



wwPDB EM Validation Summary Report ⓘ

May 7, 2026 – 04:42 PM EDT

PDB ID : 9PJ7 / pdb_00009pj7
EMDB ID : EMD-71682
Title : C. acnes 70S ribosome bound to Doxycycline
Authors : Devarkar, S.C.; Lomakin, I.B.; Bunick, C.G.
Deposited on : 2025-07-12
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

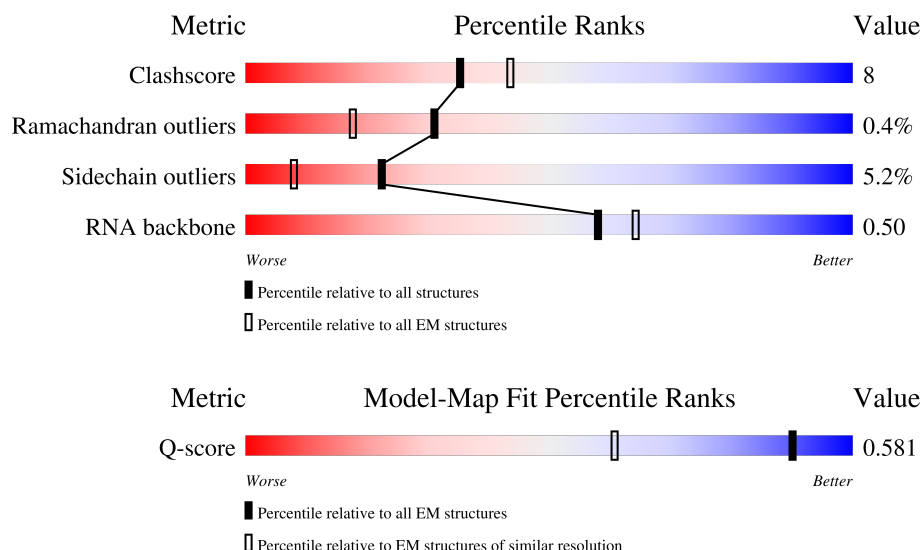
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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.












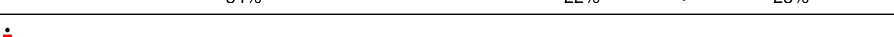
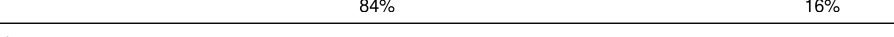

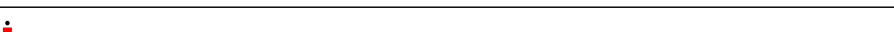



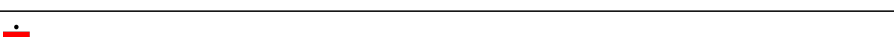

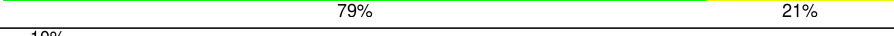






Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	0	56	
2	1	44	
3	2	68	

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Mol	Chain	Length	Quality of chain
4	3	37	
5	4	69	
6	A	1537	
7	B	283	
8	C	76	
9	D	201	
10	E	215	
11	F	96	
12	G	269	
13	H	135	
14	I	156	
15	J	173	
16	K	135	
17	L	123	
18	M	103	
19	N	123	
20	O	87	
21	P	147	
22	Q	90	
23	R	79	
24	S	61	
25	T	88	
26	U	93	
27	V	24	
28	X	33	

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Mol	Chain	Length	Quality of chain
29	Y	22	
30	a	3086	
31	b	120	
32	c	278	
33	d	223	
34	e	301	
35	f	210	
36	g	180	
37	i	147	
38	j	122	
39	k	146	
40	l	139	
41	m	187	
42	n	127	
43	o	117	
44	p	123	
45	q	102	
46	r	153	
47	s	102	
48	t	122	
49	u	205	
50	v	89	
51	w	61	
52	x	77	
53	y	60	

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Mol	Chain	Length	Quality of chain
54	z	63	<div><div></div><div>84%</div><div>11%</div><div></div></div>

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 144663 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 L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	50	Total	C	N	O	S	0	0
			423	253	91	73	6		

- Molecule 2 is a protein called 50S ribosomal protein L34.

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

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	67	Total	C	N	O	S	0	0
			513	315	110	87	1		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	37	Total	C	N	O	S	0	0
			302	184	66	47	5		

- Molecule 5 is a protein called 50S ribosomal protein L31.

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

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1512	Total	C	N	O	P	0	0
			32480	14471	5911	10586	1512		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	233	Total	C	N	O	S	0	0
			1836	1163	326	338	9		

- Molecule 8 is a RNA chain called initiator tRNA Met (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	75	Total	C	N	O	P S	0	0
			1605	716	291	522	75 1		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	200	Total	C	N	O	S	0	0
			1632	1021	313	297	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	179	Total	C	N	O	S	0	0
			1309	816	244	245	4		

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	96	Total	C	N	O	S	0	0
			785	496	134	149	6		

- Molecule 12 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	206	Total	C	N	O	S	0	0
			1613	1010	305	294	4		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	134	Total	C	N	O	S	0	0
			1021	642	182	194	3		

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	155	Total	C	N	O	S	0	0
			1225	764	235	220	6		

- Molecule 15 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	134	Total	C	N	O	S	0	0
			1012	629	204	177	2		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	117	Total	C	N	O	S	0	0
			858	532	168	154	4		

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	122	Total	C	N	O	S	0	0
			948	587	195	164	2		

- Molecule 18 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	98	Total	C	N	O	S	0	0
			786	496	146	141	3		

- Molecule 19 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	122	Total	C	N	O	S	0	0
			976	598	205	173			

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	87	Total	C	N	O	S	0	0
			708	440	140	125	3		

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	128	Total	C	N	O	S	0	0
			994	621	185	187	1		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	90	Total	C	N	O	S	0	0
			728	446	142	134	6		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	67	Total	C	N	O		0	0
			527	334	103	90			

- Molecule 24 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	60	Total	C	N	O	S	0	0
			474	298	98	73	5		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	87	Total	C	N	O		0	0
			673	408	144	121			

- Molecule 26 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	84	Total	C	N	O	S	0	0
			658	416	126	113	3		

- Molecule 27 is a protein called 50S ribosomal protein bL37.

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

- Molecule 28 is a protein called AURKAIP1/COX24 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	32	Total	C	N	O	S	0	0
			277	170	71	35	1		

- Molecule 29 is a RNA chain called mRNA 32MF.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	10	Total	C	N	O	P	0	0
			211	95	35	71	10		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2903	Total	C	N	O	P	0	0
			62408	27795	11386	20324	2903		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	63	A	G	conflict	GB CP012350
a	524	C	G	conflict	GB CP012350
a	1038	PSU	G	conflict	GB CP012350

- Molecule 31 is a RNA chain called 5S rRNA.

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

- Molecule 32 is a protein called 50S ribosomal protein L2.

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

- Molecule 33 is a protein called 50S ribosomal protein L3.

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

- Molecule 34 is a protein called 50S ribosomal protein L4.

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

- Molecule 35 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	184	Total	C	N	O	S	0	0
			1468	924	269	266	9		

- Molecule 36 is a protein called 50S ribosomal protein L6.

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

- Molecule 37 is a protein called 50S ribosomal protein L13.

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

- Molecule 38 is a protein called 50S ribosomal protein L14.

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

- Molecule 39 is a protein called 50S ribosomal protein L15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

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

- Molecule 41 is a protein called Large ribosomal subunit protein bL17.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	124	ALA	THR	conflict	UNP A0A8B2VJI7
m	185	PRO	SER	conflict	UNP A0A8B2VJI7

- Molecule 42 is a protein called 50S ribosomal protein L18.

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

- Molecule 43 is a protein called 50S ribosomal protein L19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called Large ribosomal subunit protein bL21.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	52	ALA	VAL	conflict	UNP Q6A9I3

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

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

- Molecule 48 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 49 is a protein called 50S ribosomal protein L25.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called 50S ribosomal protein L29.

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

- Molecule 53 is a protein called 50S ribosomal protein L30.

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

- Molecule 54 is a protein called 50S ribosomal protein L32.

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

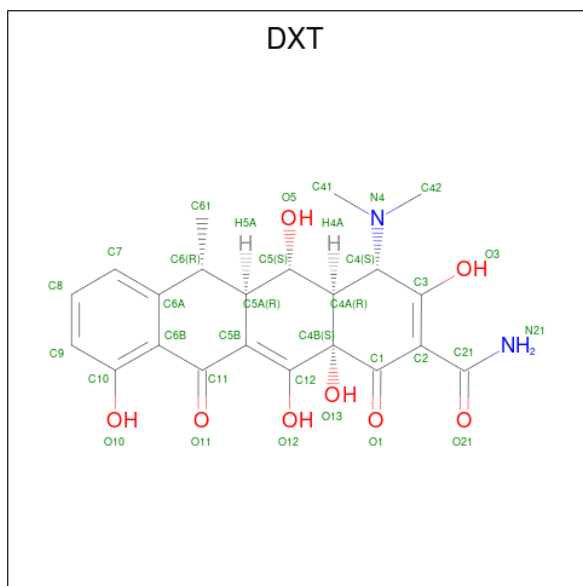
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	0	1	Total	Zn	0
			1	1	
55	3	1	Total	Zn	0
			1	1	
55	4	1	Total	Zn	0
			1	1	
55	S	1	Total	Zn	0
			1	1	
55	w	1	Total	Zn	0
			1	1	
55	z	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

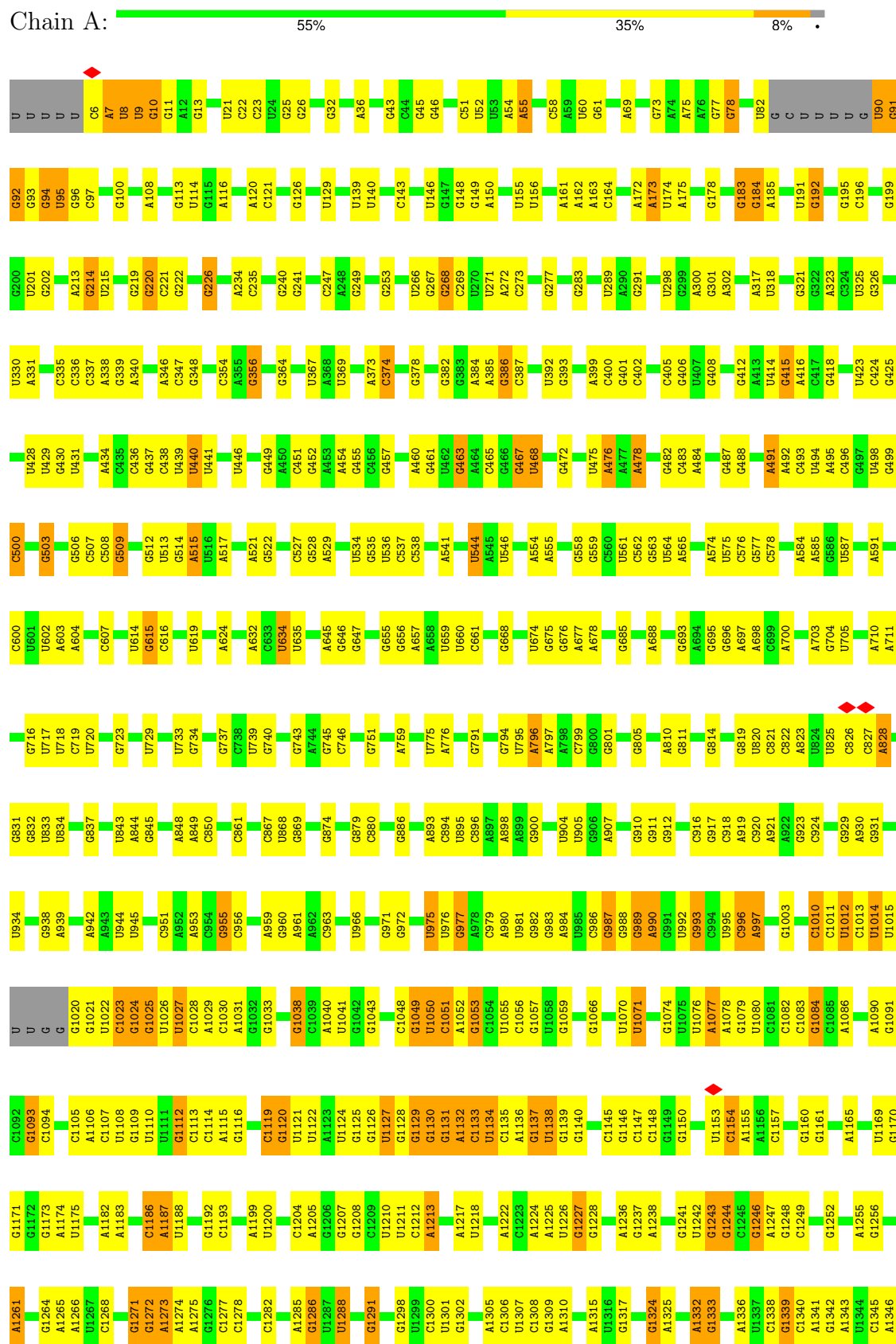
Mol	Chain	Residues	Atoms		AltConf
56	A	51	Total	Mg	0
			51	51	
56	a	230	Total	Mg	0
			230	230	
56	b	2	Total	Mg	0
			2	2	
56	c	1	Total	Mg	0
			1	1	
56	d	1	Total	Mg	0
			1	1	
56	k	1	Total	Mg	0
			1	1	
56	o	1	Total	Mg	0
			1	1	

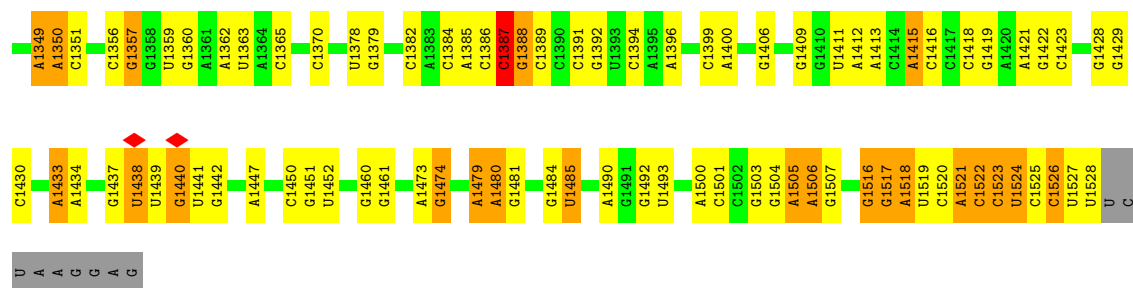
- Molecule 57 is (4S,4AR,5S,5AR,6R,12AS)-4-(DIMETHYLAMINO)-3,5,10,12,12A-PENTAHYDROXY-6-METHYL-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: DXT) (formula: $C_{22}H_{24}N_2O_8$) (labeled as "Ligand of Interest" by depositor).



