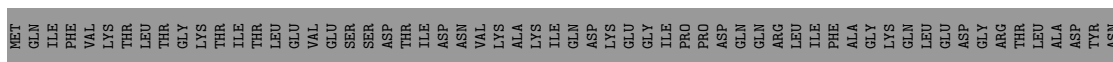
- Molecule 58: 60S ribosomal protein L39-3

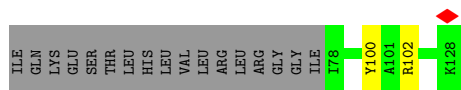
Chain X3:  90% 8%



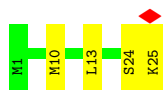
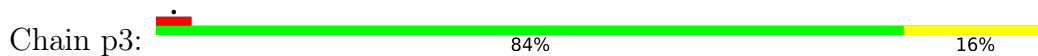
- Molecule 59: ubiquitin-60S ribosomal protein L40

Chain Y3:  38% 60%

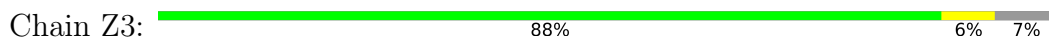




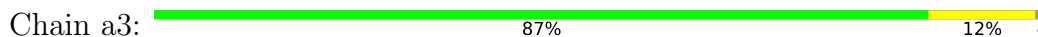
• Molecule 60: 60S ribosomal protein L41



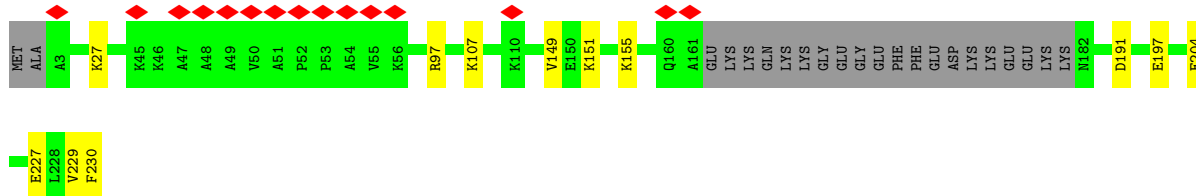
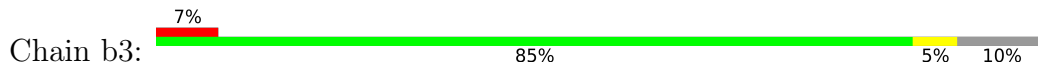
• Molecule 61: 60S ribosomal protein L44



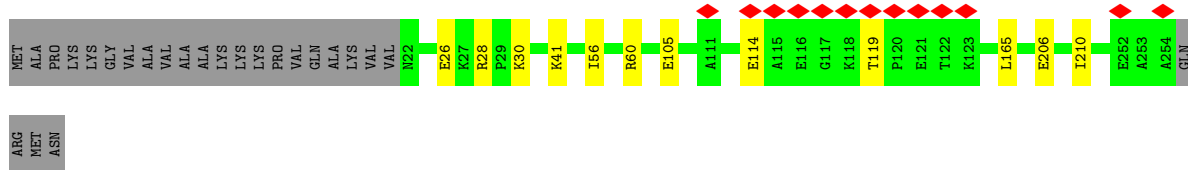
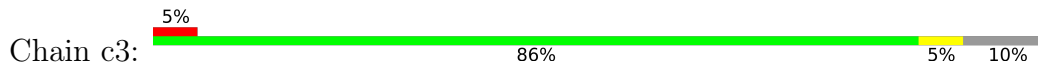
• Molecule 62: 60S ribosomal protein L37a



• Molecule 63: eL6 (60S ribosomal protein L6)



• Molecule 64: 60S ribosomal protein L7a

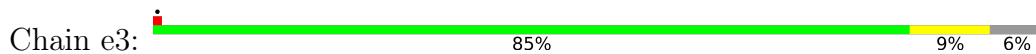


• Molecule 65: uL13 (60S ribosomal protein L13a)

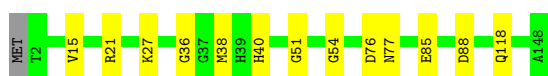
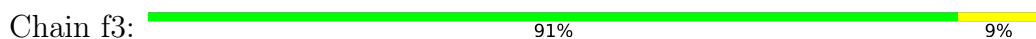




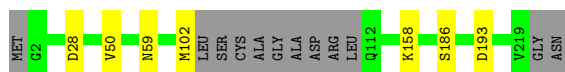
- Molecule 66: 60S ribosomal protein L23



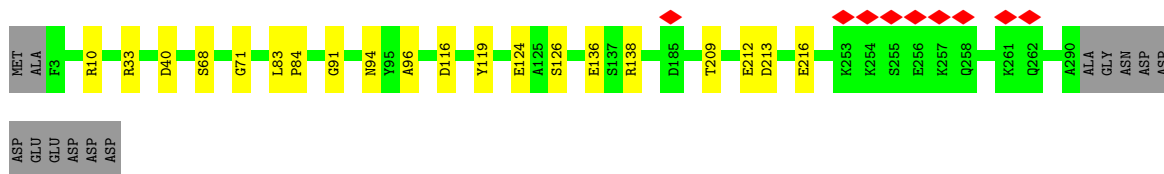
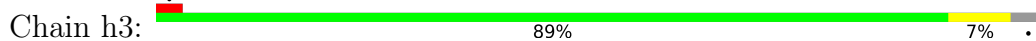
- Molecule 67: uL15 (60S ribosomal protein L27a)



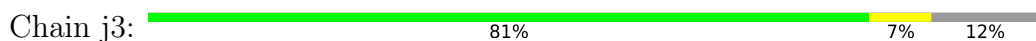
- Molecule 68: uL16 (60S ribosomal protein L10)



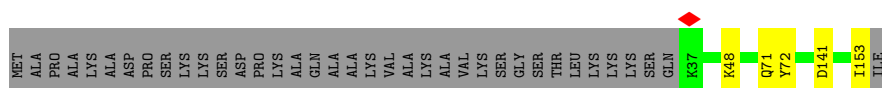
- Molecule 69: 60S ribosomal protein L5-like




- Molecule 70: 50S ribosomal protein L22, chloroplastic



- Molecule 71: 60S ribosomal protein L23a



- Molecule 72: uL24 (60S ribosomal protein L26)

Chain m3:  79% 6% 14%




- Molecule 73: 60S ribosomal protein L35-like

Chain n3:  92% 7%



- Molecule 74: uL2 (60S ribosomal protein L8)

Chain o3:  91% 6%



- Molecule 75: 60S ribosomal protein L7-4-like

Chain q3:  92% 6%



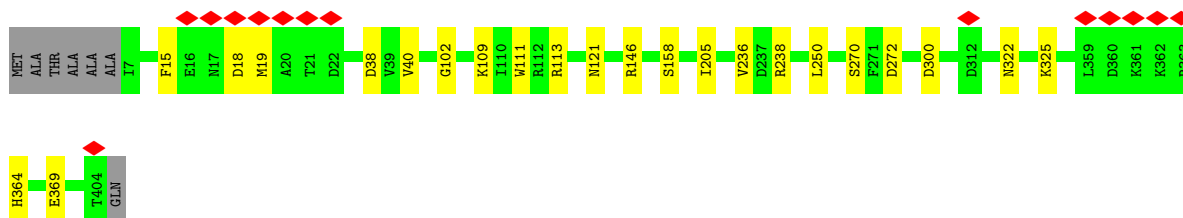
- Molecule 76: uL3 (60S ribosomal protein L3)

Chain r3:  93% 7%

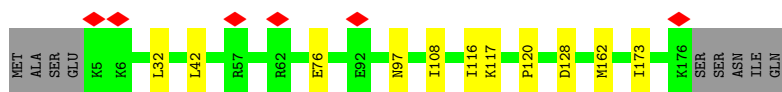
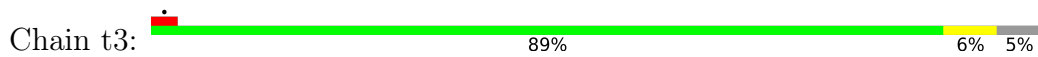


- Molecule 77: uL4 (60S ribosomal protein L4)

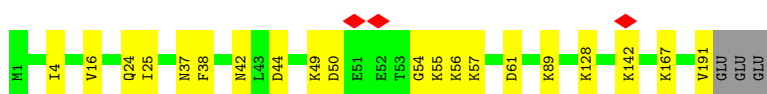
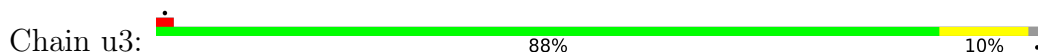
Chain s3:  93% 6%



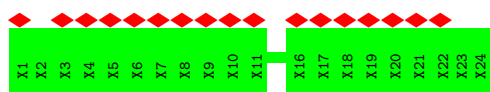
- Molecule 78: uL5 (60S ribosomal protein L11)



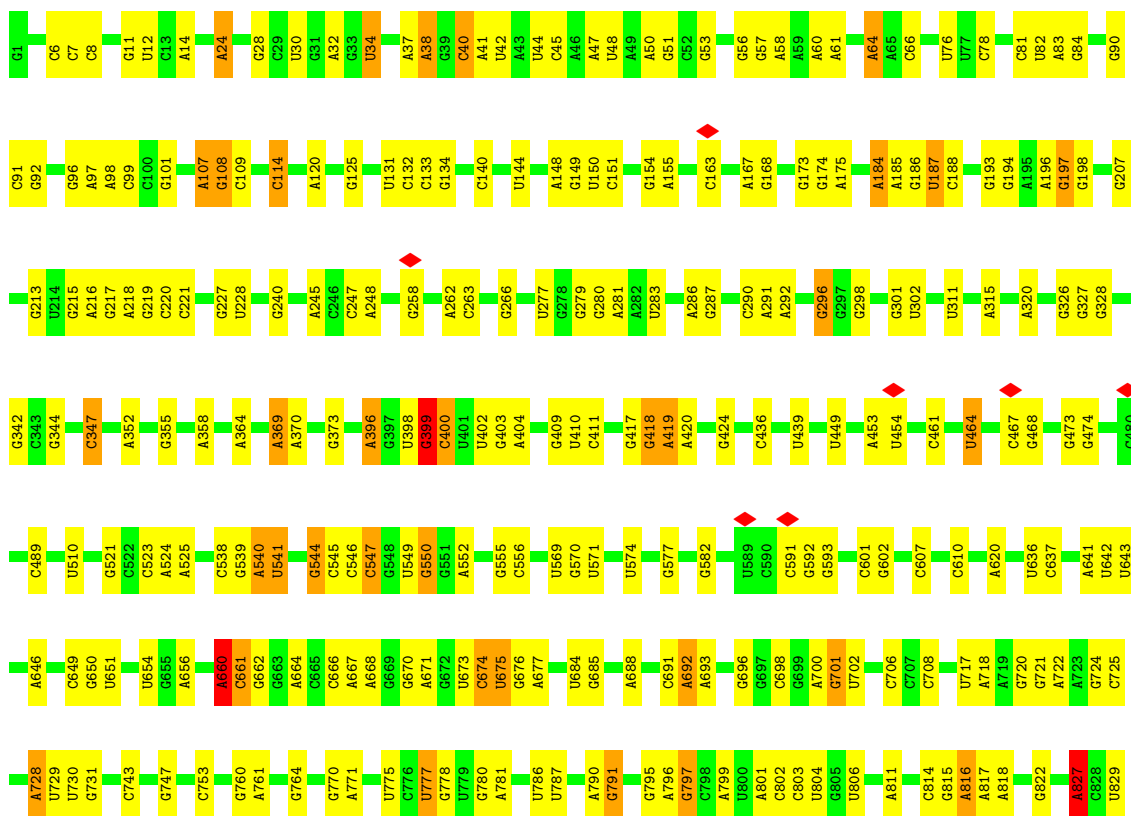
- Molecule 79: uL6 (60S ribosomal protein L9)



- Molecule 80: nascent chain



- Molecule 81: 25S rRNA







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	335291	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 ( $e^-/\text{\AA}^2$ )	27	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	14.499	Depositor
Minimum map value	-6.970	Depositor
Average map value	0.031	Depositor
Map value standard deviation	0.323	Depositor
Recommended contour level	0.6	Depositor
Map size ( $\text{\AA}$ )	381.6, 381.6, 381.6	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.848, 0.848, 0.848	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMU, 1MA, MA6, B8N, A2M, PSU, UY1, K, UR3, SPD, OMC, ZN, 5MC, 6MZ, 4AC, OMG, SPM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A1	0.11	0/2114	0.27	0/2837
2	k1	0.12	0/1875	0.30	0/2494
3	h1	0.14	1/36945 (0.0%)	0.23	0/57563
4	l1	0.11	0/794	0.25	0/1074
5	C1	0.14	0/889	0.37	0/1198
6	D1	0.15	0/973	0.31	0/1299
7	E1	0.12	0/1103	0.24	0/1480
8	F1	0.10	0/1790	0.26	0/2402
9	G1	0.10	0/662	0.25	0/891
10	H1	0.11	0/1049	0.26	0/1391
11	I1	0.10	0/589	0.24	0/789
12	J1	0.12	0/805	0.26	0/1076
13	K1	0.13	0/662	0.25	0/892
14	L1	0.13	0/496	0.32	0/661
15	M1	0.15	0/414	0.26	0/544
16	N1	0.14	0/574	0.29	0/763
17	O1	0.14	0/1560	0.33	0/2097
18	P1	0.12	0/1535	0.28	0/2050
19	Q1	0.12	0/2446	0.33	0/3324
20	R1	0.12	0/813	0.26	0/1095
21	S1	0.12	0/1010	0.27	0/1352
22	T1	0.12	0/1119	0.25	0/1487
23	U1	0.12	0/1170	0.28	0/1562
24	V1	0.14	0/453	0.23	0/605
25	W1	0.13	0/1214	0.26	0/1632
26	X1	0.11	0/1180	0.27	0/1579
27	Y1	0.12	0/1084	0.27	0/1450
28	Z1	0.14	0/1644	0.30	0/2223
29	a1	0.13	0/1684	0.30	0/2257
30	b1	0.10	0/1550	0.23	0/2073
31	c1	0.11	0/1721	0.29	0/2320

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	d1	0.11	0/1553	0.28	0/2095
33	e1	0.11	0/1050	0.26	0/1405
34	f1	0.12	0/1154	0.27	0/1542
35	B1	0.07	0/263	0.20	0/404
36	W2	0.10	0/1822	0.24	0/2840
36	i2	0.08	0/1823	0.23	0/2840
37	C3	0.08	0/2837	0.22	0/4420
38	D3	0.10	0/1635	0.25	0/2194
39	E3	0.09	0/1069	0.23	0/1427
40	F3	0.13	0/1740	0.30	0/2333
41	G3	0.12	0/1487	0.27	0/1989
42	H3	0.11	0/1548	0.28	0/2042
43	I3	0.10	0/1544	0.25	0/2071
44	J3	0.09	0/1331	0.25	0/1784
45	K3	0.11	0/819	0.27	0/1098
46	L3	0.12	0/539	0.26	0/716
47	M3	0.11	0/1118	0.24	0/1492
48	N3	0.11	0/1126	0.29	0/1508
49	O3	0.13	0/422	0.31	0/558
50	P3	0.14	0/757	0.29	0/1018
51	Q3	0.13	0/885	0.30	0/1184
52	R3	0.11	0/1053	0.27	0/1408
53	S3	0.11	0/920	0.26	0/1232
54	T3	0.10	0/939	0.24	0/1251
55	U3	0.11	0/791	0.25	0/1047
56	V3	0.14	0/714	0.29	0/949
57	W3	0.16	0/566	0.36	0/752
58	X3	0.09	0/460	0.21	0/611
59	Y3	0.12	0/427	0.27	0/562
60	p3	0.12	0/239	0.32	0/302
61	Z3	0.12	0/801	0.23	0/1058
62	a3	0.11	0/717	0.25	0/952
63	b3	0.12	0/1645	0.28	0/2210
64	c3	0.12	0/1912	0.27	0/2562
65	d3	0.12	0/1669	0.26	0/2235
66	e3	0.11	0/1001	0.29	0/1345
67	f3	0.13	0/1190	0.30	0/1591
68	g3	0.11	0/1707	0.26	0/2283
69	h3	0.11	0/2386	0.28	0/3200
70	j3	0.12	0/1270	0.32	0/1704
71	k3	0.10	0/965	0.25	0/1295
72	m3	0.09	0/1035	0.26	0/1383
73	n3	0.11	0/1009	0.22	0/1343

