Full wwPDB EM Validation Report ⓘ

Jun 2, 2024 – 09:23 AM EDT

PDB ID	:	7UVX
EMDB ID	:	EMD-26819
Title	:	A. baumannii 70S ribosome-Streptothricin-F complex
Authors	:	Morgan, C.E.; Yu, E.W.
Deposited on	:	2022-05-02
Resolution	:	2.35 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

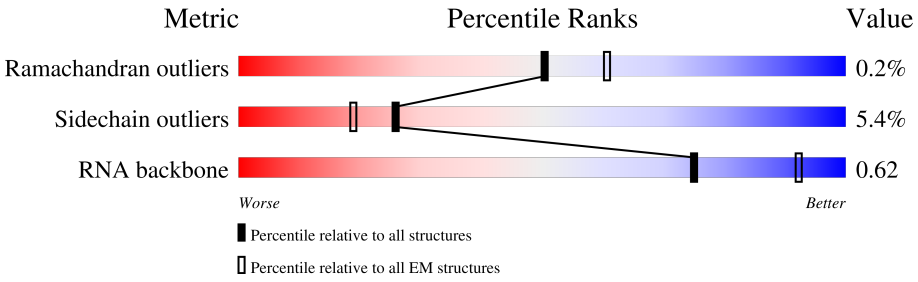
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.35 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	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	51	92% 8%
2	1	44	98%
3	2	64	97%
4	3	38	92% 8%
5	A	2918	81% 12% 7%
6	B	115	87% 13%
7	C	274	95%
8	D	212	97%

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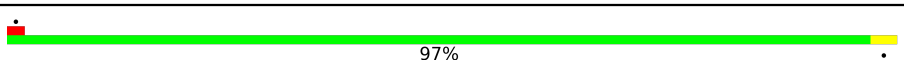
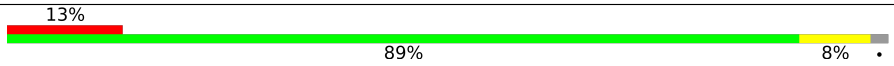
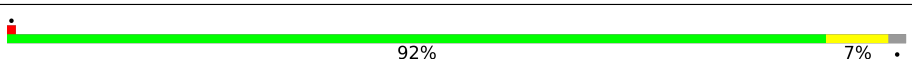
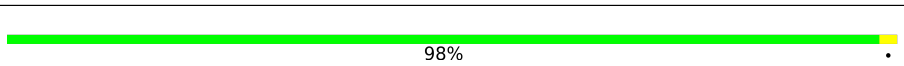
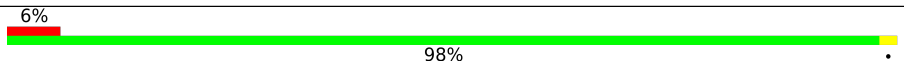
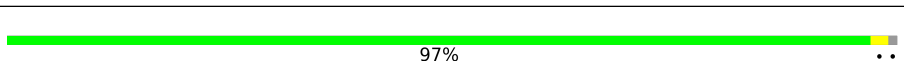
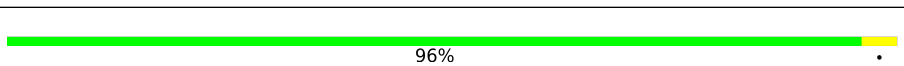
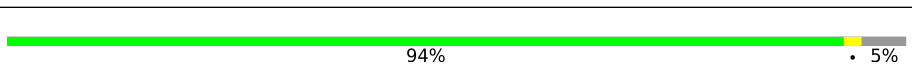
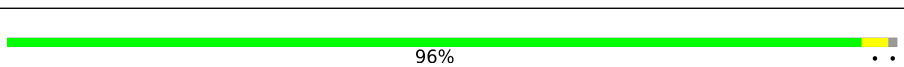
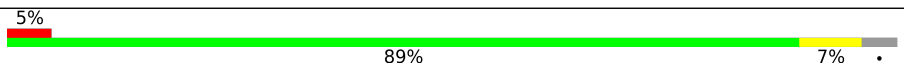
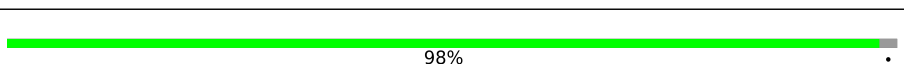
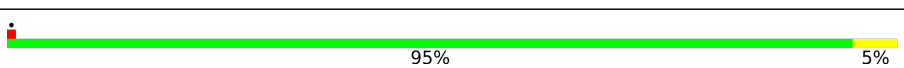
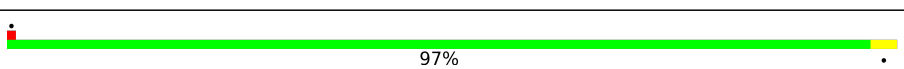
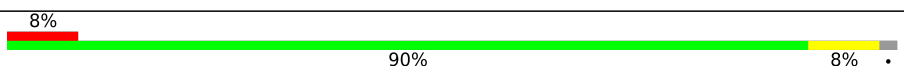
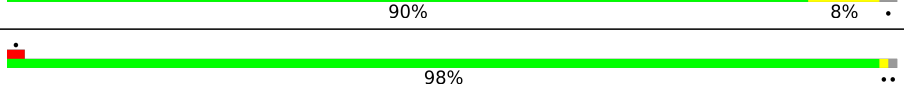
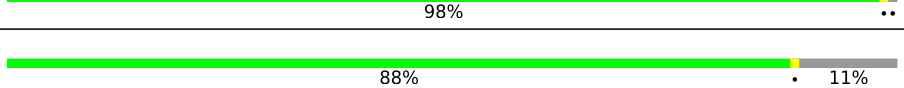
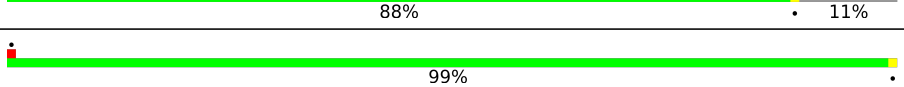
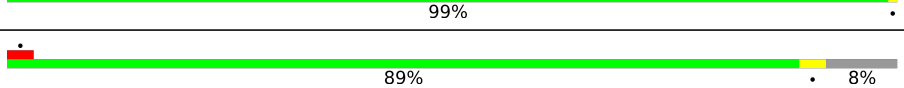
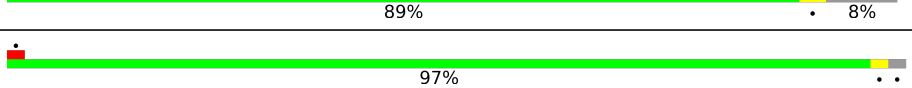
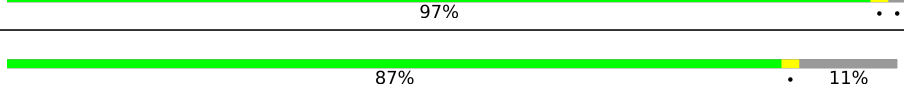
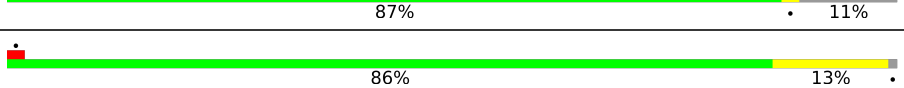
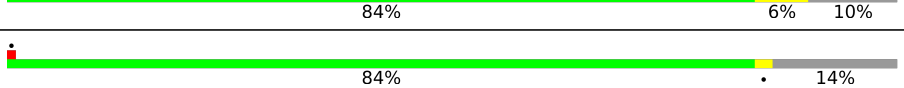
Mol	Chain	Length	Quality of chain
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26	V	85	
27	W	78	
28	X	65	
29	Y	58	
30	Z	61	
31	a	1544	
32	b	250	
33	c	250	

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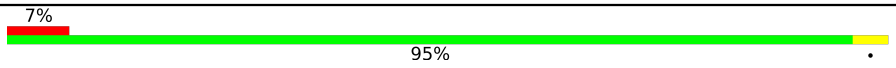
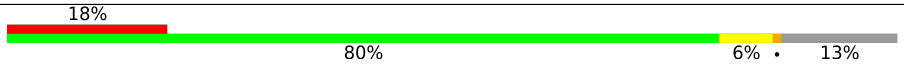
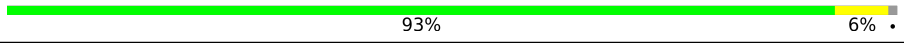
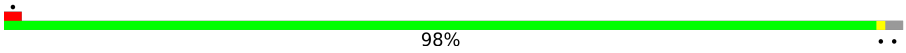
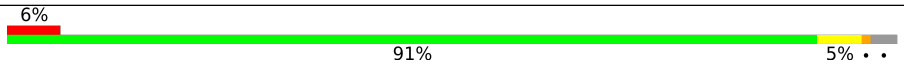
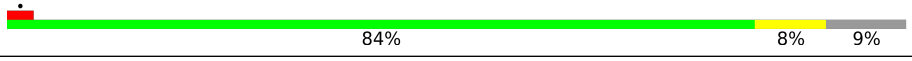
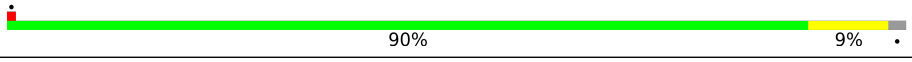
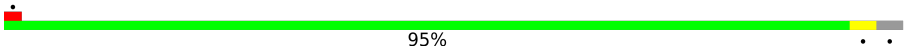
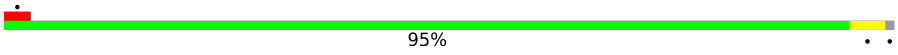
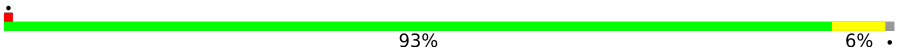
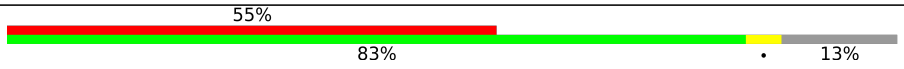
Mol	Chain	Length	Quality of chain
34	d	208	
35	e	165	
36	f	127	
37	g	156	
38	h	131	
39	i	128	
40	j	103	
41	k	128	
42	l	124	
43	m	118	
44	n	101	
45	o	89	
46	p	101	
47	q	85	
48	r	75	
49	s	91	
50	t	88	
51	u	71	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 136470 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			363	222	85	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2715	Total	C	N	O	P	0	0
			58247	25999	10665	18868	2715		

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	271	Total	C	N	O	S	0	0
			2106	1297	436	365	8		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	200	Total	C	N	O	S	0	0
			1516	952	281	278	5		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	174	Total	C	N	O	S	0	0
			1370	871	243	248	8		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	174	Total	C	N	O	S	0	0
			1318	832	236	249	1		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	122	Total	C	N	O	S	0	0
			946	592	180	169	5		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	K	144	Total	C	N	O	0	0
			1071	663	213	195		

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	137	Total	C	N	O	S	0	0
			1087	687	210	185	5		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			942	590	186	163	3		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	115	Total	C	N	O	S	0	0
			865	532	175	157	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	117	Total	C	N	O	0	0
			919	578	177	164		

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	103	Total 807	C 506	N 155	O 143	S 3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	109	Total 826	C 514	N 158	O 150	S 4	0	0

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	91	Total 710	C 452	N 128	O 129	S 1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	T	103	Total 766	C 476	N 142	O 148	0	0

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	97	Total 760	C 477	N 143	O 139	S 1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	76	Total 577	C 358	N 111	O 106	S 2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	78	Total 640	C 400	N 131	O 106	S 3	0	0

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	60	Total	C	N	O	S	0	0
			486	302	93	90	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	57	Total	C	N	O	S	0	0
			455	281	87	84	3		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	54	Total	C	N	O	S	0	0
			447	265	100	81	1		

- Molecule 31 is a RNA chain called 16s Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1528	Total	C	N	O	P	0	0
			32782	14631	5994	10630	1527		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1007	U	C	conflict	GB 1211343212
a	1034	C	U	conflict	GB 1211343212

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	225	Total	C	N	O	S	0	0
			1769	1110	328	325	6		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	215	Total	C	N	O	S	0	0
			1690	1065	318	299	8		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1631	1017	313	299	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	104	Total	C	N	O	S	0	0
			867	546	158	159	4		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	136	Total	C	N	O	S	0	0
			1073	671	201	194	7		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	130	Total	C	N	O	S	0	0
			985	615	177	187	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	126	Total	C	N	O	S	0	0
			991	618	197	175	1		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	100	Total	C	N	O	S	0	0
			801	500	150	148	3		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	117	Total	C	N	O	S	0	0
			862	535	167	159	1		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	122	Total	C	N	O	S	0	0
			945	580	193	167	5		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	115	Total	C	N	O	S	0	0
			903	558	184	158	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			705	434	144	126	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	82	Total	C	N	O	S	0	0
			644	403	128	112	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	79	Total	C	N	O	S	0	0
			621	390	116	114	1		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	52	Total 426	C 273	N 74	O 79	0	0

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total 646	C 412	N 125	O 107	S 2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	86	Total 663	C 409	N 139	O 113	S 2	0	0

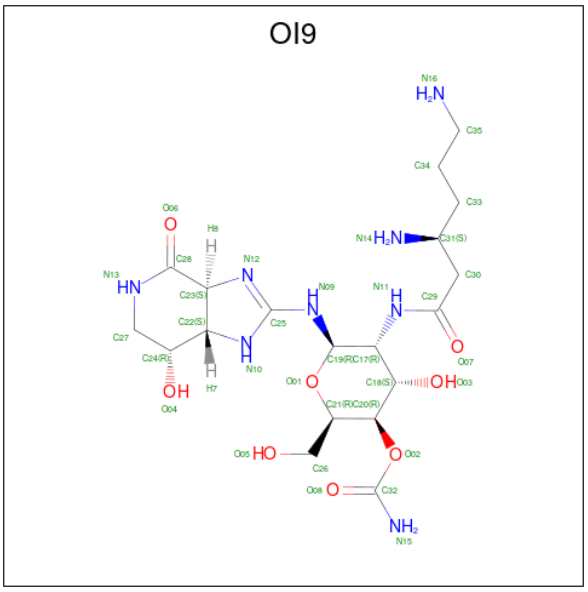
- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	62	Total 515	C 322	N 104	O 88	S 1	0	0

- Molecule 52 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	3	1	Total 1	Zn 1	0

- Molecule 53 is Streptothricin F (three-letter code: OI9) (formula: $C_{19}H_{34}N_8O_8$) (labeled as "Ligand of Interest" by depositor).



