Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 08:22 pm GMT

PDB ID	:	5OT7
EMDB ID	:	EMD-3852
Title	:	Elongation factor G-ribosome complex captures in the absence of inhibitors.
Authors	:	Mace, K.; Giudice, E.; Chat, S.; Gillet, R.
Deposited on	:	2017-08-21
Resolution	:	3.80 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 (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:

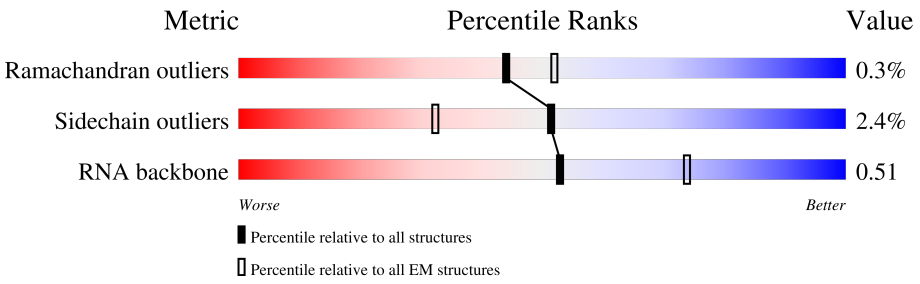
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	1	1507	72% 27%
2	2	76	22% 63% 37%
3	3	15	20% 40% 7% 33%
4	4	2901	79% 20%
5	5	119	66% 31%
6	6	178	11% 93% 7%
7	7	146	40% 97%
8	A	235	11% 95%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	B	207	18% 96%
10	C	208	98%
11	D	151	98%
12	E	101	96%
13	F	155	30% 95% 5%
14	G	138	96%
15	H	127	12% 99%
16	I	99	15% 99%
17	J	119	18% 97%
18	K	125	6% 97%
19	L	119	24% 94% 5%
20	M	60	23% 98%
21	N	88	100%
22	O	84	96%
23	P	100	98%
24	Q	70	7% 97%
25	R	88	31% 97%
26	S	99	5% 99%
27	T	25	12% 96%
28	U	687	26% 94%
29	V	78	96%
30	W	94	97%
31	X	71	94% 6%
32	Y	60	100%
33	Z	71	21% 93% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	a	59	7% 97%
35	b	50	8% 98%
36	c	48	96%
37	d	64	6% 95% 5%
38	e	37	5% 89% 11%
39	f	227	53% 100%
40	g	275	98%
41	h	205	97%
42	i	208	100%
43	j	179	7% 93% 6%
44	k	176	97%
45	l	130	25% 99%
46	m	140	21% 100%
47	n	71	63% 100%
48	o	139	100%
49	p	122	100%
50	q	150	96%
51	r	141	99%
52	s	118	97%
53	t	99	96%
54	u	138	7% 96%
55	v	117	98%
56	w	101	99%
57	x	113	97%
58	y	93	95% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
59	z	101	90% 10%

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 154665 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	1507	32391	14418	6002	10465	1506	0	0

- Molecule 2 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	76	1619	723	290	531	75	0	0

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	10	214	95	35	74	10	0	0

- Molecule 4 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	2901	62476	27807	11683	20086	2900	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1041	G	C	conflict	GB 55771382
4	2133	A	G	conflict	GB 55771382

- Molecule 5 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	5	119	2551	1136	471	826	118	0	0

- Molecule 6 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	178	1418	906	254	256	2	0	0

- Molecule 7 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	146	1136	726	201	208	1	0	0

- Molecule 8 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A	235	1901	1213	342	341	5	0	1

- Molecule 9 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	207	1613	1016	315	281	1	0	1

- Molecule 10 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	208	1703	1066	339	291	7	0	0

- Molecule 11 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	D	151	1147	724	218	201	4	0	1

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E	101	843	531	155	154	3	0	0

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	F	155	1257	781	252	218	6	0	0

- Molecule 14 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	G	138	1116	705	215	193	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	H	127	1010	639	197	174	0	0

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	I	99	795	499	157	138	1	0	1

- Molecule 17 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	J	119	885	549	168	165	3	0	0

- Molecule 18 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	K	125	971	611	196	163	1	0	1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	L	119	938	579	194	163	2	0	1

- Molecule 20 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	M	60	492	312	104	72	4	0	0

- Molecule 21 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	N	88	734	459	147	126	2	0	0

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	O	84	701	443	140	117	1	0	1

- Molecule 23 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	100	824	528	152	142	2	0	1

- Molecule 24 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	Q	70	574	367	112	95	0	0

- Molecule 25 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	88	692	440	128	122	2	0	1

- Molecule 26 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	S	99	763	470	162	129	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	T	25	209	128	51	30	0	1

- Molecule 28 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	U	661	5173	3288	884	983	18	0	0

- Molecule 29 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	V	78	617	381	130	105	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	W	94	732	460	146	125	1	0	1

- Molecule 31 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	X	71	598	370	121	106	1	0	0

- Molecule 32 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Y	60	468	298	91	78	1	0	1

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Z	71	581	364	108	104	5	0	0

- Molecule 34 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	a	59	459	288	90	76	5	0	0

- Molecule 35 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	b	50	433	270	88	71	4	0	0

- Molecule 36 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	c	48	419	257	104	56	2	0	0

- Molecule 37 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	d	64	508	326	102	78	2	0	1

- Molecule 38 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	e	37	307	188	68	47	4	0	0

- Molecule 39 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	f	227	1735	1096	318	318	3	0	0

- Molecule 40 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	g	275	2145	1353	428	361	3	0	0

- Molecule 41 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	h	205	1564	988	300	270	6	0	1

- Molecule 42 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	i	208	1624	1035	304	282	3	0	1

- Molecule 43 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	j	179	1459	931	266	258	4	0	0

- Molecule 44 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	k	176	1345	853	253	237	2	0	1

- Molecule 45 is a protein called Ribosomal protein uL10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	l	130	654	393	130	131	0	0

- Molecule 46 is a protein called Ribosomal protein uL11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	m	140	701	420	140	141	0	0

- Molecule 47 is a protein called Ribosomal protein bL12.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	n	71	356	213	71	72	0	0

- Molecule 48 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	o	139	1105	712	207	182	4	0	1

- Molecule 49 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	p	122	933	588	171	170	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	q	150	1145	712	232	198	3	0	0

- Molecule 51 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	r	141	1122	715	212	188	7	0	0

- Molecule 52 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	s	118	968	604	203	160	1	0	0

- Molecule 53 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	t	99	771	486	155	130	0	1

- Molecule 54 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	u	138	1142	710	235	196	1	0	1

- Molecule 55 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	v	117	958	604	202	151	1	0	0

- Molecule 56 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	w	101	779	501	142	135	1	0	0

- Molecule 57 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	x	113	896	563	176	155	2	0	0

- Molecule 58 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
58	y	93	726	471	132	123	0	1

- Molecule 59 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	z	101	776	500	149	123	4	0	1

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	1	126	126	126	0
60	4	322	322	322	0
60	D	1	1	1	0
60	O	2	2	2	0
60	S	1	1	1	0
60	U	1	1	1	0

Continued on next page...

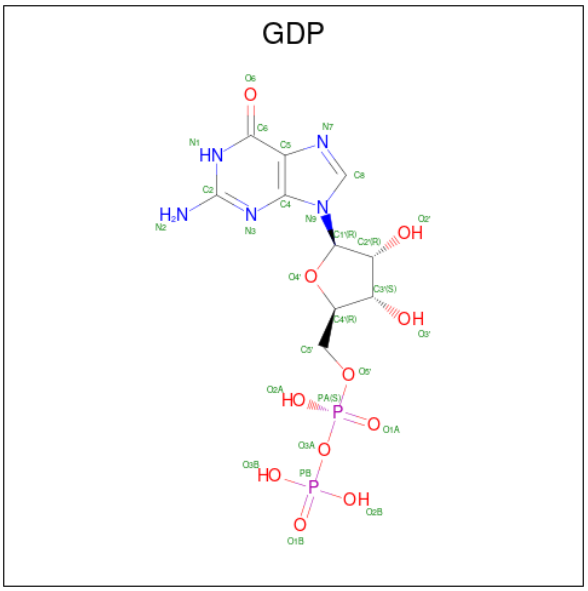
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
60	c	1	1	1	0
60	e	1	1	1	0
60	h	1	1	1	0
60	i	1	1	1	0
60	q	1	1	1	0
60	t	2	2	2	0
60	u	1	1	1	0
60	x	1	1	1	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
61	C	1	1	1	0
61	M	1	1	1	0
61	e	1	1	1	0