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
74	o3	0.11	0/1924	0.30	0/2585
75	q3	0.14	0/1992	0.29	0/2670
76	r3	0.10	0/3172	0.28	0/4249
77	s3	0.10	0/3159	0.26	0/4259
78	t3	0.12	0/1414	0.30	0/1890
79	u3	0.10	0/1539	0.29	0/2059
81	A3	0.15	4/73585 (0.0%)	0.26	0/114781
82	B3	0.13	1/3772 (0.0%)	0.26	0/5878
All	All	0.13	6/212412 (0.0%)	0.26	0/311066

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
81	A3	675	OMU	O3'-P	5.26	1.61	1.56
81	A3	2284	A2M	O3'-P	5.11	1.61	1.56
82	B3	46	A2M	O3'-P	5.10	1.61	1.56
81	A3	2483	A	C1'-N9	-5.05	1.40	1.48
3	h1	440	A2M	O3'-P	5.03	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	2074	2180	2181	14	0
2	k1	1851	1965	1969	19	0
3	h1	34741	17529	17528	280	0
4	l1	773	776	776	4	0
5	C1	878	900	905	15	0
6	D1	963	1026	1025	18	0
7	E1	1081	1091	1091	11	0
8	F1	1760	1818	1820	13	0
9	G1	652	643	645	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H1	1034	1111	1110	4	0
11	I1	583	621	620	2	0
12	J1	792	818	820	5	0
13	K1	651	656	661	7	0
14	L1	493	525	524	7	0
15	M1	409	442	440	2	0
16	N1	562	581	580	3	0
17	O1	1534	1591	1590	22	0
18	P1	1511	1570	1570	18	0
19	Q1	2394	2362	2368	38	0
20	R1	804	864	865	6	0
21	S1	998	1028	1028	7	0
22	T1	1100	1164	1165	6	0
23	U1	1153	1184	1184	10	0
24	V1	441	430	430	3	0
25	W1	1189	1278	1277	15	0
26	X1	1155	1207	1210	2	0
27	Y1	1061	1132	1131	10	0
28	Z1	1610	1623	1624	17	0
29	a1	1661	1752	1754	17	0
30	b1	1523	1595	1595	12	0
31	c1	1686	1786	1789	8	0
32	d1	1531	1572	1573	9	0
33	e1	1032	1068	1068	8	0
34	f1	1135	1197	1198	10	0
35	B1	240	120	121	2	0
36	W2	1629	822	823	23	0
36	i2	1630	822	823	9	0
37	C3	2538	1285	1285	10	0
38	D3	1605	1691	1691	7	0
39	E3	1056	1150	1150	2	0
40	F3	1701	1768	1769	13	0
41	G3	1462	1580	1581	7	0
42	H3	1529	1652	1652	18	0
43	I3	1505	1556	1557	7	0
44	J3	1306	1366	1367	9	0
45	K3	808	845	845	4	0
46	L3	526	553	554	1	0
47	M3	1099	1184	1184	6	0
48	N3	1111	1187	1186	5	0
49	O3	412	419	418	2	0
50	P3	745	781	783	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	Q3	875	934	934	1	0
52	R3	1036	1115	1116	11	0
53	S3	900	932	933	4	0
54	T3	926	1013	1013	5	0
55	U3	782	868	867	2	0
56	V3	701	726	724	2	0
57	W3	558	602	604	9	0
58	X3	448	480	480	3	0
59	Y3	421	460	459	2	0
60	p3	238	289	289	3	0
61	Z3	787	842	842	5	0
62	a3	708	745	744	8	0
63	b3	1611	1749	1749	10	0
64	c3	1879	2028	2030	11	0
65	d3	1640	1774	1776	8	0
66	e3	985	1044	1046	8	0
67	f3	1161	1200	1200	12	0
68	g3	1671	1726	1731	5	0
69	h3	2341	2374	2374	14	0
70	j3	1245	1270	1272	7	0
71	k3	950	1030	1029	5	0
72	m3	1021	1103	1103	7	0
73	n3	999	1141	1140	7	0
74	o3	1880	1911	1915	8	0
75	q3	1958	2058	2058	12	0
76	r3	3104	3223	3229	17	0
77	s3	3097	3227	3228	21	0
78	t3	1392	1444	1446	9	0
79	u3	1520	1604	1605	11	0
80	l3	120	49	34	0	0
81	A3	68518	34651	34634	525	0
82	B3	3480	1763	1764	22	0
83	A3	49	0	0	0	0
83	B1	1	0	0	0	0
83	C3	4	0	0	0	0
83	S1	1	0	0	0	0
83	U1	1	0	0	0	0
83	V3	1	0	0	0	0
83	e3	1	0	0	0	0
83	h1	73	0	0	0	0
83	j3	1	0	0	0	0
83	q3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
83	r3	2	0	0	0	0
84	A3	83	0	0	0	0
84	B3	1	0	0	0	0
84	D3	1	0	0	0	0
84	R3	1	0	0	0	0
84	S1	1	0	0	0	0
84	T1	1	0	0	0	0
84	T3	1	0	0	0	0
84	U1	1	0	0	0	0
84	V1	1	0	0	0	0
84	W1	1	0	0	0	0
84	Z3	1	0	0	0	0
84	f3	2	0	0	0	0
84	g3	1	0	0	0	0
84	h1	42	0	0	0	0
84	o3	2	0	0	0	0
84	r3	1	0	0	0	0
85	A3	10	0	19	6	0
85	h1	10	0	19	2	0
86	A3	28	52	52	1	0
86	h1	42	78	78	3	0
87	J1	1	0	0	0	0
87	N1	1	0	0	0	0
87	V1	1	0	0	0	0
87	V3	1	0	0	0	0
87	Y3	1	0	0	0	0
87	Z3	1	0	0	0	0
87	a3	1	0	0	0	0
88	A1	7	0	0	0	0
88	A3	3383	0	0	160	0
88	B1	17	0	0	1	0
88	B3	162	0	0	8	0
88	C3	91	0	0	4	0
88	D3	43	0	0	1	0
88	E1	12	0	0	0	0
88	F1	13	0	0	0	0
88	F3	105	0	0	3	0
88	G3	52	0	0	0	0
88	H3	10	0	0	0	0
88	I1	1	0	0	0	0
88	I3	14	0	0	1	0
88	J1	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	J3	27	0	0	0	0
88	K1	6	0	0	1	0
88	M1	1	0	0	0	0
88	M3	2	0	0	0	0
88	N3	10	0	0	1	0
88	O1	1	0	0	0	0
88	O3	27	0	0	2	0
88	P1	20	0	0	1	0
88	Q3	3	0	0	0	0
88	R1	12	0	0	1	0
88	R3	42	0	0	5	0
88	S1	32	0	0	1	0
88	S3	6	0	0	0	0
88	T1	43	0	0	3	0
88	T3	14	0	0	0	0
88	U1	7	0	0	0	0
88	U3	4	0	0	0	0
88	V1	4	0	0	0	0
88	V3	29	0	0	0	0
88	W1	20	0	0	2	0
88	W2	13	0	0	0	0
88	X1	21	0	0	0	0
88	X3	7	0	0	0	0
88	Y1	6	0	0	0	0
88	Y3	2	0	0	1	0
88	Z1	1	0	0	0	0
88	Z3	21	0	0	1	0
88	a3	6	0	0	1	0
88	b1	11	0	0	0	0
88	b3	1	0	0	0	0
88	c1	12	0	0	0	0
88	c3	10	0	0	1	0
88	d1	12	0	0	0	0
88	d3	13	0	0	0	0
88	e1	16	0	0	1	0
88	e3	12	0	0	0	0
88	f1	10	0	0	0	0
88	f3	48	0	0	2	0
88	g3	16	0	0	1	0
88	h1	2039	0	0	72	0
88	h3	15	0	0	0	0
88	i2	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
88	j3	16	0	0	1	0
88	k1	5	0	0	0	0
88	k3	14	0	0	1	0
88	m3	9	0	0	0	0
88	n3	15	0	0	0	0
88	o3	56	0	0	1	0
88	p3	9	0	0	0	0
88	q3	29	0	0	2	0
88	r3	27	0	0	2	0
88	s3	65	0	0	4	0
88	t3	1	0	0	0	0
88	u3	2	0	0	0	0
All	All	209834	151371	151439	1332	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 1332 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)
36:W2:56:C:N4	81:A3:2458:U:H3	1.60	0.99
81:A3:2468:G:O2'	81:A3:2469:G:O5'	1.83	0.96
3:h1:392:OMG:OP2	3:h1:427:G:O2'	1.84	0.95
81:A3:884:U:OP2	81:A3:1913:C:O2'	1.85	0.94
3:h1:76:C:O2'	3:h1:77:A:O4'	1.88	0.91

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	257/264 (97%)	254 (99%)	3 (1%)	0	100	100
2	k1	228/249 (92%)	228 (100%)	0	0	100	100
4	l1	89/208 (43%)	87 (98%)	2 (2%)	0	100	100
5	C1	115/144 (80%)	114 (99%)	1 (1%)	0	100	100
6	D1	117/149 (78%)	115 (98%)	2 (2%)	0	100	100
7	E1	134/143 (94%)	132 (98%)	2 (2%)	0	100	100
8	F1	214/261 (82%)	213 (100%)	1 (0%)	0	100	100
9	G1	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
10	H1	125/133 (94%)	123 (98%)	2 (2%)	0	100	100
11	I1	72/107 (67%)	70 (97%)	2 (3%)	0	100	100
12	J1	96/127 (76%)	96 (100%)	0	0	100	100
13	K1	82/86 (95%)	81 (99%)	1 (1%)	0	100	100
14	L1	59/65 (91%)	58 (98%)	1 (2%)	0	100	100
15	M1	48/62 (77%)	45 (94%)	3 (6%)	0	100	100
16	N1	67/156 (43%)	66 (98%)	1 (2%)	0	100	100
17	O1	186/191 (97%)	182 (98%)	4 (2%)	0	100	100
18	P1	182/224 (81%)	180 (99%)	2 (1%)	0	100	100
19	Q1	305/328 (93%)	297 (97%)	8 (3%)	0	100	100
20	R1	100/122 (82%)	98 (98%)	2 (2%)	0	100	100
21	S1	130/150 (87%)	129 (99%)	1 (1%)	0	100	100
22	T1	139/142 (98%)	136 (98%)	3 (2%)	0	100	100
23	U1	140/152 (92%)	136 (97%)	4 (3%)	0	100	100
24	V1	53/56 (95%)	53 (100%)	0	0	100	100
25	W1	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
26	X1	143/159 (90%)	141 (99%)	2 (1%)	0	100	100
27	Y1	129/152 (85%)	126 (98%)	3 (2%)	0	100	100
28	Z1	200/336 (60%)	197 (98%)	3 (2%)	0	100	100
29	a1	209/248 (84%)	201 (96%)	8 (4%)	0	100	100
30	b1	181/197 (92%)	176 (97%)	5 (3%)	0	100	100
31	c1	215/280 (77%)	210 (98%)	5 (2%)	0	100	100
32	d1	192/210 (91%)	184 (96%)	7 (4%)	1 (0%)	24	27
33	e1	127/130 (98%)	126 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	f1	139/147 (95%)	138 (99%)	1 (1%)	0	100	100
38	D3	198/206 (96%)	195 (98%)	3 (2%)	0	100	100
39	E3	128/134 (96%)	126 (98%)	2 (2%)	0	100	100
40	F3	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
41	G3	184/187 (98%)	182 (99%)	2 (1%)	0	100	100
42	H3	180/214 (84%)	179 (99%)	1 (1%)	0	100	100
43	I3	175/178 (98%)	174 (99%)	1 (1%)	0	100	100
44	J3	161/164 (98%)	160 (99%)	1 (1%)	0	100	100
45	K3	97/127 (76%)	93 (96%)	4 (4%)	0	100	100
46	L3	60/164 (37%)	57 (95%)	3 (5%)	0	100	100
47	M3	132/135 (98%)	131 (99%)	1 (1%)	0	100	100
48	N3	140/143 (98%)	136 (97%)	4 (3%)	0	100	100
49	O3	47/61 (77%)	46 (98%)	1 (2%)	0	100	100
50	P3	95/113 (84%)	94 (99%)	1 (1%)	0	100	100
51	Q3	106/120 (88%)	106 (100%)	0	0	100	100
52	R3	124/133 (93%)	123 (99%)	1 (1%)	0	100	100
53	S3	109/112 (97%)	108 (99%)	1 (1%)	0	100	100
54	T3	112/120 (93%)	111 (99%)	1 (1%)	0	100	100
55	U3	96/110 (87%)	96 (100%)	0	0	100	100
56	V3	84/95 (88%)	82 (98%)	2 (2%)	0	100	100
57	W3	66/69 (96%)	66 (100%)	0	0	100	100
58	X3	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
59	Y3	49/128 (38%)	49 (100%)	0	0	100	100
60	p3	23/25 (92%)	23 (100%)	0	0	100	100
61	Z3	96/105 (91%)	95 (99%)	1 (1%)	0	100	100
62	a3	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
63	b3	204/230 (89%)	201 (98%)	3 (2%)	0	100	100
64	c3	231/258 (90%)	228 (99%)	3 (1%)	0	100	100
65	d3	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
66	e3	129/140 (92%)	125 (97%)	4 (3%)	0	100	100
67	f3	145/148 (98%)	137 (94%)	7 (5%)	1 (1%)	18	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	g3	205/221 (93%)	202 (98%)	3 (2%)	0	100	100
69	h3	286/301 (95%)	278 (97%)	8 (3%)	0	100	100
70	j3	152/175 (87%)	150 (99%)	2 (1%)	0	100	100
71	k3	115/154 (75%)	113 (98%)	2 (2%)	0	100	100
72	m3	124/146 (85%)	120 (97%)	4 (3%)	0	100	100
73	n3	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
74	o3	243/260 (94%)	234 (96%)	9 (4%)	0	100	100
75	q3	236/242 (98%)	231 (98%)	5 (2%)	0	100	100
76	r3	384/389 (99%)	380 (99%)	4 (1%)	0	100	100
77	s3	396/405 (98%)	390 (98%)	6 (2%)	0	100	100
78	t3	170/181 (94%)	168 (99%)	2 (1%)	0	100	100
79	u3	189/194 (97%)	188 (100%)	1 (0%)	0	100	100
All	All	11033/12575 (88%)	10841 (98%)	190 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	d1	85	HIS
67	f3	15	VAL