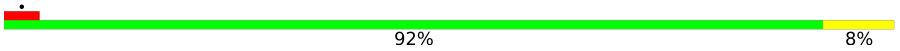
Mol	Chain	Residues	Atoms				AltConf
53	W	1	Total	C	N	O	0
			35	19	8	8	

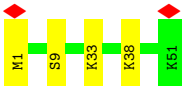
3 Residue-property plots (i)

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

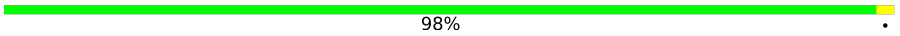
Chain 0:





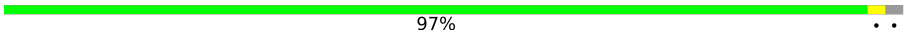
• Molecule 2: 50S ribosomal protein L34

Chain 1:



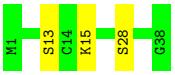
• Molecule 3: 50S ribosomal protein L35

Chain 2:



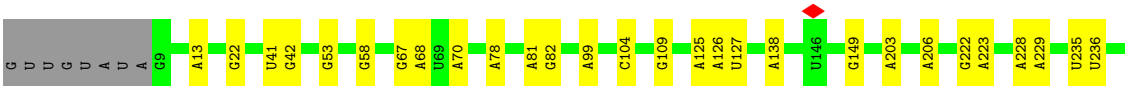
• Molecule 4: 50S ribosomal protein L36

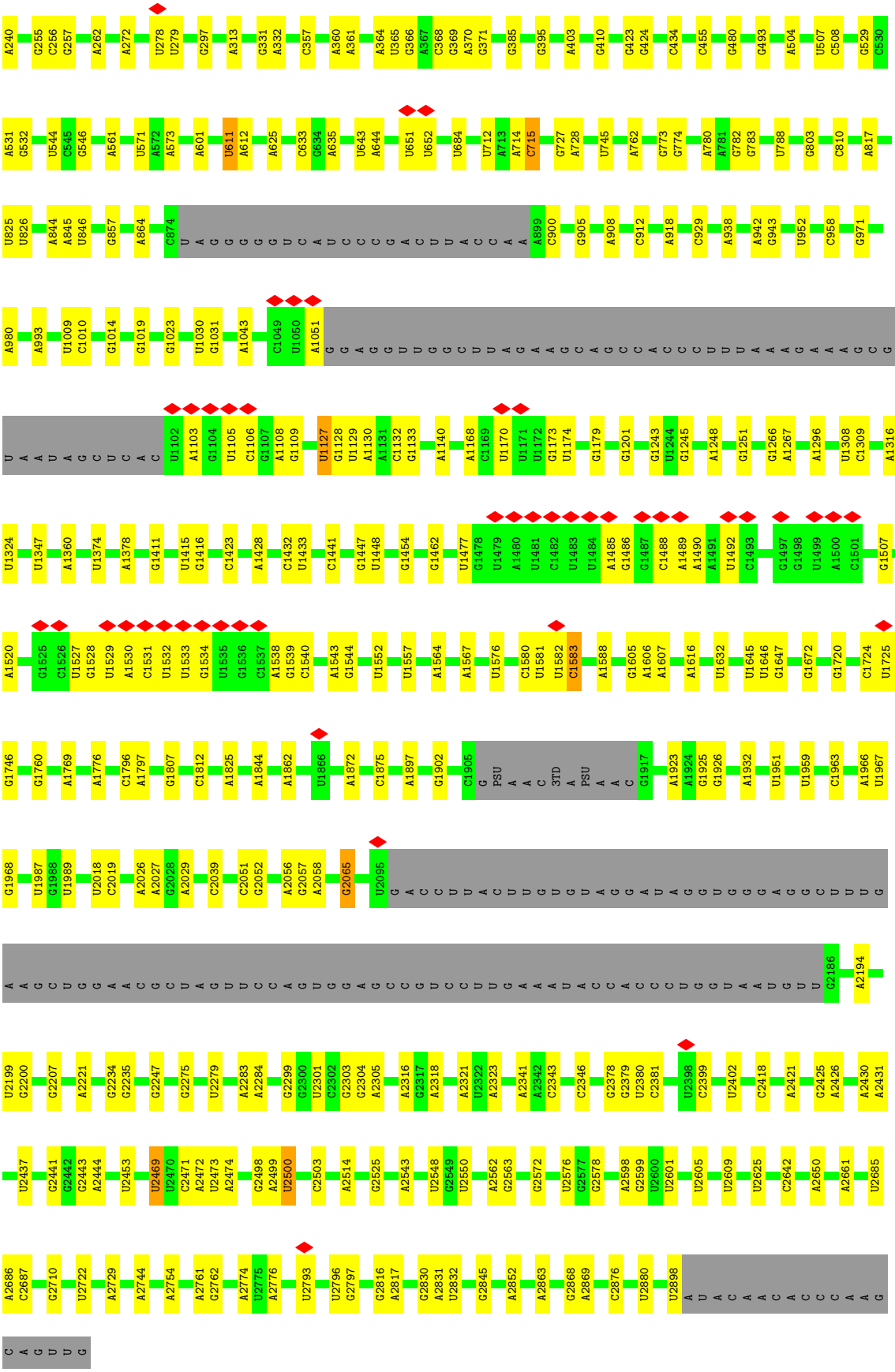
Chain 3:



• Molecule 5: 23s ribosomal RNA

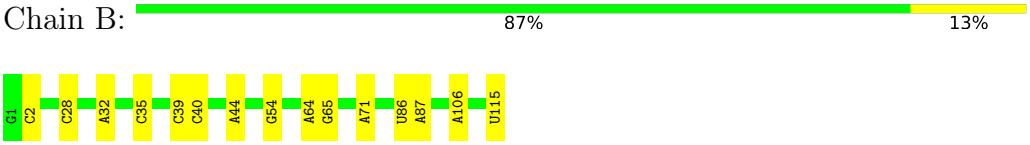
Chain A:





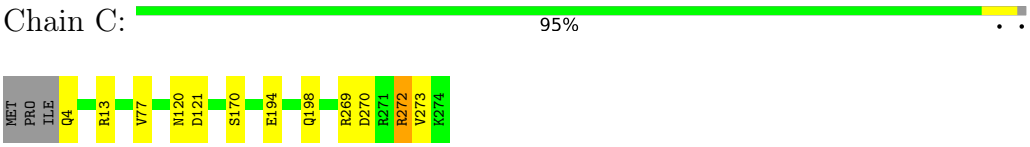
• Molecule 6: 5s ribosomal RNA

Chain B:



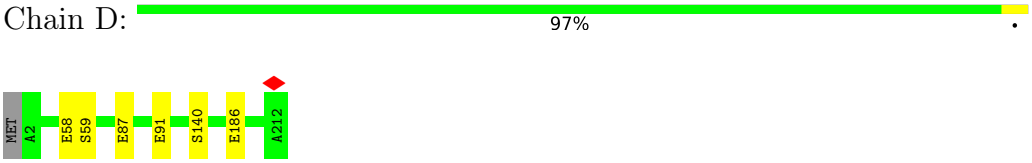
• Molecule 7: 50S ribosomal protein L2

Chain C:



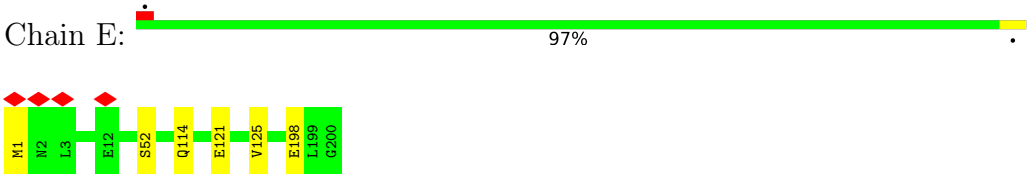
• Molecule 8: 50S ribosomal protein L3

Chain D:



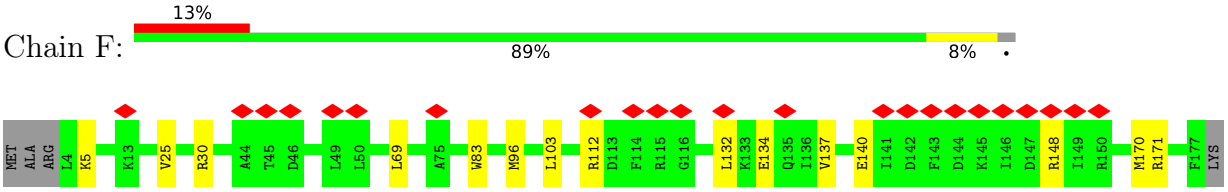
• Molecule 9: 50S ribosomal protein L4

Chain E:



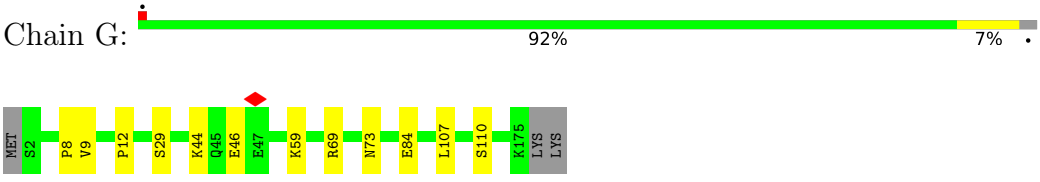
• Molecule 10: 50S ribosomal protein L5

Chain F:



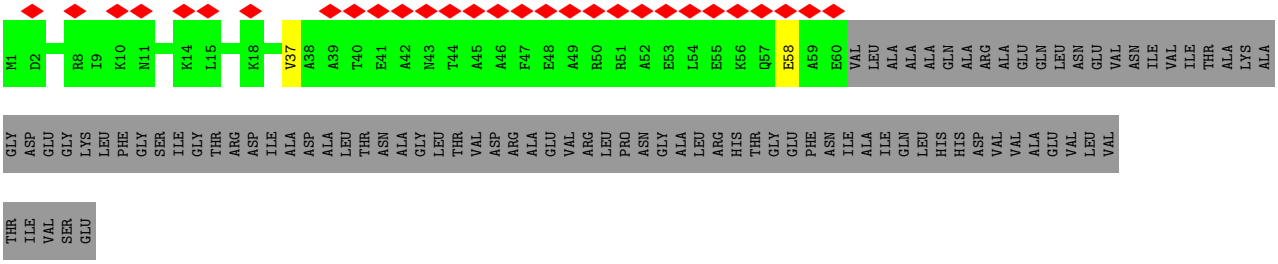
• Molecule 11: 50S ribosomal protein L6

Chain G:



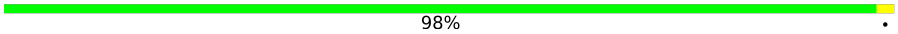
• Molecule 12: 50S ribosomal protein L9

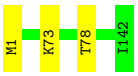
Chain H:



• Molecule 13: 50S ribosomal protein L13

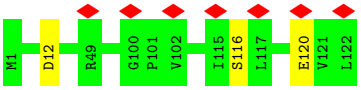
Chain I:





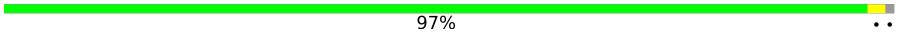
• Molecule 14: 50S ribosomal protein L14

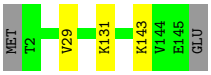
Chain J:



• Molecule 15: 50S ribosomal protein L15

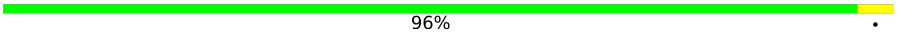
Chain K:

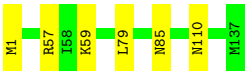




• Molecule 16: 50S ribosomal protein L16

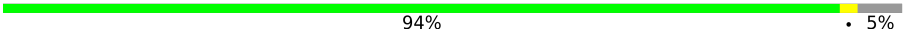
Chain L:





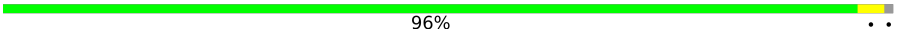
• Molecule 17: 50S ribosomal protein L17

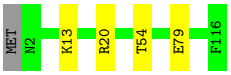
Chain M:



• Molecule 18: 50S ribosomal protein L18

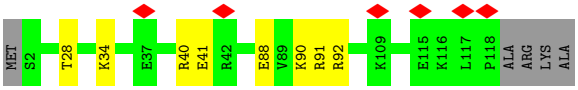
Chain N:





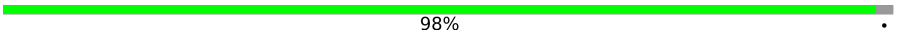
• Molecule 19: 50S ribosomal protein L19

Chain O:



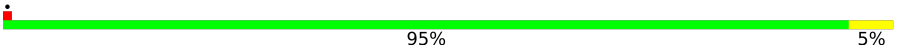
• Molecule 20: 50S ribosomal protein L20

Chain P:



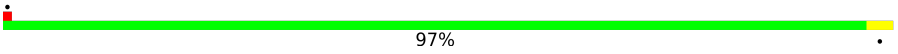
• Molecule 21: 50S ribosomal protein L21

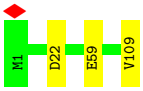
Chain Q:



• Molecule 22: 50S ribosomal protein L22

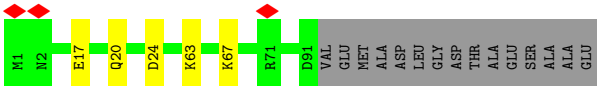
Chain R:





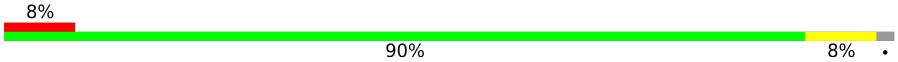
• Molecule 23: 50S ribosomal protein L23

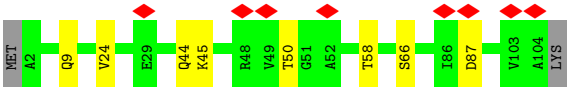
Chain S:



• Molecule 24: 50S ribosomal protein L24

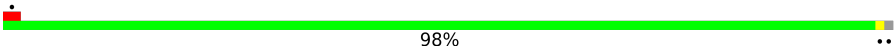
Chain T:

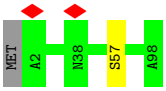




• Molecule 25: 50S ribosomal protein L25

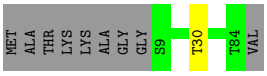
Chain U:





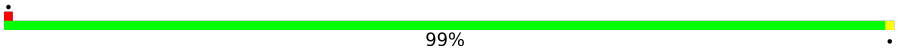
• Molecule 26: 50S ribosomal protein L27

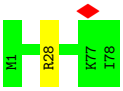
Chain V:



• Molecule 27: 50S ribosomal protein L28

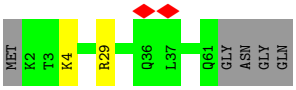
Chain W:





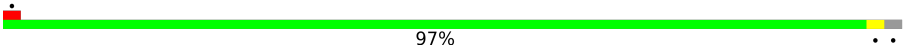
• Molecule 28: 50S ribosomal protein L29