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



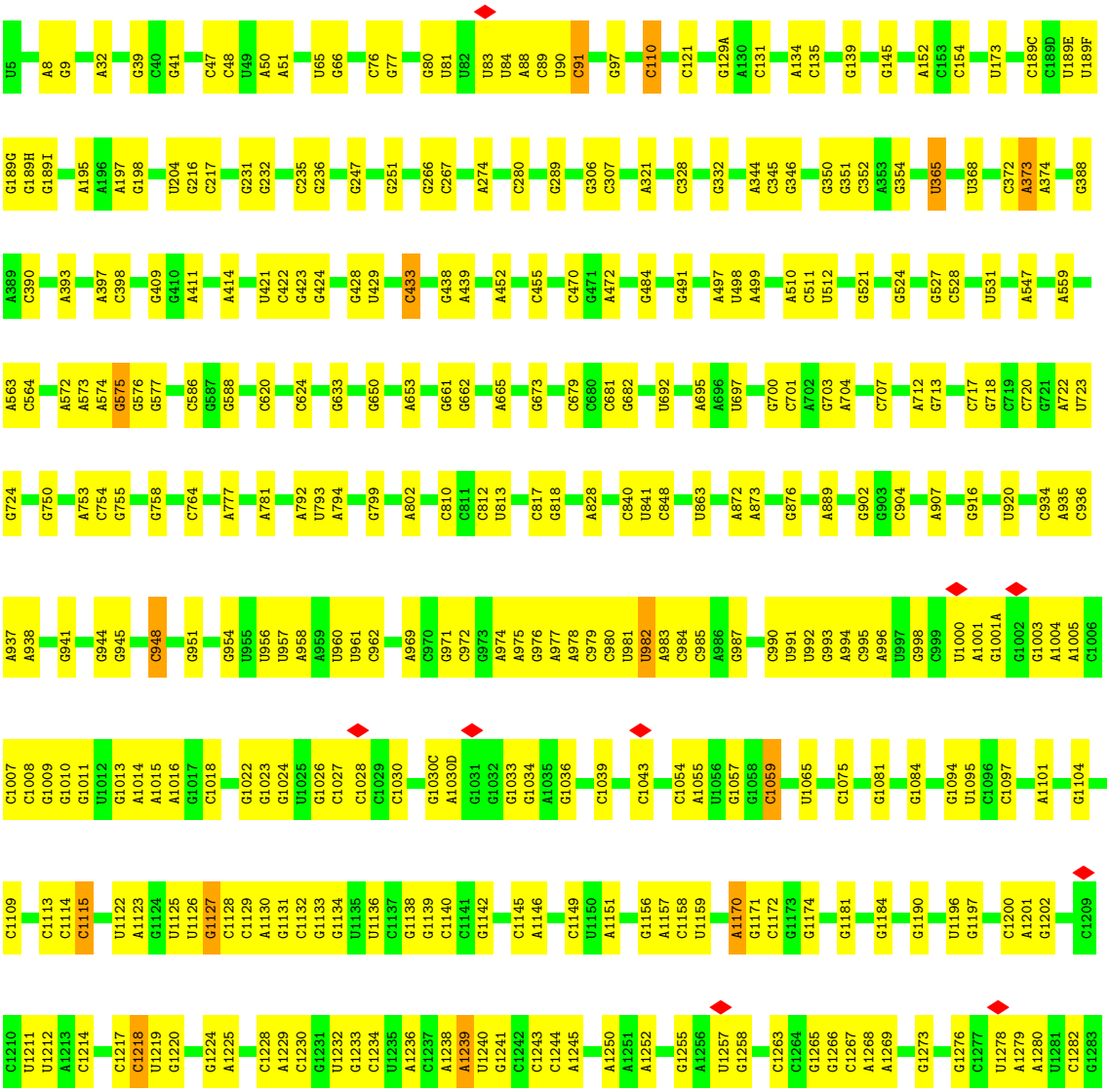
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
62	U	1	28	10	5	11	2	0

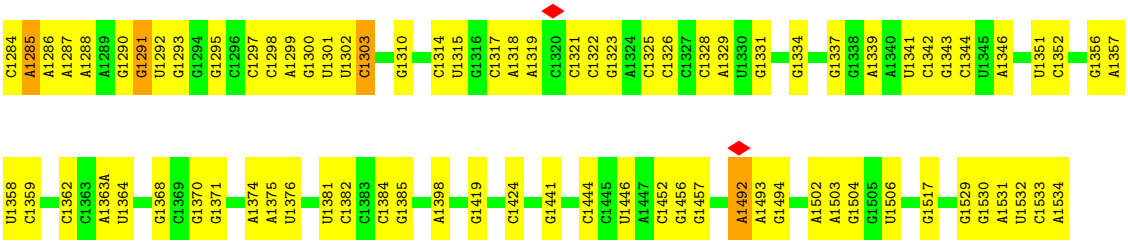
3 Residue-property plots (i)

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: 16S Ribosomal RNA

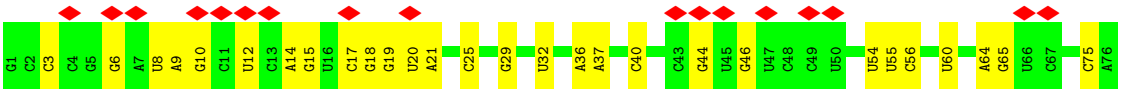
Chain 1:





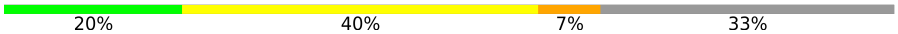
- Molecule 2: tRNA-Phe

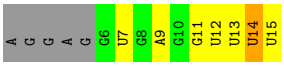
Chain 2:



- Molecule 3: mRNA

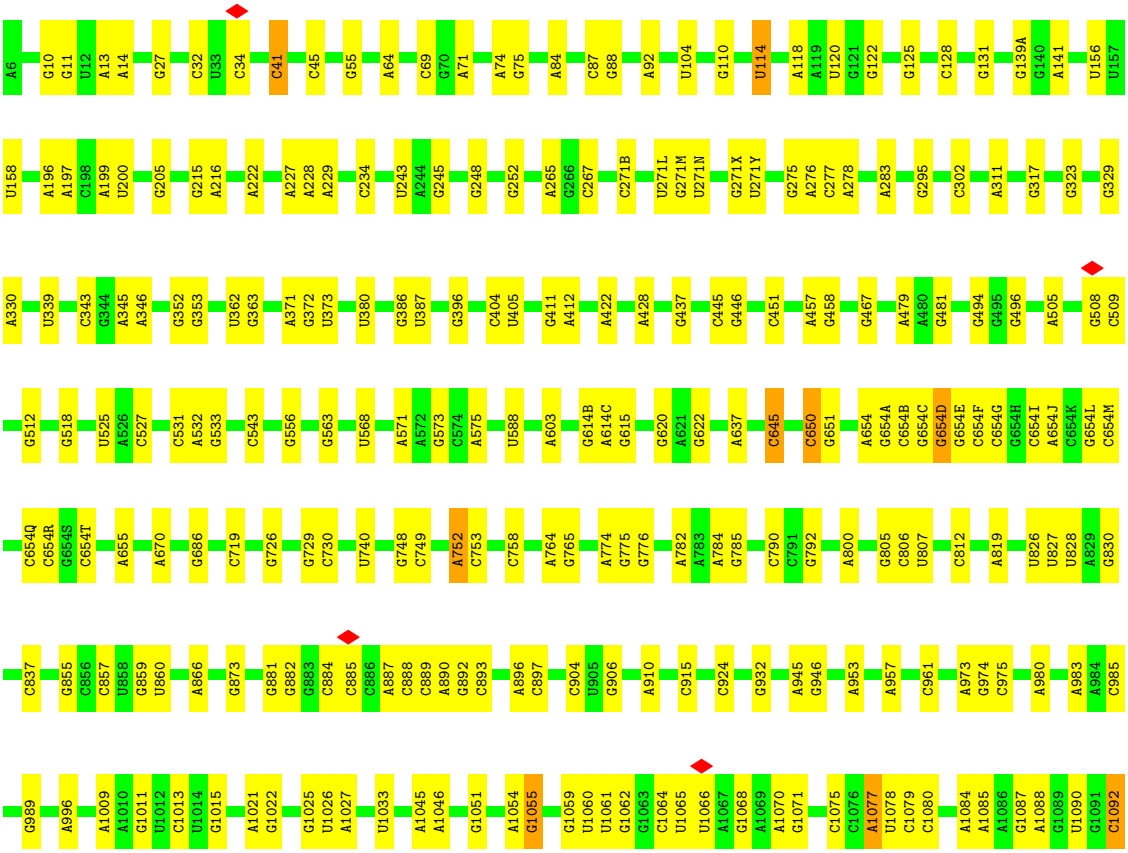
Chain 3:

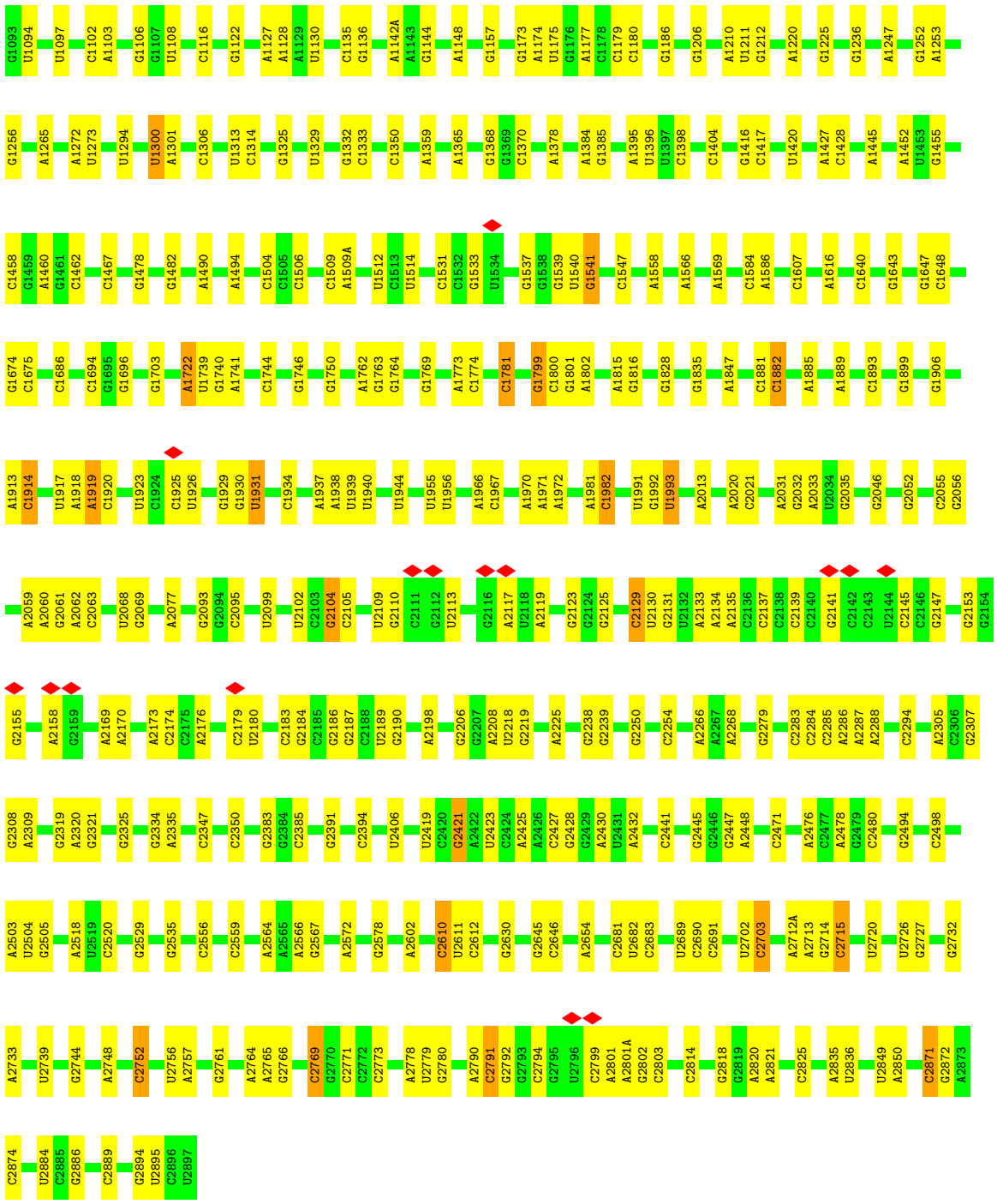




- Molecule 4: 23S Ribosomal RNA

Chain 4:



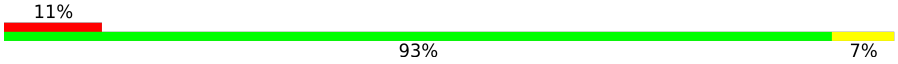


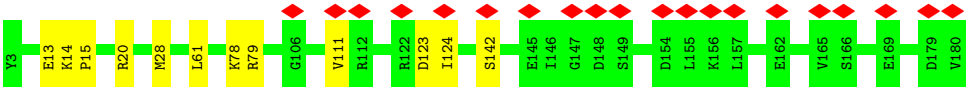
- Molecule 5: 5S Ribosomal RNA

Chain 5:

• Molecule 6: 50S ribosomal protein L25

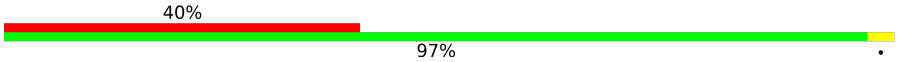
Chain 6:

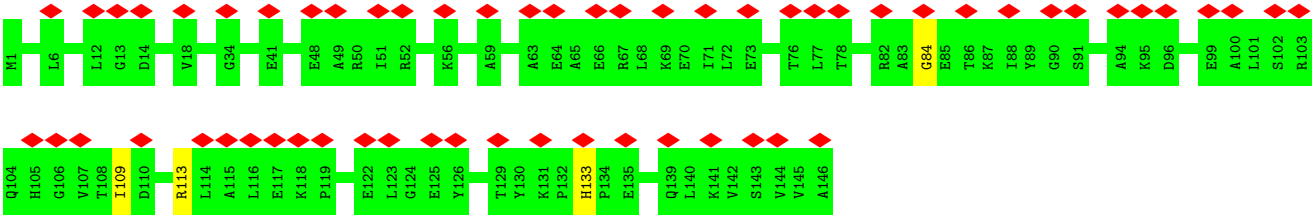




• Molecule 7: 50S ribosomal protein L9

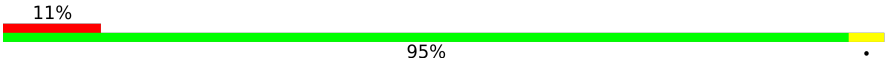
Chain 7:

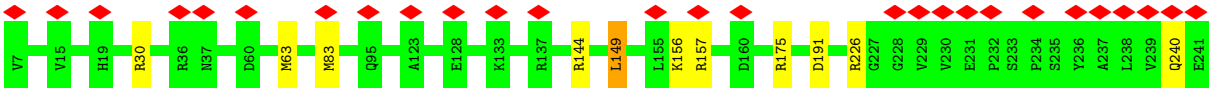




• Molecule 8: 30S ribosomal protein S2

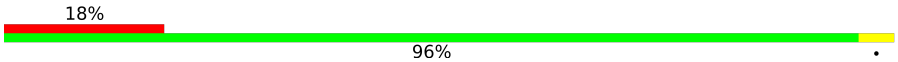
Chain A:

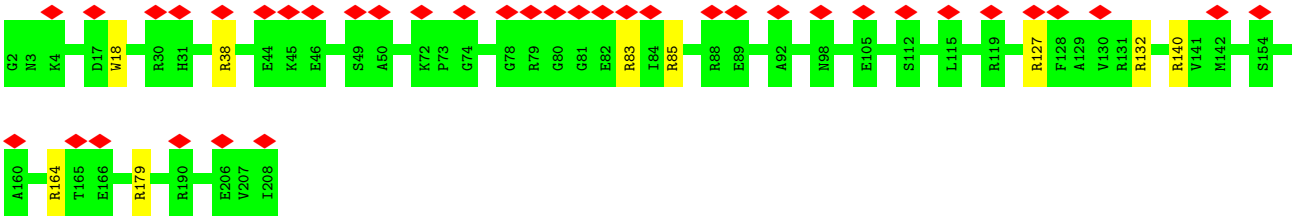




• Molecule 9: 30S ribosomal protein S3

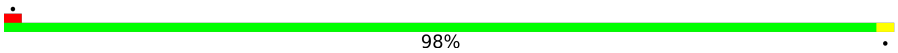
Chain B:

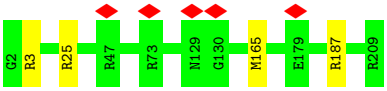




• Molecule 10: 30S ribosomal protein S4

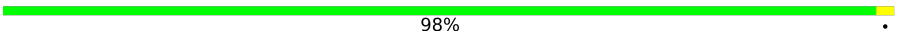
Chain C:

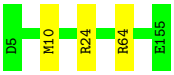




• Molecule 11: 30S ribosomal protein S5

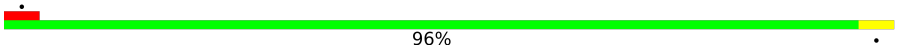
Chain D:

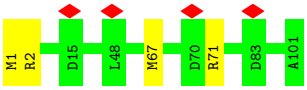




• Molecule 12: 30S ribosomal protein S6

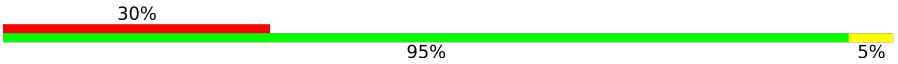
Chain E:

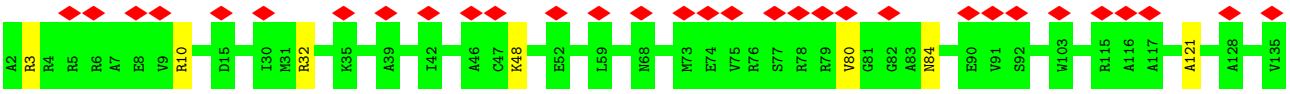


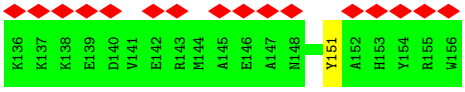


• Molecule 13: 30S ribosomal protein S7

Chain F:

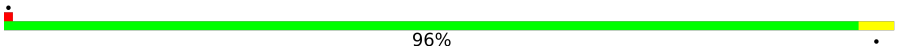


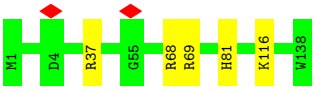




• Molecule 14: 30S ribosomal protein S8

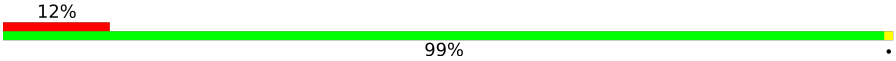
Chain G:

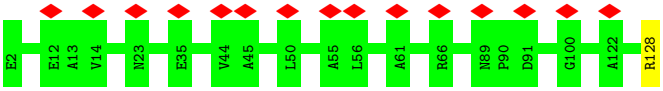




• Molecule 15: 30S ribosomal protein S9

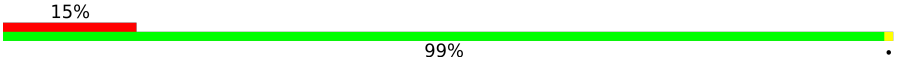
Chain H:

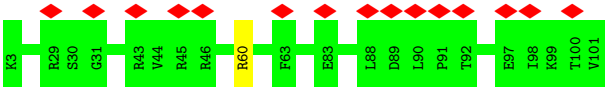




• Molecule 16: 30S ribosomal protein S10

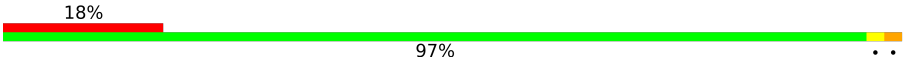
Chain I:

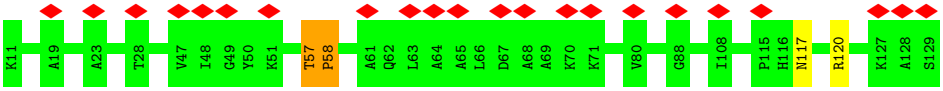




• Molecule 17: 30S ribosomal protein S11

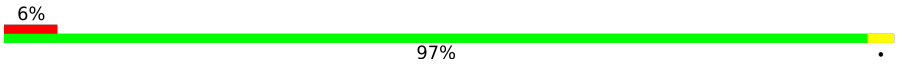
Chain J:

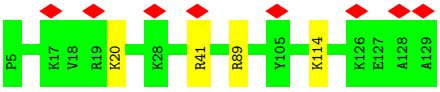




• Molecule 18: 30S ribosomal protein S12

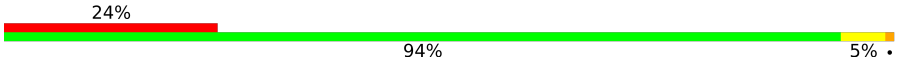
Chain K:

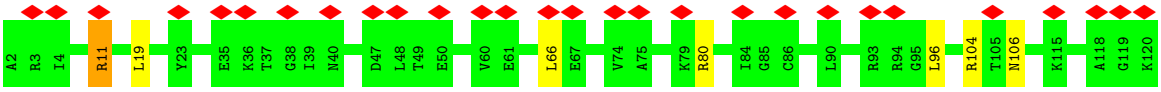




• Molecule 19: 30S ribosomal protein S13

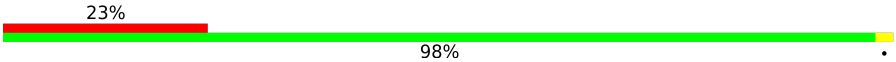
Chain L:

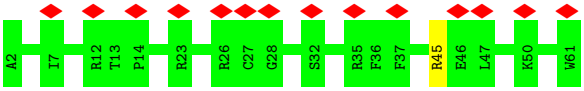




• Molecule 20: 30S ribosomal protein S14 type Z

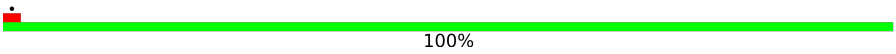
Chain M:

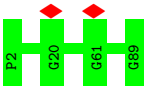




• Molecule 21: 30S ribosomal protein S15

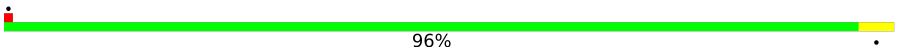
Chain N:

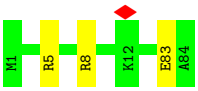




• Molecule 22: 30S ribosomal protein S16

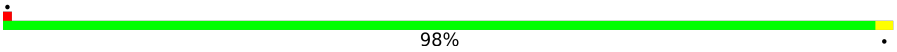
Chain O:

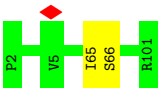




• Molecule 23: 30S ribosomal protein S17

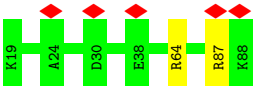
Chain P:





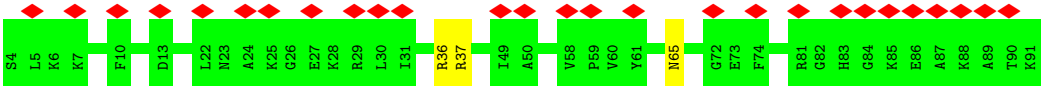
• Molecule 24: 30S ribosomal protein S18

Chain Q: 7% 97%



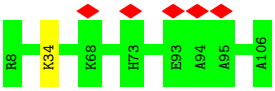
• Molecule 25: 30S ribosomal protein S19

Chain R: 31% 97%



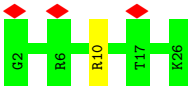
• Molecule 26: 30S ribosomal protein S20

Chain S: 5% 99%



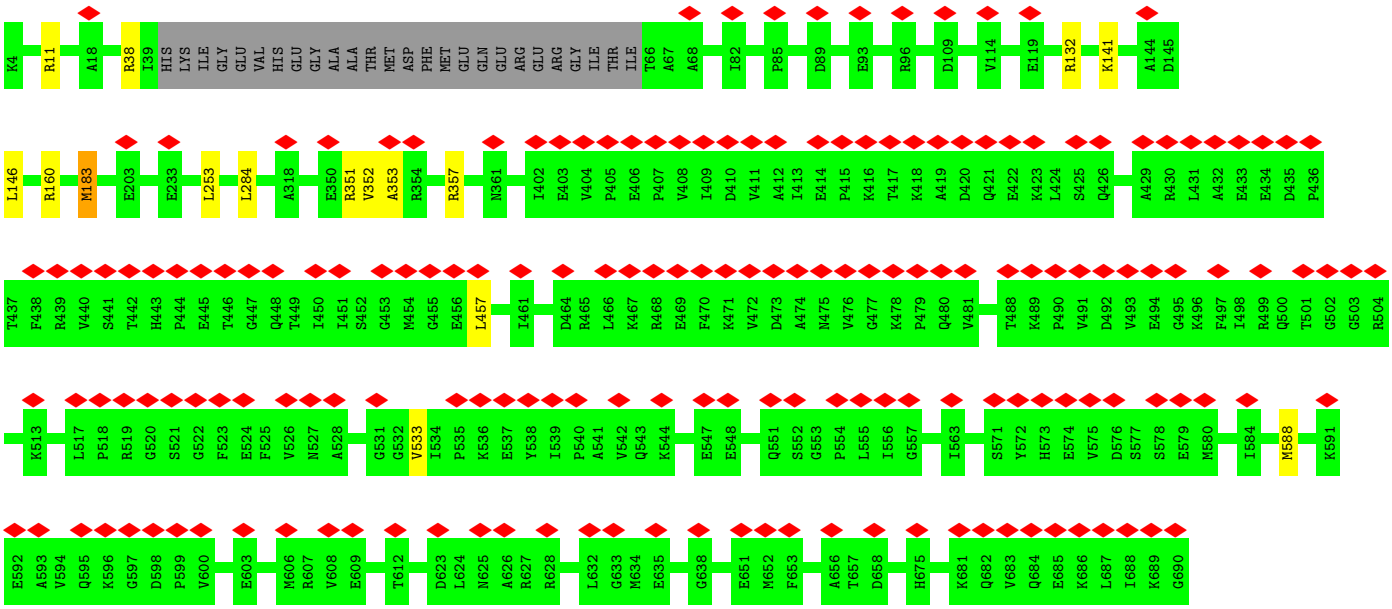
• Molecule 27: 30S ribosomal protein Thx