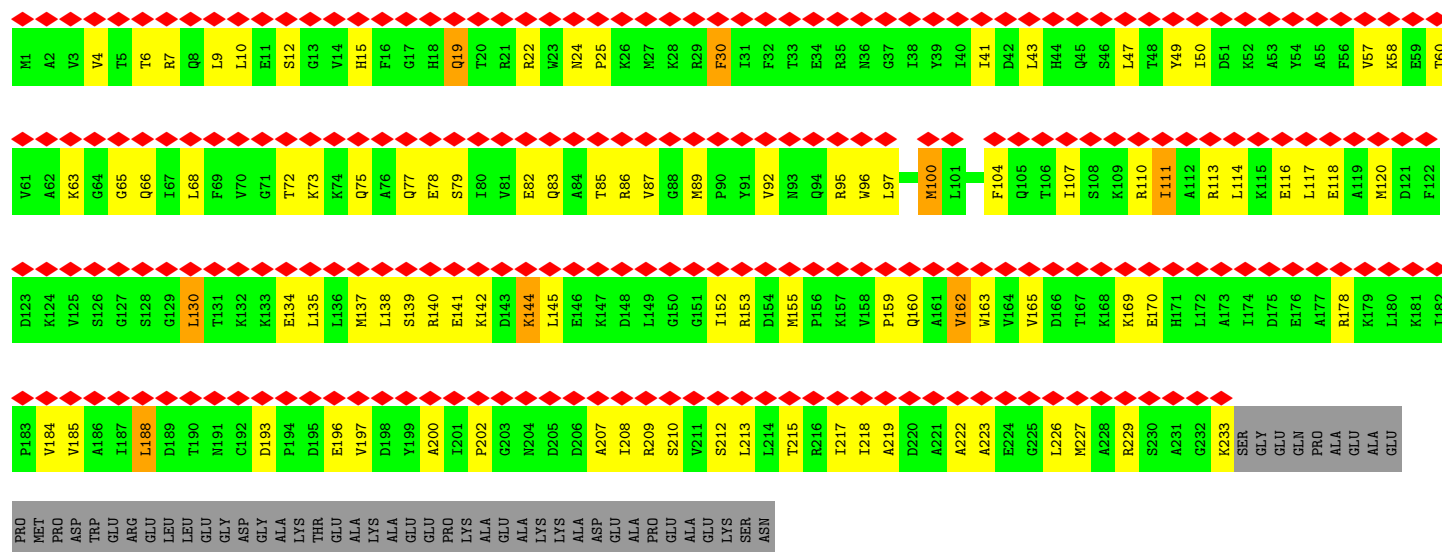
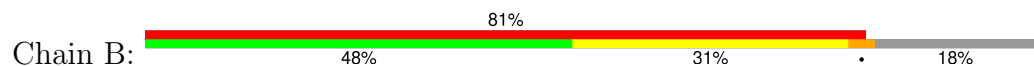
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Mol	Chain	Residues	Atoms		AltConf
58	S	1	Total 1	O 1	0
58	a	115	Total 115	O 115	0
58	b	1	Total 1	O 1	0
58	c	1	Total 1	O 1	0
58	d	1	Total 1	O 1	0
58	s	1	Total 1	O 1	0

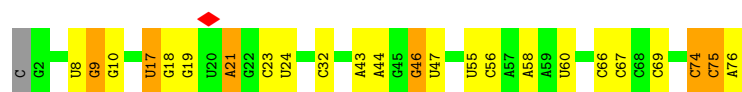




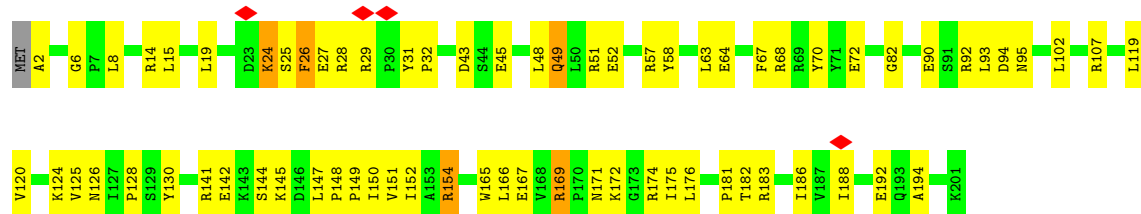
• Molecule 7: 30S ribosomal protein S2



• Molecule 8: initiator tRNA Met (76-MER)

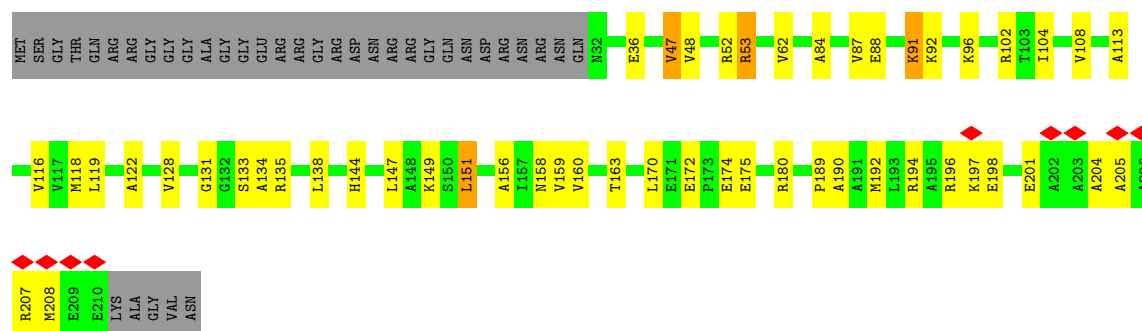


• Molecule 9: 30S ribosomal protein S4



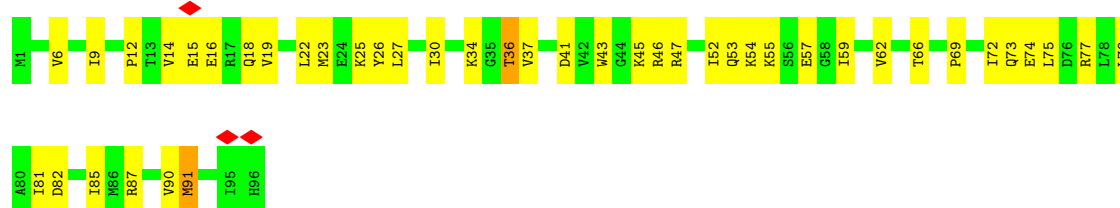
• Molecule 10: Small ribosomal subunit protein uS5

Chain E: 



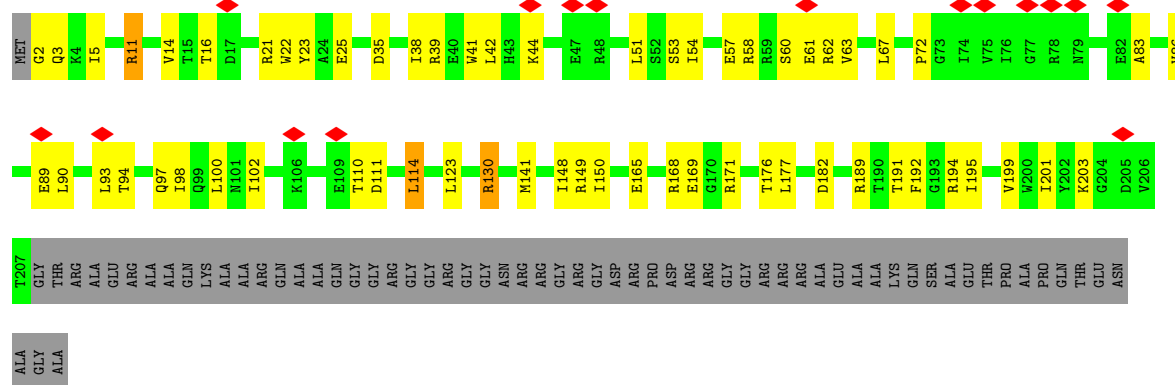
- Molecule 11: 30S ribosomal protein S6

Chain F: 




- Molecule 12: 30S ribosomal protein S3

Chain G: 

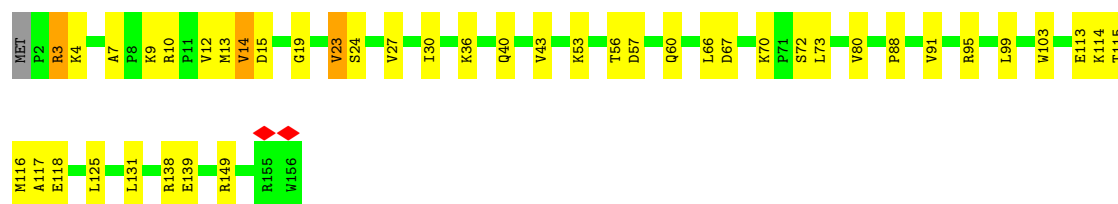


- Molecule 13: 30S ribosomal protein S8

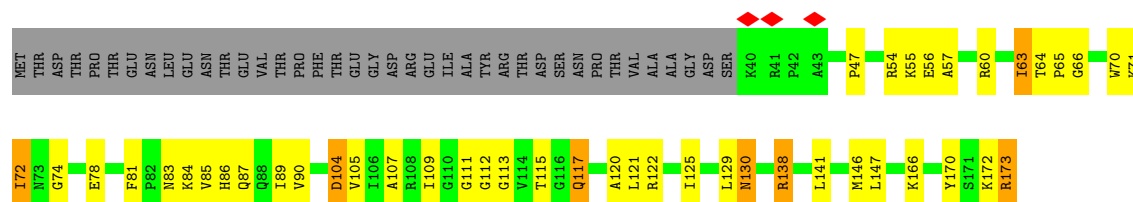
Chain H: 



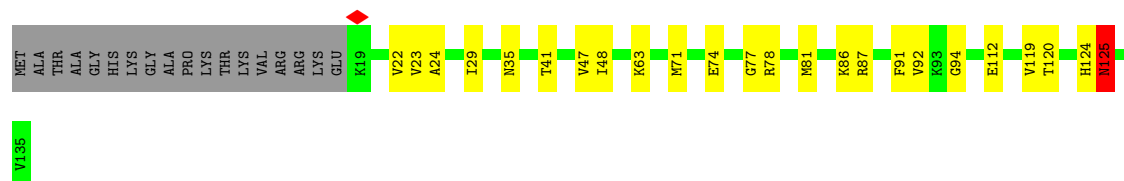
- Molecule 14: 30S ribosomal protein S7



- Molecule 15: 30S ribosomal protein S9



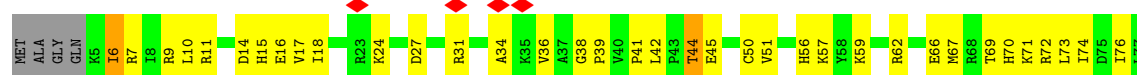
- Molecule 16: 30S ribosomal protein S11

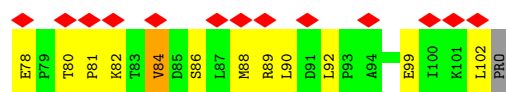


- Molecule 17: 30S ribosomal protein S12



- Molecule 18: Small ribosomal subunit protein uS10





- Molecule 19: 30S ribosomal protein S13

Chain N: 70% 28%



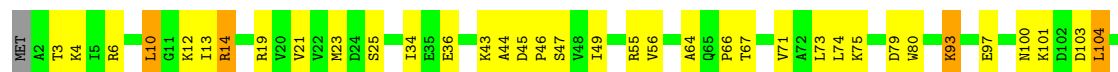
- Molecule 20: 30S ribosomal protein S15

Chain O: 79% 21%



- Molecule 21: 30S ribosomal protein S16

Chain P: 10% 54% 30% 13%



- Molecule 22: 30S ribosomal protein S17

Chain Q: 8% 79% 20%



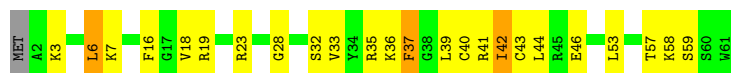
- Molecule 23: 30S ribosomal protein S18

Chain R: 8% 59% 24% 15%



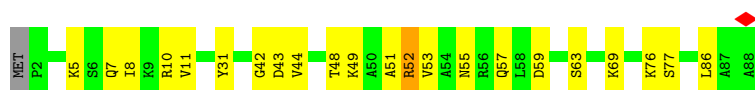
- Molecule 24: 30S ribosomal protein S14 type Z

Chain S:  59% 34% 5% .



- Molecule 25: 30S ribosomal protein S20

Chain T:  74% 24% ..




- Molecule 26: 30S ribosomal protein S19

Chain U:  58% 30% . 10%




- Molecule 27: 50S ribosomal protein bL37

Chain V:  83% 12% .




- Molecule 28: AURKAIP1/COX24 domain-containing protein

Chain X:  76% 18% . .



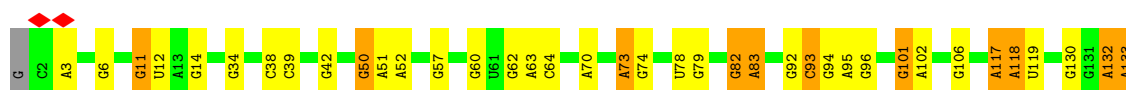
- Molecule 29: mRNA 32MF

Chain Y:  9% 9% 23% 14% 55%



- Molecule 30: 23S rRNA

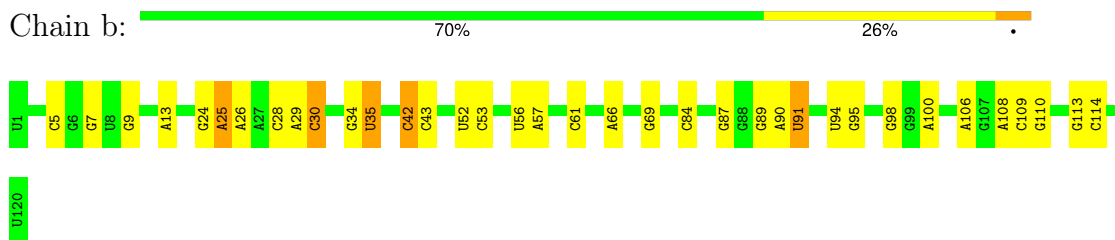
Chain a:  59% 29% 6% 6%



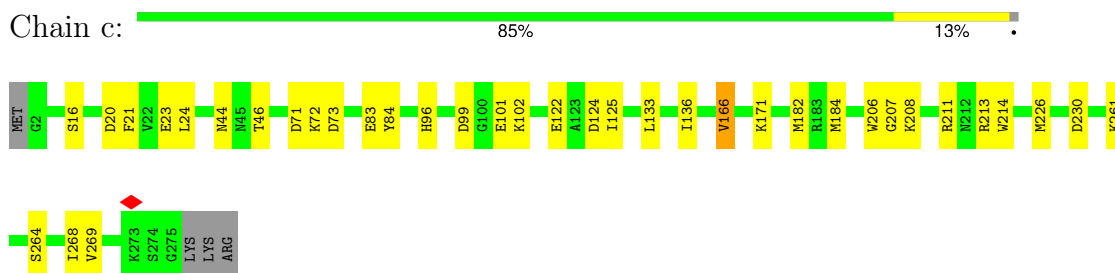


A3053	A3054	U3055	A3063	U3064	A3065	G3066	A3071	G3072	G3073	A3074	C3075	U3076	U3077	U3078	C3079	A3080	U	U	A	A	C	A
A2923	C2924	C2925	G2926	G2929	A2930	G2933	C2934	C2935	U2936	C2937	A2947	A2948	A2949	U2950	A2960	U2961	A2962	C2971	A2972	C2973	A2977	G2978
G2774	A2784	G2785	U2786	U2787	U2791	C2792	C2793	C2794	U2795	G2807	C2808	A2811	G2812	U2816	U2819	G2820	A2821	G2827	C2828	U2829	G2830	U2831
C2865	U2873	C2880	C2881	G2884	A2885	U2886	C2887	U2888	G2895	U2896	A2700	G2706	U2710	G2711	G2712	A2713	G2714	U2715	G2716	U2717	U2718	U2719
G2554	G2555	C2556	A2557	G2571	U2572	C2573	A2579	C2580	U2583	G2584	U2588	C2589	G2592	C2598	C2606	A2607	G2610	A2611	A2612	U2613	A2617	C2623
A2455	A2456	G2461	C2465	C2466	C2467	A2469	U2473	U2474	C2475	U2484	U2487	G2490	G2500	G2501	G2502	A2504	G2507	U2508	A2509	A2510	G2511	U2512
G	A	A	A	U	U	C	C	C	C	U2360	C2361	U2362	G2363	A2364	U2365	U2366	G2367	U2368	U2369	C2370	U2371	G2384
U2290	U2291	G	U	G	U	U	A	G	G	G	U	U	G	U	U	U	U	U	U	U	U	U
G2193	A2197	A2198	U2199	U2200	G2201	C2202	U2203	U2204	U2205	U2206	C2207	G2208	A2209	G2210	A2213	A2214	G2215	A2216	U2220	C2221	G2222	C2226
U2065	G2066	A2067	C2068	C2069	A2072	A2073	A2084	C2085	G2089	U2094	A2095	C2097	C2098	G2112	G2113	U2114	A2115	G2116	G2122	G2123	A2120	A2121
G1933	G1939	G1947	A1956	A1965	C1973	A1974	G1983	A1985	A1986	A1992	A1993	G1994	A1995	C1996	U1999	A2008	C2009	A2012	G2018	G2025	C2026	A2031
A1787	U1791	A1792	G1797	U1818	A1830	U1831	C1832	G1835	U1836	G1837	A1838	G1851	A1852	A1853	G1858	A1859	A1860	A1861	A1862	A1863	C1866	C1867
C1686	G1687	U1688	A1689	A1691	C1593	A1594	A1595	G1596	U1694	G1695	G1697	A1698	G1706	G1707	G1708	G1709	A1710	G1711	C1712	G1713	G1714	A1715
U	A	G	G	C1593	A1594	A1595	G1596	G1601	A1607	C1608	G1609	U1613	U1618	A1619	G1620	G1623	A1624	U1625	C1626	C1627	C1628	C1629
G	U	A	G	C1593	A1594	A1595	G1596	G1601	A1607	C1608	G1609	U1613	U1618	A1619	G1620	G1623	A1624	U1625	C1626	C1627	C1628	C1629