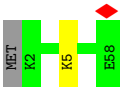
Chain X:



• Molecule 29: 50S ribosomal protein L30

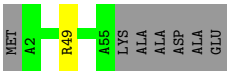
Chain Y:





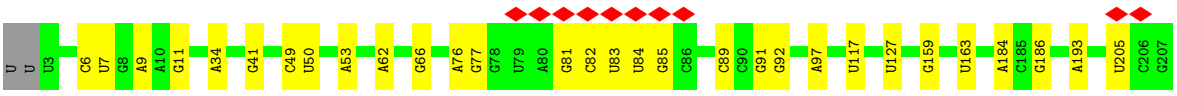
• Molecule 30: 50S ribosomal protein L32

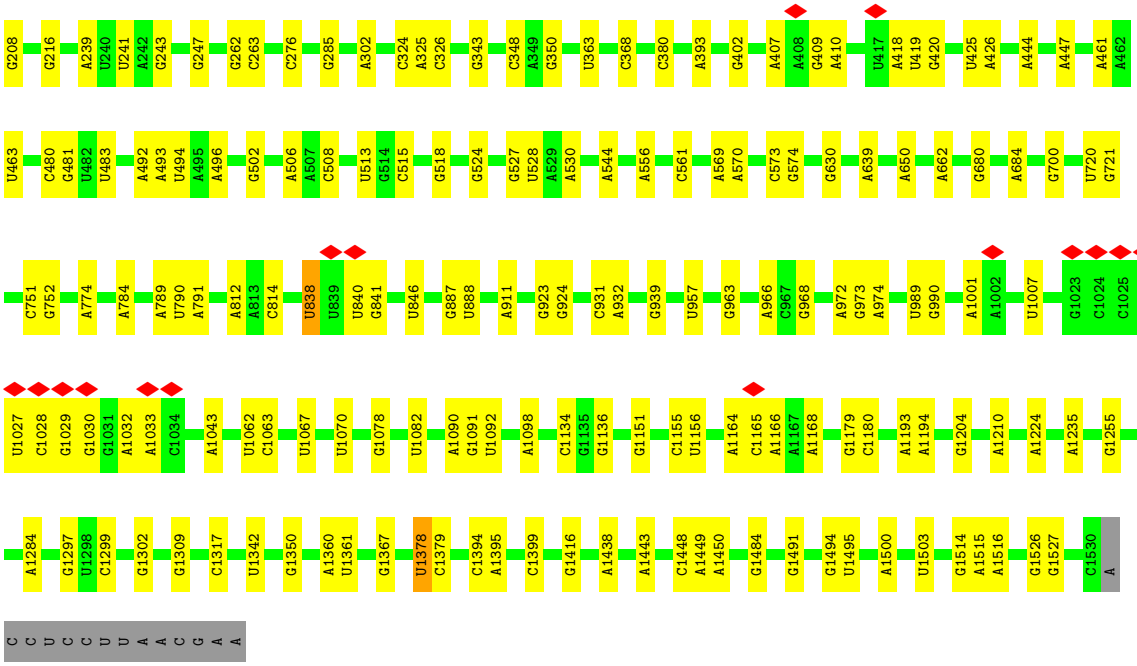
Chain Z:



• Molecule 31: 16s Ribosomal RNA

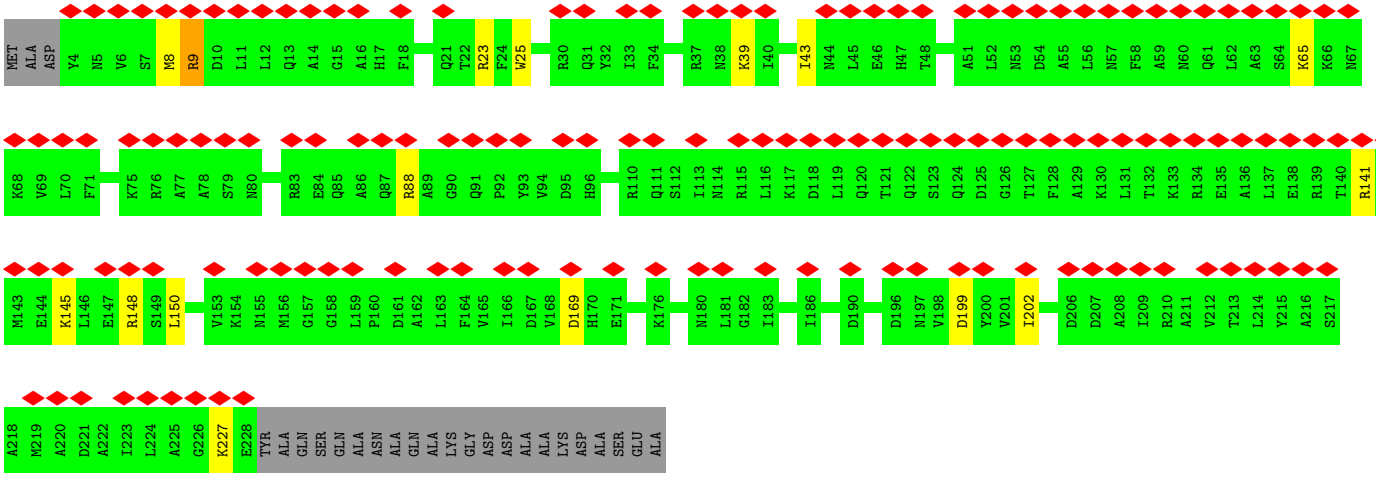
Chain a:





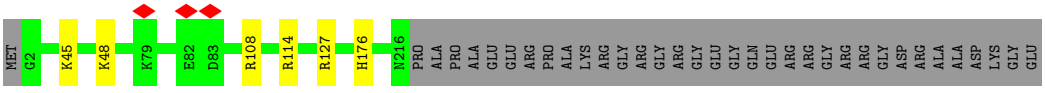
• Molecule 32: 30S ribosomal protein S2

Chain b:



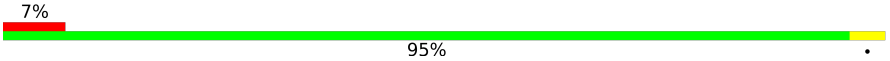
• Molecule 33: 30S ribosomal protein S3

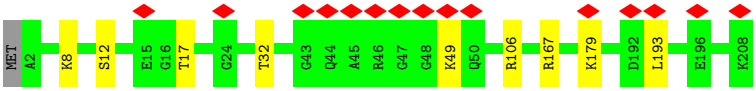
Chain c:



• Molecule 34: 30S ribosomal protein S4

Chain d:



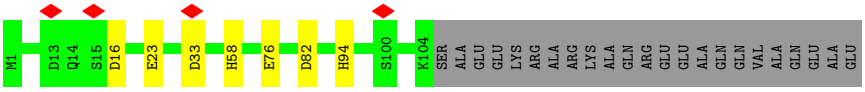


• Molecule 35: 30S ribosomal protein S5

Chain e:

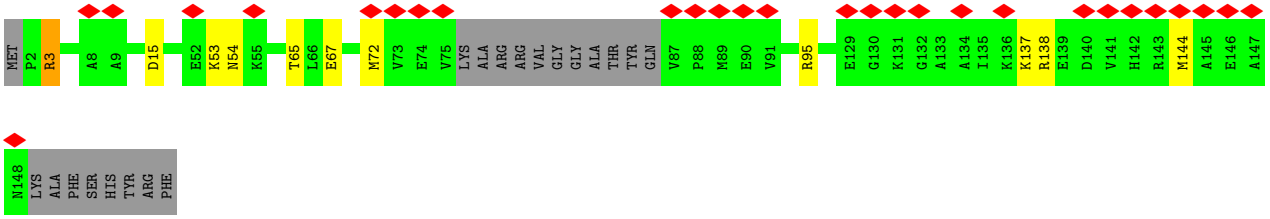
• Molecule 36: 30S ribosomal protein S6

Chain f:



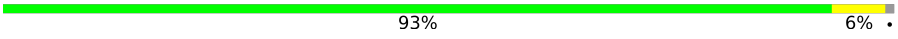
• Molecule 37: 30S ribosomal protein S7

Chain g:



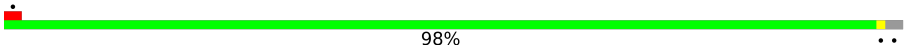
• Molecule 38: 30S ribosomal protein S8

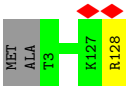
Chain h:



• Molecule 39: 30S ribosomal protein S9

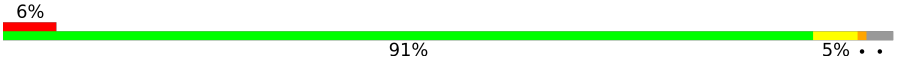
Chain i:

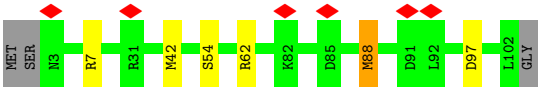




• Molecule 40: 30S ribosomal protein S10

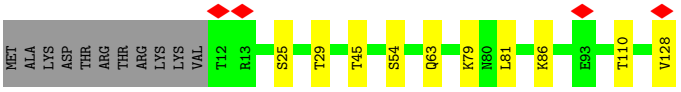
Chain j:





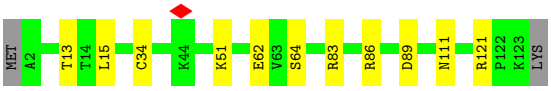
• Molecule 41: 30S ribosomal protein S11

Chain k:



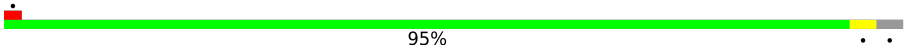
• Molecule 42: 30S ribosomal protein S12

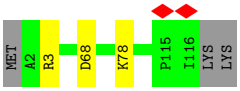
Chain l:



• Molecule 43: 30S ribosomal protein S13

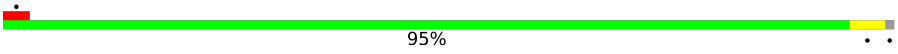
Chain m:

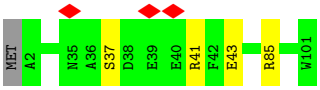




• Molecule 44: 30S ribosomal protein S14

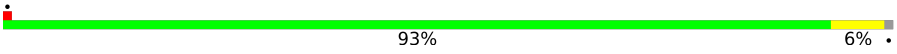
Chain n:

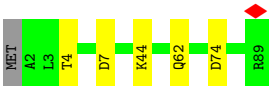




• Molecule 45: 30S ribosomal protein S15

Chain o:



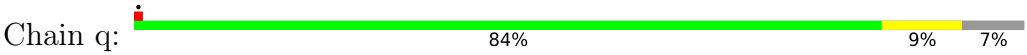


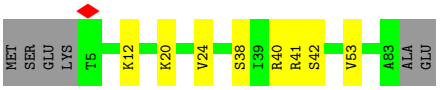
• Molecule 46: 30S ribosomal protein S16

Chain p:

• Molecule 47: 30S ribosomal protein S17

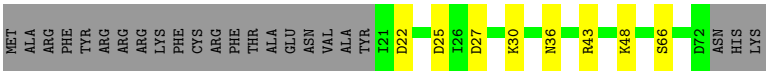
Chain q:





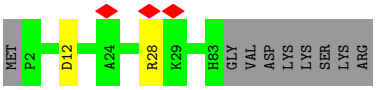
• Molecule 48: 30S ribosomal protein S18

Chain r:



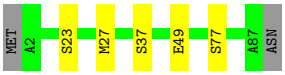
• Molecule 49: 30S ribosomal protein S19

Chain s:



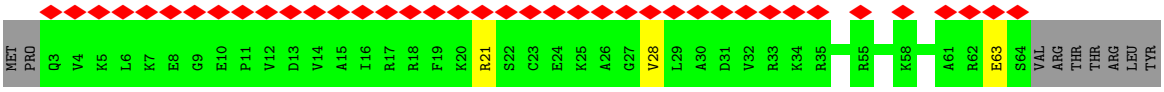
• Molecule 50: 30S ribosomal protein S20

Chain t:



• Molecule 51: 30S ribosomal protein S21

Chain u:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	135858	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.427	Depositor
Minimum map value	0.000	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	434.176, 434.176, 434.176	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.848, 0.848, 0.848	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: 5MU, PSU, 6MZ, 4OC, OMU, 5MC, UR3, 7MG, 2MG, MA6, OI9, OMG, ZN, 2MA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.27	0/434	0.54	0/573
2	1	0.25	0/367	0.64	0/481
3	2	0.26	0/515	0.57	0/678
4	3	0.26	0/296	0.56	0/389
5	A	0.36	0/64939	0.81	22/101284 (0.0%)
6	B	0.29	0/2739	0.81	0/4266
7	C	0.27	0/2146	0.59	0/2880
8	D	0.27	0/1590	0.55	0/2142
9	E	0.27	0/1537	0.53	0/2073
10	F	0.27	0/1390	0.60	0/1863
11	G	0.27	0/1337	0.50	0/1807
12	H	0.25	0/461	0.52	0/616
13	I	0.27	0/1151	0.48	0/1551
14	J	0.29	0/956	0.63	0/1286
15	K	0.26	0/1079	0.57	0/1439
16	L	0.26	0/1104	0.57	0/1475
17	M	0.26	0/956	0.57	0/1282
18	N	0.27	0/873	0.58	0/1167
19	O	0.27	0/931	0.59	0/1249
20	P	0.29	0/947	0.59	0/1262
21	Q	0.26	0/818	0.55	0/1094
22	R	0.24	0/831	0.51	0/1113
23	S	0.27	0/716	0.53	0/957
24	T	0.25	0/770	0.54	0/1034
25	U	0.27	0/770	0.53	0/1036
26	V	0.27	0/585	0.53	0/783
27	W	0.26	0/650	0.59	0/866
28	X	0.27	0/487	0.56	0/646
29	Y	0.25	0/460	0.51	0/614
30	Z	0.25	0/453	0.62	0/604
31	a	0.31	0/36476	0.79	13/56895 (0.0%)
32	b	0.29	0/1799	0.61	1/2429 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.26	0/1714	0.54	0/2304
34	d	0.27	0/1653	0.55	0/2213
35	e	0.27	0/1141	0.54	0/1537
36	f	0.28	0/882	0.62	0/1189
37	g	0.29	0/1087	0.60	0/1456
38	h	0.27	0/993	0.52	0/1331
39	i	0.28	0/1002	0.59	0/1339
40	j	0.27	0/811	0.61	1/1096 (0.1%)
41	k	0.25	0/878	0.55	0/1189
42	l	0.26	0/958	0.59	0/1284
43	m	0.24	0/913	0.56	0/1226
44	n	0.27	0/803	0.53	0/1071
45	o	0.28	0/715	0.53	0/958
46	p	0.27	0/655	0.58	0/879
47	q	0.24	0/628	0.56	0/847
48	r	0.26	0/432	0.52	0/583
49	s	0.28	0/664	0.52	0/897
50	t	0.28	0/669	0.50	0/892
51	u	0.25	0/520	0.52	0/686
All	All	0.32	0/147681	0.75	37/220811 (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
21	Q	0	1