Chain T: 12% 96%



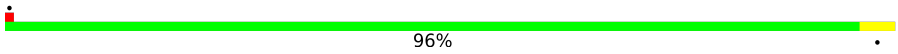
• Molecule 28: Elongation factor G

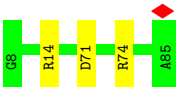
Chain U: 26% 94%



- Molecule 29: 50S ribosomal protein L27

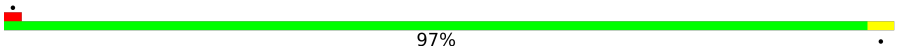
Chain V:

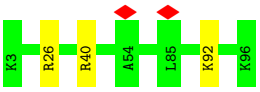




- Molecule 30: 50S ribosomal protein L28

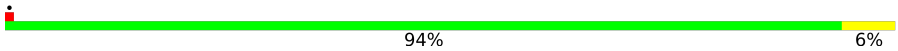
Chain W:

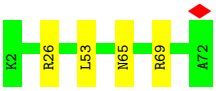




- Molecule 31: 50S ribosomal protein L29

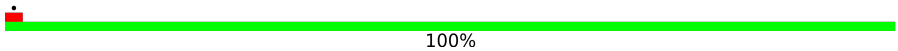
Chain X:





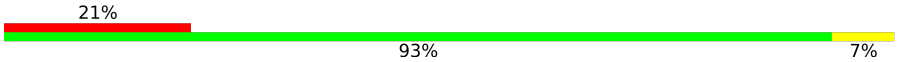
- Molecule 32: 50S ribosomal protein L30

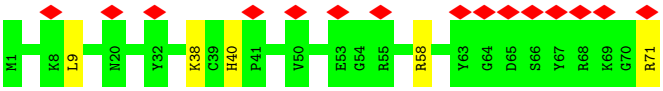
Chain Y:



- Molecule 33: 50S ribosomal protein L31

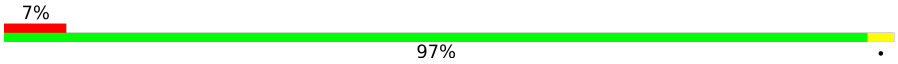
Chain Z:

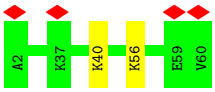




- Molecule 34: 50S ribosomal protein L32

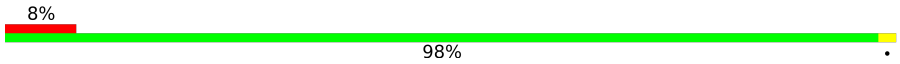
Chain a:

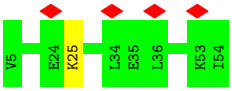




- Molecule 35: 50S ribosomal protein L33

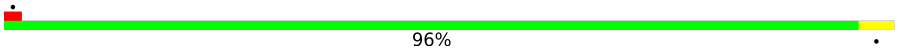
Chain b:

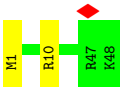




• Molecule 36: 50S ribosomal protein L34

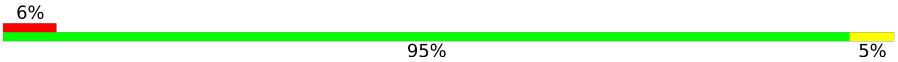
Chain c:

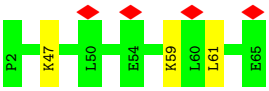




• Molecule 37: 50S ribosomal protein L35

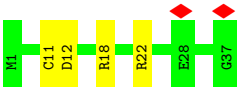
Chain d:





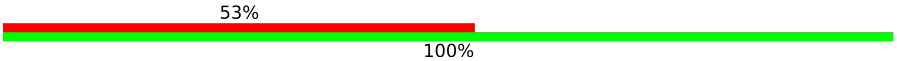
• Molecule 38: 50S ribosomal protein L36

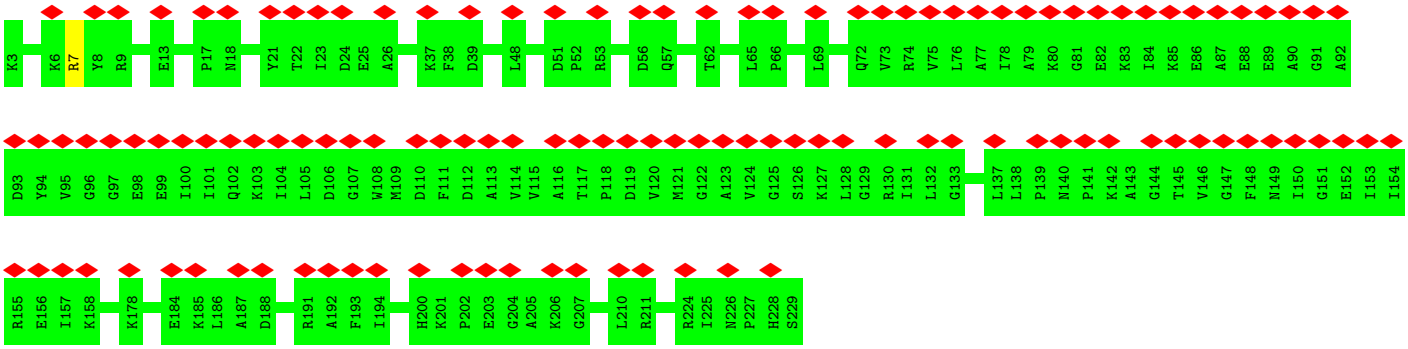
Chain e:



• Molecule 39: 50S ribosomal protein L1

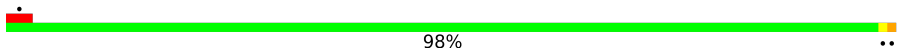
Chain f:

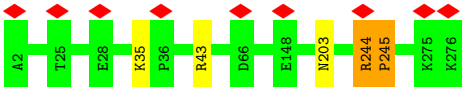




• Molecule 40: 50S ribosomal protein L2

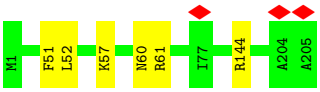
Chain g:





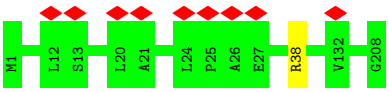
• Molecule 41: 50S ribosomal protein L3

Chain h: 97%



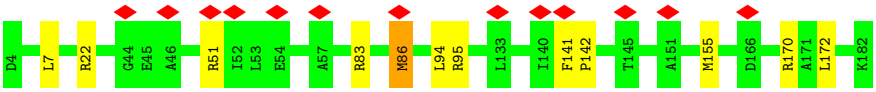
• Molecule 42: 50S ribosomal protein L4

Chain i: 100%



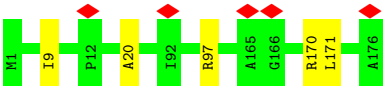
• Molecule 43: 50S ribosomal protein L5

Chain j: 7% 93% 6%



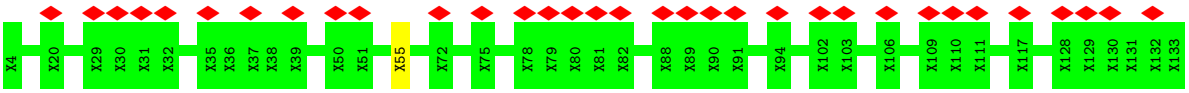
• Molecule 44: 50S ribosomal protein L6

Chain k: 97%



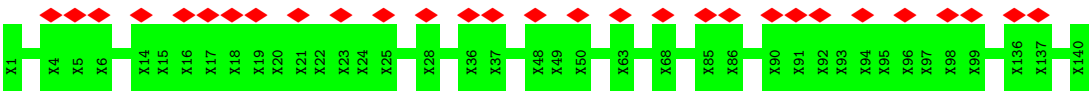
• Molecule 45: Ribosomal protein uL10

Chain l: 25% 99%



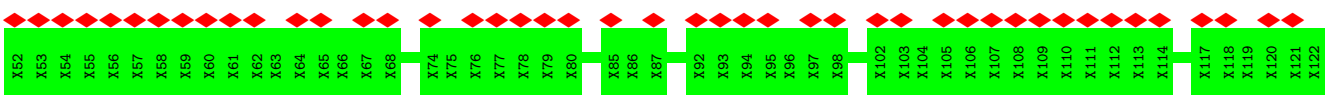
• Molecule 46: Ribosomal protein uL11

Chain m: 21% 100%



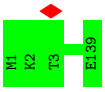
• Molecule 47: Ribosomal protein bL12

Chain n: 63% 100%



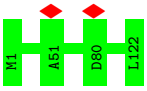
• Molecule 48: 50S ribosomal protein L13

