



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 11:58 AM UTC

PDB ID : 6WDD / pdb_00006wdd
EMDB ID : EMD-21632
Title : Cryo-EM of elongating ribosome with EF-Tu*GTP elucidates tRNA proof-reading (Cognate Structure V-A)
Authors : Loveland, A.B.; Demo, G.; Korostelev, A.A.
Deposited on : 2020-03-31
Resolution : 3.20 Å(reported)

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

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

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
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

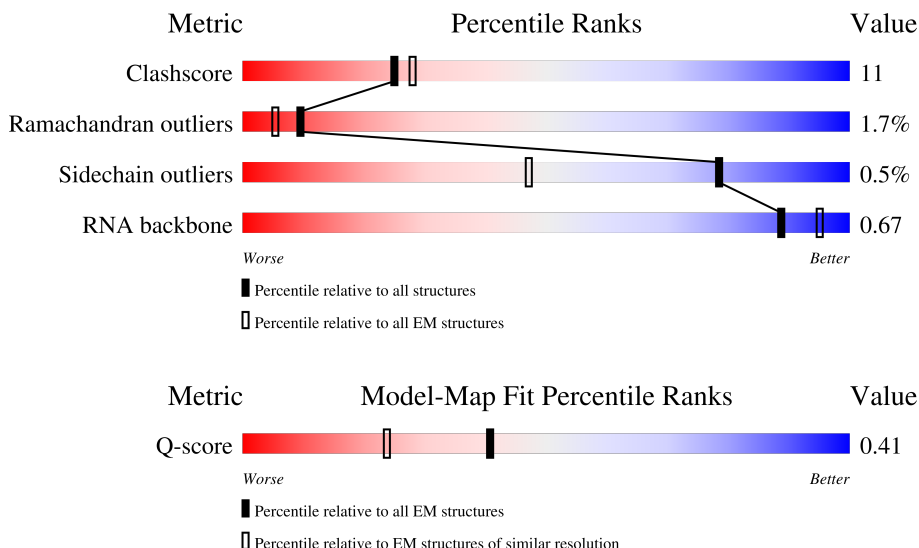
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



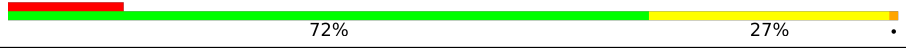
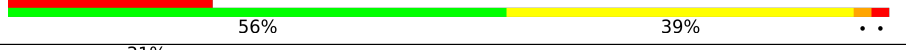
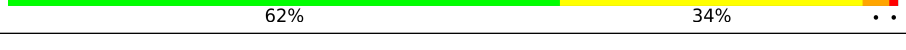
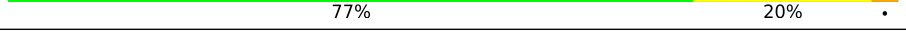
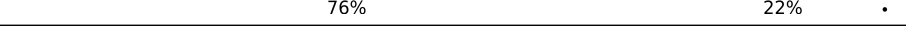
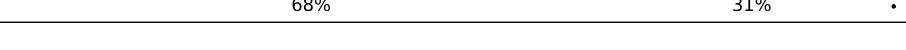
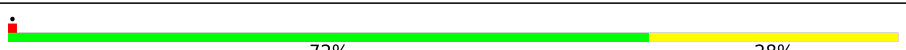
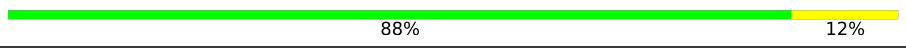
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	b	271	
2	c	209	
3	d	201	

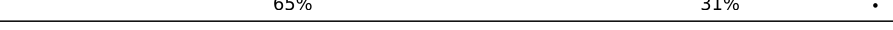
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Mol	Chain	Length	Quality of chain
4	e	177	
5	f	176	
6	g	149	
7	h	131	
8	i	141	
9	j	142	
10	k	122	
11	l	143	
12	m	136	
13	n	120	
14	o	116	
15	p	114	
16	q	117	
17	r	103	
18	s	110	
19	t	93	
20	u	102	
21	v	94	
22	w	75	
23	x	77	
24	y	63	
25	z	58	
26	B	56	
27	C	50	
28	D	46	

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Mol	Chain	Length	Quality of chain
29	E	64	
30	F	38	
31	G	225	
32	H	206	
33	I	205	
34	J	157	
35	K	100	
36	L	151	
37	M	129	
38	N	127	
39	O	98	
40	P	116	
41	Q	123	
42	R	114	
43	S	100	
44	T	88	
45	U	82	
46	V	80	
47	W	65	
48	X	79	
49	Y	85	
50	Z	65	
51	a	223	
52	3	1539	
53	1	2903	

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Mol	Chain	Length	Quality of chain
54	2	120	49% 46% 5%
55	5	77	53% 42% 5%
55	6	77	60% 36%
56	4	18	6% 67% 33%
57	7	76	62% 29% 9%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 150222 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 6 is a protein called 50S ribosomal protein L9.

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

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	131	Total	C	N	O	S	0	0
			989	625	175	184	5		

- Molecule 8 is a protein called 50S ribosomal protein L11.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

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

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

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

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

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

- Molecule 20 is a protein called 50S ribosomal protein L24.

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

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

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

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L32.

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

- Molecule 27 is a protein called 50S ribosomal protein L33.

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

- Molecule 28 is a protein called 50S ribosomal protein L34.

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

- Molecule 29 is a protein called 50S ribosomal protein L35.

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

- Molecule 30 is a protein called 50S ribosomal protein L36.

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

- Molecule 31 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	225	Total	C	N	O	S	0	0
			1757	1111	315	323	8		

- Molecule 32 is a protein called 30S ribosomal protein S3.

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

- Molecule 33 is a protein called 30S ribosomal protein S4.

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

- Molecule 34 is a protein called 30S ribosomal protein S5.

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

- Molecule 35 is a protein called 30S ribosomal protein S6.

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

- Molecule 36 is a protein called 30S ribosomal protein S7.

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

- Molecule 37 is a protein called 30S ribosomal protein S8.

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

- Molecule 38 is a protein called 30S ribosomal protein S9.

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

- Molecule 39 is a protein called 30S ribosomal protein S10.

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

- Molecule 40 is a protein called 30S ribosomal protein S11.

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

- Molecule 41 is a protein called 30S ribosomal protein S12.

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

- Molecule 42 is a protein called 30S ribosomal protein S13.

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

- Molecule 43 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	S	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 44 is a protein called 30S ribosomal protein S15.

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

- Molecule 45 is a protein called 30S ribosomal protein S16.

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

- Molecule 46 is a protein called 30S ribosomal protein S17.

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

- Molecule 47 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	W	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 48 is a protein called 30S ribosomal protein S19.

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

- Molecule 49 is a protein called 30S ribosomal protein S20.

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

- Molecule 50 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Z	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 51 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	a	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 53 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 802133627

- Molecule 54 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1266961702

- Molecule 55 is a RNA chain called tRNA^{fMet}.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	5	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
55	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

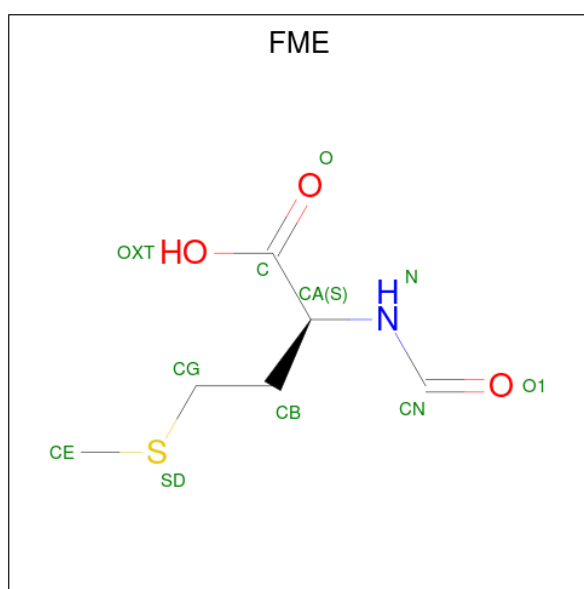
- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	18	Total	C	N	O	P	0	0
			388	175	76	120	17		

- Molecule 57 is a RNA chain called tRNA^{Phe}.

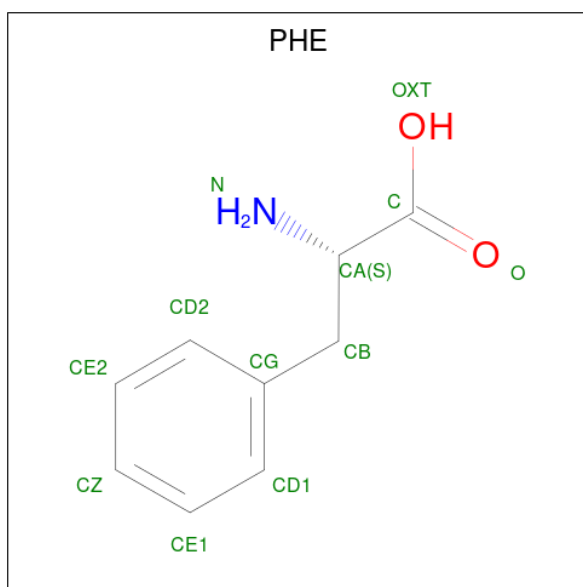
Mol	Chain	Residues	Atoms					AltConf	Trace
57	7	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

- Molecule 58 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
58	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 59 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).

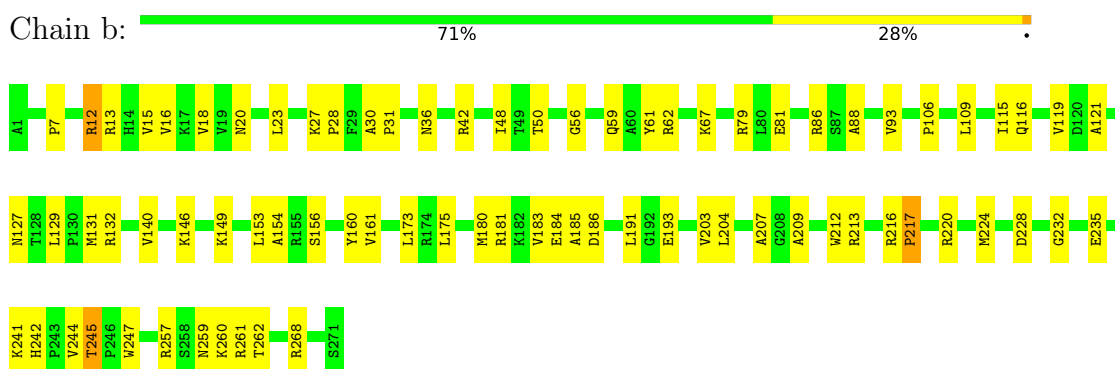


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
59	7	1	11	9	1	1	0

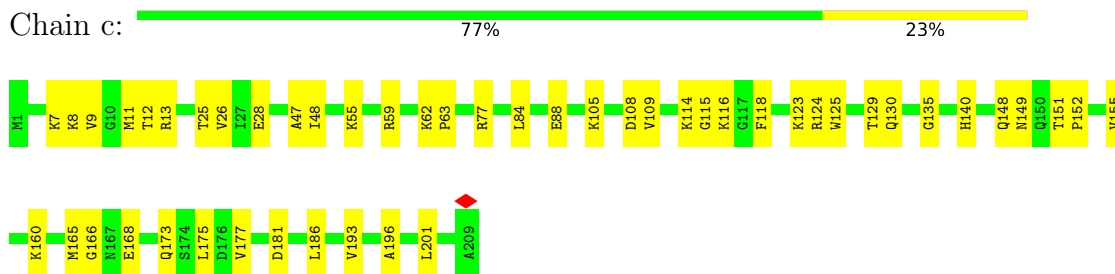
3 Residue-property plots [i](#)