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	225/228 (99%)	225 (100%)	0	100	100
2	k1	199/213 (93%)	199 (100%)	0	100	100
4	l1	85/169 (50%)	85 (100%)	0	100	100
5	C1	94/112 (84%)	94 (100%)	0	100	100
6	D1	109/124 (88%)	109 (100%)	0	100	100
7	E1	111/114 (97%)	111 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F1	195/228 (86%)	195 (100%)	0	100	100
9	G1	70/70 (100%)	70 (100%)	0	100	100
10	H1	108/113 (96%)	107 (99%)	1 (1%)	70	84
11	I1	64/89 (72%)	64 (100%)	0	100	100
12	J1	87/109 (80%)	87 (100%)	0	100	100
13	K1	76/78 (97%)	76 (100%)	0	100	100
14	L1	54/57 (95%)	54 (100%)	0	100	100
15	M1	41/49 (84%)	41 (100%)	0	100	100
16	N1	60/134 (45%)	60 (100%)	0	100	100
17	O1	169/171 (99%)	167 (99%)	2 (1%)	63	78
18	P1	158/178 (89%)	158 (100%)	0	100	100
19	Q1	266/279 (95%)	264 (99%)	2 (1%)	73	85
20	R1	93/108 (86%)	93 (100%)	0	100	100
21	S1	103/120 (86%)	102 (99%)	1 (1%)	68	81
22	T1	113/114 (99%)	112 (99%)	1 (1%)	70	84
23	U1	122/131 (93%)	122 (100%)	0	100	100
24	V1	46/47 (98%)	46 (100%)	0	100	100
25	W1	130/131 (99%)	130 (100%)	0	100	100
26	X1	124/131 (95%)	124 (100%)	0	100	100
27	Y1	115/130 (88%)	115 (100%)	0	100	100
28	Z1	171/256 (67%)	171 (100%)	0	100	100
29	a1	179/215 (83%)	178 (99%)	1 (1%)	78	89
30	b1	161/171 (94%)	161 (100%)	0	100	100
31	c1	184/226 (81%)	183 (100%)	1 (0%)	81	90
32	d1	165/175 (94%)	165 (100%)	0	100	100
33	e1	111/112 (99%)	111 (100%)	0	100	100
34	f1	116/120 (97%)	116 (100%)	0	100	100
38	D3	165/171 (96%)	164 (99%)	1 (1%)	78	89
39	E3	114/117 (97%)	113 (99%)	1 (1%)	70	84
40	F3	176/177 (99%)	175 (99%)	1 (1%)	78	89
41	G3	154/155 (99%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	H3	160/182 (88%)	160 (100%)	0	100	100
43	I3	163/164 (99%)	161 (99%)	2 (1%)	63	78
44	J3	140/141 (99%)	139 (99%)	1 (1%)	76	87
45	K3	91/109 (84%)	91 (100%)	0	100	100
46	L3	57/133 (43%)	56 (98%)	1 (2%)	51	68
47	M3	117/118 (99%)	117 (100%)	0	100	100
48	N3	123/124 (99%)	123 (100%)	0	100	100
49	O3	43/53 (81%)	43 (100%)	0	100	100
50	P3	85/98 (87%)	85 (100%)	0	100	100
51	Q3	95/106 (90%)	95 (100%)	0	100	100
52	R3	114/121 (94%)	114 (100%)	0	100	100
53	S3	98/99 (99%)	97 (99%)	1 (1%)	68	81
54	T3	100/104 (96%)	98 (98%)	2 (2%)	48	64
55	U3	83/90 (92%)	83 (100%)	0	100	100
56	V3	72/77 (94%)	71 (99%)	1 (1%)	59	75
57	W3	64/65 (98%)	62 (97%)	2 (3%)	35	48
58	X3	47/48 (98%)	47 (100%)	0	100	100
59	Y3	46/114 (40%)	46 (100%)	0	100	100
60	p3	24/24 (100%)	24 (100%)	0	100	100
61	Z3	86/92 (94%)	86 (100%)	0	100	100
62	a3	73/74 (99%)	73 (100%)	0	100	100
63	b3	175/194 (90%)	175 (100%)	0	100	100
64	c3	202/221 (91%)	202 (100%)	0	100	100
65	d3	173/174 (99%)	171 (99%)	2 (1%)	63	78
66	e3	103/109 (94%)	103 (100%)	0	100	100
67	f3	119/120 (99%)	119 (100%)	0	100	100
68	g3	173/181 (96%)	171 (99%)	2 (1%)	63	78
69	h3	244/254 (96%)	243 (100%)	1 (0%)	84	92
70	j3	135/154 (88%)	134 (99%)	1 (1%)	76	87
71	k3	106/134 (79%)	106 (100%)	0	100	100
72	m3	115/131 (88%)	113 (98%)	2 (2%)	53	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	n3	109/110 (99%)	109 (100%)	0	100	100
74	o3	190/197 (96%)	189 (100%)	1 (0%)	81	90
75	q3	207/209 (99%)	207 (100%)	0	100	100
76	r3	330/332 (99%)	328 (99%)	2 (1%)	78	89
77	s3	326/329 (99%)	325 (100%)	1 (0%)	86	93
78	t3	149/157 (95%)	148 (99%)	1 (1%)	76	87
79	u3	167/170 (98%)	165 (99%)	2 (1%)	63	78
All	All	9617/10634 (90%)	9580 (100%)	37 (0%)	81	92

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
72	m3	36	SER
79	u3	42	ASN
72	m3	55	VAL
76	r3	377	THR
43	I3	10	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
33	e1	42	GLN
77	s3	350	GLN
48	N3	86	ASN
76	r3	317	HIS
79	u3	37	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	h1	1617/1808 (89%)	223 (13%)	0
35	B1	11/12 (91%)	1 (9%)	0
36	W2	75/76 (98%)	10 (13%)	0
36	i2	75/76 (98%)	8 (10%)	0
37	C3	118/119 (99%)	8 (6%)	0
81	A3	3191/3390 (94%)	417 (13%)	19 (0%)
82	B3	162/163 (99%)	26 (16%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	5249/5644 (93%)	693 (13%)	19 (0%)

5 of 693 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	h1	2	A
3	h1	4	C
3	h1	17	C
3	h1	25	C
3	h1	26	A

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
81	A3	2482	G
81	A3	2543	A
81	A3	3123	U
81	A3	2503	U
81	A3	926	G