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1378	U	C2-N1-C1'	7.69	126.93	117.70
5	A	2469	U	C2-N1-C1'	7.16	126.30	117.70
5	A	2469	U	N1-C2-O2	7.09	127.76	122.80
31	a	1378	U	N1-C2-O2	6.92	127.64	122.80
5	A	1308	U	C2-N1-C1'	6.79	125.85	117.70
5	A	788	U	C2-N1-C1'	6.64	125.67	117.70
31	a	1378	U	N3-C2-O2	-6.53	117.63	122.20
5	A	611	U	C2-N1-C1'	6.35	125.32	117.70
31	a	838	U	C2-N1-C1'	6.30	125.26	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1127	U	P-O3'-C3'	6.26	127.22	119.70
5	A	652	U	C2-N1-C1'	6.10	125.02	117.70
5	A	2469	U	N3-C2-O2	-5.96	118.03	122.20
31	a	1379	C	C2-N1-C1'	5.76	125.14	118.80
31	a	1063	C	N1-C2-O2	5.69	122.31	118.90
5	A	434	C	C2-N1-C1'	5.69	125.06	118.80
5	A	1309	C	C2-N1-C1'	5.64	125.00	118.80
5	A	912	C	C2-N1-C1'	5.63	124.99	118.80
31	a	1063	C	C2-N1-C1'	5.57	124.93	118.80
31	a	1155	C	C2-N1-C1'	5.56	124.92	118.80
5	A	611	U	N1-C2-O2	5.46	126.62	122.80
31	a	1448	C	C2-N1-C1'	5.46	124.80	118.80
5	A	727	G	O4'-C1'-N9	5.42	112.54	108.20
31	a	326	C	N1-C2-O2	5.40	122.14	118.90
5	A	1308	U	N3-C2-O2	-5.39	118.43	122.20
5	A	715	C	C2-N1-C1'	5.36	124.70	118.80
31	a	751	C	C2-N1-C1'	5.34	124.68	118.80
32	b	9	ARG	CA-CB-CG	5.28	125.02	113.40
5	A	912	C	N1-C2-O2	5.28	122.07	118.90
31	a	1448	C	N1-C2-O2	5.27	122.06	118.90
5	A	1583	C	N1-C2-O2	5.22	122.03	118.90
5	A	1308	U	N1-C2-O2	5.18	126.43	122.80
5	A	2572	G	C4-N9-C1'	5.18	133.23	126.50
5	A	652	U	N1-C2-O2	5.14	126.40	122.80
31	a	1379	C	N1-C2-O2	5.08	121.95	118.90
40	j	88	MET	CB-CG-SD	5.07	127.62	112.40
5	A	2473	U	C2-N1-C1'	5.06	123.77	117.70
5	A	1583	C	C2-N1-C1'	5.01	124.31	118.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	Q	51	ALA	Peptide

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	49/51 (96%)	49 (100%)	0	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
7	C	269/274 (98%)	263 (98%)	5 (2%)	1 (0%)	34	38
8	D	209/212 (99%)	201 (96%)	8 (4%)	0	100	100
9	E	198/200 (99%)	197 (100%)	1 (0%)	0	100	100
10	F	172/178 (97%)	152 (88%)	17 (10%)	3 (2%)	9	7
11	G	172/177 (97%)	167 (97%)	4 (2%)	1 (1%)	25	27
12	H	58/148 (39%)	57 (98%)	1 (2%)	0	100	100
13	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
14	J	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
15	K	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
16	L	135/137 (98%)	132 (98%)	2 (2%)	1 (1%)	22	23
17	M	117/125 (94%)	116 (99%)	1 (1%)	0	100	100
18	N	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
19	O	115/122 (94%)	114 (99%)	1 (1%)	0	100	100
20	P	115/119 (97%)	114 (99%)	1 (1%)	0	100	100
21	Q	101/103 (98%)	98 (97%)	2 (2%)	1 (1%)	15	15
22	R	107/109 (98%)	107 (100%)	0	0	100	100
23	S	89/106 (84%)	88 (99%)	1 (1%)	0	100	100
24	T	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
25	U	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	V	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
27	W	76/78 (97%)	74 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	X	58/65 (89%)	57 (98%)	1 (2%)	0	100	100
29	Y	55/58 (95%)	55 (100%)	0	0	100	100
30	Z	52/61 (85%)	51 (98%)	1 (2%)	0	100	100
32	b	223/250 (89%)	208 (93%)	14 (6%)	1 (0%)	34	38
33	c	213/250 (85%)	208 (98%)	5 (2%)	0	100	100
34	d	205/208 (99%)	202 (98%)	3 (2%)	0	100	100
35	e	153/165 (93%)	153 (100%)	0	0	100	100
36	f	102/127 (80%)	100 (98%)	0	2 (2%)	7	5
37	g	132/156 (85%)	128 (97%)	3 (2%)	1 (1%)	19	20
38	h	128/131 (98%)	123 (96%)	5 (4%)	0	100	100
39	i	124/128 (97%)	120 (97%)	4 (3%)	0	100	100
40	j	98/103 (95%)	94 (96%)	4 (4%)	0	100	100
41	k	115/128 (90%)	111 (96%)	4 (4%)	0	100	100
42	l	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
45	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
46	p	80/101 (79%)	80 (100%)	0	0	100	100
47	q	77/85 (91%)	76 (99%)	1 (1%)	0	100	100
48	r	50/75 (67%)	50 (100%)	0	0	100	100
49	s	80/91 (88%)	78 (98%)	2 (2%)	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100
51	u	60/71 (84%)	59 (98%)	1 (2%)	0	100	100
All	All	5412/5872 (92%)	5275 (98%)	126 (2%)	11 (0%)	50	56

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	C	272	ARG
32	b	8	MET
36	f	33	ASP
36	f	94	HIS
37	g	3	ARG
10	F	137	VAL

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Mol	Chain	Res	Type
10	F	5	LYS
11	G	12	PRO
10	F	134	GLU
16	L	79	LEU
21	Q	52	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/47 (100%)	43 (92%)	4 (8%)	10	10
2	1	36/36 (100%)	35 (97%)	1 (3%)	43	53
3	2	52/53 (98%)	51 (98%)	1 (2%)	57	68
4	3	33/33 (100%)	30 (91%)	3 (9%)	9	8
7	C	217/220 (99%)	205 (94%)	12 (6%)	21	24
8	D	166/167 (99%)	160 (96%)	6 (4%)	35	43
9	E	155/155 (100%)	149 (96%)	6 (4%)	32	40
10	F	144/147 (98%)	132 (92%)	12 (8%)	11	11
11	G	139/142 (98%)	128 (92%)	11 (8%)	12	12
12	H	45/112 (40%)	43 (96%)	2 (4%)	28	34
13	I	118/118 (100%)	115 (98%)	3 (2%)	47	58
14	J	103/103 (100%)	100 (97%)	3 (3%)	42	52
15	K	106/108 (98%)	103 (97%)	3 (3%)	43	53
16	L	113/113 (100%)	108 (96%)	5 (4%)	28	34
17	M	96/101 (95%)	94 (98%)	2 (2%)	53	65
18	N	84/85 (99%)	80 (95%)	4 (5%)	25	30
19	O	99/102 (97%)	91 (92%)	8 (8%)	11	11
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	81 (96%)	3 (4%)	35	43
22	R	88/88 (100%)	85 (97%)	3 (3%)	37	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	S	77/87 (88%)	72 (94%)	5 (6%)	17 18
24	T	83/85 (98%)	75 (90%)	8 (10%)	8 7
25	U	79/80 (99%)	78 (99%)	1 (1%)	69 80
26	V	59/64 (92%)	58 (98%)	1 (2%)	60 72
27	W	70/70 (100%)	69 (99%)	1 (1%)	67 78
28	X	53/56 (95%)	51 (96%)	2 (4%)	33 41
29	Y	53/54 (98%)	52 (98%)	1 (2%)	57 68
30	Z	46/50 (92%)	45 (98%)	1 (2%)	52 63
32	b	185/200 (92%)	170 (92%)	15 (8%)	11 11
33	c	175/198 (88%)	169 (97%)	6 (3%)	37 46
34	d	170/171 (99%)	161 (95%)	9 (5%)	22 26
35	e	113/120 (94%)	104 (92%)	9 (8%)	12 12
36	f	94/111 (85%)	89 (95%)	5 (5%)	22 26
37	g	113/128 (88%)	102 (90%)	11 (10%)	8 7
38	h	108/109 (99%)	100 (93%)	8 (7%)	13 14
39	i	99/100 (99%)	98 (99%)	1 (1%)	76 85
40	j	89/91 (98%)	83 (93%)	6 (7%)	16 17
41	k	88/98 (90%)	78 (89%)	10 (11%)	5 5
42	l	104/106 (98%)	93 (89%)	11 (11%)	6 6
43	m	95/98 (97%)	92 (97%)	3 (3%)	39 47
44	n	81/82 (99%)	77 (95%)	4 (5%)	25 29
45	o	71/72 (99%)	66 (93%)	5 (7%)	15 15
46	p	63/77 (82%)	61 (97%)	2 (3%)	39 47
47	q	71/76 (93%)	63 (89%)	8 (11%)	6 5
48	r	46/66 (70%)	38 (83%)	8 (17%)	2 1
49	s	70/78 (90%)	68 (97%)	2 (3%)	42 52
50	t	65/67 (97%)	60 (92%)	5 (8%)	13 12
51	u	53/62 (86%)	50 (94%)	3 (6%)	20 22
All	All	4483/4756 (94%)	4240 (95%)	243 (5%)	26 25

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	1	MET
1	0	9	SER
1	0	33	LYS
1	0	38	LYS
2	1	41	SER
3	2	30	HIS
4	3	13	SER
4	3	15	LYS
4	3	28	SER
7	C	4	GLN
7	C	13	ARG
7	C	77	VAL
7	C	120	ASN
7	C	121	ASP
7	C	170	SER
7	C	194	GLU
7	C	198	GLN
7	C	269	ARG
7	C	270	ASP
7	C	272	ARG
7	C	273	VAL
8	D	58	GLU
8	D	59	SER
8	D	87	GLU
8	D	91	GLU
8	D	140	SER
8	D	186	GLU
9	E	1	MET
9	E	52	SER
9	E	114	GLN
9	E	121	GLU
9	E	125	VAL
9	E	198	GLU
10	F	25	VAL
10	F	30	ARG
10	F	69	LEU
10	F	83	TRP
10	F	96	MET
10	F	103	LEU
10	F	112	ARG
10	F	132	LEU
10	F	140	GLU
10	F	148	ARG

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Mol	Chain	Res	Type
10	F	170	MET
10	F	171	ARG
11	G	8	PRO
11	G	9	VAL
11	G	29	SER
11	G	44	LYS
11	G	46	GLU
11	G	59	LYS
11	G	69	ARG
11	G	73	ASN
11	G	84	GLU
11	G	107	LEU
11	G	110	SER
12	H	37	VAL
12	H	58	GLU
13	I	1	MET
13	I	73	LYS
13	I	78	THR
14	J	12	ASP
14	J	116	SER
14	J	120	GLU
15	K	29	VAL
15	K	131	LYS
15	K	143	LYS
16	L	1	MET
16	L	57	ARG
16	L	59	LYS
16	L	85	ASN
16	L	110	ASN
17	M	16	HIS
17	M	119	GLU
18	N	13	LYS
18	N	20	ARG
18	N	54	THR
18	N	79	GLU
19	O	28	THR
19	O	34	LYS
19	O	40	ARG
19	O	41	GLU
19	O	88	GLU
19	O	90	LYS
19	O	91	ARG

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Mol	Chain	Res	Type
19	O	92	ARG
21	Q	43	ASN
21	Q	71	LYS
21	Q	87	GLN
22	R	22	ASP
22	R	59	GLU
22	R	109	VAL
23	S	17	GLU
23	S	20	GLN
23	S	24	ASP
23	S	63	LYS
23	S	67	LYS
24	T	9	GLN
24	T	24	VAL
24	T	44	GLN
24	T	45	LYS
24	T	50	THR
24	T	58	THR
24	T	66	SER
24	T	87	ASP
25	U	57	SER
26	V	30	THR
27	W	28	ARG
28	X	4	LYS
28	X	29	ARG
29	Y	5	LYS
30	Z	49	ARG
32	b	9	ARG
32	b	23	ARG
32	b	25	TRP
32	b	39	LYS
32	b	43	ILE
32	b	65	LYS
32	b	88	ARG
32	b	141	ARG
32	b	145	LYS
32	b	148	ARG
32	b	150	LEU
32	b	169	ASP
32	b	199	ASP
32	b	202	ILE
32	b	227	LYS

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Mol	Chain	Res	Type
33	c	45	LYS
33	c	48	LYS
33	c	108	ARG
33	c	114	ARG
33	c	127	ARG
33	c	176	HIS
34	d	8	LYS
34	d	12	SER
34	d	17	THR
34	d	32	THR
34	d	49	LYS
34	d	106	ARG
34	d	167	ARG
34	d	179	LYS
34	d	193	LEU
35	e	40	ASP
35	e	60	SER
35	e	68	ARG
35	e	87	ARG
35	e	129	SER
35	e	148	SER
35	e	155	LYS
35	e	158	LYS
35	e	163	ILE
36	f	16	ASP
36	f	23	GLU
36	f	58	HIS
36	f	76	GLU
36	f	82	ASP
37	g	3	ARG
37	g	15	ASP
37	g	53	LYS
37	g	54	ASN
37	g	65	THR
37	g	67	GLU
37	g	72	MET
37	g	95	ARG
37	g	137	LYS
37	g	138	ARG
37	g	144	MET
38	h	10	MET
38	h	29	SER

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Mol	Chain	Res	Type
38	h	53	GLN
38	h	74	GLU
38	h	75	MET
38	h	107	THR
38	h	112	MET
38	h	115	ARG
39	i	128	ARG
40	j	7	ARG
40	j	42	MET
40	j	54	SER
40	j	62	ARG
40	j	88	MET
40	j	97	ASP
41	k	25	SER
41	k	29	THR
41	k	45	THR
41	k	54	SER
41	k	63	GLN
41	k	79	LYS
41	k	81	LEU
41	k	86	LYS
41	k	110	THR
41	k	128	VAL
42	l	13	THR
42	l	15	LEU
42	l	34	CYS
42	l	51	LYS
42	l	62	GLU
42	l	64	SER
42	l	83	ARG
42	l	86	ARG
42	l	89	ASP
42	l	111	ASN
42	l	121	ARG
43	m	3	ARG
43	m	68	ASP
43	m	78	LYS
44	n	37	SER
44	n	41	ARG
44	n	43	GLU
44	n	85	ARG
45	o	4	THR