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

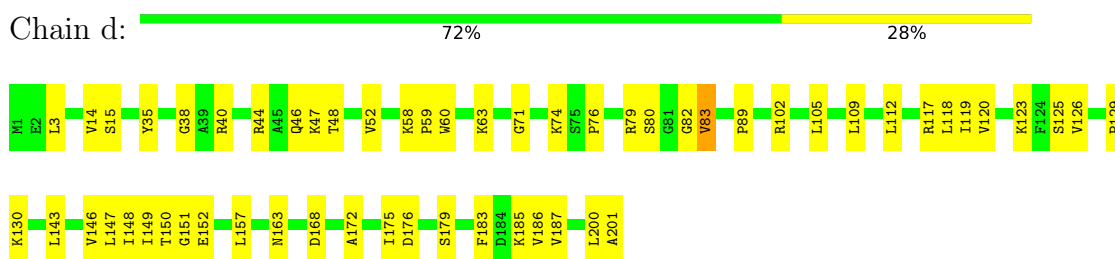
• Molecule 1: 50S ribosomal protein L2



• Molecule 2: 50S ribosomal protein L3

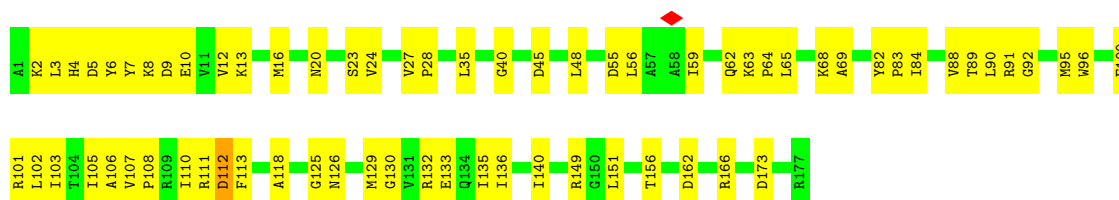


• Molecule 3: 50S ribosomal protein L4

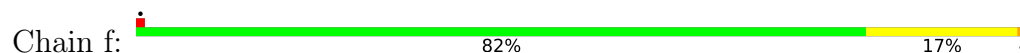


• Molecule 4: 50S ribosomal protein L5

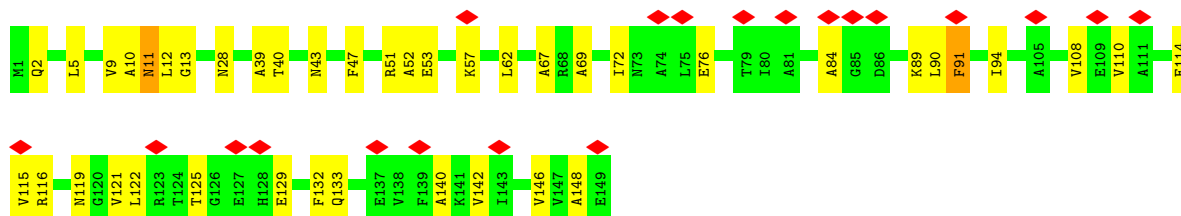
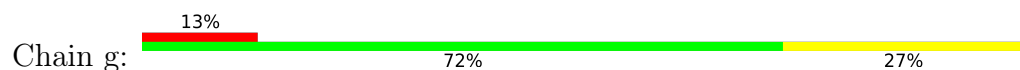




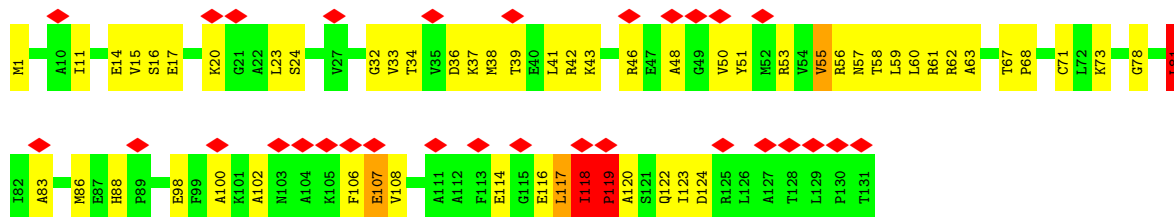
• Molecule 5: 50S ribosomal protein L6



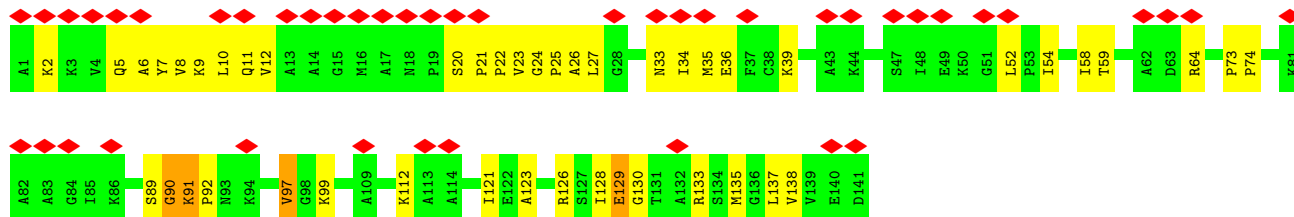
• Molecule 6: 50S ribosomal protein L9



• Molecule 7: 50S ribosomal protein L10

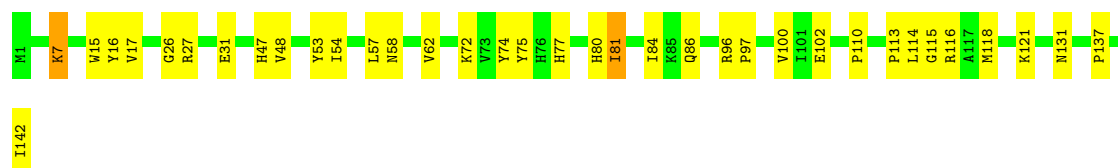


• Molecule 8: 50S ribosomal protein L11



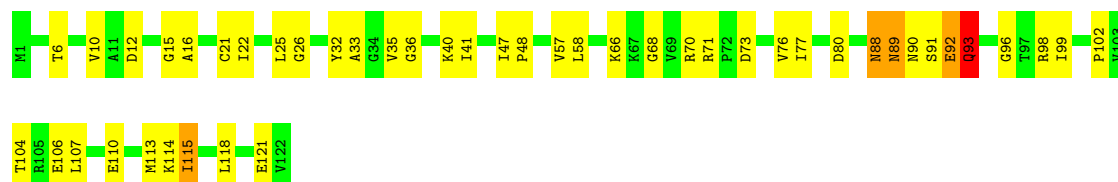
• Molecule 9: 50S ribosomal protein L13

Chain j:  75% 24%



- Molecule 10: 50S ribosomal protein L14

Chain k:  62% 34%



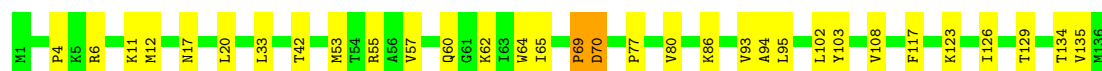
- Molecule 11: 50S ribosomal protein L15

Chain l:  77% 20%



- Molecule 12: 50S ribosomal protein L16

Chain m:  76% 22%



- Molecule 13: 50S ribosomal protein L17

Chain n:  68% 31%



- Molecule 14: 50S ribosomal protein L18

Chain o:  68% 31%





- Molecule 15: 50S ribosomal protein L19

Chain p: 74% 26%



- Molecule 16: 50S ribosomal protein L20

Chain q: 82% 18%



- Molecule 17: 50S ribosomal protein L21

Chain r: 75% 23%



- Molecule 18: 50S ribosomal protein L22

Chain s: 72% 28%



- Molecule 19: 50S ribosomal protein L23

Chain t: 72% 28%



- Molecule 20: 50S ribosomal protein L24

Chain u: 65% 34%

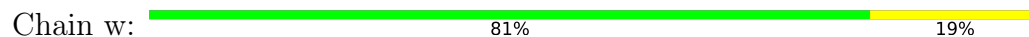


- Molecule 21: 50S ribosomal protein L25

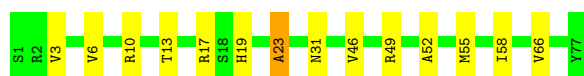
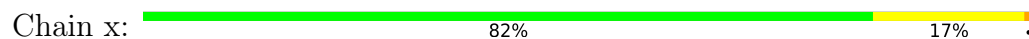
Chain v: 68% 29%



- Molecule 22: 50S ribosomal protein L27



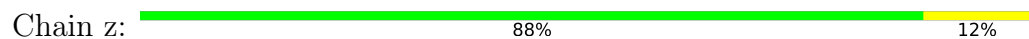
- Molecule 23: 50S ribosomal protein L28



- Molecule 24: 50S ribosomal protein L29



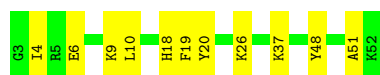
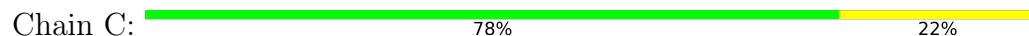
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L33

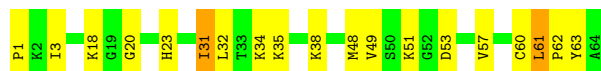


- Molecule 28: 50S ribosomal protein L34

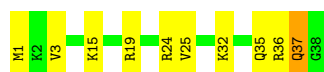




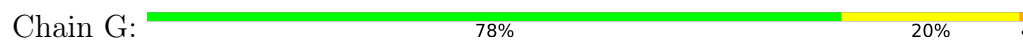
- Molecule 29: 50S ribosomal protein L35



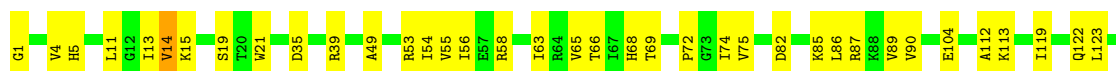
- Molecule 30: 50S ribosomal protein L36



- Molecule 31: 30S ribosomal protein S2



- Molecule 32: 30S ribosomal protein S3



- Molecule 33: 30S ribosomal protein S4





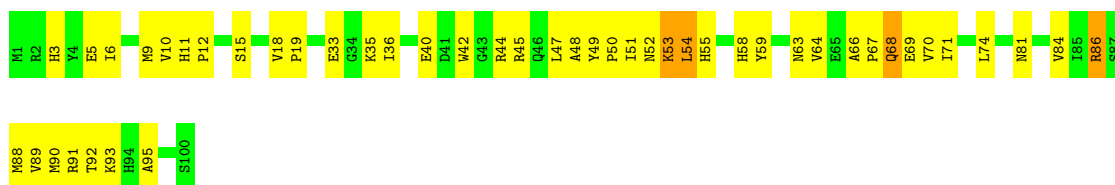
• Molecule 34: 30S ribosomal protein S5

Chain J: 71% 26% ..



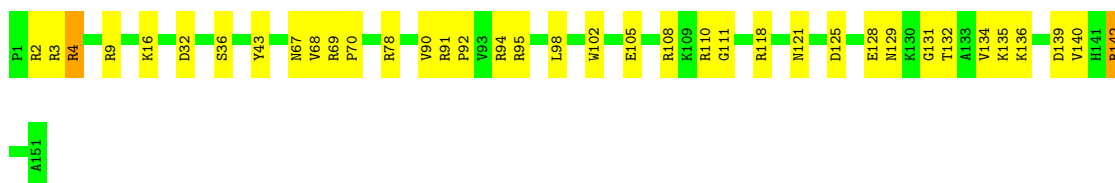
• Molecule 35: 30S ribosomal protein S6

Chain K: 53% 43% .



• Molecule 36: 30S ribosomal protein S7

Chain L: 75% 23% .



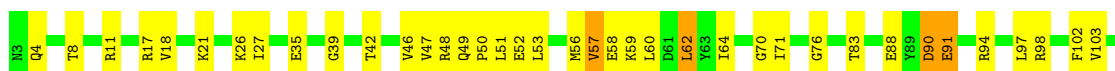
• Molecule 37: 30S ribosomal protein S8

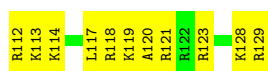
Chain M: 64% 36% .



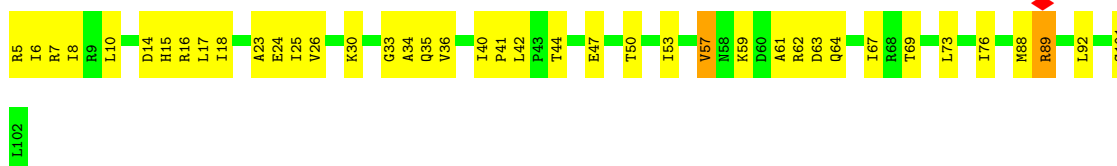
• Molecule 38: 30S ribosomal protein S9

Chain N: 61% 35% .

