



Full wwPDB EM Validation Report ⓘ

Mar 12, 2025 – 07:15 AM EDT

PDB ID : 8CVM
EMDB ID : EMD-27009
Title : Cutibacterium acnes 50S ribosomal subunit with P-site tRNA and Sarecycline bound in the local refined map
Authors : Lomakin, I.B.; Devarkar, S.C.; Bunick, C.G.
Deposited on : 2022-05-18
Resolution : 2.66 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

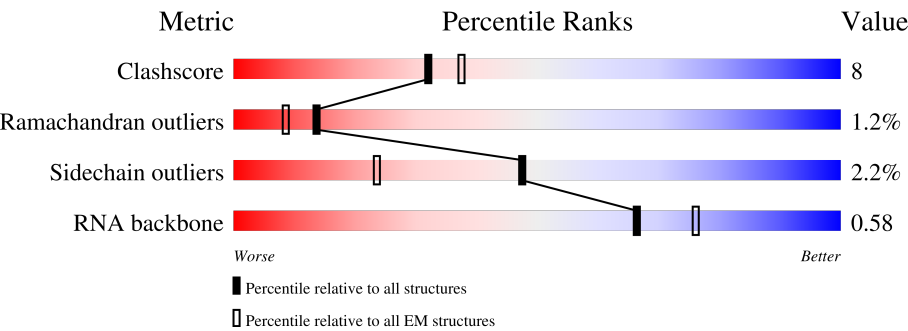
EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

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 2.66 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.



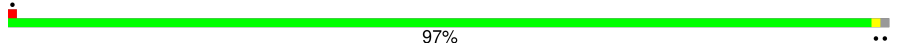
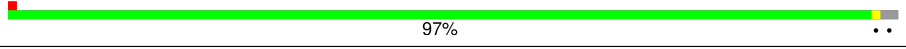

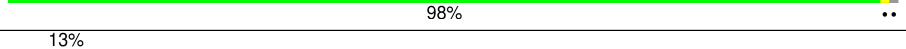
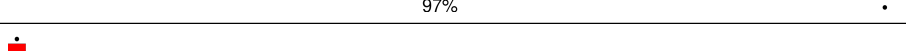
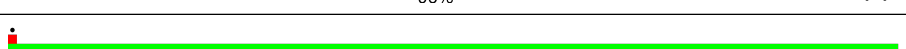





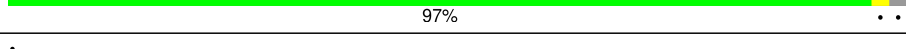
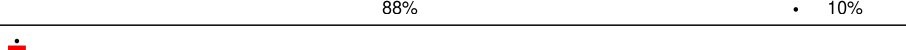
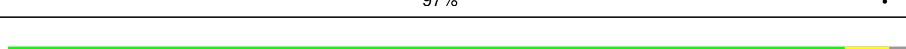
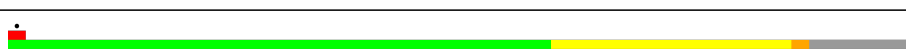



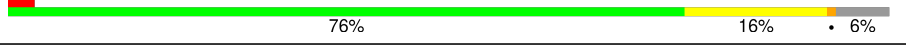
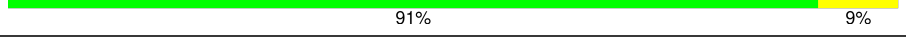





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	c	278	<div><div></div><div>98%</div><div></div></div>
2	d	223	<div><div></div><div>95%</div><div></div></div>
3	e	301	<div><div></div><div>67%</div><div>30%</div></div>
4	f	210	<div><div>12%</div><div>86%</div><div>7%</div></div>
5	g	180	<div><div>5%</div><div>93%</div><div>6%</div></div>
6	i	147	<div><div></div><div>99%</div><div></div></div>
7	j	122	<div><div></div><div>98%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
8	k	146	
9	l	139	
10	m	187	
11	n	127	
12	o	117	
13	p	123	
14	q	102	
15	r	153	
16	s	102	
17	t	122	
18	u	205	
19	v	89	
20	w	61	
21	x	77	
22	y	60	
23	z	63	
24	0	56	
25	1	44	
26	2	68	
27	4	69	
28	a	3086	
29	b	120	
30	V	24	
31	C	77	
32	3	37	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 93049 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	c	274	Total	C	N	O	S	0	0
			2091	1289	425	372	5		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	d	214	Total	C	N	O	S	0	0
			1586	984	304	291	7		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	e	210	Total	C	N	O	S	0	0
			1577	979	301	295	2		

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	203	Total	C	N	O	S	0	0
			1623	1025	299	290	9		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	177	Total	C	N	O	S	0	0
			1376	867	250	258	1		

- Molecule 6 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	i	146	Total	C	N	O	S	0	0
			1139	718	213	205	3		

- Molecule 7 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	122	Total	C	N	O	S	0	0
			946	596	177	169	4		

- Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	144	Total	C	N	O	S	0	0
			1072	675	196	199	2		

- Molecule 9 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	l	136	Total	C	N	O	S	0	0
			1082	685	210	181	6		

- Molecule 10 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	m	120	Total	C	N	O	S	0	0
			936	583	188	163	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	102	ILE	ASN	conflict	UNP A0A085AZY3

- Molecule 11 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	n	126	Total	C	N	O	S	0	0
			952	583	190	176	3		

- Molecule 12 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	o	114	Total	C	N	O	S	0	0
			896	559	174	162	1		

- Molecule 13 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	p	119	Total	C	N	O	S	0	0
			958	589	196	171	2		

- Molecule 14 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	q	102	Total	C	N	O	S	0	0
			778	487	140	150	1		

- Molecule 15 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	r	132	Total	C	N	O	S	0	0
			1017	624	204	182	7		

- Molecule 16 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	s	95	Total	C	N	O	S	0	0
			751	474	138	138	1		

- Molecule 17 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	t	107	Total	C	N	O	S	0	0
			833	516	163	153	1		

- Molecule 18 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	u	179	Total	C	N	O	S	0	0
			1376	865	240	268	3		

- Molecule 19 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	v	78	Total	C	N	O	0	0
			591	355	127	109		

- Molecule 20 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	w	60	Total	C	N	O	S	0	0
			474	290	102	77	5		

- Molecule 21 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	x	69	Total	C	N	O		0	0
			564	348	108	108			

- Molecule 22 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	y	58	Total	C	N	O	S	0	0
			467	290	91	83	3		

- Molecule 23 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	z	62	Total	C	N	O	S	0	0
			477	287	102	83	5		

- Molecule 24 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	0	50	Total	C	N	O	S	0	0
			423	253	91	73	6		

- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	44	Total	C	N	O	S	0	0
			362	213	91	56	2		

- Molecule 26 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	67	Total	C	N	O	S	0	0
			513	315	110	87	1		

- Molecule 27 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	66	Total	C	N	O	S	0	0
			512	313	97	97	5		

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2903	Total	C	N	O	P	6	0
			62531	27850	11406	20366	2909		

- Molecule 29 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	120	Total	C	N	O	P	0	0
			2567	1145	466	836	120		

- Molecule 30 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	V	23	Total	C	N	O	0	0
			183	106	50	27		

- Molecule 31 is a RNA chain called Initiator fMet RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	C	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	3	37	Total	C	N	O	S	0	0
			302	184	66	47	5		

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	c	3	Total	Mg	0
			3	3	
33	d	1	Total	Mg	0
			1	1	
33	k	2	Total	Mg	0
			2	2	

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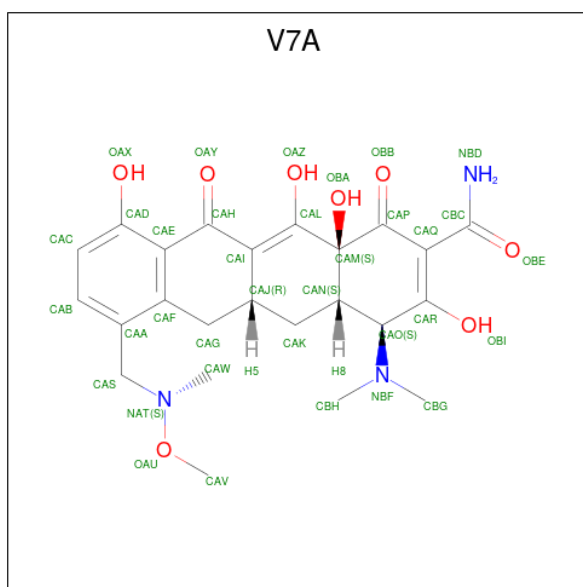
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Mol	Chain	Residues	Atoms		AltConf
33	1	1	Total	Mg	0
			1	1	
33	a	294	Total	Mg	0
			294	294	
33	b	2	Total	Mg	0
			2	2	
33	C	2	Total	Mg	0
			2	2	

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	w	1	Total	Zn	0
			1	1	
34	z	1	Total	Zn	0
			1	1	
34	0	1	Total	Zn	0
			1	1	
34	4	1	Total	Zn	0
			1	1	

- Molecule 35 is Sarecycline (three-letter code: V7A) (formula: C₂₄H₂₉N₃O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
35	a	1	Total	C	N	O	0
			35	24	3	8	

- Molecule 36 is water.

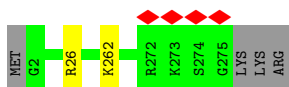
Mol	Chain	Residues	Atoms		AltConf
36	d	1	Total 1	O 1	0
36	s	1	Total 1	O 1	0
36	a	120	Total 120	O 120	0
36	b	3	Total 3	O 3	0

3 Residue-property plots

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

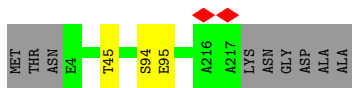
- Molecule 1: 50S ribosomal protein L2

Chain c:  98%



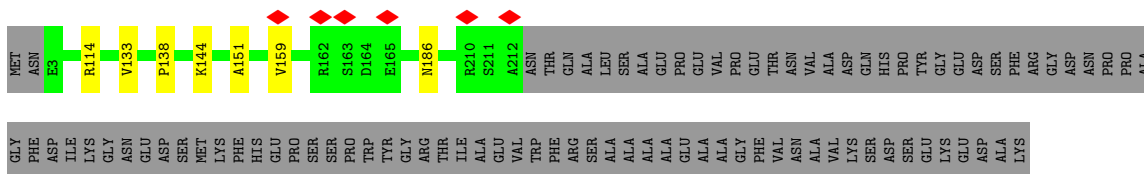
- Molecule 2: 50S ribosomal protein L3

Chain d:  95%




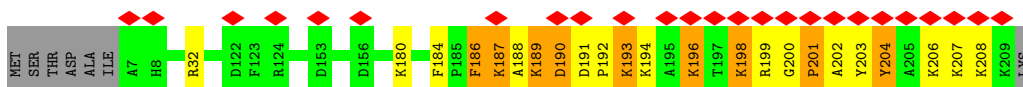
- Molecule 3: 50S ribosomal protein L4

Chain e:  67% 30%

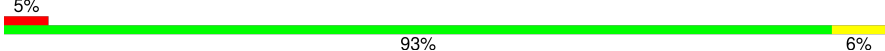


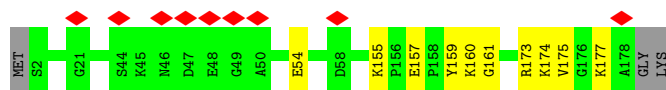
- Molecule 4: 50S ribosomal protein L5

Chain f:  12% 86% 7%



- Molecule 5: 50S ribosomal protein L6

Chain g:  5% 93% 6%



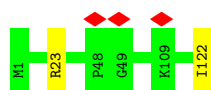
- Molecule 6: 50S ribosomal protein L13

Chain i: 99%



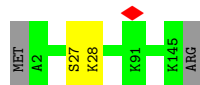
- Molecule 7: 50S ribosomal protein L14

Chain j: 98%



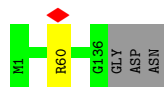
- Molecule 8: 50S ribosomal protein L15

Chain k: 97%



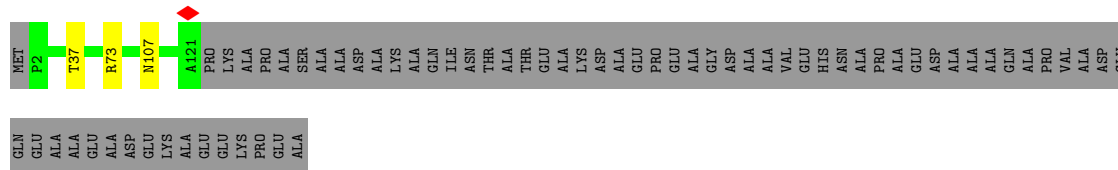
- Molecule 9: 50S ribosomal protein L16

Chain l: 97%



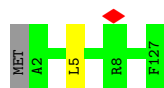
- Molecule 10: 50S ribosomal protein L17

Chain m: 63% 36%

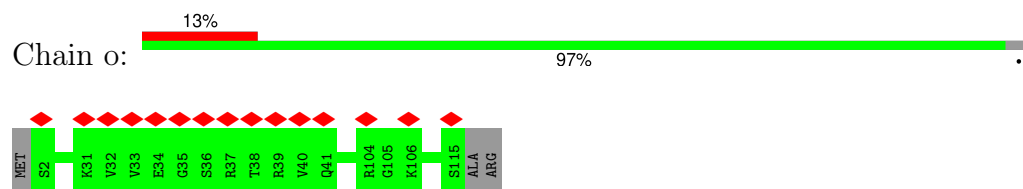


- Molecule 11: 50S ribosomal protein L18

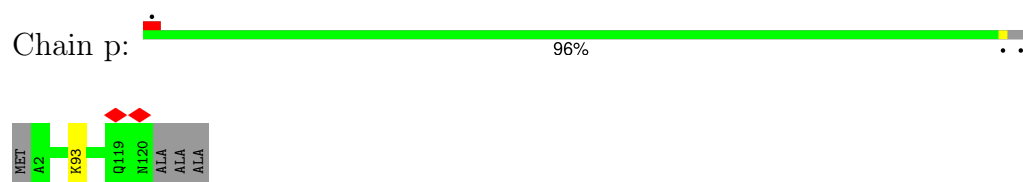
Chain n: 98%



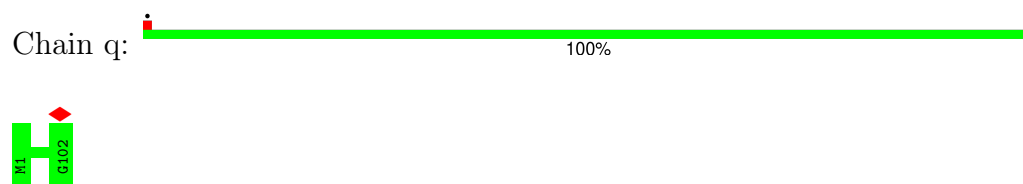
- Molecule 12: 50S ribosomal protein L19



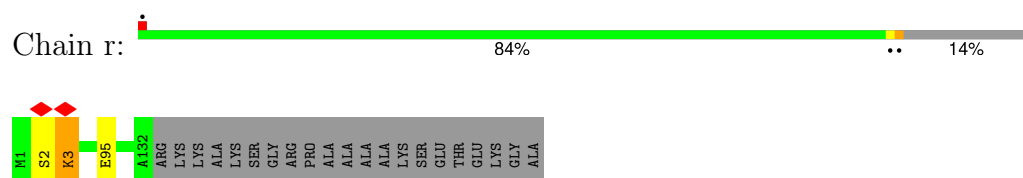
- Molecule 13: 50S ribosomal protein L20