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Mol	Chain	Res	Type
45	o	7	ASP
45	o	44	LYS
45	o	62	GLN
45	o	74	ASP
46	p	53	ARG
46	p	81	GLN
47	q	12	LYS
47	q	20	LYS
47	q	24	VAL
47	q	38	SER
47	q	40	ARG
47	q	41	ARG
47	q	42	SER
47	q	53	VAL
48	r	22	ASP
48	r	25	ASP
48	r	27	ASP
48	r	30	LYS
48	r	36	ASN
48	r	43	ARG
48	r	48	LYS
48	r	66	SER
49	s	12	ASP
49	s	28	ARG
50	t	23	SER
50	t	27	MET
50	t	37	SER
50	t	49	GLU
50	t	77	SER
51	u	21	ARG
51	u	28	VAL
51	u	63	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
10	F	135	GLN
19	O	44	GLN
33	c	25	ASN
33	c	28	GLN
34	d	36	ASN
41	k	118	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1524/1544 (98%)	184 (12%)	0
5	A	2708/2918 (92%)	330 (12%)	14 (0%)
6	B	114/115 (99%)	14 (12%)	1 (0%)
All	All	4346/4577 (94%)	528 (12%)	15 (0%)

All (528) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	13	A
5	A	22	G
5	A	41	U
5	A	42	G
5	A	53	G
5	A	58	G
5	A	67	G
5	A	68	A
5	A	70	A
5	A	78	A
5	A	81	A
5	A	82	G
5	A	99	A
5	A	104	C
5	A	109	G
5	A	125	A
5	A	126	A
5	A	127	U
5	A	138	A
5	A	149	G
5	A	203	A
5	A	206	A
5	A	222	G
5	A	223	A
5	A	228	A
5	A	229	A
5	A	235	U
5	A	236	U
5	A	240	A
5	A	255	G
5	A	257	G
5	A	262	A
5	A	272	A

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Mol	Chain	Res	Type
5	A	278	U
5	A	279	U
5	A	297	G
5	A	313	A
5	A	331	G
5	A	332	A
5	A	357	C
5	A	360	A
5	A	361	A
5	A	365	U
5	A	366	G
5	A	369	G
5	A	370	A
5	A	371	G
5	A	385	G
5	A	395	G
5	A	403	A
5	A	410	G
5	A	423	G
5	A	455	C
5	A	480	G
5	A	493	G
5	A	504	A
5	A	508	C
5	A	529	G
5	A	531	A
5	A	532	G
5	A	544	U
5	A	546	G
5	A	561	A
5	A	571	U
5	A	573	A
5	A	601	A
5	A	611	U
5	A	612	A
5	A	625	A
5	A	633	C
5	A	635	A
5	A	643	U
5	A	644	A
5	A	651	U
5	A	684	U

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Mol	Chain	Res	Type
5	A	712	U
5	A	714	A
5	A	715	C
5	A	728	A
5	A	745	U
5	A	762	A
5	A	773	G
5	A	774	G
5	A	780	A
5	A	782	G
5	A	783	G
5	A	803	G
5	A	810	C
5	A	817	A
5	A	825	U
5	A	826	U
5	A	845	A
5	A	846	U
5	A	857	G
5	A	864	A
5	A	900	C
5	A	905	G
5	A	908	A
5	A	918	A
5	A	929	C
5	A	938	A
5	A	942	A
5	A	943	G
5	A	958	C
5	A	971	G
5	A	980	A
5	A	993	A
5	A	1009	U
5	A	1010	C
5	A	1014	G
5	A	1019	G
5	A	1023	G
5	A	1030	U
5	A	1031	G
5	A	1043	A
5	A	1051	A
5	A	1103	A

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Mol	Chain	Res	Type
5	A	1105	U
5	A	1106	C
5	A	1108	A
5	A	1109	G
5	A	1128	G
5	A	1129	U
5	A	1130	A
5	A	1132	C
5	A	1133	G
5	A	1140	A
5	A	1168	A
5	A	1170	U
5	A	1173	G
5	A	1174	U
5	A	1201	G
5	A	1243	G
5	A	1245	G
5	A	1248	A
5	A	1251	G
5	A	1266	G
5	A	1267	A
5	A	1296	A
5	A	1316	A
5	A	1324	U
5	A	1347	U
5	A	1360	A
5	A	1374	U
5	A	1378	A
5	A	1411	G
5	A	1415	U
5	A	1416	G
5	A	1423	C
5	A	1428	A
5	A	1432	C
5	A	1433	U
5	A	1441	C
5	A	1447	G
5	A	1448	U
5	A	1454	G
5	A	1462	G
5	A	1477	U
5	A	1485	A

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Mol	Chain	Res	Type
5	A	1486	G
5	A	1488	C
5	A	1489	A
5	A	1490	A
5	A	1492	U
5	A	1507	G
5	A	1511	A
5	A	1519	U
5	A	1520	A
5	A	1527	U
5	A	1528	G
5	A	1529	U
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1534	G
5	A	1538	A
5	A	1539	G
5	A	1540	C
5	A	1543	A
5	A	1544	G
5	A	1552	U
5	A	1557	U
5	A	1564	A
5	A	1567	A
5	A	1576	U
5	A	1580	C
5	A	1581	U
5	A	1582	U
5	A	1583	C
5	A	1588	A
5	A	1605	G
5	A	1606	A
5	A	1607	A
5	A	1616	A
5	A	1632	U
5	A	1645	U
5	A	1646	U
5	A	1647	G
5	A	1672	G
5	A	1720	G

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Mol	Chain	Res	Type
5	A	1724	C
5	A	1725	U
5	A	1726	C
5	A	1727	G
5	A	1746	G
5	A	1760	G
5	A	1769	A
5	A	1776	A
5	A	1796	C
5	A	1797	A
5	A	1807	G
5	A	1812	C
5	A	1825	A
5	A	1844	A
5	A	1862	A
5	A	1872	A
5	A	1875	C
5	A	1897	A
5	A	1902	G
5	A	1923	A
5	A	1925	G
5	A	1926	G
5	A	1932	A
5	A	1951	U
5	A	1959	U
5	A	1963	C
5	A	1966	A
5	A	1967	U
5	A	1968	G
5	A	1987	U
5	A	1989	U
5	A	2018	U
5	A	2019	C
5	A	2027	A
5	A	2029	A
5	A	2039	C
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2058	A
5	A	2065	7MG

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Mol	Chain	Res	Type
5	A	2194	A
5	A	2199	U
5	A	2200	G
5	A	2207	G
5	A	2221	A
5	A	2234	G
5	A	2235	G
5	A	2275	G
5	A	2279	U
5	A	2283	A
5	A	2284	A
5	A	2299	G
5	A	2301	U
5	A	2303	G
5	A	2304	G
5	A	2305	A
5	A	2316	A
5	A	2318	A
5	A	2321	A
5	A	2323	A
5	A	2341	A
5	A	2343	C
5	A	2346	C
5	A	2378	G
5	A	2379	G
5	A	2380	U
5	A	2381	C
5	A	2399	C
5	A	2402	U
5	A	2418	C
5	A	2421	A
5	A	2425	G
5	A	2426	A
5	A	2430	A
5	A	2431	A
5	A	2437	U
5	A	2444	A
5	A	2469	U
5	A	2471	C
5	A	2472	A
5	A	2474	A
5	A	2498	G

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Mol	Chain	Res	Type
5	A	2500	PSU
5	A	2503	C
5	A	2514	A
5	A	2525	G
5	A	2543	A
5	A	2550	U
5	A	2562	A
5	A	2563	G
5	A	2578	G
5	A	2598	A
5	A	2599	G
5	A	2605	U
5	A	2609	U
5	A	2625	U
5	A	2642	C
5	A	2650	A
5	A	2661	A
5	A	2685	U
5	A	2686	A
5	A	2687	C
5	A	2710	G
5	A	2722	U
5	A	2729	A
5	A	2744	A
5	A	2754	A
5	A	2761	A
5	A	2762	G
5	A	2774	A
5	A	2776	A
5	A	2793	U
5	A	2796	U
5	A	2797	G
5	A	2816	G
5	A	2817	A
5	A	2830	G
5	A	2831	A
5	A	2832	U
5	A	2845	G
5	A	2852	A
5	A	2863	A
5	A	2868	G
5	A	2869	A

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Mol	Chain	Res	Type
5	A	2876	C
5	A	2880	U
5	A	2898	U
6	B	2	C
6	B	28	C
6	B	32	A
6	B	35	C
6	B	39	C
6	B	40	C
6	B	44	A
6	B	54	G
6	B	64	A
6	B	65	G
6	B	71	A
6	B	87	A
6	B	106	A
6	B	115	U
31	a	6	C
31	a	7	U
31	a	9	A
31	a	11	G
31	a	34	A
31	a	41	G
31	a	49	C
31	a	50	U
31	a	53	A
31	a	62	A
31	a	66	G
31	a	76	A
31	a	77	G
31	a	81	G
31	a	82	C
31	a	83	U
31	a	84	U
31	a	85	G
31	a	89	C
31	a	91	G
31	a	92	G
31	a	97	A
31	a	117	U
31	a	127	U
31	a	159	G

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Mol	Chain	Res	Type
31	a	163	U
31	a	184	A
31	a	186	G
31	a	193	A
31	a	205	U
31	a	208	G
31	a	216	G
31	a	239	A
31	a	241	U
31	a	243	G
31	a	247	G
31	a	262	G
31	a	263	C
31	a	276	C
31	a	285	G
31	a	302	A
31	a	324	C
31	a	325	A
31	a	343	G
31	a	348	C
31	a	350	G
31	a	363	U
31	a	368	C
31	a	380	C
31	a	393	A
31	a	402	G
31	a	407	A
31	a	409	G
31	a	410	A
31	a	418	A
31	a	419	U
31	a	420	G
31	a	425	U
31	a	426	A
31	a	444	A
31	a	447	A
31	a	461	A
31	a	463	U
31	a	480	C
31	a	481	G
31	a	483	U
31	a	492	A

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Mol	Chain	Res	Type
31	a	493	A
31	a	494	U
31	a	496	A
31	a	502	G
31	a	506	A
31	a	508	C
31	a	515	C
31	a	518	G
31	a	527	G
31	a	528	U
31	a	530	A
31	a	544	A
31	a	556	A
31	a	561	C
31	a	569	A
31	a	570	A
31	a	573	C
31	a	574	G
31	a	630	G
31	a	639	A
31	a	650	A
31	a	662	A
31	a	680	G
31	a	684	A
31	a	700	G
31	a	720	U
31	a	721	G
31	a	752	G
31	a	774	A
31	a	784	A
31	a	789	A
31	a	790	U
31	a	791	A
31	a	812	A
31	a	814	C
31	a	838	U
31	a	840	U
31	a	841	G
31	a	846	U
31	a	887	G
31	a	888	U
31	a	911	A

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Mol	Chain	Res	Type
31	a	923	G
31	a	924	G
31	a	931	C
31	a	932	A
31	a	939	G
31	a	957	U
31	a	966	A
31	a	968	G
31	a	972	A
31	a	973	G
31	a	974	A
31	a	989	U
31	a	990	G
31	a	1001	A
31	a	1007	U
31	a	1027	U
31	a	1028	C
31	a	1029	G
31	a	1030	G
31	a	1032	A
31	a	1033	A
31	a	1043	A
31	a	1062	U
31	a	1067	U
31	a	1070	U
31	a	1078	G
31	a	1082	U
31	a	1090	A
31	a	1091	G
31	a	1092	U
31	a	1098	A
31	a	1134	C
31	a	1136	G
31	a	1151	G
31	a	1156	U
31	a	1164	A
31	a	1165	C
31	a	1166	A
31	a	1168	A
31	a	1179	G
31	a	1180	C
31	a	1193	A

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Mol	Chain	Res	Type
31	a	1194	A
31	a	1210	A
31	a	1224	A
31	a	1235	A
31	a	1255	G
31	a	1277	A
31	a	1284	A
31	a	1297	G
31	a	1299	C
31	a	1302	G
31	a	1309	G
31	a	1317	C
31	a	1342	U
31	a	1350	G
31	a	1360	A
31	a	1361	U
31	a	1367	G
31	a	1378	U
31	a	1394	C
31	a	1395	A
31	a	1416	G
31	a	1438	A
31	a	1443	A
31	a	1449	A
31	a	1450	A
31	a	1484	G
31	a	1491	G
31	a	1494	G
31	a	1500	A
31	a	1503	U
31	a	1514	G
31	a	1526	G
31	a	1527	G

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	41	U
5	A	256	C
5	A	364	A
5	A	365	U
5	A	368	C

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Mol	Chain	Res	Type
5	A	424	G
5	A	507	U
5	A	782	G
5	A	844	A
5	A	1127	U
5	A	1173	G
5	A	1179	G
5	A	2379	G
5	A	2443	G
6	B	86	U

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

21 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	$\#\|Z\| > 2$
5	PSU	A	2601	5	18,21,22	1.04	1 (5%)	22,30,33	1.80	4 (18%)
5	OMG	A	2247	5	18,26,27	1.16	2 (11%)	19,38,41	0.86	1 (5%)
5	PSU	A	2453	5	18,21,22	1.04	1 (5%)	22,30,33	1.84	5 (22%)
31	UR3	a	1495	31	19,22,23	2.87	7 (36%)	26,32,35	1.28	1 (3%)
31	2MG	a	1204	31	18,26,27	1.16	2 (11%)	16,38,41	0.88	1 (6%)
31	2MG	a	963	31	18,26,27	1.13	2 (11%)	16,38,41	0.91	1 (6%)
31	MA6	a	1516	31	18,26,27	1.03	2 (11%)	19,38,41	3.46	2 (10%)
31	4OC	a	1399	31	20,23,24	3.11	8 (40%)	26,32,35	0.88	1 (3%)
5	2MG	A	2441	5	18,26,27	1.20	2 (11%)	16,38,41	0.84	1 (6%)
5	5MU	A	1935	5	19,22,23	0.50	0	28,32,35	0.51	0
5	OMU	A	2548	5	19,22,23	2.97	8 (42%)	26,31,34	1.71	5 (19%)
31	MA6	a	1515	31	18,26,27	1.03	2 (11%)	19,38,41	3.41	2 (10%)
31	5MC	a	964	31	18,22,23	0.55	0	26,32,35	0.54	0
5	PSU	A	952	5	18,21,22	1.02	1 (5%)	22,30,33	1.82	4 (18%)
5	6MZ	A	2026	5	18,25,26	1.89	3 (16%)	16,36,39	3.38	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PSU	A	2500	5	18,21,22	1.08	1 (5%)	22,30,33	1.77	4 (18%)
31	7MG	a	524	31	22,26,27	1.22	1 (4%)	29,39,42	0.81	1 (3%)
5	PSU	A	2576	5	18,21,22	1.09	2 (11%)	22,30,33	1.87	6 (27%)
31	PSU	a	513	31	18,21,22	1.08	1 (5%)	22,30,33	1.80	5 (22%)
5	7MG	A	2065	5	22,26,27	1.15	1 (4%)	29,39,42	0.84	1 (3%)
5	2MA	A	2499	5	17,25,26	2.50	5 (29%)	17,37,40	1.41	3 (17%)

