Full wwPDB EM Validation Report (i)

Apr 22, 2025 – 04:25 pm BST

PDB ID	:	9GHA / pdb_00009gha
EMDB ID	:	EMD-51350
Title	:	Fusidic acid-locked Escherichia coli 70S ribosome with Staphylococcus aureus EF-G and a tRNA in pe/E chimeric state (CHI)
Authors	:	Gonzalez-Lopez, A.; Selmer, M.
Deposited on	:	2024-08-15
Resolution	:	2.24 Å(reported)
Based on initial models	:	9GHE, 8P2H, 7N2C

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

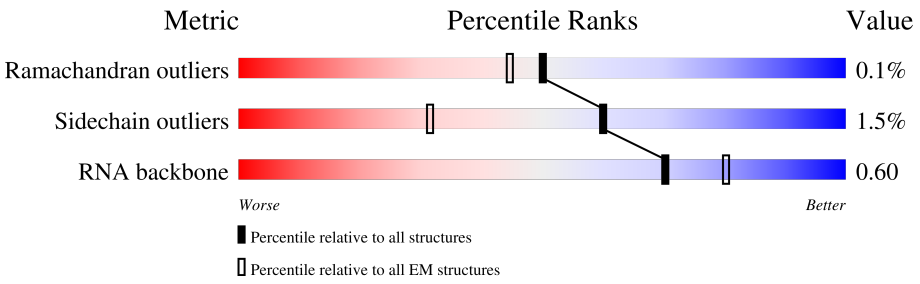
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.24 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	55	87% • 9%
2	1	46	98% •
3	2	65	95% • •
4	3	38	97% •
5	4	70	• 69% 31%
6	8	77	81% 19%
7	9	24	21% 79%
8	A	1554	• 82% 16% •

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Mol	Chain	Length	Quality of chain
9	B	241	7% 88% 8%
10	C	233	87% 12%
11	D	206	97%
12	E	167	91% 8%
13	F	135	75% 25%
14	G	179	11% 80% 16%
15	H	130	98%
16	I	130	92% 5%
17	J	103	15% 88% 5% 7%
18	K	129	90% 9%
19	L	124	94%
20	M	118	12% 96%
21	N	101	98%
22	O	89	97%
23	P	82	96%
24	Q	84	89% 5% 6%
25	R	75	85% 15%
26	S	92	91% 9%
27	T	87	98%
28	U	71	77% 23%
29	W	693	95%
30	a	2930	84% 11% 5%
31	b	119	94% 6%
32	c	273	99%
33	d	209	99%

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Mol	Chain	Length	Quality of chain
34	e	201	100%
35	f	179	94%
36	g	177	93%
37	h	149	28% 72%
38	i	142	98%
39	j	123	98%
40	k	144	99%
41	l	136	99%
42	m	127	93% 7%
43	n	117	97%
44	o	115	98%
45	p	118	98%
46	q	103	98%
47	r	110	99%
48	s	100	93% 7%
49	t	104	88% 11%
50	u	94	99%
51	v	85	88% 12%
52	w	78	97%
53	x	63	94% 5%
54	y	59	98%
55	z	57	95% 5%

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 145564 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	50	413	267	75	71	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	45	367	222	88	55	2	0	0

- Molecule 3 is a protein called 50S ribosomal protein L35.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	38	302	185	65	48	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	48	373	232	66	69	6	0	0

- Molecule 6 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	8	77	1640	732	297	535	76	0	0

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	9	5	110	49	22	34	5	0	0

- Molecule 8 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	A	1526	32757	14617	6009	10605	1526	0	0

- Molecule 9 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	222	1737	1099	312	318	8	0	0

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	206	1624	1028	305	288	3	0	0

- Molecule 11 is a protein called 30S ribosomal protein S4.

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

- Molecule 12 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E	154	1135	706	215	208	6	0	0

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	F	101	824	520	149	149	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	G	150	1176	732	226	214	4	0	0

- Molecule 15 is a protein called 30S ribosomal protein S8.

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

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	I	125	1001	622	200	176	3	0	0

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	J	96	775	487	148	139	1	0	0

- Molecule 18 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	K	117	877	540	173	161	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP P0A7R9

- Molecule 19 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	L	121	942	582	193	162	5	0	0

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	M	115	891	552	179	157	3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S14.

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

- Molecule 22 is a protein called 30S ribosomal protein S15.

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

- Molecule 23 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	79	629	394	124	110	1	0	0

- Molecule 24 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	79	641	406	120	112	3	0	0

- Molecule 25 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	64	524	330	99	94	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	S	84	668	427	127	112	2	0	0

- Molecule 27 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	T	86	670	414	138	115	3	0	0

- Molecule 28 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	U	55	460	287	95	77	1	0	0

- Molecule 29 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	W	666	5154	3232	865	1028	29	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	a	2782	59756	26665	11017	19292	2782	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	b	119	2549	1135	466	829	119	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	c	271	2082	1288	423	364	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	d	207	1552	972	286	291	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	f	177	1410	899	249	256	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	g	170	1273	803	232	236	2	0	0

- Molecule 37 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	h	41	303	194	54	54	1	0	0

- Molecule 38 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	i	141	1121	709	211	198	3	0	0

- Molecule 39 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	j	123	946	593	181	166	6	0	0

- Molecule 40 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	k	144	1053	654	207	190	2	0	0

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	l	136	1075	686	205	177	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	modified residue	UNP P0ADY7

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	m	118	945	585	194	161	5	0	0

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L19.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called 50S ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	r	109	845	526	162	154	3	0	0

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	s	93	738	466	139	131	2	0	0

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	t	93	717	452	135	130	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	u	93	745	474	136	133	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	v	75	569	353	113	102	1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L28.

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

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	x	60	491	303	96	91	1	0	0

- Molecule 54 is a protein called 50S ribosomal protein L30.

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

- Molecule 55 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	z	54	429	260	91	77	1	0	0

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
56	3	1	1	1	0
56	4	1	1	1	0

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
57	A	14	14	14	0
57	F	1	1	1	0
57	a	74	74	74	0
57	c	3	3	3	0
57	e	1	1	1	0
57	t	1	1	1	0

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
58	A	27	27	27	0
58	W	1	1	1	0
58	a	233	233	233	0

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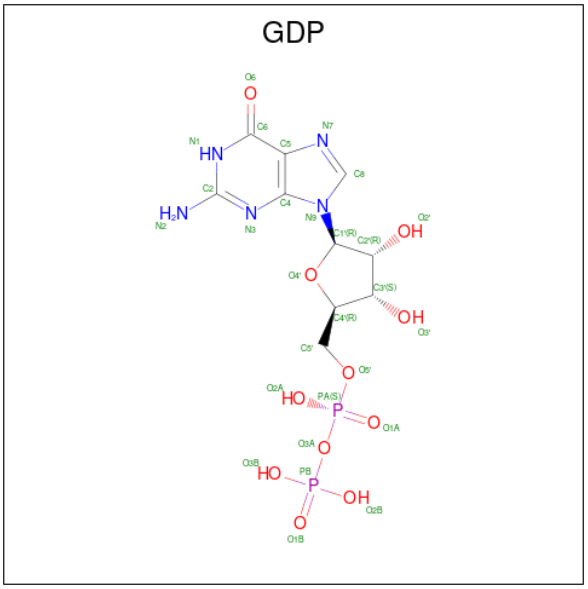
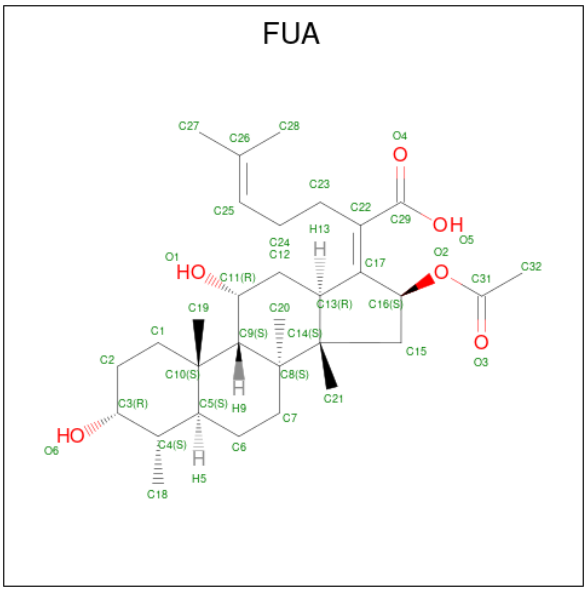
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
58	b	3	3	3	0
58	c	3	3	3	0
58	d	2	2	2	0
58	k	1	1	1	0
58	z	1	1	1	0

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	W	1	28	10	5	11	2	0

- Molecule 60 is FUSIDIC ACID (CCD ID: FUA) (formula: $C_{31}H_{48}O_6$) (labeled as "Ligand of Interest" by depositor).



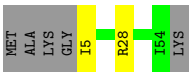
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
60	W	1	37	31	6	0

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.

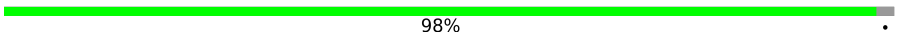
- Molecule 1: 50S ribosomal protein L33

Chain 0:



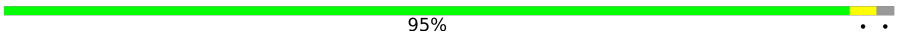
- Molecule 2: 50S ribosomal protein L34

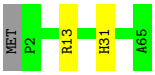
Chain 1:



- Molecule 3: 50S ribosomal protein L35

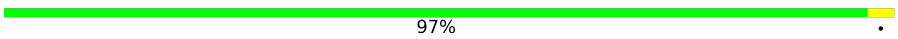
Chain 2:





- Molecule 4: 50S ribosomal protein L36

Chain 3:

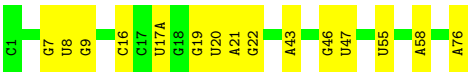


- Molecule 5: 50S ribosomal protein L31

Chain 4:

- Molecule 6: tRNA

Chain 8: 81% 19%

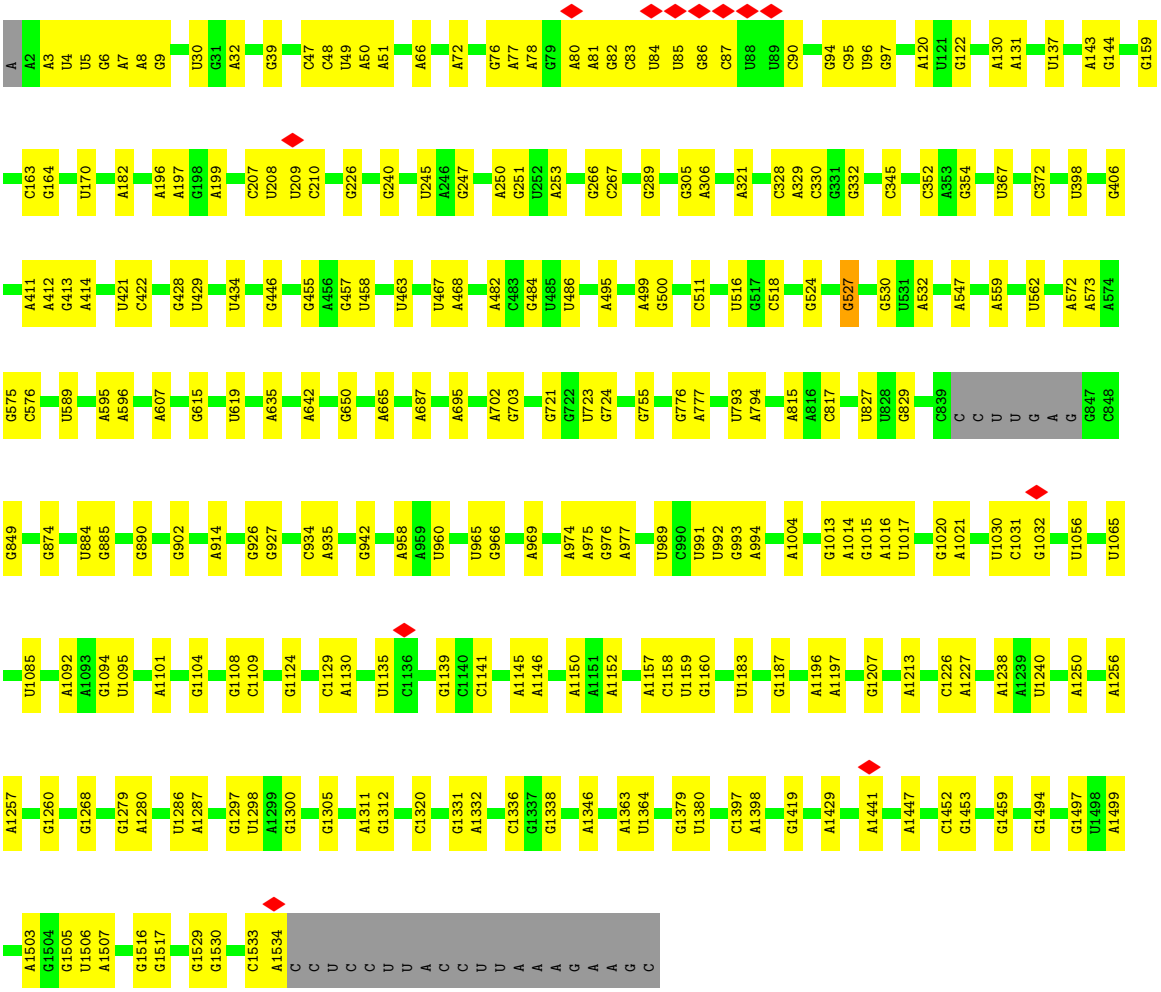


• Molecule 7: mRNA

Chain 9: 21% 79%

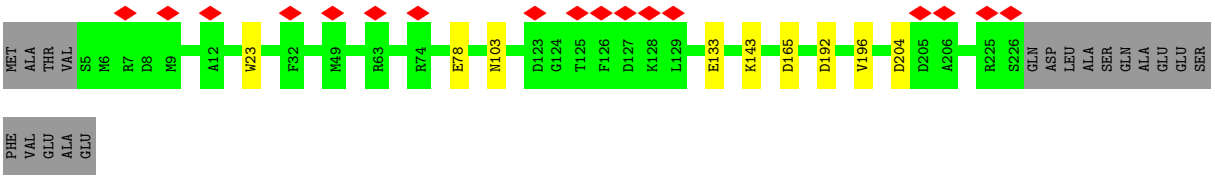
• Molecule 8: 16S rRNA

Chain A: 82% 16%



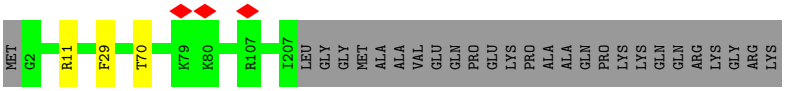
• Molecule 9: 30S ribosomal protein S2

Chain B: 7% 88% 8%



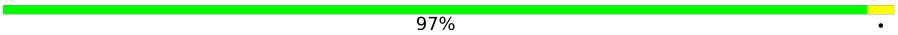
- Molecule 10: 30S ribosomal protein S3

Chain C:



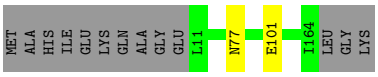
- Molecule 11: 30S ribosomal protein S4

Chain D:



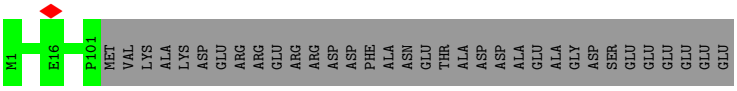
- Molecule 12: 30S ribosomal protein S5

Chain E:



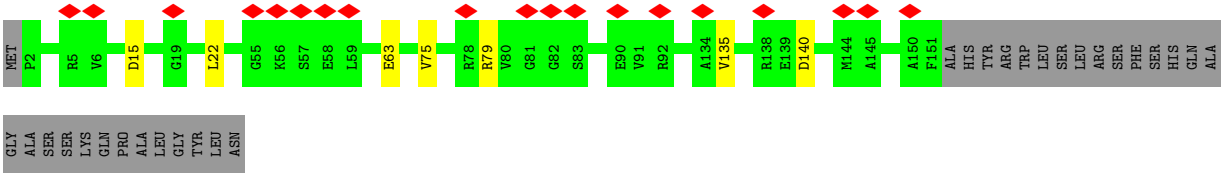
- Molecule 13: 30S ribosomal protein S6

Chain F:



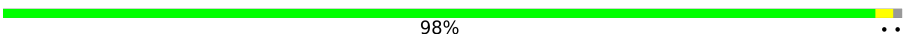
- Molecule 14: 30S ribosomal protein S7

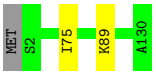
Chain G:



- Molecule 15: 30S ribosomal protein S8

Chain H:



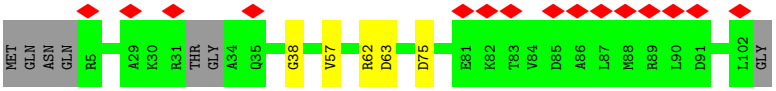


• Molecule 16: 30S ribosomal protein S9

Chain I:

• Molecule 17: 30S ribosomal protein S10

Chain J:

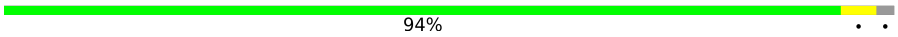


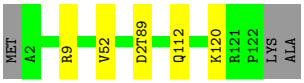
• Molecule 18: Small ribosomal subunit protein uS11

Chain K:

• Molecule 19: 30S ribosomal protein S12

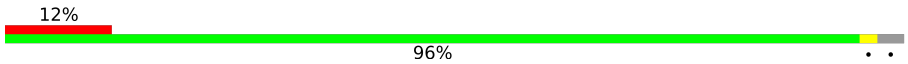
Chain L:

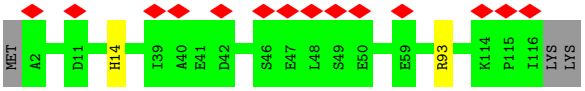




• Molecule 20: 30S ribosomal protein S13

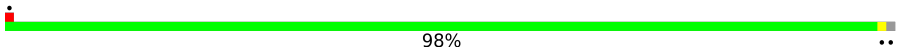
Chain M:

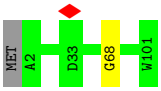




• Molecule 21: 30S ribosomal protein S14

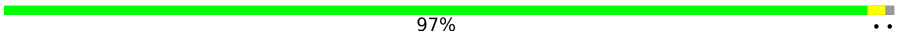
Chain N:





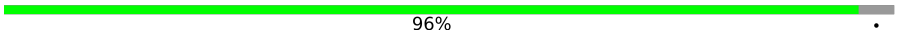
• Molecule 22: 30S ribosomal protein S15

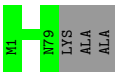
Chain O:



• Molecule 23: 30S ribosomal protein S16

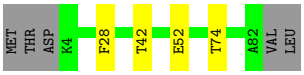
Chain P:





• Molecule 24: 30S ribosomal protein S17

Chain Q:

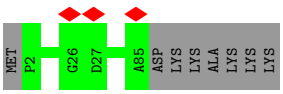


• Molecule 25: 30S ribosomal protein S18

Chain R:

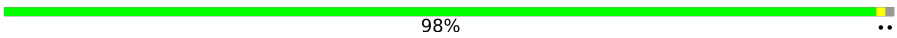
• Molecule 26: 30S ribosomal protein S19

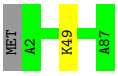
Chain S:



• Molecule 27: 30S ribosomal protein S20

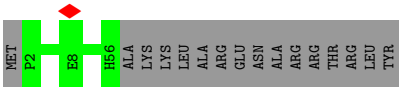
Chain T:





• Molecule 28: 30S ribosomal protein S21

Chain U:



• Molecule 29: Elongation factor G

Chain W: 95%

M1 I37 HIS LYS ILE GLY GLU THR HIS GLU GLY GLU GLY ALA SER GLN MET ASP TRP MET GLU GLN GLU GLN ASP ARG GLY ILE THR ILE T64 D87 T260 H290 M401 D419 Q447 E472 V492 N690 K691 G692 GLU

- Molecule 30: 23S rRNA

Chain a: 84% 11% 5%

G G G U U G U G A G1 A10 C11 U12 G15 U34 A71 A74 G75 A101 A118 A119 U120 A131 U139 A142 U162 A181 A196 A199 G215 A216 A221 A222 G242 G248 A272 A278 A279 U280 C281

G285 G289 A311 A330 A346 A354 G361 A362 G386 G411 U448 U451 G481 G491 A505 C509 G512 C531 A532 G533 C544 U545 U546 A547 G548 G549 A556 A563 U573 A574 A575 A586 A603 U615 A627

A637 C645 U646 G647 U653 A654 A655 U686 A716 C717 A730 G745 U746 U747 A764 C765 G775 G776 A782 A783 G784 G785 A792 G805 C812 U827 U828 A845 U846 G858 G869 A878 G G G G G U C A U C

C C G A C U U A C C A899 A910 G914 C915 U931 U934 C946 U955 C961 G974 A983 A984 C985 A996 U1012 C1013 G1022 G1026 U1033 G1041 G1047 G1059 U1060 A1070 A1077 A1080 U1083 G1087

A1088 U1097 U1101 G1112 G1116 G1128 A1129 U1130 G1131 U1132 A1133 A1134 C1135 A1142 A1143 A1144 A1151 A1169 C1170 G1171 C U U A U G C1178 G1179 U1188 A1253 G1256 G1271 A1272 G1300 A1301 A1321 U1352 A1365 A1378 U1379 A1383

C1386 U1409 G1416 A1419 C1428 C1451 G1452 A1453 C1454 G1455 U1458 G1459 U1460 G1482 A1490 C1493 A1508 A1509 G1510 A1515 U1534 A1535 C1536 G1537 G1538 A1569 U1578 U1584 C1585 A1608 A1609 A1618 U1647 U1648 G1649 G1674 A1698 G1715

U1729 C1730 G1734 G1737 G1738 A1744 C1764 A1773 U1782 C1800 A1801 A1808 C1816 A1829 G1835 A1847 A1848 A1858 C1870 A1871 A1872 C1905 G1906 G1907 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 G1929 G1930 U1931 A1936 A1937 U1955 C1967 A1970

U1971 G1972 U1991 G1992 U1993 A2020 C2023 A2030 A2031 G2032 A2033 C2043 C2055 G2056 A2060 G2061 A2062 G2069 G2093 C2096 A2097 U U G A G C C U U G A U G U G A A U A C C A G G A C C U U G G A A A U A C C A G C U U G U U G G A

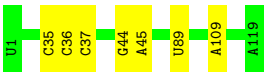
U U U G A U2192 G2193 A2198 G2204 A2211 A2225 G2238 G2251 A2268 A2273 A2278 C2283 A2287 U2305 G2308 U2312 A2322 G2325 A2333 U2334 A2335 C2347 C2350 A2366 G2383 U2384 C2385 U2402 A2406 A2425

G2429 A2430 U2431 A2435 U2441 G2445 G2446 G2447 A2448 U2449 U2457 G2458 A2459 A2469 A2476 U2477 A2478 U2491 G2502 A2503 U2504 G2505 A2518 G2529 U2546 A2547 A2566 G2567 C2573 U2580 A2602 G2603 U2604 U2605 U2609 U2613 U2629 G2661 A2662 G2663

U2689 U2690 G2714 C2715 C2716 A2726 G2744 A2748 A2749 A2750 A2757 A2765 A2778 U2798 A2799 G2803 A2809 U2818 G2819 A2820 A2821 A2883 U2884 C2902 U U A C A A C G C C G A A G C U G U U

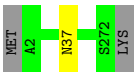
- Molecule 31: 5S rRNA

Chain b: 94% 6%



• Molecule 32: 50S ribosomal protein L2

Chain c: 99%



• Molecule 33: 50S ribosomal protein L3

Chain d: 99%

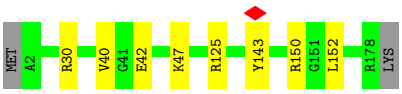
• Molecule 34: 50S ribosomal protein L4

Chain e: 100%

There are no outlier residues recorded for this chain.

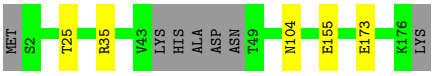
• Molecule 35: 50S ribosomal protein L5

Chain f: 94%



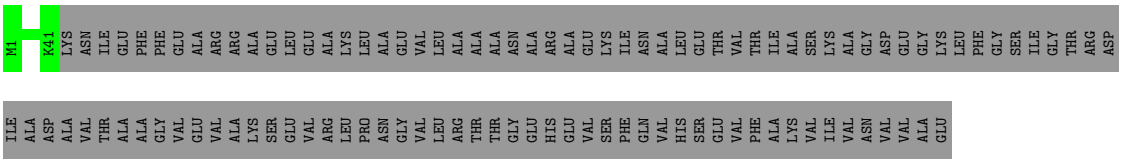
• Molecule 36: 50S ribosomal protein L6

Chain g: 93%



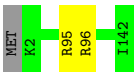
• Molecule 37: 50S ribosomal protein L9

Chain h: 28% 72%



• Molecule 38: 50S ribosomal protein L13

Chain i: 98%



• Molecule 39: 50S ribosomal protein L14

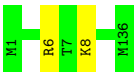
Chain j: 98%

• Molecule 40: 50S ribosomal protein L15

Chain k: 99%

• Molecule 41: 50S ribosomal protein L16

Chain l: 99%



• Molecule 42: 50S ribosomal protein L17

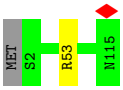
Chain m: 93% 7%

• Molecule 43: 50S ribosomal protein L18

Chain n: 97%

• Molecule 44: 50S ribosomal protein L19

Chain o: 98%



• Molecule 45: 50S ribosomal protein L20

Chain p: 98%

• Molecule 46: 50S ribosomal protein L21

Chain q: 98%

• Molecule 47: 50S ribosomal protein L22

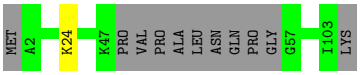
Chain r: 99%

• Molecule 48: 50S ribosomal protein L23

Chain s: 93% 7%

• Molecule 49: 50S ribosomal protein L24

Chain t: 88% 11%

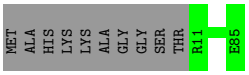


• Molecule 50: 50S ribosomal protein L25

Chain u: 99%

• Molecule 51: 50S ribosomal protein L27

Chain v: 88% 12%

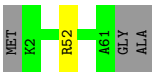


• Molecule 52: 50S ribosomal protein L28

Chain w: 97%

• Molecule 53: 50S ribosomal protein L29

Chain x: 94% 5%

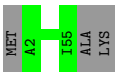


• Molecule 54: 50S ribosomal protein L30

Chain y: 98%

• Molecule 55: 50S ribosomal protein L32

Chain z: 95% 5%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88568	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.714	Depositor
Minimum map value	-0.317	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	388.8, 388.8, 388.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.648, 0.648, 0.648	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, MS6, ZN, MA6, 3TD, MEQ, MG, D2T, 4OC, H2U, 2MG, OMU, IAS, 6MZ, OMC, 5MU, 5MC, UR3, 4D4, GDP, FUA, G7M, 2MA, K, OMG, 1MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.31	0/420	0.52	0/560
2	1	0.29	0/370	0.61	0/487
3	2	0.32	0/513	0.55	0/676
4	3	0.30	0/303	0.57	0/397
5	4	0.31	0/380	0.53	0/508
6	8	0.46	0/1832	0.89	0/2855
7	9	0.55	0/123	0.86	0/190
8	A	0.44	0/36398	0.88	0/56774
9	B	0.29	0/1768	0.53	0/2381
10	C	0.28	0/1651	0.51	0/2225
11	D	0.29	0/1665	0.52	0/2227
12	E	0.29	0/1148	0.52	0/1545
13	F	0.28	0/843	0.49	0/1140
14	G	0.29	0/1190	0.53	0/1595
15	H	0.29	0/989	0.55	0/1326
16	I	0.29	0/1013	0.53	0/1350
17	J	0.28	0/784	0.59	0/1059
18	K	0.31	0/884	0.53	0/1191
19	L	0.29	0/945	0.58	0/1268
20	M	0.29	0/900	0.53	0/1204
21	N	0.30	0/817	0.51	0/1088
22	O	0.28	0/722	0.50	0/964
23	P	0.28	0/639	0.54	0/859
24	Q	0.28	0/650	0.53	0/871
25	R	0.29	0/532	0.52	0/715
26	S	0.32	0/685	0.52	0/922
27	T	0.28	0/676	0.50	0/895
28	U	0.31	0/467	0.58	0/620
29	W	0.29	0/5244	0.49	0/7091
30	a	0.42	0/66355	0.90	8/103511 (0.0%)
31	b	0.44	0/2850	0.90	0/4444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	c	0.29	0/2121	0.56	0/2852
33	d	0.29	0/1562	0.54	0/2102
34	e	0.28	0/1571	0.51	0/2113
35	f	0.29	0/1434	0.52	0/1926
36	g	0.29	0/1291	0.54	0/1747
37	h	0.30	0/306	0.53	0/413
38	i	0.28	0/1144	0.54	0/1541
39	j	0.28	0/955	0.57	0/1279
40	k	0.31	0/1062	0.54	0/1413
41	l	0.29	0/1073	0.55	0/1433
42	m	0.28	0/958	0.55	0/1281
43	n	0.29	0/902	0.54	0/1209
44	o	0.29	0/929	0.55	0/1242
45	p	0.29	0/960	0.56	0/1278
46	q	0.29	0/829	0.54	0/1107
47	r	0.28	0/852	0.56	0/1142
48	s	0.27	0/744	0.51	0/994
49	t	0.30	0/721	0.54	0/956
50	u	0.29	0/758	0.54	0/1015
51	v	0.32	0/576	0.56	0/762
52	w	0.30	0/635	0.57	0/848
53	x	0.27	0/492	0.49	0/655
54	y	0.29	0/453	0.52	0/605
55	z	0.30	0/435	0.56	0/581
All	All	0.39	0/156519	0.81	8/233432 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	2	0	1
4	3	0	1
10	C	0	1
11	D	0	1
14	G	0	1
16	I	0	2
17	J	0	2
18	K	0	1
19	L	0	1
36	g	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	i	0	1
45	p	0	1
52	w	0	1
53	x	0	1
All	All	0	16