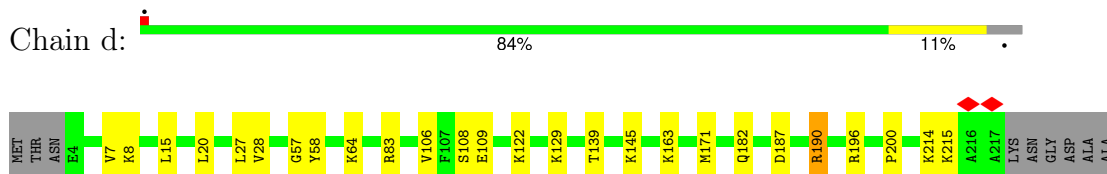
- Molecule 31: 5S rRNA



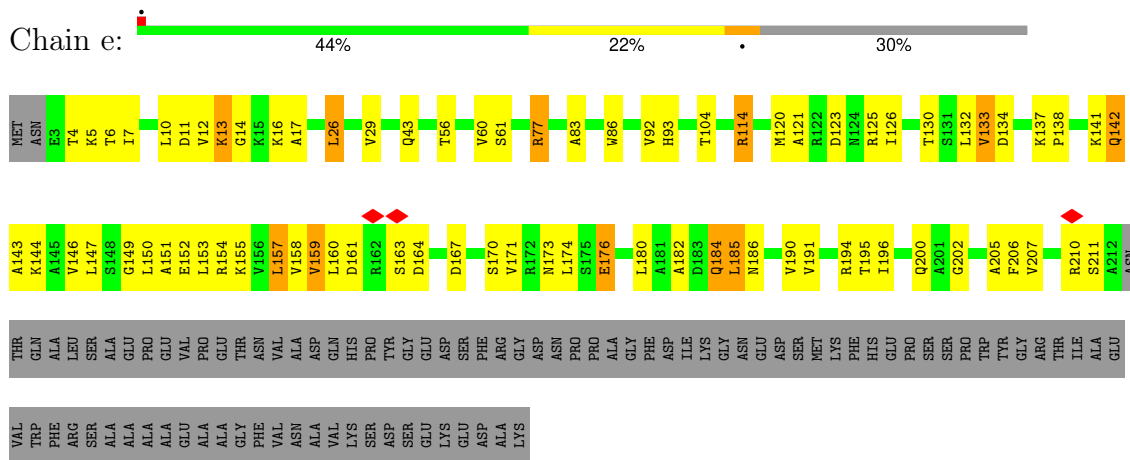
- Molecule 32: 50S ribosomal protein L2



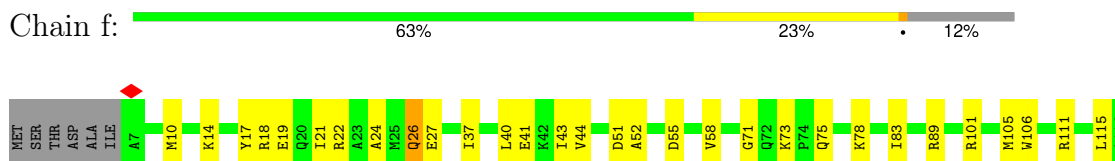
- Molecule 33: 50S ribosomal protein L3

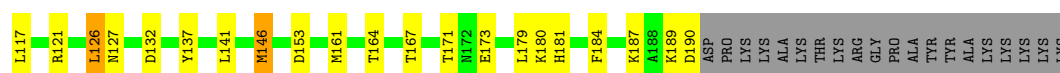


- Molecule 34: 50S ribosomal protein L4

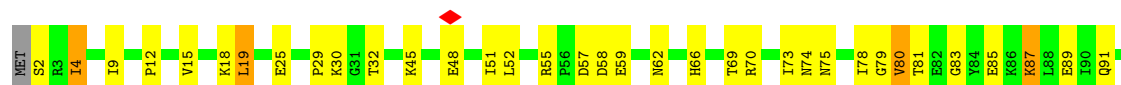


- Molecule 35: 50S ribosomal protein L5

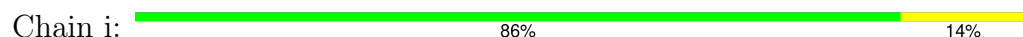




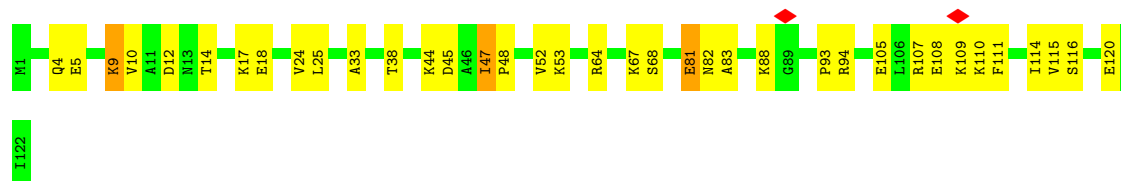
- Molecule 36: 50S ribosomal protein L6



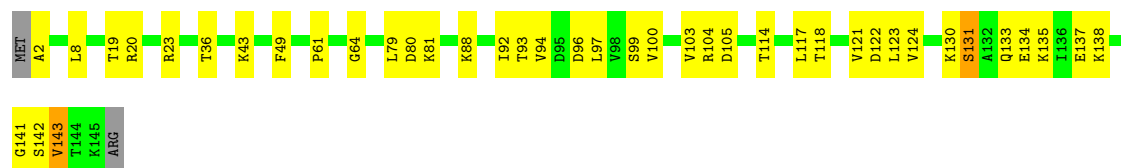
- Molecule 37: 50S ribosomal protein L13



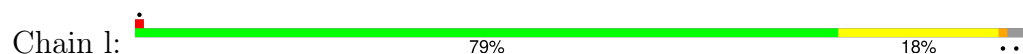
- Molecule 38: 50S ribosomal protein L14



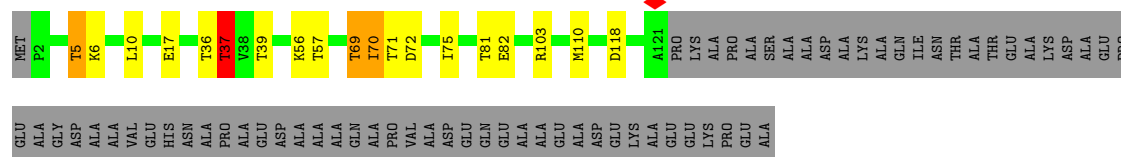
- Molecule 39: 50S ribosomal protein L15



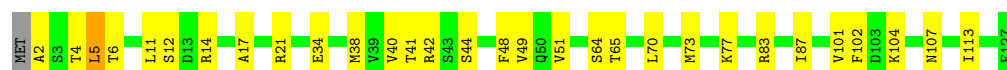
- Molecule 40: 50S ribosomal protein L16



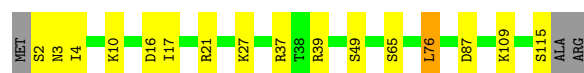
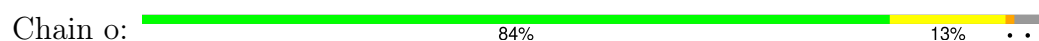
- Molecule 41: Large ribosomal subunit protein bL17



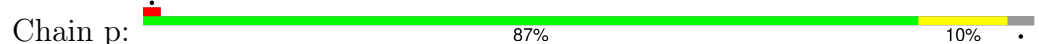
- Molecule 42: 50S ribosomal protein L18



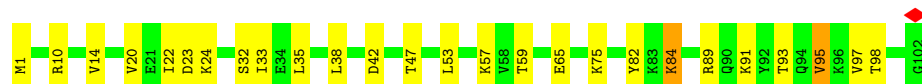
- Molecule 43: 50S ribosomal protein L19



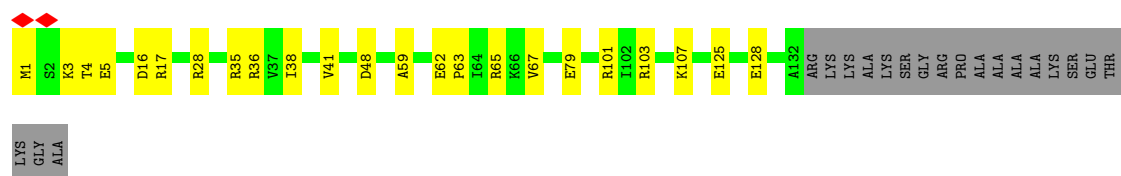
- Molecule 44: 50S ribosomal protein L20



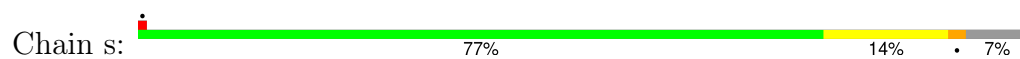
- Molecule 45: Large ribosomal subunit protein bL21



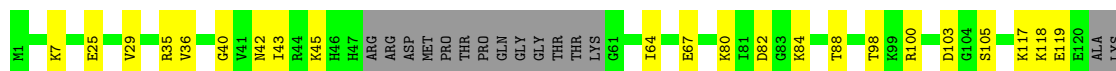
- Molecule 46: 50S ribosomal protein L22



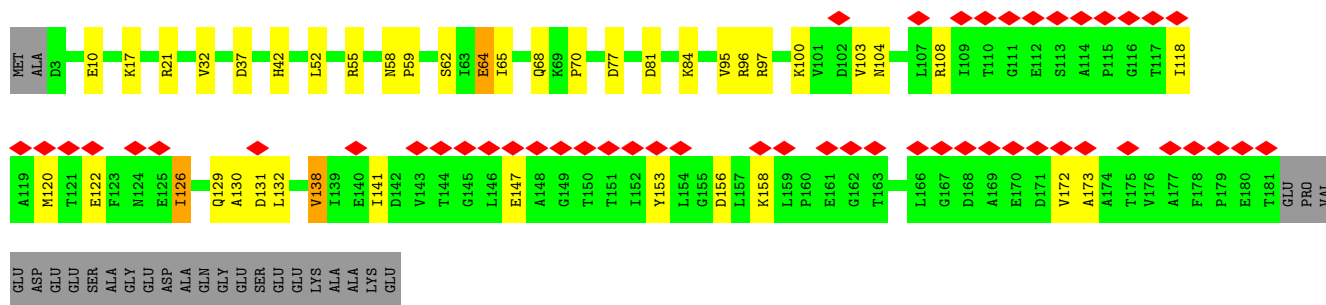
- Molecule 47: 50S ribosomal protein L23



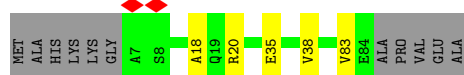
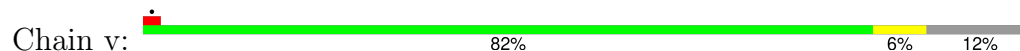
- Molecule 48: Large ribosomal subunit protein uL24



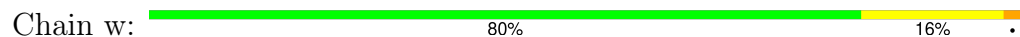
- Molecule 49: 50S ribosomal protein L25



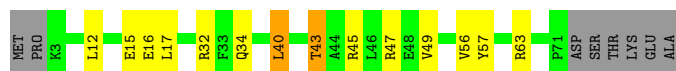
- Molecule 50: 50S ribosomal protein L27



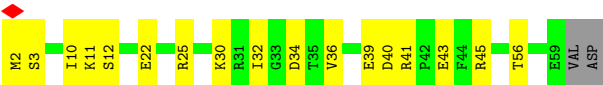
- Molecule 51: 50S ribosomal protein L28



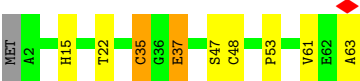
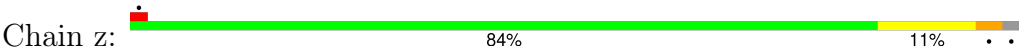
- Molecule 52: 50S ribosomal protein L29



- Molecule 53: 50S ribosomal protein L30



• Molecule 54: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103369	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.757	Depositor
Minimum map value	-0.231	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, MG, MA6, 5MU, 5MC, H2U, 4SU, 3TD, UR3, 2MA, PSU, 4OC, ZN, 2MG, OMC, G7M, OMU, DXT

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	0	0.27	0/429	0.40	0/569
2	1	0.28	0/365	0.36	0/478
3	2	0.29	0/519	0.38	0/682
4	3	0.29	0/305	0.39	0/401
5	4	0.69	0/521	0.93	0/700
6	A	0.37	0/36052	0.47	0/56250
7	B	0.17	0/1864	0.48	0/2509
8	C	0.34	0/1703	0.42	0/2655
9	D	0.26	0/1662	0.47	0/2239
10	E	0.22	0/1325	0.46	0/1789
11	F	0.24	0/794	0.50	0/1069
12	G	0.19	0/1638	0.45	0/2201
13	H	0.21	0/1036	0.38	0/1395
14	I	0.23	0/1246	0.45	0/1679
15	J	0.36	0/1027	0.58	0/1376
16	K	0.34	0/874	0.56	0/1177
17	L	0.23	0/960	0.39	0/1283
18	M	0.19	0/800	0.43	0/1080
19	N	0.21	0/985	0.43	0/1317
20	O	0.23	0/718	0.43	0/959
21	P	0.36	0/1013	0.53	0/1370
22	Q	0.27	0/734	0.47	0/978
23	R	0.20	0/532	0.42	0/713
24	S	0.34	0/484	0.46	0/644
25	T	0.23	0/676	0.30	0/897
26	U	0.19	0/675	0.50	0/908
27	V	0.30	0/184	0.46	0/236
28	X	0.22	0/277	0.39	0/355
29	Y	0.22	0/235	0.29	0/363
30	a	0.39	1/69445 (0.0%)	0.48	2/108364 (0.0%)
31	b	0.32	0/2871	0.37	0/4475

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.30	0/2132	0.44	0/2871
33	d	0.29	0/1611	0.42	0/2172
34	e	0.36	0/1600	0.60	0/2165
35	f	0.25	0/1493	0.41	0/2001
36	g	0.21	0/1398	0.41	0/1884
37	i	0.28	0/1164	0.40	0/1574
38	j	0.29	0/957	0.46	0/1282
39	k	0.28	0/1090	0.57	0/1465
40	l	0.29	0/1108	0.42	0/1488
41	m	0.29	0/949	0.43	0/1277
42	n	0.39	0/959	0.57	0/1281
43	o	0.26	0/909	0.37	0/1216
44	p	0.42	0/969	0.63	0/1292
45	q	0.37	0/785	0.50	0/1050
46	r	0.35	0/1028	0.49	0/1379
47	s	0.29	0/759	0.47	0/1022
48	t	0.21	0/840	0.37	0/1123
49	u	0.19	0/1396	0.41	0/1896
50	v	0.28	0/598	0.39	0/800
51	w	0.89	0/483	1.22	0/648
52	x	0.22	0/567	0.38	0/759
53	y	0.37	0/471	0.52	0/627
54	z	0.31	0/487	0.40	0/654
All	All	0.36	1/155702 (0.0%)	0.47	2/233037 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	D	0	1
14	I	0	1
22	Q	0	1
44	p	0	2
51	w	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2734	OMU	O3'-P	5.28	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	272	A	C1'-O4'-C4'	-5.36	104.54	109.90
30	a	271	G	C4'-C3'-C2'	-5.09	97.50	102.60

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	D	154	ARG	Sidechain
14	I	3	ARG	Sidechain
22	Q	8	ARG	Sidechain
44	p	14	ARG	Sidechain
44	p	92	ARG	Sidechain

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	0	423	0	429	8	0
2	1	362	0	388	7	0
3	2	513	0	565	7	0
4	3	302	0	330	7	0
5	4	512	0	498	17	0
6	A	32480	0	16339	377	0
7	B	1836	0	1902	69	0
8	C	1605	0	818	10	0
9	D	1632	0	1663	60	0
10	E	1309	0	1349	36	0
11	F	785	0	818	36	0
12	G	1613	0	1626	43	0
13	H	1021	0	1059	11	0
14	I	1225	0	1275	32	0
15	J	1012	0	1069	45	0
16	K	858	0	884	17	0
17	L	948	0	1031	20	0
18	M	786	0	823	36	0
19	N	976	0	1031	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	O	708	0	737	10	0
21	P	994	0	1008	36	0
22	Q	728	0	772	15	0
23	R	527	0	580	17	0
24	S	474	0	499	21	0
25	T	673	0	726	13	0
26	U	658	0	671	23	0
27	V	183	0	202	2	0
28	X	277	0	338	5	0
29	Y	211	0	106	7	0
30	a	62408	0	31296	593	0
31	b	2567	0	1297	21	0
32	c	2091	0	2150	22	0
33	d	1586	0	1634	16	0
34	e	1577	0	1619	68	0
35	f	1468	0	1487	36	0
36	g	1376	0	1421	41	0
37	i	1139	0	1163	14	0
38	j	946	0	1011	26	0
39	k	1072	0	1106	25	0
40	l	1082	0	1117	18	0
41	m	936	0	997	13	0
42	n	952	0	995	17	0
43	o	896	0	928	8	0
44	p	958	0	986	7	0
45	q	778	0	824	15	0
46	r	1017	0	1070	13	0
47	s	751	0	803	10	0
48	t	833	0	883	13	0
49	u	1376	0	1397	29	0
50	v	591	0	581	3	0
51	w	474	0	488	4	0
52	x	564	0	582	9	0
53	y	467	0	504	11	0
54	z	477	0	479	7	0
55	0	1	0	0	0	0
55	3	1	0	0	0	0
55	4	1	0	0	0	0
55	S	1	0	0	0	0
55	w	1	0	0	0	0
55	z	1	0	0	0	0
56	A	51	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	a	230	0	0	0	0
56	b	2	0	0	0	0
56	c	1	0	0	0	0
56	d	1	0	0	0	0
56	k	1	0	0	0	0
56	o	1	0	0	0	0
57	A	32	0	22	1	0
57	a	128	0	88	4	0
57	r	32	0	22	1	0
57	s	32	0	22	0	0
58	A	12	0	0	0	0
58	C	1	0	0	0	0
58	S	1	0	0	0	0
58	a	115	0	0	0	0
58	b	1	0	0	0	0
58	c	1	0	0	0	0
58	d	1	0	0	0	0
58	s	1	0	0	0	0
All	All	144663	0	96508	1858	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.