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

216 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
81	PSU	A3	902	84,83,81	18,21,22	4.65	8 (44%)	22,30,33	1.81	5 (22%)
81	A2M	A3	2284	81	22,25,26	3.89	9 (40%)	31,36,39	3.17	14 (45%)
81	PSU	A3	2257	81	18,21,22	4.64	8 (44%)	22,30,33	1.85	5 (22%)
3	PSU	h1	1190	3	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)
81	OMG	A3	2818	81	23,26,27	2.55	9 (39%)	33,38,41	2.17	12 (36%)
81	A2M	A3	369	81	22,25,26	3.93	8 (36%)	31,36,39	3.02	13 (41%)
81	PSU	A3	1135	81	18,21,22	4.64	8 (44%)	22,30,33	1.86	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
81	OMG	A3	296	81	23,26,27	2.57	8 (34%)	33,38,41	2.21	11 (33%)
81	A2M	A3	2259	81	22,25,26	3.97	9 (40%)	31,36,39	3.07	14 (45%)
81	UY1	A3	2653	81	19,22,23	4.20	7 (36%)	22,31,34	1.87	5 (22%)
81	PSU	A3	2868	81	18,21,22	4.64	8 (44%)	22,30,33	1.90	6 (27%)
3	PSU	h1	310	3	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)
81	A2M	A3	2329	81	22,25,26	3.94	8 (36%)	31,36,39	3.00	11 (35%)
3	4AC	h1	1283	3	21,24,25	3.25	11 (52%)	29,34,37	0.98	2 (6%)
3	OMC	h1	473	3	19,22,23	3.30	8 (42%)	26,31,34	0.72	0
3	PSU	h1	1304	3	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
81	OMC	A3	2200	84,81	19,22,23	3.29	8 (42%)	26,31,34	0.80	0
3	PSU	h1	1634	3	18,21,22	4.64	8 (44%)	22,30,33	1.80	5 (22%)
81	OMU	A3	3304	81	19,22,23	3.20	8 (42%)	26,31,34	1.64	4 (15%)
3	B8N	h1	1194	3	24,29,30	3.04	7 (29%)	29,42,45	1.73	6 (20%)
81	PSU	A3	150	84,81	18,21,22	4.65	8 (44%)	22,30,33	1.85	5 (22%)
81	A2M	A3	2643	81	22,25,26	3.94	9 (40%)	31,36,39	2.96	12 (38%)
81	A2M	A3	946	81	22,25,26	3.94	9 (40%)	31,36,39	3.07	14 (45%)
81	OMU	A3	1068	81	19,22,23	3.20	8 (42%)	26,31,34	1.70	5 (19%)
81	A2M	A3	2223	81	22,25,26	3.95	9 (40%)	31,36,39	2.96	11 (35%)
3	OMG	h1	246	84,3	23,26,27	2.59	8 (34%)	33,38,41	2.27	10 (30%)
81	PSU	A3	2263	81	18,21,22	4.66	8 (44%)	22,30,33	1.84	5 (22%)
3	OMG	h1	598	3	23,26,27	2.57	8 (34%)	33,38,41	2.25	10 (30%)
3	PSU	h1	103	84,3	18,21,22	4.64	8 (44%)	22,30,33	1.84	5 (22%)
81	PSU	A3	2267	81	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
81	OMC	A3	2340	81	19,22,23	3.28	8 (42%)	26,31,34	0.68	0
81	A2M	A3	1144	81	22,25,26	3.94	9 (40%)	31,36,39	3.00	13 (41%)
3	UY1	h1	603	3	19,22,23	4.17	7 (36%)	22,31,34	1.84	5 (22%)
81	OMU	A3	2738	81	19,22,23	3.21	8 (42%)	26,31,34	1.67	5 (19%)
3	PSU	h1	1308	3	18,21,22	4.64	8 (44%)	22,30,33	1.78	5 (22%)
3	PSU	h1	584	3	18,21,22	4.75	9 (50%)	22,30,33	1.79	5 (22%)
3	OMU	h1	886	3	19,22,23	3.22	8 (42%)	26,31,34	1.80	5 (19%)
3	PSU	h1	339	84,3	18,21,22	4.66	8 (44%)	22,30,33	1.80	6 (27%)
81	PSU	A3	228	81	18,21,22	4.66	8 (44%)	22,30,33	1.83	5 (22%)
81	OMG	A3	2920	81	23,26,27	2.55	8 (34%)	33,38,41	2.21	11 (33%)
3	PSU	h1	306	3	18,21,22	4.65	8 (44%)	22,30,33	1.76	5 (22%)
3	A2M	h1	440	3	22,25,26	3.94	8 (36%)	31,36,39	3.04	12 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
81	OMG	A3	1857	81	23,26,27	2.54	8 (34%)	33,38,41	2.19	11 (33%)
3	PSU	h1	121	3,83	18,21,22	4.66	8 (44%)	22,30,33	1.80	5 (22%)
81	A2M	A3	886	81	22,25,26	3.93	9 (40%)	31,36,39	2.96	13 (41%)
82	PSU	B3	96	82,84	18,21,22	4.66	8 (44%)	22,30,33	1.75	5 (22%)
81	OMC	A3	674	81	19,22,23	3.25	8 (42%)	26,31,34	0.68	0
81	PSU	A3	976	84,81	18,21,22	4.67	8 (44%)	22,30,33	1.83	5 (22%)
81	A2M	A3	1460	81	22,25,26	3.93	9 (40%)	31,36,39	2.99	12 (38%)
81	PSU	A3	2214	81	18,21,22	4.65	8 (44%)	22,30,33	1.87	5 (22%)
81	5MC	A3	2281	81	18,22,23	4.01	7 (38%)	26,32,35	1.04	2 (7%)
81	PSU	A3	2958	81	18,21,22	4.66	8 (44%)	22,30,33	1.84	5 (22%)
3	PSU	h1	258	3	18,21,22	4.66	8 (44%)	22,30,33	1.81	5 (22%)
81	PSU	A3	1482	81	18,21,22	4.62	8 (44%)	22,30,33	1.76	5 (22%)
81	PSU	A3	1134	81	18,21,22	4.60	8 (44%)	22,30,33	1.88	5 (22%)
81	OMG	A3	2622	36,81	23,26,27	2.57	8 (34%)	33,38,41	2.22	10 (30%)
3	A2M	h1	544	3	22,25,26	3.91	9 (40%)	31,36,39	2.98	13 (41%)
3	OMU	h1	1234	3	19,22,23	3.20	8 (42%)	26,31,34	1.65	4 (15%)
81	PSU	A3	717	81	18,21,22	4.65	8 (44%)	22,30,33	1.86	5 (22%)
81	PSU	A3	2137	84,81	18,21,22	4.65	8 (44%)	22,30,33	1.92	5 (22%)
3	OMU	h1	1447	3	19,22,23	3.20	8 (42%)	26,31,34	1.61	4 (15%)
81	PSU	A3	1685	81	18,21,22	4.65	8 (44%)	22,30,33	1.87	6 (27%)
3	PSU	h1	95	3	18,21,22	4.67	8 (44%)	22,30,33	1.80	5 (22%)
3	PSU	h1	753	3	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)
3	PSU	h1	1615	3	18,21,22	4.63	8 (44%)	22,30,33	1.81	5 (22%)
81	OMU	A3	48	81	19,22,23	3.19	8 (42%)	26,31,34	1.63	4 (15%)
81	OMC	A3	2839	81	19,22,23	3.28	8 (42%)	26,31,34	0.78	0
3	PSU	h1	1210	3	18,21,22	4.63	8 (44%)	22,30,33	1.83	5 (22%)
3	PSU	h1	605	3	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)
81	PSU	A3	510	81	18,21,22	4.65	8 (44%)	22,30,33	1.85	5 (22%)
81	OMG	A3	2127	81	23,26,27	2.54	9 (39%)	33,38,41	2.18	13 (39%)
81	PSU	A3	2857	81	18,21,22	4.64	8 (44%)	22,30,33	1.87	5 (22%)
81	PSU	A3	2829	81	18,21,22	4.62	8 (44%)	22,30,33	1.90	6 (27%)
81	OMG	A3	2394	81	23,26,27	2.54	9 (39%)	33,38,41	2.15	12 (36%)
3	PSU	h1	1002	3	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)
81	OMG	A3	2794	81	23,26,27	2.55	8 (34%)	33,38,41	2.14	11 (33%)
81	PSU	A3	2419	81	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
81	PSU	A3	2883	81	18,21,22	4.65	8 (44%)	22,30,33	1.85	6 (27%)
3	OMC	h1	38	3	19,22,23	3.32	8 (42%)	26,31,34	0.71	0
3	A2M	h1	468	3	22,25,26	3.95	8 (36%)	31,36,39	3.01	12 (38%)
81	1MA	A3	656	81	21,25,26	2.77	5 (23%)	31,37,40	1.73	7 (22%)
81	OMG	A3	918	84,81	23,26,27	2.57	8 (34%)	33,38,41	2.26	10 (30%)
3	OMU	h1	373	3	19,22,23	3.22	8 (42%)	26,31,34	1.66	4 (15%)
81	OMU	A3	1894	81	19,22,23	3.23	8 (42%)	26,31,34	1.71	5 (19%)
3	PSU	h1	1567	3	18,21,22	4.67	8 (44%)	22,30,33	1.83	5 (22%)
81	A2M	A3	827	84,83,81	22,25,26	3.96	9 (40%)	31,36,39	3.04	12 (38%)
81	OMC	A3	1862	81	19,22,23	3.26	8 (42%)	26,31,34	0.68	0
81	PSU	A3	2947	84,81	18,21,22	4.64	9 (50%)	22,30,33	1.85	6 (27%)
3	A2M	h1	1579	3	22,25,26	3.94	9 (40%)	31,36,39	3.04	13 (41%)
81	OMU	A3	2720	81	19,22,23	3.20	8 (42%)	26,31,34	1.64	4 (15%)
81	PSU	A3	2194	84,81	18,21,22	4.63	8 (44%)	22,30,33	1.80	5 (22%)
81	OMG	A3	2654	81	23,26,27	2.53	9 (39%)	33,38,41	2.13	13 (39%)
82	OMG	B3	78	82	23,26,27	2.56	8 (34%)	33,38,41	2.23	10 (30%)
81	PSU	A3	464	81	18,21,22	4.67	8 (44%)	22,30,33	1.80	6 (27%)
81	PSU	A3	2897	81	18,21,22	4.64	8 (44%)	22,30,33	1.80	5 (22%)
81	OMG	A3	2126	81	23,26,27	2.54	8 (34%)	33,38,41	2.20	11 (33%)
81	PSU	A3	966	81	18,21,22	4.61	8 (44%)	22,30,33	1.74	5 (22%)
81	PSU	A3	2139	81	18,21,22	4.64	8 (44%)	22,30,33	1.81	5 (22%)
3	PSU	h1	1178	3	18,21,22	4.64	8 (44%)	22,30,33	1.82	5 (22%)
81	OMC	A3	2685	81	19,22,23	3.28	8 (42%)	26,31,34	0.73	0
81	OMG	A3	2796	81	23,26,27	2.56	8 (34%)	33,38,41	2.20	11 (33%)
81	UR3	A3	2956	81	19,22,23	2.79	8 (42%)	26,32,35	1.31	2 (7%)
3	OMU	h1	614	3	19,22,23	3.21	8 (42%)	26,31,34	1.65	5 (19%)
3	OMU	h1	581	84,3	19,22,23	3.23	8 (42%)	26,31,34	1.67	4 (15%)
81	OMG	A3	399	81	23,26,27	2.60	8 (34%)	33,38,41	2.32	10 (30%)
81	OMC	A3	1480	81	19,22,23	3.30	8 (42%)	26,31,34	0.73	0
81	OMG	A3	2925	81	23,26,27	2.57	8 (34%)	33,38,41	2.25	10 (30%)
81	PSU	A3	895	81	18,21,22	4.61	8 (44%)	22,30,33	1.78	5 (22%)
81	PSU	A3	34	81	18,21,22	4.63	8 (44%)	22,30,33	1.87	5 (22%)
3	A2M	h1	1758	3	22,25,26	3.94	10 (45%)	31,36,39	2.97	12 (38%)
81	OMU	A3	3289	81	19,22,23	3.20	8 (42%)	26,31,34	1.63	4 (15%)
81	PSU	A3	684	81	18,21,22	4.64	8 (44%)	22,30,33	1.80	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	h1	1184	3	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)
3	6MZ	h1	1771	84,3,83	22,25,26	2.75	5 (22%)	30,36,39	2.45	11 (36%)
3	PSU	h1	1787	3	18,21,22	4.66	8 (44%)	22,30,33	1.84	5 (22%)
3	A2M	h1	28	3,83	22,25,26	3.93	8 (36%)	31,36,39	3.00	12 (38%)
3	OMU	h1	1272	3	19,22,23	3.23	8 (42%)	26,31,34	1.66	4 (15%)
81	OMG	A3	2398	81	23,26,27	2.53	9 (39%)	33,38,41	2.17	13 (39%)
3	PSU	h1	1120	3	18,21,22	4.64	8 (44%)	22,30,33	1.77	5 (22%)
3	PSU	h1	809	3	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
81	OMU	A3	2732	81	19,22,23	3.20	8 (42%)	26,31,34	1.61	4 (15%)
81	OMC	A3	2882	81	19,22,23	3.27	8 (42%)	26,31,34	0.75	0
81	A2M	A3	2949	81	22,25,26	3.95	9 (40%)	31,36,39	3.04	15 (48%)
81	OMU	A3	675	81	19,22,23	3.22	8 (42%)	26,31,34	1.69	5 (19%)
81	PSU	A3	970	81	18,21,22	4.66	9 (50%)	22,30,33	1.89	5 (22%)
81	PSU	A3	2261	81	18,21,22	4.65	8 (44%)	22,30,33	1.82	5 (22%)
81	PSU	A3	2317	84,81	18,21,22	4.65	8 (44%)	22,30,33	1.90	5 (22%)
3	PSU	h1	1485	3	18,21,22	4.67	8 (44%)	22,30,33	1.83	5 (22%)
81	PSU	A3	2321	83,81	18,21,22	4.65	8 (44%)	22,30,33	1.84	5 (22%)
3	PSU	h1	961	84,3	18,21,22	4.67	8 (44%)	22,30,33	1.85	5 (22%)
3	A2M	h1	424	3	22,25,26	3.95	9 (40%)	31,36,39	3.02	14 (45%)
3	PSU	h1	451	84,3	18,21,22	4.67	8 (44%)	22,30,33	1.87	6 (27%)
3	OMU	h1	1383	3,83	19,22,23	3.23	8 (42%)	26,31,34	1.67	4 (15%)
81	OMC	A3	2296	81	19,22,23	3.29	8 (42%)	26,31,34	0.74	0
82	PSU	B3	21	82,81	18,21,22	4.62	8 (44%)	22,30,33	1.78	5 (22%)
81	PSU	A3	829	81	18,21,22	4.63	8 (44%)	22,30,33	1.86	5 (22%)
3	PSU	h1	1217	3	18,21,22	4.68	8 (44%)	22,30,33	1.81	5 (22%)
82	PSU	B3	77	82	18,21,22	4.65	8 (44%)	22,30,33	1.86	5 (22%)
3	MA6	h1	1790	3	23,26,27	1.24	3 (13%)	34,38,41	2.86	14 (41%)
3	PSU	h1	635	3	18,21,22	4.62	8 (44%)	22,30,33	1.79	5 (22%)
3	A2M	h1	1329	3	22,25,26	3.95	9 (40%)	31,36,39	3.02	13 (41%)
81	OMU	A3	2886	81	19,22,23	3.21	8 (42%)	26,31,34	1.63	4 (15%)
81	OMG	A3	2239	81	23,26,27	2.59	8 (34%)	33,38,41	2.24	10 (30%)
3	PSU	h1	763	3	18,21,22	4.66	8 (44%)	22,30,33	1.83	5 (22%)
3	MA6	h1	1789	3	23,26,27	1.24	3 (13%)	34,38,41	2.82	14 (41%)
81	PSU	A3	2435	81	18,21,22	4.64	8 (44%)	22,30,33	1.90	6 (27%)
3	OMC	h1	1218	3	19,22,23	3.31	8 (42%)	26,31,34	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PSU	h1	1106	3	18,21,22	4.65	8 (44%)	22,30,33	1.82	5 (22%)
81	PSU	A3	1016	84,81	18,21,22	4.65	8 (44%)	22,30,33	1.84	5 (22%)
3	PSU	h1	762	3	18,21,22	4.65	8 (44%)	22,30,33	1.80	5 (22%)
81	OMG	A3	2412	84,81	23,26,27	2.56	8 (34%)	33,38,41	2.25	11 (33%)
81	A2M	A3	2804	81	22,25,26	3.90	8 (36%)	31,36,39	3.20	15 (48%)
81	PSU	A3	1002	81	18,21,22	4.67	8 (44%)	22,30,33	1.85	5 (22%)
81	OMG	A3	815	81	23,26,27	2.57	8 (34%)	33,38,41	2.27	11 (33%)
81	OMC	A3	2368	81	19,22,23	3.27	8 (42%)	26,31,34	0.69	0
81	A2M	A3	660	81	22,25,26	3.94	9 (40%)	31,36,39	3.12	14 (45%)
81	PSU	A3	786	81	18,21,22	4.66	8 (44%)	22,30,33	1.73	5 (22%)
81	OMG	A3	1461	81	23,26,27	2.55	8 (34%)	33,38,41	2.26	12 (36%)
81	OMU	A3	2413	84,81	19,22,23	3.17	8 (42%)	26,31,34	1.59	4 (15%)
81	PSU	A3	1056	81	18,21,22	4.65	8 (44%)	22,30,33	1.84	5 (22%)
81	PSU	A3	311	84,81	18,21,22	4.66	8 (44%)	22,30,33	1.73	5 (22%)
3	PSU	h1	362	3	18,21,22	4.62	8 (44%)	22,30,33	1.81	5 (22%)
81	OMC	A3	1852	81	19,22,23	3.31	8 (42%)	26,31,34	0.74	0
3	PSU	h1	470	3	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
3	OMG	h1	392	3	23,26,27	2.59	8 (34%)	33,38,41	2.24	10 (30%)
81	OMU	A3	804	81	19,22,23	3.22	8 (42%)	26,31,34	1.69	5 (19%)
81	A2M	A3	2324	81	22,25,26	3.94	9 (40%)	31,36,39	3.01	13 (41%)
81	OMU	A3	2424	81	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
81	A2M	A3	817	81	22,25,26	3.91	9 (40%)	31,36,39	3.05	14 (45%)
81	OMG	A3	2291	81	23,26,27	2.56	8 (34%)	33,38,41	2.24	10 (30%)
81	OMC	A3	1448	81	19,22,23	3.29	8 (42%)	26,31,34	0.87	1 (3%)
3	PSU	h1	417	3	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
81	A2M	A3	2914	81	22,25,26	3.93	9 (40%)	31,36,39	3.07	12 (38%)
3	PSU	h1	1535	3	18,21,22	4.67	8 (44%)	22,30,33	1.80	5 (22%)
81	OMU	A3	144	81	19,22,23	3.21	8 (42%)	26,31,34	1.65	4 (15%)
81	OMU	A3	44	84,81	19,22,23	3.23	8 (42%)	26,31,34	1.63	4 (15%)
3	PSU	h1	606	3	18,21,22	4.61	8 (44%)	22,30,33	1.79	5 (22%)
3	PSU	h1	607	3	18,21,22	4.66	8 (44%)	22,30,33	1.86	6 (27%)
3	PSU	h1	1524	3	18,21,22	4.69	8 (44%)	22,30,33	1.75	5 (22%)
3	PSU	h1	1027	3	18,21,22	4.68	9 (50%)	22,30,33	1.81	5 (22%)
3	OMC	h1	1645	3	19,22,23	3.30	8 (42%)	26,31,34	0.71	0
81	PSU	A3	277	81	18,21,22	4.62	8 (44%)	22,30,33	1.83	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
81	PSU	A3	1064	81	18,21,22	4.64	8 (44%)	22,30,33	1.85	5 (22%)
81	PSU	A3	2926	84,81	18,21,22	4.65	8 (44%)	22,30,33	1.88	5 (22%)
81	OMU	A3	2350	81	19,22,23	3.23	8 (42%)	26,31,34	1.67	5 (19%)
3	OMG	h1	1274	3	23,26,27	2.58	8 (34%)	33,38,41	2.25	10 (30%)
3	A2M	h1	622	3,83	22,25,26	3.91	9 (40%)	31,36,39	3.11	14 (45%)
3	4AC	h1	1781	3	21,24,25	3.26	11 (52%)	29,34,37	1.04	3 (10%)
3	OMU	h1	123	3	19,22,23	3.21	8 (42%)	26,31,34	1.66	5 (19%)
81	OMC	A3	1849	81	19,22,23	3.25	8 (42%)	26,31,34	0.70	0
81	PSU	A3	1133	81	18,21,22	4.63	8 (44%)	22,30,33	1.82	5 (22%)
81	OMU	A3	1537	81	19,22,23	3.21	8 (42%)	26,31,34	1.63	4 (15%)
3	A2M	h1	977	3	22,25,26	3.94	9 (40%)	31,36,39	2.94	12 (38%)
3	A2M	h1	800	3	22,25,26	3.94	9 (40%)	31,36,39	2.98	12 (38%)
82	A2M	B3	46	82	22,25,26	3.93	9 (40%)	31,36,39	3.01	14 (45%)
81	A2M	A3	1378	81	22,25,26	3.93	9 (40%)	31,36,39	2.96	12 (38%)
3	OMC	h1	140	3	19,22,23	3.31	8 (42%)	26,31,34	0.72	0
3	PSU	h1	950	3	18,21,22	4.64	8 (44%)	22,30,33	1.79	5 (22%)
81	PSU	A3	3113	81	18,21,22	4.63	8 (44%)	22,30,33	1.77	5 (22%)
81	PSU	A3	2978	81	18,21,22	4.65	8 (44%)	22,30,33	1.80	5 (22%)
3	OMC	h1	418	3	19,22,23	3.30	8 (42%)	26,31,34	0.89	1 (3%)
81	5MC	A3	2873	84,81	18,22,23	4.02	7 (38%)	26,32,35	1.09	1 (3%)
81	OMC	A3	2962	81	19,22,23	3.25	8 (42%)	26,31,34	0.77	0
3	OMG	h1	1433	3,83	23,26,27	2.55	8 (34%)	33,38,41	2.19	11 (33%)
81	A2M	A3	2129	81	22,25,26	3.96	9 (40%)	31,36,39	3.01	12 (38%)
3	OMU	h1	1012	3	19,22,23	3.20	8 (42%)	26,31,34	1.67	4 (15%)
81	PSU	A3	1474	81	18,21,22	4.64	8 (44%)	22,30,33	1.82	5 (22%)
81	PSU	A3	2747	81	18,21,22	4.62	8 (44%)	22,30,33	1.80	5 (22%)
81	OMC	A3	40	81	19,22,23	3.27	8 (42%)	26,31,34	0.89	1 (3%)
3	A2M	h1	162	3	22,25,26	3.95	9 (40%)	31,36,39	3.01	13 (41%)
81	PSU	A3	2269	81	18,21,22	4.68	8 (44%)	22,30,33	1.78	5 (22%)
81	OMC	A3	2951	81	19,22,23	3.23	8 (42%)	26,31,34	0.78	0
3	PSU	h1	1293	3	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
81	PSU	A3	42	84,81	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
81	OMU	A3	787	81	19,22,23	3.21	8 (42%)	26,31,34	1.65	5 (19%)
81	OMU	A3	2924	84,81	19,22,23	3.21	8 (42%)	26,31,34	1.68	4 (15%)