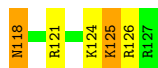
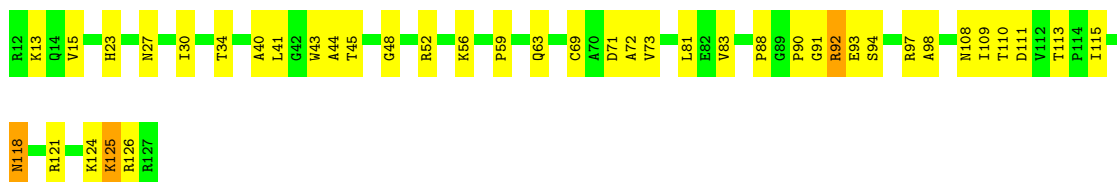




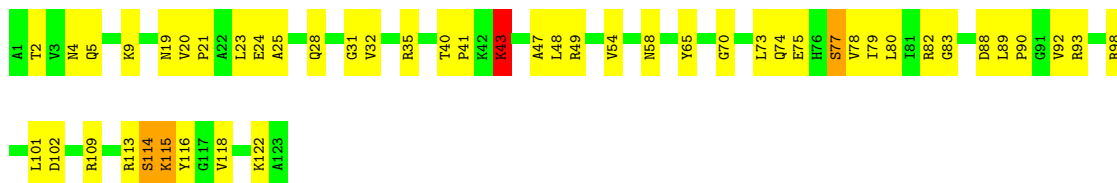
- Molecule 39: 30S ribosomal protein S10



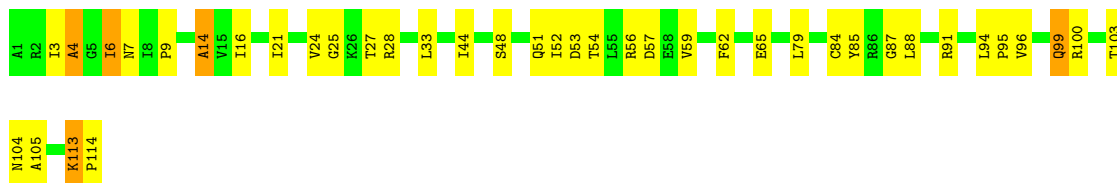
- Molecule 40: 30S ribosomal protein S11



- Molecule 41: 30S ribosomal protein S12

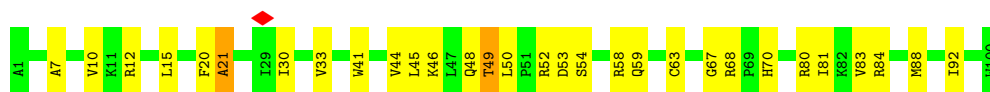


- Molecule 42: 30S ribosomal protein S13



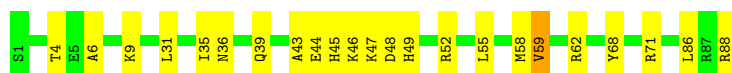
- Molecule 43: 30S ribosomal protein S14





- Molecule 44: 30S ribosomal protein S15

Chain T: 74% 25%



- Molecule 45: 30S ribosomal protein S16

Chain U: 61% 35%



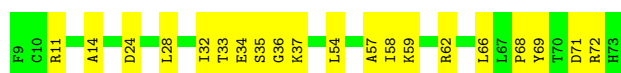
- Molecule 46: 30S ribosomal protein S17

Chain V: 59% 39%



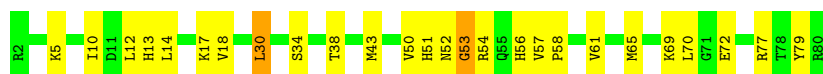
- Molecule 47: 30S ribosomal protein S18

Chain W: 69% 31%



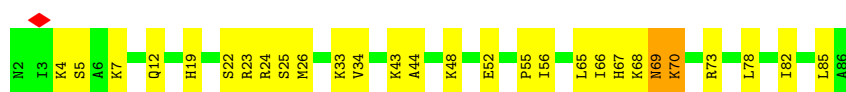
- Molecule 48: 30S ribosomal protein S19

Chain X: 67% 30%



- Molecule 49: 30S ribosomal protein S20

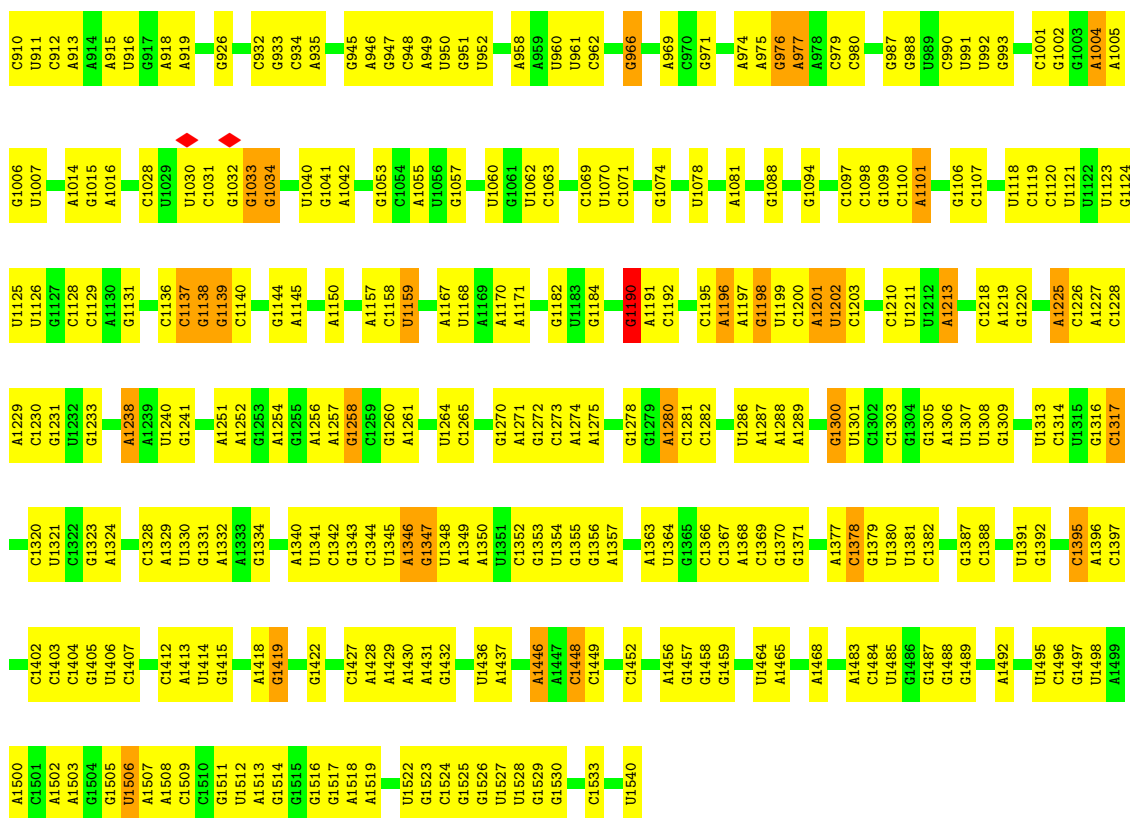
Chain Y: 67% 31%



- Molecule 50: 30S ribosomal protein S21

Chain Z: 32% 55% 12%

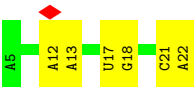




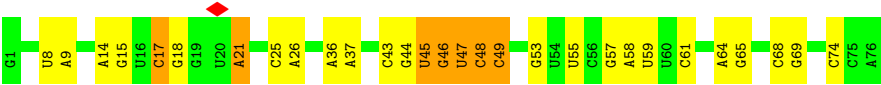
C2055	C2056	A2059	G2060	A2061	A2062	C2066	G2067	G2068	U2069	A2070	A2071	C2072	C2073	U2074	U2075	A2080	U2081	A2082	G2083	U2086	G2087	A2088	C2096	A2097	U2098	U2106	G2107	G2110	G2112	A2114	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	G2125	A2126	G2128	C2129	U2132	G2133	A2134	U2139						
U1963	G1964	C1965	A1966	C1967	G1968	A1969	G1970	G1971	G1972	U1979	G1980	U1991	G1992	U1993	C1997	A1998	C1999	G2000	C2001	U2007	C2008	A2009	G2010	U2011	A2012	A2013	A2020	C2021	U2022	C2023	G2024	C2025	U2026	G2027	U2028	G2029	A2030	A2031	G2032	C2036	G2040	U2041	A2042	C2043	C2044	C2045	U1955	U1956	C1957	C1958	G1959	
A1877	A1885	A1889	A1890	G1891	C1892	A1893	A1900	A1901	C1902	G1903	G1904	C1905	G1906	G1907	C1908	C1909	U1910	U1911	A2082	A1912	A1913	C1914	U1915	A1916	U1917	A1918	A1919	C1920	G1921	G1922	U1923	C1924	C1925	G1929	G1930	U1931	A1932	G1933	C1934	A1935	A1936	A1937	A1938	U1943	U1944	C1947	G1948	U1955	U1956	C1957	C1958	G1959
A1785	A1786	C1790	A1791	A1794	U1795	U1796	G1797	U1798	G1799	C1800	A1801	G1807	A1808	A1809	A1810	G1811	U1812	G1813	A1814	A1815	C1816	G1817	U1818	G1824	U1825	G1826	U1827	G1828	A1829	C1833	U1834	C1837	C1838	G1839	G1846	A1847	U1856	G1857	A1858	U1859	G1860	G1861	G1862	G1863	A1871	A1872	G1873	U1874	C1875	A1876		
U1683	G1684	A1689	A1690	C1691	G1695	G1696	G1699	C1704	A1705	U1715	U1720	G1721	U1729	C1730	U1736	G1737	A1738	A1739	G1740	U1636	A1637	C1638	C1639	G1645	U1646	U1647	U1648	G1651	A1654	A1655	C1656	U1657	C1658	U1662	G1663	G1666	G1667	A1672	G1673	G1674	C1675	A1676	A1677	A1678	A1679	U1779	A1780	U1781	U1782	A1783	A1784	
G1568	A1569	A1570	A1571	G1581	G1587	C1592	A1593	U1594	C1595	U1599	C1600	A1603	C1607	A1608	A1609	A1610	C1611	A1616	U1636	A1637	C1638	C1639	G1645	U1646	U1647	U1648	G1651	A1654	A1655	C1656	U1657	C1658	U1662	G1663	G1666	G1667	A1672	G1673	G1674	C1675	A1676	A1677	A1678	A1679	U1779	A1780	U1781	U1782	A1783	A1784		
U1468	A1469	A1470	A1471	G1475	U1476	G1479	C1480	U1481	G1482	A1490	G1491	A1494	C1498	U1506	C1507	A1508	A1509	G1510	A1515	G1516	G1517	C1517	U1522	A1523	G1524	A1528	G1529	C1533	U1534	A1535	C1536	G1537	U1538	U1539	G1540	A1548	A1549	C1550	G1555	G1560	C1561	U1562	U1563	C1564	C1565	A1566	G1567					
C1363	G1364	A1365	A1366	A1367	G1368	G1369	C1370	G1371	A1373	A1378	U1379	G1380	A1383	A1384	A1385	C1386	U1394	G1401	U1402	U1415	G1416	C1417	G1418	A1419	A1420	G1421	A1427	G1430	A1431	A1434	G1435	G1436	C1437	U1438	G1441	U1442	U1443	G1444	C1447	G1448	C1451	U1452	U1453	C1454	C1461							
G1286	U1287	A1288	G1289	G1290	G1291	A1292	U1293	G1294	A1295	G1296	C1297	C1298	G1299	A1300	A1301	A1302	G1309	C1319	C1320	U1326	A1327	A1328	C1329	C1330	G1331	G1332	U1340	G1341	A1342	G1343	U1344	C1345	C1348	C1349	A1354	G1355	G1356	C1357	G1358	A1359	C1361	C1362										
U1132	A1133	A1134	C1135	G1138	C1139	U1140	U1141	A1142	A1143	G1149	C1150	A1151	C1152	C1153	G1157	C1161	G1162	U1175	U1176	G1177	C1178	G1179	U1180	U1181	G1182	U1183	G1186	G1187	U1188	A1189	G1190	G1191	U1199	C1200	G1206	G1210	G1211	G1212	A1213	G1236	A1237	G1238	G1250	C1251	A1253	G1256						
C1045	A1046	A1047	A1048	C1053	A1054	G1055	U1060	U1061	G1062	U1065	U1066	A1070	G1071	A1077	U1078	C1079	A1080	U1083	A1084	A1085	A1086	G1087	A1088	A1089	A1090	G1091	C1092	G1093	U1094	A1095	A1098	A1103	C1104	U1105	G1106	G1107	U1108	C1109	G1110	A1111	G1112	U1113	C1114	G1115	G1122	G1125	U1130	G1131				
G940	A941	G942	A943	C946	A947	C948	G949	G953	G954	U955	C961	G962	U967	C968	G969	U970	A972	A973	G974	A975	A983	A984	C985	C986	C987	A988	G989	A990	C995	A996	G997	A1001	G1002	U1012	C1013	U1019	A1020	A1021	G1022	U1023	G1026	A1027	A1028	U1033	A1040							
C737	G738	A739	A742	A743	U744	G745	U746	C747	G748	A751	A752	G759	G760	A761	G762	G763	A764	C765	U766	G767	U768	U769	G770	G771	G774	G775	G776	G780	A781	A782	A783	G784	G785	C786	C787	A788	G799	A800	G801	A802	G805	C806	U807	G808	C812	U813	C814	C817	G818	A819		