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	512	G	O4'-C1'-N9	7.53	114.23	108.20
30	a	2447	G	C3'-C2'-C1'	-5.94	96.75	101.50
30	a	2546	U	O3'-P-O5'	-5.94	92.71	104.00
30	a	512	G	C1'-O4'-C4'	-5.93	105.16	109.90
30	a	1936	A	C1'-O4'-C4'	-5.50	105.50	109.90
30	a	1936	A	O4'-C1'-N9	5.34	112.47	108.20
30	a	1905	C	O3'-P-O5'	-5.10	94.32	104.00
30	a	242	G	C3'-C2'-C1'	-5.01	97.50	101.50

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	13	ARG	Sidechain
4	3	36	ARG	Sidechain
10	C	11	ARG	Sidechain
11	D	184	ARG	Sidechain
14	G	79	ARG	Sidechain
16	I	41	ARG	Sidechain
16	I	95	ARG	Sidechain
17	J	38	GLY	Peptide
17	J	62	ARG	Sidechain
18	K	118	HIS	Peptide
19	L	9	ARG	Sidechain
36	g	35	ARG	Sidechain
38	i	96	ARG	Sidechain
45	p	51	ARG	Sidechain
52	w	74	ARG	Sidechain
53	x	52	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	48/55 (87%)	48 (100%)	0	0	100	100
2	1	43/46 (94%)	43 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	46/70 (66%)	45 (98%)	1 (2%)	0	100	100
9	B	220/241 (91%)	214 (97%)	5 (2%)	1 (0%)	25	24
10	C	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
11	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
12	E	152/167 (91%)	148 (97%)	4 (3%)	0	100	100
13	F	99/135 (73%)	95 (96%)	4 (4%)	0	100	100
14	G	148/179 (83%)	145 (98%)	3 (2%)	0	100	100
15	H	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	16	13
16	I	123/130 (95%)	118 (96%)	5 (4%)	0	100	100
17	J	92/103 (89%)	88 (96%)	3 (3%)	1 (1%)	12	8
18	K	113/129 (88%)	107 (95%)	6 (5%)	0	100	100
19	L	118/124 (95%)	111 (94%)	7 (6%)	0	100	100
20	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
21	N	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	13	9
22	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
23	P	77/82 (94%)	74 (96%)	3 (4%)	0	100	100
24	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	R	62/75 (83%)	62 (100%)	0	0	100	100
26	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
27	T	84/87 (97%)	84 (100%)	0	0	100	100
28	U	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
29	W	662/693 (96%)	647 (98%)	15 (2%)	0	100	100
32	c	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
33	d	204/209 (98%)	198 (97%)	6 (3%)	0	100	100
34	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
35	f	175/179 (98%)	170 (97%)	4 (2%)	1 (1%)	22	20
36	g	166/177 (94%)	164 (99%)	2 (1%)	0	100	100
37	h	39/149 (26%)	37 (95%)	2 (5%)	0	100	100
38	i	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
39	j	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
40	k	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	19	17
41	l	132/136 (97%)	129 (98%)	3 (2%)	0	100	100
42	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
43	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
44	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
45	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
46	q	101/103 (98%)	100 (99%)	0	1 (1%)	13	9
47	r	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
48	s	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
49	t	89/104 (86%)	88 (99%)	1 (1%)	0	100	100
50	u	91/94 (97%)	88 (97%)	3 (3%)	0	100	100
51	v	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
52	w	75/78 (96%)	75 (100%)	0	0	100	100
53	x	58/63 (92%)	58 (100%)	0	0	100	100
54	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
55	z	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
All	All	6064/6606 (92%)	5915 (98%)	142 (2%)	7 (0%)	50	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	J	57	VAL
35	f	42	GLU
9	B	165	ASP
40	k	29	LYS
15	H	75	ILE
46	q	44	GLY
21	N	68	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	44 (96%)	2 (4%)	25	26
2	1	37/38 (97%)	37 (100%)	0	100	100
3	2	51/52 (98%)	50 (98%)	1 (2%)	50	57
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	44/62 (71%)	44 (100%)	0	100	100
9	B	184/199 (92%)	176 (96%)	8 (4%)	25	26
10	C	170/190 (90%)	168 (99%)	2 (1%)	67	75
11	D	172/173 (99%)	167 (97%)	5 (3%)	37	43
12	E	117/126 (93%)	115 (98%)	2 (2%)	56	64
13	F	88/116 (76%)	88 (100%)	0	100	100
14	G	124/147 (84%)	118 (95%)	6 (5%)	21	21
15	H	104/105 (99%)	103 (99%)	1 (1%)	73	79
16	I	103/107 (96%)	99 (96%)	4 (4%)	27	30
17	J	85/90 (94%)	83 (98%)	2 (2%)	44	50
18	K	89/98 (91%)	89 (100%)	0	100	100
19	L	101/103 (98%)	98 (97%)	3 (3%)	36	42
20	M	93/96 (97%)	91 (98%)	2 (2%)	47	54
21	N	83/84 (99%)	83 (100%)	0	100	100
22	O	76/77 (99%)	74 (97%)	2 (3%)	41	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	P	64/65 (98%)	64 (100%)	0	100	100
24	Q	73/78 (94%)	69 (94%)	4 (6%)	18	16
25	R	55/65 (85%)	55 (100%)	0	100	100
26	S	72/79 (91%)	72 (100%)	0	100	100
27	T	65/66 (98%)	64 (98%)	1 (2%)	60	69
28	U	48/61 (79%)	48 (100%)	0	100	100
29	W	556/579 (96%)	549 (99%)	7 (1%)	65	73
32	c	216/218 (99%)	215 (100%)	1 (0%)	86	90
33	d	162/163 (99%)	162 (100%)	0	100	100
34	e	165/165 (100%)	165 (100%)	0	100	100
35	f	148/150 (99%)	141 (95%)	7 (5%)	22	23
36	g	132/138 (96%)	128 (97%)	4 (3%)	36	42
37	h	32/114 (28%)	32 (100%)	0	100	100
38	i	115/116 (99%)	114 (99%)	1 (1%)	75	82
39	j	104/104 (100%)	102 (98%)	2 (2%)	52	60
40	k	103/103 (100%)	103 (100%)	0	100	100
41	l	107/107 (100%)	105 (98%)	2 (2%)	52	60
42	m	98/103 (95%)	98 (100%)	0	100	100
43	n	86/87 (99%)	83 (96%)	3 (4%)	31	35
44	o	99/100 (99%)	98 (99%)	1 (1%)	73	79
45	p	89/90 (99%)	89 (100%)	0	100	100
46	q	84/84 (100%)	83 (99%)	1 (1%)	67	75
47	r	92/93 (99%)	92 (100%)	0	100	100
48	s	80/84 (95%)	80 (100%)	0	100	100
49	t	76/85 (89%)	75 (99%)	1 (1%)	65	73
50	u	77/78 (99%)	77 (100%)	0	100	100
51	v	56/63 (89%)	56 (100%)	0	100	100
52	w	67/68 (98%)	67 (100%)	0	100	100
53	x	54/55 (98%)	54 (100%)	0	100	100
54	y	48/49 (98%)	48 (100%)	0	100	100
55	z	46/48 (96%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5070/5404 (94%)	4995 (98%)	75 (2%)	60 69

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	5	ILE
1	0	28	ARG
3	2	31	HIS
9	B	23	TRP
9	B	78	GLU
9	B	103	ASN
9	B	133	GLU
9	B	143	LYS
9	B	192	ASP
9	B	196	VAL
9	B	204	ASP
10	C	29	PHE
10	C	70	THR
11	D	44	ARG
11	D	45	LYS
11	D	58	LYS
11	D	145	ILE
11	D	147	GLU
12	E	77	ASN
12	E	101	GLU
14	G	15	ASP
14	G	22	LEU
14	G	63	GLU
14	G	75	VAL
14	G	135	VAL
14	G	140	ASP
15	H	89	LYS
16	I	63	LEU
16	I	66	THR
16	I	72	ILE
16	I	123	ARG
17	J	63	ASP
17	J	75	ASP
19	L	52	VAL
19	L	112	GLN
19	L	120	LYS
20	M	14	HIS

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Mol	Chain	Res	Type
20	M	93	ARG
22	O	17	ARG
22	O	89	ARG
24	Q	28	PHE
24	Q	42	THR
24	Q	52	GLU
24	Q	74	THR
27	T	49	LYS
29	W	87	ASP
29	W	260	THR
29	W	290	HIS
29	W	401	MET
29	W	447	GLN
29	W	472	GLU
29	W	492	VAL
32	c	37	ASN
35	f	30	ARG
35	f	40	VAL
35	f	47	LYS
35	f	125	ARG
35	f	143	TYR
35	f	150	ARG
35	f	152	LEU
36	g	25	THR
36	g	104	ASN
36	g	155	GLU
36	g	173	GLU
38	i	95	ARG
39	j	49	ARG
39	j	58	LEU
41	l	6	ARG
41	l	8	LYS
43	n	49	VAL
43	n	56	LYS
43	n	90	VAL
44	o	53	ARG
46	q	55	ASP
49	t	24	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
5	4	41	HIS
9	B	42	ASN
9	B	103	ASN
9	B	146	ASN
10	C	100	GLN
10	C	139	GLN
10	C	140	ASN
11	D	71	GLN
11	D	152	GLN
12	E	77	ASN
12	E	82	GLN
14	G	148	ASN
17	J	58	ASN
19	L	112	GLN
21	N	66	GLN
22	O	35	GLN
25	R	31	ASN
26	S	52	HIS
27	T	61	GLN
27	T	68	HIS
27	T	84	ASN
29	W	447	GLN
32	c	37	ASN
35	f	23	ASN
35	f	27	GLN
37	h	18	GLN
43	n	116	GLN
45	p	44	GLN
46	q	12	HIS
46	q	43	ASN
49	t	40	ASN
50	u	5	ASN
50	u	49	ASN
53	x	45	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	a	2774/2930 (94%)	298 (10%)	0
31	b	118/119 (99%)	7 (5%)	0
6	8	76/77 (98%)	15 (19%)	3 (3%)
7	9	4/24 (16%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	A	1521/1554 (97%)	233 (15%)	47 (3%)
All	All	4493/4704 (95%)	553 (12%)	50 (1%)

All (553) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	8	7	G
6	8	8	U
6	8	9	G
6	8	16	C
6	8	17(A)	U
6	8	19	G
6	8	20	U
6	8	21	A
6	8	22	G
6	8	43	A
6	8	46	G
6	8	47	U
6	8	55	U
6	8	58	A
6	8	76	A
8	A	3	A
8	A	4	U
8	A	5	U
8	A	6	G
8	A	7	A
8	A	8	A
8	A	9	G
8	A	32	A
8	A	39	G
8	A	47	C
8	A	48	C
8	A	49	U
8	A	50	A
8	A	51	A
8	A	66	A
8	A	72	A
8	A	76	G
8	A	77	A
8	A	78	A
8	A	80	A
8	A	81	A

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Mol	Chain	Res	Type
8	A	82	G
8	A	83	C
8	A	84	U
8	A	85	U
8	A	86	G
8	A	87	C
8	A	90	C
8	A	94	G
8	A	95	C
8	A	96	U
8	A	97	G
8	A	120	A
8	A	122	G
8	A	130	A
8	A	131	A
8	A	137	U
8	A	143	A
8	A	144	G
8	A	159	G
8	A	163	C
8	A	164	G
8	A	170	U
8	A	182	A
8	A	196	A
8	A	197	A
8	A	207	C
8	A	208	U
8	A	209	U
8	A	210	C
8	A	226	G
8	A	240	G
8	A	245	U
8	A	247	G
8	A	250	A
8	A	251	G
8	A	253	A
8	A	266	G
8	A	267	C
8	A	289	G
8	A	305	G
8	A	306	A
8	A	321	A

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Mol	Chain	Res	Type
8	A	328	C
8	A	329	A
8	A	330	C
8	A	332	G
8	A	352	C
8	A	354	G
8	A	367	U
8	A	372	C
8	A	398	U
8	A	406	G
8	A	411	A
8	A	412	A
8	A	413	G
8	A	414	A
8	A	421	U
8	A	422	C
8	A	429	U
8	A	455	G
8	A	457	G
8	A	458	U
8	A	463	U
8	A	467	U
8	A	468	A
8	A	482	A
8	A	484	G
8	A	486	U
8	A	495	A
8	A	499	A
8	A	500	G
8	A	511	C
8	A	518	C
8	A	524	G
8	A	527	G7M
8	A	530	G
8	A	532	A
8	A	547	A
8	A	559	A
8	A	562	U
8	A	572	A
8	A	573	A
8	A	576	C
8	A	589	U

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Mol	Chain	Res	Type
8	A	596	A
8	A	607	A
8	A	615	G
8	A	619	U
8	A	635	A
8	A	642	A
8	A	650	G
8	A	665	A
8	A	687	A
8	A	695	A
8	A	702	A
8	A	703	G
8	A	721	G
8	A	723	U
8	A	724	G
8	A	755	G
8	A	777	A
8	A	793	U
8	A	794	A
8	A	815	A
8	A	817	C
8	A	829	G
8	A	849	G
8	A	874	G
8	A	884	U
8	A	885	G
8	A	890	G
8	A	902	G
8	A	914	A
8	A	926	G
8	A	927	G
8	A	934	C
8	A	935	A
8	A	942	G
8	A	958	A
8	A	960	U
8	A	965	U
8	A	969	A
8	A	975	A
8	A	976	G
8	A	977	A
8	A	989	U