The worst 5 of 1858 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)
30:a:1281:C:H5	30:a:1318:G:H1	1.07	0.98
30:a:2282:G:H1	30:a:2371:U:H3	1.09	0.97
34:e:133:VAL:HG21	34:e:138:PRO:HD2	1.47	0.96
34:e:160:LEU:HB3	34:e:164:ASP:HB2	1.47	0.96
30:a:2706:G:H1	30:a:2721:C:H5	1.07	0.95

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	48/56 (86%)	45 (94%)	3 (6%)	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	65/68 (96%)	64 (98%)	1 (2%)	0	100	100
4	3	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
5	4	64/69 (93%)	54 (84%)	9 (14%)	1 (2%)	7	11
7	B	231/283 (82%)	207 (90%)	23 (10%)	1 (0%)	30	43
9	D	198/201 (98%)	185 (93%)	12 (6%)	1 (0%)	24	37
10	E	177/215 (82%)	168 (95%)	8 (4%)	1 (1%)	21	32
11	F	94/96 (98%)	91 (97%)	2 (2%)	1 (1%)	11	18
12	G	204/269 (76%)	195 (96%)	9 (4%)	0	100	100
13	H	132/135 (98%)	128 (97%)	4 (3%)	0	100	100
14	I	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
15	J	132/173 (76%)	120 (91%)	12 (9%)	0	100	100
16	K	115/135 (85%)	105 (91%)	8 (7%)	2 (2%)	7	10
17	L	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
18	M	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	12	20
19	N	120/123 (98%)	110 (92%)	10 (8%)	0	100	100
20	O	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
21	P	126/147 (86%)	113 (90%)	12 (10%)	1 (1%)	16	25
22	Q	88/90 (98%)	81 (92%)	7 (8%)	0	100	100
23	R	65/79 (82%)	61 (94%)	4 (6%)	0	100	100
24	S	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
25	T	85/88 (97%)	85 (100%)	0	0	100	100
26	U	82/93 (88%)	76 (93%)	5 (6%)	1 (1%)	10	16
27	V	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
28	X	30/33 (91%)	28 (93%)	1 (3%)	1 (3%)	3	2
32	c	272/278 (98%)	259 (95%)	13 (5%)	0	100	100
33	d	212/223 (95%)	202 (95%)	9 (4%)	1 (0%)	24	37
34	e	208/301 (69%)	179 (86%)	26 (12%)	3 (1%)	9	13
35	f	182/210 (87%)	174 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	g	175/180 (97%)	163 (93%)	12 (7%)	0	100	100
37	i	144/147 (98%)	142 (99%)	2 (1%)	0	100	100
38	j	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
39	k	142/146 (97%)	119 (84%)	22 (16%)	1 (1%)	18	28
40	l	134/139 (96%)	130 (97%)	4 (3%)	0	100	100
41	m	118/187 (63%)	111 (94%)	5 (4%)	2 (2%)	7	10
42	n	124/127 (98%)	118 (95%)	5 (4%)	1 (1%)	16	25
43	o	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
44	p	117/123 (95%)	114 (97%)	2 (2%)	1 (1%)	14	22
45	q	100/102 (98%)	97 (97%)	3 (3%)	0	100	100
46	r	130/153 (85%)	126 (97%)	4 (3%)	0	100	100
47	s	93/102 (91%)	85 (91%)	7 (8%)	1 (1%)	11	18
48	t	103/122 (84%)	95 (92%)	7 (7%)	1 (1%)	12	20
49	u	177/205 (86%)	164 (93%)	13 (7%)	0	100	100
50	v	76/89 (85%)	73 (96%)	3 (4%)	0	100	100
51	w	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	7	10
52	x	67/77 (87%)	63 (94%)	4 (6%)	0	100	100
53	y	56/60 (93%)	54 (96%)	2 (4%)	0	100	100
54	z	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
All	All	5646/6322 (89%)	5302 (94%)	321 (6%)	23 (0%)	31	43

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	K	125	ASN
28	X	4	VAL
34	e	133	VAL
34	e	151	ALA
34	e	159	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	0	47/51 (92%)	45 (96%)	2 (4%)	26	44
2	1	36/36 (100%)	33 (92%)	3 (8%)	10	17
3	2	54/55 (98%)	54 (100%)	0	100	100
4	3	35/35 (100%)	34 (97%)	1 (3%)	37	60
5	4	56/59 (95%)	48 (86%)	8 (14%)	3	4
7	B	197/234 (84%)	184 (93%)	13 (7%)	15	26
9	D	175/176 (99%)	169 (97%)	6 (3%)	32	54
10	E	130/155 (84%)	124 (95%)	6 (5%)	24	41
11	F	89/89 (100%)	86 (97%)	3 (3%)	32	54
12	G	160/200 (80%)	153 (96%)	7 (4%)	25	43
13	H	108/109 (99%)	103 (95%)	5 (5%)	24	41
14	I	132/133 (99%)	125 (95%)	7 (5%)	20	36
15	J	97/131 (74%)	89 (92%)	8 (8%)	10	18
16	K	88/101 (87%)	85 (97%)	3 (3%)	32	54
17	L	103/104 (99%)	98 (95%)	5 (5%)	22	39
18	M	89/93 (96%)	85 (96%)	4 (4%)	24	42
19	N	99/100 (99%)	94 (95%)	5 (5%)	21	37
20	O	74/74 (100%)	70 (95%)	4 (5%)	20	35
21	P	103/115 (90%)	93 (90%)	10 (10%)	8	12
22	Q	81/81 (100%)	77 (95%)	4 (5%)	22	39
23	R	55/65 (85%)	53 (96%)	2 (4%)	31	52
24	S	48/49 (98%)	42 (88%)	6 (12%)	4	6
25	T	68/69 (99%)	65 (96%)	3 (4%)	25	43
26	U	72/80 (90%)	65 (90%)	7 (10%)	8	12
27	V	16/17 (94%)	15 (94%)	1 (6%)	16	29
28	X	28/29 (97%)	27 (96%)	1 (4%)	31	52
32	c	216/220 (98%)	210 (97%)	6 (3%)	38	60
33	d	166/172 (96%)	161 (97%)	5 (3%)	36	58
34	e	165/237 (70%)	150 (91%)	15 (9%)	9	14
35	f	154/175 (88%)	146 (95%)	8 (5%)	21	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	g	150/152 (99%)	142 (95%)	8 (5%)	20	36
37	i	118/120 (98%)	116 (98%)	2 (2%)	53	74
38	j	101/101 (100%)	96 (95%)	5 (5%)	22	38
39	k	111/113 (98%)	103 (93%)	8 (7%)	13	23
40	l	108/110 (98%)	101 (94%)	7 (6%)	15	27
41	m	100/142 (70%)	95 (95%)	5 (5%)	22	38
42	n	95/96 (99%)	91 (96%)	4 (4%)	26	45
43	o	97/99 (98%)	88 (91%)	9 (9%)	8	14
44	p	98/99 (99%)	96 (98%)	2 (2%)	48	70
45	q	84/84 (100%)	78 (93%)	6 (7%)	13	23
46	r	105/118 (89%)	99 (94%)	6 (6%)	18	33
47	s	84/89 (94%)	81 (96%)	3 (4%)	31	52
48	t	91/103 (88%)	86 (94%)	5 (6%)	19	34
49	u	149/168 (89%)	144 (97%)	5 (3%)	32	54
50	v	60/67 (90%)	58 (97%)	2 (3%)	33	55
51	w	52/53 (98%)	50 (96%)	2 (4%)	29	49
52	x	61/68 (90%)	58 (95%)	3 (5%)	22	39
53	y	53/55 (96%)	51 (96%)	2 (4%)	29	49
54	z	51/52 (98%)	49 (96%)	2 (4%)	28	48
All	All	4709/5133 (92%)	4465 (95%)	244 (5%)	22	36

5 of 244 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	U	13	GLU
47	s	81	THR
34	e	134	ASP
46	r	103	ARG
51	w	54	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
35	f	127	ASN

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Mol	Chain	Res	Type
39	k	44	ASN
36	g	22	GLN
37	i	47	HIS
44	p	20	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	Y	9/22 (40%)	6 (66%)	0
30	a	2894/3086 (93%)	511 (17%)	0
31	b	117/120 (97%)	13 (11%)	0
6	A	1511/1537 (98%)	300 (19%)	27 (1%)
8	C	74/76 (97%)	10 (13%)	1 (1%)
All	All	4605/4841 (95%)	840 (18%)	28 (0%)

5 of 840 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	7	A
6	A	8	U
6	A	9	U
6	A	10	G
6	A	11	G

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	1051	C
8	C	74	C
6	A	1109	G
6	A	1387	5MC
6	A	1070	U

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

34 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$
6	5MC	A	1391	6	19,22,23	4.29	8 (42%)	26,32,35	1.03	2 (7%)
8	5MC	C	32	8	19,22,23	0.79	1 (5%)	26,32,35	0.48	0
30	PSU	a	2786	30	18,21,22	0.93	1 (5%)	21,30,33	0.68	0
30	PSU	a	2686	30	18,21,22	0.94	1 (5%)	21,30,33	0.76	1 (4%)
30	5MU	a	2122	30	19,22,23	0.30	0	27,32,35	0.31	0
30	OMC	a	2680	30,56	19,22,23	3.11	8 (42%)	25,31,34	0.88	0
6	5MC	A	1387	6	19,22,23	4.38	8 (42%)	26,32,35	1.04	2 (7%)
6	2MG	A	1503	6	23,26,27	0.33	0	33,38,41	0.55	0
6	5MC	A	1394	6	19,22,23	4.21	8 (42%)	26,32,35	0.97	2 (7%)
30	2MG	a	2018	30	23,26,27	3.01	8 (34%)	33,38,41	2.59	12 (36%)
30	OMU	a	2734	30	19,22,23	0.27	0	25,31,34	0.46	0
6	5MC	A	951	6	19,22,23	0.82	1 (5%)	26,32,35	0.48	0
30	H2U	a	2631	30	18,21,22	2.93	5 (27%)	19,30,33	1.52	4 (21%)
30	3TD	a	2098	30	19,22,23	4.15	7 (36%)	23,32,35	1.86	5 (21%)
30	PSU	a	2100	30	18,21,22	0.94	1 (5%)	21,30,33	0.66	0
30	OMG	a	2433	8,30,56	23,26,27	2.46	9 (39%)	32,38,41	2.31	11 (34%)
8	4SU	C	8	8	18,21,22	3.73	8 (44%)	25,30,33	2.27	5 (20%)
30	PSU	a	2094	30	18,21,22	0.94	1 (5%)	21,30,33	0.63	0
30	2MA	a	2685	30,56	22,25,26	3.46	8 (36%)	32,37,40	2.05	8 (25%)
6	4OC	A	1389	6	20,23,24	3.01	8 (40%)	25,32,35	0.94	1 (4%)
8	PSU	C	55	8	18,21,22	0.95	1 (5%)	21,30,33	0.64	0
6	PSU	A	498	6	18,21,22	0.93	1 (5%)	21,30,33	0.61	0
30	PSU	a	2787	30	18,21,22	0.94	1 (5%)	21,30,33	0.59	0
6	MA6	A	1506	6	23,26,27	0.27	0	33,38,41	0.69	1 (3%)
6	2MG	A	950	6	23,26,27	0.36	0	33,38,41	0.41	0
30	PSU	a	2762	30	18,21,22	0.94	1 (5%)	21,30,33	0.72	0
30	PSU	a	2639	30	18,21,22	0.93	1 (5%)	21,30,33	0.75	0
30	PSU	a	1038	30	18,21,22	0.92	1 (5%)	21,30,33	0.75	0
8	5MU	C	54	8	19,22,23	0.25	0	27,32,35	0.27	0
6	G7M	A	509	6	23,26,27	2.62	9 (39%)	34,39,42	1.70	7 (20%)
6	UR3	A	1485	6	19,22,23	2.70	8 (42%)	26,32,35	1.66	3 (11%)
30	5MC	a	2145	30	19,22,23	4.18	8 (42%)	26,32,35	1.14	2 (7%)
30	2MG	a	2627	30	23,26,27	2.98	8 (34%)	33,38,41	2.43	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MA6	A	1505	6	23,26,27	0.27	0	33,38,41	0.63	1 (3%)

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
6	5MC	A	1391	6	-	0/7/25/26	0/2/2/2
8	5MC	C	32	8	-	0/7/25/26	0/2/2/2
30	PSU	a	2786	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2686	30	-	0/7/25/26	0/2/2/2
30	5MU	a	2122	30	-	0/7/25/26	0/2/2/2
30	OMC	a	2680	30,56	-	0/9/27/28	0/2/2/2
6	5MC	A	1387	6	-	3/7/25/26	0/2/2/2
6	2MG	A	1503	6	-	0/9/27/28	0/3/3/3
6	5MC	A	1394	6	-	0/7/25/26	0/2/2/2
30	2MG	a	2018	30	-	2/9/27/28	0/3/3/3
30	OMU	a	2734	30	-	0/9/27/28	0/2/2/2
6	5MC	A	951	6	-	0/7/25/26	0/2/2/2
30	H2U	a	2631	30	-	0/7/38/39	0/2/2/2
30	3TD	a	2098	30	-	2/7/25/26	0/2/2/2
30	PSU	a	2100	30	-	0/7/25/26	0/2/2/2
30	OMG	a	2433	8,30,56	-	0/9/27/28	0/3/3/3
8	4SU	C	8	8	-	0/7/25/26	0/2/2/2
30	PSU	a	2094	30	-	0/7/25/26	0/2/2/2
30	2MA	a	2685	30,56	-	1/7/25/26	0/3/3/3
6	4OC	A	1389	6	-	1/9/29/30	0/2/2/2
8	PSU	C	55	8	-	0/7/25/26	0/2/2/2
6	PSU	A	498	6	-	0/7/25/26	0/2/2/2
30	PSU	a	2787	30	-	0/7/25/26	0/2/2/2
6	MA6	A	1506	6	-	0/11/29/30	0/3/3/3
6	2MG	A	950	6	-	0/9/27/28	0/3/3/3
30	PSU	a	2762	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2639	30	-	0/7/25/26	0/2/2/2
30	PSU	a	1038	30	-	0/7/25/26	0/2/2/2
8	5MU	C	54	8	-	0/7/25/26	0/2/2/2
6	G7M	A	509	6	-	2/7/25/26	0/3/3/3
6	UR3	A	1485	6	-	0/7/25/26	0/2/2/2
30	5MC	a	2145	30	-	0/7/25/26	0/2/2/2
30	2MG	a	2627	30	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MA6	A	1505	6	-	0/11/29/30	0/3/3/3

The worst 5 of 130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2098	3TD	C6-C5	12.87	1.49	1.35
30	a	2685	2MA	C4-N3	10.46	1.47	1.34
6	A	1387	5MC	C6-C5	9.43	1.50	1.34
6	A	1394	5MC	C6-C5	9.15	1.49	1.34
6	A	1391	5MC	C6-C5	9.14	1.49	1.34

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	8	4SU	C4-N3-C2	-7.87	119.78	127.31
30	a	2018	2MG	C2-N3-C4	7.44	121.30	112.00
30	a	2627	2MG	C2-N3-C4	6.59	120.25	112.00
30	a	2685	2MA	C5-C4-N3	-6.37	120.47	127.18
30	a	2018	2MG	C5-C4-N3	-6.31	118.35	128.39