• Molecule 56: mRNA



• Molecule 57: tRNAPhe



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32253	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	28.501	Depositor
Minimum map value	-14.672	Depositor
Average map value	0.119	Depositor
Map value standard deviation	1.117	Depositor
Recommended contour level	1	Depositor
Map size (Å)	383.904, 383.904, 383.904	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.333, 1.333, 1.333	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME

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	b	0.30	0/2122	0.91	8/2852 (0.3%)
2	c	0.29	0/1586	0.82	0/2134
3	d	0.29	0/1571	0.81	0/2113
4	e	0.34	0/1435	0.82	0/1926
5	f	0.31	0/1343	0.84	2/1816 (0.1%)
6	g	0.32	0/1122	0.93	4/1515 (0.3%)
7	h	0.37	0/1002	1.08	9/1350 (0.7%)
8	i	0.38	0/1046	0.99	5/1410 (0.4%)
9	j	0.29	0/1152	0.90	5/1551 (0.3%)
10	k	0.28	0/948	0.95	7/1268 (0.6%)
11	l	0.30	0/1054	0.96	1/1403 (0.1%)
12	m	0.30	0/1093	0.85	1/1460 (0.1%)
13	n	0.30	0/974	0.93	5/1301 (0.4%)
14	o	0.30	0/902	0.90	3/1209 (0.2%)
15	p	0.30	0/929	0.80	1/1242 (0.1%)
16	q	0.29	0/960	0.88	3/1278 (0.2%)
17	r	0.31	0/829	0.80	0/1107
18	s	0.28	0/864	0.86	1/1156 (0.1%)
19	t	0.29	0/745	0.80	0/994
20	u	0.31	0/788	0.88	1/1051 (0.1%)
21	v	0.29	0/766	0.91	5/1025 (0.5%)
22	w	0.28	0/582	0.82	0/769
23	x	0.27	0/635	0.91	1/848 (0.1%)
24	y	0.27	0/510	0.83	0/677
25	z	0.30	0/453	0.77	0/605
26	B	0.28	0/450	0.78	1/599 (0.2%)
27	C	0.32	0/417	0.76	0/554
28	D	0.32	0/380	0.89	1/498 (0.2%)
29	E	0.32	0/513	0.98	2/676 (0.3%)
30	F	0.31	0/303	0.88	0/397
31	G	0.30	0/1788	0.87	8/2408 (0.3%)
32	H	0.31	0/1652	0.84	2/2225 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.31	0/1665	0.91	5/2227 (0.2%)
34	J	0.36	1/1170 (0.1%)	0.86	3/1573 (0.2%)
35	K	0.33	0/836	0.91	3/1128 (0.3%)
36	L	0.31	0/1196	0.92	2/1602 (0.1%)
37	M	0.31	0/989	0.93	4/1326 (0.3%)
38	N	0.30	0/1034	0.91	4/1375 (0.3%)
39	O	0.34	0/797	0.89	0/1077
40	P	0.32	0/886	0.98	2/1195 (0.2%)
41	Q	0.32	0/969	1.00	7/1300 (0.5%)
42	R	0.32	0/893	0.89	1/1193 (0.1%)
43	S	0.30	0/817	0.89	3/1088 (0.3%)
44	T	0.30	0/722	0.91	3/964 (0.3%)
45	U	0.33	0/659	0.91	3/884 (0.3%)
46	V	0.30	0/658	0.86	2/881 (0.2%)
47	W	0.31	0/545	0.91	1/731 (0.1%)
48	X	0.33	0/653	0.90	1/877 (0.1%)
49	Y	0.30	0/671	0.99	6/888 (0.7%)
50	Z	0.33	0/551	1.01	3/728 (0.4%)
51	a	0.33	0/1034	0.85	1/1387 (0.1%)
52	3	0.42	0/36963	0.48	3/57662 (0.0%)
53	1	0.40	0/69796	0.48	3/108888 (0.0%)
54	2	0.42	0/2872	0.48	0/4479
55	5	0.42	0/1832	0.46	0/2855
55	6	0.42	0/1832	0.48	0/2855
56	4	0.42	0/436	0.46	0/679
57	7	0.41	0/1809	0.46	0/2819
All	All	0.38	1/163199 (0.0%)	0.61	136/244078 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	J	55	VAL	CA-CB	5.58	1.57	1.54

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	E	61	LEU	CA-C-N	8.57	127.89	118.97
29	E	61	LEU	C-N-CA	8.57	127.89	118.97
37	M	67	GLY	N-CA-C	-8.47	102.01	113.37
43	S	49	THR	N-CA-C	-8.35	101.71	112.23
49	Y	5	SER	N-CA-C	-8.18	102.85	112.92

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	b	2083	0	2157	59	0
2	c	1565	0	1616	34	0
3	d	1552	0	1619	46	0
4	e	1411	0	1447	62	0
5	f	1323	0	1374	23	0
6	g	1111	0	1148	27	0
7	h	989	0	1025	58	0
8	i	1032	0	1088	43	0
9	j	1129	0	1162	25	0
10	k	939	0	1012	38	0
11	l	1045	0	1117	21	0
12	m	1074	0	1157	23	0
13	n	961	0	1000	23	0
14	o	892	0	923	29	0
15	p	917	0	965	25	0
16	q	947	0	1022	16	0
17	r	816	0	839	20	0
18	s	857	0	922	21	0
19	t	739	0	807	23	0
20	u	780	0	834	21	0
21	v	753	0	780	18	0
22	w	575	0	592	11	0
23	x	625	0	655	10	0
24	y	509	0	543	17	0
25	z	449	0	491	6	0
26	B	444	0	461	14	0
27	C	410	0	440	9	0
28	D	377	0	418	20	0
29	E	504	0	574	18	0
30	F	302	0	343	12	0
31	G	1757	0	1787	30	0
32	H	1625	0	1699	44	0
33	I	1643	0	1710	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	J	1157	0	1199	34	0
35	K	818	0	808	36	0
36	L	1182	0	1240	29	0
37	M	979	0	1034	32	0
38	N	1022	0	1070	41	0
39	O	787	0	828	27	0
40	P	870	0	878	31	0
41	Q	955	0	1019	35	0
42	R	884	0	944	46	0
43	S	805	0	847	26	0
44	T	714	0	737	18	0
45	U	649	0	666	31	0
46	V	649	0	691	26	0
47	W	536	0	552	17	0
48	X	638	0	665	17	0
49	Y	665	0	714	20	0
50	Z	545	0	579	41	0
51	a	1027	0	1092	30	0
52	3	33012	0	16618	556	0
53	1	62317	0	31346	904	0
54	2	2568	0	1303	59	0
55	5	1640	0	836	23	0
55	6	1640	0	837	22	0
56	4	388	0	196	5	0
57	7	1619	0	821	23	0
58	5	10	0	10	0	0
59	7	11	0	8	1	0
All	All	150222	0	101265	2648	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 11.

The worst 5 of 2648 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)
53:1:45:G:H5''	53:1:46:G:H5'	1.19	1.16
7:h:73:LYS:HE2	7:h:120:ALA:HA	1.36	1.06
53:1:2432:A:H1'	55:6:75:C:H5'	1.39	1.05
12:m:12:MET:HA	53:1:910:A:H62	1.22	1.02
36:L:4:ARG:H	36:L:4:ARG:HD2	1.21	1.02

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	b	269/271 (99%)	235 (87%)	33 (12%)	1 (0%)	30	62
2	c	207/209 (99%)	189 (91%)	17 (8%)	1 (0%)	24	59
3	d	199/201 (99%)	180 (90%)	17 (8%)	2 (1%)	12	45
4	e	175/177 (99%)	156 (89%)	17 (10%)	2 (1%)	11	43
5	f	174/176 (99%)	160 (92%)	12 (7%)	2 (1%)	11	43
6	g	147/149 (99%)	126 (86%)	18 (12%)	3 (2%)	6	31
7	h	129/131 (98%)	95 (74%)	30 (23%)	4 (3%)	3	22
8	i	139/141 (99%)	124 (89%)	13 (9%)	2 (1%)	9	39
9	j	140/142 (99%)	133 (95%)	6 (4%)	1 (1%)	18	52
10	k	120/122 (98%)	98 (82%)	17 (14%)	5 (4%)	2	16
11	l	141/143 (99%)	119 (84%)	15 (11%)	7 (5%)	1	13
12	m	134/136 (98%)	113 (84%)	19 (14%)	2 (2%)	8	37
13	n	118/120 (98%)	106 (90%)	10 (8%)	2 (2%)	7	35
14	o	114/116 (98%)	106 (93%)	7 (6%)	1 (1%)	14	47
15	p	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
16	q	115/117 (98%)	107 (93%)	8 (7%)	0	100	100
17	r	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	3	23
18	s	108/110 (98%)	95 (88%)	10 (9%)	3 (3%)	4	25
19	t	91/93 (98%)	83 (91%)	8 (9%)	0	100	100
20	u	100/102 (98%)	84 (84%)	13 (13%)	3 (3%)	3	23
21	v	92/94 (98%)	85 (92%)	6 (6%)	1 (1%)	11	43
22	w	73/75 (97%)	64 (88%)	9 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	x	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
24	y	61/63 (97%)	58 (95%)	2 (3%)	1 (2%)	7	36
25	z	56/58 (97%)	51 (91%)	5 (9%)	0	100	100
26	B	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
27	C	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
28	D	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
29	E	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	7	36
30	F	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	4	25
31	G	223/225 (99%)	202 (91%)	20 (9%)	1 (0%)	30	62
32	H	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
33	I	203/205 (99%)	184 (91%)	15 (7%)	4 (2%)	6	31
34	J	155/157 (99%)	124 (80%)	27 (17%)	4 (3%)	4	26
35	K	98/100 (98%)	81 (83%)	12 (12%)	5 (5%)	1	13
36	L	149/151 (99%)	131 (88%)	17 (11%)	1 (1%)	18	52
37	M	127/129 (98%)	112 (88%)	13 (10%)	2 (2%)	7	36
38	N	125/127 (98%)	103 (82%)	18 (14%)	4 (3%)	3	21
39	O	96/98 (98%)	80 (83%)	11 (12%)	5 (5%)	1	12
40	P	114/116 (98%)	94 (82%)	17 (15%)	3 (3%)	4	26
41	Q	121/123 (98%)	94 (78%)	21 (17%)	6 (5%)	1	13
42	R	112/114 (98%)	98 (88%)	10 (9%)	4 (4%)	2	19
43	S	98/100 (98%)	76 (78%)	22 (22%)	0	100	100
44	T	86/88 (98%)	78 (91%)	6 (7%)	2 (2%)	5	29
45	U	80/82 (98%)	71 (89%)	8 (10%)	1 (1%)	9	40
46	V	78/80 (98%)	64 (82%)	12 (15%)	2 (3%)	4	26
47	W	63/65 (97%)	57 (90%)	5 (8%)	1 (2%)	7	36
48	X	77/79 (98%)	65 (84%)	10 (13%)	2 (3%)	4	26
49	Y	83/85 (98%)	80 (96%)	3 (4%)	0	100	100
50	Z	63/65 (97%)	47 (75%)	9 (14%)	7 (11%)	0	2
51	a	130/223 (58%)	124 (95%)	6 (5%)	0	100	100
All	All	5919/6112 (97%)	5192 (88%)	625 (11%)	102 (2%)	9	35

