



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 02:41 pm BST

PDB ID : 5LZC
EMDB ID : EMD-4123
Title : Structure of SelB-Sec-tRNA^{Sec} bound to the 70S ribosome in the codon reading state (CR)
Authors : Fischer, N.; Neumann, P.; Bock, L.V.; Maracci, C.; Wang, Z.; Paleskava, A.; Konevega, A.L.; Schroeder, G.F.; Grubmueller, H.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on : 2016-09-29
Resolution : 4.80 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:

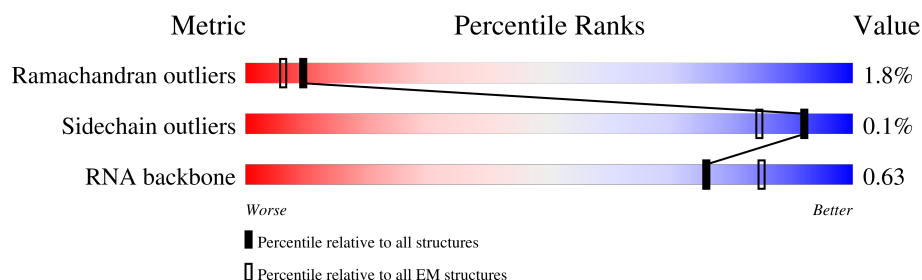
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 4.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	a	1539	
2	b	218	
3	c	206	
4	d	205	
5	e	157	
6	f	100	
7	g	151	
8	h	129	

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Mol	Chain	Length	Quality of chain
9	i	127	17% 94% 6%
10	j	98	23% 93% 6% .
11	k	116	7% 97% .
12	l	123	14% 94% 5% .
13	m	114	14% 94% 6%
14	n	100	16% 96% ..
15	o	88	7% 94% 6%
16	p	82	16% 96% .
17	q	80	14% 96% .
18	r	65	9% 92% 8%
19	s	79	16% 97% ..
20	t	85	9% 100%
21	u	65	32% 94% 6%
22	v	77	. 65% 31% .
23	x	48	31% 38% 29% 33%
24	y	95	13% 58% 37% 5%
25	z	614	50% 96% ..
26	A	2903	. 77% 21% .
27	B	120	82% 14% .
28	C	271	11% 98% .
29	D	209	13% 98% .
30	E	201	18% 99% .
31	F	177	16% 97% .
32	G	176	9% 98% ..
33	I	141	77% 98% ..

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Mol	Chain	Length	Quality of chain
34	H	149	74% 94% 6%
35	J	142	10% 99% .
36	K	122	14% 99% .
37	L	143	14% 99% .
38	M	136	12% 99% .
39	N	120	13% 99% .
40	O	116	9% 98% .
41	P	114	11% 100% .
42	Q	117	7% 99% .
43	R	103	11% 98% .
44	S	110	7% 97% .
45	T	93	13% 99% .
46	U	102	19% 95% ..
47	V	94	13% 99% .
48	W	75	9% 99% .
49	X	77	14% 97% .
50	Y	63	5% 97% .
51	Z	58	17% 97% .
52	0	56	18% 98% .
53	1	50	44% 100% .
54	2	46	13% 100% .
55	3	64	8% 98% .
56	4	38	13% 95% 5%
57	6	66	21% 94% 5%
58	w	3	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	G7M	a	527	X	-	-	-
26	G7M	A	2069	X	-	-	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 152981 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	65	Total	C	N	O	0	0
			505	317	96	92		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	65	Total	C	N	O	S	0	0
			496	307	100	88	1		

- Molecule 22 is a RNA chain called fMet-tRNA^{fMet}.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

- Molecule 23 is a RNA chain called SECIS mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	48	Total	C	N	O	P	0	0
			1025	457	183	337	48		

- Molecule 24 is a RNA chain called Sec-tRNA^{Sec}.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	95	Total	C	N	O	P	0	0
			2031	907	357	672	95		

- Molecule 25 is a protein called Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	z	614	Total	C	N	O	S	0	0
			4853	3043	901	892	17		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	2903	Total	C	N	O	P	0	0
			62335	27815	11467	20150	2903		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 28 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 30 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 31 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	F	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	H	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	K	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	N	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	T	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	U	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	1	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

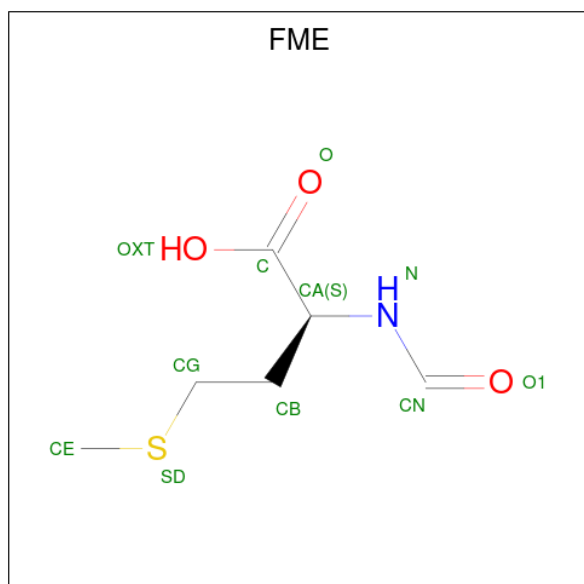
- Molecule 57 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	6	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 58 is a RNA chain called CCA 3' end of E-site tRNA^{Sec} (low occupancy).

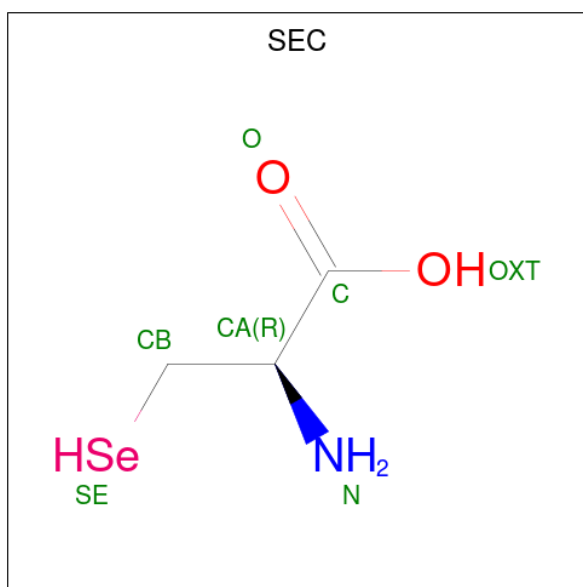
Mol	Chain	Residues	Atoms					AltConf	Trace
58	w	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



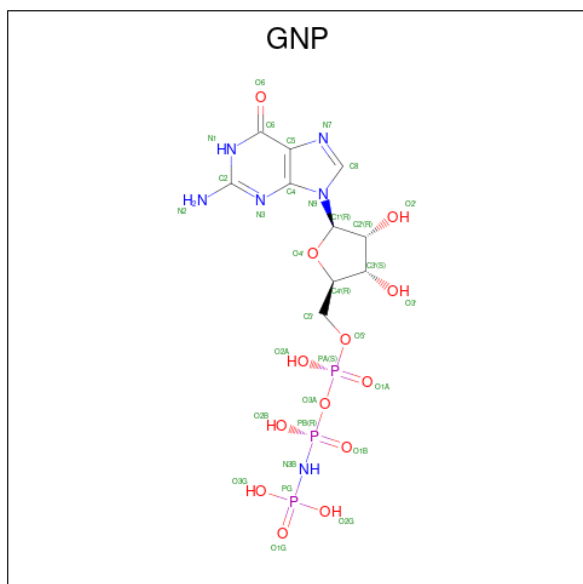
Mol	Chain	Residues	Atoms					AltConf
59	v	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is SELENOCYSTEINE (three-letter code: SEC) (formula: C₃H₇NO₂Se).



Mol	Chain	Residues	Atoms					AltConf
60	y	1	Total	C	N	O	Se	0
			6	3	1	1	1	

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
61	z	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	z	1	Total	Mg	0
			1	1	

- Molecule 63 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
63	4	1	Total	Zn	0
			1	1	
63	6	1	Total	Zn	0
			1	1	

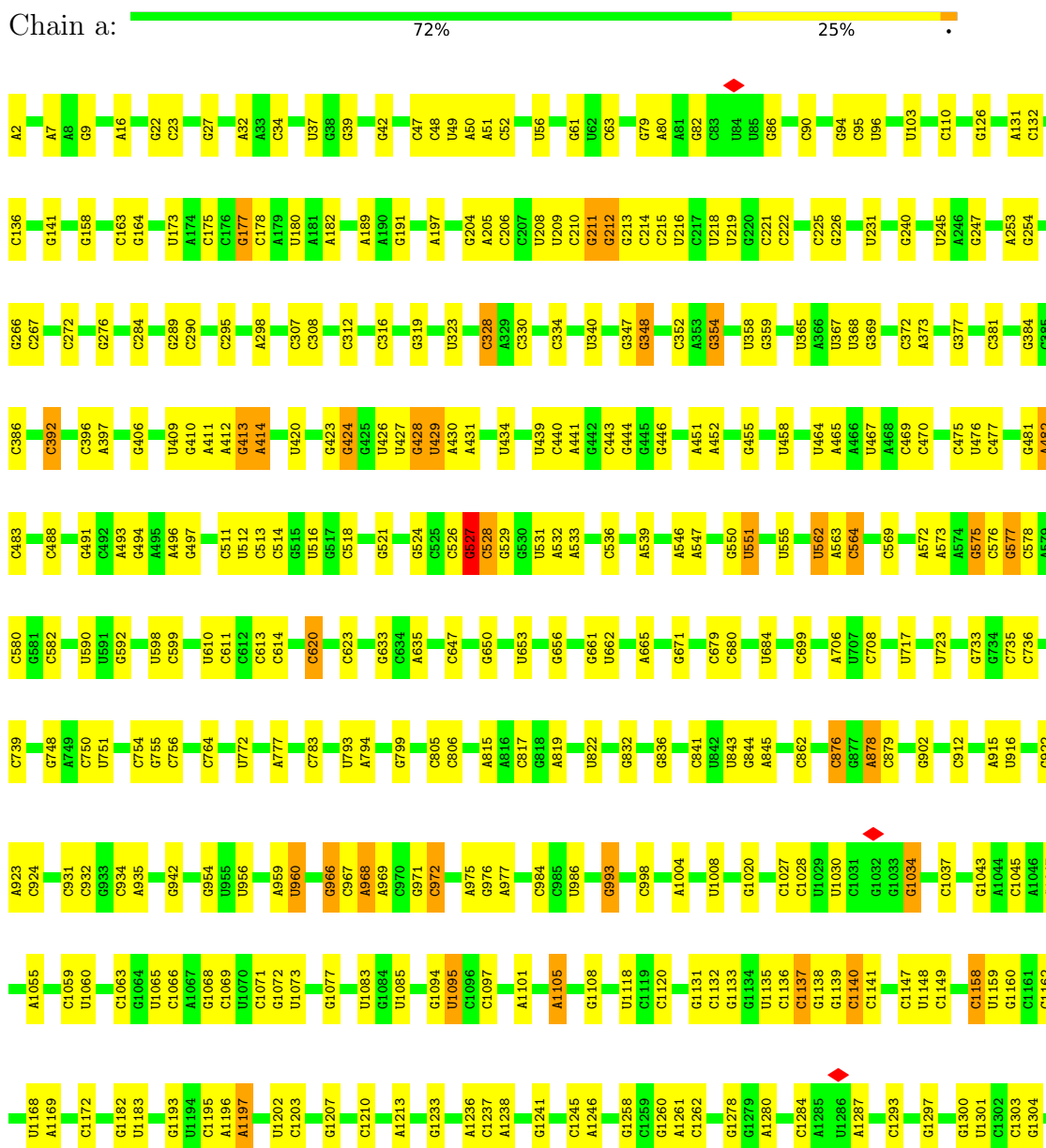
- Molecule 64 is water.

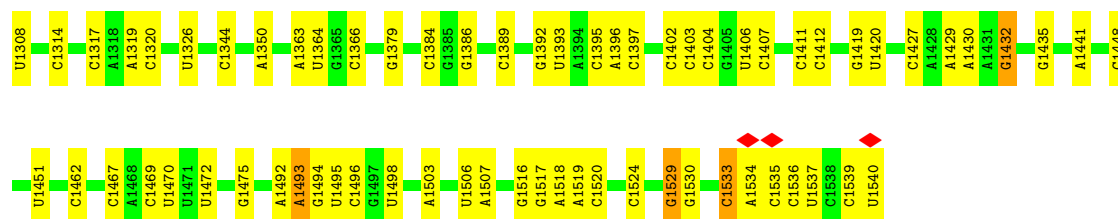
Mol	Chain	Residues	Atoms		AltConf
64	z	2	Total	O	0
			2	2	

3 Residue-property plots

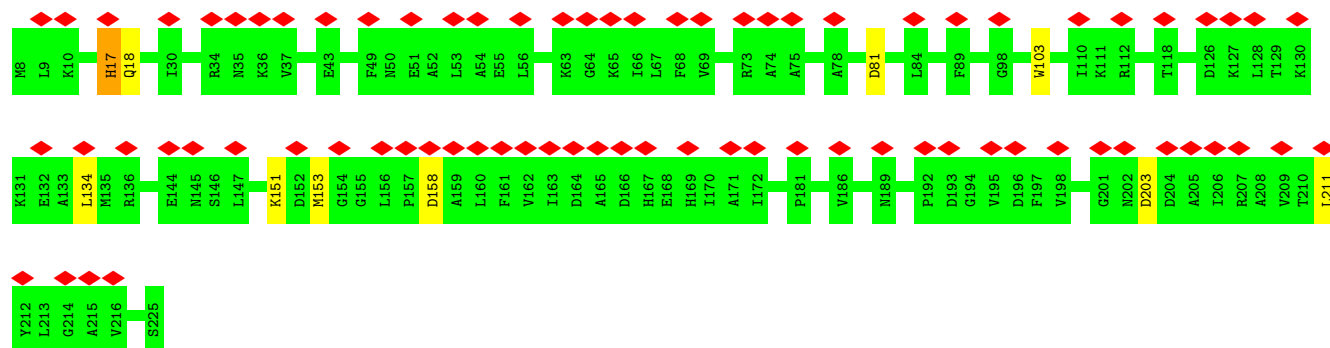
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S ribosomal RNA