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1387	5MC	O4'-C4'-C5'-O5'
30	a	2098	3TD	O4'-C4'-C5'-O5'
30	a	2098	3TD	C3'-C4'-C5'-O5'
6	A	509	G7M	C3'-C4'-C5'-O5'
6	A	1387	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1387	5MC	2	0
6	A	1503	2MG	1	0
30	a	2631	H2U	1	0
30	a	2098	3TD	2	0
30	a	2094	PSU	2	0
6	A	1506	MA6	7	0
6	A	509	G7M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1485	UR3	2	0
30	a	2627	2MG	1	0
6	A	1505	MA6	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 300 ligands modelled in this entry, 293 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	$\# Z > 2$
57	DXT	a	3146	56	34,35,35	1.13	2 (5%)	42,57,57	0.95	2 (4%)
57	DXT	a	3138	56	34,35,35	1.13	2 (5%)	42,57,57	0.97	1 (2%)
57	DXT	r	201	56	34,35,35	1.11	2 (5%)	42,57,57	1.08	3 (7%)
57	DXT	A	1615	56	34,35,35	1.11	2 (5%)	42,57,57	1.04	2 (4%)
57	DXT	s	201	56	34,35,35	1.11	2 (5%)	42,57,57	0.88	1 (2%)
57	DXT	a	3123	56	34,35,35	1.12	2 (5%)	42,57,57	0.95	2 (4%)
57	DXT	a	3130	56	34,35,35	1.12	2 (5%)	42,57,57	1.38	6 (14%)

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
57	DXT	a	3146	56	-	1/8/74/74	0/4/4/4
57	DXT	a	3138	56	-	3/8/74/74	0/4/4/4
57	DXT	r	201	56	-	8/8/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	DXT	A	1615	56	-	2/8/74/74	0/4/4/4
57	DXT	s	201	56	-	4/8/74/74	0/4/4/4
57	DXT	a	3123	56	-	1/8/74/74	0/4/4/4
57	DXT	a	3130	56	-	7/8/74/74	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	a	3138	DXT	C21-N21	5.02	1.47	1.33
57	a	3130	DXT	C21-N21	4.99	1.47	1.33
57	a	3123	DXT	C21-N21	4.96	1.47	1.33
57	a	3146	DXT	C21-N21	4.96	1.47	1.33
57	s	201	DXT	C21-N21	4.94	1.47	1.33

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	a	3130	DXT	C4B-C1-C2	3.79	121.77	115.75
57	A	1615	DXT	C21-C2-C1	3.10	124.64	120.97
57	a	3130	DXT	C4B-C12-C5B	2.99	126.10	123.06
57	a	3130	DXT	O13-C4B-C12	-2.96	105.41	110.14
57	r	201	DXT	C4B-C1-C2	2.80	120.19	115.75

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	A	1615	DXT	C4A-C4-N4-C42
57	a	3123	DXT	C4A-C4-N4-C41
57	a	3130	DXT	C1-C2-C21-O21
57	a	3130	DXT	C1-C2-C21-N21
57	a	3130	DXT	C3-C2-C21-O21

There are no ring outliers.

5 monomers are involved in 6 short contacts:

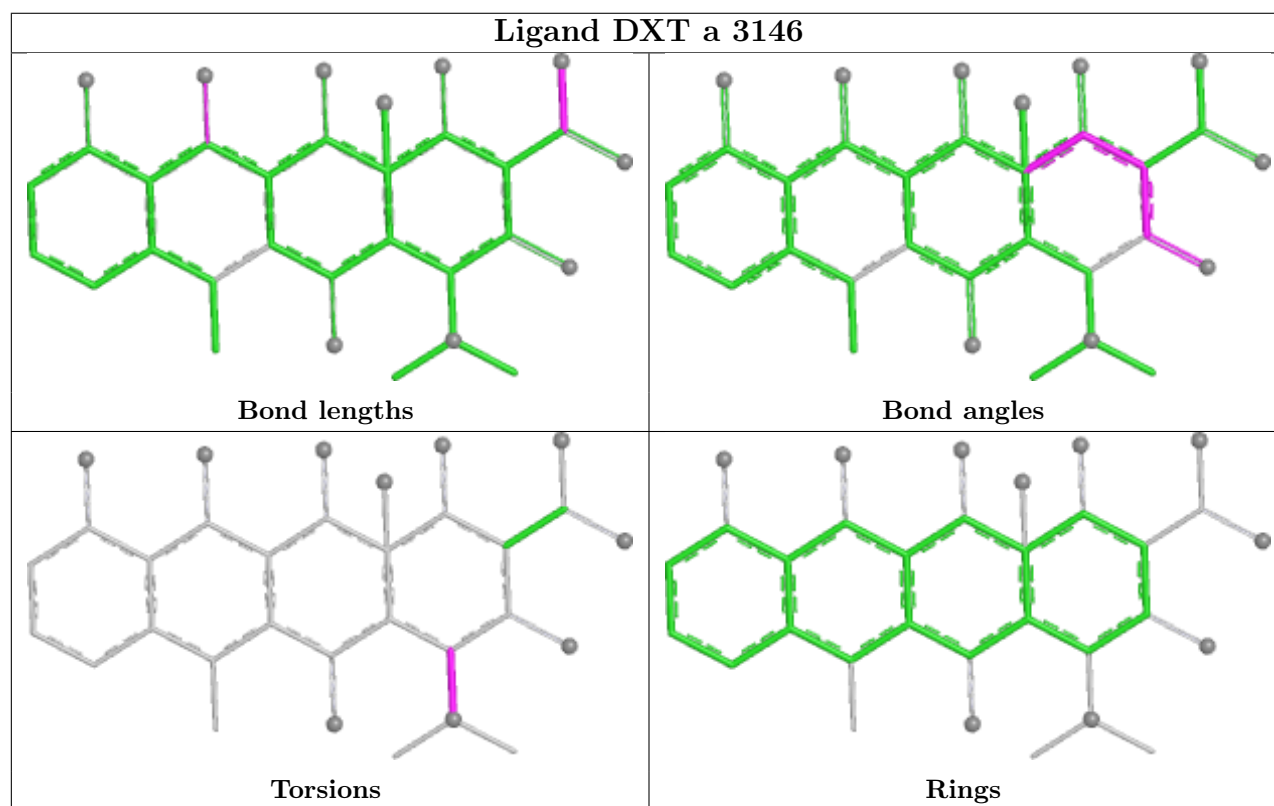
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	a	3146	DXT	1	0
57	a	3138	DXT	1	0
57	r	201	DXT	1	0

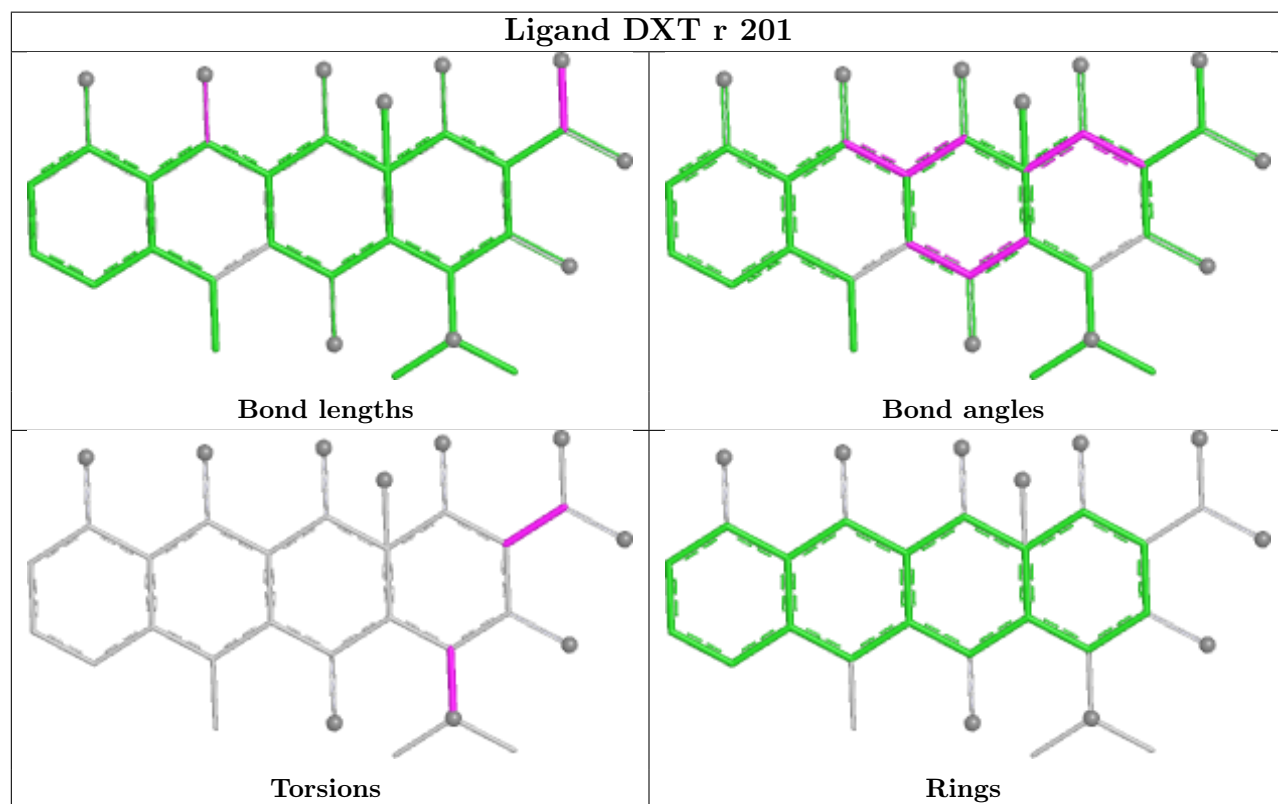
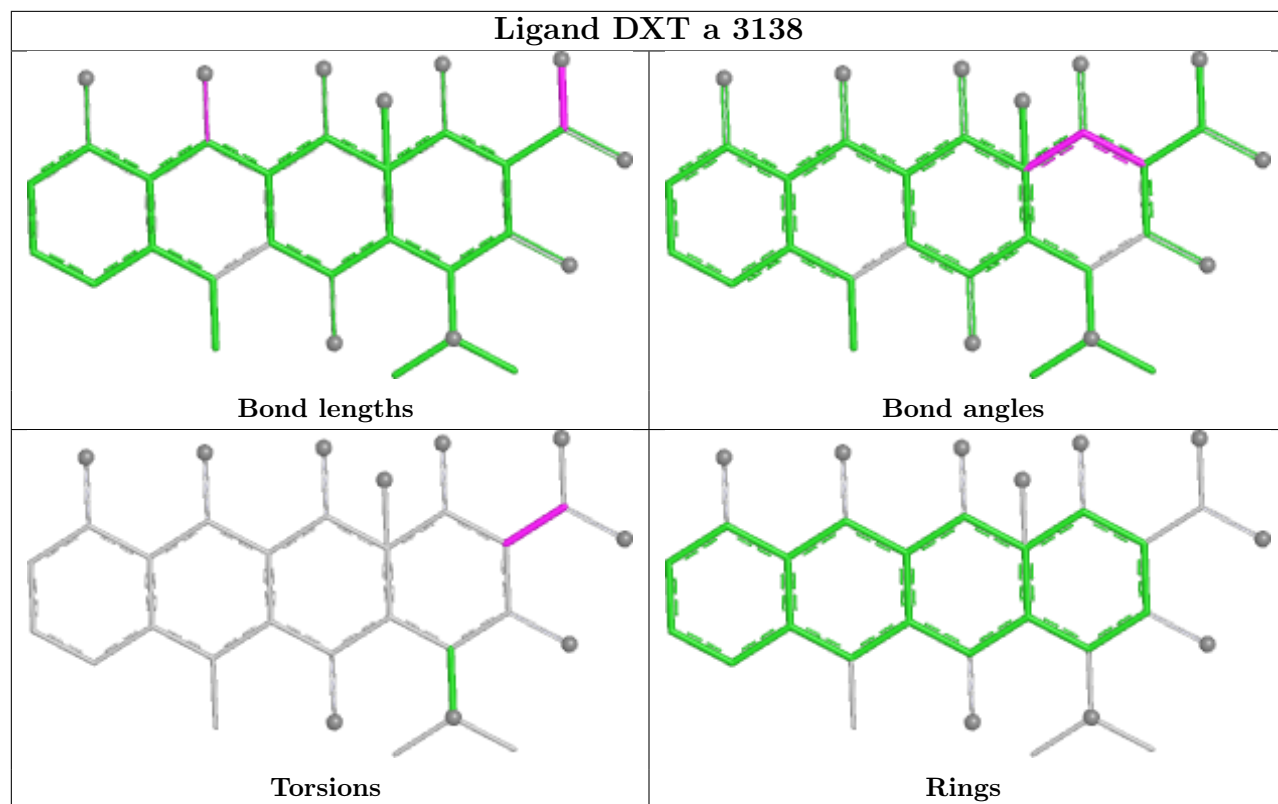
Continued on next page...

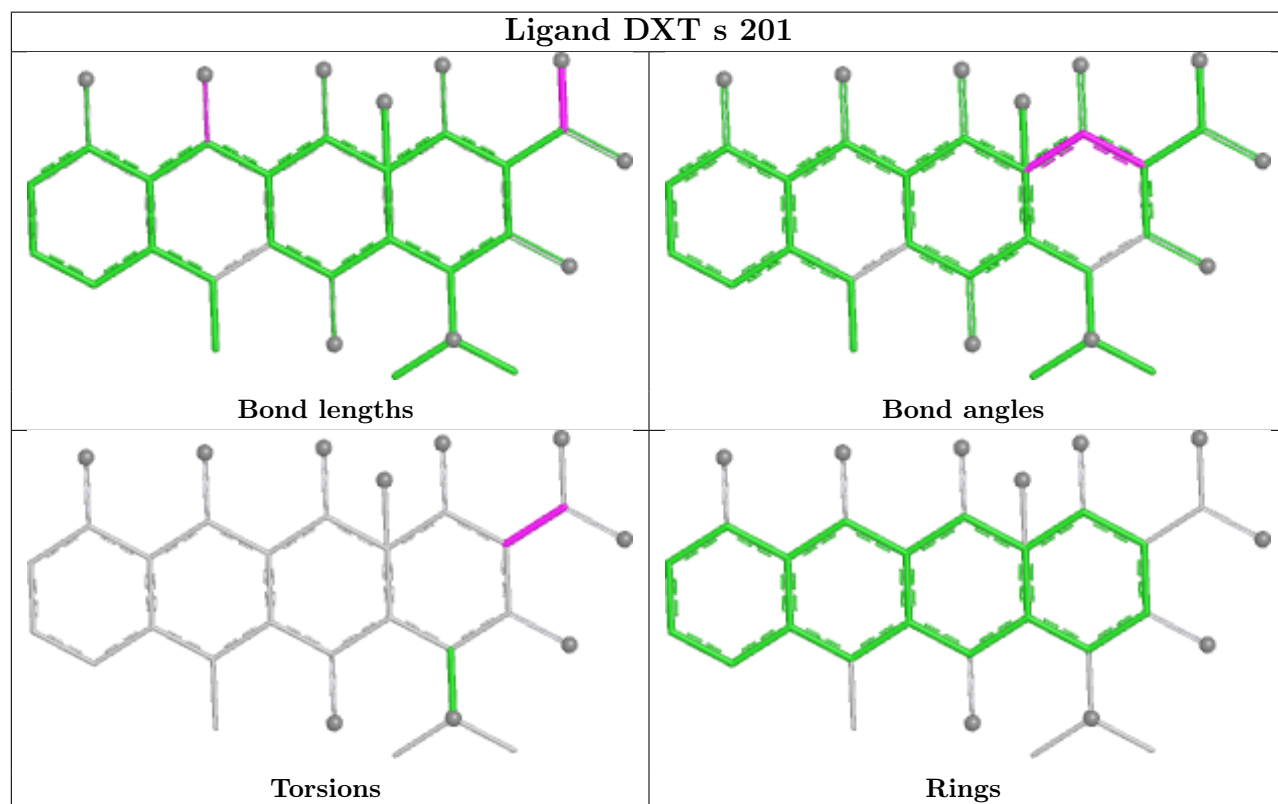
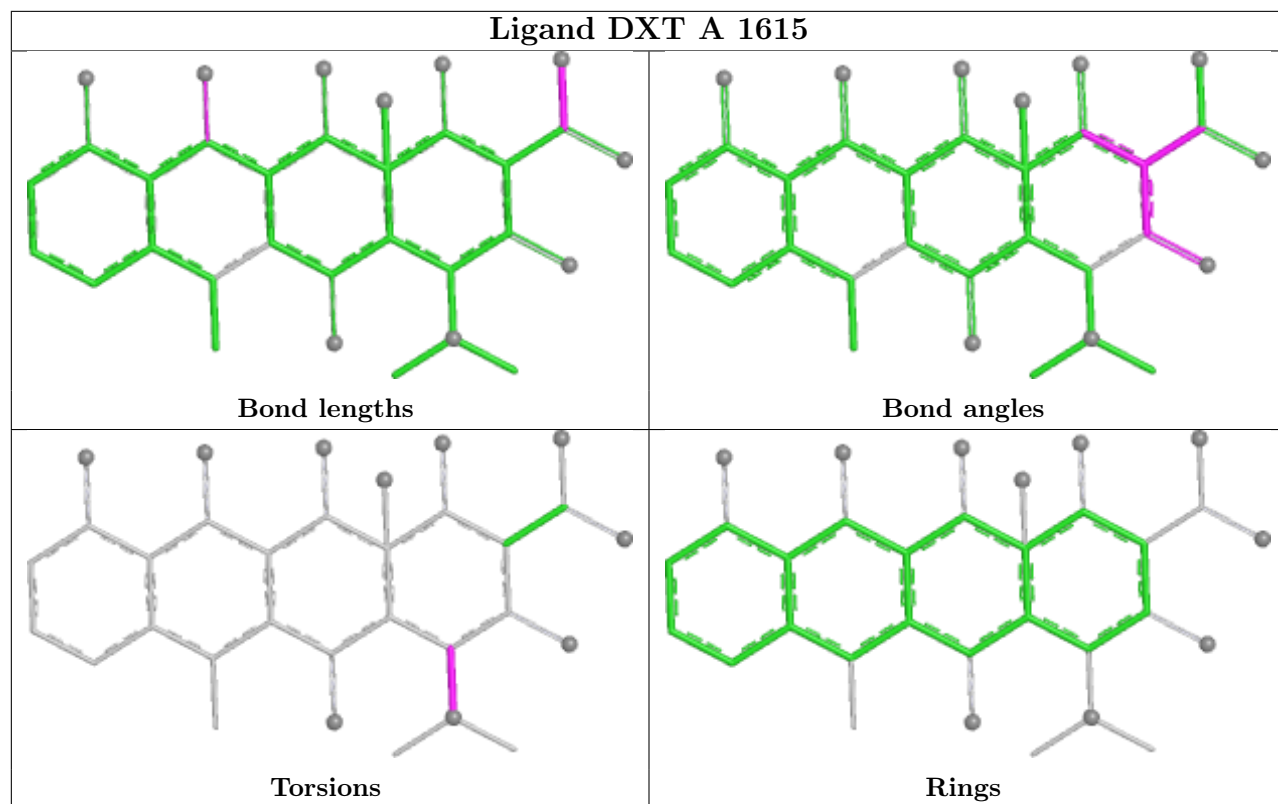
Continued from previous page...