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	b	232	GLY
5	f	45	ALA
5	f	174	LYS
6	g	9	VAL
7	h	81	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	216/216 (100%)	215 (100%)	1 (0%)	81	85
2	c	164/164 (100%)	164 (100%)	0	100	100
3	d	165/165 (100%)	165 (100%)	0	100	100
4	e	148/148 (100%)	146 (99%)	2 (1%)	59	77
5	f	137/137 (100%)	137 (100%)	0	100	100
6	g	114/114 (100%)	114 (100%)	0	100	100
7	h	100/100 (100%)	97 (97%)	3 (3%)	36	66
8	i	109/109 (100%)	108 (99%)	1 (1%)	70	81
9	j	116/116 (100%)	116 (100%)	0	100	100
10	k	103/103 (100%)	102 (99%)	1 (1%)	68	80
11	l	102/102 (100%)	101 (99%)	1 (1%)	68	80
12	m	109/109 (100%)	108 (99%)	1 (1%)	70	81
13	n	100/100 (100%)	100 (100%)	0	100	100
14	o	86/86 (100%)	85 (99%)	1 (1%)	63	79
15	p	99/99 (100%)	99 (100%)	0	100	100
16	q	89/89 (100%)	89 (100%)	0	100	100
17	r	84/84 (100%)	84 (100%)	0	100	100
18	s	93/93 (100%)	93 (100%)	0	100	100
19	t	80/80 (100%)	79 (99%)	1 (1%)	61	78
20	u	83/83 (100%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	v	78/78 (100%)	77 (99%)	1 (1%)	61	78
22	w	57/57 (100%)	57 (100%)	0	100	100
23	x	67/67 (100%)	67 (100%)	0	100	100
24	y	55/55 (100%)	55 (100%)	0	100	100
25	z	48/48 (100%)	48 (100%)	0	100	100
26	B	47/47 (100%)	47 (100%)	0	100	100
27	C	45/45 (100%)	45 (100%)	0	100	100
28	D	38/38 (100%)	38 (100%)	0	100	100
29	E	51/51 (100%)	51 (100%)	0	100	100
30	F	34/34 (100%)	34 (100%)	0	100	100
31	G	186/186 (100%)	186 (100%)	0	100	100
32	H	170/170 (100%)	169 (99%)	1 (1%)	78	84
33	I	172/172 (100%)	171 (99%)	1 (1%)	78	84
34	J	119/119 (100%)	118 (99%)	1 (1%)	73	82
35	K	87/87 (100%)	86 (99%)	1 (1%)	65	79
36	L	124/124 (100%)	124 (100%)	0	100	100
37	M	104/104 (100%)	103 (99%)	1 (1%)	68	80
38	N	105/105 (100%)	105 (100%)	0	100	100
39	O	86/86 (100%)	83 (96%)	3 (4%)	32	64
40	P	89/89 (100%)	88 (99%)	1 (1%)	65	79
41	Q	103/103 (100%)	103 (100%)	0	100	100
42	R	92/92 (100%)	91 (99%)	1 (1%)	65	79
43	S	83/83 (100%)	83 (100%)	0	100	100
44	T	76/76 (100%)	76 (100%)	0	100	100
45	U	65/65 (100%)	65 (100%)	0	100	100
46	V	74/74 (100%)	74 (100%)	0	100	100
47	W	56/56 (100%)	56 (100%)	0	100	100
48	X	70/70 (100%)	70 (100%)	0	100	100
49	Y	65/65 (100%)	65 (100%)	0	100	100
50	Z	55/55 (100%)	54 (98%)	1 (2%)	51	74
51	a	110/174 (63%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4908/4972 (99%)	4884 (100%)	24 (0%)	78 85

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	I	31	CYS
37	M	103	VAL
35	K	88	MET
39	O	57	VAL
8	i	33	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
20	u	73	ASN
49	Y	69	ASN
31	G	38	HIS
49	Y	12	GLN
43	S	48	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	3	1538/1539 (99%)	141 (9%)	4 (0%)
53	1	2902/2903 (99%)	332 (11%)	14 (0%)
54	2	119/120 (99%)	11 (9%)	1 (0%)
55	5	76/77 (98%)	10 (13%)	0
55	6	76/77 (98%)	7 (9%)	0
56	4	17/18 (94%)	2 (11%)	0
57	7	75/76 (98%)	10 (13%)	0
All	All	4803/4810 (99%)	513 (10%)	19 (0%)

5 of 513 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	3	6	G
52	3	9	G
52	3	32	A
52	3	39	G
52	3	48	C

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	1	2296	U
53	1	2756	U
54	2	88	C
53	1	2391	G
53	1	859	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
59	PHE	7	101	57	10,11,12	1.22	1 (10%)	8,13,15	0.64	0
58	FME	5	101	55	8,9,10	0.63	0	8,9,11	0.95	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
59	PHE	7	101	57	-	0/5/6/8	0/1/1/1
58	FME	5	101	55	-	2/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	7	101	PHE	CB-CG	-2.82	1.44	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	5	101	FME	O1-CN-N-CA
58	5	101	FME	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	7	101	PHE	1	0

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.

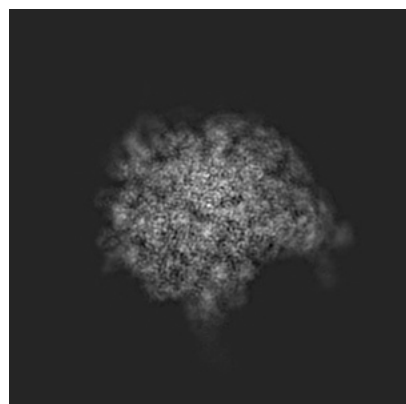
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21632. These allow visual inspection of the internal detail of the map and identification of artifacts.

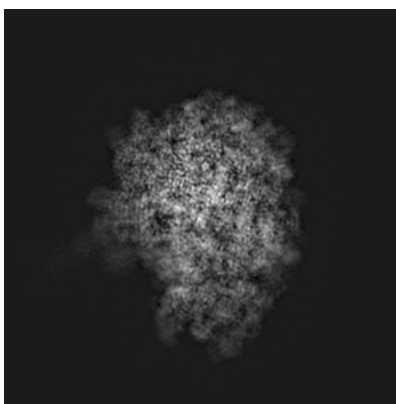
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

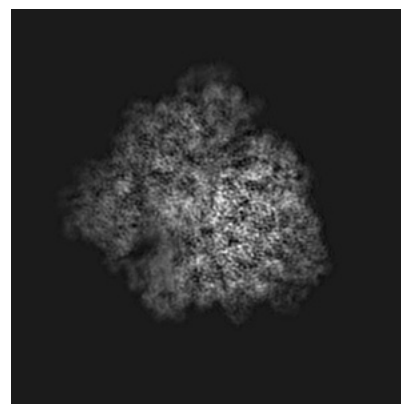
6.1.1 Primary map



X

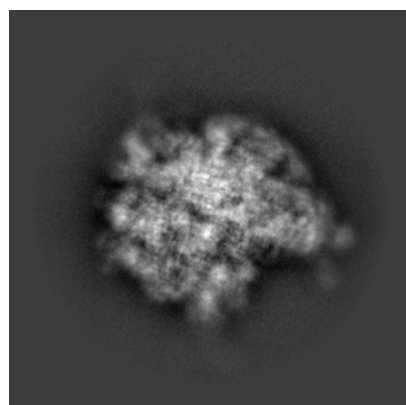


Y

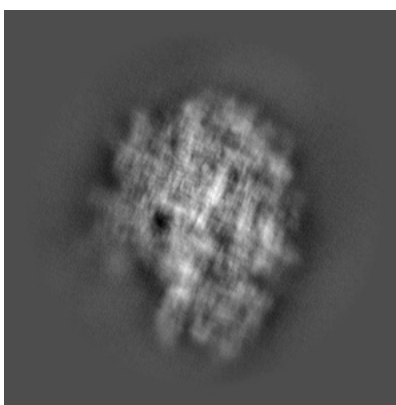


Z

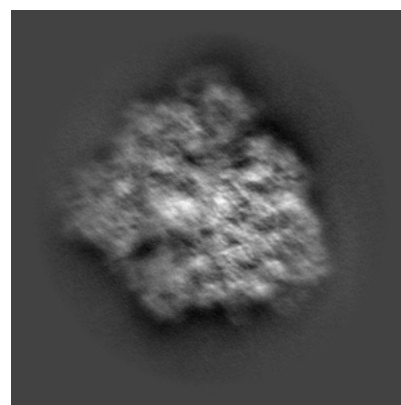
6.1.2 Raw map



X



Y

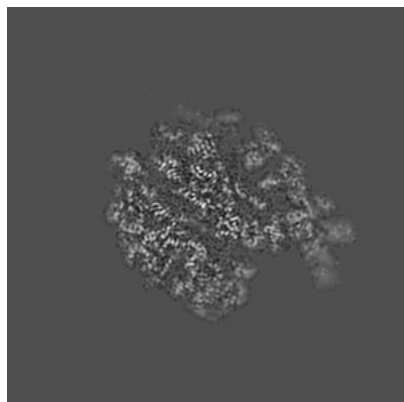


Z

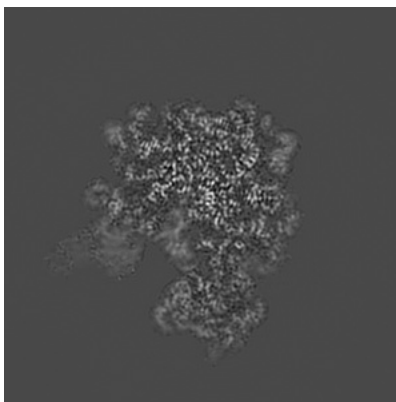
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

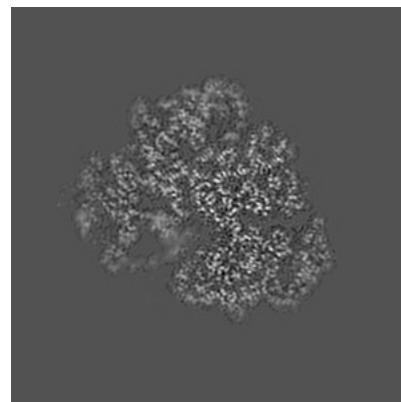
6.2.1 Primary map



X Index: 144

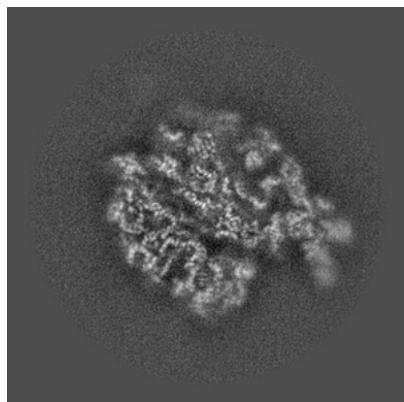


Y Index: 144

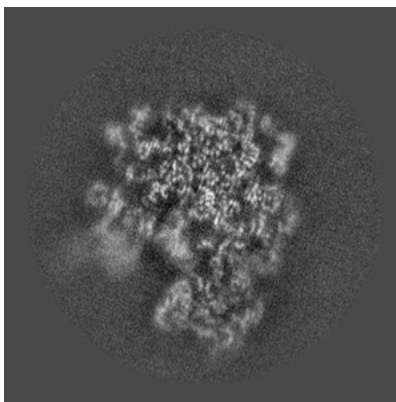


Z Index: 144

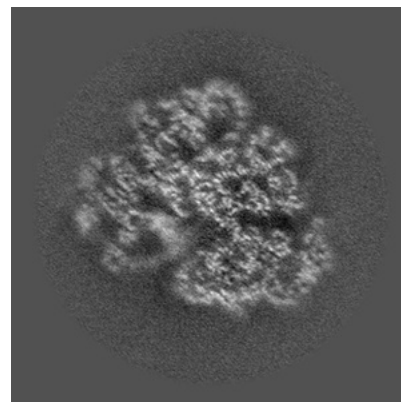
6.2.2 Raw map



X Index: 144



Y Index: 144

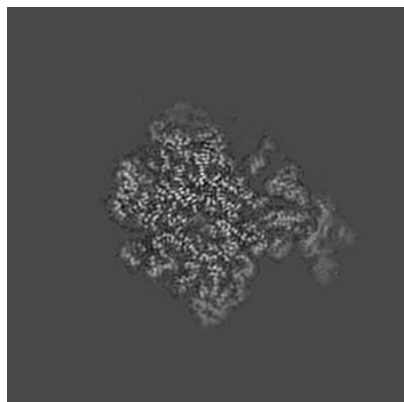


Z Index: 144

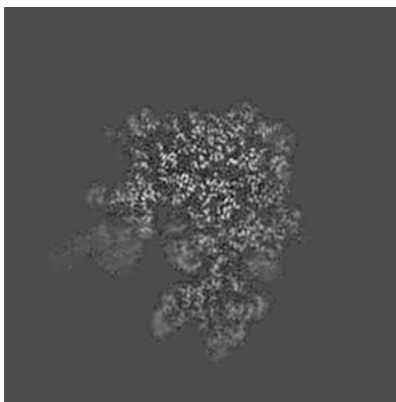
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