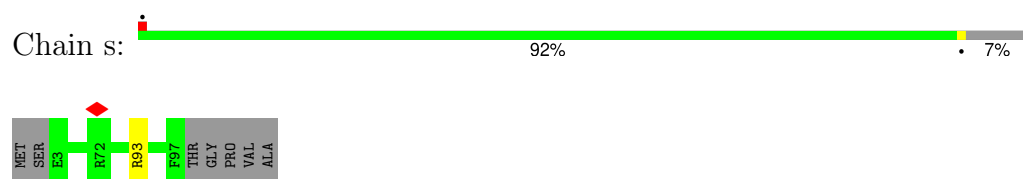
- Molecule 14: 50S ribosomal protein L21



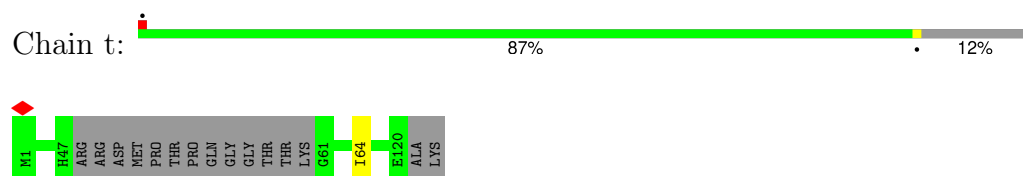
- Molecule 15: 50S ribosomal protein L22



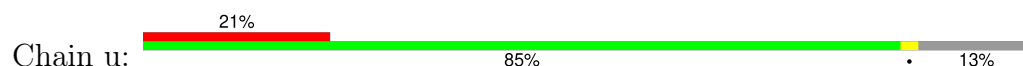
- Molecule 16: 50S ribosomal protein L23

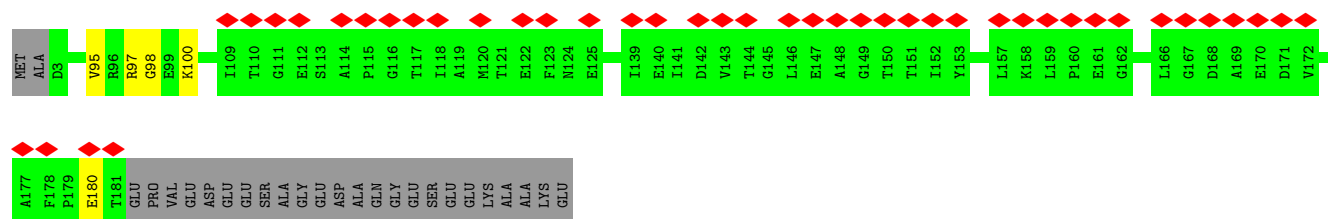


- Molecule 17: 50S ribosomal protein L24

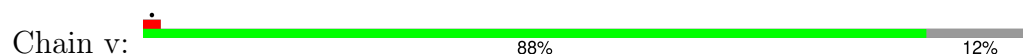


- Molecule 18: 50S ribosomal protein L25

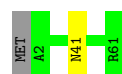




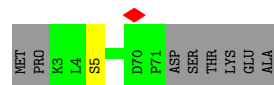
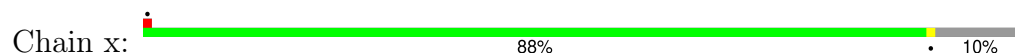
- Molecule 19: 50S ribosomal protein L27



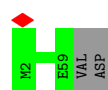
- Molecule 20: 50S ribosomal protein L28



- Molecule 21: 50S ribosomal protein L29



- Molecule 22: 50S ribosomal protein L30



- Molecule 23: 50S ribosomal protein L32



- Molecule 24: 50S ribosomal protein L33





- Molecule 25: 50S ribosomal protein L34

Chain 1: 91% 9%



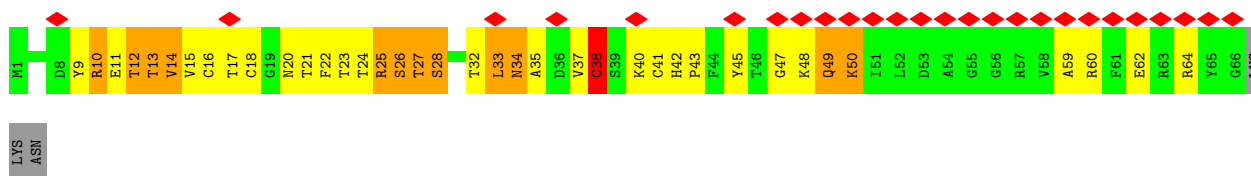
- Molecule 26: 50S ribosomal protein L35

Chain 2: 85% 13%



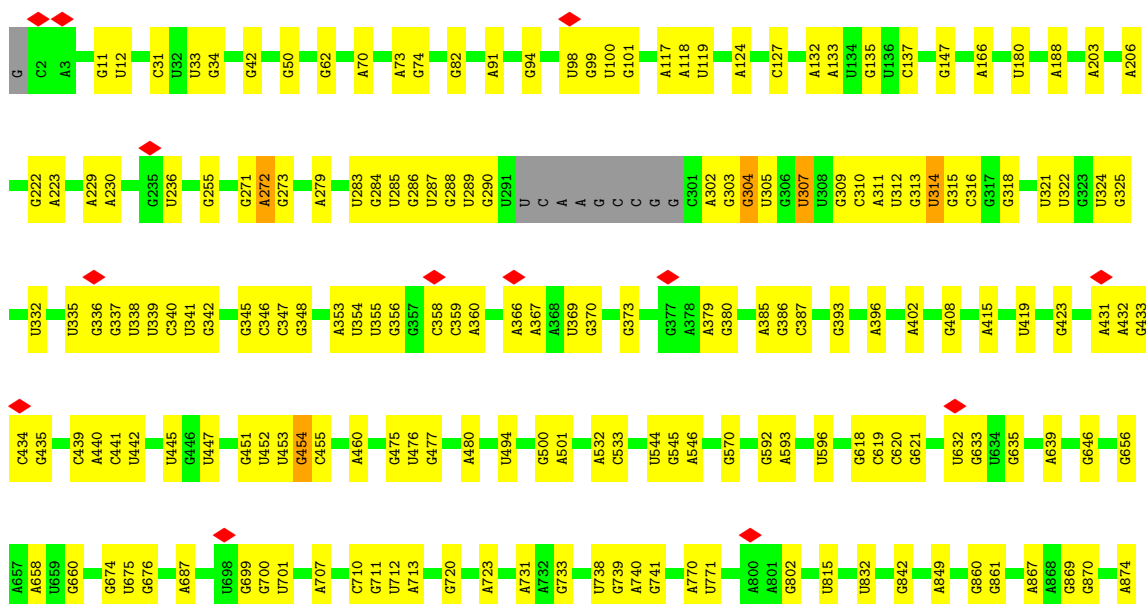
- Molecule 27: 50S ribosomal protein L31

Chain 4: 38% 41% 36% 17%

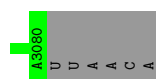


- Molecule 28: 23S ribosomal RNA

Chain a: 76% 16% 6%



C2886	A2887	U2894	G2900	C2908	C2911	U2915	U2916	U2917	G2926	A2930	C2937	U2938	A2939	A2940	G2944	A2947	G2948	A2960	U2961	A2962	C2971	A2972	C2973	U2979	U2980	U2981	U2982	C2983	G3000	A3015	G3041	G3052	A3063	U3064	A3065	G3066	G3073	A3074	C3075																		
C2662	G2663	A2664	U2673	U2674	A2679	G2684	U2685	U2686	G2687	U2688	A2700	U2701	C2702	G2708	C2709	U2710	U2711	G2716	G2717	U2718	U2719	C2720	C2721	C2722	U2734	U2748	G2749	C2755	U2762	U2767	A2784	U2786	U2787	U2795	U2796	U2797	A2811	U2871	U2872	C2873																	
G2490	U2491	G2501	G2503	A2504	G2507	A2517	A2518	U2525	U2526	U2527	A2528	C2529	U2532	U2536	A2567	U2587	U2588	A2607	G2611	A2612	U2613	A2617	C2623	G2627	A2630	U2631	U2639	A2651	G2652	C2653	G2654	U2656	C2657	U2658	U2659	A2660	G2661																				
U	G	G	G	A	G	C	C	U	G	G	A	A	A	U	U	C	C	U	U	C	U	U	U	U	U	U	U	U	U	C	G	G	C	C	A	C	G	U	C	U	G																
U2360	U2361	U2362	U2363	A2364	U2365	U2366	U2367	U2368	U2369	G2384	U2385	U2386	G2393	A2394	A2407	G2420	G2421	G2433	G2461	G2464	C2465	A2469	U2487																																		
U2055	G2056	C2057	A2068	G2089	U2094	A2095	A2096	C2097	3TD2098	A2099	U2100	A2101	A2102	C2103	G2112	G2113	A2119	A2120	A2121	U2138	U2146	C2150	A2153	U2154	G2155	U2174	G2175	U2176	G2186	U2204	U2205	A2206	G2210	A2214	G2215	A2216	G2222	C2226	C2238	G2239	A2243																
U1818	A1830	U1831	C1832	G1833	G1837	A1838	G1858	G1897	C1898	U1904	G1903	G1911	U1912	G1913	C1914	G1915	G1916	G1921	G1939	G1947	A1956	C1965	A1969	A1974	C1983	G1984	A1985	U1999	A2012	G2018	A2031	G2041	A2049	G2050	U2051	G2052	U2053	A2054																			
U1638	U1639	G1640	U1641	C1642	G1648	G1663	U1673	A1674	U1677	G1689	A1690	A1691	G1692	A1697	G1698	G1706	A1710	G1711	C1712	G1713	C1714	G1717	G1718	U1719	U1720	G1721	G1725	U1726	G1727	U1730	A1743	G1749	A1752	G1761	A1768	G1769	C1774	G1777	A1792																		
U1116	G1117	U1118	G1119	U1128	A1129	G1130	C1135	C1136	A1137	G1138	G1139	A1140	G1141	G1142	U1143	U1144	G1145	G1146	U1147	U1148	U1149	G1150	G1151	A1152	A1153	G1154	C1155	A1156	G1157	C1158	C1159	U1160	U1161	C1162	C1163	U1164	U1165	G1166	A1167	A1168	A1169	G1170	A1171	G1172	U1173	G1174	C1175	G1176	U1177	A1178	A1179	U1180	A1181	G1182	C1183	U1184	C1185
U875	C876	A877	G890	C897	U911	U912	G931	U932	G944	G968	C969	U970	U971	A972	U973	C974	G975	U978	U979	A980	C981	G990	C991	A994	A1016	A1028	G1029	U1038	A1042	A1043	G1044	G1057	A1066	A1073	A1079	G1096	G1105	G1109																			



- Molecule 29: 5S ribosomal RNA

Chain b: 91% 9%



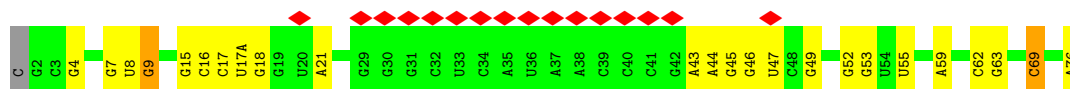
- Molecule 30: 50S ribosomal protein bL37

Chain V: 88% 8% .



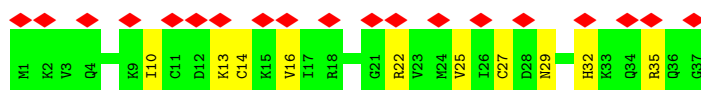
- Molecule 31: Initiator fMet RNA

Chain C: 21% 68% 29% . .



- Molecule 32: 50S ribosomal protein L36

Chain 3: 51% 73% 27%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70853	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.56	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.651	Depositor
Minimum map value	-0.589	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	363.12, 363.12, 363.12	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, 3TD, 4SU, V7A, 5MU, ZN, OMU, OMG, MG, 2MG, H2U, 5MC, 2MA, OMC

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	c	0.33	0/2132	0.59	0/2871
2	d	0.35	0/1611	0.58	0/2172
3	e	0.35	0/1600	0.62	0/2165
4	f	0.35	0/1652	0.62	0/2210
5	g	0.32	0/1398	0.56	0/1884
6	i	0.34	0/1164	0.50	0/1574
7	j	0.33	0/957	0.59	0/1282
8	k	0.36	0/1090	0.58	0/1465
9	l	0.32	0/1108	0.56	0/1488
10	m	0.32	0/949	0.58	0/1277
11	n	0.27	0/959	0.59	0/1281
12	o	0.30	0/909	0.57	0/1216
13	p	0.31	0/969	0.53	0/1292
14	q	0.32	0/785	0.57	0/1050
15	r	0.34	0/1028	0.60	0/1379
16	s	0.31	0/759	0.57	0/1022
17	t	0.29	0/840	0.58	0/1123
18	u	0.29	0/1396	0.56	0/1896
19	v	0.33	0/598	0.61	0/800
20	w	0.31	0/483	0.58	0/648
21	x	0.29	0/567	0.57	0/759
22	y	0.29	0/471	0.58	0/627
23	z	0.33	0/487	0.53	0/654
24	0	0.34	0/429	0.63	0/569
25	1	0.29	0/365	0.67	0/478
26	2	0.30	0/519	0.58	0/682
27	4	0.52	0/521	0.73	1/700 (0.1%)
28	a	0.50	1/69579 (0.0%)	0.78	97/108567 (0.1%)
29	b	0.40	0/2871	0.68	0/4475
30	V	0.28	0/184	0.66	0/236
31	C	0.20	0/1725	0.67	0/2689
32	3	0.25	0/305	0.56	0/401

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.46	1/100410 (0.0%)	0.74	98/150932 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	445	U	C1'-N1	5.70	1.57	1.48