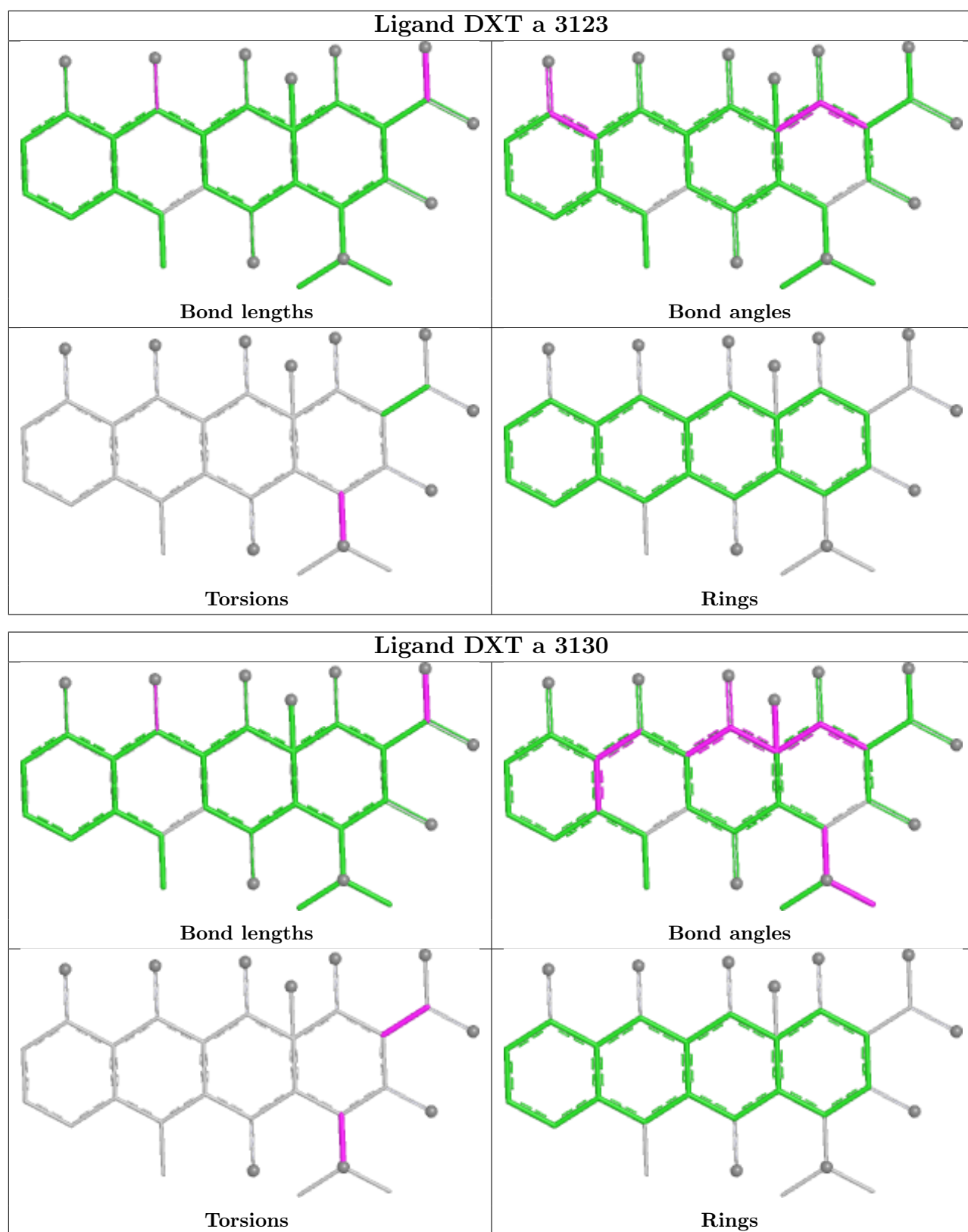
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	A	1615	DXT	1	0
57	a	3123	DXT	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

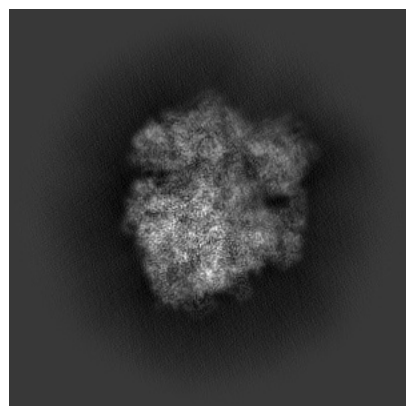
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71682. These allow visual inspection of the internal detail of the map and identification of artifacts.

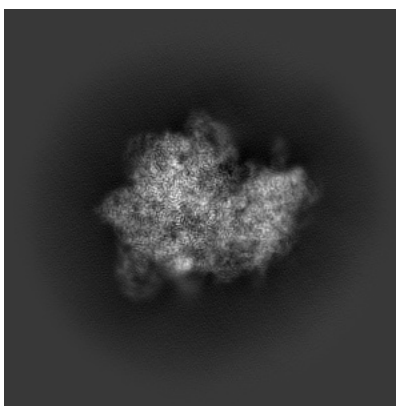
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

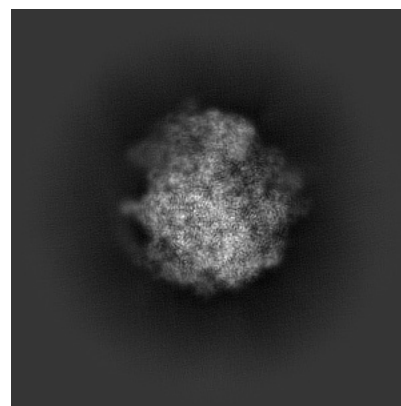
6.1.1 Primary map



X

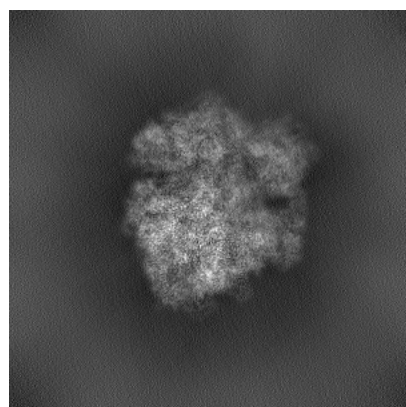


Y

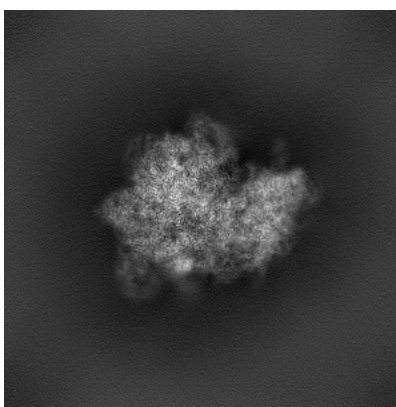


Z

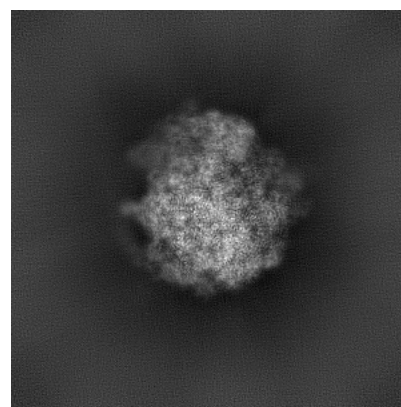
6.1.2 Raw map



X



Y

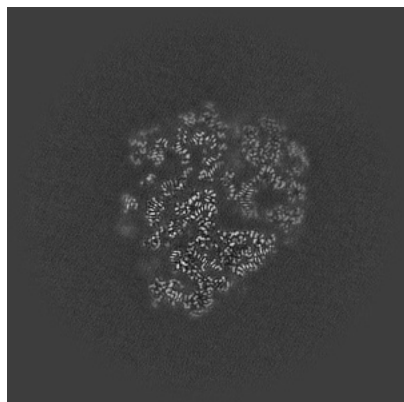


Z

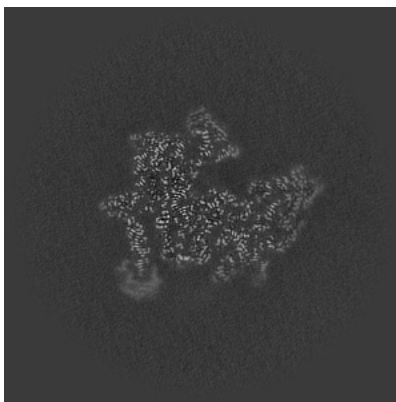
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

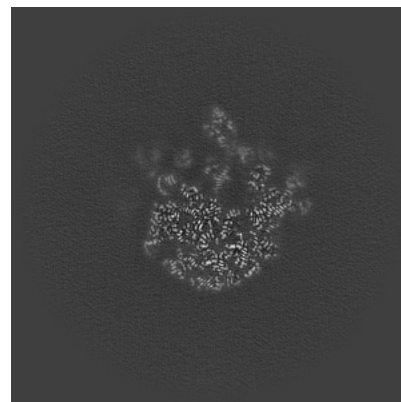
6.2.1 Primary map



X Index: 220

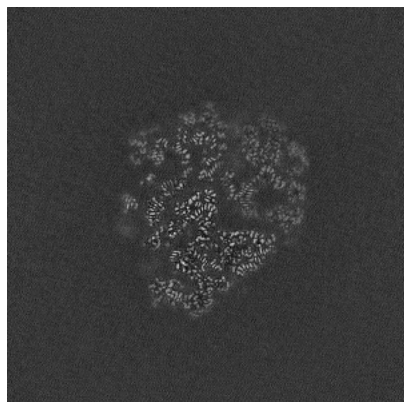


Y Index: 220

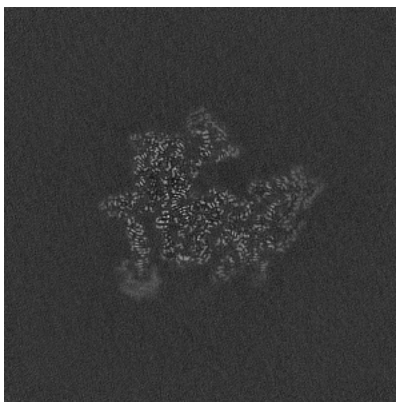


Z Index: 220

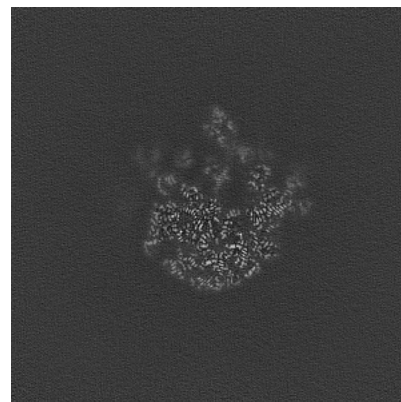
6.2.2 Raw map



X Index: 220



Y Index: 220

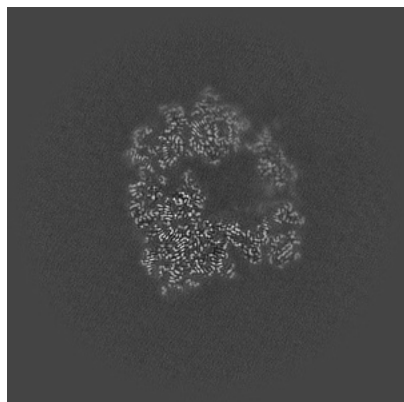


Z Index: 220

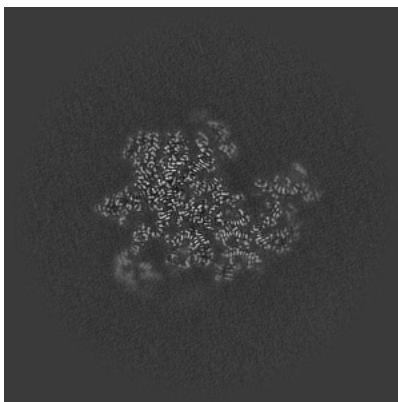
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

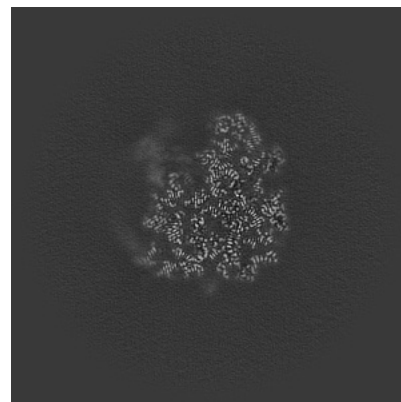
6.3.1 Primary map



X Index: 242

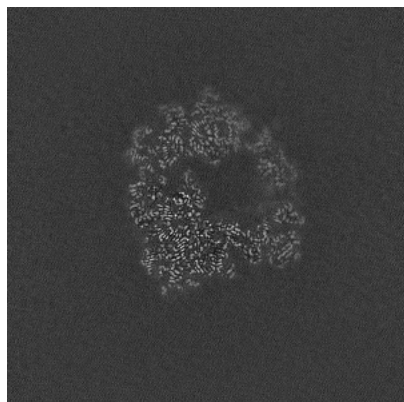


Y Index: 211

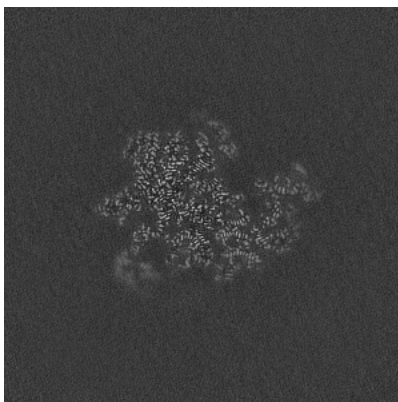


Z Index: 190

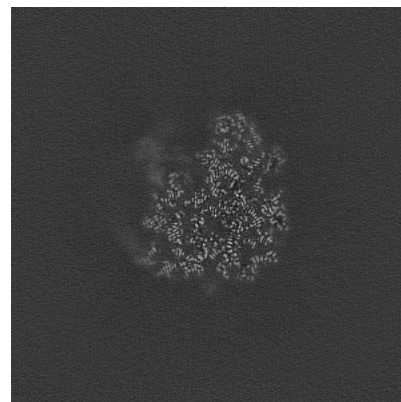
6.3.2 Raw map



X Index: 242



Y Index: 211

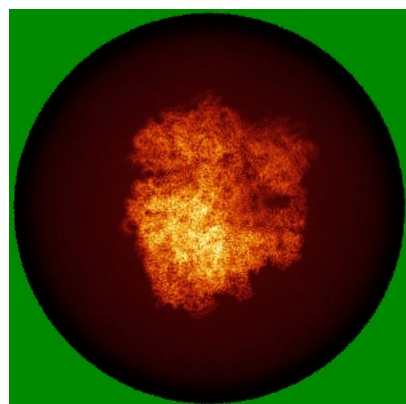


Z Index: 190

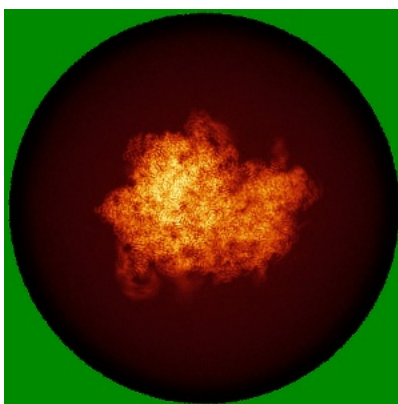
The images above show the largest variance slices of the map in three orthogonal directions.