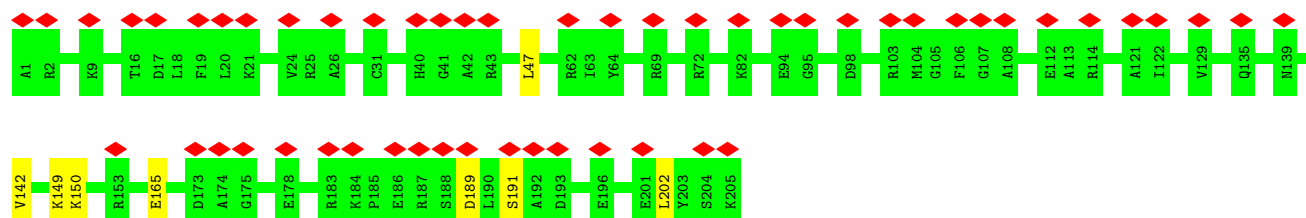
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3




• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5



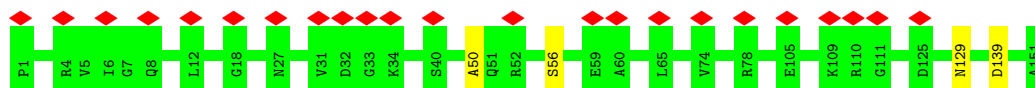
• Molecule 6: 30S ribosomal protein S6

Chain f:  89% 10%



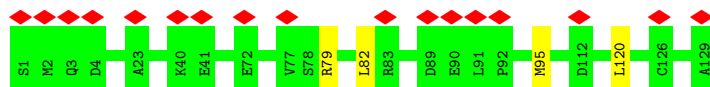
- Molecule 7: 30S ribosomal protein S7

Chain g:  15% 97%



- Molecule 8: 30S ribosomal protein S8

Chain h:  13% 97%

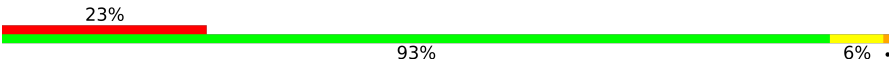


- Molecule 9: 30S ribosomal protein S9

Chain i:  17% 94% 6%



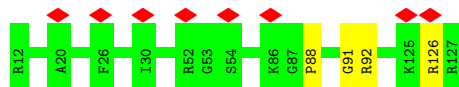
- Molecule 10: 30S ribosomal protein S10

Chain j:  23% 93% 6%



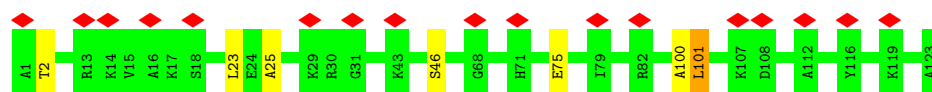
- Molecule 11: 30S ribosomal protein S11

Chain k:  7% 97%

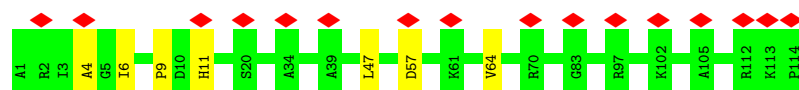


- Molecule 12: 30S ribosomal protein S12

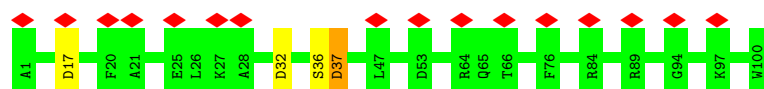
Chain l:  14% 94% 5%



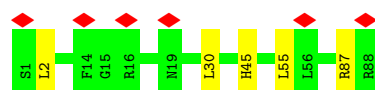
- Molecule 13: 30S ribosomal protein S13



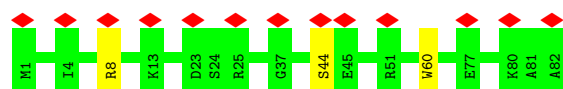
- Molecule 14: 30S ribosomal protein S14



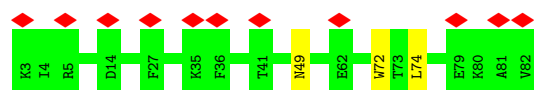
- Molecule 15: 30S ribosomal protein S15



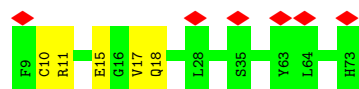
- Molecule 16: 30S ribosomal protein S16



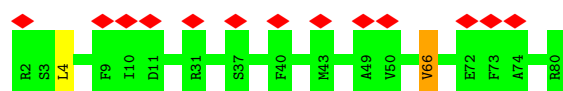
- Molecule 17: 30S ribosomal protein S17



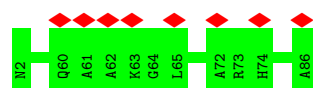
- Molecule 18: 30S ribosomal protein S18



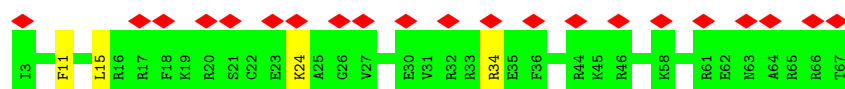
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



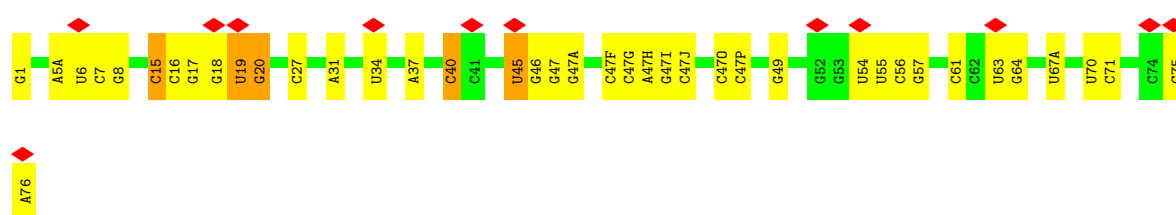
- Molecule 22: fMet-tRNA^{fMet}



- Molecule 23: SECIS mRNA

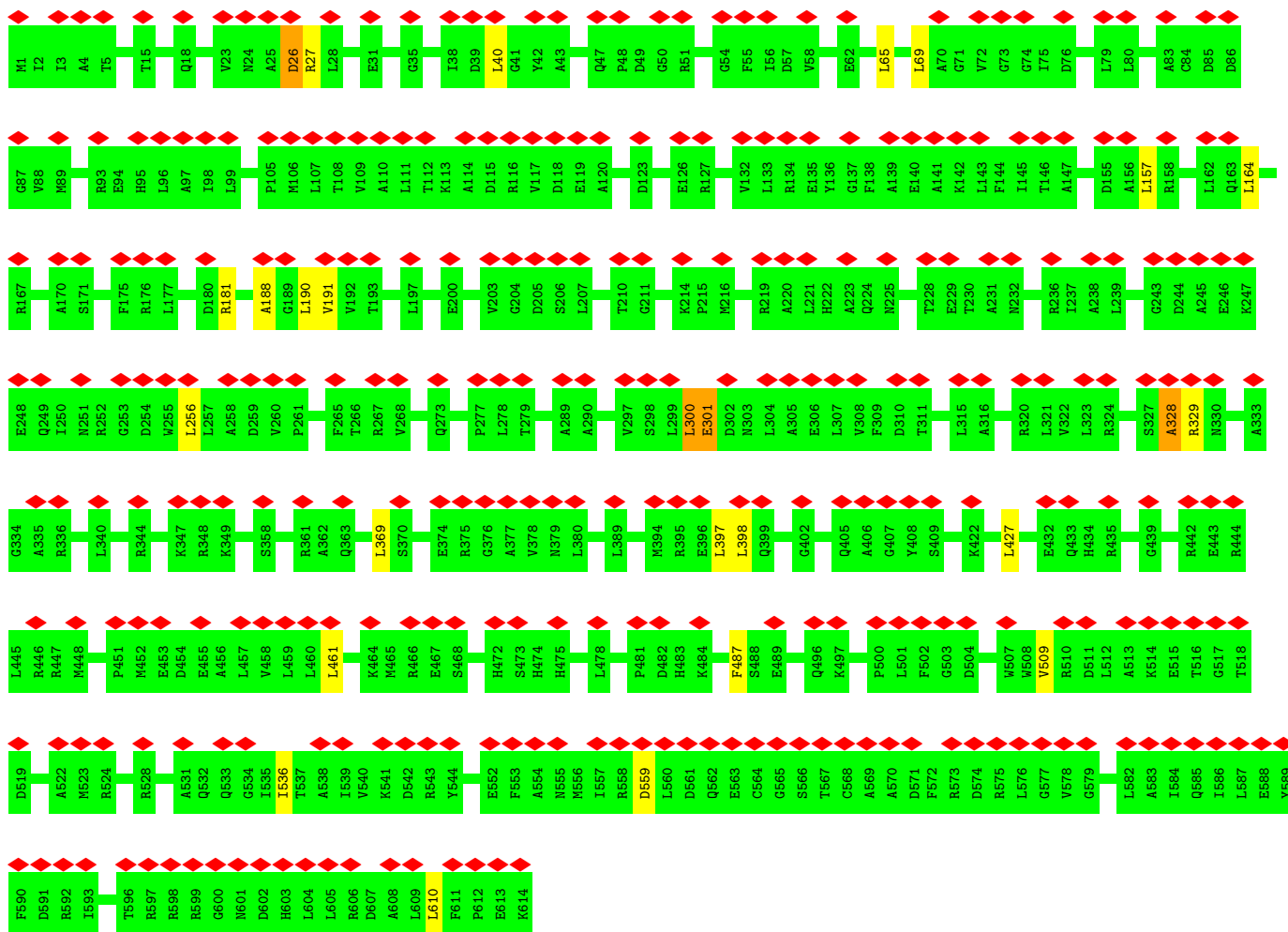


- Molecule 24: Sec-tRNA^{Sec}



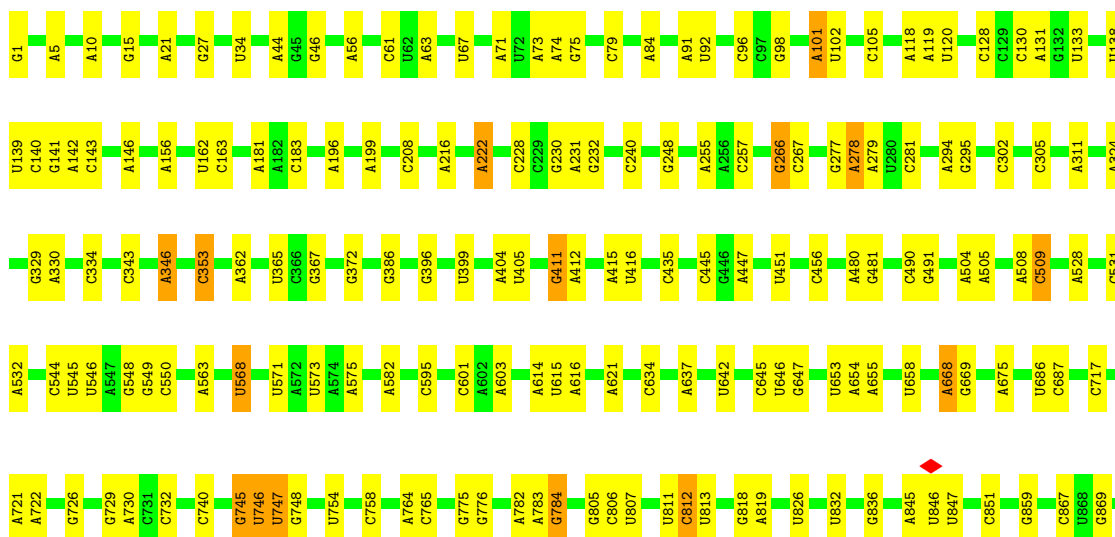
- Molecule 25: Selenocysteine-specific elongation factor






• Molecule 26: 23S ribosomal RNA

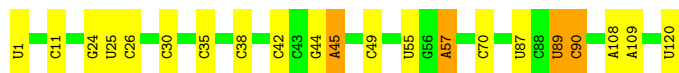
Chain A: 77% 21%.