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
81	PSU	A3	902	84,83,81	-	0/7/25/26	0/2/2/2
81	A2M	A3	2284	81	-	3/9/27/28	0/3/3/3
81	PSU	A3	2257	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	1190	3	-	0/7/25/26	0/2/2/2
81	OMG	A3	2818	81	-	0/9/27/28	0/3/3/3
81	A2M	A3	369	81	-	1/9/27/28	0/3/3/3
81	PSU	A3	1135	81	-	0/7/25/26	0/2/2/2
81	OMG	A3	296	81	-	2/9/27/28	0/3/3/3
81	A2M	A3	2259	81	-	2/9/27/28	0/3/3/3
81	UY1	A3	2653	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	2868	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	310	3	-	0/7/25/26	0/2/2/2
81	A2M	A3	2329	81	-	0/9/27/28	0/3/3/3
3	4AC	h1	1283	3	-	0/11/29/30	0/2/2/2
3	OMC	h1	473	3	-	0/9/27/28	0/2/2/2
3	PSU	h1	1304	3	-	0/7/25/26	0/2/2/2
81	OMC	A3	2200	84,81	-	4/9/27/28	0/2/2/2
3	PSU	h1	1634	3	-	0/7/25/26	0/2/2/2
81	OMU	A3	3304	81	-	0/9/27/28	0/2/2/2
3	B8N	h1	1194	3	-	3/16/34/35	0/2/2/2
81	PSU	A3	150	84,81	-	0/7/25/26	0/2/2/2
81	A2M	A3	2643	81	-	0/9/27/28	0/3/3/3
81	A2M	A3	946	81	-	2/9/27/28	0/3/3/3
81	OMU	A3	1068	81	-	0/9/27/28	0/2/2/2
81	A2M	A3	2223	81	-	0/9/27/28	0/3/3/3
3	OMG	h1	246	84,3	-	0/9/27/28	0/3/3/3
81	PSU	A3	2263	81	-	1/7/25/26	0/2/2/2
3	OMG	h1	598	3	-	3/9/27/28	0/3/3/3
3	PSU	h1	103	84,3	-	0/7/25/26	0/2/2/2
81	PSU	A3	2267	81	-	0/7/25/26	0/2/2/2
81	OMC	A3	2340	81	-	0/9/27/28	0/2/2/2
81	A2M	A3	1144	81	-	0/9/27/28	0/3/3/3
3	UY1	h1	603	3	-	0/9/27/28	0/2/2/2
81	OMU	A3	2738	81	-	0/9/27/28	0/2/2/2
3	PSU	h1	1308	3	-	2/7/25/26	0/2/2/2
3	PSU	h1	584	3	-	6/7/25/26	0/2/2/2
3	OMU	h1	886	3	-	3/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	h1	339	84,3	-	0/7/25/26	0/2/2/2
81	PSU	A3	228	81	-	1/7/25/26	0/2/2/2
81	OMG	A3	2920	81	-	0/9/27/28	0/3/3/3
3	PSU	h1	306	3	-	0/7/25/26	0/2/2/2
3	A2M	h1	440	3	-	0/9/27/28	0/3/3/3
81	OMG	A3	1857	81	-	0/9/27/28	0/3/3/3
3	PSU	h1	121	3,83	-	0/7/25/26	0/2/2/2
81	A2M	A3	886	81	-	0/9/27/28	0/3/3/3
82	PSU	B3	96	82,84	-	2/7/25/26	0/2/2/2
81	OMC	A3	674	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	976	84,81	-	0/7/25/26	0/2/2/2
81	A2M	A3	1460	81	-	0/9/27/28	0/3/3/3
81	PSU	A3	2214	81	-	0/7/25/26	0/2/2/2
81	5MC	A3	2281	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	2958	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	258	3	-	1/7/25/26	0/2/2/2
81	PSU	A3	1482	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	1134	81	-	0/7/25/26	0/2/2/2
81	OMG	A3	2622	36,81	-	0/9/27/28	0/3/3/3
3	A2M	h1	544	3	-	2/9/27/28	0/3/3/3
3	OMU	h1	1234	3	-	2/9/27/28	0/2/2/2
81	PSU	A3	717	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	2137	84,81	-	0/7/25/26	0/2/2/2
3	OMU	h1	1447	3	-	0/9/27/28	0/2/2/2
81	PSU	A3	1685	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	95	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	753	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	1615	3	-	0/7/25/26	0/2/2/2
81	OMU	A3	48	81	-	0/9/27/28	0/2/2/2
81	OMC	A3	2839	81	-	0/9/27/28	0/2/2/2
3	PSU	h1	1210	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	605	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	510	81	-	0/7/25/26	0/2/2/2
81	OMG	A3	2127	81	-	0/9/27/28	0/3/3/3
81	PSU	A3	2857	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	2829	81	-	0/7/25/26	0/2/2/2
81	OMG	A3	2394	81	-	0/9/27/28	0/3/3/3
3	PSU	h1	1002	3	-	0/7/25/26	0/2/2/2
81	OMG	A3	2794	81	-	0/9/27/28	0/3/3/3
81	PSU	A3	2419	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	2883	81	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	h1	38	3	-	2/9/27/28	0/2/2/2
3	A2M	h1	468	3	-	0/9/27/28	0/3/3/3
81	1MA	A3	656	81	-	2/7/25/26	0/3/3/3
81	OMG	A3	918	84,81	-	2/9/27/28	0/3/3/3
3	OMU	h1	373	3	-	0/9/27/28	0/2/2/2
81	OMU	A3	1894	81	-	0/9/27/28	0/2/2/2
3	PSU	h1	1567	3	-	0/7/25/26	0/2/2/2
81	A2M	A3	827	84,83,81	-	3/9/27/28	0/3/3/3
81	OMC	A3	1862	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	2947	84,81	-	2/7/25/26	0/2/2/2
3	A2M	h1	1579	3	-	2/9/27/28	0/3/3/3
81	OMU	A3	2720	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	2194	84,81	-	0/7/25/26	0/2/2/2
81	OMG	A3	2654	81	-	0/9/27/28	0/3/3/3
82	OMG	B3	78	82	-	2/9/27/28	0/3/3/3
81	PSU	A3	464	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	2897	81	-	0/7/25/26	0/2/2/2
81	OMG	A3	2126	81	-	0/9/27/28	0/3/3/3
81	PSU	A3	966	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	2139	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	1178	3	-	0/7/25/26	0/2/2/2
81	OMC	A3	2685	81	-	0/9/27/28	0/2/2/2
81	OMG	A3	2796	81	-	0/9/27/28	0/3/3/3
81	UR3	A3	2956	81	-	2/7/25/26	0/2/2/2
3	OMU	h1	614	3	-	3/9/27/28	0/2/2/2
3	OMU	h1	581	84,3	-	2/9/27/28	0/2/2/2
81	OMG	A3	399	81	-	2/9/27/28	0/3/3/3
81	OMC	A3	1480	81	-	0/9/27/28	0/2/2/2
81	OMG	A3	2925	81	-	0/9/27/28	0/3/3/3
81	PSU	A3	895	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	34	81	-	0/7/25/26	0/2/2/2
3	A2M	h1	1758	3	-	0/9/27/28	0/3/3/3
81	OMU	A3	3289	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	684	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	1184	3	-	0/7/25/26	0/2/2/2
3	6MZ	h1	1771	84,3,83	-	0/9/27/28	0/3/3/3
3	PSU	h1	1787	3	-	2/7/25/26	0/2/2/2
3	A2M	h1	28	3,83	-	0/9/27/28	0/3/3/3
3	OMU	h1	1272	3	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	OMG	A3	2398	81	-	0/9/27/28	0/3/3/3
3	PSU	h1	1120	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	809	3	-	0/7/25/26	0/2/2/2
81	OMU	A3	2732	81	-	0/9/27/28	0/2/2/2
81	OMC	A3	2882	81	-	0/9/27/28	0/2/2/2
81	A2M	A3	2949	81	-	0/9/27/28	0/3/3/3
81	OMU	A3	675	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	970	81	-	1/7/25/26	0/2/2/2
81	PSU	A3	2261	81	-	1/7/25/26	0/2/2/2
81	PSU	A3	2317	84,81	-	3/7/25/26	0/2/2/2
3	PSU	h1	1485	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	2321	83,81	-	2/7/25/26	0/2/2/2
3	PSU	h1	961	84,3	-	0/7/25/26	0/2/2/2
3	A2M	h1	424	3	-	0/9/27/28	0/3/3/3
3	PSU	h1	451	84,3	-	0/7/25/26	0/2/2/2
3	OMU	h1	1383	3,83	-	0/9/27/28	0/2/2/2
81	OMC	A3	2296	81	-	0/9/27/28	0/2/2/2
82	PSU	B3	21	82,81	-	0/7/25/26	0/2/2/2
81	PSU	A3	829	81	-	0/7/25/26	0/2/2/2
3	PSU	h1	1217	3	-	0/7/25/26	0/2/2/2
82	PSU	B3	77	82	-	0/7/25/26	0/2/2/2
3	MA6	h1	1790	3	-	4/11/29/30	0/3/3/3
3	PSU	h1	635	3	-	0/7/25/26	0/2/2/2
3	A2M	h1	1329	3	-	0/9/27/28	0/3/3/3
81	OMU	A3	2886	81	-	0/9/27/28	0/2/2/2
81	OMG	A3	2239	81	-	0/9/27/28	0/3/3/3
3	PSU	h1	763	3	-	0/7/25/26	0/2/2/2
3	MA6	h1	1789	3	-	0/11/29/30	0/3/3/3
81	PSU	A3	2435	81	-	0/7/25/26	0/2/2/2
3	OMC	h1	1218	3	-	0/9/27/28	0/2/2/2
3	PSU	h1	1106	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	1016	84,81	-	0/7/25/26	0/2/2/2
3	PSU	h1	762	3	-	0/7/25/26	0/2/2/2
81	OMG	A3	2412	84,81	-	1/9/27/28	0/3/3/3
81	A2M	A3	2804	81	-	4/9/27/28	0/3/3/3
81	PSU	A3	1002	81	-	2/7/25/26	0/2/2/2
81	OMG	A3	815	81	-	0/9/27/28	0/3/3/3
81	OMC	A3	2368	81	-	3/9/27/28	0/2/2/2
81	A2M	A3	660	81	-	2/9/27/28	0/3/3/3
81	PSU	A3	786	81	-	3/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
81	OMG	A3	1461	81	-	1/9/27/28	0/3/3/3
81	OMU	A3	2413	84,81	-	2/9/27/28	0/2/2/2
81	PSU	A3	1056	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	311	84,81	-	0/7/25/26	0/2/2/2
3	PSU	h1	362	3	-	0/7/25/26	0/2/2/2
81	OMC	A3	1852	81	-	0/9/27/28	0/2/2/2
3	PSU	h1	470	3	-	0/7/25/26	0/2/2/2
3	OMG	h1	392	3	-	2/9/27/28	0/3/3/3
81	OMU	A3	804	81	-	0/9/27/28	0/2/2/2
81	A2M	A3	2324	81	-	0/9/27/28	0/3/3/3
81	OMU	A3	2424	81	-	0/9/27/28	0/2/2/2
81	A2M	A3	817	81	-	1/9/27/28	0/3/3/3
81	OMG	A3	2291	81	-	2/9/27/28	0/3/3/3
81	OMC	A3	1448	81	-	3/9/27/28	0/2/2/2
3	PSU	h1	417	3	-	0/7/25/26	0/2/2/2
81	A2M	A3	2914	81	-	5/9/27/28	0/3/3/3
3	PSU	h1	1535	3	-	0/7/25/26	0/2/2/2
81	OMU	A3	144	81	-	1/9/27/28	0/2/2/2
81	OMU	A3	44	84,81	-	0/9/27/28	0/2/2/2
3	PSU	h1	606	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	607	3	-	0/7/25/26	0/2/2/2
3	PSU	h1	1524	3	-	2/7/25/26	0/2/2/2
3	PSU	h1	1027	3	-	1/7/25/26	0/2/2/2
3	OMC	h1	1645	3	-	0/9/27/28	0/2/2/2
81	PSU	A3	277	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	1064	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	2926	84,81	-	3/7/25/26	0/2/2/2
81	OMU	A3	2350	81	-	0/9/27/28	0/2/2/2
3	OMG	h1	1274	3	-	2/9/27/28	0/3/3/3
3	A2M	h1	622	3,83	-	4/9/27/28	0/3/3/3
3	4AC	h1	1781	3	-	0/11/29/30	0/2/2/2
3	OMU	h1	123	3	-	2/9/27/28	0/2/2/2
81	OMC	A3	1849	81	-	0/9/27/28	0/2/2/2
81	PSU	A3	1133	81	-	0/7/25/26	0/2/2/2
81	OMU	A3	1537	81	-	0/9/27/28	0/2/2/2
3	A2M	h1	977	3	-	0/9/27/28	0/3/3/3
3	A2M	h1	800	3	-	0/9/27/28	0/3/3/3
82	A2M	B3	46	82	-	0/9/27/28	0/3/3/3
81	A2M	A3	1378	81	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	h1	140	3	-	2/9/27/28	0/2/2/2
3	PSU	h1	950	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	3113	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	2978	81	-	0/7/25/26	0/2/2/2
3	OMC	h1	418	3	-	2/9/27/28	0/2/2/2
81	5MC	A3	2873	84,81	-	4/7/25/26	0/2/2/2
81	OMC	A3	2962	81	-	0/9/27/28	0/2/2/2
3	OMG	h1	1433	3,83	-	1/9/27/28	0/3/3/3
81	A2M	A3	2129	81	-	0/9/27/28	0/3/3/3
3	OMU	h1	1012	3	-	0/9/27/28	0/2/2/2
81	PSU	A3	1474	81	-	0/7/25/26	0/2/2/2
81	PSU	A3	2747	81	-	0/7/25/26	0/2/2/2
81	OMC	A3	40	81	-	1/9/27/28	0/2/2/2
3	A2M	h1	162	3	-	0/9/27/28	0/3/3/3
81	PSU	A3	2269	81	-	2/7/25/26	0/2/2/2
81	OMC	A3	2951	81	-	0/9/27/28	0/2/2/2
3	PSU	h1	1293	3	-	0/7/25/26	0/2/2/2
81	PSU	A3	42	84,81	-	0/7/25/26	0/2/2/2
81	OMU	A3	787	81	-	0/9/27/28	0/2/2/2
81	OMU	A3	2924	84,81	-	0/9/27/28	0/2/2/2

The worst 5 of 1749 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	h1	1524	PSU	C6-C5	12.36	1.49	1.35
3	h1	584	PSU	C6-C5	12.34	1.49	1.35
81	A3	2137	PSU	C6-C5	12.29	1.49	1.35
81	A3	2269	PSU	C6-C5	12.27	1.49	1.35
3	h1	1217	PSU	C6-C5	12.25	1.49	1.35

The worst 5 of 1383 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	h1	1790	MA6	N1-C6-N6	-8.65	107.62	117.08
3	h1	1789	MA6	N1-C6-N6	-8.41	107.89	117.08
81	A3	2284	A2M	N6-C6-N1	-7.11	102.77	118.35
81	A3	946	A2M	N6-C6-N1	-6.92	103.20	118.35
81	A3	2804	A2M	N6-C6-N1	-6.86	103.32	118.35

There are no chirality outliers.

5 of 139 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	B3	78	OMG	O4'-C4'-C5'-O5'
82	B3	78	OMG	C3'-C4'-C5'-O5'
82	B3	96	PSU	C3'-C4'-C5'-O5'
82	B3	96	PSU	O4'-C4'-C5'-O5'
3	h1	38	OMC	C3'-C4'-C5'-O5'

There are no ring outliers.

57 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	A3	2284	A2M	2	0
3	h1	1190	PSU	1	0
81	A3	369	A2M	3	0
81	A3	2653	UY1	1	0
3	h1	1283	4AC	1	0
3	h1	1304	PSU	1	0
3	h1	1194	B8N	3	0
81	A3	2223	A2M	2	0
81	A3	1144	A2M	1	0
3	h1	1308	PSU	1	0
81	A3	674	OMC	3	0
81	A3	1460	A2M	1	0
81	A3	1482	PSU	1	0
3	h1	1447	OMU	1	0
81	A3	2839	OMC	1	0
81	A3	2883	PSU	1	0
81	A3	918	OMG	1	0
81	A3	827	A2M	1	0
81	A3	2947	PSU	1	0
81	A3	2194	PSU	1	0
81	A3	464	PSU	1	0
3	h1	614	OMU	1	0
81	A3	399	OMG	1	0
81	A3	34	PSU	1	0
3	h1	1758	A2M	1	0
81	A3	3289	OMU	2	0
3	h1	1787	PSU	1	0
3	h1	28	A2M	1	0
81	A3	2398	OMG	1	0
81	A3	2732	OMU	1	0
81	A3	675	OMU	1	0
81	A3	970	PSU	1	0
81	A3	2261	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
81	A3	2317	PSU	1	0
3	h1	961	PSU	1	0
3	h1	1383	OMU	1	0
3	h1	1790	MA6	2	0
81	A3	2886	OMU	3	0
81	A3	2239	OMG	1	0
3	h1	1789	MA6	3	0
3	h1	1106	PSU	1	0
3	h1	762	PSU	1	0
81	A3	2412	OMG	1	0
81	A3	2804	A2M	1	0
81	A3	2368	OMC	1	0
81	A3	660	A2M	2	0
81	A3	2413	OMU	1	0
3	h1	392	OMG	2	0
3	h1	1645	OMC	1	0
3	h1	1781	4AC	2	0
3	h1	977	A2M	1	0
3	h1	140	OMC	1	0
81	A3	2873	5MC	2	0
81	A3	2962	OMC	1	0
81	A3	2747	PSU	1	0
81	A3	40	OMC	3	0
81	A3	2951	OMC	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 290 ligands modelled in this entry, 283 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
85	SPD	h1	2016	-	9,9,9	0.33	0	8,8,8	0.66	0
85	SPD	A3	3450	-	9,9,9	0.31	0	8,8,8	0.51	0
86	SPM	A3	3451	-	13,13,13	0.35	0	12,12,12	1.05	0
86	SPM	A3	3452	-	13,13,13	0.37	0	12,12,12	1.03	0
86	SPM	h1	2017	-	13,13,13	0.47	0	12,12,12	0.95	0
86	SPM	h1	2019	-	13,13,13	0.42	0	12,12,12	1.03	0
86	SPM	h1	2018	-	13,13,13	0.38	0	12,12,12	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
85	SPD	h1	2016	-	-	4/7/7/7	-
85	SPD	A3	3450	-	-	2/7/7/7	-
86	SPM	A3	3451	-	-	5/11/11/11	-
86	SPM	A3	3452	-	-	7/11/11/11	-
86	SPM	h1	2017	-	-	5/11/11/11	-
86	SPM	h1	2019	-	-	2/11/11/11	-
86	SPM	h1	2018	-	-	3/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
86	A3	3452	SPM	N10-C11-C12-C13
86	A3	3452	SPM	C7-C8-C9-N10
86	h1	2017	SPM	C7-C8-C9-N10
85	h1	2016	SPD	C3-C4-C5-N6
85	h1	2016	SPD	N6-C7-C8-C9

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	h1	2016	SPD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	A3	3450	SPD	6	0
86	A3	3451	SPM	1	0
86	h1	2017	SPM	2	0
86	h1	2019	SPM	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
81	A3	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A3	2973:C	O3'	2974:A	P	4.08

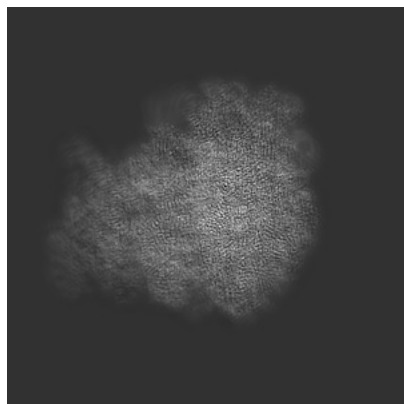
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15806. These allow visual inspection of the internal detail of the map and identification of artifacts.