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

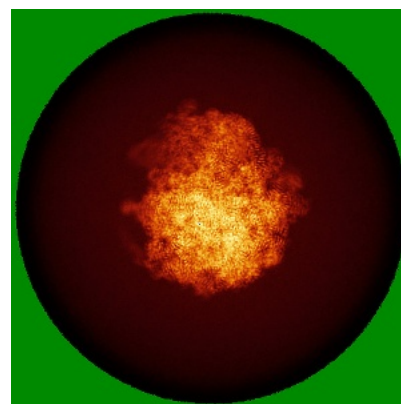
6.4.1 Primary map



X

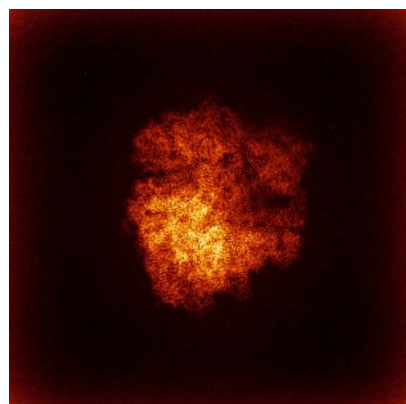


Y

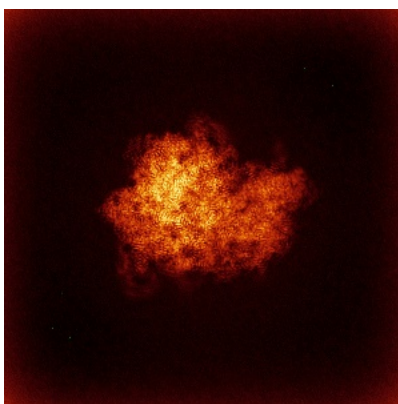


Z

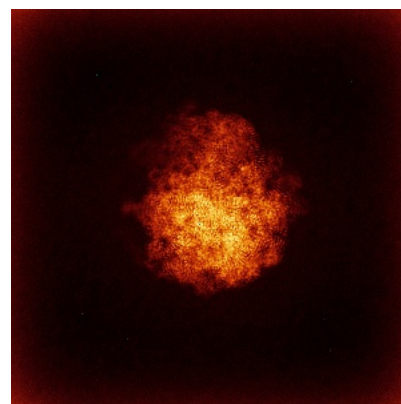
6.4.2 Raw map



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



X



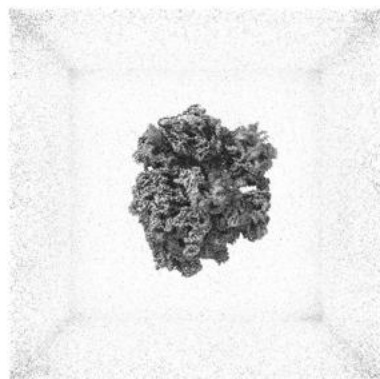
Y



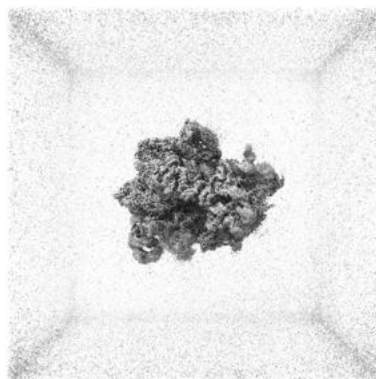
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

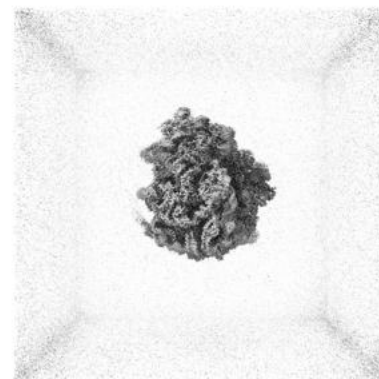
6.5.2 Raw map



X



Y



Z

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.

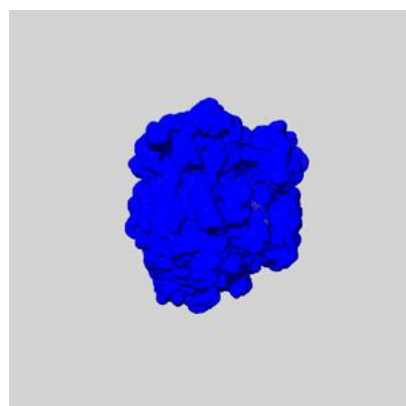
6.6 Mask visualisation [i](#)

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

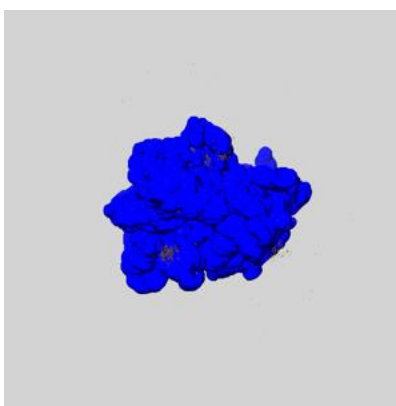
A mask typically either:

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

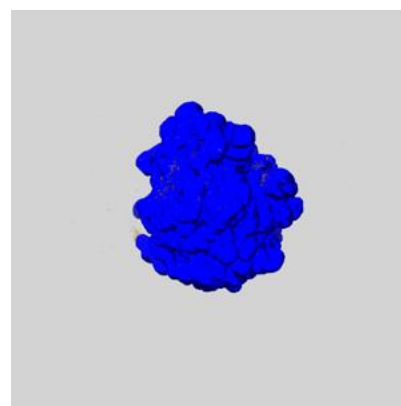
6.6.1 emd_71682_msk_1.map [i](#)



X



Y

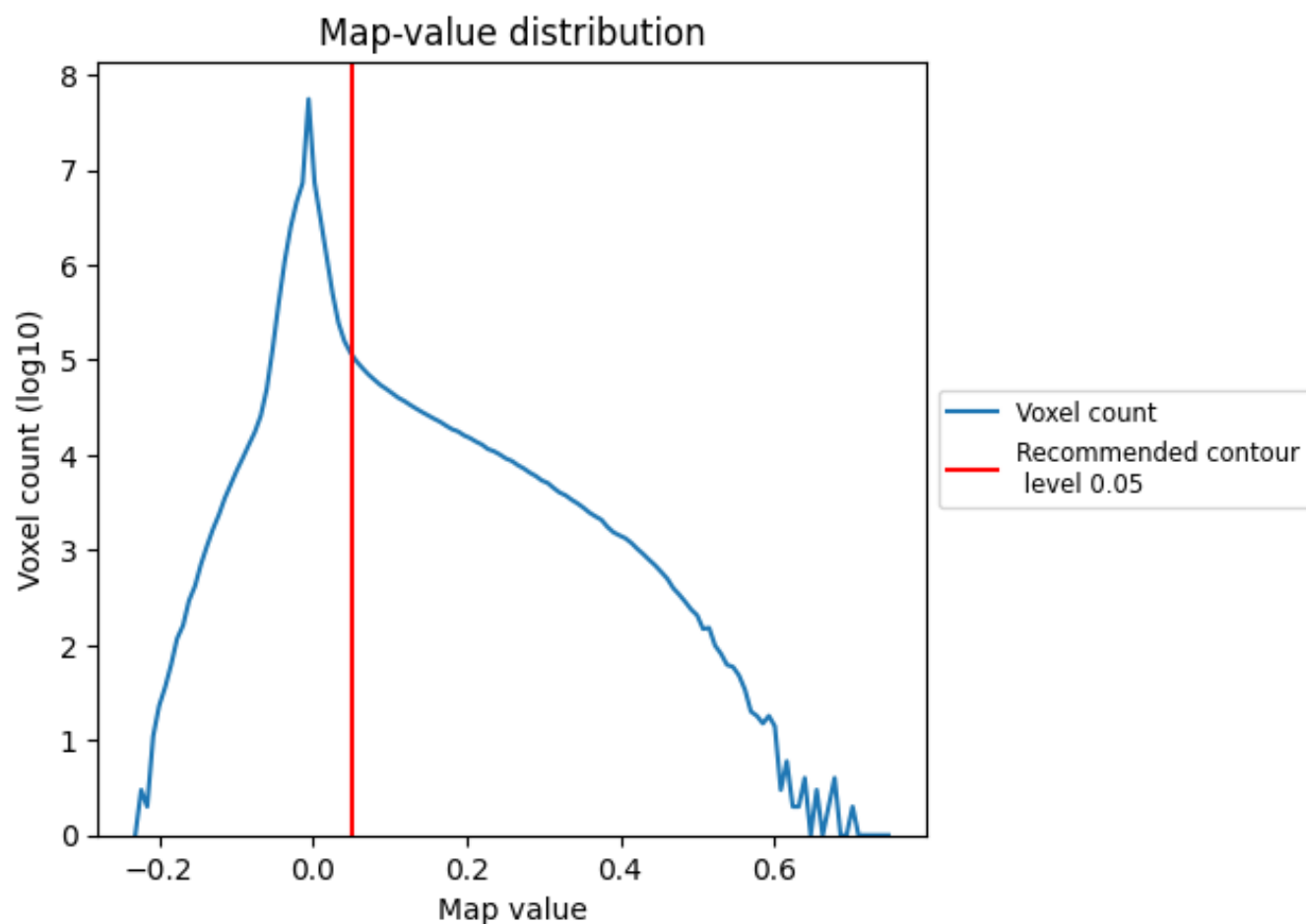


Z

7 Map analysis [i](#)

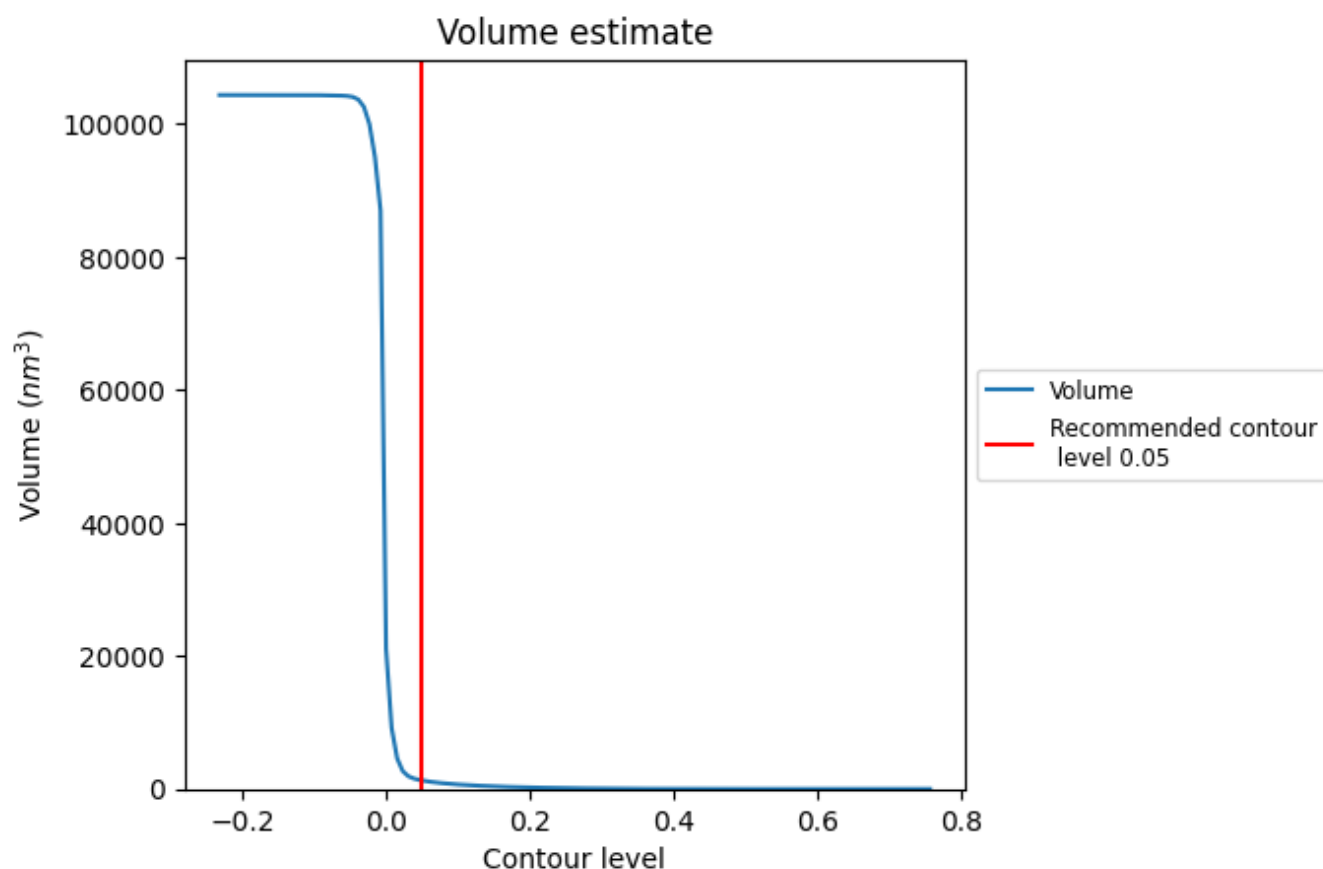
This section contains the results of statistical analysis of the map.

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.