A2800	U2609	U2457	A2309	U2194	G2110	U1982	C1843	U1648	G1455	U1273	U1101	G1022	G882
C2805	U2613	C2466	C2310	U2195	U2111	C1990	A1847	G1649	U1458	A1287	C1102	U1023	G883
C2815	U2617	C2467	A2322	A2198	G2112	U1991	A1654	A1654	U1459	U1294	A1103	G1026	U884
U2818	U2629	A2468	G2325	A2199	U2113	U1992	A1655	A1655	A1655	U1297	U1105	U1033	C885
A2821	G2630	A2469	A2333	C2200	A2117	U1993	U1657	U1657	U1460	C1298	C1040	A1040	A886
C2826	U2473	U2334	U2334	G2204	U2118	C1994	G1658	G1658	U1468	G1299	U1108	A1044	C887
C2827	U2474	A2469	A2335	C2205	A2119	U1997	G1660	G1660	C1472	G1298	C1109	C1044	C888
U2833	U2475	U2342	U2342	C2206	A2120	C1999	G1669	G1669	U1482	G1299	U1110	C1044	C889
A2839	A2476	U2343	U2343	C2207	U2121	C2006	C1670	C1670	U1484	G1299	U1111	C1045	C890
C2840	G2484	U2344	U2344	A2211	U2122	U2011	C1892	C1892	U1484	C1305	U1112	A1046	C891
U2849	C2498	C2347	C2347	U2212	G2125	U2022	C1894	G1674	C1493	U1313	C1114	A1046	A892
A2850	U2502	U2347	U2347	U2213	A2126	U2023	C1902	C1675	C1494	C1314	C1123	A1049	C901
A2872	G2502	C2350	C2350	C2214	G2127	C2023	C1906	U1680	U1497	U1329	A1133	C1052	A910
A2873	A2503	G2354	G2354	C2215	U2130	A2030	U1911	G1715	U1515	U1340	A1134	A1054	U919
U2884	U2504	C2359	C2359	G2216	U2131	A2031	A1912	G1723	A1535	C1345	C1135	G1055	U931
C2888	U2505	G2379	G2379	G2217	U2132	A2033	A1913	G1738	C1536	C1346	G1138	A1057	U932
G2895	U2506	C2380	C2380	A2227	G2133	A2036	C1914	G1738	G1537	C1348	U1142	U1058	A933
U2903	A2513	G2388	G2388	A2227	A2134	A2037	3TD1915	C1744	U1539	C1349	A1143	G1059	A941
C2895	U2518	G2388	G2388	G2238	A2135	C2043	A1916	A1744	U1539	G1358	U1159	U1060	U1061
U2903	U2519	U2383	U2383	G2239	G2141	C2044	A1917	C1752	C1557	G1359	C1150	G1062	C946
C2895	G2520	C2385	C2385	C2248	A2142	G2049	A1919	U1758	C1564	A1365	G1157	G1063	U955
U2903	U2529	G2388	G2388	G2251	C2143	C2050	C1920	C1758	C1565	U1378	U1159	U1066	U955
C2895	A2547	U2388	U2388	G2252	G2144	C2055	G1929	G1763	C1565	A1378	G1171	A1067	A959
U2903	U2552	C2394	C2394	G2253	C2145	G2056	G1930	C1764	A1566	G1380	C1172	A1067	A960
U2903	G2553	U2402	U2402	G2254	A2147	C2061	U1931	C1771	C1566	U1379	C1173	A1068	C961
U2903	U2554	C2403	C2403	C2255	C2150	A2062	A1936	A1772	U1578	G1383	U1176	A1069	G962
U2903	U2555	G2416	G2416	G2256	U2151	C2063	A1937	A1773	C1582	C1386	G1177	G1071	C965
U2903	C2556	C2417	C2417	G2257	G2152	C2064	U1939	A1784	U1583	U1396	C1178	A1072	C968
U2903	U2562	C2420	C2420	G2275	C2153	C2065	U1940	C1787	U1584	U1396	G1179	G1074	A973
U2903	G2567	G2428	G2428	C2276	G2157	C2066	G1945	C1788	C1585	U1397	U1180	C1075	G974
U2903	A2572	A2429	A2429	A2278	A2158	G2069	U1955	A1791	C1595	C1398	C1200	C1076	C974
U2903	G2576	G2430	G2430	G2279	G2160	A2070	U1956	C1795	A1598	U1399	G1206	C1077	C982
U2903	C2579	U2431	U2431	G2280	C2161	C2071	C1957	C1799	U1599	C1399	U1210	C1078	A983
U2903	U2580	A2434	A2434	A2281	G2162	C2072	C1958	G1799	C1600	U1402	G1211	A1080	A984
U2903	C2581	G2435	G2435	G2282	A2163	A2077	G1959	C1800	C1607	G1416	C1243	U1081	A990
U2903	U2582	U2436	U2436	C2283	A2164	C2080	A1960	A1801	U1608	C1417	C1244	U1082	C991
U2903	G2583	G2441	G2441	A2287	G2168	A2080	C1961	A1802	A1609	A1420	A1254	A1083	A996
U2903	C2584	C2442	C2442	U2292	U2172	C2089	U1963	A1808	A1616	C1428	A1253	A1084	C1006
U2903	U2591	G2445	G2445	C2300	A2173	G2093	G1964	C1816	C1617	C1447	U1255	A1085	C1087
U2903	A2602	G2446	G2446	C2301	C2174	G2105	U1967	C1829	A1618	G1452	U1256	A1086	A1009
U2903	G2603	U2447	U2447	U2302	G2175	U2106	C1967	C1830	C1639	G1452	G1257	A1087	U1012
U2903	U2604	A2448	A2448	U2305	A2176	U2107	A1970	C1839	C1646	G1452	C1257	C1092	C1013
U2903	U2605	U2449	U2449	U2306	U2177	U2108	U1971	C1839	U1647	G1452	G1271	G1093	A1021
U2903	U2605	U2449	U2449	U2307	U2180	U2109	G1972	G1835	U1647	G1452	A1272	U1097	A1021

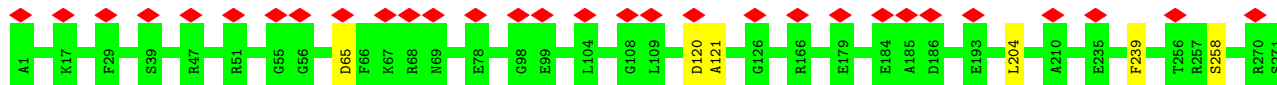
- Molecule 27: 5S ribosomal RNA

Chain B:  82% 14%



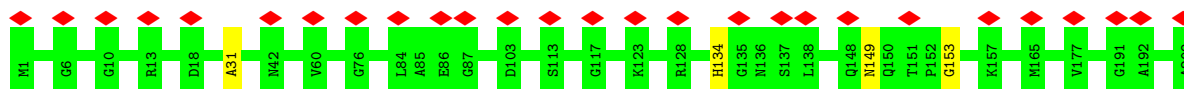
- Molecule 28: 50S ribosomal protein L2

Chain C:  11% 98%



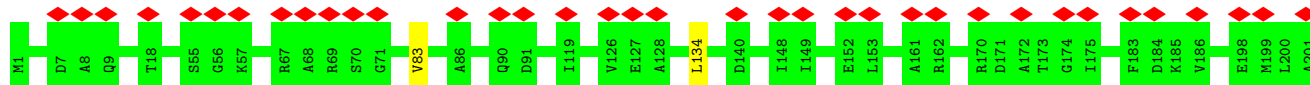
- Molecule 29: 50S ribosomal protein L3

Chain D:  13% 98%



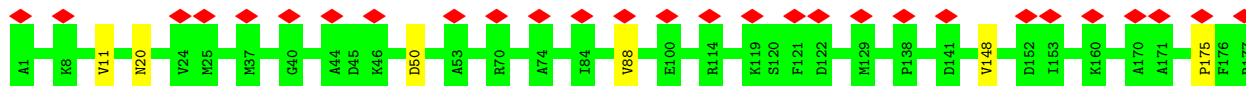
- Molecule 30: 50S ribosomal protein L4

Chain E:  18% 99%



- Molecule 31: 50S ribosomal protein L5

Chain F:  16% 97%

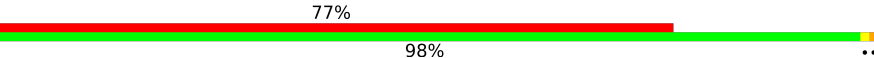


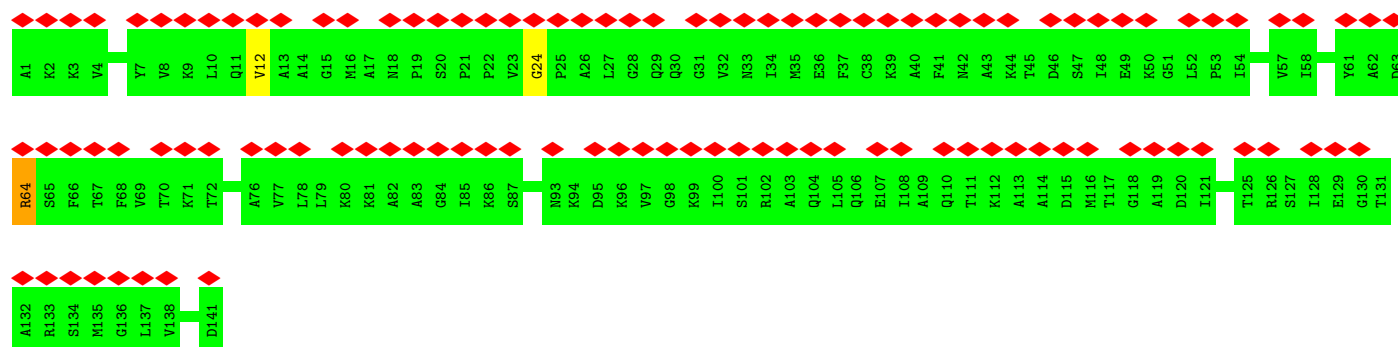
- Molecule 32: 50S ribosomal protein L6

Chain G:  9% 98%

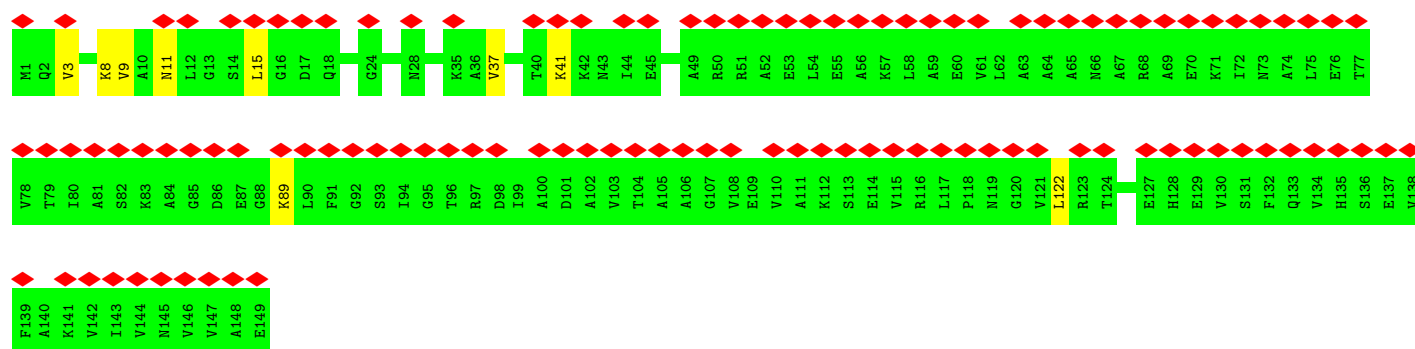
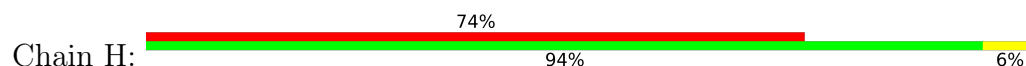


- Molecule 33: 50S ribosomal protein L11

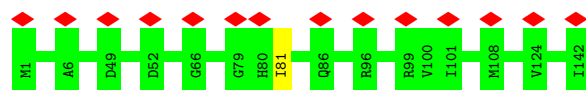
Chain I:  77% 98%



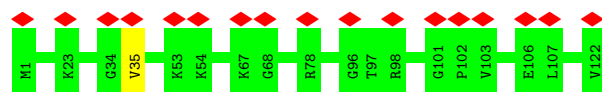
• Molecule 34: 50S ribosomal protein L9



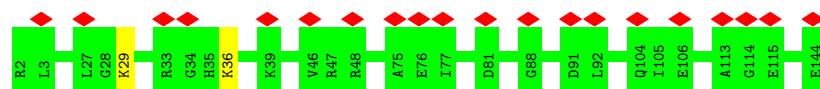
• Molecule 35: 50S ribosomal protein L13



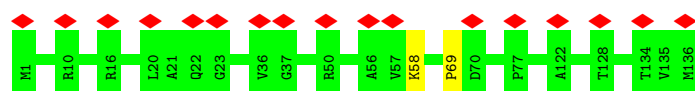
• Molecule 36: 50S ribosomal protein L14



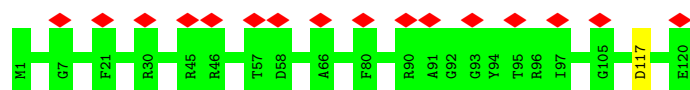
• Molecule 37: 50S ribosomal protein L15



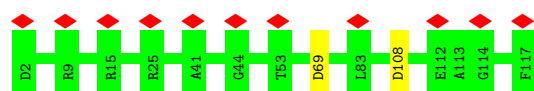
• Molecule 38: 50S ribosomal protein L16



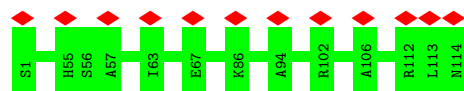
- Molecule 39: 50S ribosomal protein L17



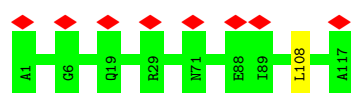
- Molecule 40: 50S ribosomal protein L18



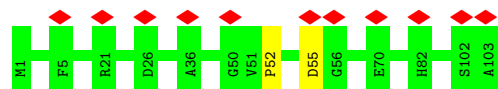
- Molecule 41: 50S ribosomal protein L19



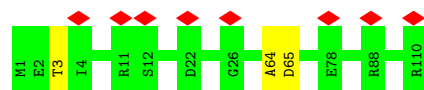
- Molecule 42: 50S ribosomal protein L20



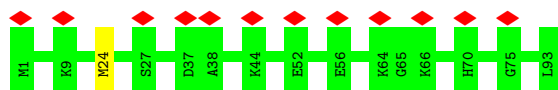
- Molecule 43: 50S ribosomal protein L21



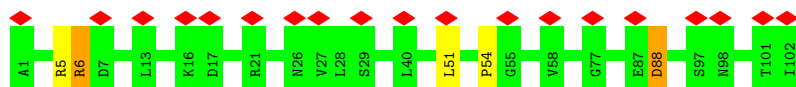
- Molecule 44: 50S ribosomal protein L22



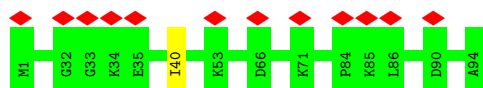
• Molecule 45: 50S ribosomal protein L23



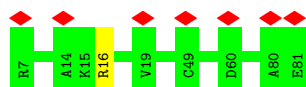
• Molecule 46: 50S ribosomal protein L24



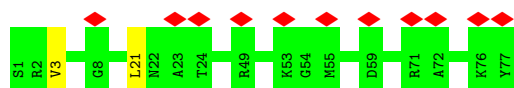
• Molecule 47: 50S ribosomal protein L25



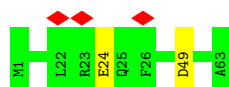
• Molecule 48: 50S ribosomal protein L27



• Molecule 49: 50S ribosomal protein L28

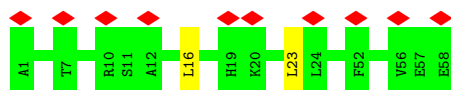


• Molecule 50: 50S ribosomal protein L29

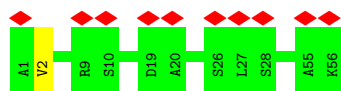


• Molecule 51: 50S ribosomal protein L30

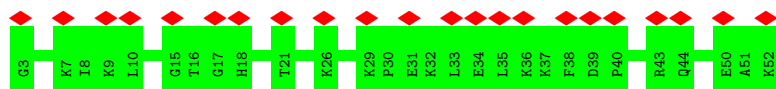




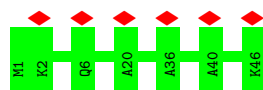
- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33