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
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
5	OMG	A	2247	5	-	1/5/27/28	0/3/3/3
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2
31	2MG	a	1204	31	-	0/5/27/28	0/3/3/3
31	2MG	a	963	31	-	0/5/27/28	0/3/3/3
31	MA6	a	1516	31	-	0/7/29/30	0/3/3/3
31	4OC	a	1399	31	-	2/9/29/30	0/2/2/2
5	2MG	A	2441	5	-	2/5/27/28	0/3/3/3
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
5	OMU	A	2548	5	-	0/9/27/28	0/2/2/2
31	MA6	a	1515	31	-	0/7/29/30	0/3/3/3
31	5MC	a	964	31	-	0/7/25/26	0/2/2/2
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
5	6MZ	A	2026	5	-	2/5/27/28	0/3/3/3
5	PSU	A	2500	5	-	2/7/25/26	0/2/2/2
31	7MG	a	524	31	-	1/7/37/38	0/3/3/3
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
31	PSU	a	513	31	-	0/7/25/26	0/2/2/2
5	7MG	A	2065	5	-	1/7/37/38	0/3/3/3
5	2MA	A	2499	5	-	2/3/25/26	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2499	2MA	C2-N3	7.20	1.46	1.31
31	a	1495	UR3	C2-N1	6.86	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2548	OMU	C2-N1	6.78	1.49	1.38
31	a	1495	UR3	C6-C5	6.74	1.50	1.35
31	a	1399	4OC	C4-N3	6.71	1.44	1.32
5	A	2548	OMU	C2-N3	6.54	1.49	1.38
5	A	2026	6MZ	C6-N6	6.49	1.45	1.35
31	a	1399	4OC	C6-C5	6.22	1.49	1.35
31	a	1399	4OC	C2-N3	6.06	1.48	1.36
31	a	1495	UR3	C2-N3	5.71	1.50	1.39
5	A	2548	OMU	C6-C5	5.64	1.48	1.35
5	A	2499	2MA	C4-N3	5.11	1.49	1.37
31	a	524	7MG	C5-N7	5.10	1.41	1.35
31	a	1399	4OC	C4-N4	4.77	1.45	1.35
5	A	2065	7MG	C5-N7	4.76	1.41	1.35
31	a	1399	4OC	C2-N1	4.11	1.48	1.40
5	A	2548	OMU	C4-N3	4.00	1.45	1.38
31	a	1399	4OC	C5-C4	3.77	1.48	1.40
5	A	2500	PSU	C6-C5	3.45	1.39	1.35
31	a	513	PSU	C6-C5	3.44	1.39	1.35
31	a	1495	UR3	C6-N1	3.38	1.46	1.38
5	A	2576	PSU	C6-C5	3.29	1.39	1.35
5	A	2601	PSU	C6-C5	3.28	1.39	1.35
31	a	1399	4OC	C6-N1	3.22	1.45	1.38
5	A	2453	PSU	C6-C5	3.21	1.39	1.35
5	A	2441	2MG	C8-N7	-3.12	1.29	1.35
5	A	952	PSU	C6-C5	3.08	1.38	1.35
5	A	2548	OMU	O4-C4	-3.06	1.18	1.24
5	A	2247	OMG	C8-N7	-3.01	1.29	1.35
31	a	1204	2MG	C8-N7	-2.97	1.30	1.35
5	A	2499	2MA	C6-N1	2.95	1.44	1.38
31	a	963	2MG	C8-N7	-2.88	1.30	1.35
5	A	2548	OMU	C6-N1	2.84	1.44	1.38
5	A	2499	2MA	C5-C4	-2.78	1.36	1.43
31	a	1399	4OC	O2-C2	-2.77	1.18	1.23
5	A	2026	6MZ	C5-C4	-2.73	1.33	1.40
31	a	1515	MA6	C5-C4	-2.68	1.33	1.40
31	a	1516	MA6	C5-C4	-2.67	1.33	1.40
5	A	2548	OMU	O2-C2	-2.55	1.18	1.23
5	A	2499	2MA	C2-N1	2.50	1.44	1.36
31	a	1515	MA6	C2-N3	2.50	1.36	1.32
5	A	2441	2MG	C5-C6	-2.42	1.42	1.47
5	A	2026	6MZ	C2-N3	2.42	1.36	1.32
5	A	2247	OMG	C5-C6	-2.41	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	1516	MA6	C2-N3	2.41	1.36	1.32
31	a	1204	2MG	C5-C6	-2.38	1.42	1.47
5	A	2548	OMU	C5-C4	2.33	1.48	1.43
31	a	963	2MG	C5-C6	-2.28	1.42	1.47
31	a	1495	UR3	C5-C4	2.23	1.49	1.43
31	a	1495	UR3	C4-N3	2.20	1.45	1.40
5	A	2576	PSU	O4'-C1'	-2.04	1.41	1.43
31	a	1495	UR3	O2-C2	-2.03	1.18	1.22

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1516	MA6	N1-C6-N6	-13.81	102.53	117.06
31	a	1515	MA6	N1-C6-N6	-13.59	102.76	117.06
5	A	2026	6MZ	C1'-N9-C4	-12.05	105.47	126.64
31	a	1516	MA6	N3-C2-N1	-5.51	120.06	128.68
31	a	1515	MA6	N3-C2-N1	-5.51	120.06	128.68
5	A	2548	OMU	C4-N3-C2	-5.32	119.56	126.58
5	A	2026	6MZ	N3-C2-N1	-5.05	120.79	128.68
31	a	1495	UR3	C4-N3-C2	-4.73	120.11	124.56
5	A	2576	PSU	N1-C2-N3	4.73	120.49	115.13
5	A	2453	PSU	N1-C2-N3	4.73	120.48	115.13
5	A	952	PSU	C4-N3-C2	-4.72	119.54	126.34
5	A	2601	PSU	C4-N3-C2	-4.67	119.61	126.34
5	A	952	PSU	N1-C2-N3	4.67	120.42	115.13
5	A	2453	PSU	C4-N3-C2	-4.63	119.67	126.34
5	A	2601	PSU	N1-C2-N3	4.61	120.36	115.13
31	a	513	PSU	N1-C2-N3	4.58	120.32	115.13
5	A	2500	PSU	C4-N3-C2	-4.57	119.75	126.34
5	A	2500	PSU	N1-C2-N3	4.53	120.26	115.13
31	a	513	PSU	C4-N3-C2	-4.48	119.88	126.34
5	A	2576	PSU	C4-N3-C2	-4.48	119.89	126.34
5	A	2548	OMU	N3-C2-N1	3.85	120.00	114.89
5	A	2499	2MA	C5-C6-N1	3.67	120.35	114.02
5	A	2548	OMU	C5-C4-N3	3.46	120.01	114.84
5	A	2499	2MA	C8-N7-C5	3.01	108.72	102.99
5	A	2548	OMU	O4-C4-C5	-2.81	120.22	125.16
5	A	2453	PSU	O2-C2-N1	-2.79	119.72	122.79
5	A	952	PSU	O2-C2-N1	-2.68	119.84	122.79
5	A	2500	PSU	O2-C2-N1	-2.64	119.88	122.79
31	a	513	PSU	O2-C2-N1	-2.60	119.93	122.79
5	A	2576	PSU	O2-C2-N1	-2.57	119.96	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2576	PSU	O4'-C1'-C2'	2.55	108.75	105.14
5	A	2026	6MZ	C2-N1-C6	2.50	118.73	116.59
5	A	2247	OMG	O6-C6-C5	2.47	129.20	124.37
5	A	2576	PSU	C6-N1-C2	-2.47	120.16	122.68
31	a	513	PSU	C6-N1-C2	-2.41	120.22	122.68
5	A	2065	7MG	C5-C4-N9	2.33	109.38	106.35
5	A	2453	PSU	C6-N1-C2	-2.32	120.31	122.68
5	A	2601	PSU	O2-C2-N1	-2.30	120.26	122.79
5	A	952	PSU	C6-N1-C2	-2.28	120.35	122.68
31	a	513	PSU	O4'-C1'-C2'	2.26	108.34	105.14
31	a	963	2MG	O6-C6-C5	2.26	128.78	124.37
5	A	2548	OMU	O2-C2-N1	-2.24	119.81	122.79
31	a	1399	4OC	C6-C5-C4	2.24	119.70	116.96
5	A	2441	2MG	O6-C6-C5	2.23	128.73	124.37
5	A	2500	PSU	C6-N1-C2	-2.21	120.42	122.68
31	a	524	7MG	C5-C4-N9	2.19	109.19	106.35
5	A	2601	PSU	C6-N1-C2	-2.18	120.45	122.68
5	A	2576	PSU	C6-C5-C4	2.16	119.71	118.20
31	a	1204	2MG	O6-C6-C5	2.15	128.56	124.37
5	A	2453	PSU	O4'-C1'-C2'	2.10	108.10	105.14
5	A	2499	2MA	CM2-C2-N1	2.09	120.87	116.23

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2026	6MZ	O4'-C4'-C5'-O5'
5	A	2499	2MA	O4'-C4'-C5'-O5'
5	A	2026	6MZ	C3'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
5	A	2441	2MG	C3'-C4'-C5'-O5'
5	A	2500	PSU	O4'-C4'-C5'-O5'
31	a	1399	4OC	O4'-C4'-C5'-O5'
31	a	524	7MG	C3'-C4'-C5'-O5'
5	A	2500	PSU	C3'-C4'-C5'-O5'
5	A	2247	OMG	C1'-C2'-O2'-CM2
5	A	2441	2MG	O4'-C4'-C5'-O5'
31	a	1399	4OC	C3'-C4'-C5'-O5'
5	A	2065	7MG	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
53	OI9	W	101	-	34,37,37	1.42	6 (17%)	38,52,52	1.87	6 (15%)

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
53	OI9	W	101	-	-	4/22/67/67	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	W	101	OI9	C28-N13	3.92	1.40	1.33
53	W	101	OI9	C27-C24	3.16	1.55	1.52
53	W	101	OI9	C27-N13	3.13	1.49	1.46
53	W	101	OI9	C24-C22	-3.02	1.50	1.53
53	W	101	OI9	C29-N11	2.32	1.39	1.34
53	W	101	OI9	C32-N15	2.19	1.37	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	W	101	OI9	C24-C27-N13	6.52	116.59	109.83
53	W	101	OI9	C22-N10-C25	-4.92	107.84	112.56
53	W	101	OI9	C22-C23-N12	4.33	108.69	104.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	W	101	OI9	C30-C29-N11	-3.22	112.11	116.33
53	W	101	OI9	C22-C23-C28	-3.13	105.00	116.61
53	W	101	OI9	O06-C28-N13	2.46	125.80	122.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

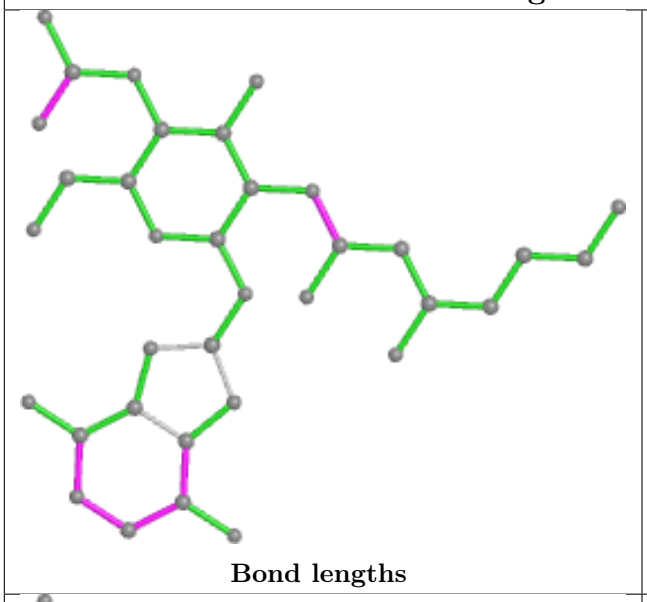
Mol	Chain	Res	Type	Atoms
53	W	101	OI9	C18-C20-O02-C32
53	W	101	OI9	C21-C20-O02-C32
53	W	101	OI9	N15-C32-O02-C20
53	W	101	OI9	O08-C32-O02-C20

There are no ring outliers.

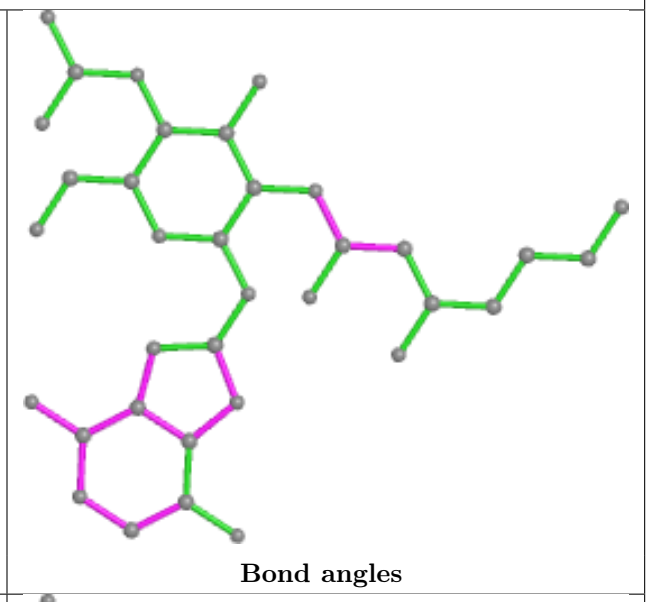
No monomer is involved in short contacts.

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.