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	127	C	C5-C6-N1	15.97	128.99	121.00
28	a	127	C	C4-C5-C6	13.26	124.03	117.40
28	a	1349	U	P-O3'-C3'	-11.91	105.41	119.70
28	a	315	G	P-O3'-C3'	-11.90	105.42	119.70
28	a	2661	G	P-O3'-C3'	-11.46	105.95	119.70
28	a	2653	C	P-O3'-C3'	-11.26	106.19	119.70
28	a	2940	A	P-O3'-C3'	-11.06	106.43	119.70
28	a	660	G	P-O3'-C3'	-10.76	106.79	119.70
28	a	2937	C	P-O3'-C3'	10.29	132.05	119.70
28	a	2052	G	P-O3'-C3'	-10.22	107.44	119.70
28	a	2250	G	P-O3'-C3'	-10.18	107.48	119.70
28	a	440	A	P-O3'-C3'	-10.09	107.60	119.70
28	a	454	G	P-O3'-C3'	-10.06	107.62	119.70
28	a	452	U	P-O3'-C3'	-10.01	107.69	119.70
28	a	314	U	P-O3'-C3'	-9.96	107.75	119.70
28	a	2249	C	P-O3'-C3'	-9.93	107.79	119.70
28	a	2715	U	P-O3'-C3'	-9.85	107.88	119.70
28	a	2652	G	P-O3'-C3'	-9.79	107.96	119.70
28	a	1118	U	P-O3'-C3'	-9.64	108.14	119.70
28	a	2657	C	P-O3'-C3'	-9.62	108.15	119.70
28	a	2051	U	P-O3'-C3'	-9.62	108.16	119.70
28	a	2050	G	P-O3'-C3'	-9.50	108.30	119.70
28	a	2939	A	P-O3'-C3'	-9.45	108.36	119.70
28	a	2654	G	P-O3'-C3'	-9.34	108.49	119.70
28	a	712	U	P-O3'-C3'	-9.27	108.58	119.70
28	a	2588	U	P-O3'-C3'	-9.26	108.59	119.70
28	a	1189	G	P-O3'-C3'	-9.13	108.75	119.70
28	a	2714	G	P-O3'-C3'	-9.10	108.78	119.70
28	a	990	G	P-O3'-C3'	-9.03	108.86	119.70
28	a	2718	G	P-O3'-C3'	-9.02	108.87	119.70
28	a	2053	U	P-O3'-C3'	-9.01	108.89	119.70
28	a	911	U	P-O3'-C3'	-8.91	109.01	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2659	U	P-O3'-C3'	-8.90	109.02	119.70
28	a	2248	C	P-O3'-C3'	-8.71	109.25	119.70
28	a	127	C	C6-N1-C2	8.70	123.78	120.30
28	a	2719	U	P-O3'-C3'	-8.67	109.30	119.70
28	a	2887	A	P-O3'-C3'	-8.65	109.32	119.70
28	a	2662	C	P-O3'-C3'	-8.62	109.36	119.70
28	a	2655	C	P-O3'-C3'	-8.59	109.40	119.70
28	a	2721	C	P-O3'-C3'	-8.54	109.46	119.70
28	a	711	G	P-O3'-C3'	-8.46	109.55	119.70
28	a	2886	C	P-O3'-C3'	-8.33	109.71	119.70
28	a	2894	U	P-O3'-C3'	-8.30	109.74	119.70
28	a	304	G	P-O3'-C3'	-8.29	109.75	119.70
28	a	2153	A	P-O3'-C3'	-8.23	109.83	119.70
28	a	2525	U	P-O3'-C3'	-8.22	109.83	119.70
28	a	2711	G	P-O3'-C3'	-8.20	109.86	119.70
28	a	2055	U	P-O3'-C3'	-8.19	109.88	119.70
28	a	442	U	P-O3'-C3'	-8.12	109.96	119.70
28	a	1637	G	P-O3'-C3'	-8.10	109.98	119.70
28	a	1832	C	P-O3'-C3'	-8.07	110.02	119.70
28	a	2651	A	P-O3'-C3'	-8.05	110.04	119.70
28	a	441	C	P-O3'-C3'	-8.04	110.05	119.70
28	a	2658	A	P-O3'-C3'	-8.02	110.08	119.70
28	a	2660	A	P-O3'-C3'	-7.96	110.15	119.70
28	a	2054	A	P-O3'-C3'	-7.88	110.24	119.70
28	a	303	G	P-O3'-C3'	-7.85	110.28	119.70
28	a	2056	G	P-O3'-C3'	-7.82	110.31	119.70
28	a	1914	C	C2-N1-C1'	7.76	127.34	118.80
28	a	2961	U	O4'-C1'-N1	7.55	114.24	108.20
28	a	272	A	P-O3'-C3'	-7.46	110.75	119.70
28	a	2587	U	P-O3'-C3'	-7.46	110.75	119.70
28	a	2712	G	P-O3'-C3'	-7.42	110.80	119.70
28	a	1348	G	P-O3'-C3'	-7.20	111.06	119.70
28	a	2612	A	P-O3'-C3'	-7.19	111.07	119.70
28	a	1914	C	N1-C2-O2	7.17	123.20	118.90
28	a	2710	U	P-O3'-C3'	-7.17	111.09	119.70
28	a	2049	A	P-O3'-C3'	-7.04	111.25	119.70
28	a	2717	G	P-O3'-C3'	-6.93	111.39	119.70
28	a	2961	U	N1-C1'-C2'	6.80	122.83	114.00
28	a	1638	U	P-O3'-C3'	-6.79	111.55	119.70
28	a	1389	U	C2-N1-C1'	6.72	125.76	117.70
28	a	1833	G	P-O3'-C3'	-6.69	111.67	119.70
28	a	1187	C	P-O3'-C3'	-6.57	111.82	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	272	A	C1'-O4'-C4'	-6.55	104.66	109.90
28	a	738	U	P-O3'-C3'	-6.52	111.87	119.70
28	a	439	C	P-O3'-C3'	-6.43	111.98	119.70
28	a	302	A	P-O3'-C3'	-6.39	112.03	119.70
28	a	271	G	C3'-C2'-C1'	-6.38	96.39	101.50
28	a	932	U	C2-N1-C1'	6.38	125.35	117.70
28	a	1730	U	C1'-O4'-C4'	6.05	114.74	109.90
28	a	2716	C	P-O3'-C3'	-5.93	112.58	119.70
28	a	307	U	C2-N1-C1'	5.92	124.80	117.70
28	a	2611	G	P-O3'-C3'	-5.71	112.84	119.70
28	a	1914	C	C6-N1-C1'	-5.69	113.97	120.80
28	a	271	G	C2'-C3'-O3'	5.67	122.76	113.70
28	a	1188	U	P-O3'-C3'	-5.59	112.99	119.70
28	a	2708	G	P-O3'-C3'	-5.56	113.03	119.70
28	a	455	C	P-O3'-C3'	-5.39	113.23	119.70
28	a	710	C	P-O3'-C3'	-5.38	113.24	119.70
28	a	932	U	N1-C2-O2	5.36	126.55	122.80
28	a	451	G	P-O3'-C3'	-5.33	113.31	119.70
28	a	2722	C	P-O3'-C3'	-5.30	113.34	119.70
28	a	1914	C	N3-C2-O2	-5.27	118.21	121.90
28	a	271	G	C4'-C3'-C2'	-5.22	97.38	102.60
28	a	2503	G	C4-N9-C1'	5.21	133.28	126.50
27	4	38	CYS	CB-CA-C	-5.18	100.04	110.40
28	a	2720	C	P-O3'-C3'	-5.11	113.57	119.70

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	c	2091	0	2150	0	0
2	d	1586	0	1634	0	0
3	e	1577	0	1619	0	0
4	f	1623	0	1665	0	0
5	g	1376	0	1421	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	i	1139	0	1163	0	0
7	j	946	0	1011	0	0
8	k	1072	0	1106	0	0
9	l	1082	0	1117	0	0
10	m	936	0	997	0	0
11	n	952	0	995	0	0
12	o	896	0	928	0	0
13	p	958	0	986	0	0
14	q	778	0	824	0	0
15	r	1017	0	1070	0	0
16	s	751	0	803	0	0
17	t	833	0	883	0	0
18	u	1376	0	1397	0	0
19	v	591	0	581	0	0
20	w	474	0	487	0	0
21	x	564	0	582	0	0
22	y	467	0	504	0	0
23	z	477	0	479	0	0
24	0	423	0	429	14	0
25	1	362	0	387	2	0
26	2	513	0	565	4	0
27	4	512	0	497	39	0
28	a	62531	0	31359	0	0
29	b	2567	0	1297	0	0
30	V	183	0	202	1	0
31	C	1625	0	829	10	0
32	3	302	0	333	5	0
33	1	1	0	0	0	0
33	C	2	0	0	0	0
33	a	294	0	0	0	0
33	b	2	0	0	0	0
33	c	3	0	0	0	0
33	d	1	0	0	0	0
33	k	2	0	0	0	0
34	0	1	0	0	0	0
34	4	1	0	0	0	0
34	w	1	0	0	0	0
34	z	1	0	0	0	0
35	a	35	0	0	0	0
36	a	120	0	0	0	0
36	b	3	0	0	0	0
36	d	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	s	1	0	0	0	0
All	All	93049	0	60300	75	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 8.

All (75) 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)
27:4:38:CYS:SG	27:4:41:CYS:HB2	1.83	1.10
27:4:16:CYS:HA	27:4:35:ALA:HB3	1.51	0.92
24:0:8:VAL:HA	24:0:30:ARG:HH21	1.35	0.88
27:4:49:GLN:O	27:4:50:LYS:HB2	1.72	0.87
27:4:11:GLU:HA	27:4:25:ARG:HA	1.69	0.74
27:4:47:GLY:HA2	27:4:50:LYS:NZ	2.05	0.72
27:4:18:CYS:HB2	27:4:41:CYS:SG	2.31	0.70
25:1:24:THR:HG23	25:1:27:GLY:H	1.59	0.66
27:4:47:GLY:HA2	27:4:50:LYS:HZ2	1.63	0.64
27:4:9:TYR:HD1	27:4:27:THR:HG23	1.64	0.63
27:4:45:TYR:C	27:4:47:GLY:H	2.05	0.60
27:4:16:CYS:CA	27:4:35:ALA:HB3	2.30	0.59
27:4:16:CYS:O	27:4:16:CYS:SG	2.61	0.59
31:C:4:G:H1	31:C:69:C:H42	1.50	0.58
24:0:36:ARG:NH2	24:0:53:ARG:HE	2.03	0.57
27:4:22:PHE:CG	27:4:23:THR:N	2.73	0.56
27:4:47:GLY:CA	27:4:50:LYS:NZ	2.69	0.55
27:4:13:THR:O	27:4:32:THR:HA	2.07	0.55
26:2:8:SER:HA	26:2:11:LYS:HE2	1.89	0.55
27:4:45:TYR:C	27:4:47:GLY:N	2.57	0.54
27:4:18:CYS:SG	27:4:41:CYS:HB2	2.48	0.54
27:4:41:CYS:SG	27:4:41:CYS:O	2.65	0.54
32:3:14:CYS:SG	32:3:27:CYS:SG	3.04	0.53
27:4:43:PRO:HB3	27:4:48:LYS:O	2.09	0.53
27:4:18:CYS:CB	27:4:41:CYS:SG	2.96	0.53
24:0:38:GLU:OE2	24:0:53:ARG:NH1	2.37	0.52
27:4:13:THR:HA	27:4:23:THR:HA	1.92	0.52
27:4:38:CYS:O	27:4:42:HIS:HB2	2.10	0.51
27:4:14:VAL:O	27:4:21:THR:HA	2.11	0.51
31:C:52:G:H2'	31:C:53:G:H8	1.75	0.51
24:0:36:ARG:NH1	24:0:54:GLU:O	2.45	0.50
27:4:43:PRO:HG3	27:4:48:LYS:NZ	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:0:30:ARG:HH22	24:0:31:ARG:NH2	2.10	0.50
27:4:10:ARG:HH22	27:4:26:SER:C	2.16	0.49
25:1:16:HIS:HB2	25:1:44:ALA:HB3	1.93	0.49
31:C:7:G:O2'	31:C:49:G:OP2	2.21	0.49
32:3:16:VAL:HG22	32:3:25:VAL:HG22	1.95	0.49
27:4:43:PRO:HA	27:4:48:LYS:HB3	1.96	0.48
30:V:21:ARG:HG3	30:V:22:PRO:HD2	1.96	0.48
32:3:10:ILE:HB	32:3:32:HIS:CD2	2.49	0.48
31:C:52:G:H2'	31:C:53:G:C8	2.49	0.47
27:4:37:VAL:HG11	27:4:42:HIS:HD2	1.78	0.47
31:C:43:A:H2'	31:C:44:A:C8	2.50	0.47
31:C:62:C:H2'	31:C:63:G:H8	1.80	0.47
27:4:15:VAL:HG22	27:4:17:THR:H	1.80	0.46
24:0:12:ILE:HB	24:0:54:GLU:HG3	1.97	0.46
27:4:20:ASN:HB3	27:4:40:LYS:HZ1	1.81	0.45
24:0:7:ASP:OD1	24:0:7:ASP:N	2.49	0.45
24:0:11:LYS:HE2	24:0:11:LYS:HB2	1.79	0.45
26:2:26:LYS:HD3	26:2:48:THR:HB	1.98	0.45
24:0:35:ASP:OD1	24:0:35:ASP:N	2.47	0.44
27:4:20:ASN:ND2	27:4:38:CYS:SG	2.78	0.44
27:4:15:VAL:O	27:4:34:ASN:HA	2.17	0.44
24:0:32:ASN:N	24:0:32:ASN:HD22	2.16	0.44
31:C:15:G:H2'	31:C:59:A:N1	2.33	0.44
31:C:4:G:H1	31:C:69:C:N4	2.16	0.43
24:0:20:LYS:N	24:0:20:LYS:HD2	2.34	0.43
31:C:9:G:N3	31:C:45:G:H2'	2.34	0.43
24:0:29:ASN:O	24:0:31:ARG:N	2.48	0.43
27:4:59:ALA:HA	27:4:62:GLU:OE2	2.19	0.43
27:4:11:GLU:CD	27:4:12:THR:H	2.22	0.42
24:0:14:LEU:HD21	24:0:39:MET:SD	2.59	0.42
26:2:50:LEU:HD23	26:2:54:GLU:HB3	2.01	0.42
27:4:60:ARG:O	27:4:64:ARG:HG2	2.19	0.42
32:3:22:ARG:HD3	32:3:35:ARG:HD3	2.00	0.42
31:C:62:C:H2'	31:C:63:G:C8	2.55	0.42
27:4:33:LEU:HD12	27:4:33:LEU:HA	1.77	0.42
27:4:9:TYR:CD1	27:4:27:THR:HG23	2.48	0.41
27:4:49:GLN:HG3	27:4:50:LYS:N	2.35	0.41
32:3:29:ASN:HB3	32:3:32:HIS:ND1	2.35	0.41
26:2:29:LYS:HD2	26:2:41:THR:HG23	2.02	0.41
27:4:13:THR:HB	27:4:23:THR:HG22	2.02	0.41
27:4:20:ASN:HB3	27:4:40:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:0:29:ASN:C	24:0:31:ARG:H	2.23	0.40
27:4:42:HIS:HA	27:4:43:PRO:HD3	1.95	0.40

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	c	272/278 (98%)	254 (93%)	16 (6%)	2 (1%)	19	31
2	d	212/223 (95%)	198 (93%)	13 (6%)	1 (0%)	25	40
3	e	208/301 (69%)	185 (89%)	18 (9%)	5 (2%)	5	8
4	f	201/210 (96%)	168 (84%)	19 (10%)	14 (7%)	1	0
5	g	175/180 (97%)	162 (93%)	12 (7%)	1 (1%)	22	35
6	i	144/147 (98%)	139 (96%)	5 (4%)	0	100	100
7	j	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
8	k	142/146 (97%)	120 (84%)	22 (16%)	0	100	100
9	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
10	m	118/187 (63%)	112 (95%)	5 (4%)	1 (1%)	16	28
11	n	124/127 (98%)	120 (97%)	3 (2%)	1 (1%)	16	28
12	o	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
13	p	117/123 (95%)	109 (93%)	7 (6%)	1 (1%)	14	25
14	q	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
15	r	130/153 (85%)	123 (95%)	6 (5%)	1 (1%)	16	28
16	s	93/102 (91%)	87 (94%)	5 (5%)	1 (1%)	12	19
17	t	103/122 (84%)	99 (96%)	3 (3%)	1 (1%)	13	21
18	u	177/205 (86%)	168 (95%)	7 (4%)	2 (1%)	12	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	v	76/89 (85%)	73 (96%)	3 (4%)	0	100	100
20	w	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	7	12
21	x	67/77 (87%)	62 (92%)	4 (6%)	1 (2%)	8	14
22	y	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
23	z	60/63 (95%)	55 (92%)	3 (5%)	2 (3%)	3	5
24	0	48/56 (86%)	42 (88%)	6 (12%)	0	100	100
25	1	42/44 (96%)	42 (100%)	0	0	100	100
26	2	65/68 (96%)	65 (100%)	0	0	100	100
27	4	64/69 (93%)	50 (78%)	11 (17%)	3 (5%)	2	2
30	V	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
32	3	35/37 (95%)	35 (100%)	0	0	100	100
All	All	3274/3632 (90%)	3048 (93%)	188 (6%)	38 (1%)	14	18