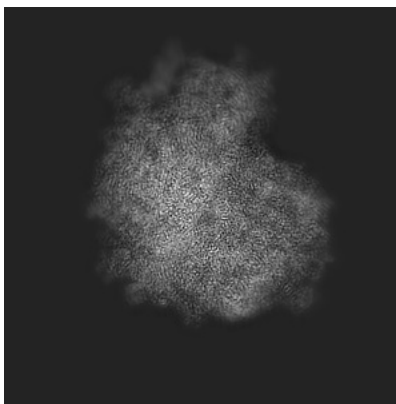
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

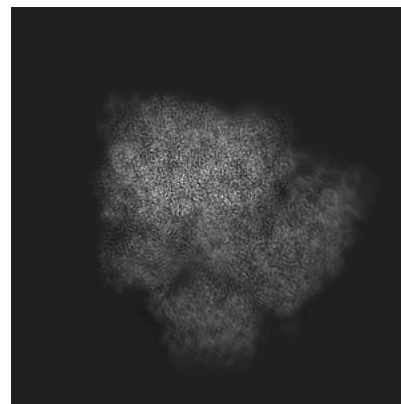
#### 6.1.1 Primary map



X

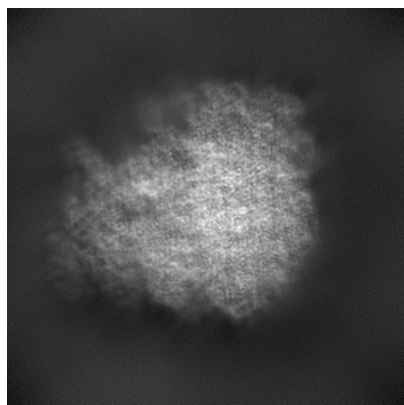


Y

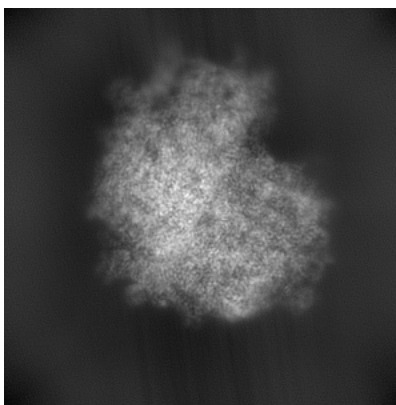


Z

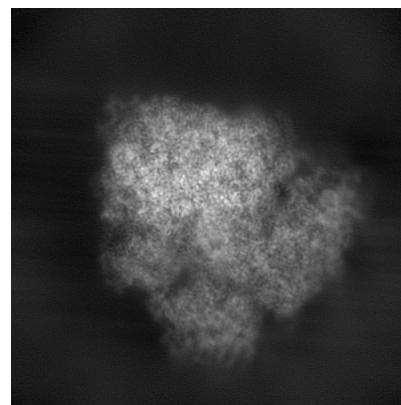
#### 6.1.2 Raw map



X



Y

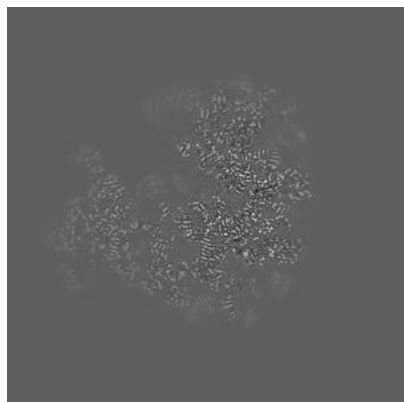


Z

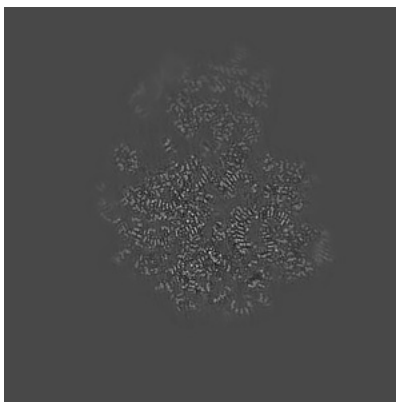
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

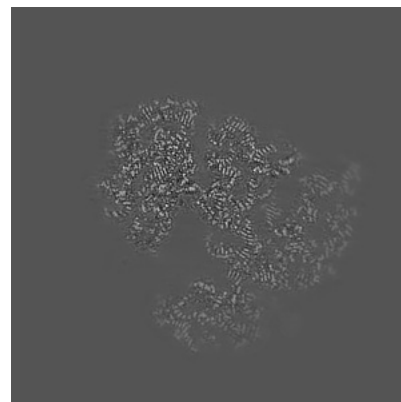
### 6.2.1 Primary map



X Index: 225

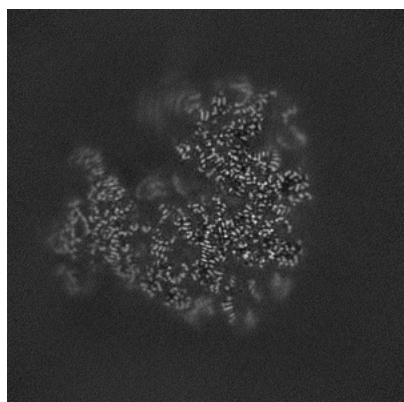


Y Index: 225

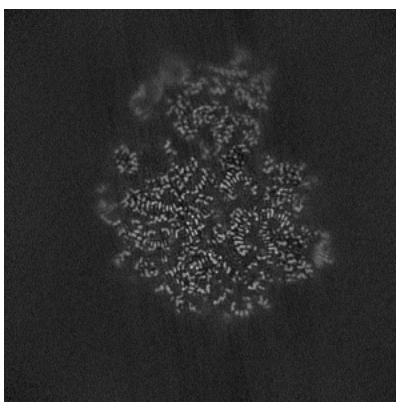


Z Index: 225

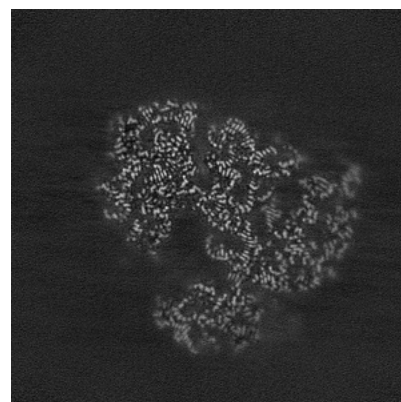
### 6.2.2 Raw map



X Index: 225



Y Index: 225

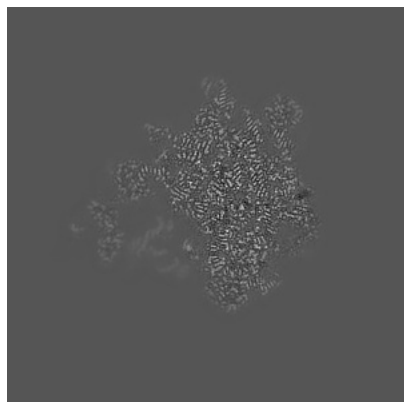


Z Index: 225

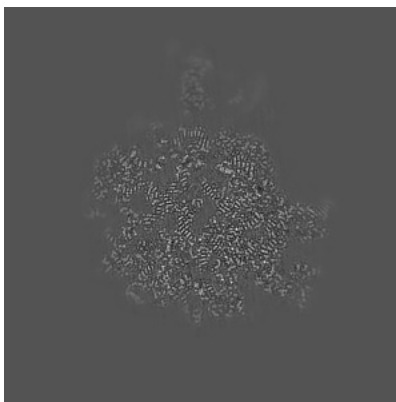
The images above show central slices of the map in three orthogonal directions.

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

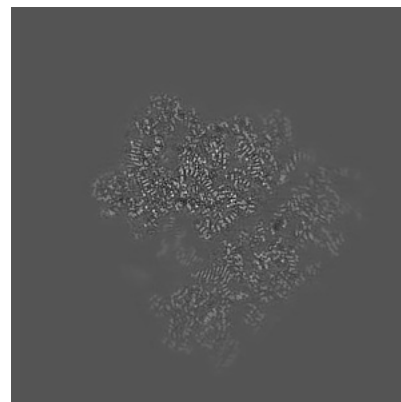
### 6.3.1 Primary map



X Index: 169

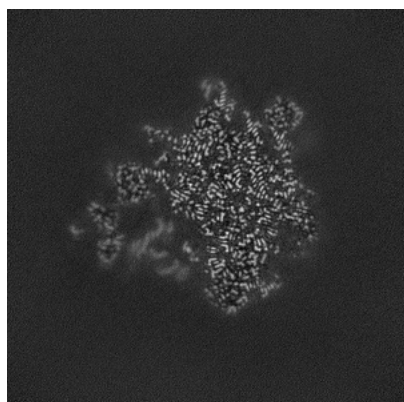


Y Index: 262

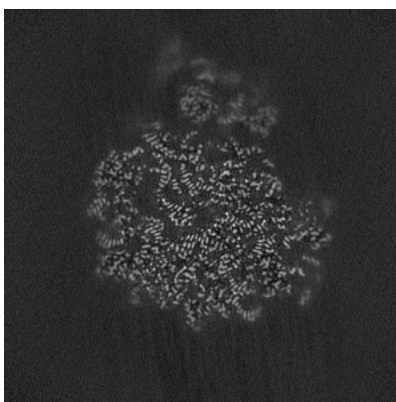


Z Index: 206

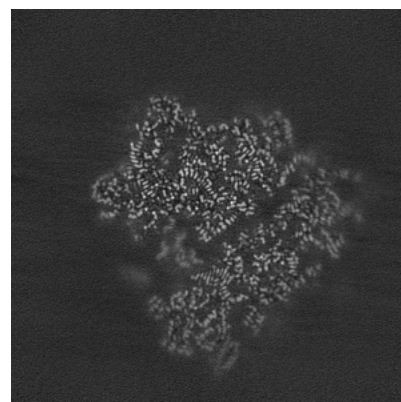
### 6.3.2 Raw map



X Index: 169



Y Index: 254

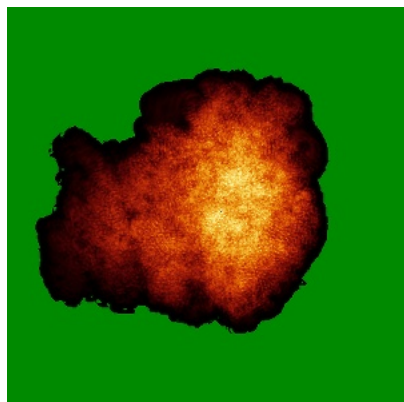


Z Index: 206

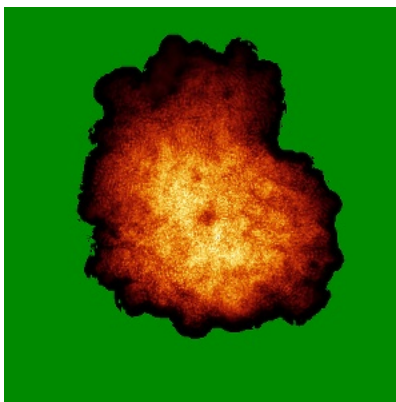
The images above show the largest variance slices of the map in three orthogonal directions.

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

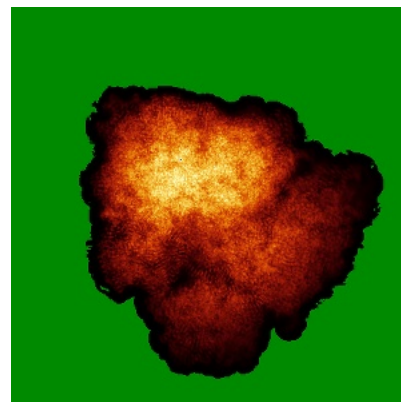
### 6.4.1 Primary map



X

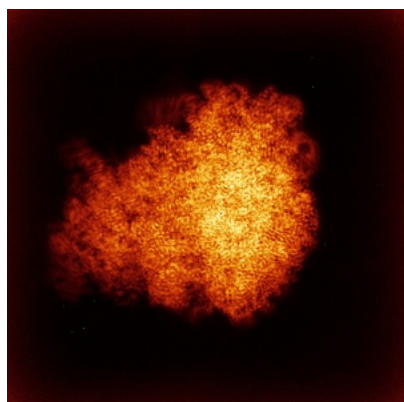


Y

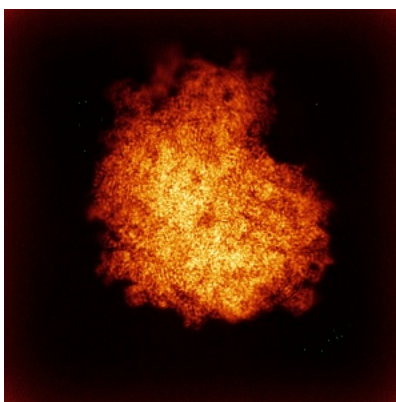


Z

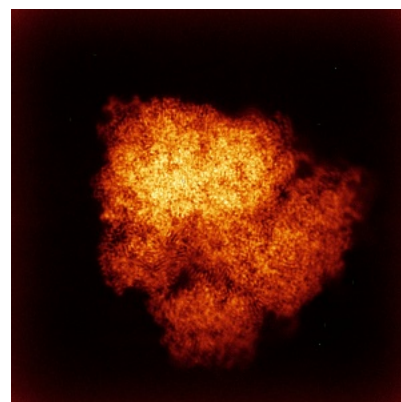
### 6.4.2 Raw map



X



Y

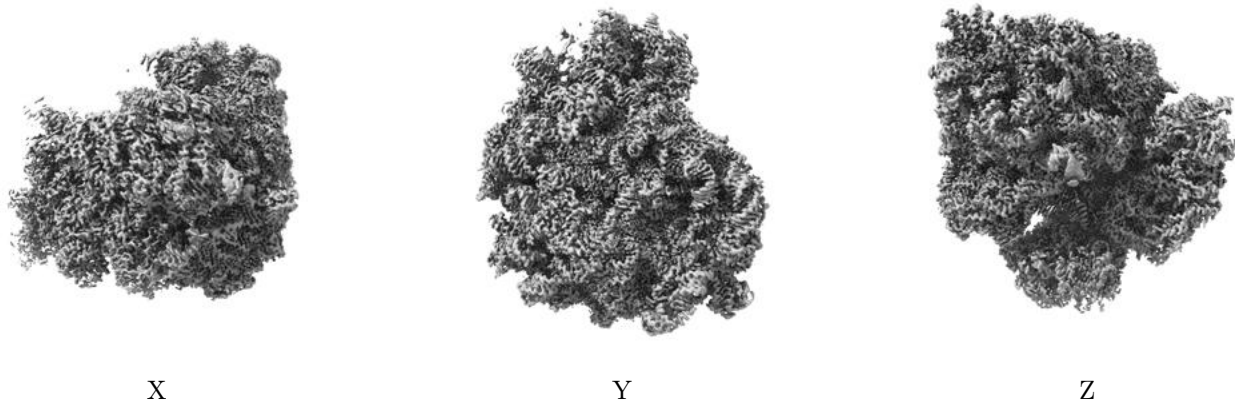


Z

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.