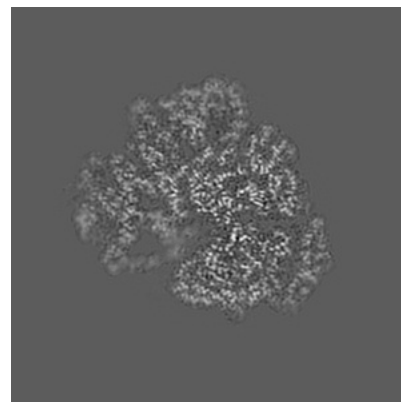
6.3.1 Primary map



X Index: 149

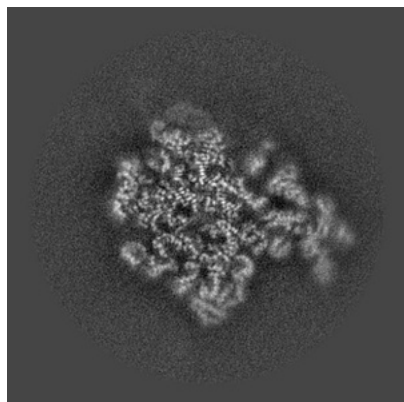


Y Index: 149

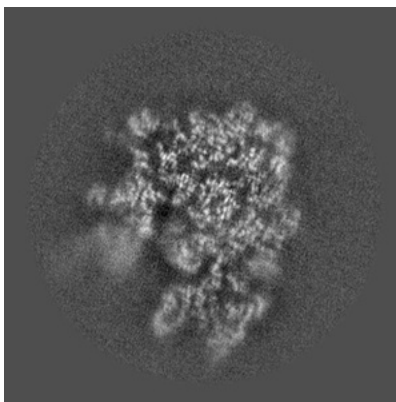


Z Index: 143

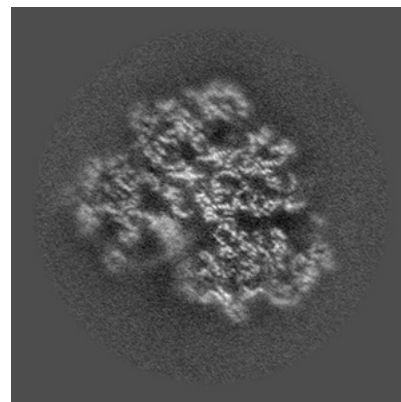
6.3.2 Raw map



X Index: 149



Y Index: 149

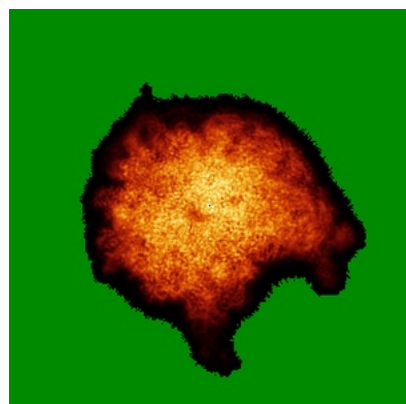


Z Index: 146

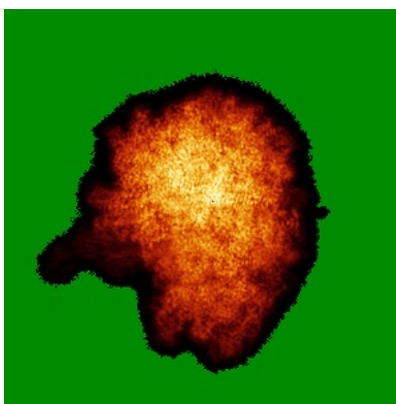
The images above show the largest variance slices of the map in three orthogonal directions.

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

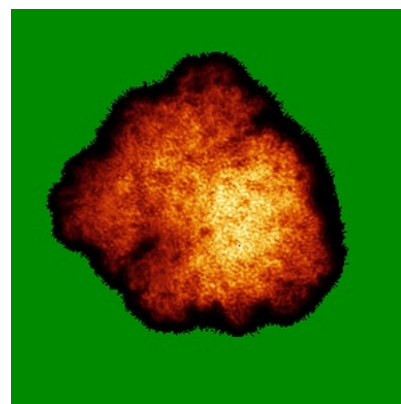
6.4.1 Primary map



X

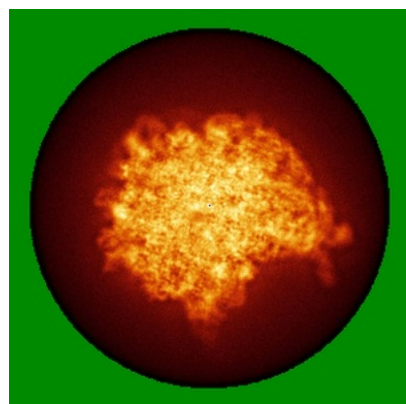


Y

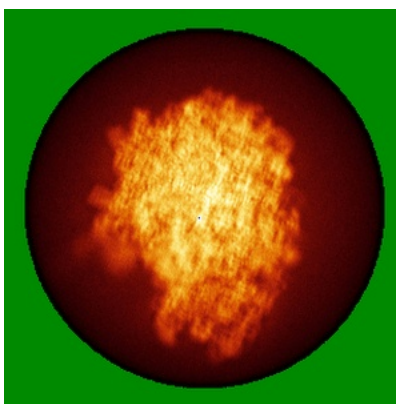


Z

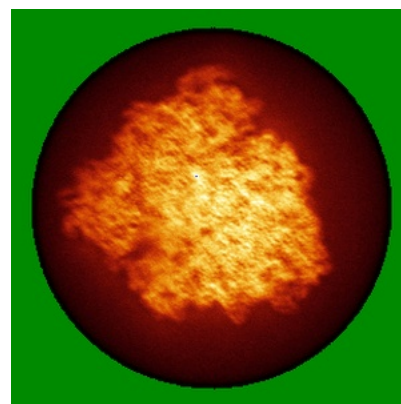
6.4.2 Raw map



X



Y

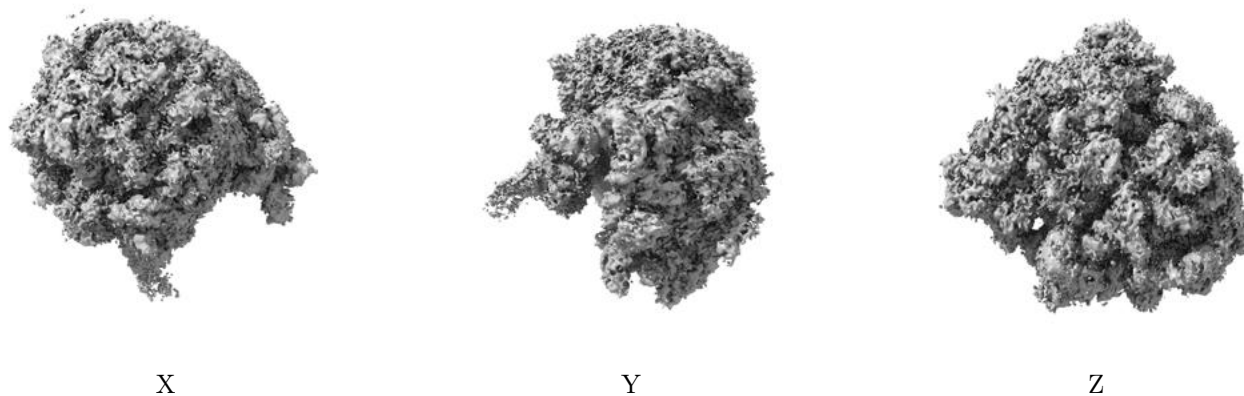


Z

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.

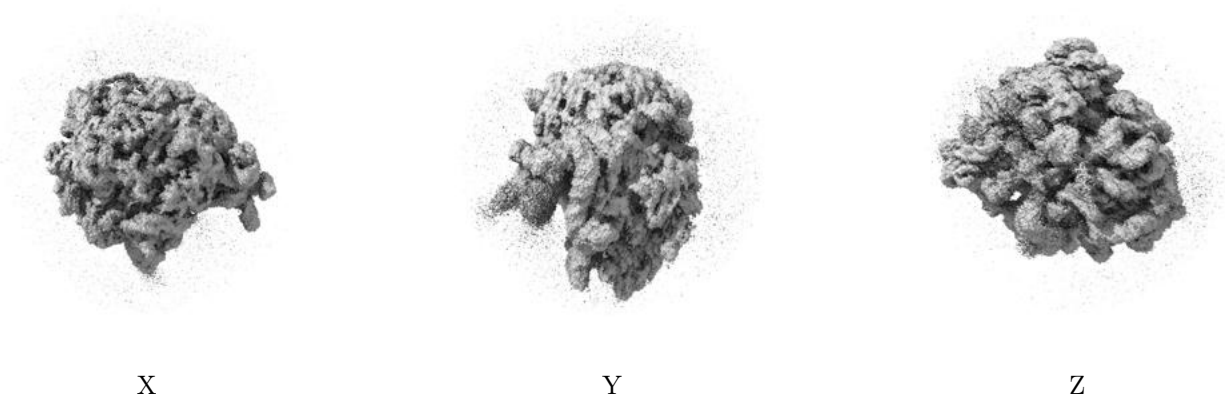
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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.

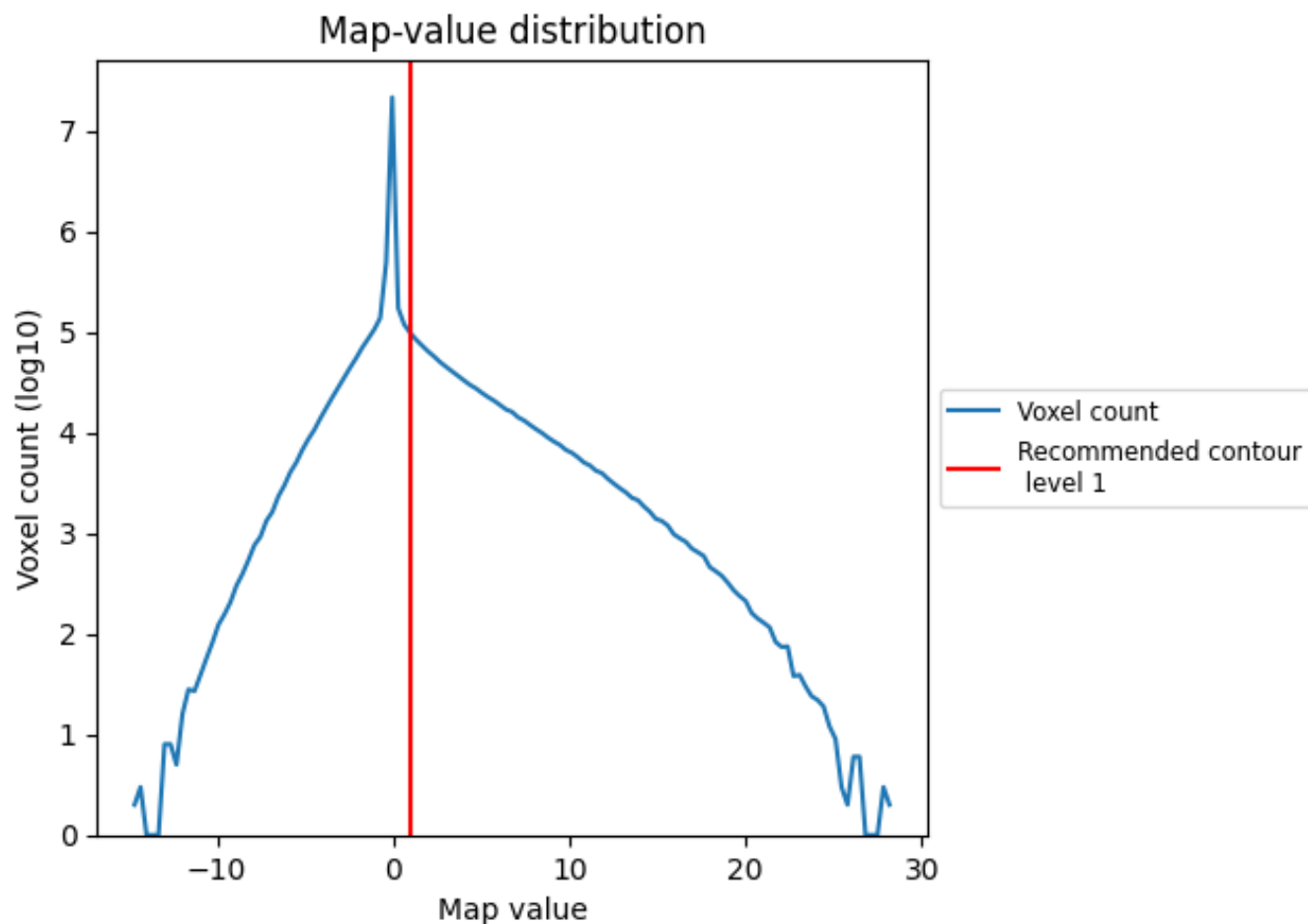
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