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	c	26	ARG
3	e	151	ALA
3	e	159	VAL
3	e	186	ASN
4	f	188	ALA
4	f	189	LYS
4	f	190	ASP
4	f	191	ASP
4	f	192	PRO
4	f	204	TYR
13	p	93	LYS
27	4	49	GLN
27	4	50	LYS
3	e	133	VAL
4	f	186	PHE
4	f	187	LYS
4	f	193	LYS
4	f	196	LYS
4	f	198	LYS
4	f	200	GLY
11	n	5	LEU
15	r	3	LYS

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Mol	Chain	Res	Type
18	u	97	ARG
20	w	41	ASN
23	z	56	ASP
4	f	202	ALA
27	4	28	SER
16	s	93	ARG
1	c	262	LYS
3	e	138	PRO
10	m	37	THR
2	d	95	GLU
17	t	64	ILE
18	u	98	GLY
21	x	5	SER
4	f	201	PRO
5	g	161	GLY
23	z	55	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	c	216/220 (98%)	216 (100%)	0	100	100
2	d	166/172 (96%)	164 (99%)	2 (1%)	67	82
3	e	165/237 (70%)	163 (99%)	2 (1%)	67	82
4	f	169/175 (97%)	151 (89%)	18 (11%)	5	8
5	g	150/152 (99%)	141 (94%)	9 (6%)	16	28
6	i	118/120 (98%)	118 (100%)	0	100	100
7	j	101/101 (100%)	99 (98%)	2 (2%)	50	71
8	k	111/113 (98%)	109 (98%)	2 (2%)	54	73
9	l	108/110 (98%)	107 (99%)	1 (1%)	75	87
10	m	100/142 (70%)	98 (98%)	2 (2%)	50	71
11	n	95/96 (99%)	95 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	o	97/99 (98%)	97 (100%)	0	100	100
13	p	98/99 (99%)	98 (100%)	0	100	100
14	q	84/84 (100%)	84 (100%)	0	100	100
15	r	105/118 (89%)	102 (97%)	3 (3%)	37	58
16	s	84/89 (94%)	84 (100%)	0	100	100
17	t	91/103 (88%)	91 (100%)	0	100	100
18	u	149/168 (89%)	146 (98%)	3 (2%)	50	71
19	v	60/67 (90%)	60 (100%)	0	100	100
20	w	52/53 (98%)	52 (100%)	0	100	100
21	x	61/68 (90%)	61 (100%)	0	100	100
22	y	53/55 (96%)	53 (100%)	0	100	100
23	z	51/52 (98%)	50 (98%)	1 (2%)	50	71
24	0	47/51 (92%)	46 (98%)	1 (2%)	48	70
25	1	36/36 (100%)	36 (100%)	0	100	100
26	2	54/55 (98%)	53 (98%)	1 (2%)	52	72
27	4	56/59 (95%)	44 (79%)	12 (21%)	1	0
30	V	16/17 (94%)	16 (100%)	0	100	100
32	3	35/35 (100%)	34 (97%)	1 (3%)	37	58
All	All	2728/2946 (93%)	2668 (98%)	60 (2%)	47	68

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	d	45	THR
2	d	94	SER
3	e	114	ARG
3	e	144	LYS
4	f	32	ARG
4	f	180	LYS
4	f	184	PHE
4	f	186	PHE
4	f	187	LYS
4	f	189	LYS
4	f	190	ASP
4	f	193	LYS
4	f	194	LYS

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Mol	Chain	Res	Type
4	f	196	LYS
4	f	198	LYS
4	f	199	ARG
4	f	201	PRO
4	f	203	TYR
4	f	204	TYR
4	f	206	LYS
4	f	207	LYS
4	f	208	LYS
5	g	54	GLU
5	g	155	LYS
5	g	157	GLU
5	g	159	TYR
5	g	160	LYS
5	g	173	ARG
5	g	174	LYS
5	g	175	VAL
5	g	177	LYS
7	j	23	ARG
7	j	122	ILE
8	k	27	SER
8	k	28	LYS
9	l	60	ARG
10	m	73	ARG
10	m	107	ASN
15	r	2	SER
15	r	3	LYS
15	r	95	GLU
18	u	95	VAL
18	u	100	LYS
18	u	180	GLU
23	z	57	ARG
24	0	20	LYS
26	2	68	ARG
27	4	10	ARG
27	4	12	THR
27	4	13	THR
27	4	14	VAL
27	4	24	THR
27	4	25	ARG
27	4	26	SER
27	4	27	THR

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Mol	Chain	Res	Type
27	4	28	SER
27	4	33	LEU
27	4	34	ASN
27	4	38	CYS
32	3	13	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	d	55	GLN
3	e	142	GLN
8	k	75	GLN
15	r	56	GLN
18	u	58	ASN
24	0	29	ASN
24	0	32	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	a	2885/3086 (93%)	484 (16%)	0
29	b	118/120 (98%)	11 (9%)	0
31	C	75/77 (97%)	10 (13%)	1 (1%)
All	All	3078/3283 (93%)	505 (16%)	1 (0%)

All (505) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	a	11	G
28	a	12	U
28	a	31	C
28	a	33	U
28	a	34	G
28	a	42	G
28	a	50	G
28	a	62	G
28	a	70	A
28	a	73	A
28	a	74	G
28	a	82	G

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Mol	Chain	Res	Type
28	a	91	A
28	a	94	G
28	a	98	U
28	a	99	G
28	a	100	U
28	a	101	G
28	a	117	A
28	a	118	A
28	a	119	U
28	a	124	A
28	a	132	A
28	a	133	A
28	a	135	G
28	a	137	C
28	a	147	G
28	a	166	A
28	a	180	U
28	a	188	A
28	a	203	A
28	a	206	A
28	a	222	G
28	a	223	A
28	a	229	A
28	a	230	A
28	a	236	U
28	a	255	G
28	a	272	A
28	a	273	G
28	a	279	A
28	a	283	U
28	a	284	G
28	a	285	U
28	a	286	G
28	a	287	U
28	a	288	G
28	a	289	U
28	a	290	G
28	a	304	G
28	a	305	U
28	a	307	U
28	a	309	G
28	a	310	C

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Mol	Chain	Res	Type
28	a	311	A
28	a	312	U
28	a	313	G
28	a	314	U
28	a	316	C
28	a	318	G
28	a	321	U
28	a	322	U
28	a	324	U
28	a	325	G
28	a	332	U
28	a	335	U
28	a	336	G
28	a	337	G
28	a	338	U
28	a	339	U
28	a	340	C
28	a	341	U
28	a	342	G
28	a	345	G
28	a	346	C
28	a	347	C
28	a	348	G
28	a	353	A
28	a	354	U
28	a	355	U
28	a	356	G
28	a	358	C
28	a	359	C
28	a	360	A
28	a	366	A
28	a	367	A
28	a	369	U
28	a	370	G
28	a	373	G
28	a	379	A
28	a	380	G
28	a	385	A
28	a	386	G
28	a	387	C
28	a	393	G
28	a	396	A

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Mol	Chain	Res	Type
28	a	402	A
28	a	408	G
28	a	415	A
28	a	419	U
28	a	423	G
28	a	431	A
28	a	432	A
28	a	433	G
28	a	434	C
28	a	435	G
28	a	447	U
28	a	453	U
28	a	454	G
28	a	460	A
28	a	475	G
28	a	476	U
28	a	477	G
28	a	480	A
28	a	494	U
28	a	500	G
28	a	501	A
28	a	532	A
28	a	533	C
28	a	544	U
28	a	545	G
28	a	546	A
28	a	570	G
28	a	592	G
28	a	593	A
28	a	596	U
28	a	618	G
28	a	619	C
28	a	620	C
28	a	621	G
28	a	632	U
28	a	633	G
28	a	635	G
28	a	639	A
28	a	646	G
28	a	656	G
28	a	658	A
28	a	674	G

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Mol	Chain	Res	Type
28	a	675	U
28	a	676	G
28	a	687	A
28	a	699	G
28	a	700	G
28	a	701	U
28	a	707	A
28	a	713	A
28	a	720	G
28	a	723	A
28	a	731	A
28	a	733	G
28	a	739	G
28	a	740	A
28	a	741	G
28	a	770	A
28	a	771	U
28	a	802	G
28	a	815	U
28	a	832	U
28	a	842	G
28	a	849	A
28	a	860	G
28	a	861	G
28	a	867	A
28	a	869	G
28	a	870	G
28	a	874	A
28	a	875	U
28	a	877	A
28	a	890	G
28	a	897	C
28	a	912	U
28	a	931	G
28	a	944	G
28	a	968	G
28	a	969	C
28	a	970	U
28	a	972	A
28	a	973	U
28	a	974	C
28	a	975	G

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Mol	Chain	Res	Type
28	a	978	U
28	a	979	U
28	a	980	A
28	a	981	C
28	a	991	C
28	a	994	A
28	a	1016	A
28	a	1028	A
28	a	1029	G
28	a	1042	A
28	a	1044	G
28	a	1057	G
28	a	1066	A
28	a	1073	A
28	a	1079	A
28	a	1096	G
28	a	1105	G
28	a	1109	G
28	a	1116	U
28	a	1119	G
28	a	1128	U
28	a	1129	A
28	a	1130	G
28	a	1141	G
28	a	1142	G
28	a	1144	U
28	a	1145	G
28	a	1149	U
28	a	1150	G
28	a	1151	G
28	a	1152	A
28	a	1153	A
28	a	1154	G
28	a	1156	A
28	a	1157	G
28	a	1161	U
28	a	1165	U
28	a	1172	G
28	a	1173	U
28	a	1177	U
28	a	1178	A
28	a	1179	A

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Mol	Chain	Res	Type
28	a	1181	A
28	a	1189	G
28	a	1190	G
28	a	1193	A
28	a	1195	G
28	a	1196	U
28	a	1215	U
28	a	1216	A
28	a	1218	C
28	a	1225	U
28	a	1226	A
28	a	1227	A
28	a	1254	G
28	a	1255	U
28	a	1256	G
28	a	1257	U
28	a	1283	G
28	a	1297	G
28	a	1306	U
28	a	1307	G
28	a	1327	G
28	a	1330	A
28	a	1333	G
28	a	1348	G
28	a	1350	G
28	a	1351	U
28	a	1365	C
28	a	1376	A
28	a	1377	U
28	a	1390	C
28	a	1428	U
28	a	1441	A
28	a	1455	U
28	a	1460	A
28	a	1471	A
28	a	1472	U
28	a	1595	A
28	a	1601	G
28	a	1607	A
28	a	1608	C
28	a	1625	U
28	a	1626	C

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Mol	Chain	Res	Type
28	a	1630	G
28	a	1633	G
28	a	1637	G
28	a	1639	U
28	a	1641	U
28	a	1642	C
28	a	1648	C
28	a	1663	G
28	a	1673	U
28	a	1674	A
28	a	1677	U
28	a	1689	G
28	a	1690	A
28	a	1691	A
28	a	1692	G
28	a	1697	A
28	a	1698	G
28	a	1706	G
28	a	1710	A
28	a	1712	C
28	a	1714	C
28	a	1717	G
28	a	1718	G
28	a	1719	U
28	a	1720	U
28	a	1721	G
28	a	1725	G
28	a	1726	U
28	a	1727	G
28	a	1743	A
28	a	1749	G
28	a	1752	A
28	a	1761	G
28	a	1768	A
28	a	1769	G
28	a	1774	C
28	a	1777	G
28	a	1792	A
28	a	1818	U
28	a	1830	A
28	a	1832	C
28	a	1837	G

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Mol	Chain	Res	Type
28	a	1838	A
28	a	1858	G
28	a	1897	G
28	a	1898	C
28	a	1904	U
28	a	1911	G
28	a	1912	U
28	a	1913	G
28	a	1914	C
28	a	1915	G
28	a	1916	G
28	a	1921	G
28	a	1939	G
28	a	1947	G
28	a	1956	A
28	a	1965	C
28	a	1969	A
28	a	1974	A
28	a	1983	C
28	a	1984	G
28	a	1985	A
28	a	1999	U
28	a	2012	A
28	a	2031	A
28	a	2041	G
28	a	2052	G
28	a	2053	U
28	a	2054	A
28	a	2055	U
28	a	2056	G
28	a	2057	C
28	a	2068	A
28	a	2089	G
28	a	2096	A
28	a	2112	G
28	a	2113	G
28	a	2119	A
28	a	2120	A
28	a	2121	A
28	a	2138	U
28	a	2146	U
28	a	2150	C

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Mol	Chain	Res	Type
28	a	2153	A
28	a	2154	U
28	a	2155	G
28	a	2174	U
28	a	2176	U
28	a	2186	G
28	a	2204	U
28	a	2206	A
28	a	2210	G
28	a	2214	A
28	a	2215	G
28	a	2216	A
28	a	2222	G
28	a	2226	C
28	a	2238	C
28	a	2239	G
28	a	2243	A
28	a	2250	G
28	a	2275	G
28	a	2279	A
28	a	2283	G
28	a	2287	G
28	a	2289	U
28	a	2364	A
28	a	2365	U
28	a	2366	U
28	a	2367	G
28	a	2368	U
28	a	2369	U
28	a	2384	G
28	a	2385	U
28	a	2386	G
28	a	2393	G
28	a	2394	A
28	a	2407	A
28	a	2420	G
28	a	2421	G
28	a	2461	G
28	a	2464	G
28	a	2465	C
28	a	2469	A
28	a	2487	U

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Mol	Chain	Res	Type
28	a	2490	G
28	a	2491	U
28	a	2501	G
28	a	2502	U
28	a	2503	G
28	a	2504	A
28	a	2507	G
28	a	2517	A
28	a	2518	A
28	a	2527	G
28	a	2529	C
28	a	2532	U
28	a	2536	A
28	a	2543	G
28	a	2565	G
28	a	2567	A
28	a	2588	U
28	a	2607	A
28	a	2611	G
28	a	2612	A
28	a	2613	U
28	a	2617	A
28	a	2623	C
28	a	2630	A
28	a	2652	G
28	a	2653	C
28	a	2654	G
28	a	2655	C
28	a	2656	U
28	a	2657	C
28	a	2658	A
28	a	2659	U
28	a	2660	A
28	a	2661	G
28	a	2663	G
28	a	2664	A
28	a	2673	U
28	a	2674	U
28	a	2679	A
28	a	2684	G
28	a	2687	G
28	a	2688	U