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Mol	Chain	Res	Type
8	A	991	U
8	A	992	U
8	A	993	G
8	A	994	A
8	A	1004	A
8	A	1013	G
8	A	1014	A
8	A	1015	G
8	A	1016	A
8	A	1017	U
8	A	1020	G
8	A	1021	A
8	A	1030	U
8	A	1031	C
8	A	1032	G
8	A	1056	U
8	A	1065	U
8	A	1085	U
8	A	1092	A
8	A	1094	G
8	A	1095	U
8	A	1101	A
8	A	1104	G
8	A	1108	G
8	A	1109	C
8	A	1124	G
8	A	1130	A
8	A	1135	U
8	A	1139	G
8	A	1141	C
8	A	1146	A
8	A	1150	A
8	A	1152	A
8	A	1157	A
8	A	1158	C
8	A	1159	U
8	A	1160	G
8	A	1183	U
8	A	1196	A
8	A	1197	A
8	A	1213	A
8	A	1226	C

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Mol	Chain	Res	Type
8	A	1227	A
8	A	1238	A
8	A	1240	U
8	A	1250	A
8	A	1256	A
8	A	1257	A
8	A	1260	G
8	A	1268	G
8	A	1279	G
8	A	1280	A
8	A	1286	U
8	A	1287	A
8	A	1297	G
8	A	1298	U
8	A	1300	G
8	A	1305	G
8	A	1311	A
8	A	1312	G
8	A	1320	C
8	A	1331	G
8	A	1332	A
8	A	1336	C
8	A	1338	G
8	A	1346	A
8	A	1363	A
8	A	1364	U
8	A	1379	G
8	A	1398	A
8	A	1419	G
8	A	1429	A
8	A	1441	A
8	A	1453	G
8	A	1494	G
8	A	1497	G
8	A	1499	A
8	A	1503	A
8	A	1505	G
8	A	1506	U
8	A	1507	A
8	A	1517	G
8	A	1529	G
8	A	1530	G

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Mol	Chain	Res	Type
8	A	1533	C
8	A	1534	A
30	a	10	A
30	a	12	U
30	a	15	G
30	a	34	U
30	a	71	A
30	a	74	A
30	a	75	G
30	a	101	A
30	a	118	A
30	a	119	A
30	a	120	U
30	a	131	A
30	a	139	U
30	a	142	A
30	a	162	U
30	a	181	A
30	a	196	A
30	a	199	A
30	a	215	G
30	a	216	A
30	a	221	A
30	a	222	A
30	a	248	G
30	a	272	A
30	a	278	A
30	a	279	A
30	a	281	C
30	a	285	G
30	a	289	G
30	a	311	A
30	a	330	A
30	a	346	A
30	a	354	A
30	a	361	G
30	a	362	A
30	a	386	G
30	a	411	G
30	a	448	U
30	a	451	U
30	a	481	G

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Mol	Chain	Res	Type
30	a	491	G
30	a	505	A
30	a	509	C
30	a	531	C
30	a	532	A
30	a	533	G
30	a	544	C
30	a	545	U
30	a	547	A
30	a	548	G
30	a	549	G
30	a	556	A
30	a	563	A
30	a	573	U
30	a	574	A
30	a	575	A
30	a	586	A
30	a	603	A
30	a	615	U
30	a	627	A
30	a	637	A
30	a	645	C
30	a	647	G
30	a	653	U
30	a	654	A
30	a	655	A
30	a	686	U
30	a	716	A
30	a	717	C
30	a	730	A
30	a	747	5MU
30	a	764	A
30	a	765	C
30	a	775	G
30	a	776	G
30	a	782	A
30	a	784	G
30	a	785	G
30	a	792	A
30	a	805	G
30	a	812	C
30	a	827	U

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Mol	Chain	Res	Type
30	a	828	U
30	a	845	A
30	a	846	U
30	a	858	G
30	a	869	G
30	a	910	A
30	a	914	G
30	a	915	C
30	a	931	U
30	a	934	U
30	a	946	C
30	a	961	C
30	a	974	G
30	a	983	A
30	a	984	A
30	a	985	C
30	a	996	A
30	a	1012	U
30	a	1013	C
30	a	1022	G
30	a	1026	G
30	a	1033	U
30	a	1041	G
30	a	1047	G
30	a	1059	G
30	a	1060	U
30	a	1070	A
30	a	1077	A
30	a	1080	A
30	a	1083	U
30	a	1087	G
30	a	1088	A
30	a	1097	U
30	a	1101	U
30	a	1112	G
30	a	1116	G
30	a	1128	G
30	a	1129	A
30	a	1130	U
30	a	1132	U
30	a	1133	A
30	a	1134	A

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Mol	Chain	Res	Type
30	a	1135	C
30	a	1142	A
30	a	1144	A
30	a	1151	A
30	a	1169	A
30	a	1170	C
30	a	1179	G
30	a	1188	U
30	a	1253	A
30	a	1256	G
30	a	1271	G
30	a	1272	A
30	a	1300	G
30	a	1301	A
30	a	1321	A
30	a	1352	U
30	a	1365	A
30	a	1378	A
30	a	1379	U
30	a	1383	A
30	a	1386	C
30	a	1409	U
30	a	1416	G
30	a	1419	A
30	a	1428	C
30	a	1451	C
30	a	1452	G
30	a	1453	A
30	a	1455	G
30	a	1458	U
30	a	1460	U
30	a	1482	G
30	a	1490	A
30	a	1493	C
30	a	1508	A
30	a	1509	A
30	a	1510	G
30	a	1515	A
30	a	1534	U
30	a	1535	A
30	a	1536	C
30	a	1537	G

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Mol	Chain	Res	Type
30	a	1538	G
30	a	1569	A
30	a	1578	U
30	a	1585	C
30	a	1608	A
30	a	1609	A
30	a	1647	U
30	a	1648	U
30	a	1649	G
30	a	1674	G
30	a	1698	A
30	a	1715	G
30	a	1729	U
30	a	1730	C
30	a	1734	G
30	a	1737	G
30	a	1738	G
30	a	1744	A
30	a	1764	C
30	a	1773	A
30	a	1782	U
30	a	1800	C
30	a	1801	A
30	a	1808	A
30	a	1816	C
30	a	1829	A
30	a	1847	A
30	a	1848	A
30	a	1858	A
30	a	1870	C
30	a	1871	A
30	a	1872	A
30	a	1906	G
30	a	1907	G
30	a	1913	A
30	a	1914	C
30	a	1929	G
30	a	1930	G
30	a	1931	U
30	a	1937	A
30	a	1955	U
30	a	1967	C

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Mol	Chain	Res	Type
30	a	1970	A
30	a	1971	U
30	a	1972	G
30	a	1991	U
30	a	1993	U
30	a	2020	A
30	a	2023	C
30	a	2031	A
30	a	2033	A
30	a	2043	C
30	a	2055	C
30	a	2056	G
30	a	2060	A
30	a	2061	G
30	a	2062	A
30	a	2069	G7M
30	a	2093	G
30	a	2096	C
30	a	2193	G
30	a	2198	A
30	a	2204	G
30	a	2211	A
30	a	2225	A
30	a	2238	G
30	a	2268	A
30	a	2273	A
30	a	2278	A
30	a	2283	C
30	a	2287	A
30	a	2305	U
30	a	2308	G
30	a	2312	U
30	a	2322	A
30	a	2325	G
30	a	2333	A
30	a	2335	A
30	a	2347	C
30	a	2350	C
30	a	2366	A
30	a	2383	G
30	a	2385	C
30	a	2402	U

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Mol	Chain	Res	Type
30	a	2406	A
30	a	2425	A
30	a	2429	G
30	a	2430	A
30	a	2431	U
30	a	2435	A
30	a	2441	U
30	a	2448	A
30	a	2459	A
30	a	2469	A
30	a	2476	A
30	a	2478	A
30	a	2491	U
30	a	2502	G
30	a	2504	PSU
30	a	2505	G
30	a	2518	A
30	a	2529	G
30	a	2547	A
30	a	2566	A
30	a	2567	G
30	a	2573	C
30	a	2602	A
30	a	2609	U
30	a	2613	U
30	a	2629	U
30	a	2661	G
30	a	2663	G
30	a	2689	U
30	a	2690	U
30	a	2714	G
30	a	2716	C
30	a	2726	A
30	a	2744	G
30	a	2748	A
30	a	2750	A
30	a	2757	A
30	a	2765	A
30	a	2778	A
30	a	2798	U
30	a	2799	A
30	a	2803	G

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Mol	Chain	Res	Type
30	a	2809	A
30	a	2818	U
30	a	2820	A
30	a	2821	A
30	a	2883	A
30	a	2884	U
31	b	35	C
31	b	36	C
31	b	37	C
31	b	44	G
31	b	45	A
31	b	89	U
31	b	109	A

All (50) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	8	7	G
6	8	17(A)	U
6	8	20	U
8	A	7	A
8	A	30	U
8	A	84	U
8	A	86	G
8	A	182	A
8	A	199	A
8	A	305	G
8	A	329	A
8	A	345	C
8	A	411	A
8	A	428	G
8	A	434	U
8	A	446	G
8	A	499	A
8	A	575	G
8	A	595	A
8	A	702	A
8	A	776	G
8	A	827	U
8	A	884	U
8	A	958	A
8	A	974	A

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Mol	Chain	Res	Type
8	A	991	U
8	A	993	G
8	A	1013	G
8	A	1031	C
8	A	1092	A
8	A	1101	A
8	A	1108	G
8	A	1124	G
8	A	1129	C
8	A	1145	A
8	A	1157	A
8	A	1159	U
8	A	1160	G
8	A	1187	G
8	A	1256	A
8	A	1297	G
8	A	1320	C
8	A	1331	G
8	A	1364	U
8	A	1380	U
8	A	1397	C
8	A	1447	A
8	A	1452	C
8	A	1459	G
8	A	1505	G

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

39 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	$\#\|Z\| > 2$
8	4OC	A	1402	8	20,23,24	0.39	0	26,32,35	0.42	0
8	2MG	A	1207	8	18,26,27	1.04	2 (11%)	16,38,41	0.73	0
30	PSU	a	2604	30	18,21,22	0.91	1 (5%)	22,30,33	0.75	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	2MG	A	1516	8	18,26,27	1.02	2 (11%)	16,38,41	0.82	0
30	6MZ	a	2030	30	18,25,26	0.70	0	16,36,39	0.75	1 (6%)
30	OMC	a	2498	30,58	19,22,23	0.28	0	26,31,34	0.53	0
30	PSU	a	2504	57,30	18,21,22	0.85	1 (5%)	22,30,33	0.76	0
19	D2T	L	89	19	7,9,10	0.94	0	6,11,13	1.85	4 (66%)
30	PSU	a	955	30	18,21,22	0.88	1 (5%)	22,30,33	0.65	0
30	2MA	a	2503	57,30,58	19,25,26	0.99	1 (5%)	21,37,40	1.78	5 (23%)
8	G7M	A	527	8	20,26,27	1.13	2 (10%)	17,39,42	0.30	0
30	PSU	a	1911	30	18,21,22	0.92	1 (5%)	22,30,33	0.66	0
30	OMU	a	2552	30	19,22,23	0.21	0	26,31,34	0.40	0
8	5MC	A	1407	8	18,22,23	0.32	0	26,32,35	0.54	0
41	4D4	l	81	41	9,11,12	0.55	0	8,13,15	0.70	0
30	PSU	a	2457	30	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
18	IAS	K	119	18	6,7,8	0.91	0	6,8,10	0.99	0
30	OMG	a	2251	57,30	18,26,27	1.00	2 (11%)	19,38,41	0.69	0
30	6MZ	a	1618	30	18,25,26	0.66	0	16,36,39	0.74	1 (6%)
30	5MU	a	1939	57,30	19,22,23	0.30	0	28,32,35	0.37	0
33	MEQ	d	150	33	8,9,10	0.43	0	5,10,12	0.54	0
30	2MG	a	2445	30	18,26,27	1.01	2 (11%)	16,38,41	0.75	0
8	5MC	A	967	8	18,22,23	0.33	0	26,32,35	0.49	0
30	2MG	a	1835	30	18,26,27	1.02	2 (11%)	16,38,41	0.70	0
8	UR3	A	1498	8	19,22,23	0.28	0	26,32,35	0.64	0
30	PSU	a	746	30,58	18,21,22	0.95	1 (5%)	22,30,33	0.60	0
30	PSU	a	2580	57,30	18,21,22	0.90	1 (5%)	22,30,33	0.85	1 (4%)
30	5MU	a	747	30	19,22,23	0.26	0	28,32,35	0.42	0
8	MA6	A	1519	8	18,26,27	0.73	0	19,38,41	0.58	0
30	PSU	a	1917	30	18,21,22	0.89	1 (5%)	22,30,33	0.52	0
30	H2U	a	2449	30	18,21,22	0.60	0	21,30,33	0.88	2 (9%)
30	PSU	a	2605	30	18,21,22	0.90	1 (5%)	22,30,33	0.75	0
30	5MC	a	1962	30	18,22,23	0.34	0	26,32,35	0.50	0
30	G7M	a	2069	30	20,26,27	1.11	3 (15%)	17,39,42	0.55	0
30	3TD	a	1915	30	18,22,23	0.98	1 (5%)	22,32,35	0.62	0
8	PSU	A	516	8	18,21,22	0.91	1 (5%)	22,30,33	0.59	0
8	2MG	A	966	8	18,26,27	1.02	2 (11%)	16,38,41	0.70	0
30	1MG	a	745	30	18,26,27	0.97	1 (5%)	19,39,42	0.52	0
8	MA6	A	1518	8	18,26,27	0.75	0	19,38,41	0.45	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
8	4OC	A	1402	8	-	0/9/29/30	0/2/2/2
8	2MG	A	1207	8	-	0/5/27/28	0/3/3/3
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2
8	2MG	A	1516	8	-	0/5/27/28	0/3/3/3
30	6MZ	a	2030	30	-	2/5/27/28	0/3/3/3
30	OMC	a	2498	30,58	-	0/9/27/28	0/2/2/2
30	PSU	a	2504	57,30	-	2/7/25/26	0/2/2/2
19	D2T	L	89	19	-	4/7/12/14	-
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
30	2MA	a	2503	57,30,58	-	1/3/25/26	0/3/3/3
8	G7M	A	527	8	-	2/3/25/26	0/3/3/3
30	PSU	a	1911	30	-	2/7/25/26	0/2/2/2
30	OMU	a	2552	30	-	0/9/27/28	0/2/2/2
8	5MC	A	1407	8	-	0/7/25/26	0/2/2/2
41	4D4	l	81	41	-	1/11/12/14	-
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2
18	IAS	K	119	18	-	2/7/7/8	-
30	OMG	a	2251	57,30	-	1/5/27/28	0/3/3/3
30	6MZ	a	1618	30	-	0/5/27/28	0/3/3/3
30	5MU	a	1939	57,30	-	0/7/25/26	0/2/2/2
33	MEQ	d	150	33	-	2/8/9/11	-
30	2MG	a	2445	30	-	1/5/27/28	0/3/3/3
8	5MC	A	967	8	-	0/7/25/26	0/2/2/2
30	2MG	a	1835	30	-	0/5/27/28	0/3/3/3
8	UR3	A	1498	8	-	0/7/25/26	0/2/2/2
30	PSU	a	746	30,58	-	2/7/25/26	0/2/2/2
30	PSU	a	2580	57,30	-	0/7/25/26	0/2/2/2
30	5MU	a	747	30	-	1/7/25/26	0/2/2/2
8	MA6	A	1519	8	-	0/7/29/30	0/3/3/3
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2
30	H2U	a	2449	30	-	0/7/38/39	0/2/2/2
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
30	5MC	a	1962	30	-	2/7/25/26	0/2/2/2
30	G7M	a	2069	30	-	2/3/25/26	0/3/3/3
30	3TD	a	1915	30	-	0/7/25/26	0/2/2/2
8	PSU	A	516	8	-	0/7/25/26	0/2/2/2
8	2MG	A	966	8	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	1MG	a	745	30	-	0/3/25/26	0/3/3/3
8	MA6	A	1518	8	-	0/7/29/30	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	746	PSU	C6-C5	3.77	1.39	1.35
30	a	1915	3TD	C6-C5	3.71	1.39	1.35
30	a	1911	PSU	C6-C5	3.65	1.39	1.35
8	A	516	PSU	C6-C5	3.58	1.39	1.35
30	a	2580	PSU	C6-C5	3.58	1.39	1.35
30	a	2604	PSU	C6-C5	3.53	1.39	1.35
30	a	1917	PSU	C6-C5	3.52	1.39	1.35
8	A	527	G7M	C8-N9	3.50	1.39	1.33
30	a	2605	PSU	C6-C5	3.49	1.39	1.35
30	a	2457	PSU	C6-C5	3.47	1.39	1.35
30	a	955	PSU	C6-C5	3.41	1.39	1.35
30	a	2504	PSU	C6-C5	3.36	1.39	1.35
30	a	2069	G7M	C8-N9	3.35	1.39	1.33
30	a	2251	OMG	C5-C6	-2.55	1.42	1.47
8	A	1207	2MG	C5-C6	-2.50	1.42	1.47
30	a	1835	2MG	C5-C6	-2.49	1.42	1.47
8	A	527	G7M	C8-N7	2.46	1.37	1.33
8	A	966	2MG	C5-C6	-2.45	1.42	1.47
8	A	1516	2MG	C5-C6	-2.43	1.42	1.47
30	a	2445	2MG	C5-C6	-2.37	1.42	1.47
30	a	2069	G7M	C8-N7	2.36	1.37	1.33
30	a	745	1MG	C5-C4	-2.22	1.37	1.43
30	a	2445	2MG	C8-N7	-2.14	1.31	1.35
8	A	1207	2MG	C8-N7	-2.10	1.31	1.35
30	a	2069	G7M	C5-C6	-2.08	1.40	1.45
30	a	1835	2MG	C8-N7	-2.06	1.31	1.35
8	A	966	2MG	C8-N7	-2.05	1.31	1.35
30	a	2251	OMG	C8-N7	-2.05	1.31	1.35
8	A	1516	2MG	C8-N7	-2.03	1.31	1.35
30	a	2503	2MA	C6-N1	2.02	1.37	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	2503	2MA	C5-C6-N1	-5.42	117.45	121.01
30	a	2503	2MA	C5-C6-N6	4.25	126.81	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	2580	PSU	C3'-C2'-C1'	2.75	104.84	101.64
19	L	89	D2T	OD1-CG-CB	-2.58	117.03	122.44
30	a	2503	2MA	CM2-C2-N1	2.37	120.85	117.15
30	a	2449	H2U	O2-C2-N1	-2.36	120.15	123.11
30	a	2449	H2U	N3-C2-N1	2.28	119.06	116.65
30	a	2503	2MA	C2-N1-C6	2.27	121.62	118.08
19	L	89	D2T	CB-CA-N	2.24	113.87	109.10
30	a	2503	2MA	N3-C2-N1	-2.23	121.65	125.73
30	a	1618	6MZ	C2-N1-C6	2.23	118.50	116.59
30	a	2030	6MZ	C2-N1-C6	2.22	118.49	116.59
19	L	89	D2T	OD2-CG-CB	2.07	117.62	113.15
19	L	89	D2T	O-C-CA	-2.03	119.46	124.78
30	a	2604	PSU	C2'-C3'-C4'	-2.01	98.74	102.64