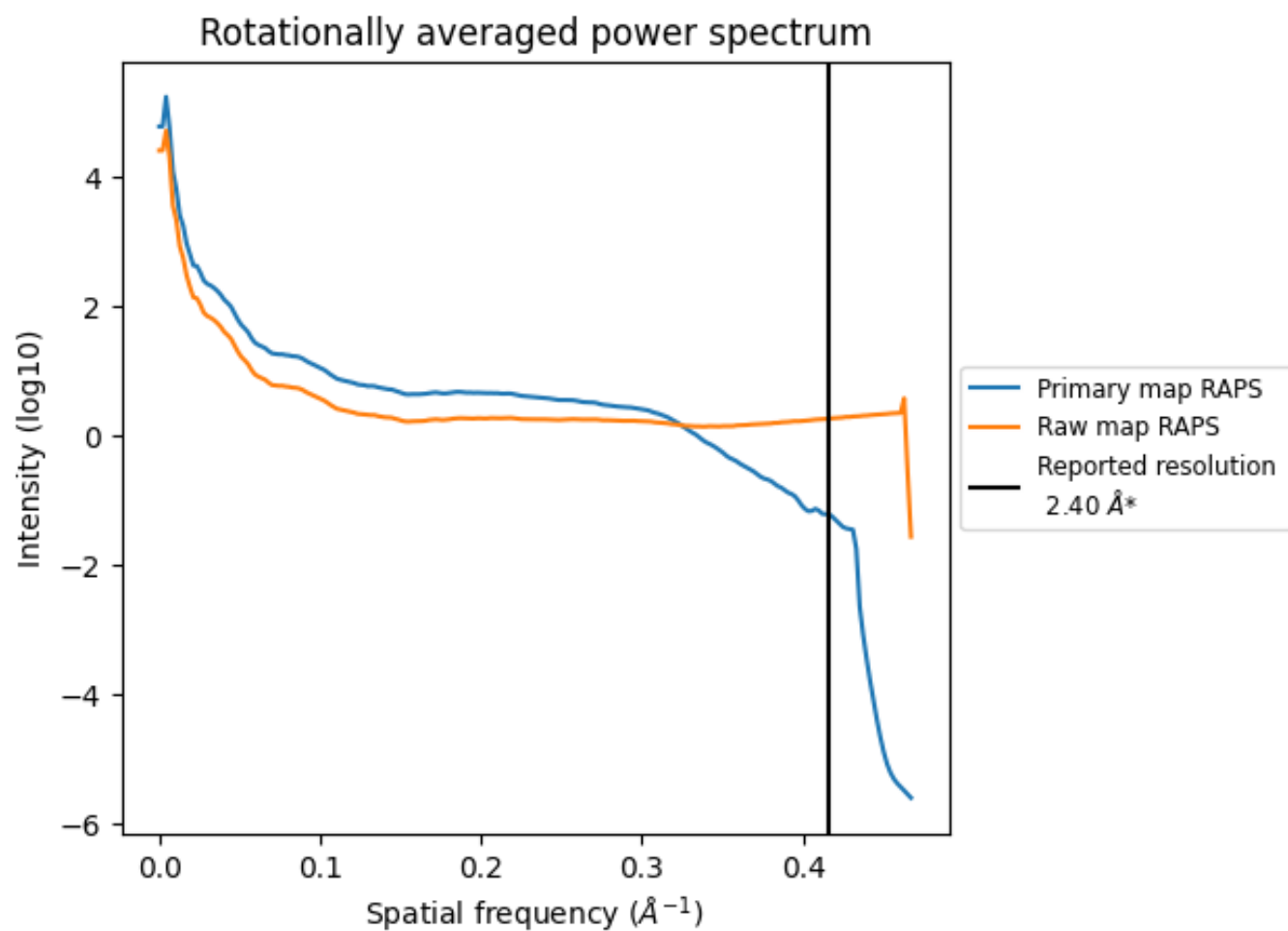
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1284 nm^3 ; this corresponds to an approximate mass of 1160 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 ⓘ

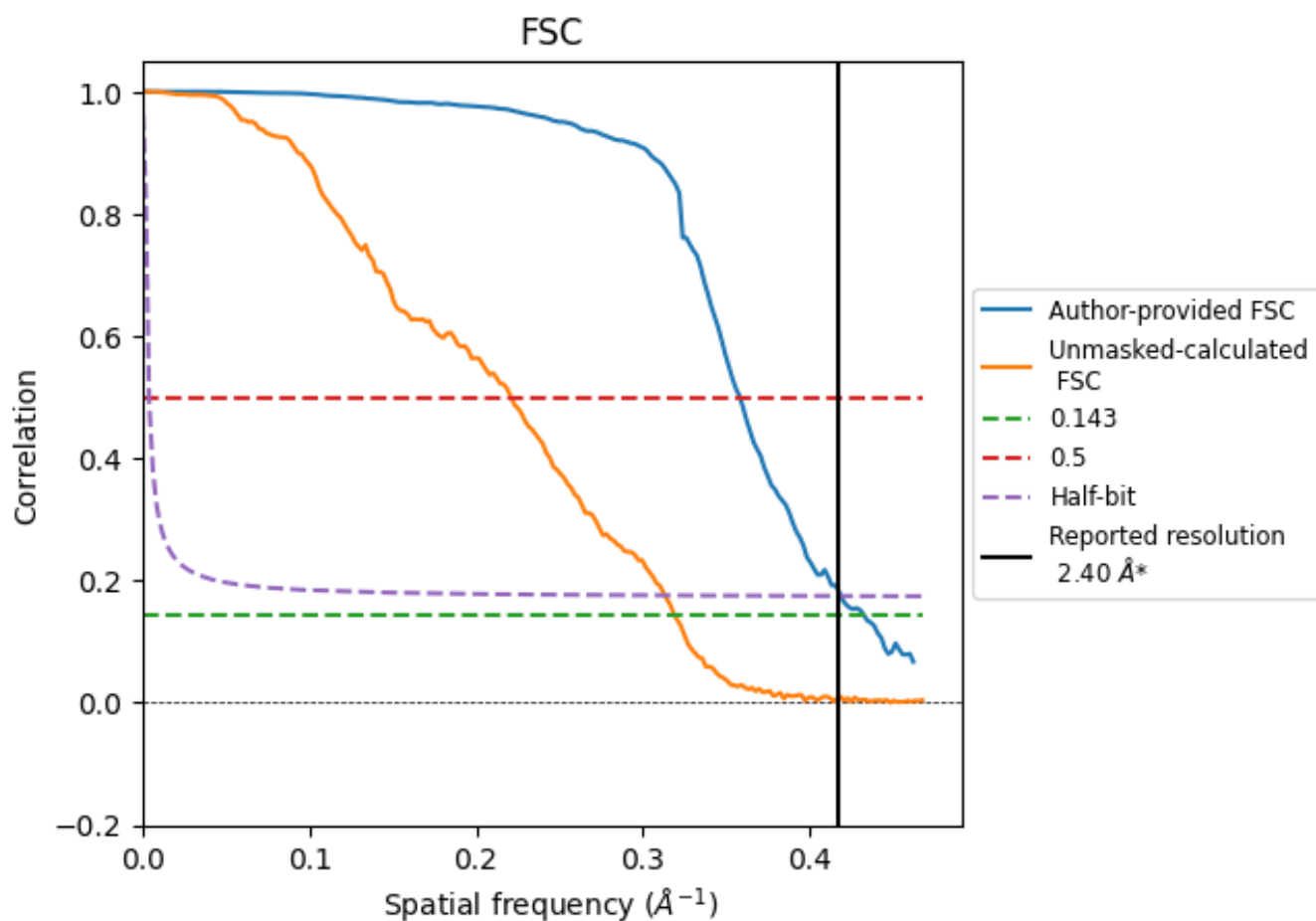


*Reported resolution corresponds to spatial frequency of 0.417 \AA^{-1}

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 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

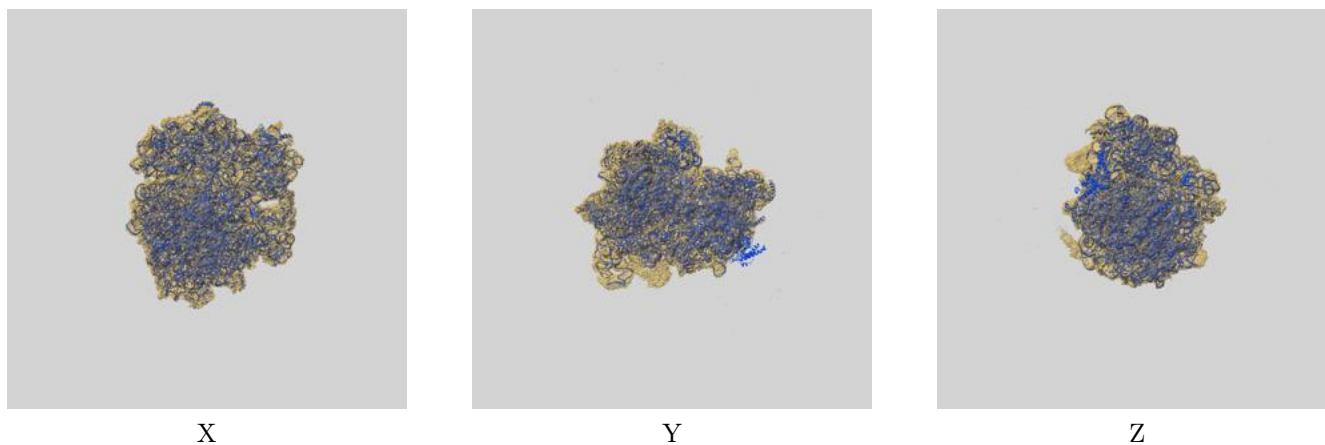
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.31	2.79	2.39
Unmasked-calculated*	3.14	4.52	3.19

*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 3.14 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

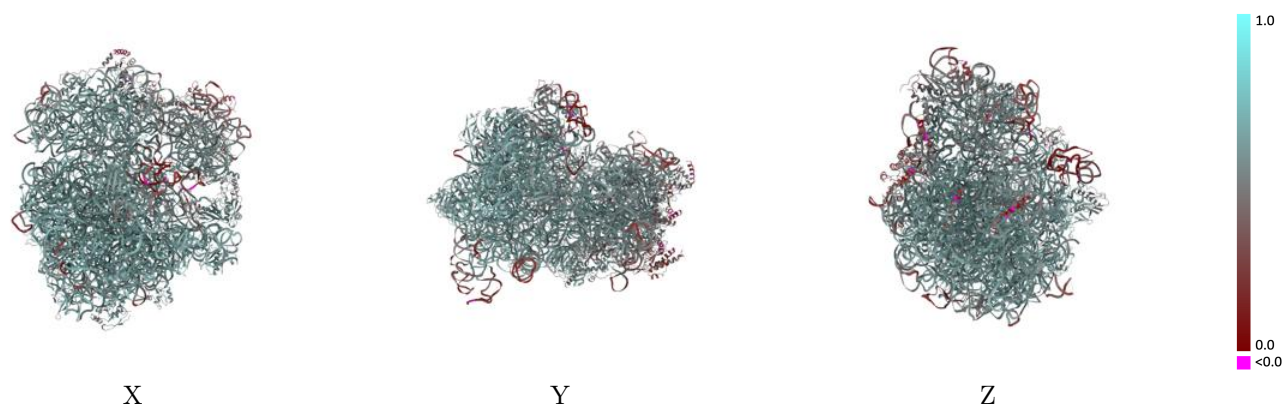
This section contains information regarding the fit between EMDB map EMD-71682 and PDB model 9PJ7. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



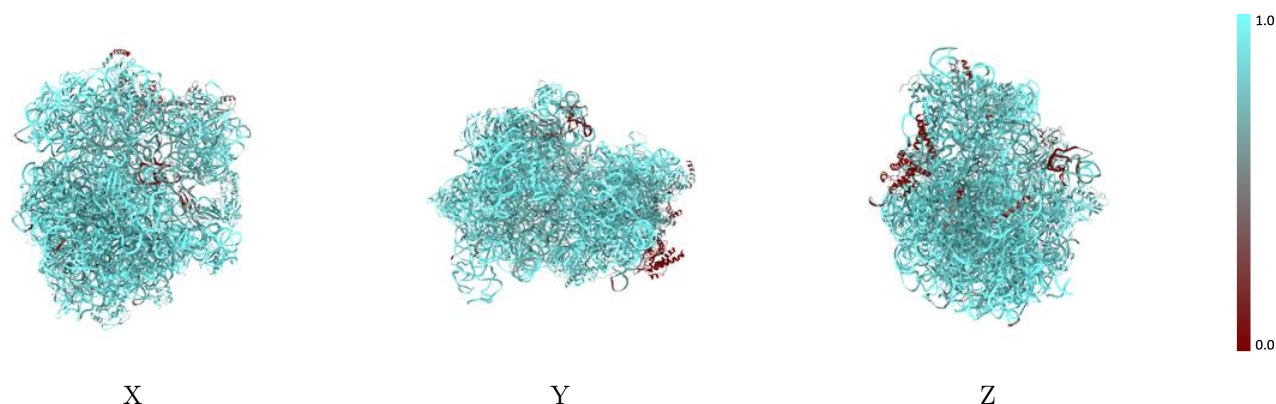
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



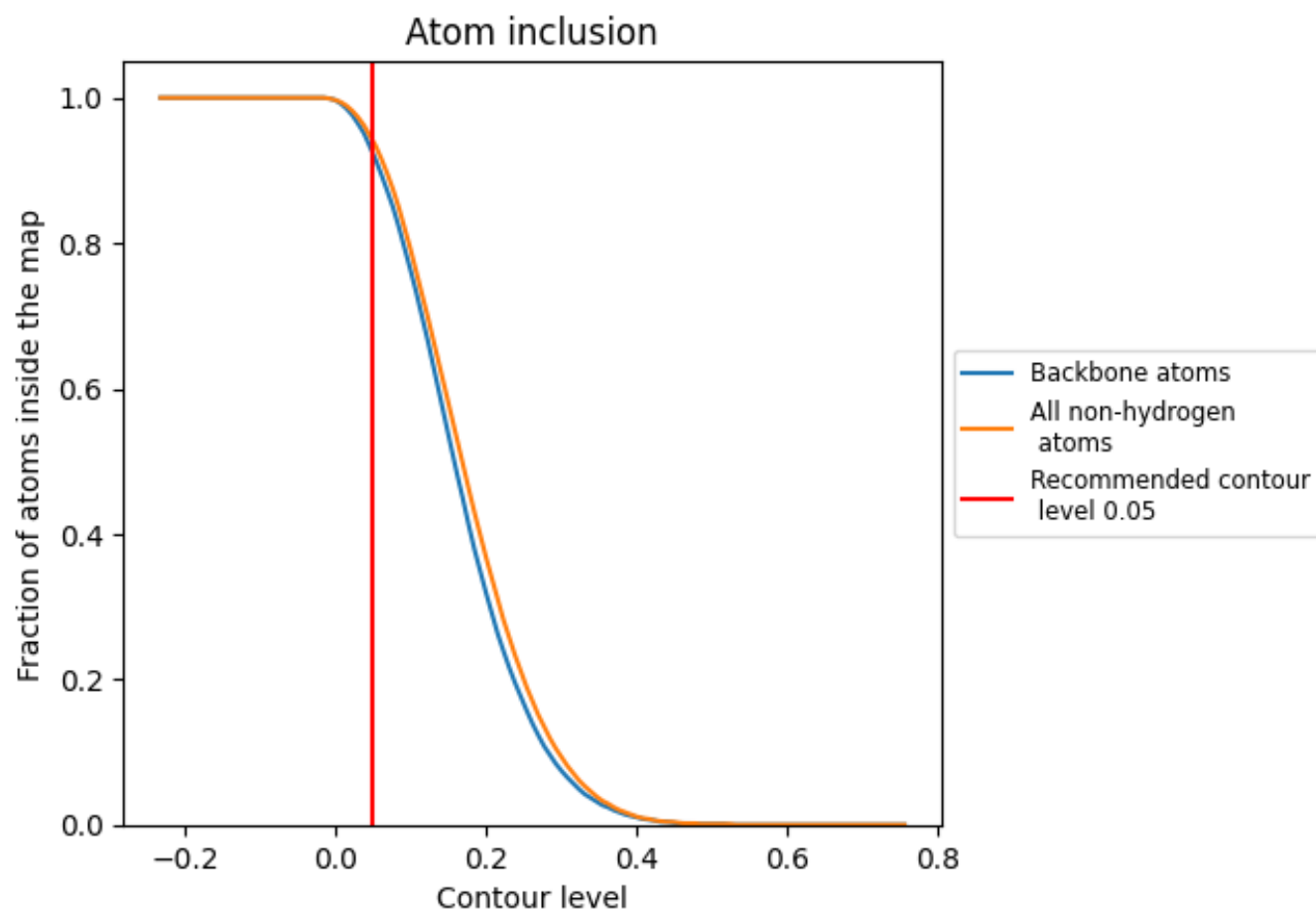
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 94% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9420	 0.5810
0	 0.9580	 0.6150
1	 0.9910	 0.6610
2	 0.9700	 0.6420
3	 0.9560	 0.6240
4	 0.8590	 0.5050
A	 0.9830	 0.5710
B	 0.0430	 0.3090
C	 0.9600	 0.5800
D	 0.8910	 0.5340
E	 0.8340	 0.5490
F	 0.8920	 0.5300
G	 0.7750	 0.4970
H	 0.9440	 0.5860
I	 0.8960	 0.5260
J	 0.8600	 0.4820
K	 0.9320	 0.5650
L	 0.9360	 0.6020
M	 0.6470	 0.4270
N	 0.8800	 0.5360
O	 0.9360	 0.5710
P	 0.8370	 0.4950
Q	 0.8720	 0.5580
R	 0.8450	 0.5280
S	 0.8840	 0.5550
T	 0.9290	 0.5730
U	 0.9180	 0.5210
V	 0.9770	 0.6560
X	 0.9270	 0.6150
Y	 0.7680	 0.4690
a	 0.9690	 0.5980
b	 0.9950	 0.6110
c	 0.9710	 0.6390
d	 0.9700	 0.6280
e	 0.9380	 0.5870



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Chain	Atom inclusion	Q-score
f	 0.9430	 0.5750
g	 0.9120	 0.5240
i	 0.9730	 0.6380
j	 0.9490	 0.6170
k	 0.9590	 0.6140
l	 0.9650	 0.6280
m	 0.9620	 0.6230
n	 0.9720	 0.5940
o	 0.9450	 0.6270
p	 0.9600	 0.6350
q	 0.9490	 0.6150
r	 0.9530	 0.6240
s	 0.9490	 0.6010
t	 0.9370	 0.5940
u	 0.6770	 0.4910
v	 0.9540	 0.6360
w	 0.9720	 0.6380
x	 0.9270	 0.5780
y	 0.9470	 0.6150
z	 0.9630	 0.6280