Chain o: 100%



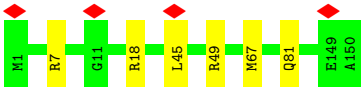
• Molecule 49: 50S ribosomal protein L14

Chain p: 100%



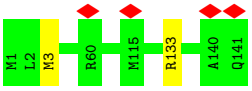
• Molecule 50: 50S ribosomal protein L15

Chain q: 96%



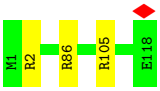
• Molecule 51: 50S ribosomal protein L16

Chain r: 99%



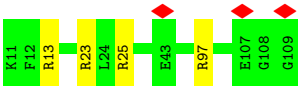
• Molecule 52: 50S ribosomal protein L17

Chain s: 97%



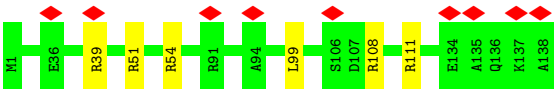
• Molecule 53: 50S ribosomal protein L18

Chain t: 96%

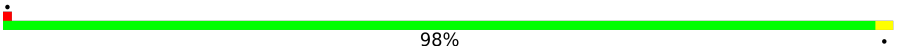


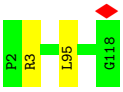
• Molecule 54: 50S ribosomal protein L19

Chain u: 7% 96%

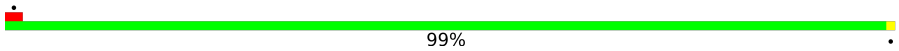


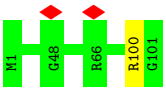
• Molecule 55: 50S ribosomal protein L20

Chain v: 

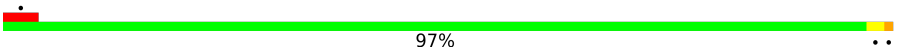


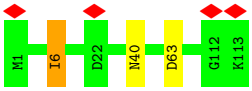
• Molecule 56: 50S ribosomal protein L21

Chain w: 

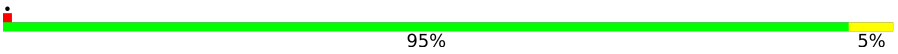


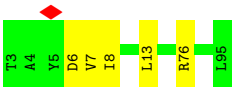
• Molecule 57: 50S ribosomal protein L22

Chain x: 



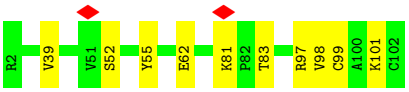
• Molecule 58: 50S ribosomal protein L23

Chain y: 



• Molecule 59: 50S ribosomal protein L24

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32383	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 ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	120443	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.453	Depositor
Minimum map value	-0.272	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	463.05, 463.05, 463.05	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1025, 1.1025, 1.1025	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: ZN, GDP, MG

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	1	0.28	0/36259	0.99	100/56593 (0.2%)
2	2	0.25	0/1809	0.96	3/2819 (0.1%)
3	3	0.32	0/238	1.04	1/369 (0.3%)
4	4	0.29	0/69975	1.00	185/109242 (0.2%)
5	5	0.33	0/2853	1.07	12/4451 (0.3%)
6	6	0.28	0/1450	0.69	3/1970 (0.2%)
7	7	0.28	0/1151	0.66	2/1558 (0.1%)
8	A	0.27	0/1936	0.61	2/2611 (0.1%)
9	B	0.28	0/1637	0.63	0/2207
10	C	0.27	0/1733	0.55	0/2318
11	D	0.27	0/1163	0.58	0/1566
12	E	0.26	0/856	0.55	0/1154
13	F	0.31	0/1276	0.63	0/1709
14	G	0.26	0/1136	0.56	0/1527
15	H	0.29	0/1029	0.62	0/1379
16	I	0.27	0/808	0.58	0/1087
17	J	0.32	0/900	0.67	2/1213 (0.2%)
18	K	0.27	0/987	0.54	0/1322
19	L	0.27	0/948	0.65	3/1272 (0.2%)
20	M	0.29	0/501	0.60	0/664
21	N	0.26	0/745	0.57	0/992
22	O	0.24	0/717	0.52	0/965
23	P	0.26	0/837	0.62	0/1119
24	Q	0.27	0/579	0.53	0/768
25	R	0.26	0/706	0.58	0/950
26	S	0.25	0/765	0.56	0/1007
27	T	0.24	0/213	0.50	0/279
28	U	0.27	0/5270	0.60	2/7135 (0.0%)
29	V	0.28	0/625	0.60	0/832
30	W	0.27	0/739	0.58	0/983
31	X	0.26	0/600	0.55	0/793
32	Y	0.24	0/473	0.55	0/636

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Z	0.29	0/594	0.76	1/795 (0.1%)
34	a	0.29	0/473	0.60	0/639
35	b	0.29	0/440	0.76	0/586
36	c	0.24	0/427	0.47	0/561
37	d	0.30	0/516	0.66	1/681 (0.1%)
38	e	0.32	0/310	0.71	1/407 (0.2%)
39	f	0.28	0/1766	0.63	0/2380
40	g	0.28	0/2195	0.59	1/2955 (0.0%)
41	h	0.29	0/1597	0.64	2/2155 (0.1%)
42	i	0.27	0/1659	0.57	0/2246
43	j	0.30	0/1483	0.76	3/1994 (0.2%)
44	k	0.27	0/1371	0.60	1/1853 (0.1%)
45	l	0.17	0/7	0.20	0/8
48	o	0.26	0/1132	0.58	0/1527
49	p	0.28	0/943	0.53	0/1269
50	q	0.28	0/1162	0.72	1/1544 (0.1%)
51	r	0.25	0/1143	0.49	0/1527
52	s	0.27	0/982	0.63	0/1312
53	t	0.28	0/779	0.70	0/1038
54	u	0.29	0/1156	0.63	0/1544
55	v	0.26	0/975	0.53	0/1297
56	w	0.26	0/790	0.60	0/1057
57	x	0.28	0/907	0.61	1/1216 (0.1%)
58	y	0.27	0/740	0.59	1/995 (0.1%)
59	z	0.36	0/789	0.86	2/1053 (0.2%)
All	All	0.28	0/165250	0.90	330/246129 (0.1%)

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
6	6	0	3
7	7	0	1
8	A	0	2
9	B	0	1
13	F	0	2
14	G	0	1
23	P	0	1
28	U	0	3
29	V	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
33	Z	0	1
40	g	0	2
41	h	0	3
43	j	0	2
44	k	0	2
45	l	0	1
50	q	0	1
57	x	0	1
58	y	0	2
59	z	0	5
All	All	0	35

There are no bond length outliers.