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	L	89	D2T	CA-CB-CG-OD1
19	L	89	D2T	CA-CB-CG-OD2
30	a	746	PSU	C2'-C1'-C5-C4
30	a	1911	PSU	O4'-C1'-C5-C4
30	a	1911	PSU	O4'-C1'-C5-C6
30	a	2030	6MZ	O4'-C4'-C5'-O5'
30	a	2251	OMG	C1'-C2'-O2'-CM2
8	A	527	G7M	O4'-C4'-C5'-O5'
8	A	527	G7M	C3'-C4'-C5'-O5'
33	d	150	MEQ	OE1-CD-CG-CB
30	a	2030	6MZ	C3'-C4'-C5'-O5'
33	d	150	MEQ	NE2-CD-CG-CB
19	L	89	D2T	CG-CB-SB-CB1
30	a	2445	2MG	C3'-C4'-C5'-O5'
30	a	2504	PSU	O4'-C4'-C5'-O5'
8	A	966	2MG	O4'-C4'-C5'-O5'
18	K	119	IAS	CA-CB-CG-OD1
18	K	119	IAS	O-C-CA-N
30	a	2069	G7M	C4'-C5'-O5'-P
30	a	1962	5MC	C2'-C1'-N1-C6
8	A	966	2MG	C3'-C4'-C5'-O5'
19	L	89	D2T	SB-CB-CG-OD2
30	a	1962	5MC	O4'-C1'-N1-C6
30	a	747	5MU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
30	a	746	PSU	O4'-C1'-C5-C6
30	a	2504	PSU	C3'-C4'-C5'-O5'
30	a	2069	G7M	O4'-C4'-C5'-O5'
30	a	2503	2MA	O4'-C4'-C5'-O5'
41	l	81	4D4	O-C-CA-CB

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 369 ligands modelled in this entry, 367 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
60	FUA	W	703	-	39,40,40	1.48	2 (5%)	49,64,64	0.91	2 (4%)
59	GDP	W	701	58	24,30,30	0.95	2 (8%)	30,47,47	0.63	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
60	FUA	W	703	-	-	7/15/92/92	0/4/4/4
59	GDP	W	701	58	-	1/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	W	703	FUA	C29-C22	-8.49	1.35	1.47
59	W	701	GDP	C5-C6	-2.61	1.42	1.47
60	W	703	FUA	O5-C29	-2.32	1.23	1.30
59	W	701	GDP	C8-N7	-2.09	1.31	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	W	703	FUA	C14-C8-C9	-2.20	105.10	109.40
60	W	703	FUA	C16-O2-C31	2.16	120.34	117.06

There are no chirality outliers.

All (8) torsion outliers are listed below:

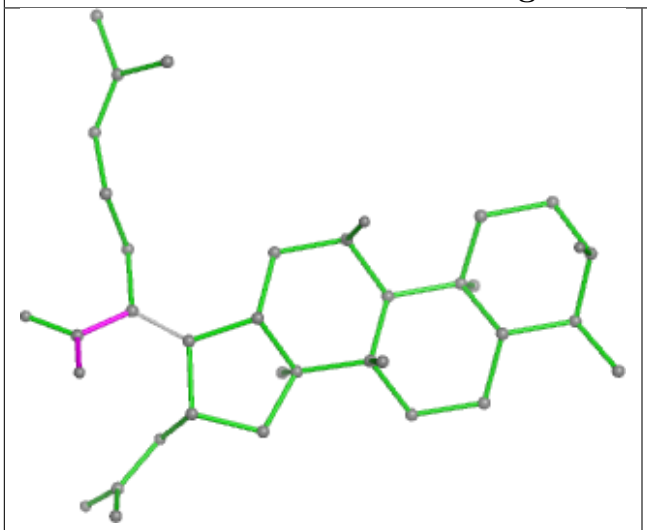
Mol	Chain	Res	Type	Atoms
60	W	703	FUA	C13-C17-C22-C29
60	W	703	FUA	C32-C31-O2-C16
60	W	703	FUA	O3-C31-O2-C16
60	W	703	FUA	C29-C22-C23-C24
60	W	703	FUA	C17-C22-C29-O4
60	W	703	FUA	C17-C22-C29-O5
59	W	701	GDP	O4'-C4'-C5'-O5'
60	W	703	FUA	C17-C16-O2-C31

There are no ring outliers.

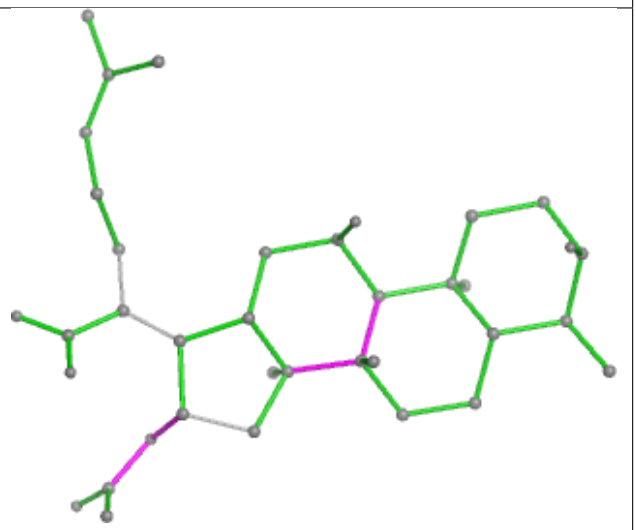
No monomer is involved in short contacts.

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 then 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.

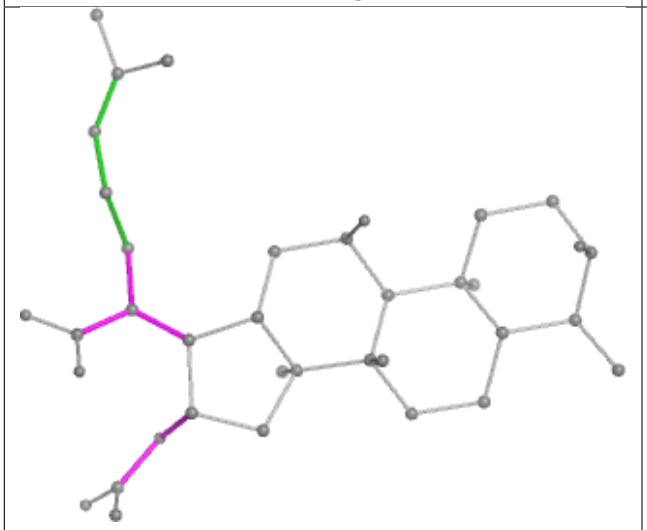
Ligand FUA W 703



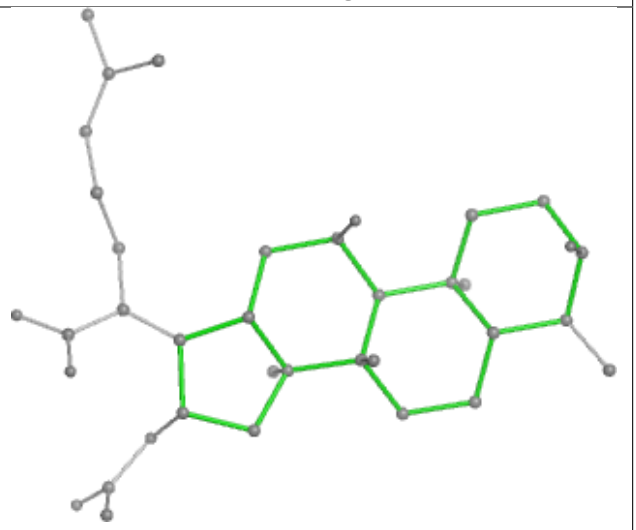
Bond lengths



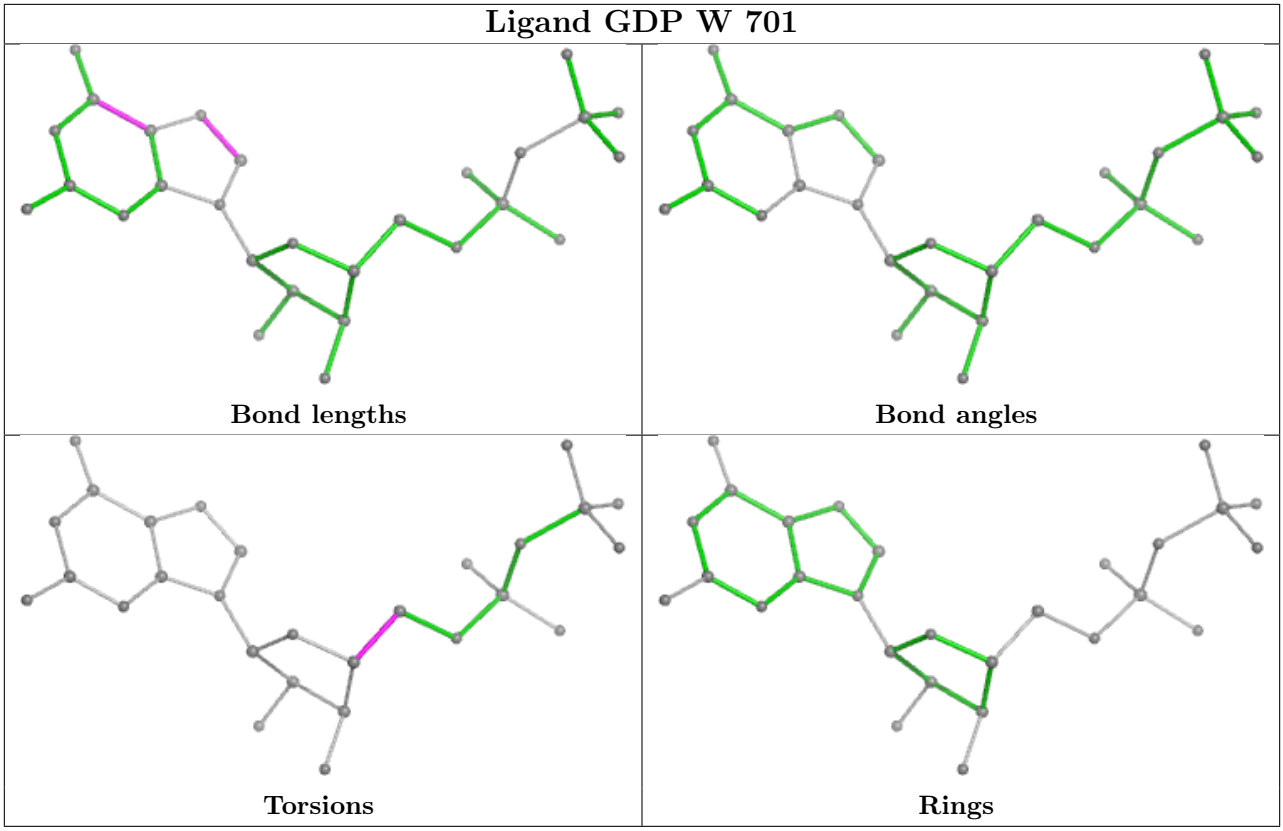
Bond angles



Torsions



Rings



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.