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Mol	Chain	Res	Type
28	a	2700	A
28	a	2702	C
28	a	2711	G
28	a	2712	G
28	a	2713	A
28	a	2714	G
28	a	2716	C
28	a	2717	G
28	a	2720	C
28	a	2721	C
28	a	2722	C
28	a	2748	A
28	a	2749	G
28	a	2755	C
28	a	2767	U
28	a	2784	A
28	a	2795	U
28	a	2797	U
28	a	2811	A
28	a	2871	U
28	a	2872	G
28	a	2873	C
28	a	2900	G
28	a	2908	C
28	a	2911	C
28	a	2915	U
28	a	2917	G
28	a	2926	G
28	a	2930	A
28	a	2939	A
28	a	2944	G
28	a	2947	A
28	a	2948	G
28	a	2960	A
28	a	2962	A
28	a	2971	C
28	a	2972	A
28	a	2973	C
28	a	2979	U
28	a	2981	U
28	a	2982	U
28	a	2983	C

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Mol	Chain	Res	Type
28	a	3000	G
28	a	3015	A
28	a	3041	G
28	a	3052	G
28	a	3063	A
28	a	3064	U
28	a	3066	G
28	a	3073	G
28	a	3074	A
28	a	3075	C
29	b	24	G
29	b	25	A
29	b	35	U
29	b	45	A
29	b	56	U
29	b	57	A
29	b	84	C
29	b	90	A
29	b	100	A
29	b	109	C
29	b	110	G
31	C	9	G
31	C	16	C
31	C	17	C
31	C	17(A)	U
31	C	18	G
31	C	21	A
31	C	46	G
31	C	47	U
31	C	69	C
31	C	76	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
31	C	17(A)	U

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

22 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$
28	2MG	a	2627	28	18,26,27	1.24	3 (16%)	16,38,41	0.88	1 (6%)
28	PSU	a	2787	28	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
28	2MA	a	2685	28,33	18,25,26	3.33	6 (33%)	20,37,40	1.77	3 (15%)
28	OMG	a	2433	28,31	19,26,27	1.24	3 (15%)	21,38,41	0.82	1 (4%)
28	5MC	a	2145	28	19,22,23	0.58	0	26,32,35	0.70	0
28	PSU	a	2686	28	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
31	4SU	C	8	31	18,21,22	3.80	7 (38%)	25,30,33	2.30	5 (20%)
31	5MC	C	32	31	19,22,23	0.49	0	26,32,35	0.61	0
28	PSU	a	2639	28	18,21,22	1.08	2 (11%)	21,30,33	2.02	5 (23%)
28	2MG	a	2018	28	18,26,27	1.20	2 (11%)	16,38,41	0.92	1 (6%)
28	OMU	a	2734	28	19,22,23	2.91	7 (36%)	25,31,34	1.85	5 (20%)
28	PSU	a	2786	28	18,21,22	1.09	1 (5%)	21,30,33	1.98	5 (23%)
28	PSU	a	2094	28	18,21,22	1.12	1 (5%)	21,30,33	1.93	5 (23%)
28	OMC	a	2680	28,33	19,22,23	0.62	0	25,31,34	0.74	0
28	H2U	a	2631	28	18,21,22	0.48	0	19,30,33	1.08	1 (5%)
31	PSU	C	55	31	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
28	PSU	a	1038	28	18,21,22	1.03	1 (5%)	21,30,33	2.01	3 (14%)
31	5MU	C	54	31	19,22,23	0.38	0	27,32,35	0.62	0
28	PSU	a	2100	28	18,21,22	1.13	1 (5%)	21,30,33	1.88	4 (19%)
28	PSU	a	2762	28	18,21,22	1.11	2 (11%)	21,30,33	1.96	5 (23%)
28	3TD	a	2098	28	19,22,23	4.27	6 (31%)	23,32,35	1.81	4 (17%)
28	5MU	a	2122	28	19,22,23	0.47	0	27,32,35	0.47	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
28	2MG	a	2627	28	-	1/5/27/28	0/3/3/3
28	PSU	a	2787	28	-	0/7/25/26	0/2/2/2
28	2MA	a	2685	28,33	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	OMG	a	2433	28,31	-	1/5/27/28	0/3/3/3
28	5MC	a	2145	28	-	1/7/25/26	0/2/2/2
28	PSU	a	2686	28	-	0/7/25/26	0/2/2/2
31	4SU	C	8	31	-	0/7/25/26	0/2/2/2
31	5MC	C	32	31	-	0/7/25/26	0/2/2/2
28	PSU	a	2639	28	-	0/7/25/26	0/2/2/2
28	2MG	a	2018	28	-	0/5/27/28	0/3/3/3
28	OMU	a	2734	28	-	0/9/27/28	0/2/2/2
28	PSU	a	2786	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2094	28	-	0/7/25/26	0/2/2/2
28	OMC	a	2680	28,33	-	0/9/27/28	0/2/2/2
28	H2U	a	2631	28	-	0/7/38/39	0/2/2/2
31	PSU	C	55	31	-	0/7/25/26	0/2/2/2
28	PSU	a	1038	28	-	0/7/25/26	0/2/2/2
31	5MU	C	54	31	-	0/7/25/26	0/2/2/2
28	PSU	a	2100	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2762	28	-	0/7/25/26	0/2/2/2
28	3TD	a	2098	28	-	2/7/25/26	0/2/2/2
28	5MU	a	2122	28	-	0/7/25/26	0/2/2/2

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2098	3TD	C6-C5	13.12	1.49	1.35
28	a	2098	3TD	C2-N1	9.47	1.48	1.37
28	a	2685	2MA	C4-N3	8.22	1.48	1.35
31	C	8	4SU	C2-N3	7.39	1.50	1.38
31	C	8	4SU	C2-N1	7.23	1.49	1.38
31	C	8	4SU	C4-N3	7.04	1.44	1.37
28	a	2734	OMU	C2-N1	6.90	1.49	1.38
28	a	2685	2MA	C2-N3	6.89	1.45	1.34
28	a	2685	2MA	C2-N1	6.86	1.45	1.34
28	a	2734	OMU	C2-N3	6.60	1.49	1.38
31	C	8	4SU	C5-C4	6.15	1.49	1.42
28	a	2098	3TD	C6-N1	6.14	1.46	1.36
28	a	2734	OMU	C6-C5	5.79	1.48	1.35
31	C	8	4SU	C6-C5	5.61	1.48	1.35
31	C	8	4SU	C4-S4	-4.83	1.60	1.68
28	a	2098	3TD	C2-N3	4.77	1.48	1.38
28	a	2685	2MA	C6-N1	3.97	1.41	1.33
31	C	55	PSU	C6-C5	3.79	1.39	1.35
28	a	2100	PSU	C6-C5	3.76	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2094	PSU	C6-C5	3.68	1.39	1.35
28	a	2734	OMU	C4-N3	3.47	1.44	1.38
28	a	2686	PSU	C6-C5	3.43	1.39	1.35
28	a	2762	PSU	C6-C5	3.33	1.39	1.35
28	a	2786	PSU	C6-C5	3.30	1.38	1.35
28	a	2787	PSU	C6-C5	3.24	1.38	1.35
28	a	2627	2MG	C8-N7	-3.24	1.29	1.34
28	a	1038	PSU	C6-C5	3.17	1.38	1.35
28	a	2639	PSU	C6-C5	3.11	1.38	1.35
28	a	2018	2MG	C8-N7	-3.11	1.30	1.34
28	a	2433	OMG	C8-N7	-3.06	1.30	1.34
28	a	2098	3TD	C4-N3	2.98	1.46	1.40
28	a	2734	OMU	O2-C2	-2.84	1.18	1.23
28	a	2685	2MA	C6-C5	2.84	1.54	1.43
28	a	2734	OMU	O4-C4	-2.77	1.19	1.24
28	a	2433	OMG	C5-C6	-2.75	1.42	1.47
31	C	8	4SU	C6-N1	2.74	1.44	1.38
28	a	2627	2MG	C5-C6	-2.54	1.42	1.47
28	a	2018	2MG	C5-C6	-2.50	1.42	1.47
28	a	2685	2MA	C6-N6	-2.41	1.25	1.34
28	a	2098	3TD	O4-C4	-2.20	1.18	1.23
28	a	2627	2MG	C5-C4	-2.13	1.37	1.43
28	a	2762	PSU	C4-C5	-2.09	1.38	1.44
28	a	2433	OMG	C5-C4	-2.08	1.38	1.43
28	a	2734	OMU	C5-C4	2.06	1.48	1.43
28	a	2639	PSU	C4-C5	-2.01	1.38	1.44

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	8	4SU	C4-N3-C2	-7.91	119.73	127.31
28	a	2734	OMU	C4-N3-C2	-5.81	119.40	126.61
28	a	2098	3TD	N1-C2-N3	5.73	120.30	116.13
28	a	2685	2MA	C2-N3-C4	5.70	120.06	115.46
28	a	1038	PSU	C4-N3-C2	-5.51	118.78	126.37
31	C	8	4SU	C5-C4-N3	5.39	119.76	114.75
28	a	2639	PSU	N1-C2-N3	5.09	120.53	115.17
28	a	2786	PSU	C4-N3-C2	-5.05	119.41	126.37
28	a	2787	PSU	C4-N3-C2	-5.02	119.46	126.37
28	a	1038	PSU	N1-C2-N3	4.98	120.42	115.17
28	a	2762	PSU	C4-N3-C2	-4.96	119.53	126.37
28	a	2639	PSU	C4-N3-C2	-4.89	119.64	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2786	PSU	N1-C2-N3	4.88	120.31	115.17
28	a	2686	PSU	C4-N3-C2	-4.87	119.66	126.37
28	a	2686	PSU	N1-C2-N3	4.85	120.28	115.17
28	a	2094	PSU	C4-N3-C2	-4.83	119.72	126.37
28	a	2762	PSU	N1-C2-N3	4.82	120.25	115.17
31	C	55	PSU	C4-N3-C2	-4.82	119.73	126.37
28	a	2094	PSU	N1-C2-N3	4.79	120.22	115.17
28	a	2100	PSU	C4-N3-C2	-4.78	119.78	126.37
28	a	2787	PSU	N1-C2-N3	4.77	120.20	115.17
31	C	55	PSU	N1-C2-N3	4.74	120.17	115.17
28	a	2100	PSU	N1-C2-N3	4.70	120.12	115.17
28	a	2098	3TD	C4-N3-C2	-4.15	120.22	124.61
28	a	2734	OMU	N3-C2-N1	3.87	119.93	114.89
31	C	8	4SU	C5-C4-S4	-3.86	119.90	124.31
31	C	8	4SU	N3-C2-N1	3.81	119.85	114.89
28	a	2734	OMU	C5-C4-N3	3.77	120.08	114.80
28	a	2631	H2U	C5-C4-N3	-3.41	113.06	116.69
28	a	2685	2MA	N3-C2-N1	-3.34	119.92	125.77
28	a	2734	OMU	O4-C4-C5	-2.98	120.02	125.16
28	a	2639	PSU	O2-C2-N1	-2.91	119.78	122.79
28	a	2686	PSU	O2-C2-N1	-2.84	119.86	122.79
28	a	2094	PSU	O2-C2-N1	-2.79	119.91	122.79
31	C	55	PSU	O2-C2-N1	-2.77	119.93	122.79
28	a	2639	PSU	C6-N1-C2	-2.67	120.21	122.69
28	a	2762	PSU	O2-C2-N1	-2.67	120.04	122.79
28	a	2786	PSU	O2-C2-N1	-2.61	120.10	122.79
28	a	2100	PSU	O2-C2-N1	-2.60	120.10	122.79
28	a	2639	PSU	C6-C5-C4	2.57	119.91	118.17
28	a	2787	PSU	O2-C2-N1	-2.46	120.25	122.79
28	a	2686	PSU	C6-N1-C2	-2.43	120.43	122.69
28	a	2094	PSU	C6-N1-C2	-2.42	120.45	122.69
28	a	2098	3TD	C6-C5-C4	2.41	119.81	118.19
28	a	1038	PSU	O2-C2-N1	-2.36	120.35	122.79
28	a	2433	OMG	O6-C6-C5	2.36	129.01	124.32
28	a	2762	PSU	C6-N1-C2	-2.35	120.51	122.69
28	a	2786	PSU	C6-C5-C4	2.33	119.75	118.17
31	C	55	PSU	C6-N1-C2	-2.33	120.53	122.69
28	a	2762	PSU	C6-C5-C4	2.31	119.73	118.17
28	a	2627	2MG	O6-C6-C5	2.28	128.84	124.32
28	a	2786	PSU	C6-N1-C2	-2.24	120.61	122.69
28	a	2100	PSU	C6-N1-C2	-2.22	120.63	122.69
28	a	2734	OMU	O2-C2-N1	-2.20	119.93	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2787	PSU	C6-N1-C2	-2.16	120.69	122.69
28	a	2094	PSU	C6-C5-C4	2.15	119.62	118.17
31	C	8	4SU	O2-C2-N1	-2.11	120.05	122.80
31	C	55	PSU	C6-C5-C4	2.10	119.59	118.17
28	a	2018	2MG	O6-C6-C5	2.10	128.48	124.32
28	a	2098	3TD	C1'-C5-C4	2.08	120.77	117.61
28	a	2685	2MA	CM2-C2-N1	2.08	120.23	117.13

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	a	2098	3TD	O4'-C4'-C5'-O5'
28	a	2433	OMG	C1'-C2'-O2'-CM2
28	a	2098	3TD	C3'-C4'-C5'-O5'
28	a	2685	2MA	O4'-C4'-C5'-O5'
28	a	2685	2MA	C3'-C4'-C5'-O5'
28	a	2627	2MG	C3'-C4'-C5'-O5'
28	a	2145	5MC	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 310 ligands modelled in this entry, 309 are monoatomic - leaving 1 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
35	V7A	a	3101	-	37,38,38	1.05	2 (5%)	43,60,60	0.89	2 (4%)

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
35	V7A	a	3101	-	-	8/13/72/72	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	a	3101	V7A	CBC-NBD	4.99	1.47	1.33
35	a	3101	V7A	OAY-CAH	2.24	1.27	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	3101	V7A	CAM-CAP-CAQ	2.46	119.65	115.75
35	a	3101	V7A	CAP-CAM-CAL	2.09	112.33	109.88

There are no chirality outliers.