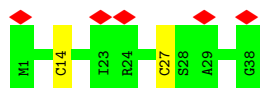
- Molecule 54: 50S ribosomal protein L34



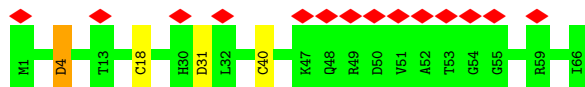
- Molecule 55: 50S ribosomal protein L35



- Molecule 56: 50S ribosomal protein L36



- Molecule 57: 50S ribosomal protein L31



- Molecule 58: CCA 3' end of E-site tRNA^{Sec} (low occupancy)

Chain w:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11658	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Local CTF correction, after MSA based classification and averaging of local power spectra	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.975	Depositor
Minimum map value	-0.877	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.191	Depositor
Recommended contour level	0.37	Depositor
Map size (\AA)	315.52, 315.52, 315.52	wwPDB
Map dimensions	272, 272, 272	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.16, 1.16, 1.16	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MG, 5MU, 2MG, OMU, PSU, UR3, 6MZ, OMG, MG, 3TD, H2U, G7M, 4OC, 4SU, ZN, SEC, FME, 2MA, OMC, GNP, 5MC, 6IA, MA6

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.60	4/36701 (0.0%)	1.38	560/57246 (1.0%)
2	b	0.49	0/1736	0.88	4/2338 (0.2%)
3	c	0.41	0/1652	0.75	3/2225 (0.1%)
4	d	0.57	0/1665	0.98	4/2227 (0.2%)
5	e	0.46	0/1170	0.86	1/1573 (0.1%)
6	f	0.52	1/836 (0.1%)	0.92	3/1128 (0.3%)
7	g	0.47	0/1196	0.79	1/1602 (0.1%)
8	h	0.46	0/989	0.83	4/1326 (0.3%)
9	i	0.48	0/1034	0.86	2/1375 (0.1%)
10	j	0.45	0/797	0.91	2/1077 (0.2%)
11	k	0.54	0/886	0.86	0/1195
12	l	0.49	0/969	0.80	1/1300 (0.1%)
13	m	0.42	0/893	0.85	3/1193 (0.3%)
14	n	0.45	0/806	0.80	2/1074 (0.2%)
15	o	0.40	0/722	0.76	2/964 (0.2%)
16	p	0.52	0/659	0.86	1/884 (0.1%)
17	q	0.44	0/658	0.84	1/881 (0.1%)
18	r	0.38	0/512	0.84	1/689 (0.1%)
19	s	0.38	0/653	0.77	1/877 (0.1%)
20	t	0.46	0/671	0.75	0/888
21	u	0.42	0/501	0.79	1/668 (0.1%)
22	v	0.65	1/1745 (0.1%)	1.47	33/2716 (1.2%)
23	x	0.92	2/1145 (0.2%)	1.88	45/1781 (2.5%)
24	y	0.70	1/2168 (0.0%)	1.52	35/3375 (1.0%)
25	z	0.50	0/4952	0.97	23/6712 (0.3%)
26	A	0.57	16/69240 (0.0%)	1.25	623/108014 (0.6%)
27	B	0.56	1/2873 (0.0%)	1.21	16/4478 (0.4%)
28	C	0.42	0/2122	0.75	1/2852 (0.0%)
29	D	0.47	0/1586	0.73	0/2134
30	E	0.45	0/1571	0.74	1/2113 (0.0%)
31	F	0.54	1/1435 (0.1%)	0.85	3/1926 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	G	0.55	0/1343	0.89	1/1816 (0.1%)
33	I	0.49	0/1046	0.96	2/1410 (0.1%)
34	H	0.41	0/1122	0.78	2/1515 (0.1%)
35	J	0.43	0/1152	0.66	0/1551
36	K	0.45	0/948	0.74	0/1268
37	L	0.43	0/1054	0.76	0/1403
38	M	0.42	0/1093	0.73	0/1460
39	N	0.45	0/974	0.68	0/1301
40	O	0.43	0/902	0.73	2/1209 (0.2%)
41	P	0.45	0/929	0.68	0/1242
42	Q	0.42	0/960	0.63	1/1278 (0.1%)
43	R	0.45	0/829	0.76	0/1107
44	S	0.41	0/864	0.73	0/1156
45	T	0.46	0/745	0.78	0/994
46	U	0.46	0/788	0.86	3/1051 (0.3%)
47	V	0.44	0/766	0.73	1/1025 (0.1%)
48	W	0.39	0/582	0.72	0/769
49	X	0.36	0/635	0.74	2/848 (0.2%)
50	Y	0.49	0/510	0.90	1/677 (0.1%)
51	Z	0.38	0/453	0.71	2/605 (0.3%)
52	0	0.36	0/450	0.76	0/599
53	1	0.35	0/417	0.75	0/554
54	2	0.43	0/380	0.75	0/498
55	3	0.41	0/513	0.70	1/676 (0.1%)
56	4	0.60	1/303 (0.3%)	0.86	1/397 (0.3%)
57	6	0.44	0/532	0.87	2/709 (0.3%)
58	w	0.41	0/68	1.01	0/103
All	All	0.55	28/164901 (0.0%)	1.19	1398/246052 (0.6%)

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
1	a	2	0
2	b	0	1
6	f	0	1
9	i	0	2
12	l	0	2
14	n	0	2
18	r	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	z	0	2
26	A	2	0
28	C	0	1
34	H	0	1
46	U	0	1
All	All	4	14

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	B	1	U	OP3-P	-10.72	1.48	1.61
24	y	1	G	OP3-P	-10.71	1.48	1.61
26	A	1	G	OP3-P	-10.60	1.48	1.61
23	x	87	A	OP3-P	-10.53	1.48	1.61
22	v	1	C	OP3-P	-10.48	1.48	1.61

The worst 5 of 1398 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1044	C	N1-C2-O2	18.02	129.71	118.90
1	a	452	A	O5'-P-OP1	-17.50	89.70	110.70
26	A	1044	C	C6-N1-C2	-16.95	113.52	120.30
26	A	1071	G	C5-C6-N1	16.75	119.88	111.50
26	A	1071	G	C2-N3-C4	16.40	120.10	111.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C3',C4'
26	A	2069	G7M	C3',C4'

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	b	17	HIS	Mainchain
6	f	93	LYS	Peptide
9	i	101	GLY	Mainchain
9	i	56	MET	Mainchain
12	l	100	ALA	Mainchain

5.2 Too-close contacts ⓘ

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

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	
2	b	216/218 (99%)	186 (86%)	24 (11%)	6 (3%)	4	24
3	c	204/206 (99%)	192 (94%)	9 (4%)	3 (2%)	8	39
4	d	203/205 (99%)	187 (92%)	12 (6%)	4 (2%)	6	31
5	e	155/157 (99%)	142 (92%)	9 (6%)	4 (3%)	4	25
6	f	98/100 (98%)	86 (88%)	5 (5%)	7 (7%)	1	11
7	g	149/151 (99%)	139 (93%)	7 (5%)	3 (2%)	6	31
8	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
9	i	125/127 (98%)	111 (89%)	10 (8%)	4 (3%)	3	21
10	j	96/98 (98%)	83 (86%)	7 (7%)	6 (6%)	1	13
11	k	114/116 (98%)	103 (90%)	7 (6%)	4 (4%)	3	20
12	l	121/123 (98%)	110 (91%)	6 (5%)	5 (4%)	2	18
13	m	112/114 (98%)	102 (91%)	6 (5%)	4 (4%)	3	20
14	n	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	13	48
15	o	86/88 (98%)	76 (88%)	7 (8%)	3 (4%)	3	20
16	p	80/82 (98%)	72 (90%)	6 (8%)	2 (2%)	4	26
17	q	78/80 (98%)	69 (88%)	7 (9%)	2 (3%)	4	25
18	r	63/65 (97%)	58 (92%)	2 (3%)	3 (5%)	2	16
19	s	77/79 (98%)	70 (91%)	5 (6%)	2 (3%)	4	25
20	t	83/85 (98%)	78 (94%)	5 (6%)	0	100	100
21	u	63/65 (97%)	55 (87%)	5 (8%)	3 (5%)	2	16
25	z	612/614 (100%)	588 (96%)	18 (3%)	6 (1%)	13	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	C	269/271 (99%)	252 (94%)	13 (5%)	4 (2%)	8	39
29	D	207/209 (99%)	191 (92%)	12 (6%)	4 (2%)	6	32
30	E	199/201 (99%)	190 (96%)	8 (4%)	1 (0%)	25	64
31	F	175/177 (99%)	157 (90%)	15 (9%)	3 (2%)	7	35
32	G	174/176 (99%)	167 (96%)	5 (3%)	2 (1%)	12	46
33	I	139/141 (99%)	121 (87%)	15 (11%)	3 (2%)	5	29
34	H	147/149 (99%)	134 (91%)	7 (5%)	6 (4%)	2	18
35	J	140/142 (99%)	135 (96%)	4 (3%)	1 (1%)	19	56
36	K	120/122 (98%)	114 (95%)	5 (4%)	1 (1%)	16	53
37	L	141/143 (99%)	128 (91%)	11 (8%)	2 (1%)	9	40
38	M	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	8	39
39	N	118/120 (98%)	111 (94%)	6 (5%)	1 (1%)	16	53
40	O	114/116 (98%)	105 (92%)	9 (8%)	0	100	100
41	P	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
42	Q	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
43	R	101/103 (98%)	92 (91%)	7 (7%)	2 (2%)	6	31
44	S	108/110 (98%)	103 (95%)	2 (2%)	3 (3%)	4	24
45	T	91/93 (98%)	81 (89%)	9 (10%)	1 (1%)	12	46
46	U	100/102 (98%)	89 (89%)	8 (8%)	3 (3%)	3	22
47	V	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
48	W	73/75 (97%)	69 (94%)	3 (4%)	1 (1%)	9	40
49	X	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
50	Y	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	8	37
51	Z	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
52	0	54/56 (96%)	51 (94%)	2 (4%)	1 (2%)	6	32
53	1	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
54	2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
55	3	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
56	4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
57	6	64/66 (97%)	57 (89%)	4 (6%)	3 (5%)	2	17
All	All	6329/6431 (98%)	5850 (92%)	362 (6%)	117 (2%)	9	34

5 of 117 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	17	HIS
2	b	18	GLN
2	b	103	TRP
5	e	89	THR
6	f	92	THR

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	
2	b	180/180 (100%)	180 (100%)	0	100	100
3	c	170/170 (100%)	170 (100%)	0	100	100
4	d	172/172 (100%)	172 (100%)	0	100	100
5	e	119/119 (100%)	119 (100%)	0	100	100
6	f	87/87 (100%)	87 (100%)	0	100	100
7	g	124/124 (100%)	124 (100%)	0	100	100
8	h	104/104 (100%)	104 (100%)	0	100	100
9	i	105/105 (100%)	105 (100%)	0	100	100
10	j	86/86 (100%)	86 (100%)	0	100	100
11	k	89/89 (100%)	89 (100%)	0	100	100
12	l	103/103 (100%)	102 (99%)	1 (1%)	73	82
13	m	92/92 (100%)	92 (100%)	0	100	100
14	n	79/83 (95%)	79 (100%)	0	100	100
15	o	76/76 (100%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	74/74 (100%)	74 (100%)	0	100	100
18	r	48/56 (86%)	48 (100%)	0	100	100
19	s	70/70 (100%)	70 (100%)	0	100	100
20	t	65/65 (100%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	u	44/55 (80%)	44 (100%)	0	100	100
25	z	501/501 (100%)	499 (100%)	2 (0%)	89	91
28	C	216/216 (100%)	216 (100%)	0	100	100
29	D	164/164 (100%)	164 (100%)	0	100	100
30	E	165/165 (100%)	165 (100%)	0	100	100
31	F	148/148 (100%)	148 (100%)	0	100	100
32	G	137/137 (100%)	135 (98%)	2 (2%)	60	75
33	I	109/109 (100%)	109 (100%)	0	100	100
34	H	114/114 (100%)	114 (100%)	0	100	100
35	J	116/116 (100%)	116 (100%)	0	100	100
36	K	103/103 (100%)	103 (100%)	0	100	100
37	L	102/102 (100%)	102 (100%)	0	100	100
38	M	109/109 (100%)	109 (100%)	0	100	100
39	N	100/100 (100%)	100 (100%)	0	100	100
40	O	86/86 (100%)	86 (100%)	0	100	100
41	P	99/99 (100%)	99 (100%)	0	100	100
42	Q	89/89 (100%)	89 (100%)	0	100	100
43	R	84/84 (100%)	84 (100%)	0	100	100
44	S	93/93 (100%)	93 (100%)	0	100	100
45	T	80/80 (100%)	80 (100%)	0	100	100
46	U	83/83 (100%)	83 (100%)	0	100	100
47	V	78/78 (100%)	78 (100%)	0	100	100
48	W	57/57 (100%)	57 (100%)	0	100	100
49	X	67/67 (100%)	67 (100%)	0	100	100
50	Y	55/55 (100%)	55 (100%)	0	100	100
51	Z	48/48 (100%)	48 (100%)	0	100	100
52	0	47/47 (100%)	47 (100%)	0	100	100
53	1	45/45 (100%)	45 (100%)	0	100	100
54	2	38/38 (100%)	38 (100%)	0	100	100
55	3	51/51 (100%)	51 (100%)	0	100	100
56	4	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	6	59/59 (100%)	59 (100%)	0	100	100
All	All	5229/5252 (100%)	5224 (100%)	5 (0%)	92	94

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	l	23	LEU
25	z	26	ASP
25	z	27	ARG
32	G	104	LEU
32	G	157	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
30	E	90	GLN
32	G	142	GLN
32	G	72	ASN
33	I	42	ASN
20	t	60	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	176 (11%)	0
22	v	76/77 (98%)	7 (9%)	0
23	x	47/48 (97%)	27 (57%)	0
24	y	93/95 (97%)	20 (21%)	0
26	A	2898/2903 (99%)	381 (13%)	10 (0%)
27	B	119/120 (99%)	14 (11%)	0
58	w	2/3 (66%)	0	0
All	All	4770/4785 (99%)	625 (13%)	10 (0%)