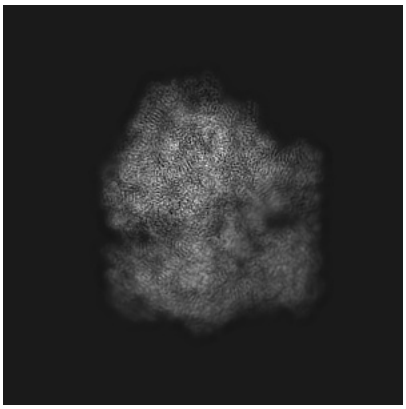
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-51350. These allow visual inspection of the internal detail of the map and identification of artifacts.

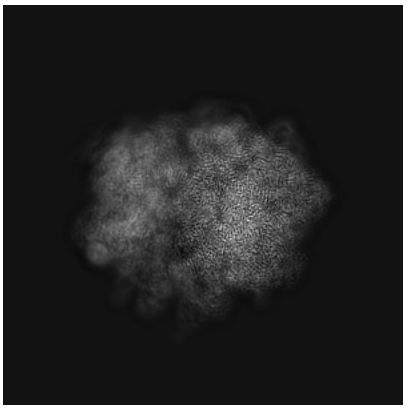
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

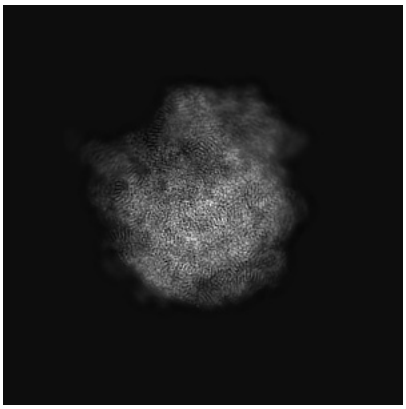
6.1.1 Primary map



X

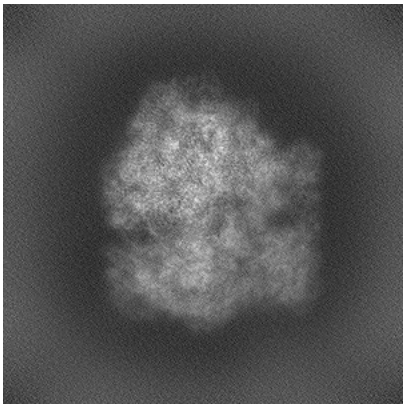


Y

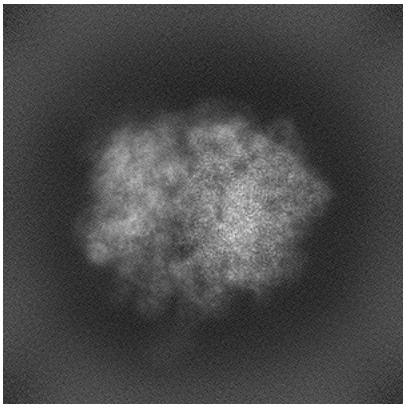


Z

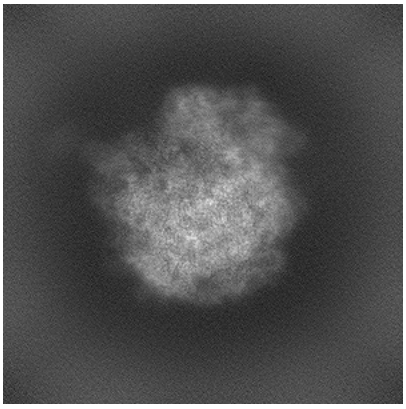
6.1.2 Raw map



X



Y

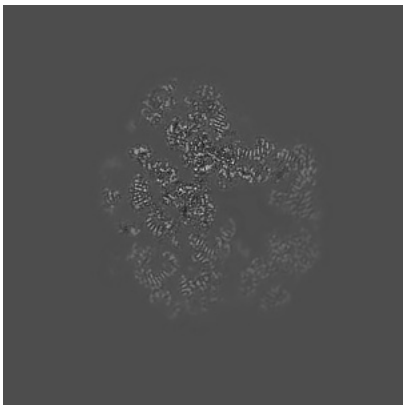


Z

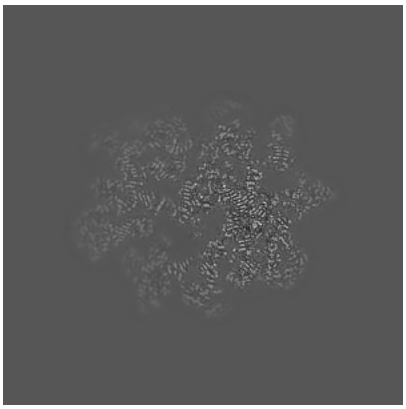
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

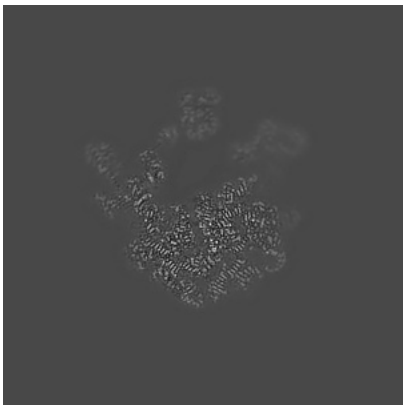
6.2.1 Primary map



X Index: 300

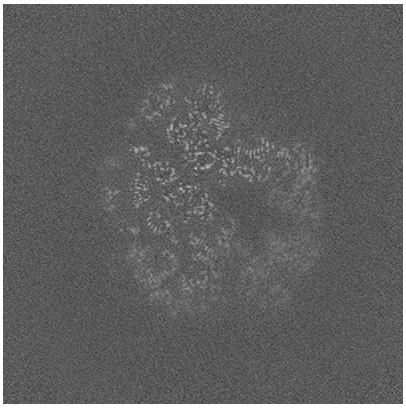


Y Index: 300

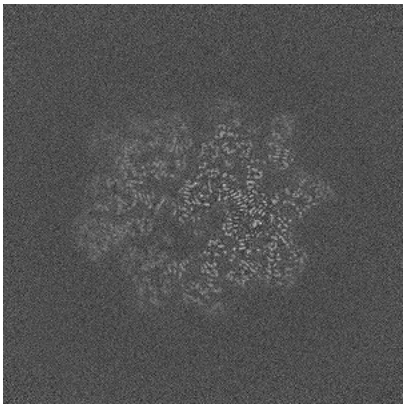


Z Index: 300

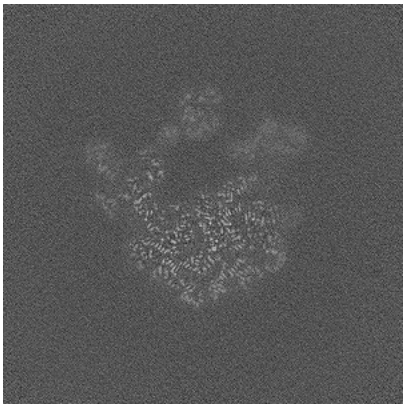
6.2.2 Raw map



X Index: 300



Y Index: 300

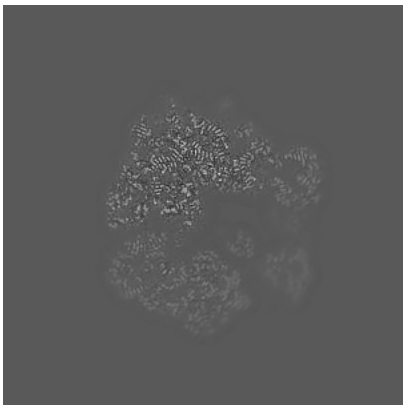


Z Index: 300

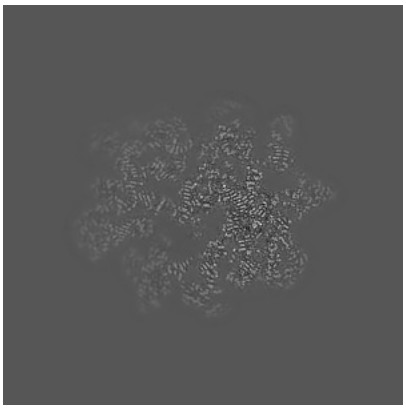
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

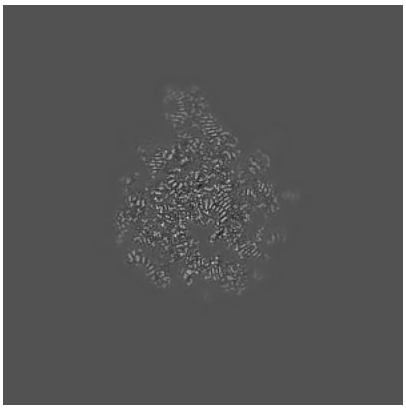
6.3.1 Primary map



X Index: 268

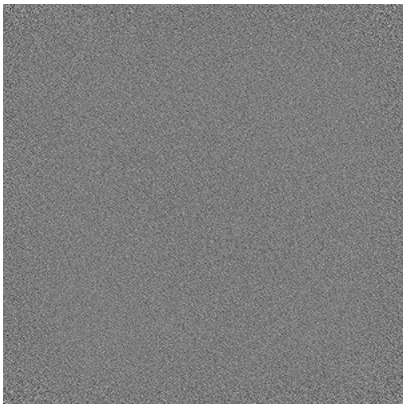


Y Index: 300

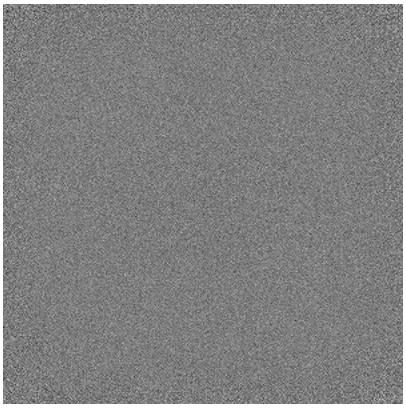


Z Index: 372

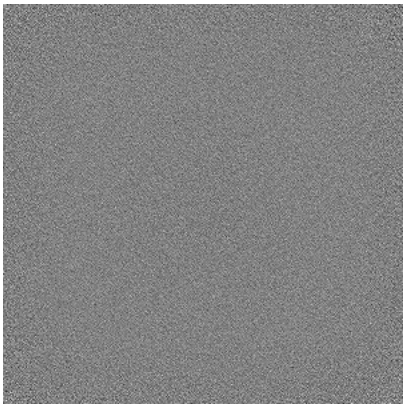
6.3.2 Raw map



X Index: 0



Y Index: 0

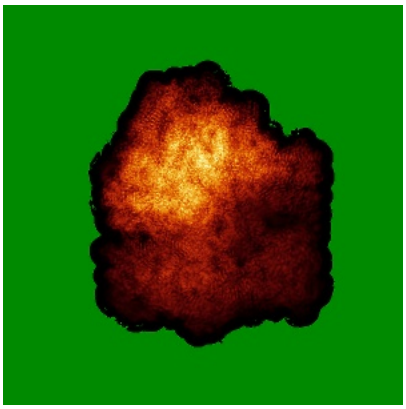


Z Index: 0

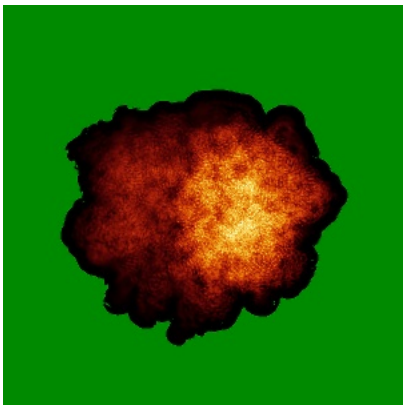
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

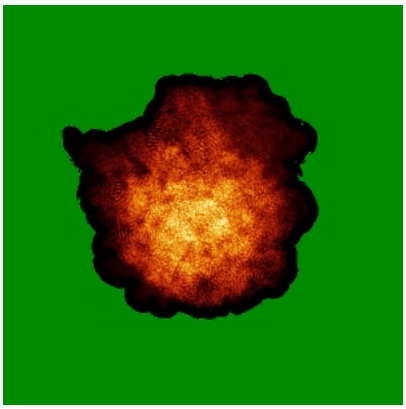
6.4.1 Primary map



X

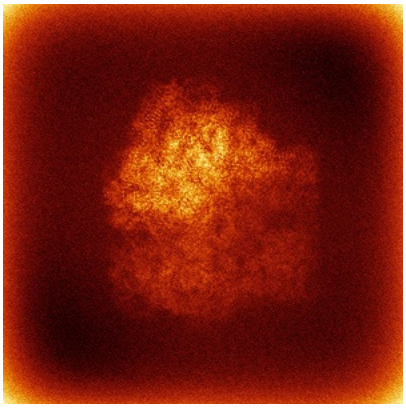


Y

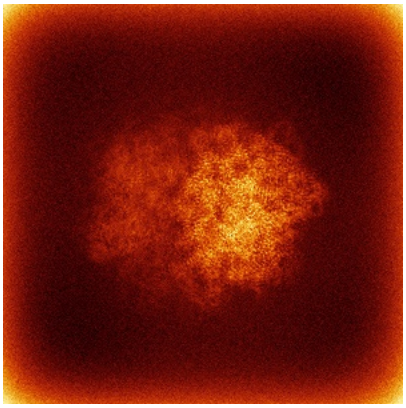


Z

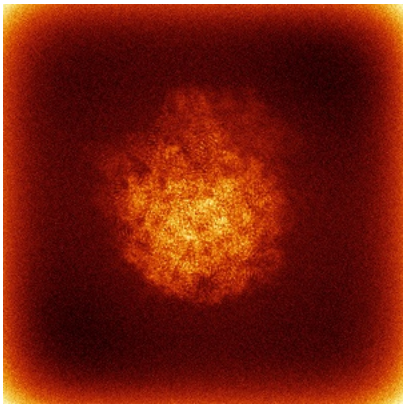
6.4.2 Raw map



X



Y



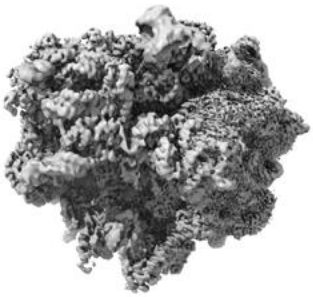
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