All (8) torsion outliers are listed below:

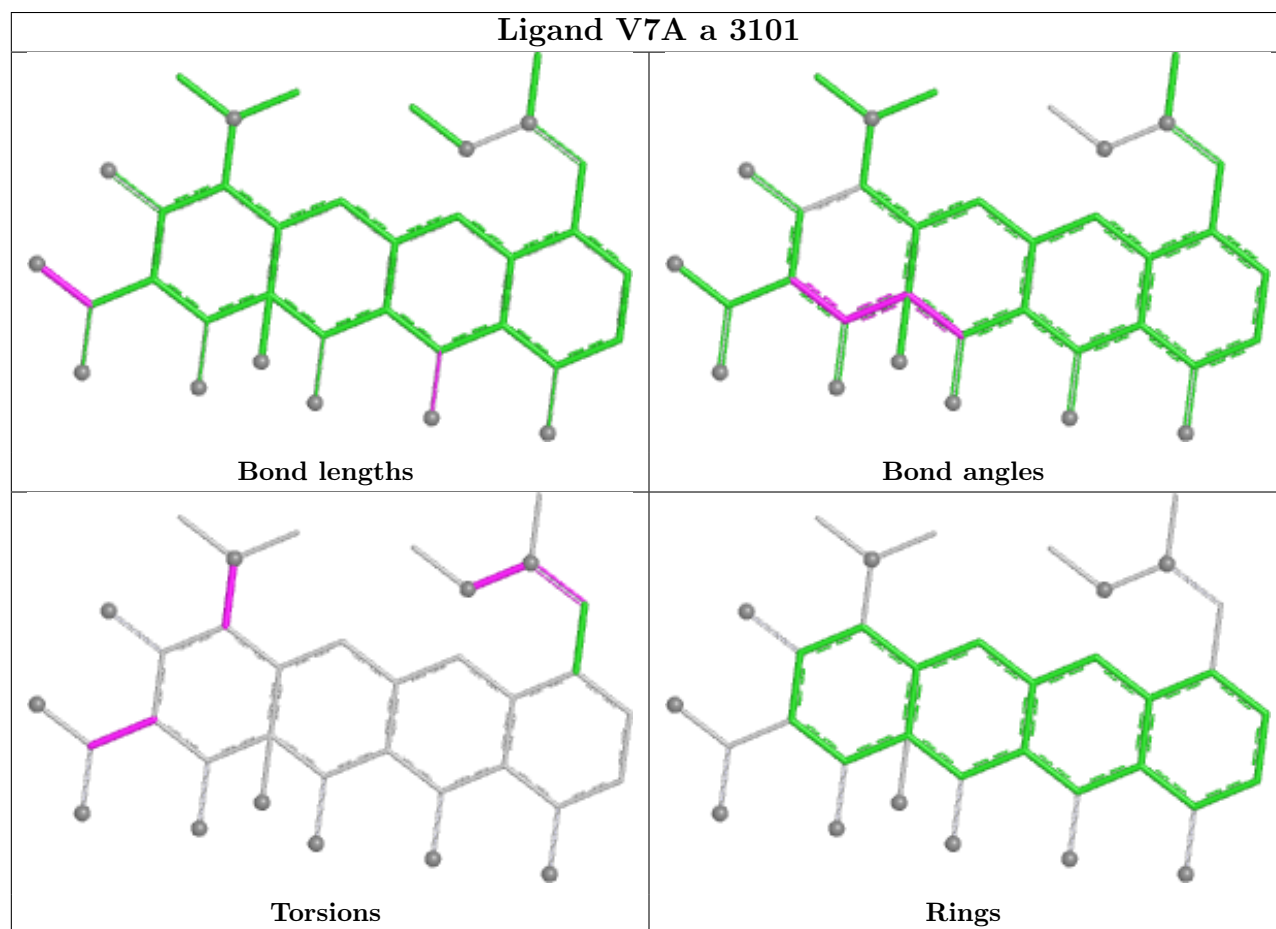
Mol	Chain	Res	Type	Atoms
35	a	3101	V7A	CAN-CAO-NBF-CBH
35	a	3101	V7A	CAP-CAQ-CBC-OBE
35	a	3101	V7A	CAR-CAQ-CBC-NBD
35	a	3101	V7A	CAR-CAQ-CBC-OBE
35	a	3101	V7A	CAA-CAS-NAT-CAW
35	a	3101	V7A	CAA-CAS-NAT-OAU
35	a	3101	V7A	CAW-NAT-OAU-CAV
35	a	3101	V7A	CAP-CAQ-CBC-NBD

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

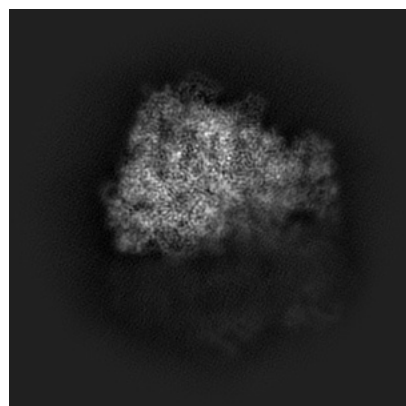
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27009. These allow visual inspection of the internal detail of the map and identification of artifacts.

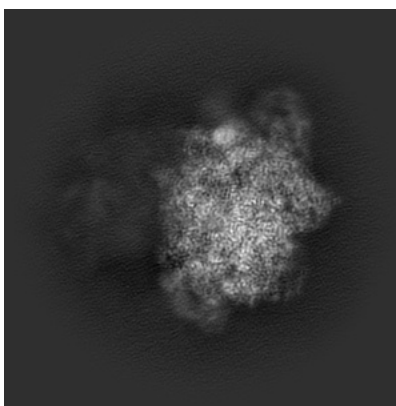
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

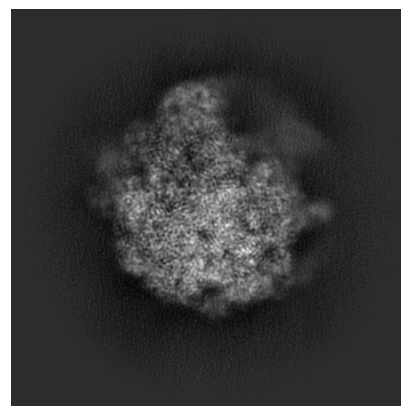
6.1.1 Primary map



X

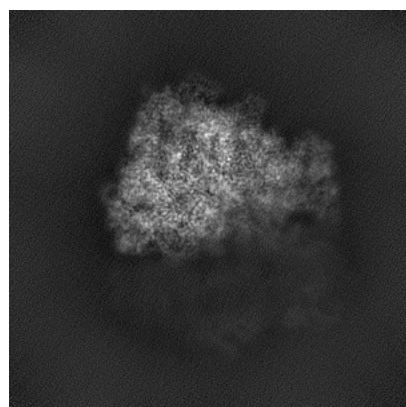


Y

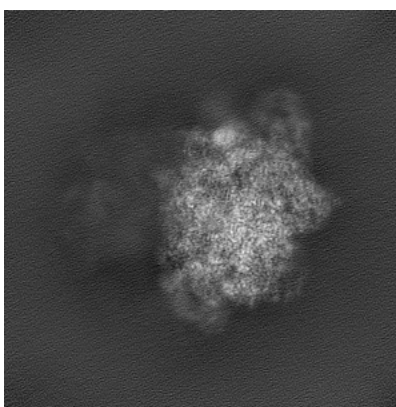


Z

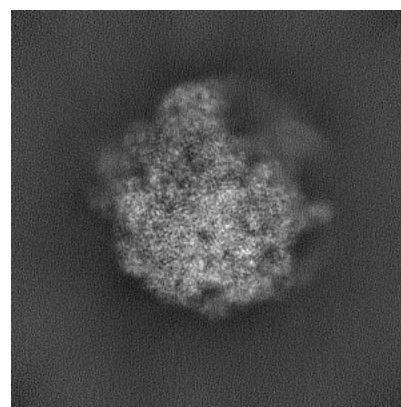
6.1.2 Raw map



X



Y

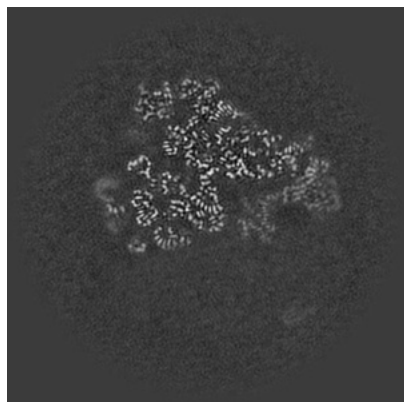


Z

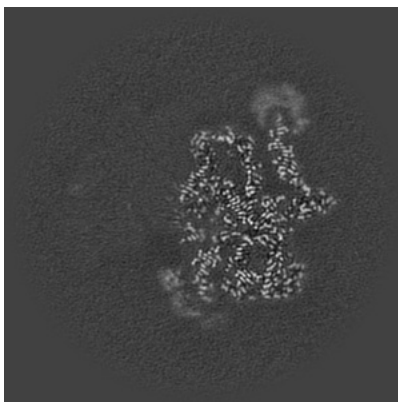
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

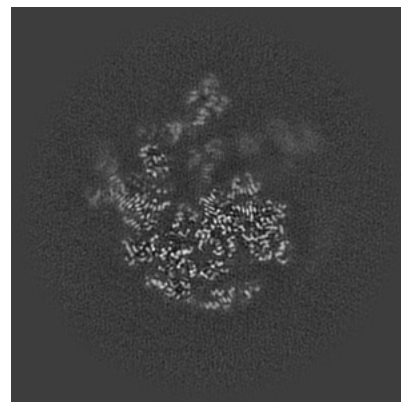
6.2.1 Primary map



X Index: 170

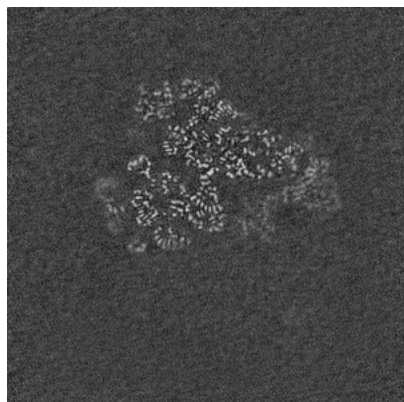


Y Index: 170

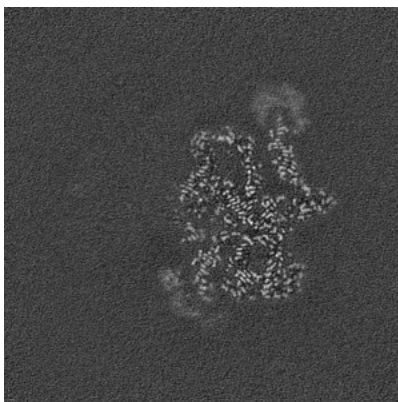


Z Index: 170

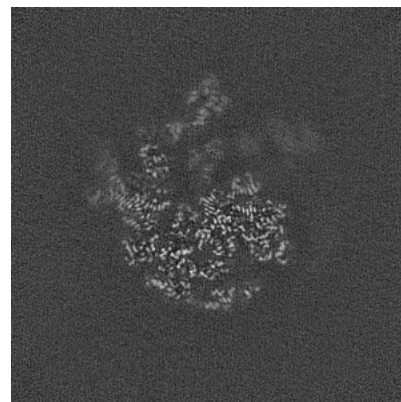
6.2.2 Raw map



X Index: 170



Y Index: 170

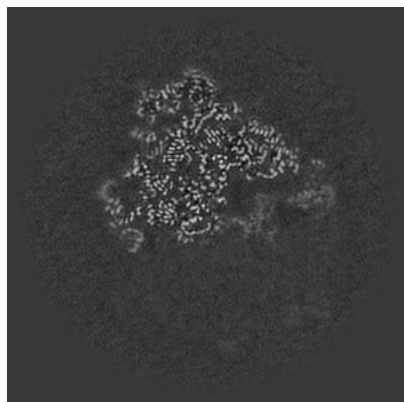


Z Index: 170

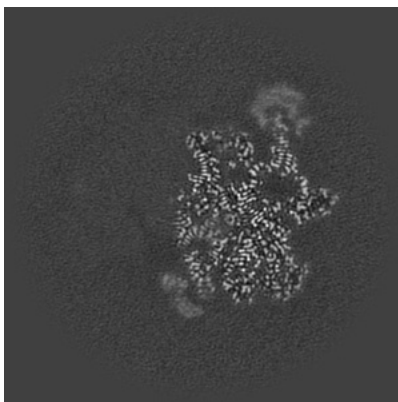
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

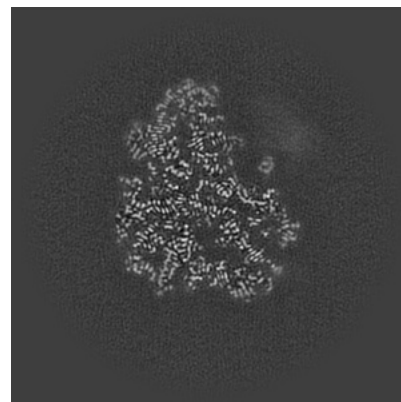
6.3.1 Primary map



X Index: 176

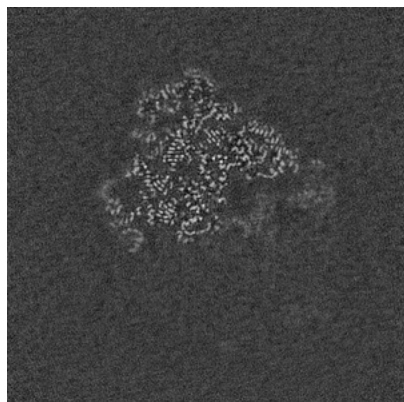


Y Index: 166

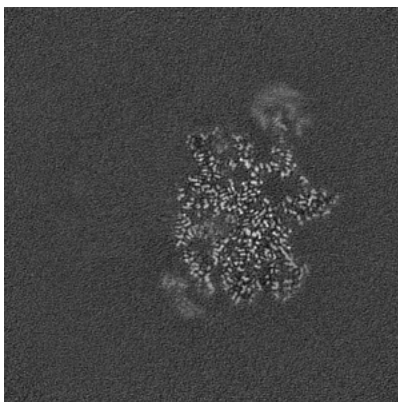


Z Index: 203

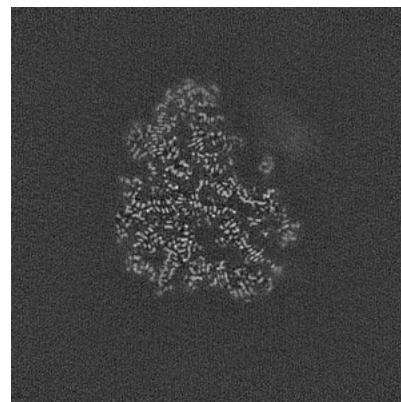
6.3.2 Raw map



X Index: 176



Y Index: 165

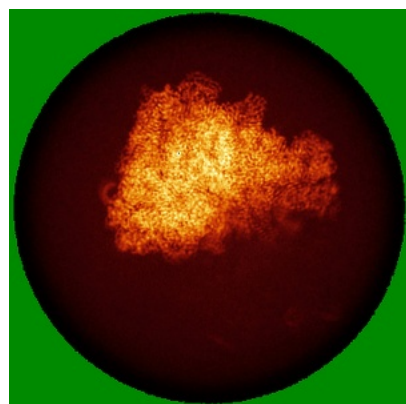


Z Index: 203

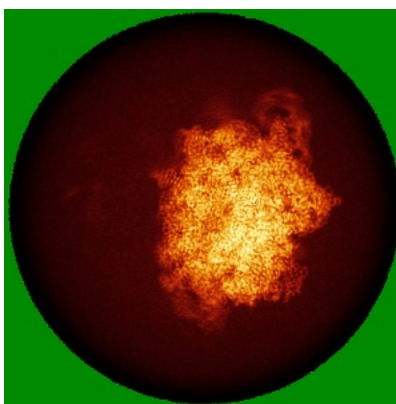
The images above show the largest variance slices of the map in three orthogonal directions.