5 of 625 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	7	A
1	a	9	G
1	a	22	G

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Mol	Chain	Res	Type
1	a	32	A
1	a	39	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	1358	G
26	A	1875	G
26	A	2756	U
26	A	960	A
26	A	1045	C

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

43 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	$\# Z > 2$
1	5MC	a	1407	1	18,22,23	1.03	2 (11%)	26,32,35	1.54	4 (15%)
26	5MU	A	1939	26	19,22,23	1.38	5 (26%)	28,32,35	2.02	6 (21%)
26	PSU	A	1911	26	18,21,22	1.42	4 (22%)	22,30,33	2.00	4 (18%)
26	OMC	A	2498	26	19,22,23	0.88	0	26,31,34	1.22	3 (11%)
1	MA6	a	1518	1	18,26,27	0.92	1 (5%)	19,38,41	1.91	4 (21%)
22	5MU	v	54	22	19,22,23	1.52	6 (31%)	28,32,35	2.09	9 (32%)
26	OMU	A	2552	26	19,22,23	1.23	3 (15%)	26,31,34	1.88	7 (26%)
1	2MG	a	1516	1	18,26,27	0.92	1 (5%)	16,38,41	1.07	2 (12%)
26	PSU	A	2605	26	18,21,22	1.39	3 (16%)	22,30,33	1.93	4 (18%)
24	5MU	y	54	24	19,22,23	1.47	5 (26%)	28,32,35	1.86	7 (25%)
24	6IA	y	37	24	22,29,30	0.82	1 (4%)	22,41,44	2.39	5 (22%)
22	4SU	v	8	22	18,21,22	1.82	4 (22%)	26,30,33	2.67	6 (23%)
24	H2U	y	19	24	18,21,22	0.99	2 (11%)	21,30,33	1.37	3 (14%)
1	MA6	a	1519	1	18,26,27	0.97	1 (5%)	19,38,41	1.89	6 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	2MG	A	1835	26	18,26,27	0.92	1 (5%)	16,38,41	1.19	2 (12%)
26	PSU	A	2504	26	18,21,22	1.35	3 (16%)	22,30,33	1.74	4 (18%)
1	G7M	a	527	1	20,26,27	1.57	3 (15%)	17,39,42	1.74	5 (29%)
22	H2U	v	20	22	18,21,22	1.05	2 (11%)	21,30,33	1.44	3 (14%)
26	H2U	A	2449	26	18,21,22	1.16	3 (16%)	21,30,33	1.30	3 (14%)
26	3TD	A	1915	26	18,22,23	4.07	7 (38%)	22,32,35	1.76	3 (13%)
26	1MG	A	745	26	18,26,27	0.83	1 (5%)	19,39,42	1.15	2 (10%)
26	PSU	A	746	26	18,21,22	1.37	2 (11%)	22,30,33	1.98	4 (18%)
26	PSU	A	1917	26	18,21,22	1.47	3 (16%)	22,30,33	1.83	4 (18%)
1	UR3	a	1498	1	19,22,23	1.13	1 (5%)	26,32,35	1.81	5 (19%)
26	PSU	A	2580	26	18,21,22	1.37	3 (16%)	22,30,33	1.84	3 (13%)
26	2MG	A	2445	26	18,26,27	0.97	1 (5%)	16,38,41	1.18	3 (18%)
24	PSU	y	55	24	18,21,22	1.41	3 (16%)	22,30,33	1.84	4 (18%)
26	6MZ	A	2030	26	18,25,26	0.99	1 (5%)	16,36,39	1.82	3 (18%)
26	2MA	A	2503	26	17,25,26	1.04	2 (11%)	17,37,40	1.24	2 (11%)
26	5MC	A	1962	26	18,22,23	0.95	1 (5%)	26,32,35	1.47	4 (15%)
26	PSU	A	955	26	18,21,22	1.40	2 (11%)	22,30,33	2.01	3 (13%)
26	PSU	A	2457	26	18,21,22	1.41	3 (16%)	22,30,33	1.98	4 (18%)
26	OMG	A	2251	26,22	18,26,27	0.97	1 (5%)	19,38,41	1.10	2 (10%)
1	4OC	a	1402	1	20,23,24	0.76	0	26,32,35	1.18	3 (11%)
1	2MG	a	966	1	18,26,27	1.06	2 (11%)	16,38,41	1.38	3 (18%)
1	PSU	a	516	1	18,21,22	1.37	2 (11%)	22,30,33	2.13	5 (22%)
26	G7M	A	2069	26	20,26,27	1.57	3 (15%)	17,39,42	1.52	3 (17%)
22	PSU	v	55	22	18,21,22	1.48	3 (16%)	22,30,33	1.90	4 (18%)
1	5MC	a	967	1	18,22,23	1.04	1 (5%)	26,32,35	0.91	0
26	PSU	A	2604	26	18,21,22	1.45	4 (22%)	22,30,33	1.96	3 (13%)
26	6MZ	A	1618	26	18,25,26	0.97	1 (5%)	16,36,39	2.08	4 (25%)
26	5MU	A	747	26	19,22,23	1.50	6 (31%)	28,32,35	2.10	8 (28%)
1	2MG	a	1207	1	18,26,27	0.91	1 (5%)	16,38,41	1.12	2 (12%)

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
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
26	5MU	A	1939	26	-	0/7/25/26	0/2/2/2
26	PSU	A	1911	26	-	0/7/25/26	0/2/2/2
26	OMC	A	2498	26	-	0/9/27/28	0/2/2/2
1	MA6	a	1518	1	-	3/7/29/30	0/3/3/3
22	5MU	v	54	22	-	2/7/25/26	0/2/2/2
26	OMU	A	2552	26	-	2/9/27/28	0/2/2/2
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
24	5MU	y	54	24	-	0/7/25/26	0/2/2/2
24	6IA	y	37	24	-	0/9/31/32	0/3/3/3
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
24	H2U	y	19	24	-	4/7/38/39	0/2/2/2
1	MA6	a	1519	1	-	2/7/29/30	0/3/3/3
26	2MG	A	1835	26	-	0/5/27/28	0/3/3/3
26	PSU	A	2504	26	-	2/7/25/26	0/2/2/2
1	G7M	a	527	1	2/2/5/5	2/3/25/26	0/3/3/3
22	H2U	v	20	22	-	1/7/38/39	0/2/2/2
26	H2U	A	2449	26	-	0/7/38/39	0/2/2/2
26	3TD	A	1915	26	-	3/7/25/26	0/2/2/2
26	1MG	A	745	26	-	2/3/25/26	0/3/3/3
26	PSU	A	746	26	-	4/7/25/26	0/2/2/2
26	PSU	A	1917	26	-	2/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	3/7/25/26	0/2/2/2
26	PSU	A	2580	26	-	0/7/25/26	0/2/2/2
26	2MG	A	2445	26	-	2/5/27/28	0/3/3/3
24	PSU	y	55	24	-	2/7/25/26	0/2/2/2
26	6MZ	A	2030	26	-	2/5/27/28	0/3/3/3
26	2MA	A	2503	26	-	2/3/25/26	0/3/3/3
26	5MC	A	1962	26	-	5/7/25/26	0/2/2/2
26	PSU	A	955	26	-	0/7/25/26	0/2/2/2
26	PSU	A	2457	26	-	0/7/25/26	0/2/2/2
26	OMG	A	2251	26,22	-	0/5/27/28	0/3/3/3
1	4OC	a	1402	1	-	3/9/29/30	0/2/2/2
1	2MG	a	966	1	-	0/5/27/28	0/3/3/3
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
26	G7M	A	2069	26	2/2/5/5	1/3/25/26	0/3/3/3
22	PSU	v	55	22	-	2/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PSU	A	2604	26	-	0/7/25/26	0/2/2/2
26	6MZ	A	1618	26	-	2/5/27/28	0/3/3/3
26	5MU	A	747	26	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	1/5/27/28	0/3/3/3

The worst 5 of 104 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1915	3TD	C6-C5	11.60	1.48	1.35
26	A	1915	3TD	C2-N1	9.14	1.49	1.37
26	A	1915	3TD	C6-N1	6.02	1.46	1.36
22	v	8	4SU	C4-S4	-4.72	1.59	1.68
1	a	527	G7M	C5-C4	4.61	1.48	1.39

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	37	6IA	C2-N1-C6	7.57	123.09	116.59
22	v	8	4SU	C4-N3-C2	-7.31	120.24	127.34
1	a	516	PSU	N1-C2-N3	6.73	122.75	115.13
22	v	8	4SU	C5-C4-S4	-6.52	116.06	124.47
26	A	955	PSU	N1-C2-N3	6.41	122.39	115.13

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	a	527	G7M	C3'
1	a	527	G7M	C4'
26	A	2069	G7M	C3'
26	A	2069	G7M	C4'

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1518	MA6	C5-C6-N6-C9
1	a	1518	MA6	N1-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C9
22	v	54	5MU	C3'-C4'-C5'-O5'
22	v	54	5MU	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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
61	GNP	z	701	62	29,34,34	1.65	5 (17%)	33,54,54	2.05	11 (33%)
60	SEC	y	701	24	2,5,6	0.77	0	0,5,7	-	-
59	FME	v	101	22	8,9,10	0.92	0	7,9,11	0.90	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
61	GNP	z	701	62	-	2/14/38/38	0/3/3/3
60	SEC	y	701	24	-	0/0/4/6	-
59	FME	v	101	22	-	1/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	z	701	GNP	PG-N3B	4.10	1.74	1.63
61	z	701	GNP	PB-N3B	3.94	1.73	1.63
61	z	701	GNP	C5-C6	3.87	1.48	1.41
61	z	701	GNP	O4'-C1'	2.76	1.44	1.41
61	z	701	GNP	C5-C4	2.42	1.47	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	z	701	GNP	C2-N3-C4	4.92	120.97	115.36
61	z	701	GNP	C2-N1-C6	3.99	122.28	115.93
61	z	701	GNP	C5-C6-N1	-3.87	118.14	123.43
61	z	701	GNP	C4-C5-C6	-3.57	117.39	120.80
61	z	701	GNP	N3-C2-N1	-3.26	122.87	127.22

There are no chirality outliers.

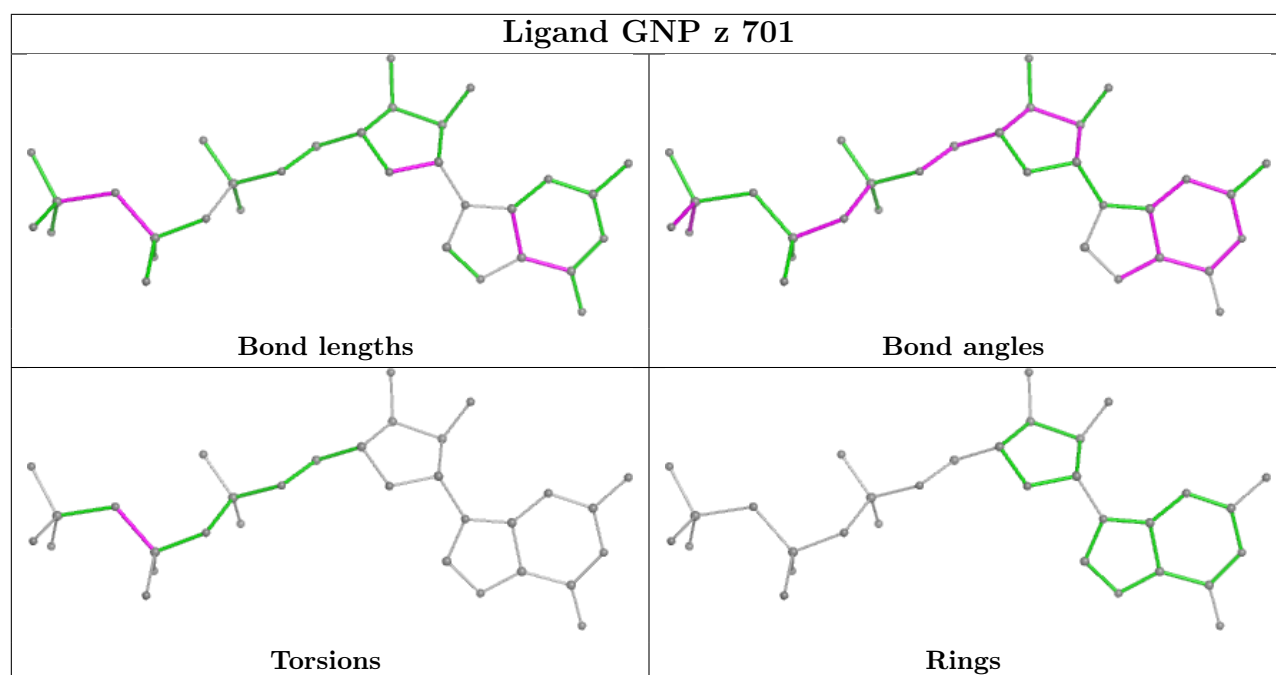
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	v	101	FME	O1-CN-N-CA
61	z	701	GNP	PG-N3B-PB-O1B
61	z	701	GNP	PG-N3B-PB-O3A

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.

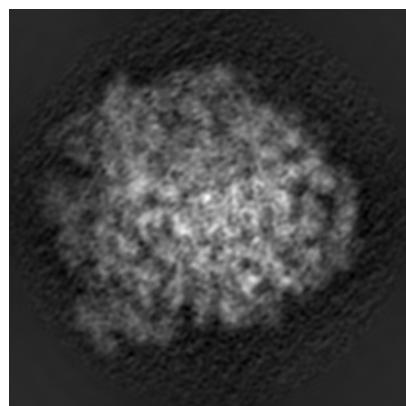
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4123. These allow visual inspection of the internal detail of the map and identification of artifacts.