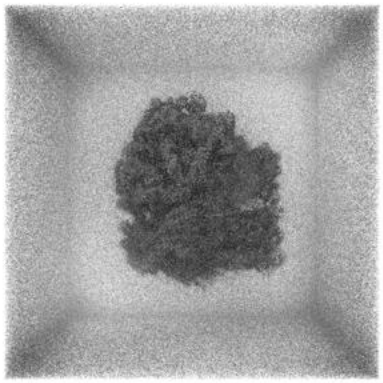


Y

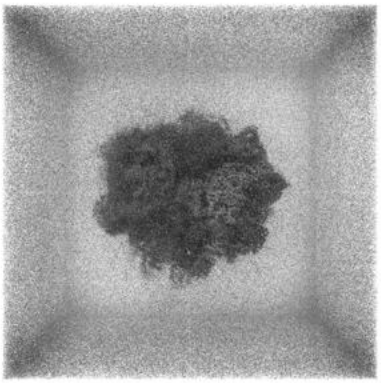
Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

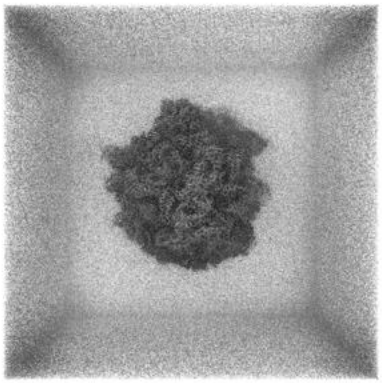
6.5.2 Raw map



X



Y



Z

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

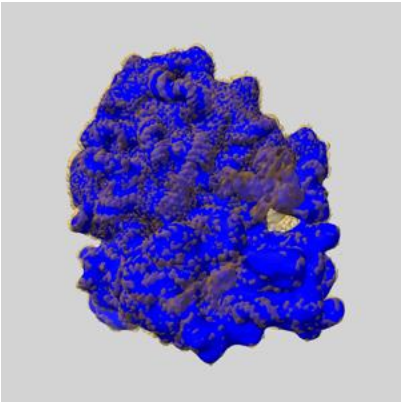
6.6 Mask visualisation (i)

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

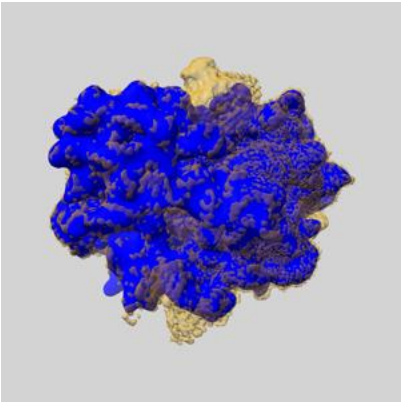
A mask typically either:

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

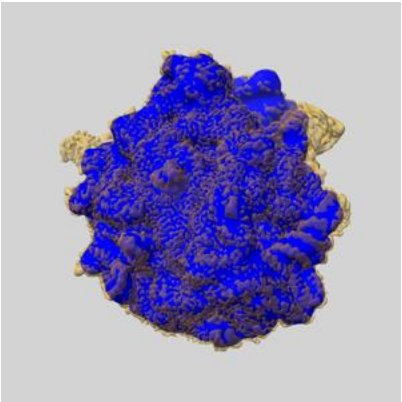
6.6.1 emd_51350_msk_1.map (i)



X



Y

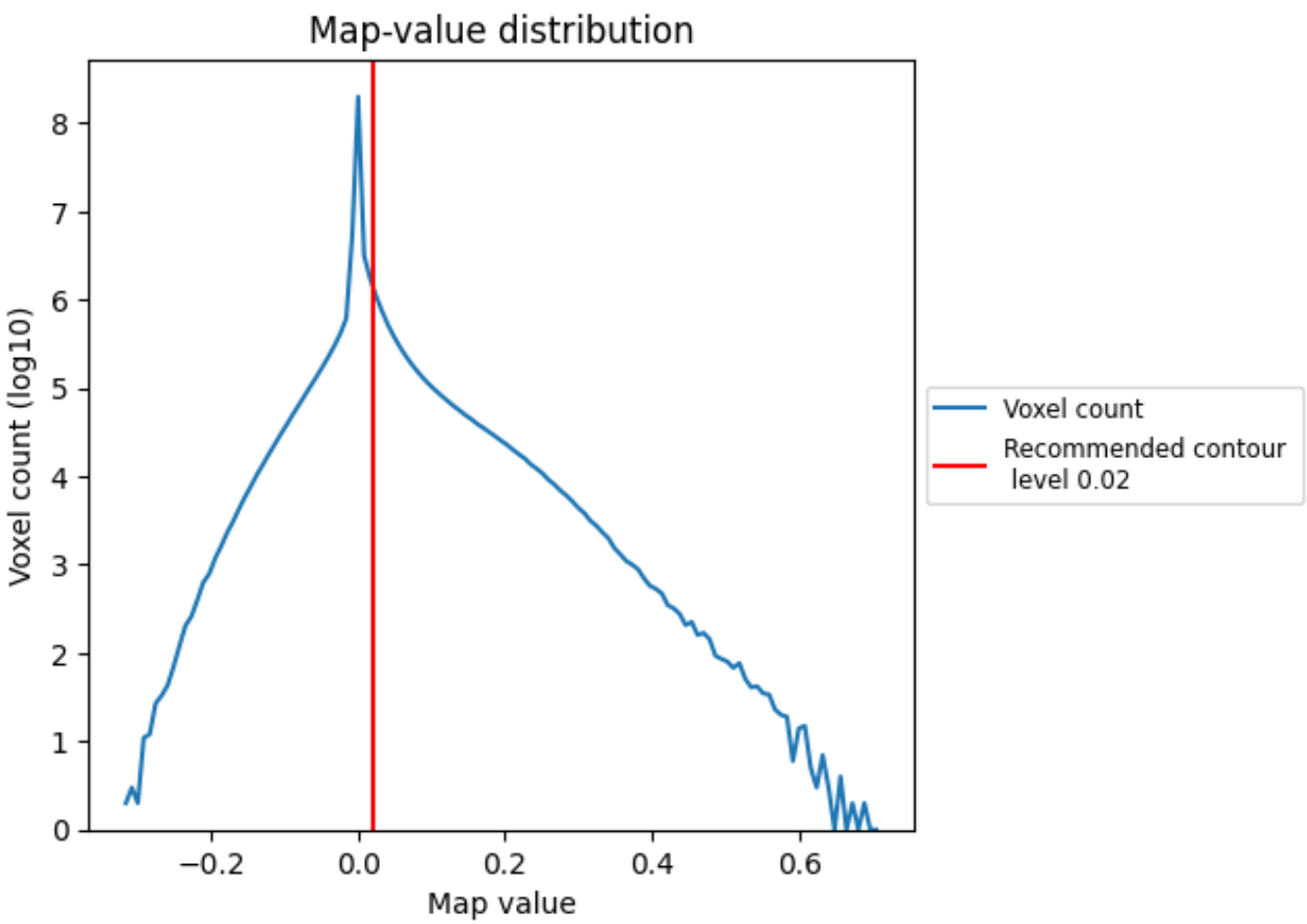


Z

7 Map analysis (i)

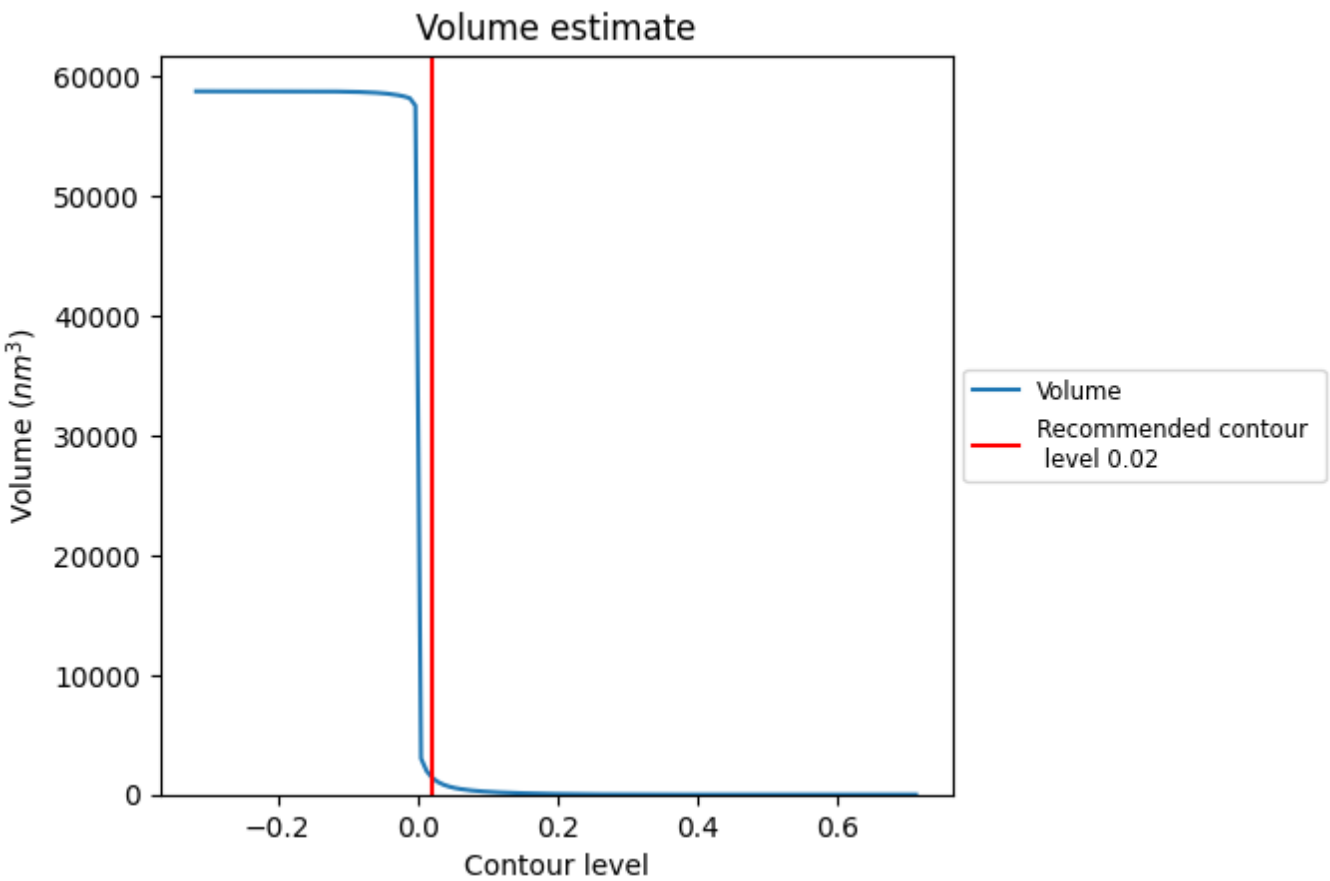
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

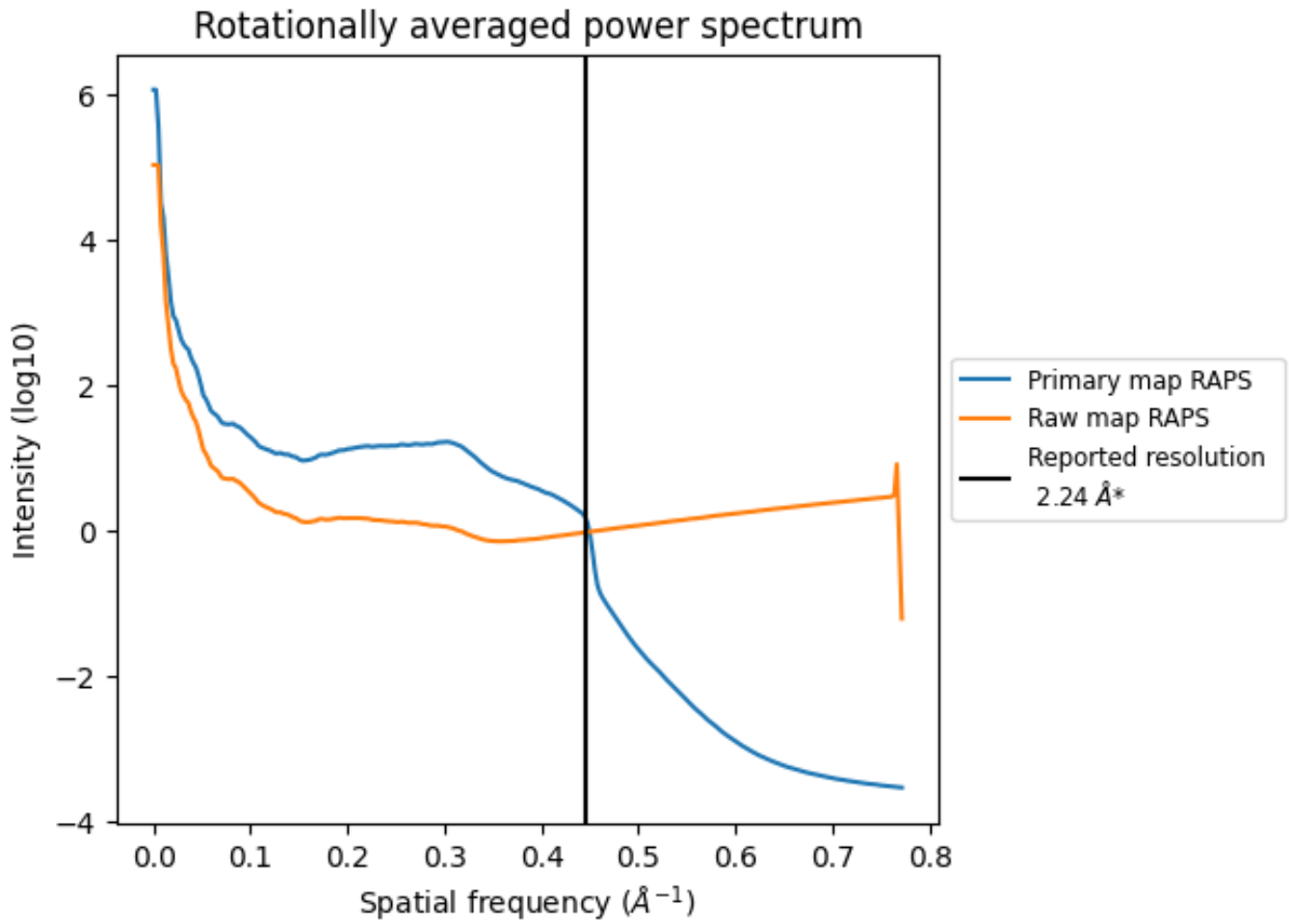
7.2 Volume estimate (i)



The volume at the recommended contour level is 1500 nm^3; this corresponds to an approximate mass of 1355 kDa.