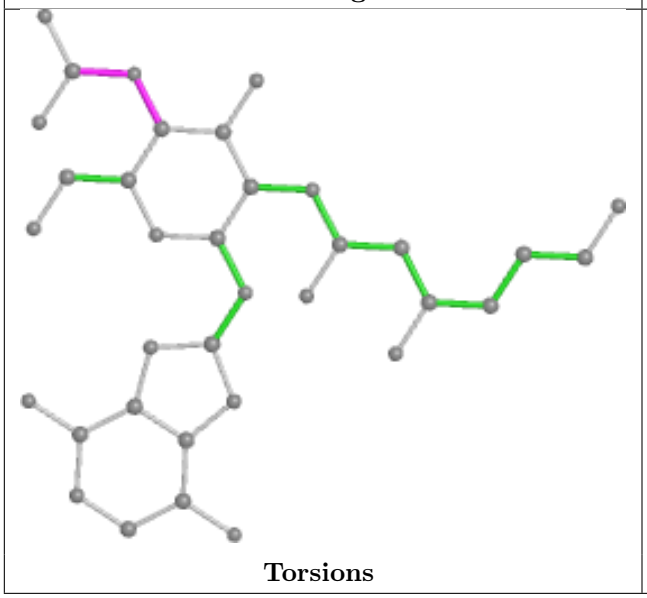
Ligand OI9 W 101



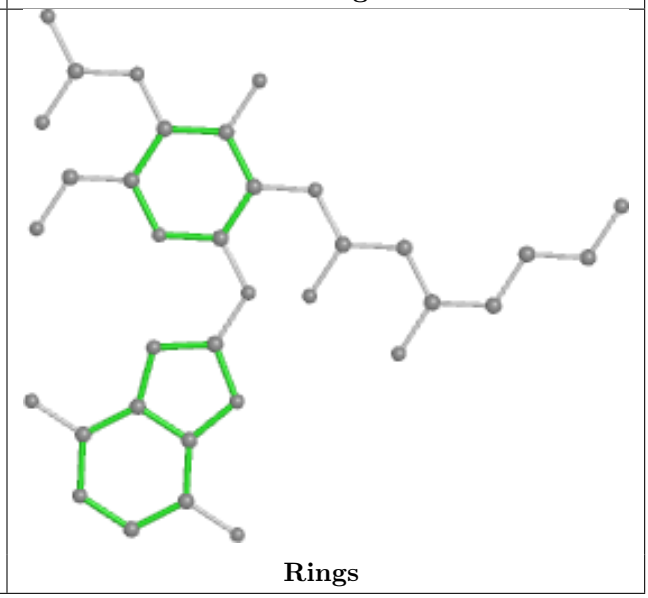
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

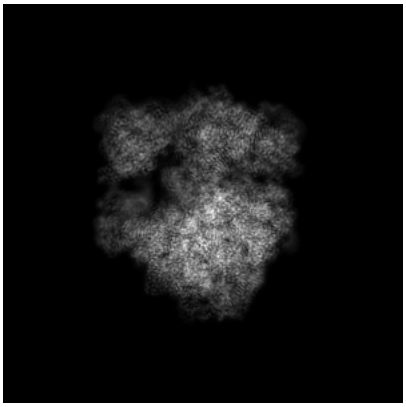
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26819. These allow visual inspection of the internal detail of the map and identification of artifacts.

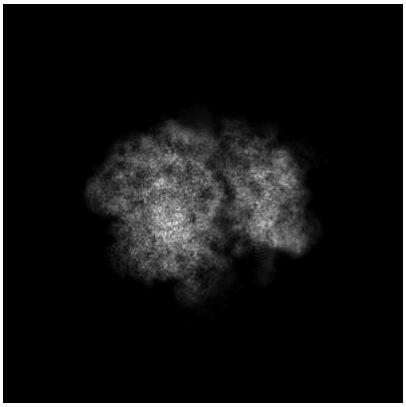
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

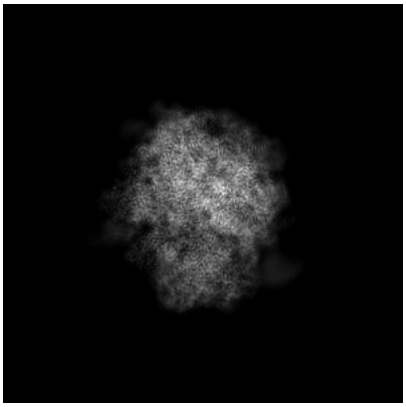
6.1.1 Primary map



X



Y



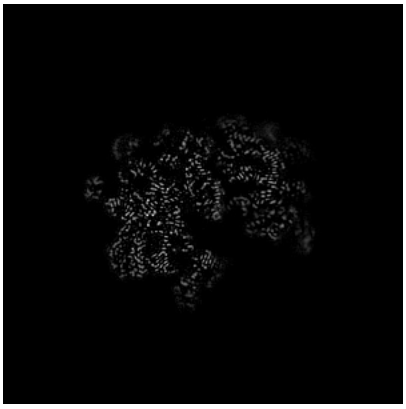
Z

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

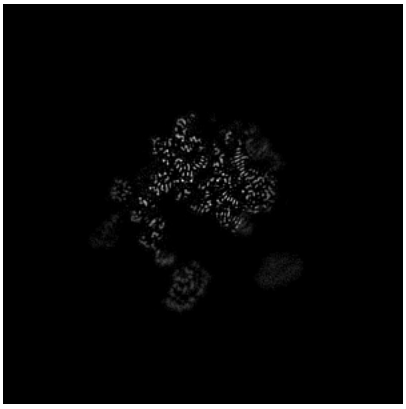
6.2 Central slices

6.2.1 Primary map

X Index: 256



Y Index: 256

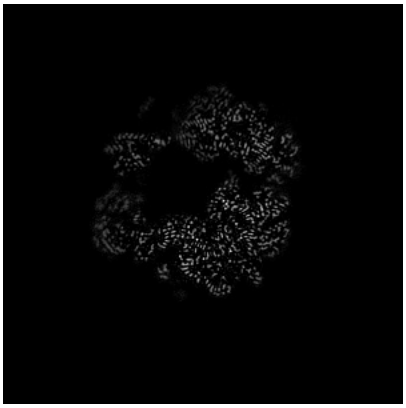


Z Index: 256

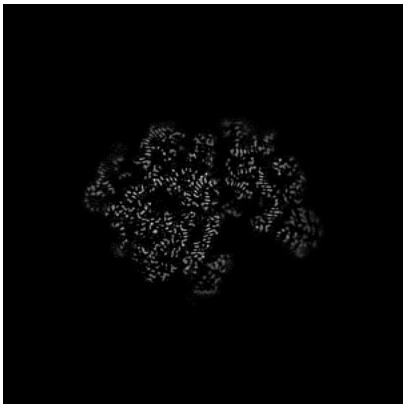
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

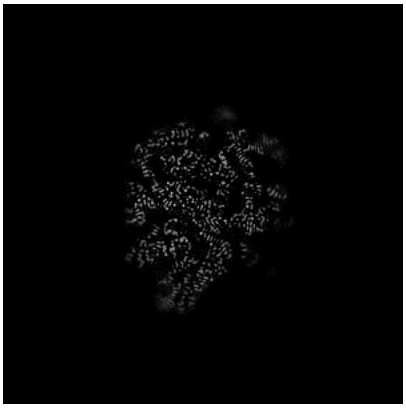
6.3.1 Primary map



X Index: 229



Y Index: 276

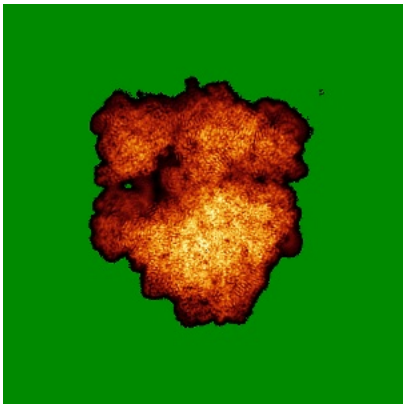


Z Index: 208

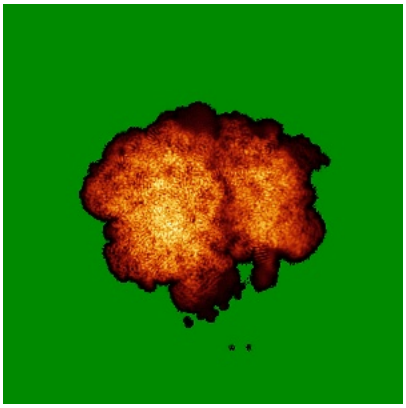
The images above show the largest variance slices of the map in three orthogonal directions.

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

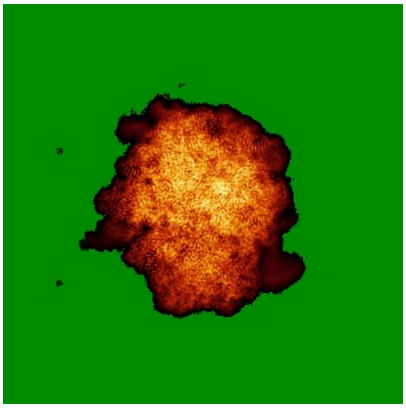
6.4.1 Primary map



X



Y



Z

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 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

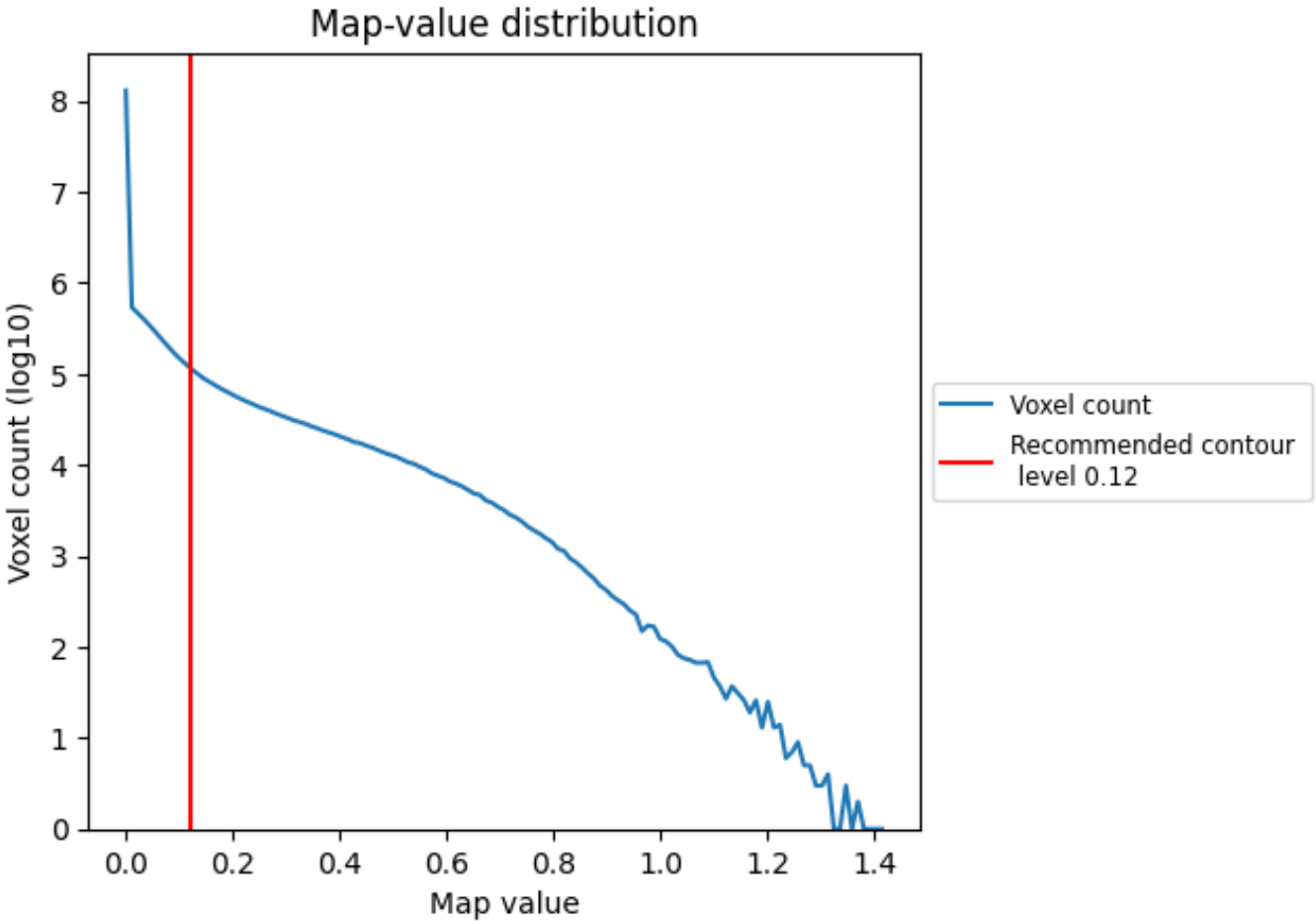
6.6 Mask visualisation (i)

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

7 Map analysis

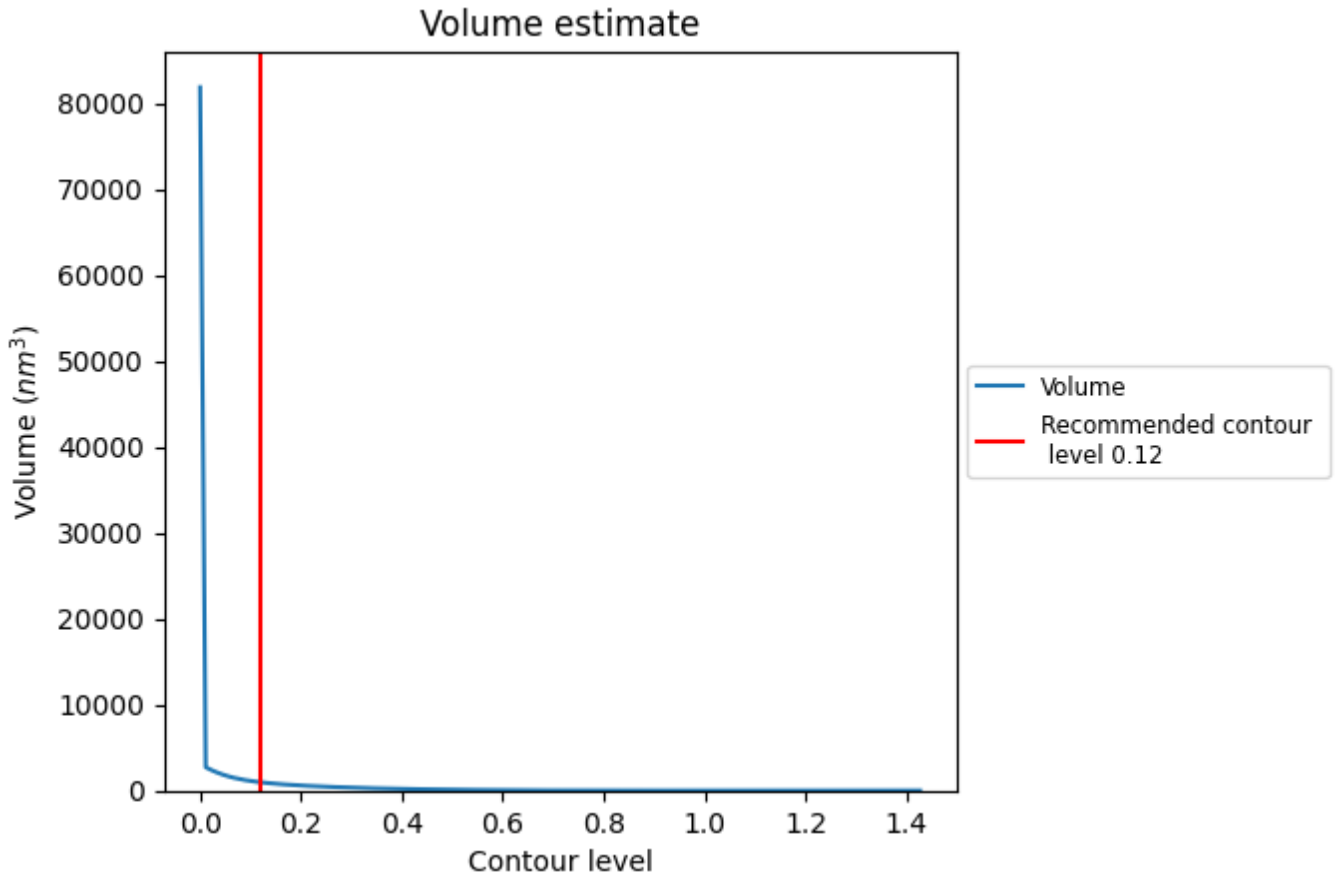
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