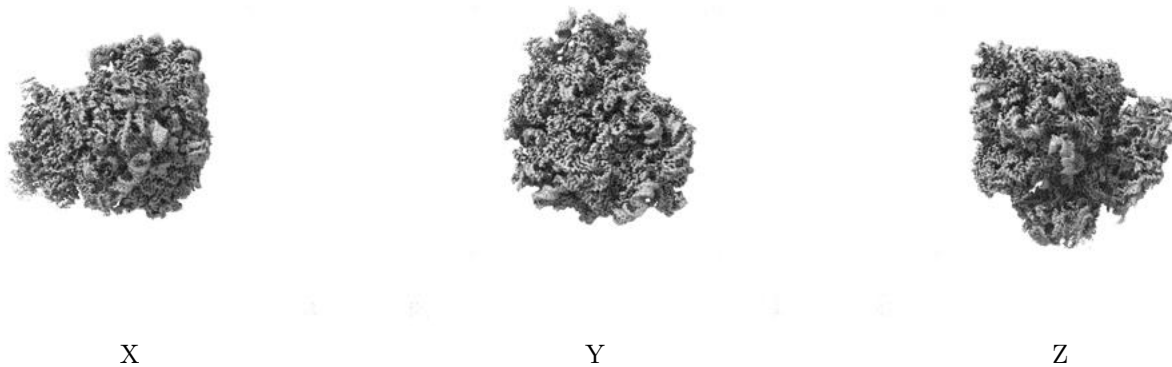
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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.

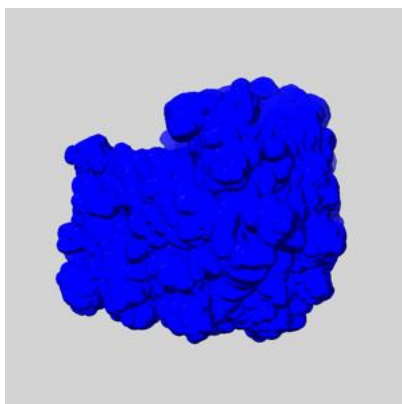
## 6.6 Mask visualisation [i](#)

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

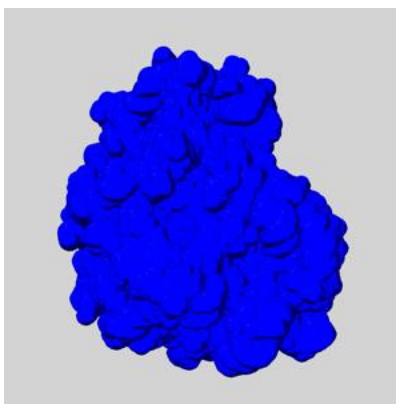
A mask typically either:

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

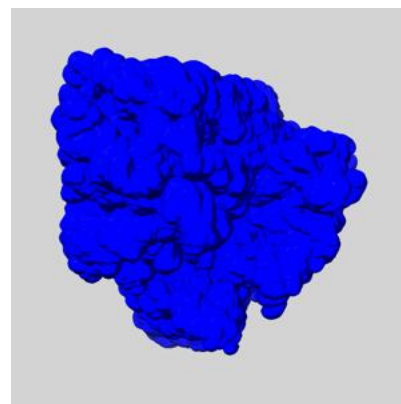
### 6.6.1 emd\_15806\_msk\_1.map [i](#)



X



Y

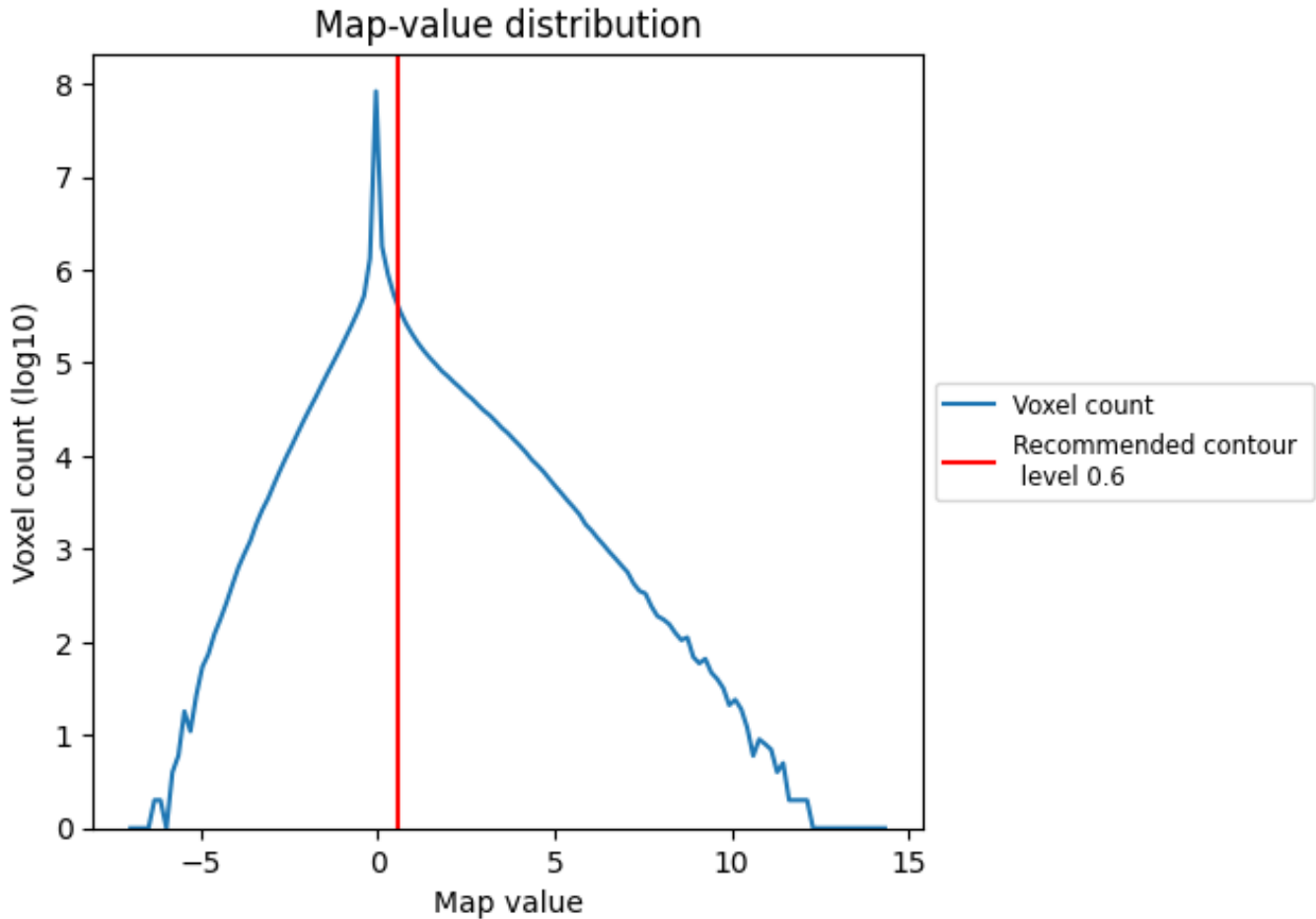


Z

## 7 Map analysis [i](#)

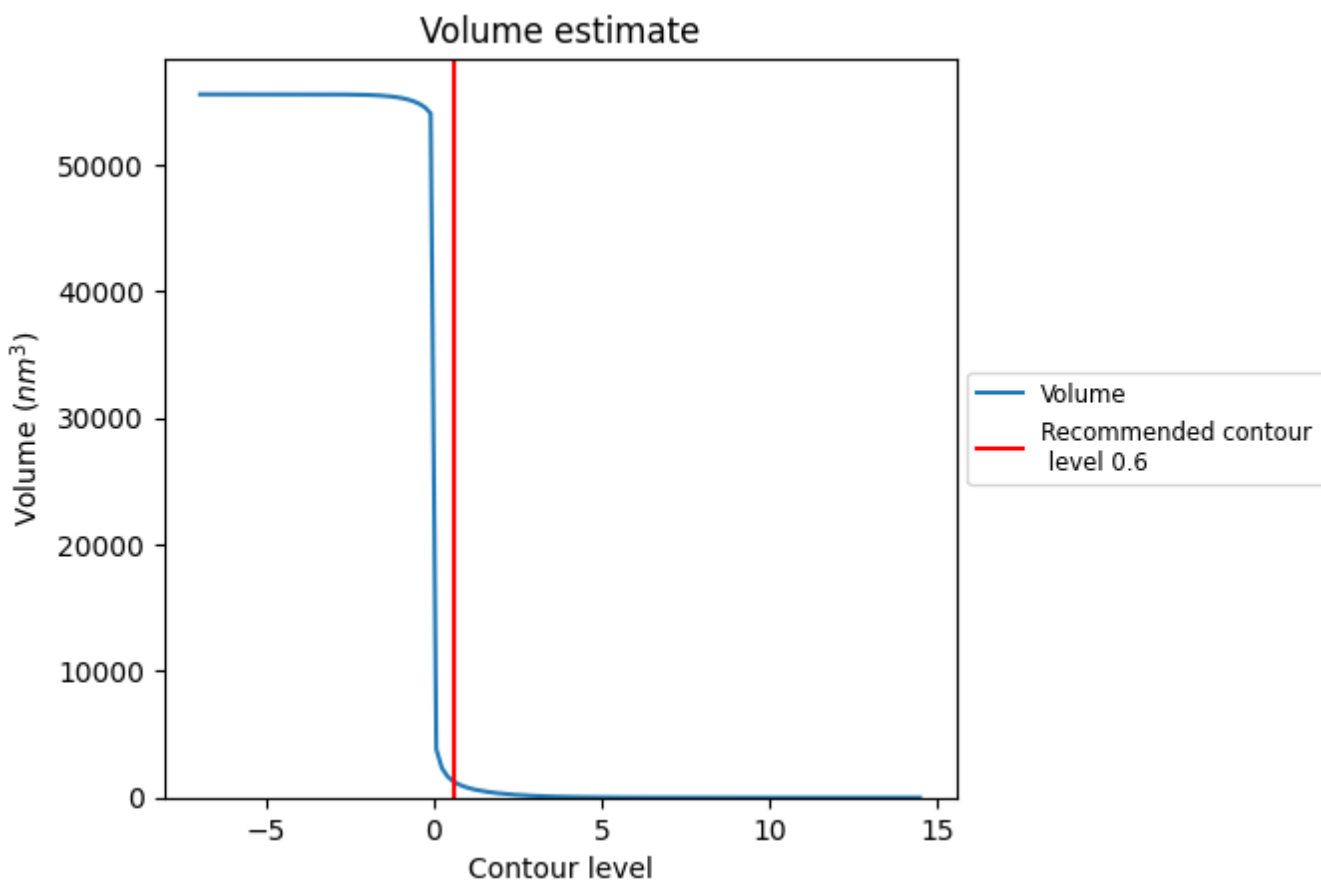
This section contains the results of statistical analysis of the map.

### 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.

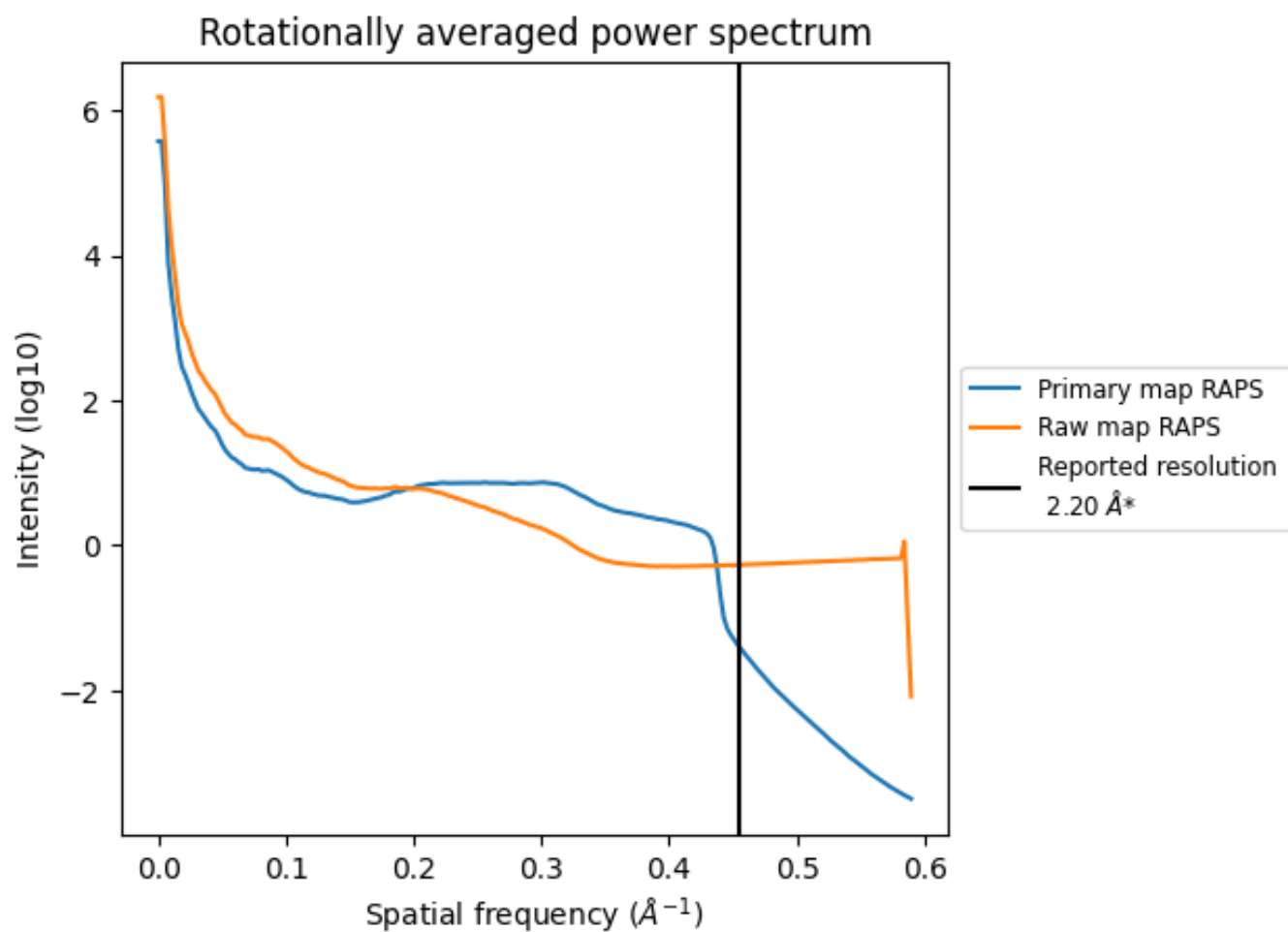
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1255 nm<sup>3</sup>; this corresponds to an approximate mass of 1133 kDa.