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

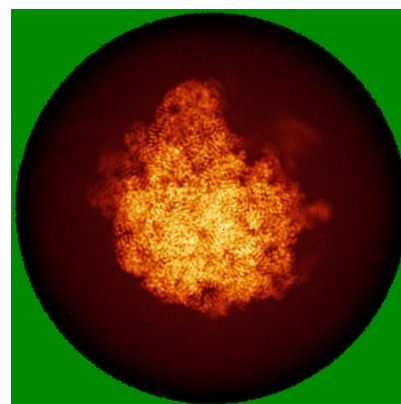
6.4.1 Primary map



X

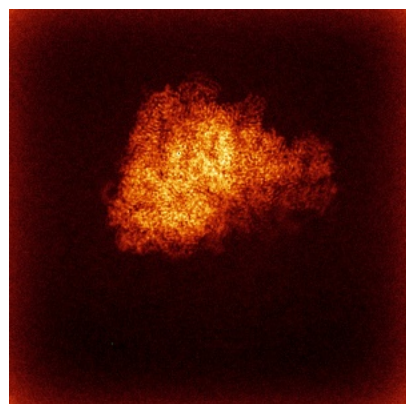


Y

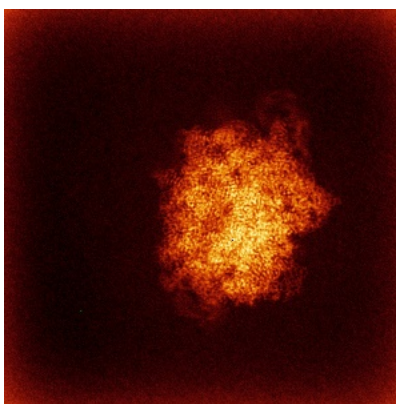


Z

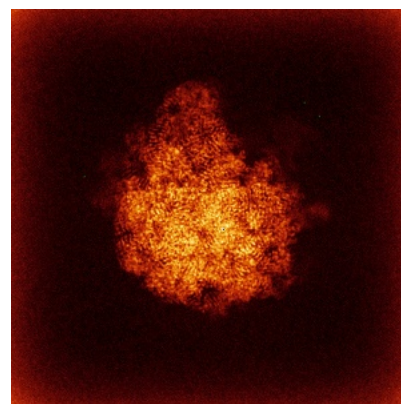
6.4.2 Raw map



X



Y

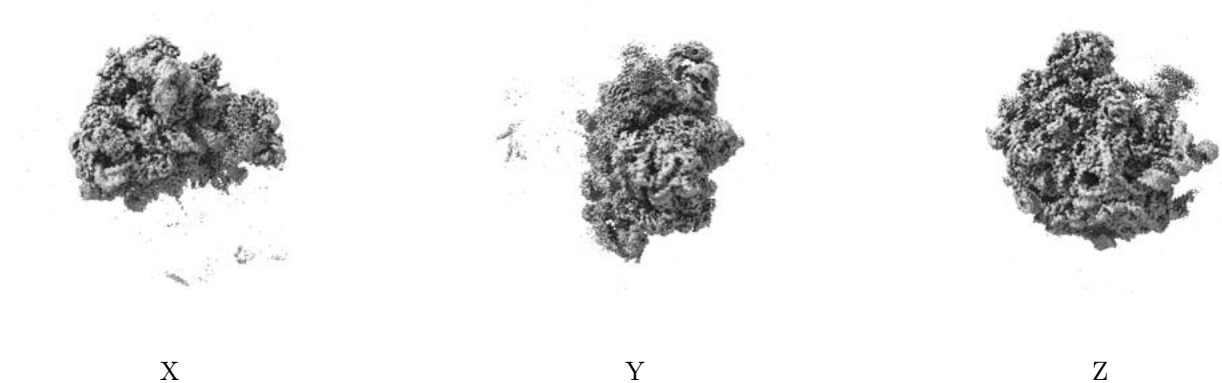


Z

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.

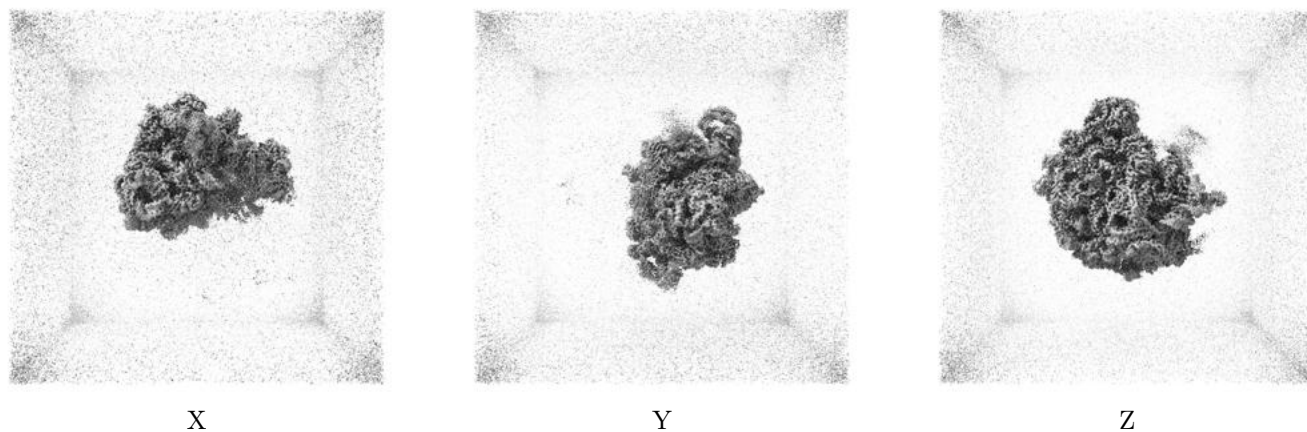
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

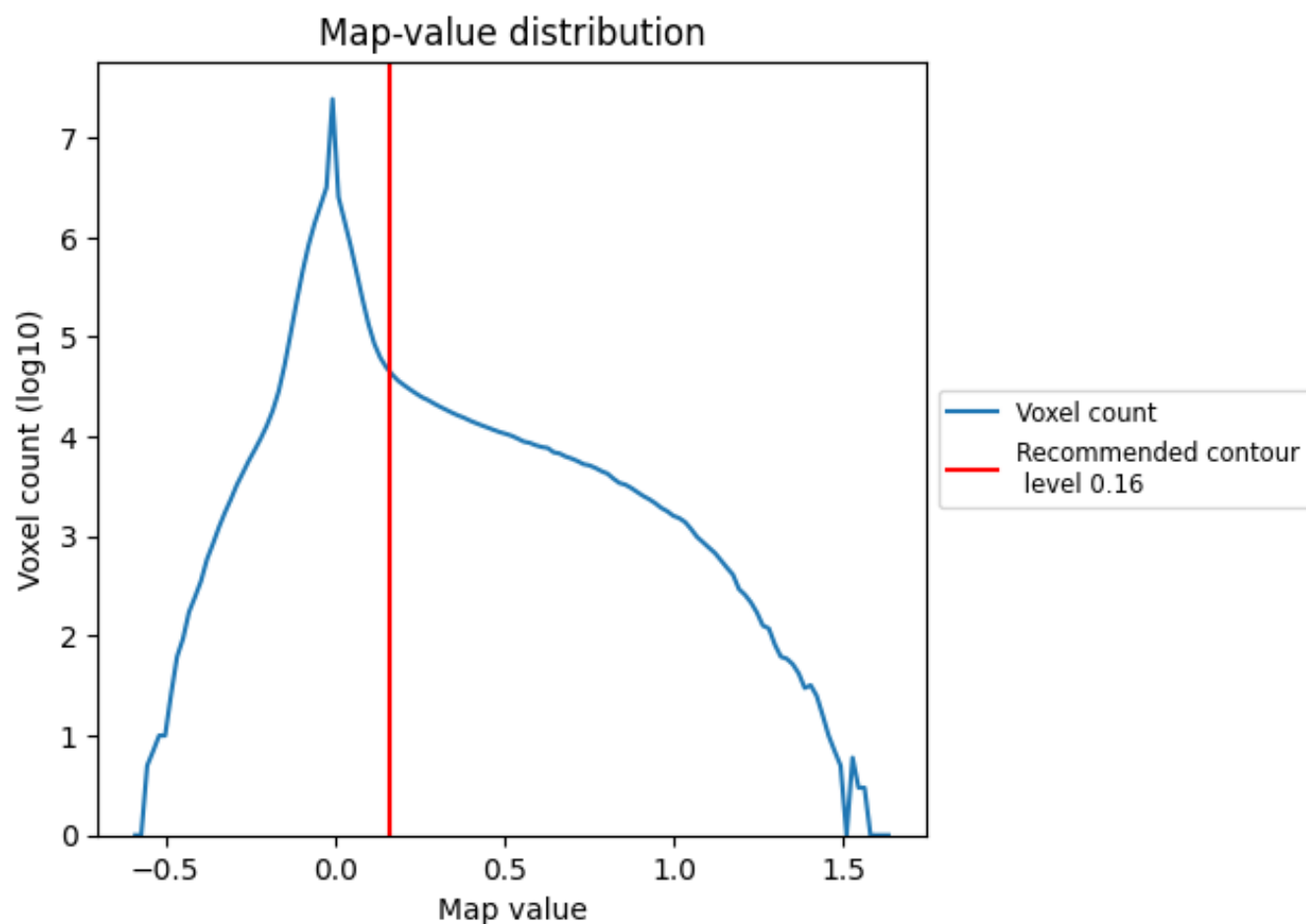
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

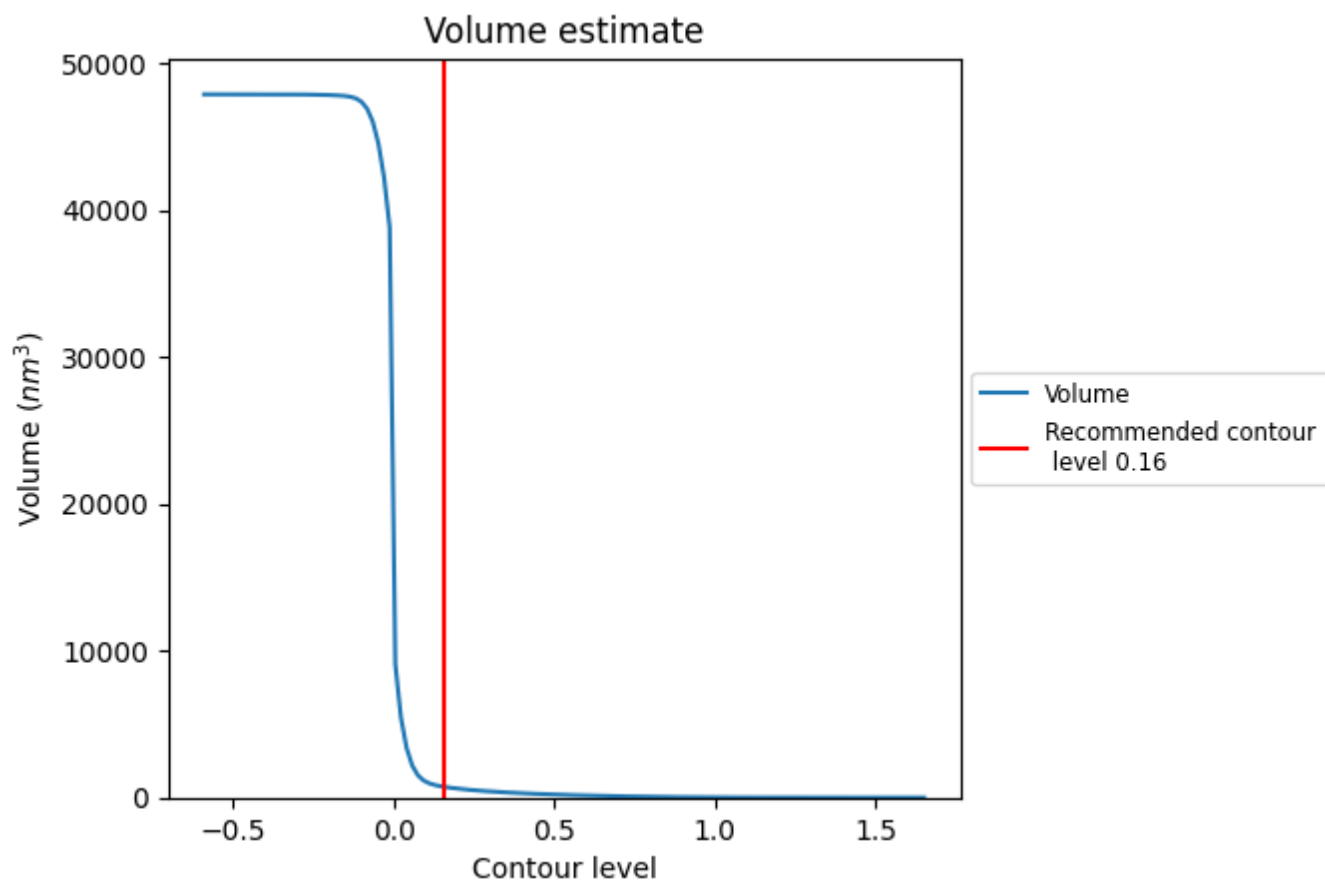
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

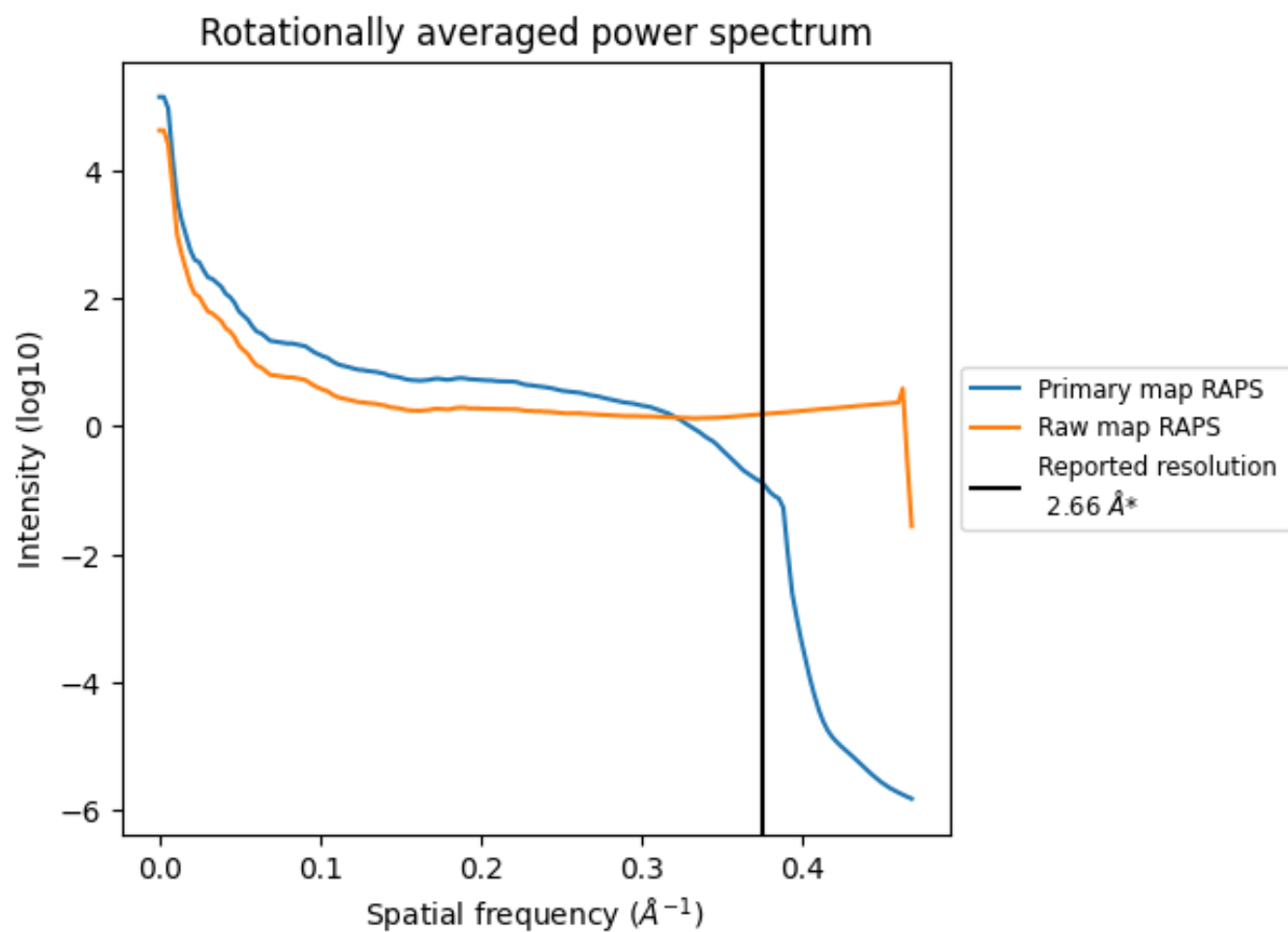
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 722 nm³; this corresponds to an approximate mass of 652 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