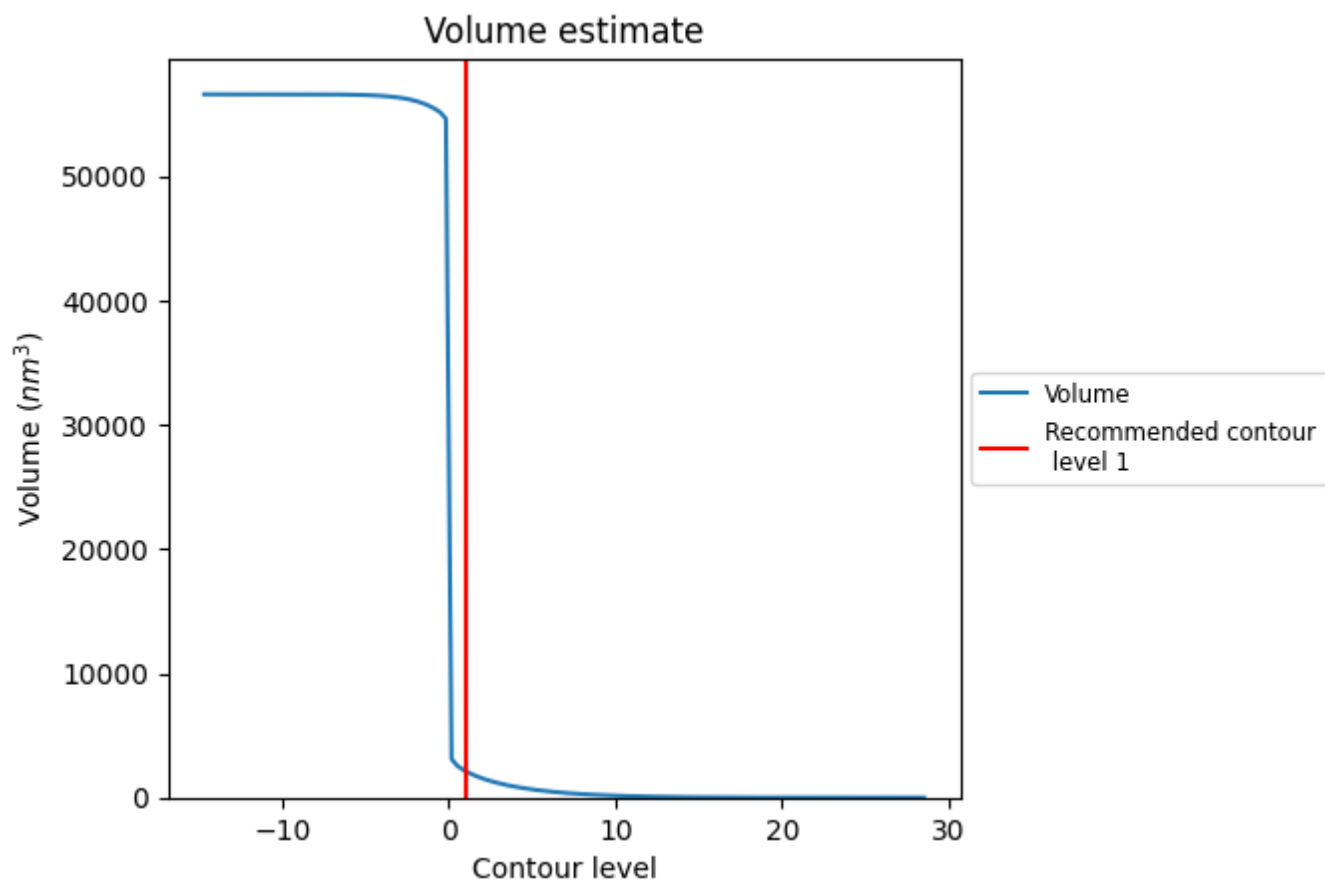
This section contains the results of statistical analysis of the map.

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.

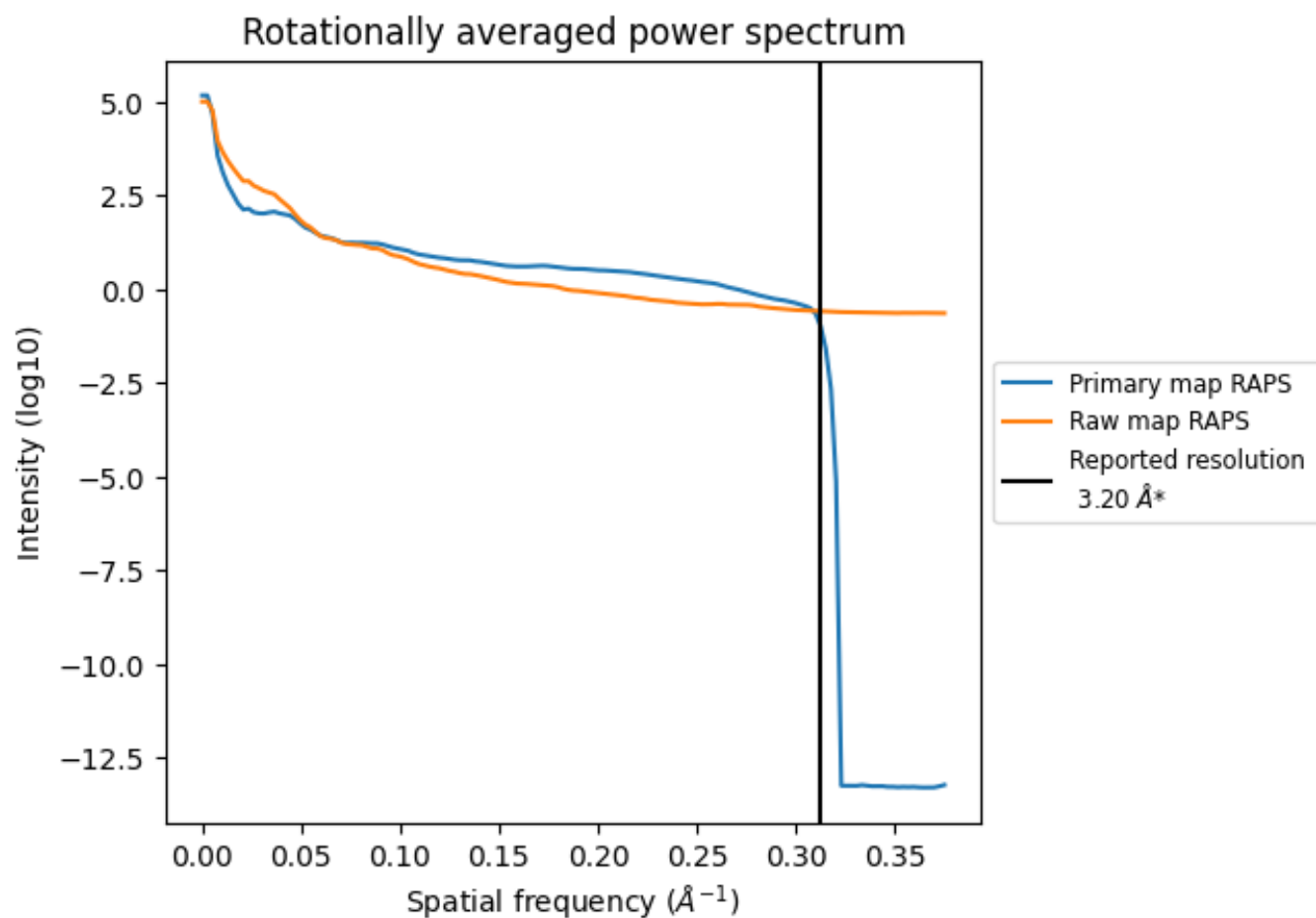
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2140 nm³; this corresponds to an approximate mass of 1933 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 ⓘ

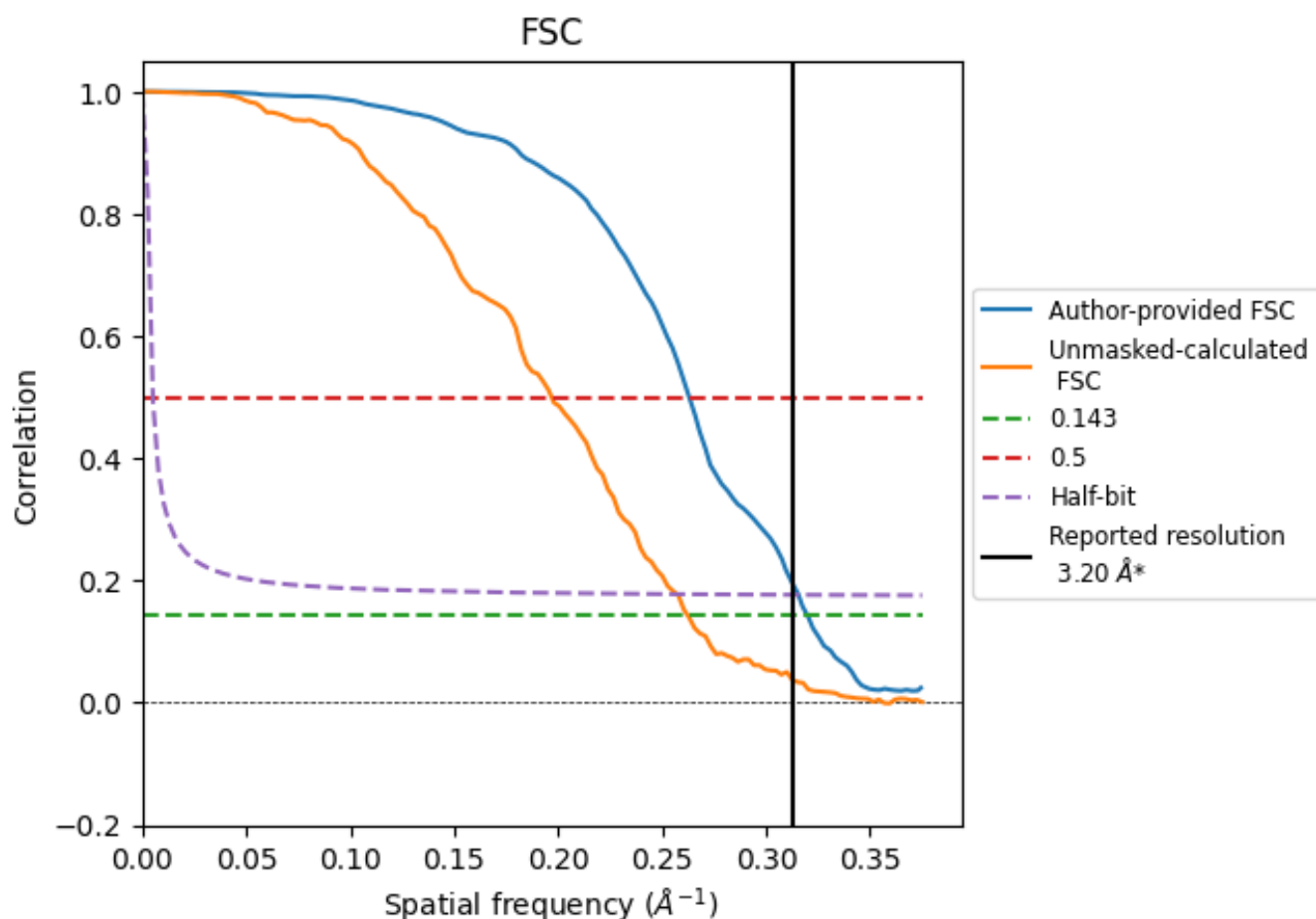


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.312 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