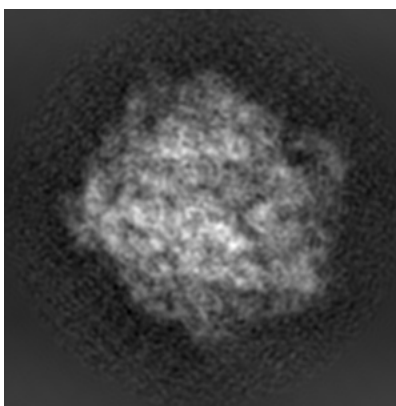
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

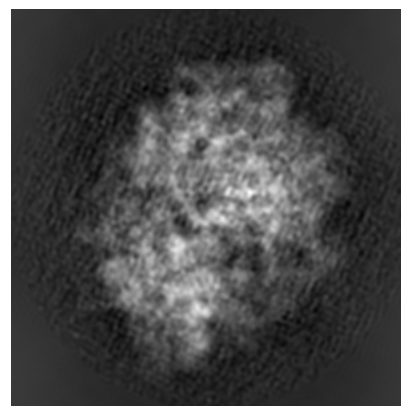
6.1.1 Primary map



X

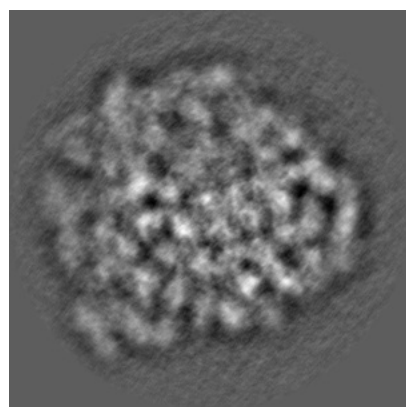


Y

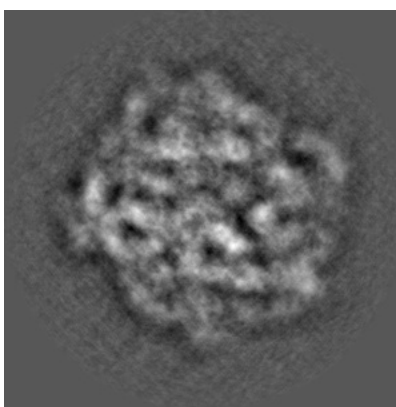


Z

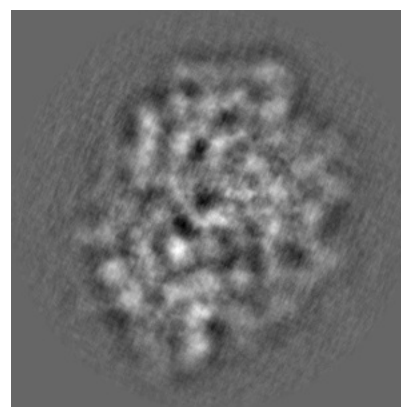
6.1.2 Raw map



X



Y

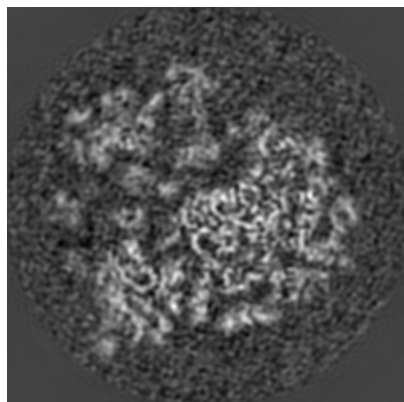


Z

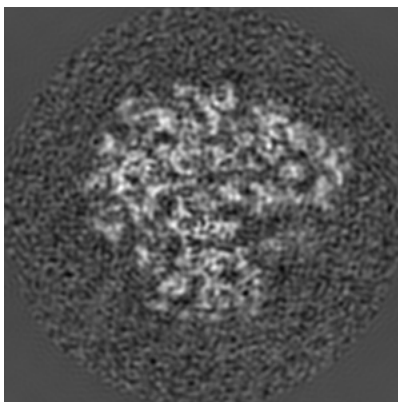
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

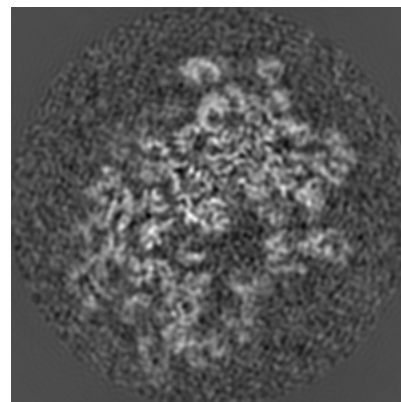
6.2.1 Primary map



X Index: 136

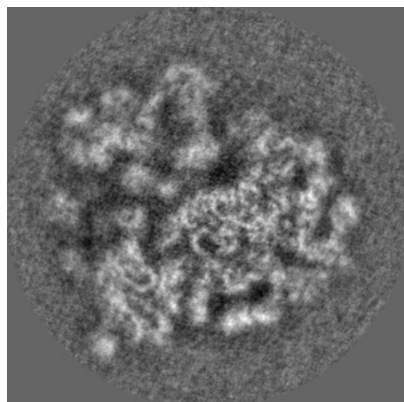


Y Index: 136

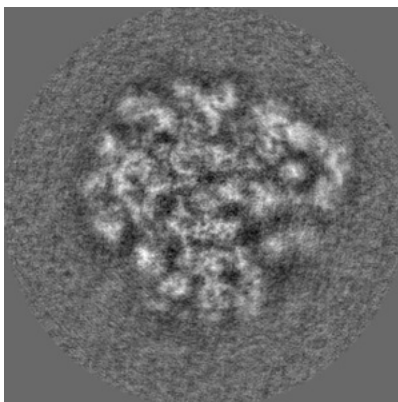


Z Index: 136

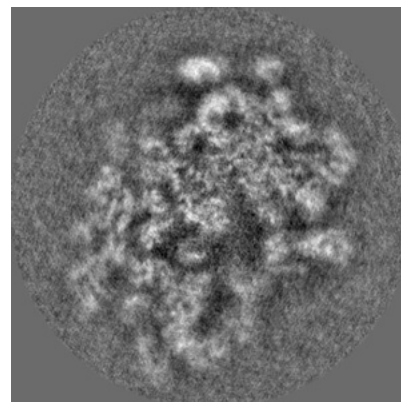
6.2.2 Raw map



X Index: 136



Y Index: 136

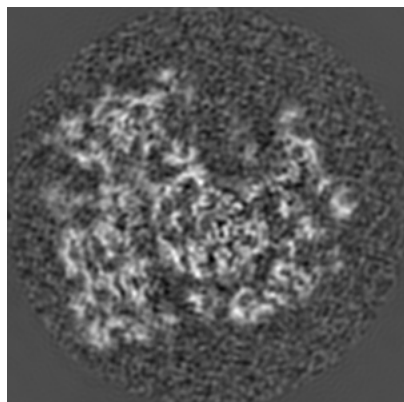


Z Index: 136

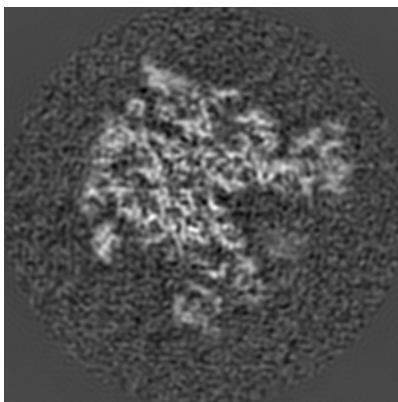
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

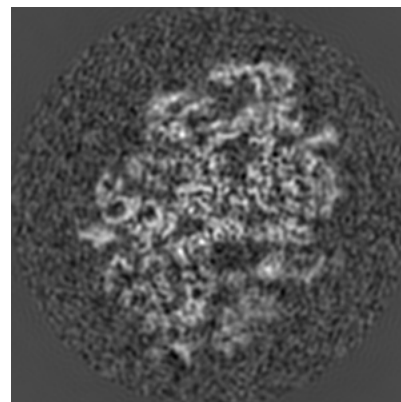
6.3.1 Primary map



X Index: 126

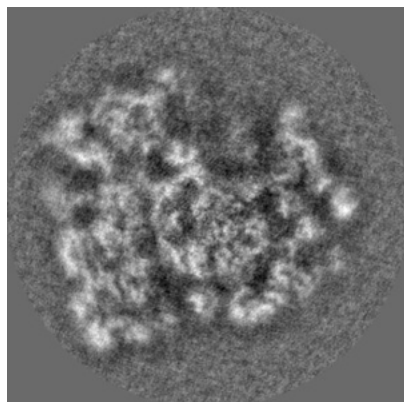


Y Index: 147

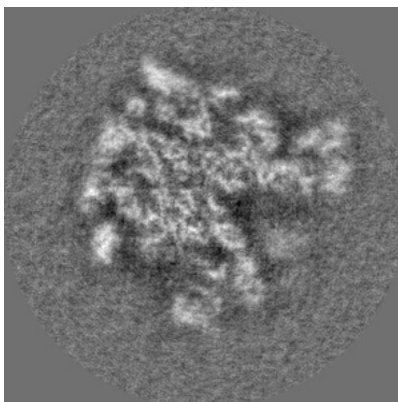


Z Index: 122

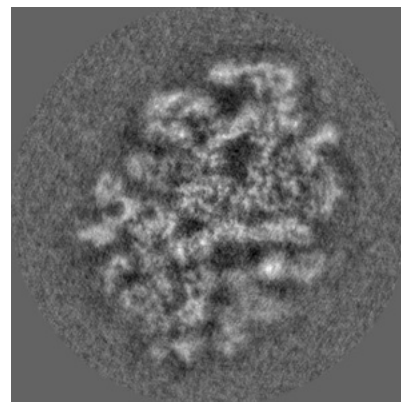
6.3.2 Raw map



X Index: 126



Y Index: 147

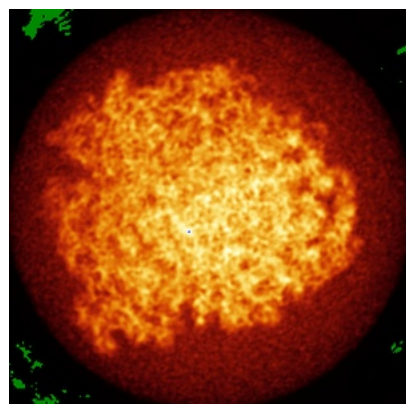


Z Index: 121

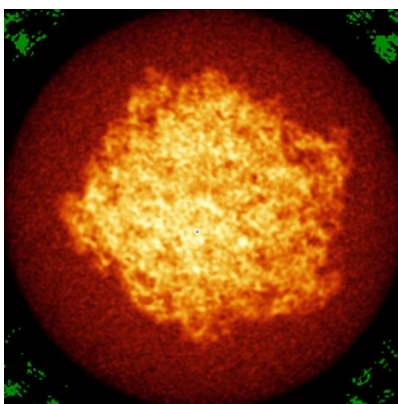
The images above show the largest variance slices of the map in three orthogonal directions.

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

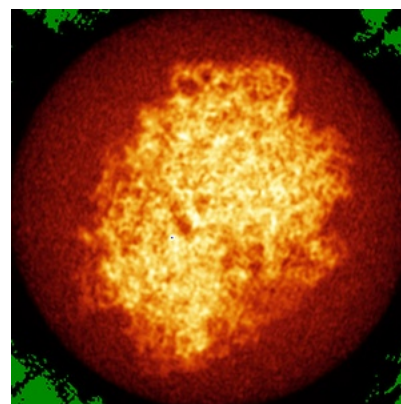
6.4.1 Primary map



X

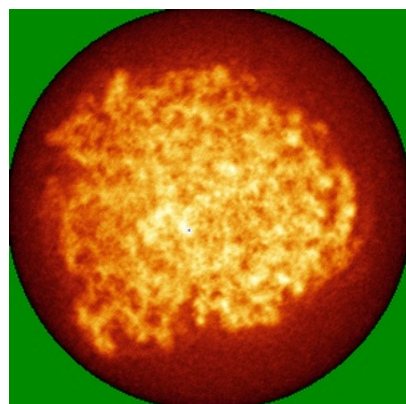


Y

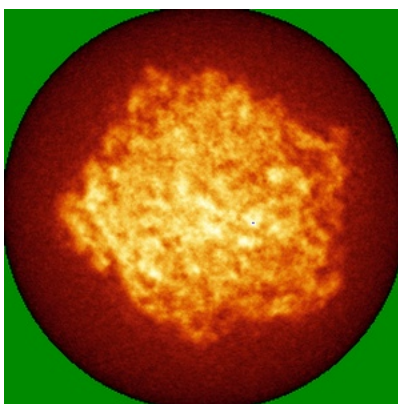


Z

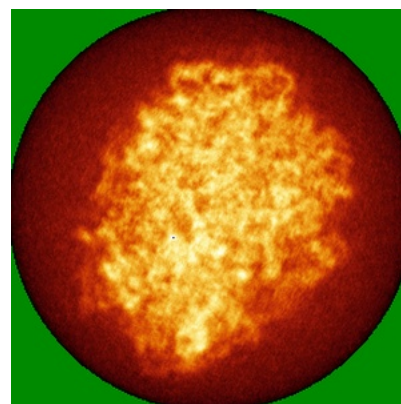
6.4.2 Raw map



X



Y

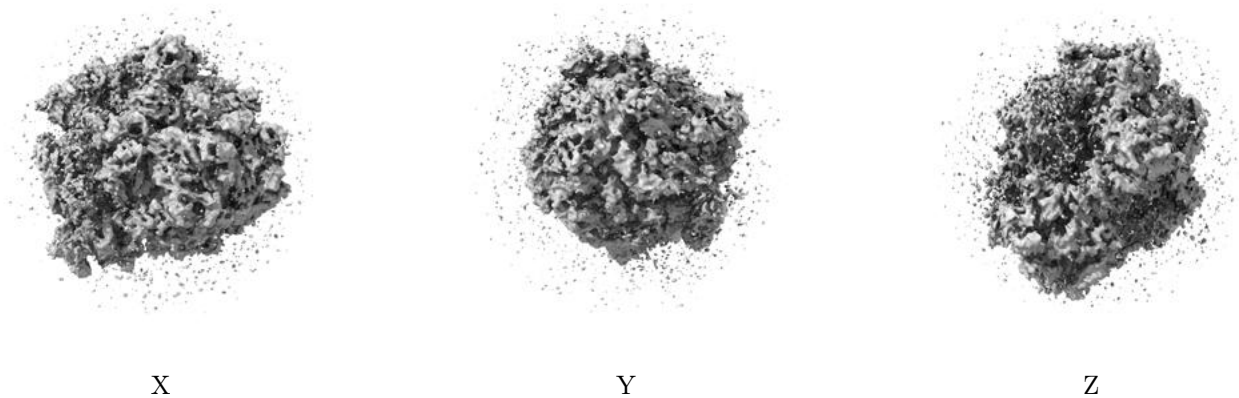


Z

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.