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

7.3 Rotationally averaged power spectrum (i)

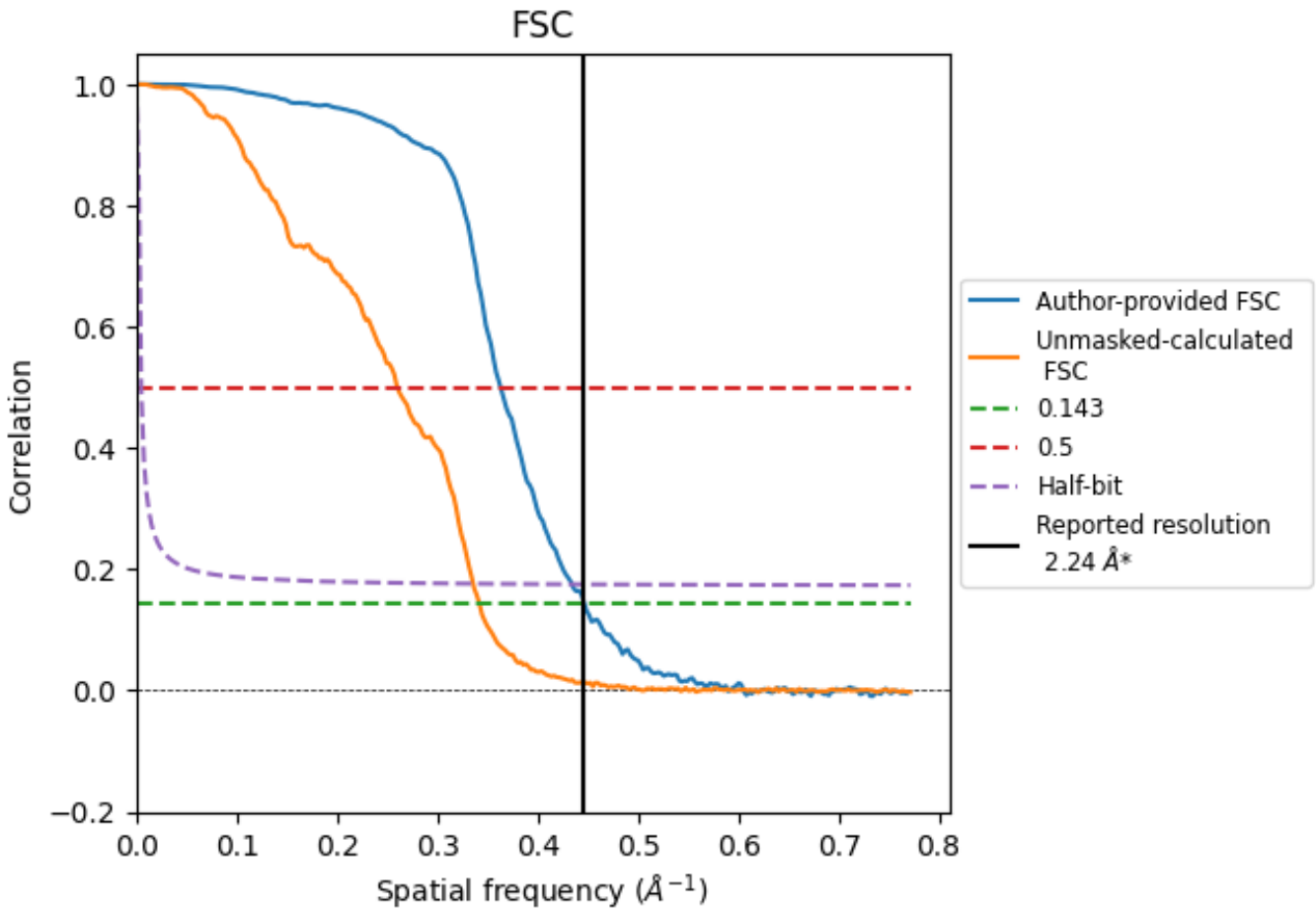


*Reported resolution corresponds to spatial frequency of 0.446 Å^{-1}

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 0.446 Å^{-1}

8.2 Resolution estimates (i)

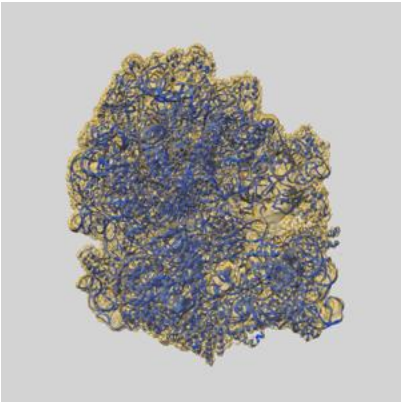
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.24	2.75	2.30
Unmasked-calculated*	2.92	3.84	2.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.92 differs from the reported value 2.24 by more than 10 %

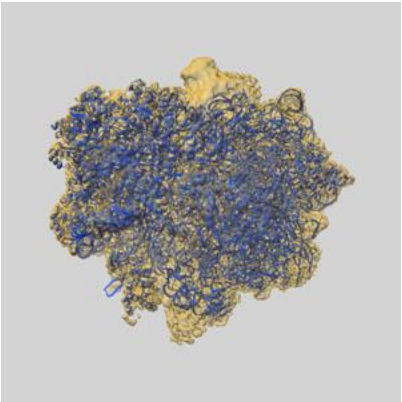
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-51350 and PDB model 9GHA. Per-residue inclusion information can be found in section 3 on page 16.

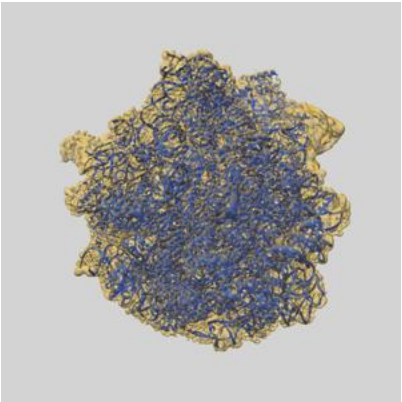
9.1 Map-model overlay (i)



X



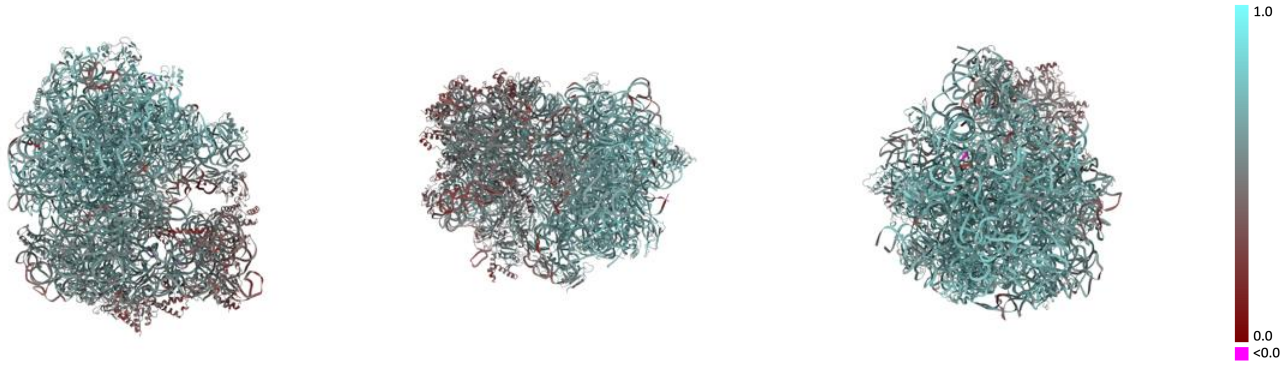
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

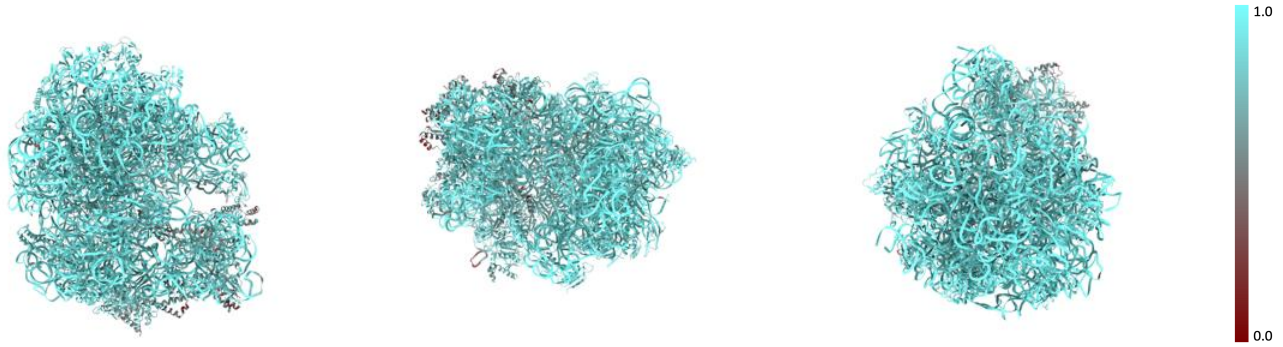
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

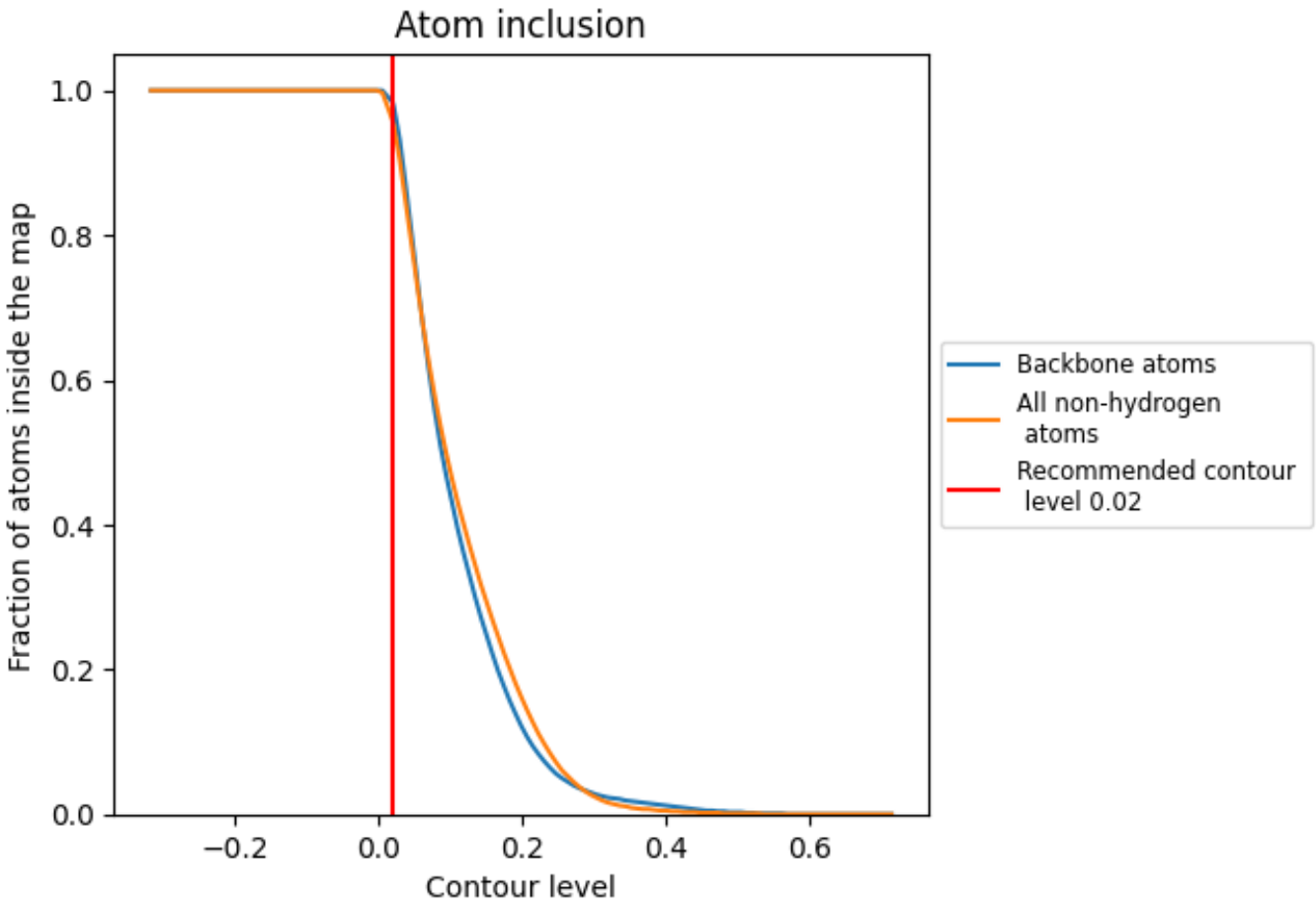
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.02).

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 (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9570	0.6150
0	0.9460	0.6380
1	0.9970	0.7540
2	0.9940	0.7340
3	0.9930	0.6730
4	0.7980	0.3930
8	0.9290	0.4840
9	0.8730	0.5040
A	0.9740	0.5540
B	0.6740	0.3880
C	0.8280	0.4780
D	0.8720	0.4780
E	0.9200	0.5390
F	0.8780	0.4970
G	0.6590	0.3370
H	0.9170	0.5450
I	0.8110	0.4350
J	0.7150	0.4190
K	0.9040	0.5440
L	0.9340	0.5650
M	0.7040	0.4140
N	0.8820	0.4880
O	0.9250	0.5580
P	0.9490	0.5510
Q	0.9330	0.5690
R	0.9180	0.5330
S	0.8220	0.4580
T	0.9360	0.5530
U	0.8500	0.5020
W	0.8390	0.4790
a	0.9930	0.6860
b	0.9950	0.6280
c	0.9890	0.7120
d	0.9730	0.7060
e	0.9590	0.6740

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Chain	Atom inclusion	Q-score
f	0.8550	0.4730
g	0.9410	0.5910
h	0.9430	0.5840
i	0.9790	0.7090
j	0.9780	0.6920
k	0.9800	0.7030
l	0.9760	0.6830
m	0.9970	0.7360
n	0.9570	0.6110
o	0.9550	0.6700
p	0.9920	0.7360
q	0.9510	0.6680
r	0.9810	0.7100
s	0.9520	0.6460
t	0.9660	0.6480
u	0.9340	0.6210
v	0.9730	0.6990
w	0.9770	0.6920
x	0.9400	0.6260
y	0.9660	0.6950
z	0.9830	0.7150