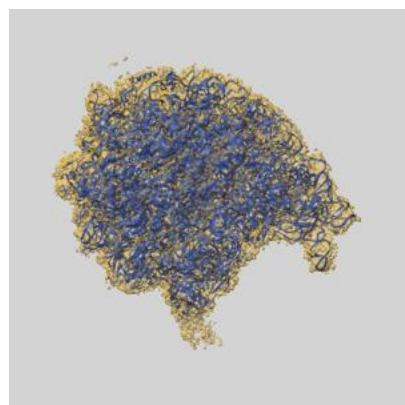
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.13	3.80	3.17
Unmasked-calculated*	3.81	5.08	3.89

*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 3.81 differs from the reported value 3.2 by more than 10 %

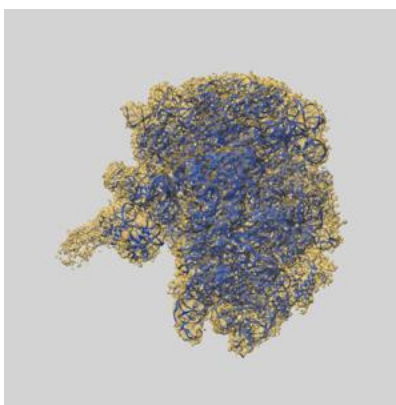
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21632 and PDB model 6WDD. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

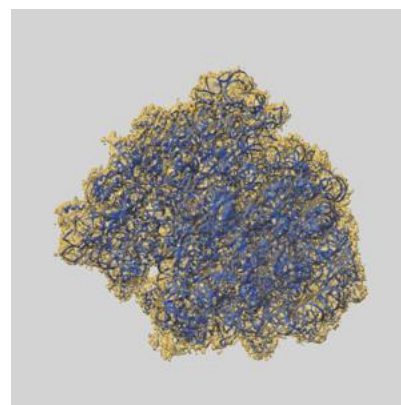
9.1 Map-model overlay [i](#)



X



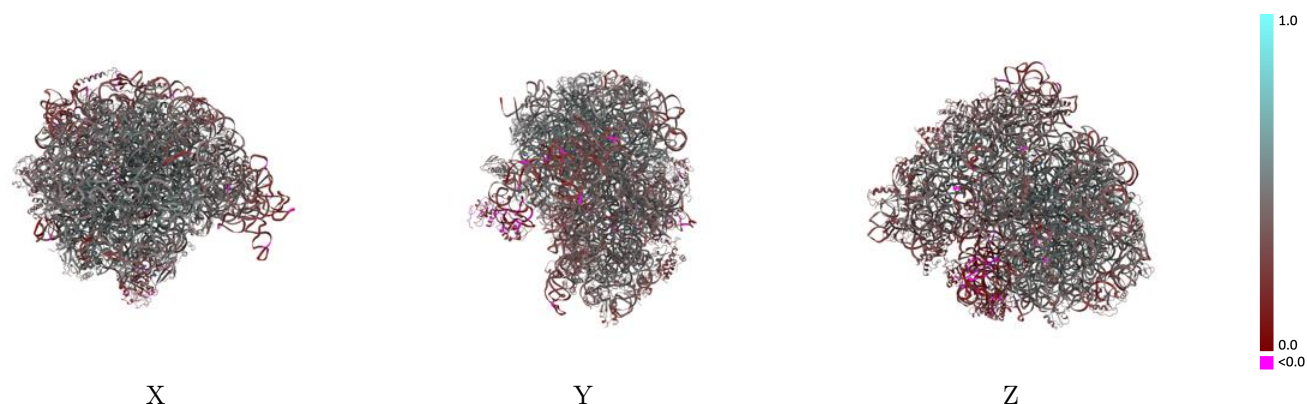
Y



Z

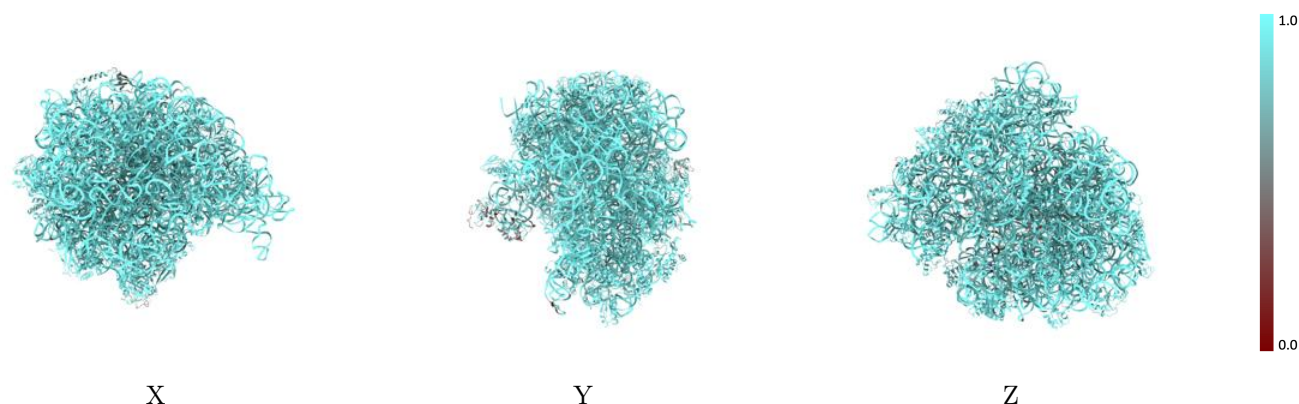
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



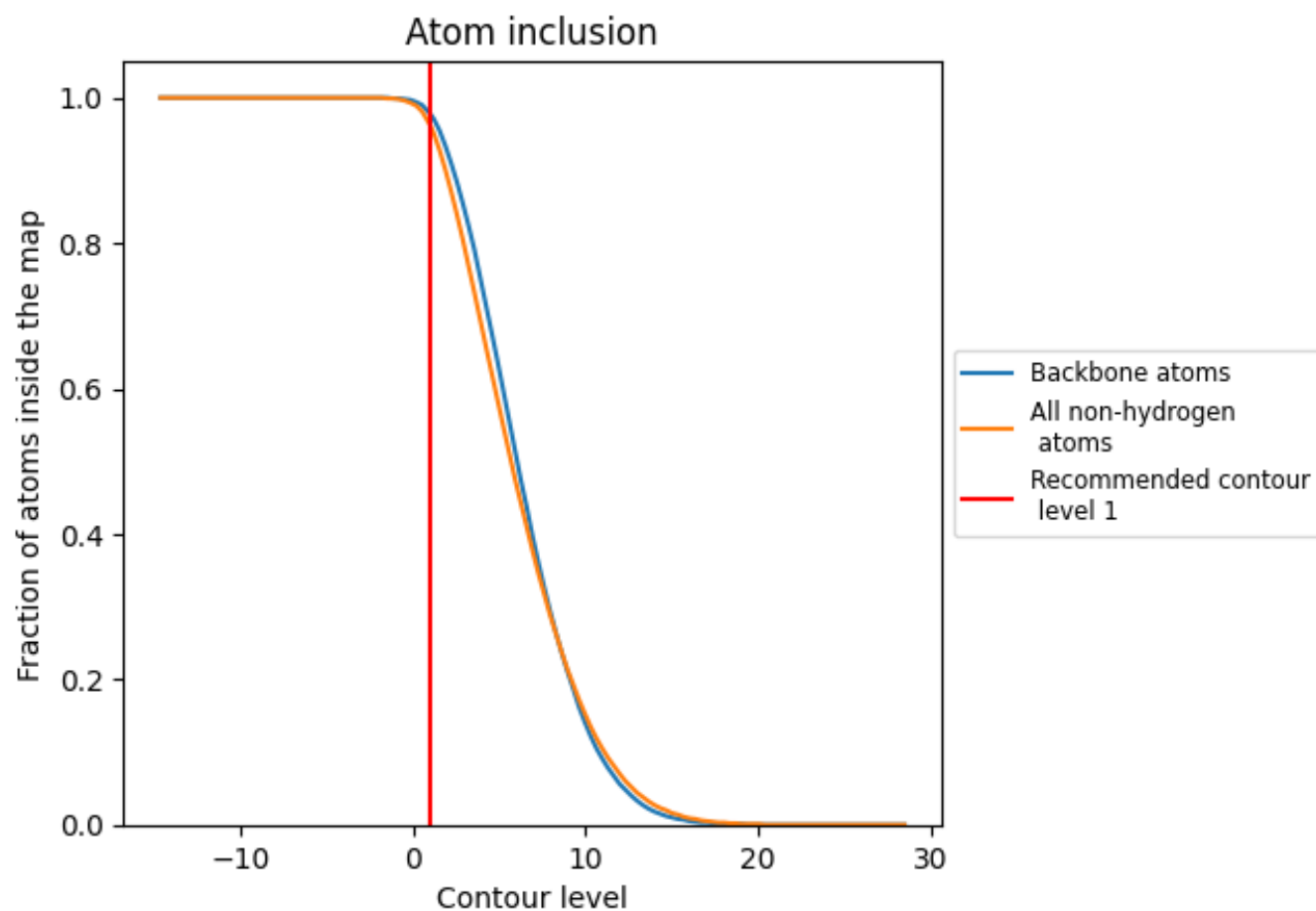
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9610	 0.4100
1	 0.9820	 0.4400
2	 0.9830	 0.3580
3	 0.9780	 0.3940
4	 0.9230	 0.3160
5	 0.8470	 0.2010
6	 0.8510	 0.1520
7	 0.9360	 0.2670
B	 0.9580	 0.4890
C	 0.8980	 0.4300
D	 0.9580	 0.5150
E	 0.9590	 0.5090
F	 0.9010	 0.4580
G	 0.9050	 0.3700
H	 0.9350	 0.4320
I	 0.9180	 0.3740
J	 0.9440	 0.4360
K	 0.9590	 0.4070
L	 0.9420	 0.3480
M	 0.9490	 0.4310
N	 0.9420	 0.3840
O	 0.8780	 0.3620
P	 0.9590	 0.4170
Q	 0.9520	 0.4730
R	 0.9460	 0.3280
S	 0.9170	 0.3920
T	 0.9680	 0.4170
U	 0.9030	 0.3780
V	 0.9590	 0.4190
W	 0.9280	 0.3950
X	 0.9570	 0.3460
Y	 0.9400	 0.3790
Z	 0.8650	 0.3220
a	 0.8970	 0.1760
b	 0.9700	 0.5070



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Chain	Atom inclusion	Q-score
c	 0.9630	 0.4940
d	 0.9500	 0.4390
e	 0.9210	 0.2490
f	 0.9650	 0.3780
g	 0.7640	 0.2830
h	 0.6460	 0.1480
i	 0.6350	 0.1380
j	 0.9630	 0.4930
k	 0.9650	 0.4840
l	 0.9510	 0.4650
m	 0.9440	 0.4790
n	 0.9660	 0.4960
o	 0.9570	 0.3980
p	 0.9580	 0.4730
q	 0.9640	 0.4970
r	 0.9640	 0.4650
s	 0.9460	 0.4920
t	 0.9470	 0.4630
u	 0.9440	 0.4160
v	 0.9620	 0.4420
w	 0.9640	 0.4880
x	 0.9800	 0.4940
y	 0.9400	 0.3980
z	 0.9680	 0.4740