All (330) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	76	C	N1-C2-O2	13.27	126.86	118.90
1	1	76	C	N3-C2-O2	-12.51	113.14	121.90
1	1	754	C	C2-N1-C1'	11.57	131.53	118.80
1	1	373	A	OP1-P-O3'	-11.47	79.96	105.20
1	1	231	G	OP1-P-O3'	-11.35	80.24	105.20
4	4	2769	C	N1-C2-O2	11.06	125.53	118.90
1	1	754	C	N1-C2-O2	10.76	125.36	118.90
1	1	76	C	C2-N1-C1'	10.65	130.51	118.80
1	1	76	C	C6-N1-C2	-10.08	116.27	120.30
4	4	2769	C	N3-C2-O2	-9.50	115.25	121.90
4	4	2129	C	N1-C2-O2	8.92	124.25	118.90
1	1	1282	C	N1-C2-O2	8.90	124.24	118.90
1	1	1282	C	C2-N1-C1'	8.84	128.52	118.80
4	4	2874	C	C2-N1-C1'	8.80	128.48	118.80
1	1	754	C	N3-C2-O2	-8.74	115.78	121.90
1	1	1109	C	N1-C2-O2	8.72	124.14	118.90
4	4	2769	C	C2-N1-C1'	8.69	128.36	118.80
4	4	2105	C	N1-C2-O2	8.42	123.95	118.90
4	4	2769	C	C6-N1-C2	-8.40	116.94	120.30
4	4	2683	C	N1-C2-O2	8.15	123.79	118.90
1	1	231	G	OP2-P-O3'	-8.12	87.35	105.20
2	2	3	C	N3-C2-O2	-8.07	116.25	121.90
1	1	373	A	OP2-P-O3'	-8.01	87.59	105.20
4	4	1079	C	C2-N1-C1'	7.96	127.56	118.80
4	4	41	C	N3-C2-O2	-7.95	116.34	121.90
1	1	1097	C	N1-C2-O2	7.92	123.65	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	754	C	C6-N1-C2	-7.91	117.14	120.30
1	1	754	C	C6-N1-C1'	-7.88	111.34	120.80
1	1	1218	C	N3-C2-O2	-7.83	116.42	121.90
4	4	1541	G	C4-N9-C1'	7.82	136.66	126.50
4	4	527	C	C6-N1-C2	-7.81	117.17	120.30
4	4	445	C	N3-C2-O2	-7.79	116.45	121.90
28	U	253	LEU	CA-CB-CG	7.77	133.18	115.30
4	4	2129	C	C2-N1-C1'	7.61	127.17	118.80
4	4	1541	G	N3-C4-C5	-7.60	124.80	128.60
4	4	87	C	N3-C2-O2	-7.57	116.60	121.90
4	4	2321	G	N3-C4-C5	-7.51	124.85	128.60
4	4	1541	G	N3-C4-N9	7.48	130.49	126.00
4	4	1075	C	C2-N1-C1'	7.42	126.97	118.80
4	4	2129	C	N3-C2-O2	-7.41	116.71	121.90
4	4	41	C	C6-N1-C2	-7.38	117.35	120.30
1	1	1127	G	N3-C4-C5	-7.35	124.92	128.60
1	1	1097	C	C2-N1-C1'	7.34	126.88	118.80
4	4	2321	G	C4-N9-C1'	7.26	135.94	126.50
4	4	2104	G	C4-N9-C1'	7.24	135.92	126.50
33	Z	9	LEU	CA-CB-CG	7.23	131.93	115.30
2	2	3	C	N1-C2-O2	7.19	123.22	118.90
4	4	2105	C	C2-N1-C1'	7.19	126.70	118.80
1	1	1109	C	N3-C2-O2	-7.11	116.92	121.90
1	1	77	G	N3-C4-N9	7.09	130.26	126.00
1	1	374	A	OP1-P-OP2	7.09	130.24	119.60
1	1	77	G	N3-C4-C5	-7.09	125.06	128.60
1	1	77	G	C4-N9-C1'	7.08	135.71	126.50
8	A	191	ASP	CB-CG-OD1	7.07	124.67	118.30
4	4	1180	C	C2-N1-C1'	7.04	126.55	118.80
4	4	1774	C	N1-C2-O2	7.03	123.12	118.90
4	4	2063	C	N1-C2-O2	6.97	123.08	118.90
4	4	2610	C	OP2-P-O3'	6.95	120.49	105.20
4	4	114	U	C2-N1-C1'	6.95	126.04	117.70
4	4	2129	C	C6-N1-C2	-6.94	117.52	120.30
1	1	1282	C	N3-C2-O2	-6.94	117.04	121.90
1	1	920	U	N1-C2-O2	6.93	127.65	122.80
4	4	2559	C	C2-N1-C1'	6.90	126.39	118.80
4	4	2099	U	N1-C2-O2	6.90	127.63	122.80
4	4	1077	A	P-O3'-C3'	6.86	127.94	119.70
4	4	2683	C	N3-C2-O2	-6.84	117.11	121.90
4	4	1462	C	N3-C2-O2	-6.84	117.11	121.90
4	4	2874	C	C6-N1-C2	-6.83	117.57	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	z	99	CYS	CA-CB-SG	6.82	126.27	114.00
1	1	1127	G	N3-C4-N9	6.81	130.08	126.00
4	4	1462	C	N1-C2-O2	6.81	122.98	118.90
50	q	45	LEU	CA-CB-CG	6.79	130.91	115.30
1	1	1127	G	C4-N9-C1'	6.79	135.32	126.50
5	5	31	C	C2-N1-C1'	6.79	126.26	118.80
4	4	2610	C	P-O3'-C3'	6.76	127.81	119.70
1	1	232	G	OP1-P-OP2	6.74	129.71	119.60
1	1	982	U	P-O3'-C3'	6.73	127.78	119.70
1	1	307	C	N1-C2-O2	6.70	122.92	118.90
5	5	30	C	N1-C2-O2	6.69	122.92	118.90
4	4	2683	C	C2-N1-C1'	6.68	126.15	118.80
4	4	2703	C	C2-N1-C1'	6.67	126.14	118.80
4	4	1108	U	N3-C2-O2	-6.66	117.54	122.20
1	1	365	U	C2-N1-C1'	6.66	125.69	117.70
4	4	2099	U	N3-C2-O2	-6.64	117.55	122.20
4	4	1108	U	N1-C2-O2	6.64	127.44	122.80
1	1	948	C	N1-C2-O2	6.61	122.87	118.90
1	1	110	C	N1-C2-O2	6.61	122.86	118.90
4	4	1541	G	C8-N9-C1'	-6.60	118.42	127.00
4	4	1079	C	N1-C2-O2	6.59	122.86	118.90
5	5	37	C	N1-C2-O2	6.58	122.85	118.90
41	h	52	LEU	CA-CB-CG	6.58	130.43	115.30
4	4	1893	C	N1-C2-O2	6.57	122.84	118.90
1	1	154	C	N1-C2-O2	6.53	122.82	118.90
4	4	1774	C	N3-C2-O2	-6.51	117.34	121.90
4	4	275	G	N3-C4-C5	-6.49	125.36	128.60
1	1	754	C	C5-C6-N1	6.48	124.24	121.00
3	3	14	U	P-O3'-C3'	6.47	127.47	119.70
1	1	1109	C	C2-N1-C1'	6.47	125.92	118.80
43	j	7	LEU	CA-CB-CG	6.46	130.16	115.30
4	4	1092	C	C2-N1-C1'	6.45	125.90	118.80
4	4	2769	C	C5-C6-N1	6.43	124.21	121.00
4	4	1799	G	P-O3'-C3'	6.43	127.41	119.70
4	4	2179	C	C2-N1-C1'	6.42	125.86	118.80
4	4	837	C	N1-C2-O2	6.42	122.75	118.90
4	4	1774	C	C6-N1-C2	-6.41	117.74	120.30
4	4	543	C	C2-N1-C1'	6.40	125.84	118.80
1	1	76	C	C6-N1-C1'	-6.39	113.13	120.80
4	4	2703	C	C5-C6-N1	6.39	124.20	121.00
4	4	2556	C	N1-C2-O2	6.38	122.73	118.90
4	4	275	G	C4-N9-C1'	6.38	134.80	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1218	C	C6-N1-C2	-6.37	117.75	120.30
4	4	1934	C	C2-N1-C1'	6.35	125.78	118.80
4	4	2559	C	C6-N1-C2	-6.33	117.77	120.30
4	4	2254	C	N1-C2-O2	6.31	122.69	118.90
1	1	1239	A	P-O3'-C3'	6.28	127.24	119.70
4	4	275	G	N3-C4-N9	6.26	129.76	126.00
4	4	837	C	N3-C2-O2	-6.24	117.53	121.90
1	1	575	G	P-O3'-C3'	6.23	127.18	119.70
4	4	2874	C	N1-C2-O2	6.23	122.64	118.90
4	4	2771	C	N1-C2-O2	6.23	122.64	118.90
4	4	2105	C	N3-C2-O2	-6.22	117.55	121.90