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

### 7.3 Rotationally averaged power spectrum i

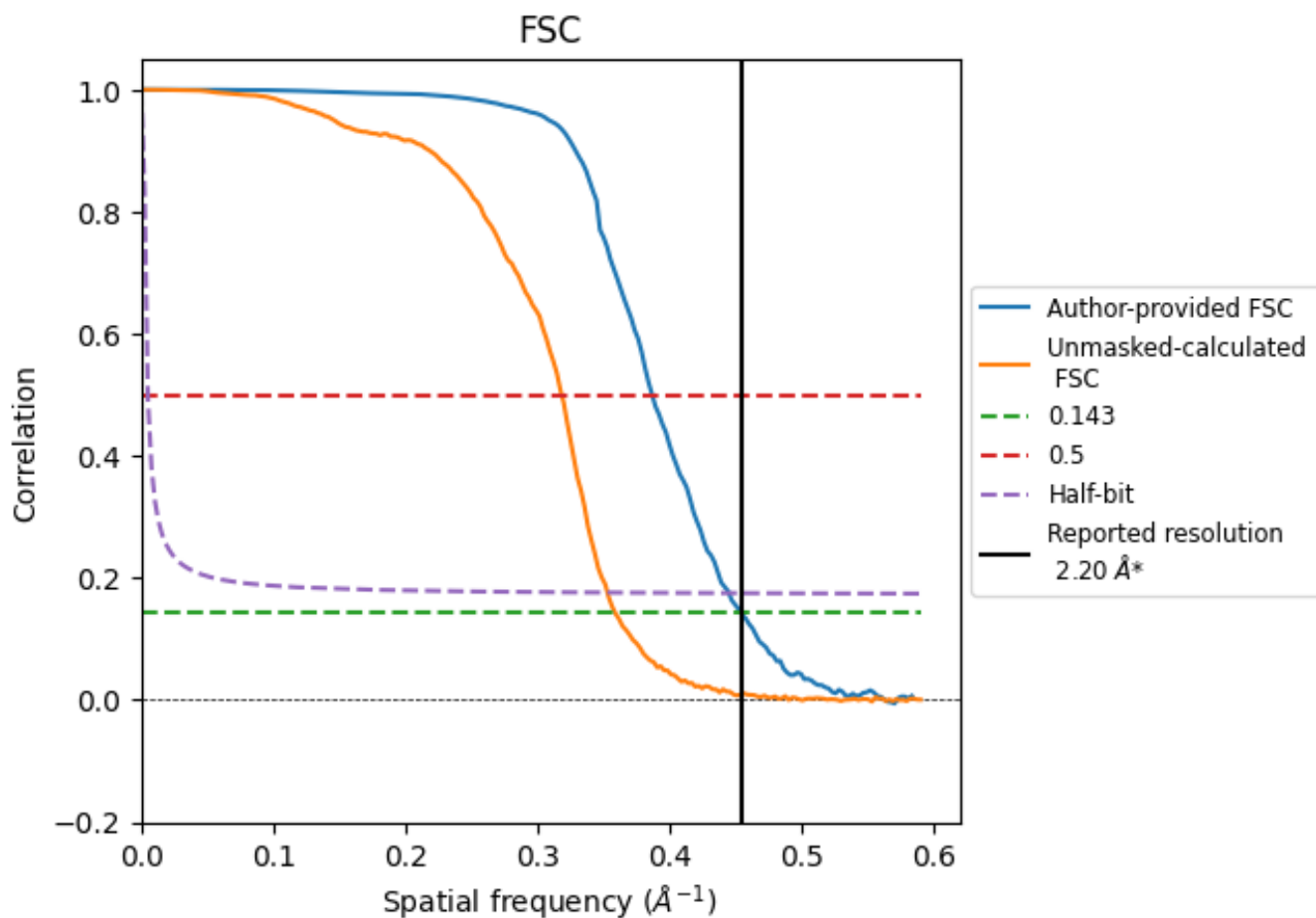


\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

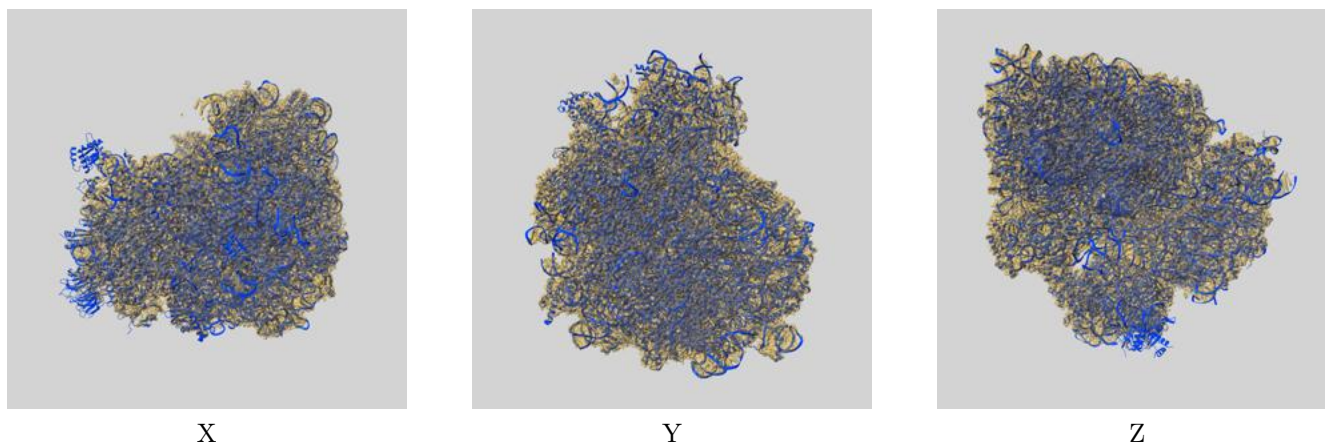
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.20	2.59	2.25
Unmasked-calculated*	2.79	3.14	2.83

\*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 2.2 by more than 10 %

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

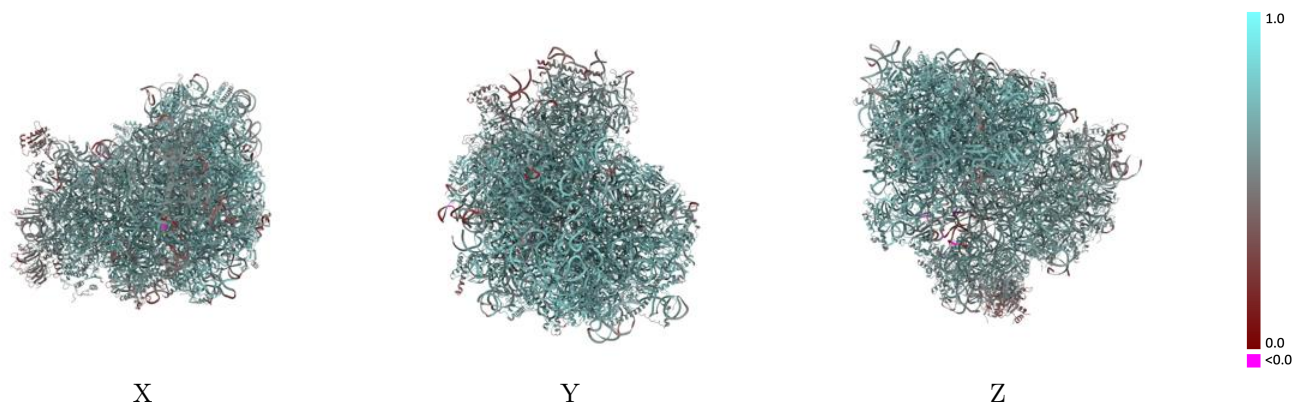
This section contains information regarding the fit between EMDB map EMD-15806 and PDB model 8B2L. Per-residue inclusion information can be found in section 3 on page 26.

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



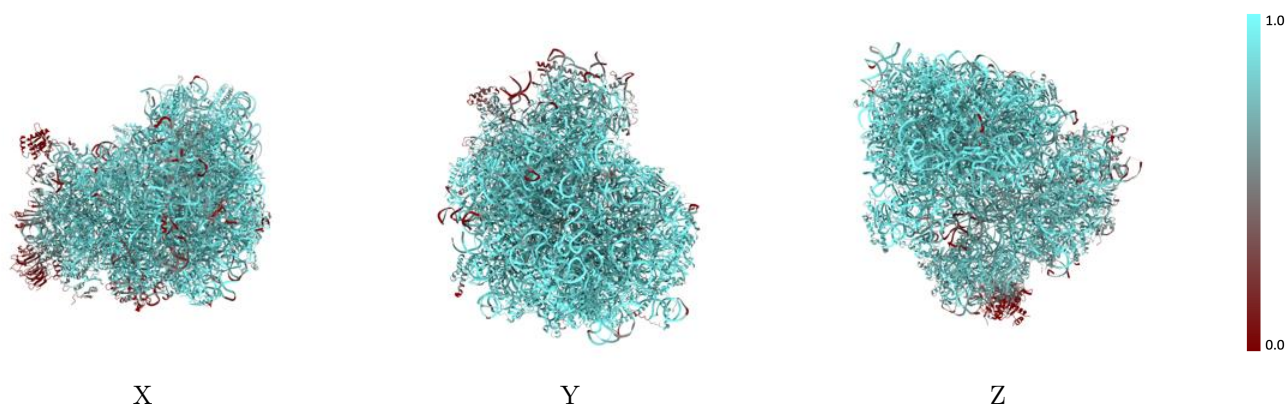
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



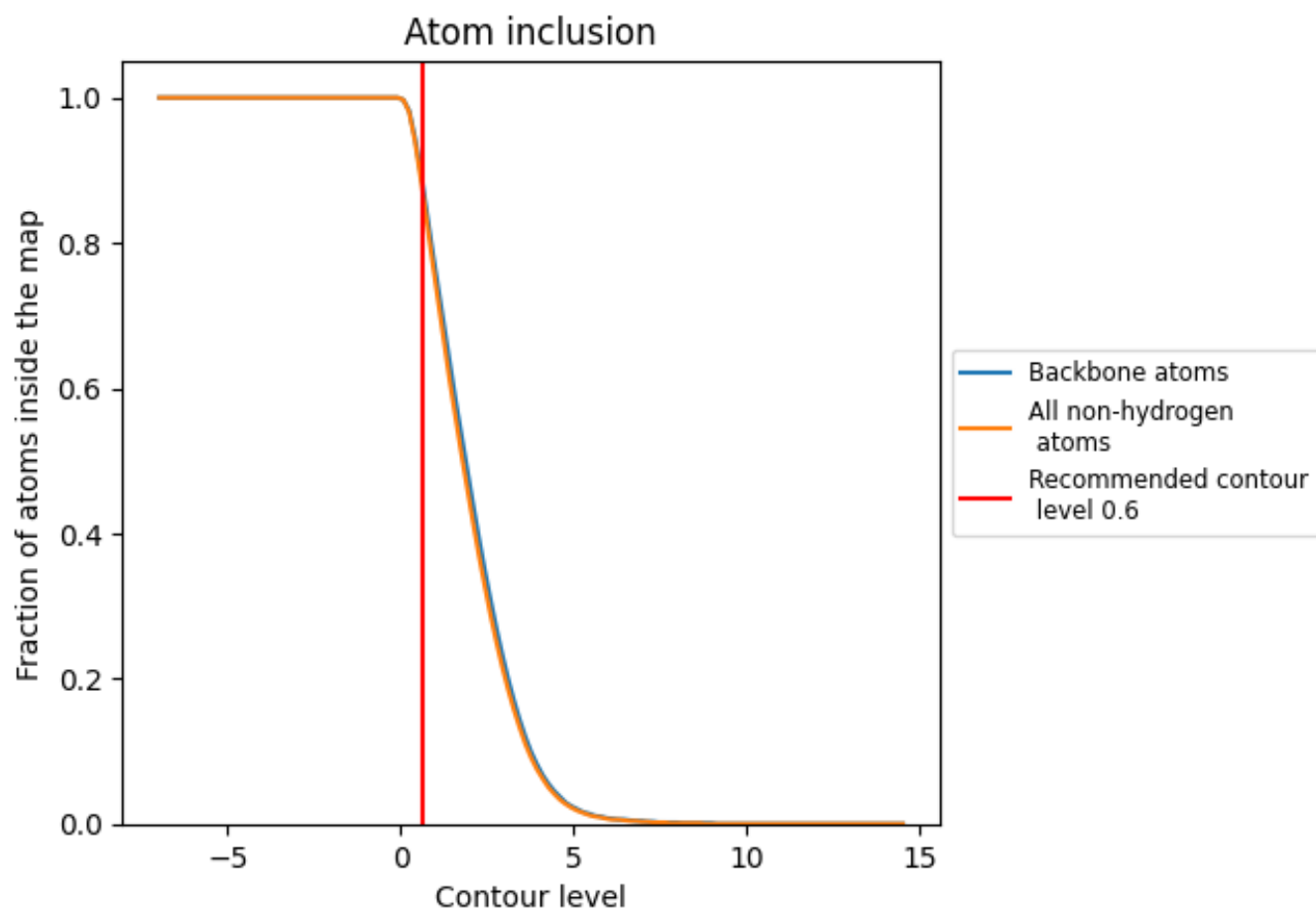
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8810	 0.6390
A1	 0.8190	 0.5960
A3	 0.9420	 0.6580
B1	 0.8630	 0.5920
B3	 0.9250	 0.6540
C1	 0.0330	 0.3580
C3	 0.9920	 0.6690
D1	 0.5440	 0.5170
D3	 0.9470	 0.6870
E1	 0.7930	 0.5800
E3	 0.9330	 0.6720
F1	 0.8900	 0.6410
F3	 0.9950	 0.7280
G1	 0.8220	 0.6030
G3	 0.9850	 0.7180
H1	 0.6990	 0.5590
H3	 0.8540	 0.6410
I1	 0.6890	 0.5490
I3	 0.9690	 0.6980
J1	 0.9250	 0.6660
J3	 0.9700	 0.6940
K1	 0.7610	 0.5970
K3	 0.7590	 0.5600
L1	 0.7270	 0.5640
L3	 0.9570	 0.6940
M1	 0.7750	 0.6010
M3	 0.9300	 0.6620
N1	 0.1380	 0.4170
N3	 0.9490	 0.6890
O1	 0.5500	 0.5350
O3	 0.9770	 0.7160
P1	 0.8080	 0.5880
P3	 0.9180	 0.6510
Q1	 0.1780	 0.4430
Q3	 0.8990	 0.6680

















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Chain	Atom inclusion	Q-score
R1	0.5160	0.5290
R3	0.9800	0.7230
S1	0.9260	0.6540
S3	0.9820	0.7150
T1	0.9500	0.6840
T3	0.9280	0.6820
U1	0.8230	0.6030
U3	0.9420	0.6640
V1	0.8900	0.6270
V3	0.9940	0.7270
W1	0.8970	0.6440
W2	0.7580	0.4970
W3	0.8320	0.6110
X1	0.8990	0.6400
X3	0.9840	0.7200
Y1	0.7710	0.5880
Y3	0.9610	0.6930
Z1	0.8330	0.6130
Z3	0.9730	0.7140
a1	0.6660	0.5540
a3	0.9650	0.7040
b1	0.8110	0.5990
b3	0.8580	0.6320
c1	0.8940	0.6520
c3	0.8650	0.6390
d1	0.7620	0.5730
d3	0.9680	0.7060
e1	0.9660	0.6780
e3	0.9690	0.7020
f1	0.7230	0.5770
f3	0.9620	0.7020
g3	0.9640	0.6900
h1	0.9020	0.6130
h3	0.8880	0.6410
i2	0.6690	0.5070
j3	0.9670	0.7050
k1	0.6380	0.5290
k3	0.9520	0.6830
l1	0.5510	0.5210
l3	0.3670	0.3350
m3	0.9560	0.6860
n3	0.9210	0.6620

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Chain	Atom inclusion	Q-score
o3	 0.9910	 0.7270
p3	 0.9360	 0.6640
q3	 0.9460	 0.6940
r3	 0.9710	 0.7100
s3	 0.9290	 0.6870
t3	 0.8750	 0.6240
u3	 0.9090	 0.6590