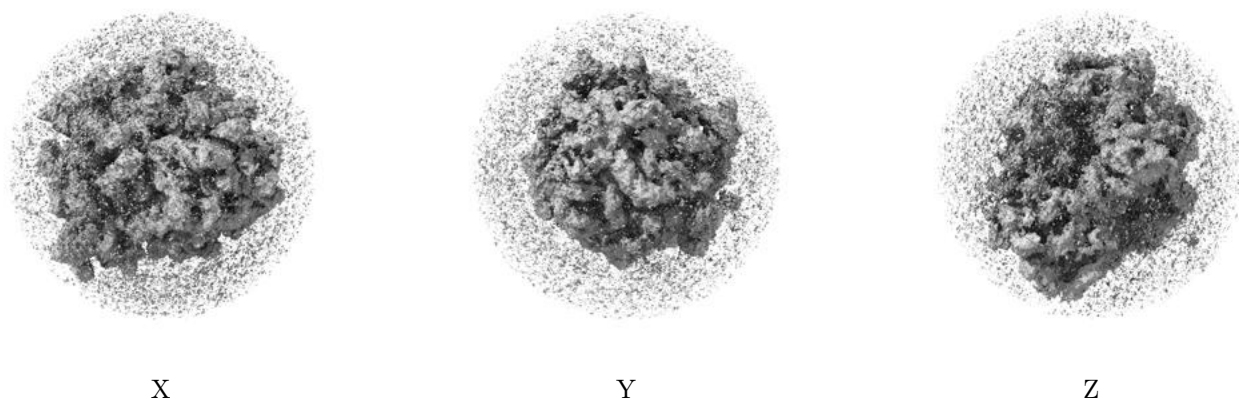
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.37. 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.

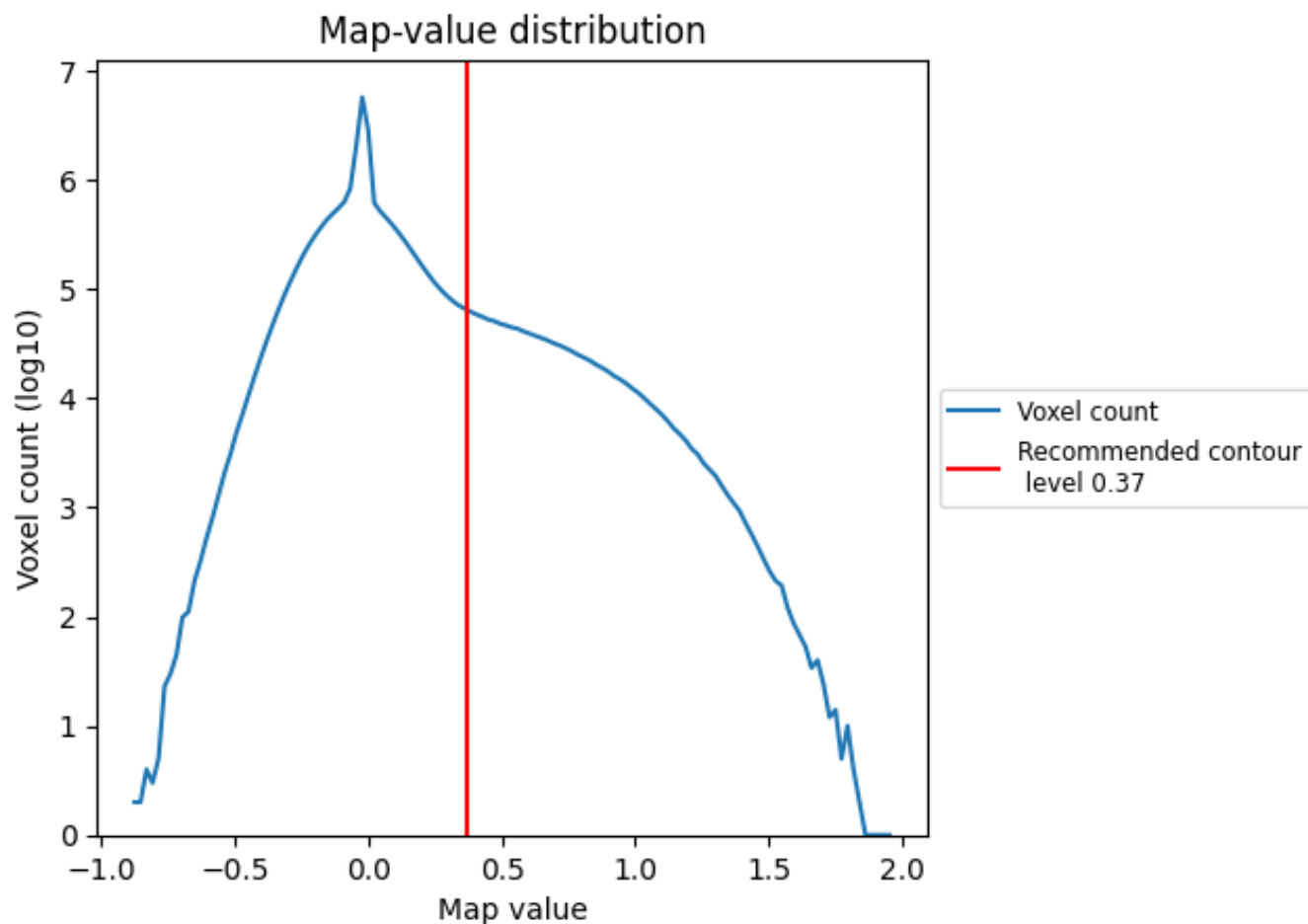
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

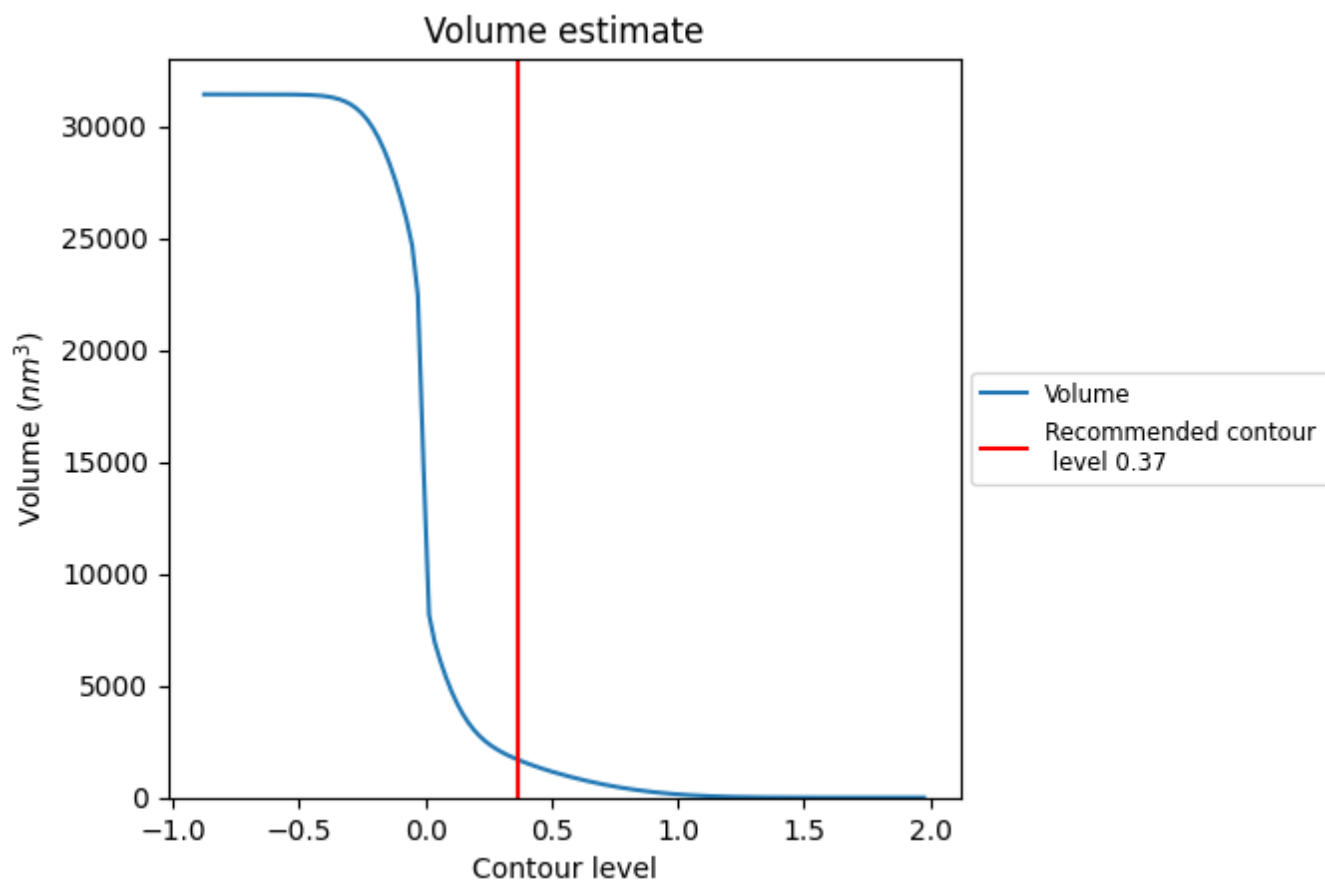
This section contains the results of statistical analysis of the map.

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.

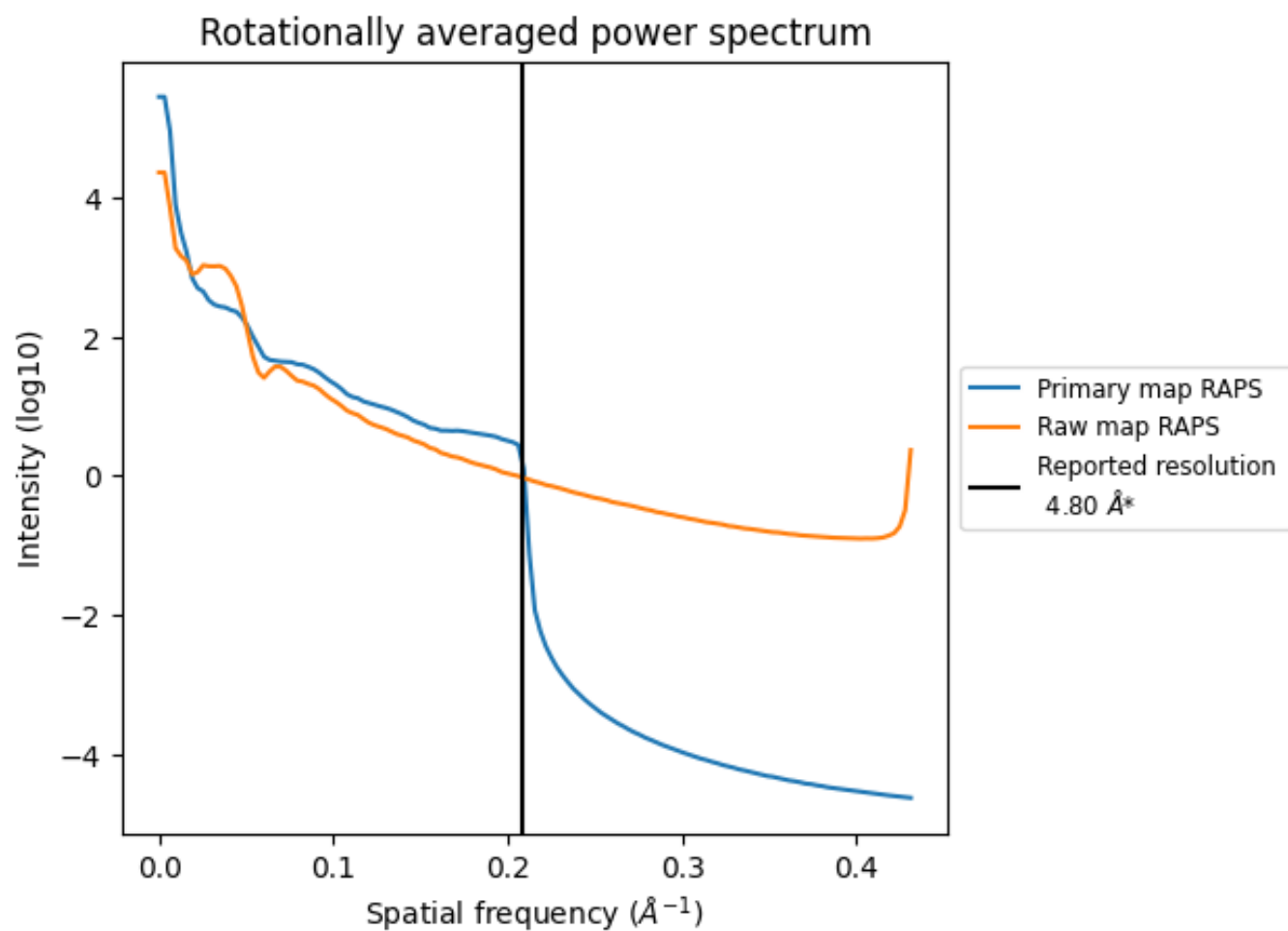
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1674 nm³; this corresponds to an approximate mass of 1512 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 ⓘ