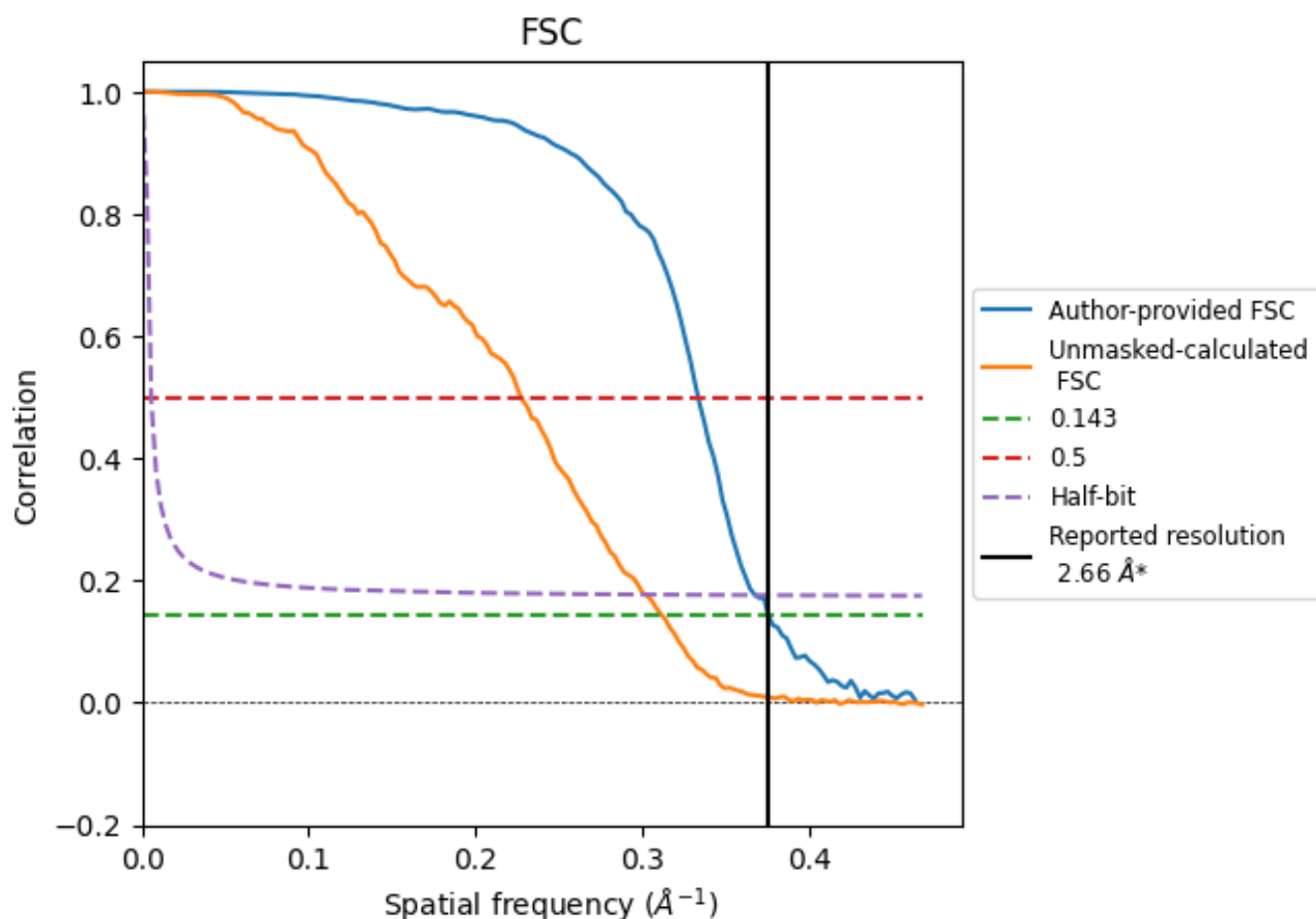


*Reported resolution corresponds to spatial frequency of 0.376 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.376 \AA^{-1}

8.2 Resolution estimates [i](#)

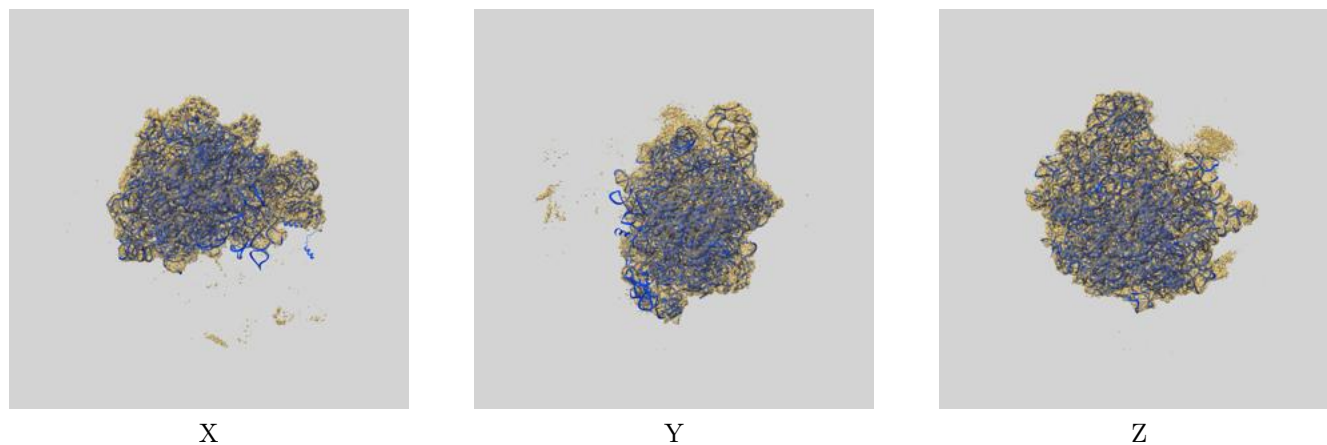
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.66	3.00	2.72
Unmasked-calculated*	3.21	4.40	3.31

*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 3.21 differs from the reported value 2.66 by more than 10 %

9 Map-model fit [i](#)

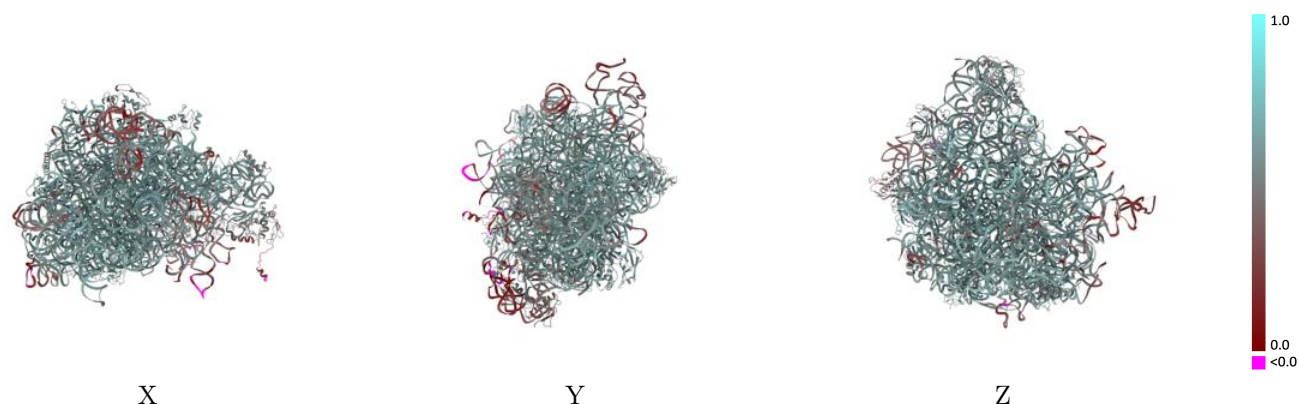
This section contains information regarding the fit between EMDB map EMD-27009 and PDB model 8CVM. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



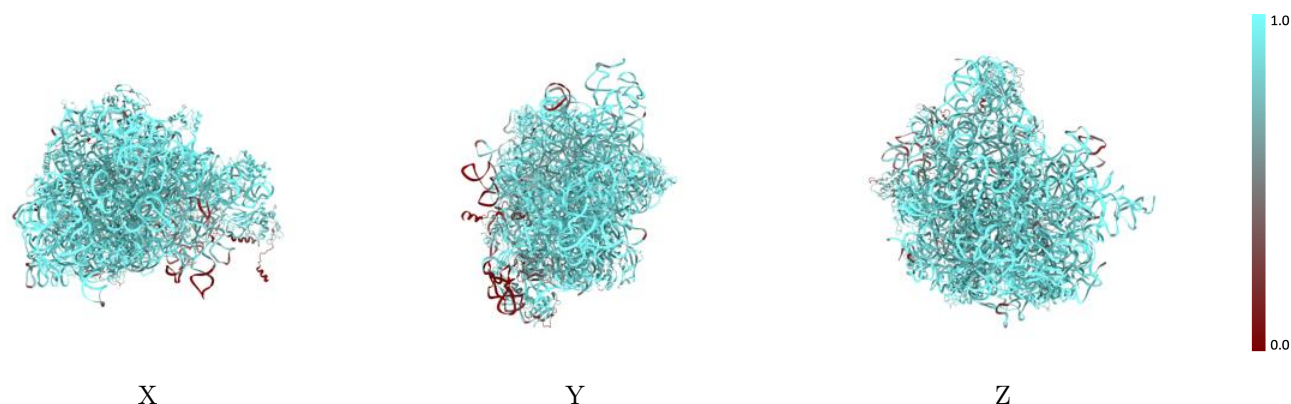
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



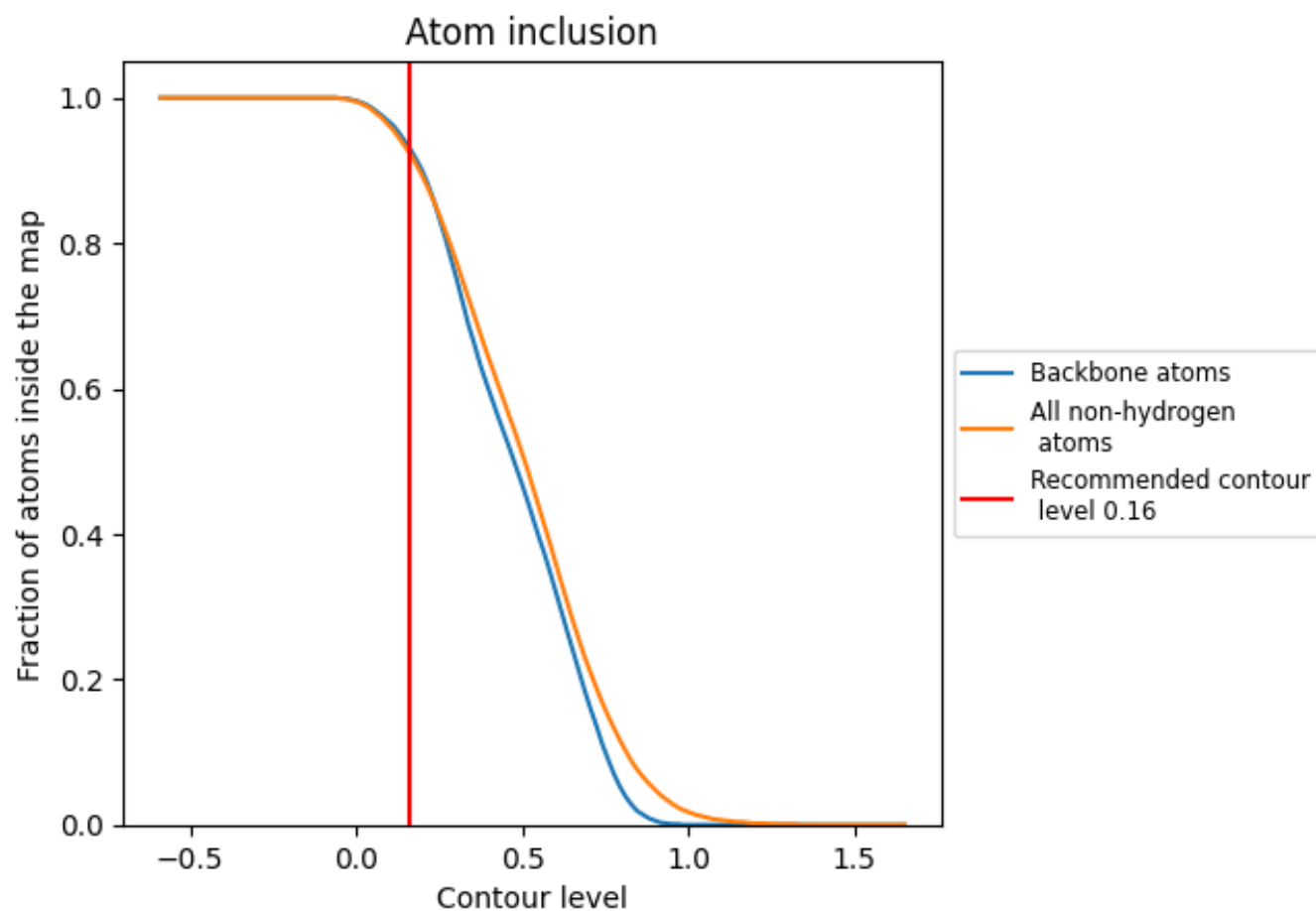
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 92% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.5650
0	 0.8910	 0.5770
1	 0.9670	 0.6300
2	 0.9640	 0.6170
3	 0.4250	 0.5010
4	 0.4580	 0.3200
C	 0.6210	 0.4180
V	 0.9590	 0.6280
a	 0.9460	 0.5700
b	 0.9950	 0.5750
c	 0.9520	 0.6070
d	 0.9540	 0.5990
e	 0.9210	 0.5550
f	 0.7690	 0.4600
g	 0.7380	 0.4150
i	 0.9640	 0.6110
j	 0.8690	 0.5740
k	 0.9390	 0.5800
l	 0.9550	 0.6050
m	 0.9490	 0.5980
n	 0.9190	 0.5450
o	 0.8000	 0.5590
p	 0.9610	 0.6110
q	 0.9170	 0.5840
r	 0.9410	 0.5960
s	 0.9300	 0.5820
t	 0.9380	 0.5690
u	 0.6720	 0.4910
v	 0.9560	 0.6090
w	 0.9780	 0.6210
x	 0.9140	 0.5560
y	 0.9600	 0.5950
z	 0.9480	 0.6040