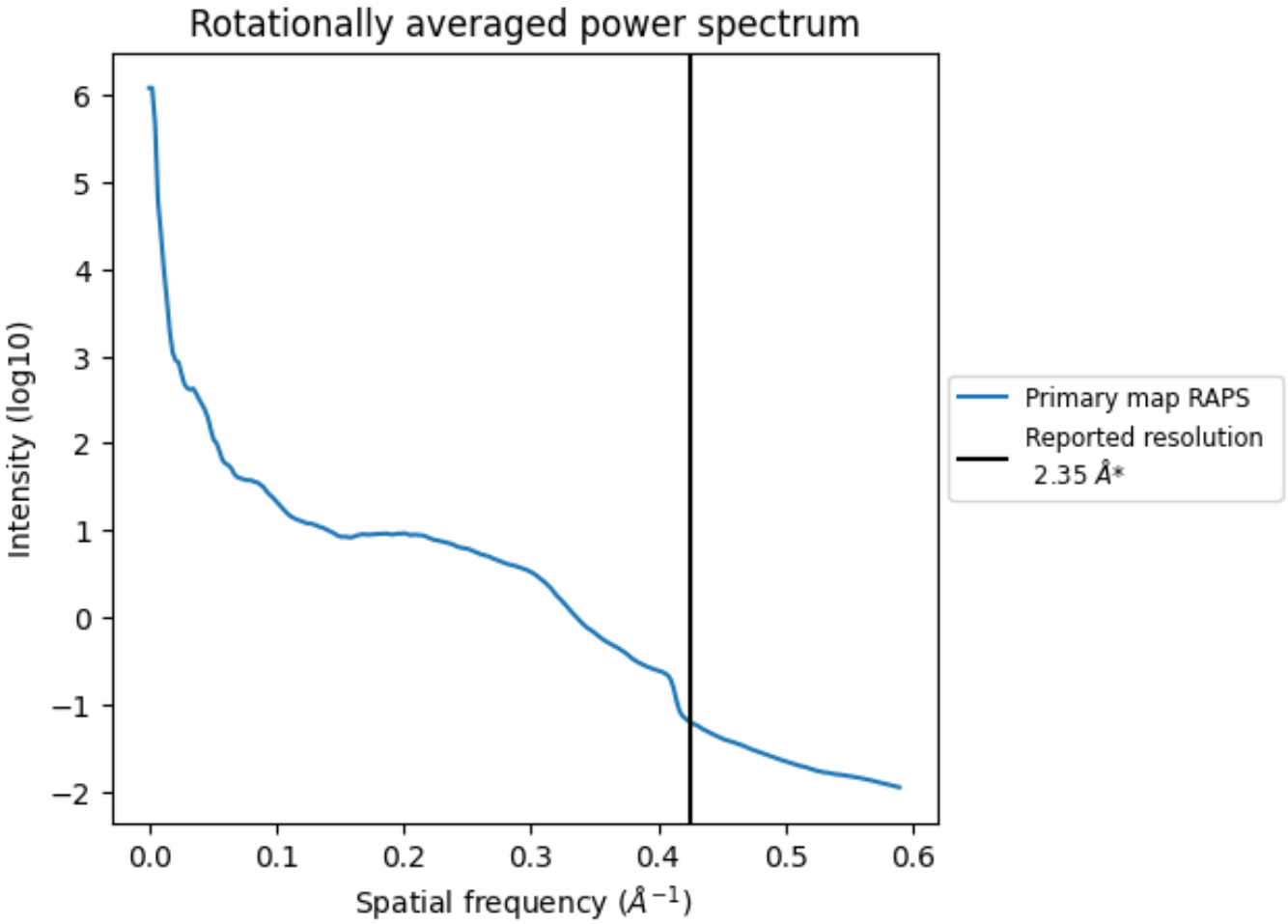
7.2 Volume estimate



The volume at the recommended contour level is 963 nm^3; this corresponds to an approximate mass of 870 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 0.426 Å^{-1}

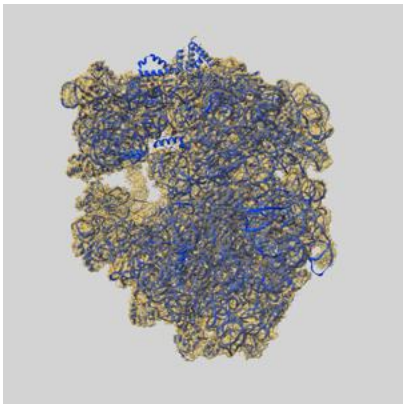
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

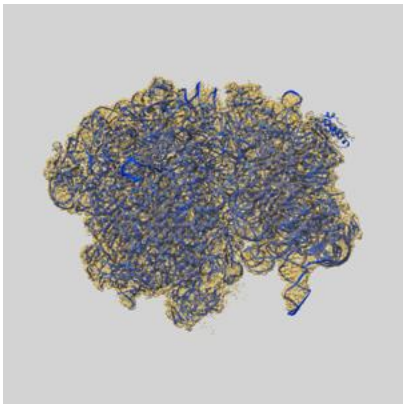
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26819 and PDB model 7UVX. Per-residue inclusion information can be found in section 3 on page 14.

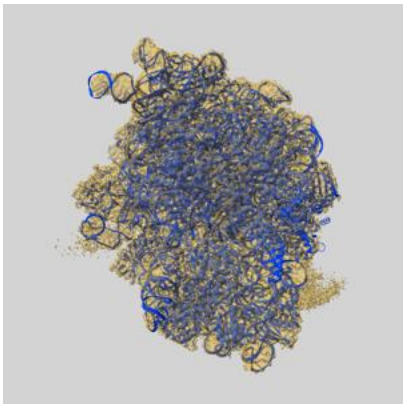
9.1 Map-model overlay



X



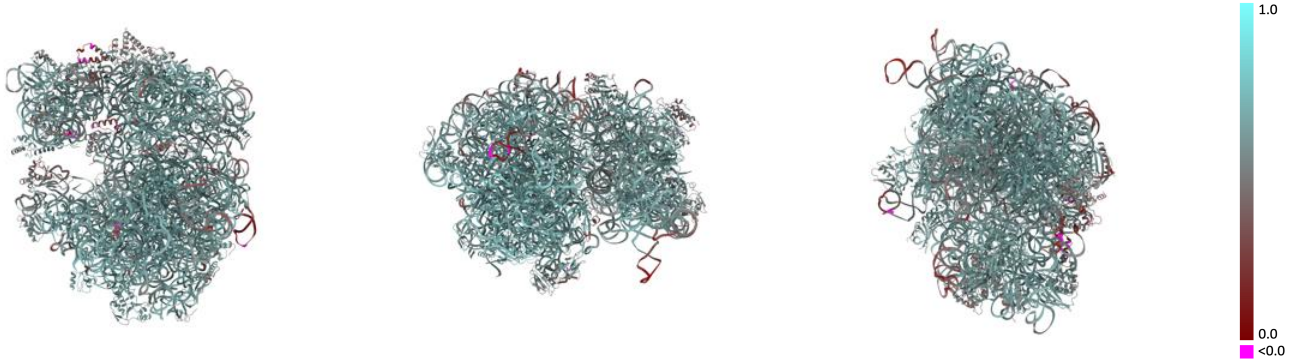
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

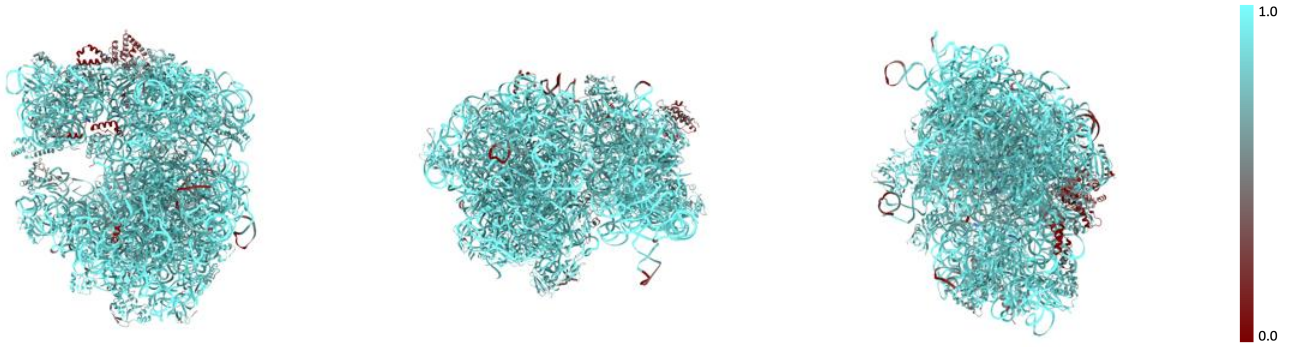
9.2 Q-score mapped to coordinate model (i)



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.

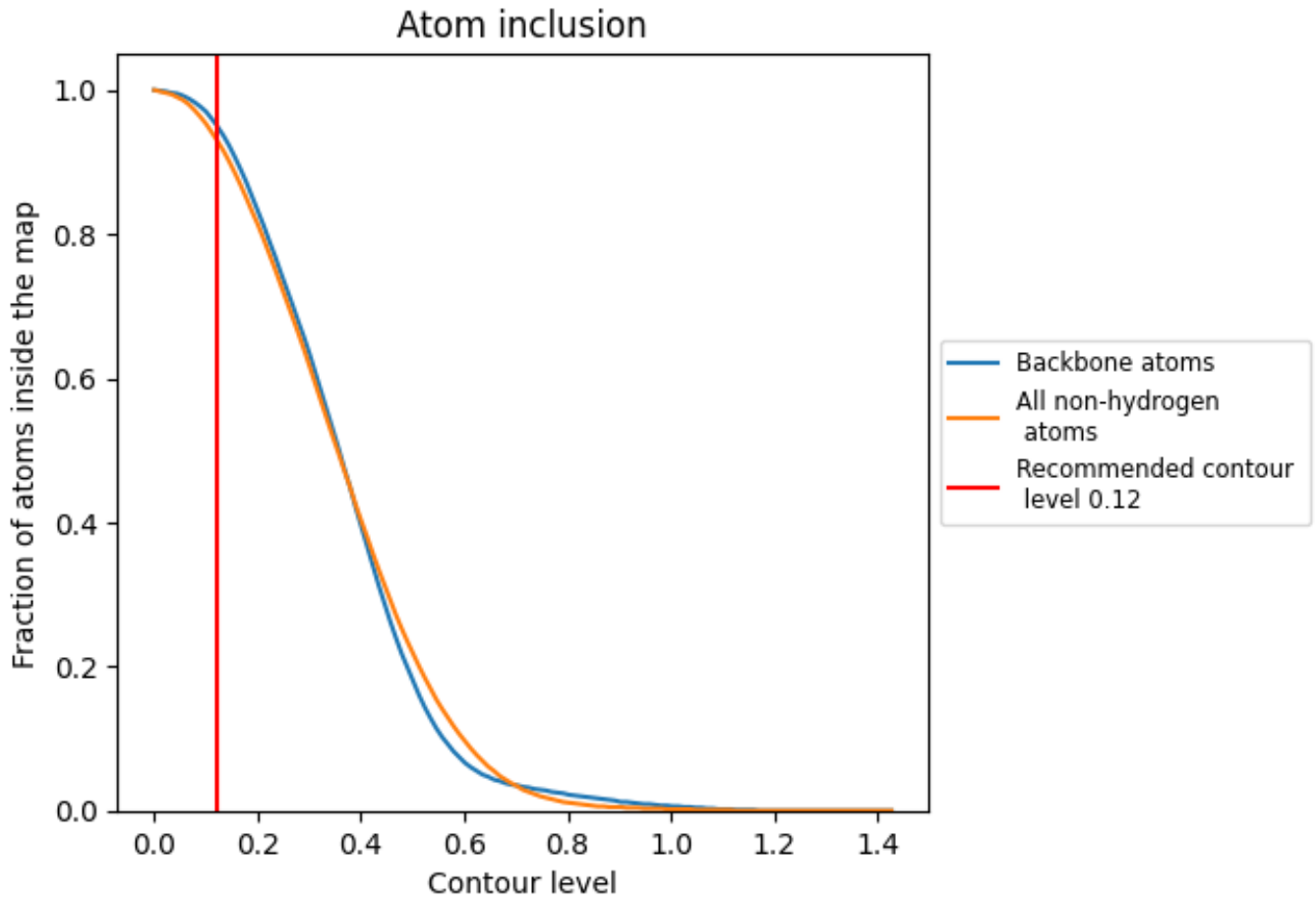
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9320	0.6180
0	0.9090	0.6520
1	0.9680	0.7010
2	0.9920	0.7030
3	0.9650	0.6650
A	0.9700	0.6430
B	0.9820	0.5840
C	0.9480	0.6700
D	0.9590	0.6840
E	0.9130	0.6540
F	0.6590	0.4210
G	0.8460	0.5650
H	0.4360	0.4290
I	0.9560	0.6790
J	0.8430	0.6020
K	0.9640	0.6800
L	0.9440	0.6680
M	0.9820	0.6930
N	0.9190	0.5840
O	0.8780	0.6230
P	0.9890	0.6960
Q	0.9580	0.6650
R	0.9520	0.6770
S	0.8650	0.6220
T	0.8410	0.5890
U	0.9110	0.6320
V	0.9770	0.6940
W	0.9310	0.6610
X	0.8110	0.5470
Y	0.9460	0.6720
Z	0.9410	0.6810
a	0.9620	0.5970
b	0.3140	0.4450
c	0.8570	0.5880
d	0.7560	0.5070

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Chain	Atom inclusion	Q-score
e	0.9270	0.6180
f	0.7710	0.5220
g	0.6230	0.4640
h	0.9450	0.6330
i	0.8970	0.6070
j	0.8200	0.5800
k	0.7790	0.5290
l	0.8580	0.6080
m	0.9000	0.5970
n	0.8950	0.6150
o	0.9390	0.6190
p	0.9530	0.6370
q	0.8930	0.5980
r	0.9030	0.6030
s	0.9290	0.6110
t	0.9390	0.6130
u	0.3030	0.4060