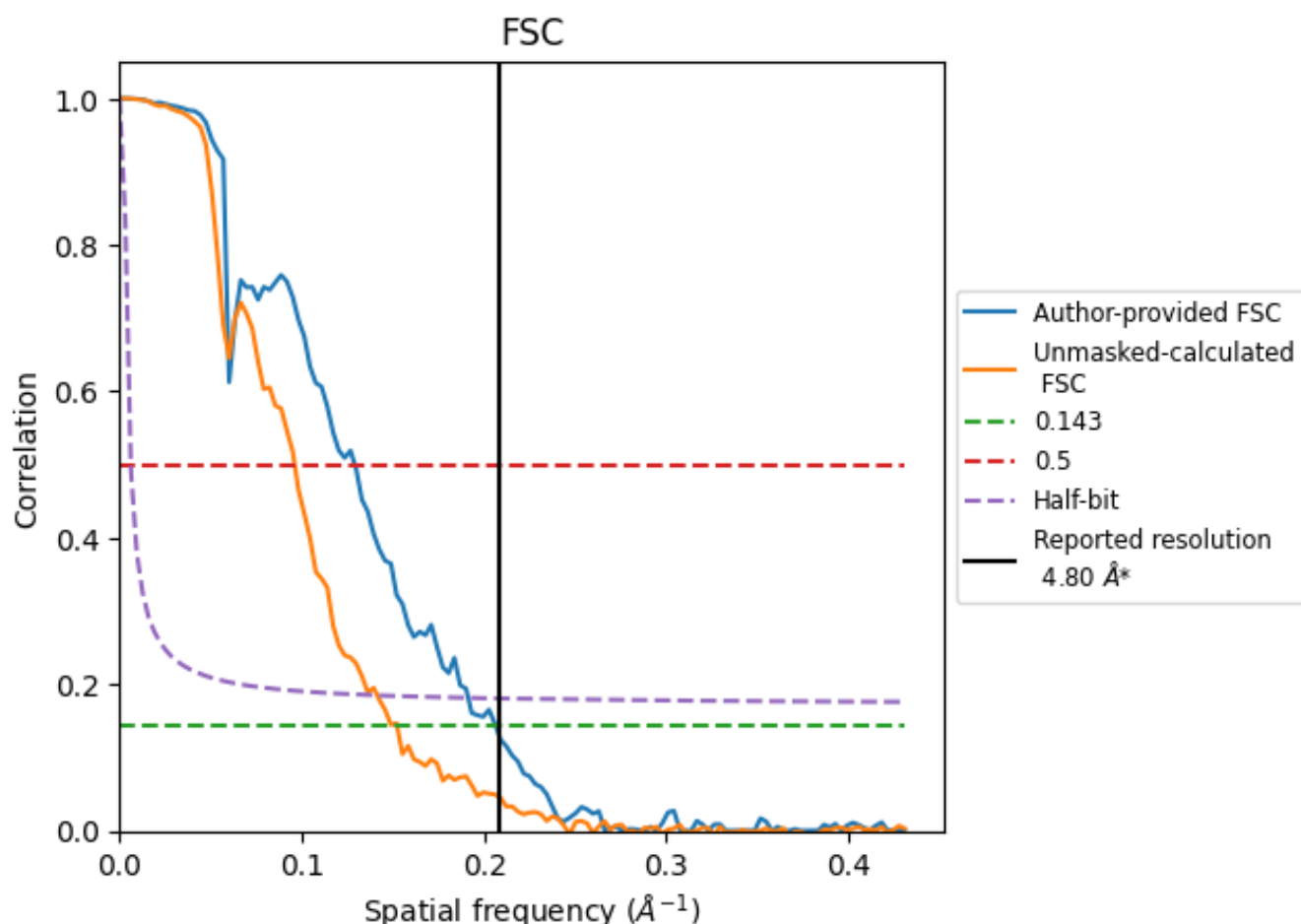


*Reported resolution corresponds to spatial frequency of 0.208 \AA^{-1}

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 0.208 \AA^{-1}

8.2 Resolution estimates [i](#)

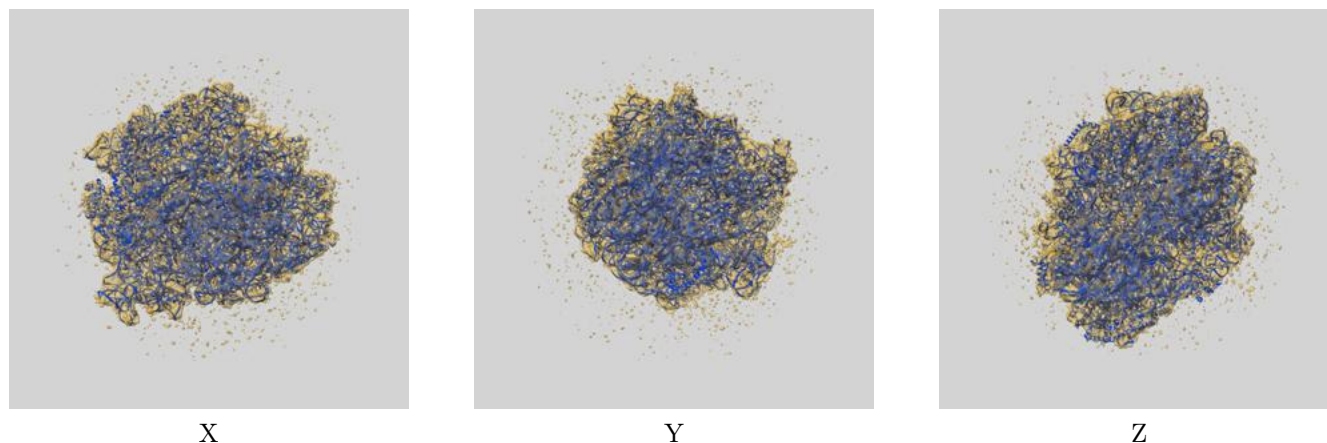
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.84	7.74	5.22
Unmasked-calculated*	6.56	10.41	7.07

*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 6.56 differs from the reported value 4.8 by more than 10 %

9 Map-model fit [i](#)

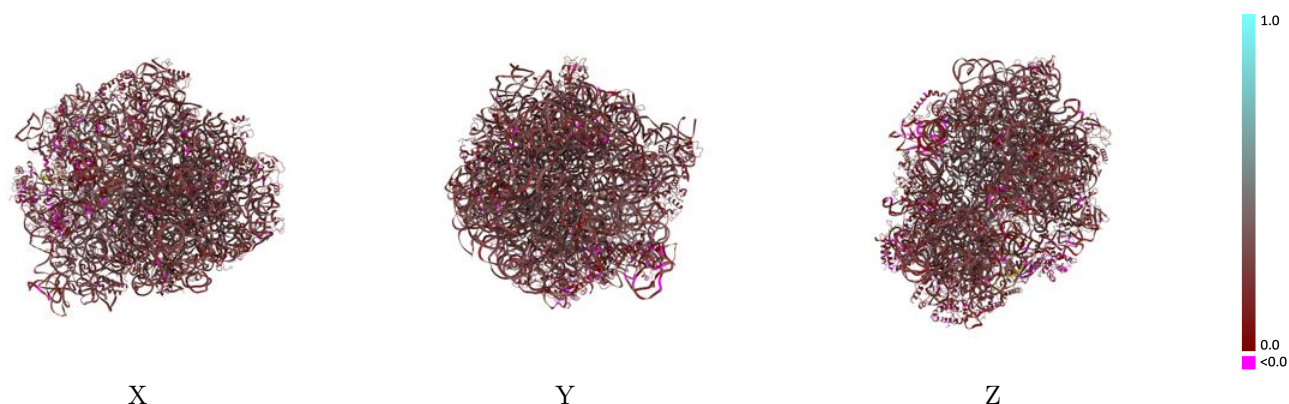
This section contains information regarding the fit between EMDB map EMD-4123 and PDB model 5LZC. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



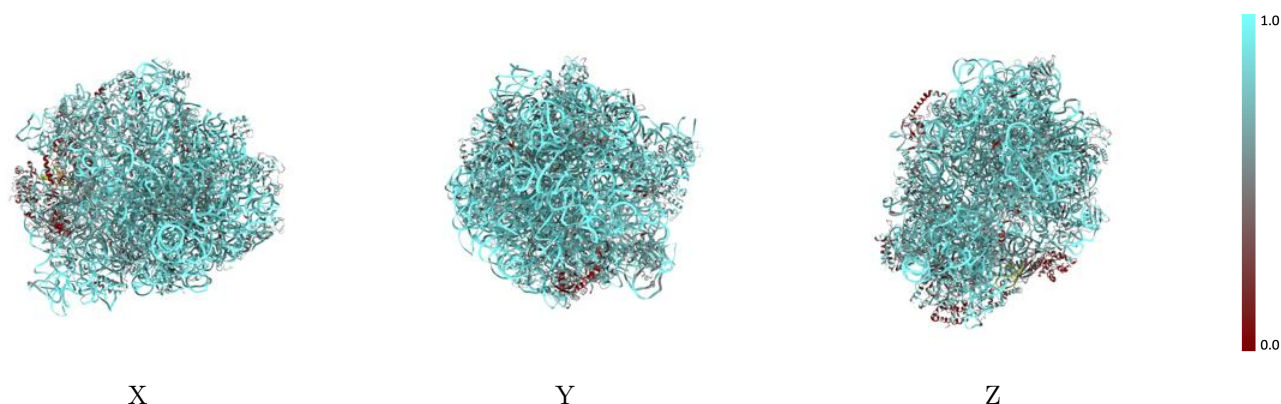
The images above show the 3D surface view of the map at the recommended contour level 0.37 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



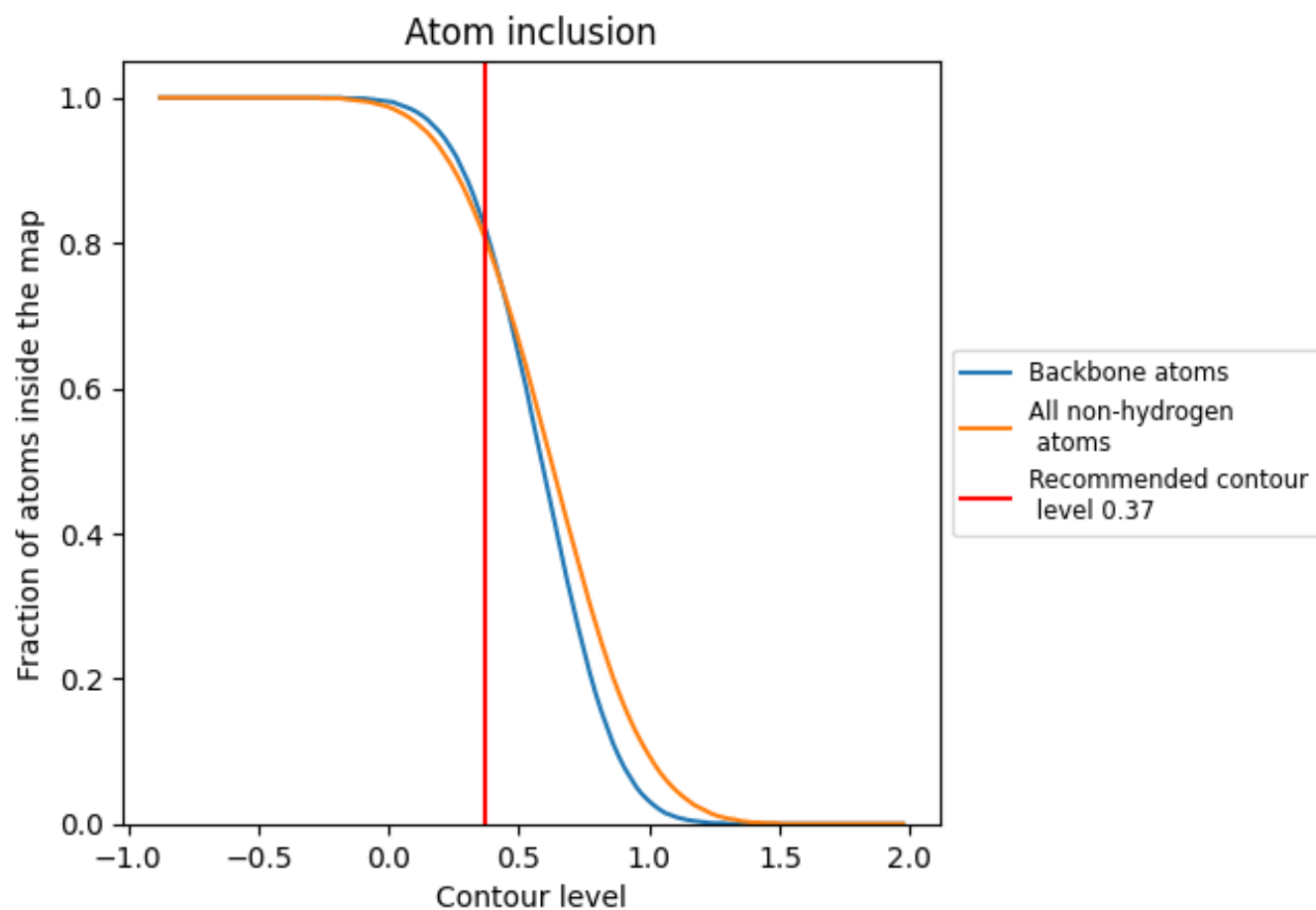
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.37).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.37) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.2510
0	 0.6450	 0.2350
1	 0.4630	 0.1860
2	 0.6510	 0.2380
3	 0.6930	 0.2550
4	 0.6180	 0.2460
6	 0.6590	 0.1940
A	 0.9180	 0.2790
B	 0.9270	 0.2640
C	 0.6690	 0.2420
D	 0.6340	 0.2230
E	 0.6320	 0.2130
F	 0.6580	 0.1830
G	 0.7020	 0.2550
H	 0.2310	 0.1310
I	 0.2120	 0.1410
J	 0.6740	 0.2240
K	 0.6270	 0.2370
L	 0.6470	 0.2340
M	 0.6630	 0.2370
N	 0.6400	 0.2000
O	 0.6700	 0.2100
P	 0.6420	 0.2200
Q	 0.6540	 0.2140
R	 0.6810	 0.2320
S	 0.6480	 0.2170
T	 0.6360	 0.2250
U	 0.6200	 0.2120
V	 0.6190	 0.1930
W	 0.6390	 0.2340
X	 0.6750	 0.2180
Y	 0.6400	 0.1780
Z	 0.6060	 0.2000
a	 0.9170	 0.2700
b	 0.5000	 0.1590



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Chain	Atom inclusion	Q-score
c	 0.6470	 0.2110
d	 0.5960	 0.2200
e	 0.6330	 0.2340
f	 0.7240	 0.2250
g	 0.6440	 0.1920
h	 0.6620	 0.2030
i	 0.6080	 0.1910
j	 0.5590	 0.2000
k	 0.7090	 0.2290
l	 0.6790	 0.2370
m	 0.6780	 0.1940
n	 0.6290	 0.2080
o	 0.7130	 0.2200
p	 0.6490	 0.2390
q	 0.6590	 0.1970
r	 0.7020	 0.2330
s	 0.6330	 0.1990
t	 0.6660	 0.2040
u	 0.5560	 0.1800
v	 0.8860	 0.2590
w	 0.6450	 0.2080
x	 0.5100	 0.1590
y	 0.6740	 0.1570
z	 0.4280	 0.1690