5	5	31	C	N1-C2-O2	6.21	122.63	118.90
4	4	2321	G	N3-C4-N9	6.21	129.73	126.00
4	4	645	C	C2-N1-C1'	6.20	125.62	118.80
5	5	38	C	N1-C2-O2	6.20	122.62	118.90
4	4	343	C	C2-N1-C1'	6.20	125.62	118.80
4	4	2703	C	N1-C2-O2	6.16	122.60	118.90
1	1	1170	A	C2-N3-C4	6.15	113.67	110.60
4	4	2129	C	C5-C6-N1	6.14	124.07	121.00
1	1	1115	C	C2-N1-C1'	6.12	125.53	118.80
4	4	1108	U	C2-N1-C1'	6.11	125.03	117.70
1	1	1352	C	N1-C2-O2	6.11	122.56	118.90
4	4	2104	G	C8-N9-C1'	-6.10	119.07	127.00
1	1	1282	C	C6-N1-C1'	-6.09	113.49	120.80
1	1	920	U	N3-C2-O2	-6.09	117.94	122.20
4	4	1956	U	N3-C2-O2	-6.09	117.94	122.20
4	4	2294	C	C2-N1-C1'	6.08	125.49	118.80
59	z	52	SER	C-N-CD	-6.07	107.25	120.60
1	1	76	C	C5-C6-N1	6.06	124.03	121.00
4	4	2063	C	N3-C2-O2	-6.05	117.67	121.90
5	5	66	A	P-O3'-C3'	6.03	126.93	119.70
4	4	1506	C	C2-N1-C1'	6.01	125.41	118.80
1	1	365	U	N1-C2-O2	6.01	127.00	122.80
4	4	2814	C	N1-C2-O2	6.00	122.50	118.90
4	4	1179	C	C2-N1-C1'	5.98	125.38	118.80
4	4	2063	C	C6-N1-C2	-5.97	117.91	120.30
4	4	1300	U	P-O3'-C3'	5.96	126.86	119.70
4	4	1686	C	C2-N1-C1'	5.96	125.36	118.80
1	1	1424	C	C2-N1-C1'	5.96	125.35	118.80
4	4	1512	U	N1-C2-O2	5.95	126.97	122.80
4	4	69	C	C2-N1-C1'	5.93	125.33	118.80
1	1	920	U	C2-N1-C1'	5.93	124.81	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	2179	C	N1-C2-O2	5.93	122.46	118.90
1	1	77	G	C8-N9-C1'	-5.92	119.30	127.00
4	4	1923	U	N1-C2-O2	5.92	126.94	122.80
4	4	1062	G	N3-C4-N9	5.92	129.55	126.00
1	1	1097	C	C6-N1-C2	-5.90	117.94	120.30
4	4	1675	C	N1-C2-O2	5.89	122.44	118.90
4	4	2683	C	C6-N1-C2	-5.89	117.94	120.30
1	1	1109	C	C6-N1-C2	-5.88	117.95	120.30
4	4	2394	C	N1-C2-O2	5.86	122.41	118.90
6	6	78	LYS	C-N-CA	5.85	136.33	121.70
1	1	1097	C	N3-C2-O2	-5.84	117.81	121.90
4	4	1079	C	C6-N1-C1'	-5.83	113.81	120.80
4	4	2874	C	C6-N1-C1'	-5.82	113.82	120.80
1	1	1218	C	N1-C2-O2	5.81	122.38	118.90
1	1	1282	C	C6-N1-C2	-5.81	117.98	120.30
4	4	2874	C	C5-C6-N1	5.79	123.90	121.00
1	1	1291	G	P-O3'-C3'	5.79	126.65	119.70
4	4	104	U	N1-C2-O2	5.79	126.85	122.80
37	d	61	LEU	CA-CB-CG	5.78	128.60	115.30
4	4	1512	U	N3-C2-O2	-5.78	118.16	122.20
4	4	1956	U	N1-C2-O2	5.78	126.84	122.80
4	4	2889	C	C2-N1-C1'	5.77	125.15	118.80
4	4	904	C	C2-N1-C1'	5.77	125.15	118.80
4	4	234	C	N1-C2-O2	5.75	122.35	118.90
4	4	645	C	N1-C2-O2	5.75	122.35	118.90
4	4	2825	C	N1-C2-O2	5.75	122.35	118.90
1	1	863	U	C2-N1-C1'	5.74	124.59	117.70
4	4	2791	C	N1-C2-O2	5.74	122.34	118.90
58	y	13	LEU	CA-CB-CG	5.74	128.50	115.30
4	4	2105	C	C6-N1-C2	-5.71	118.02	120.30
1	1	1075	C	N1-C2-O2	5.70	122.32	118.90
17	J	58	PRO	N-CA-C	5.69	126.90	112.10
4	4	860	U	C2-N1-C1'	5.69	124.53	117.70
4	4	2321	G	C8-N9-C1'	-5.67	119.62	127.00
4	4	654(D)	G	C4-N9-C1'	5.66	133.86	126.50
4	4	752	A	P-O3'-C3'	5.66	126.49	119.70
1	1	1115	C	N1-C2-O2	5.66	122.29	118.90
1	1	1344	C	N1-C2-O2	5.64	122.28	118.90
1	1	1352	C	N3-C2-O2	-5.64	117.95	121.90
5	5	38	C	C2-N1-C1'	5.64	125.00	118.80
4	4	1294	U	N1-C2-O2	5.63	126.74	122.80
1	1	692	U	O4'-C1'-N1	5.62	112.70	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	1882	C	C2-N1-C1'	5.61	124.97	118.80
4	4	1919	A	P-O3'-C3'	5.59	126.41	119.70
1	1	1059	C	C2-N1-C1'	5.58	124.94	118.80
4	4	1914	C	N1-C2-O2	5.58	122.25	118.90
4	4	2104	G	N3-C4-N9	5.58	129.35	126.00
1	1	948	C	C2-N1-C1'	5.57	124.92	118.80
44	k	171	LEU	CA-CB-CG	5.55	128.07	115.30
4	4	69	C	N1-C2-O2	5.55	122.23	118.90
4	4	2814	C	N3-C2-O2	-5.55	118.02	121.90
6	6	61	LEU	CA-CB-CG	5.54	128.04	115.30
1	1	620	C	N1-C2-O2	5.54	122.22	118.90
4	4	1180	C	N1-C2-O2	5.54	122.22	118.90
4	4	2421	G	C4-N9-C1'	5.53	133.69	126.50
4	4	1404	C	C2-N1-C1'	5.52	124.88	118.80
1	1	110	C	N3-C2-O2	-5.52	118.03	121.90
4	4	758	C	N1-C2-O2	5.51	122.21	118.90
4	4	1075	C	N1-C2-O2	5.51	122.21	118.90
5	5	31	C	C6-N1-C2	-5.51	118.10	120.30
4	4	2321	G	C2-N3-C4	5.50	114.65	111.90
1	1	624	C	N3-C2-O2	-5.50	118.05	121.90
4	4	807	U	N1-C2-O2	5.50	126.65	122.80
1	1	1170	A	N3-C4-N9	5.49	131.79	127.40
1	1	697	U	N1-C2-O2	5.49	126.64	122.80
4	4	1993	U	N3-C2-O2	-5.48	118.36	122.20
4	4	1294	U	N3-C2-O2	-5.48	118.36	122.20
4	4	2771	C	N3-C2-O2	-5.47	118.07	121.90
4	4	1931	U	N1-C2-O2	5.46	126.62	122.80
1	1	307	C	N3-C2-O2	-5.46	118.08	121.90
4	4	758	C	N3-C2-O2	-5.46	118.08	121.90
4	4	1021	A	C2-N3-C4	5.45	113.33	110.60
4	4	1923	U	N3-C2-O2	-5.45	118.39	122.20
4	4	2063	C	C2-N1-C1'	5.45	124.79	118.80
4	4	1075	C	C6-N1-C2	-5.44	118.12	120.30
17	J	57	THR	N-CA-C	5.43	125.65	111.00
4	4	650	C	N1-C2-O2	5.42	122.15	118.90
4	4	2752	C	N1-C2-O2	5.42	122.15	118.90
1	1	1127	G	C8-N9-C1'	-5.40	119.98	127.00
4	4	1055	G	C4-N9-C1'	5.40	133.52	126.50
1	1	1097	C	C5-C6-N1	5.39	123.70	121.00
40	g	244	ARG	CA-CB-CG	5.39	125.27	113.40
4	4	114	U	N1-C2-O2	5.39	126.57	122.80
4	4	2720	U	N3-C2-O2	-5.39	118.43	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	7	109	ILE	CG1-CB-CG2	-5.38	99.57	111.40
4	4	527	C	N3-C2-O2	-5.38	118.14	121.90
1	1	1285	A	C2-N3-C4	5.37	113.29	110.60
4	4	2104	G	N3-C4-C5	-5.37	125.92	128.60
4	4	1881	C	C2-N1-C1'	5.37	124.70	118.80
5	5	24	G	P-O3'-C3'	5.37	126.14	119.70
4	4	2179	C	C6-N1-C2	-5.37	118.15	120.30
1	1	91	C	N1-C2-O2	5.36	122.11	118.90
4	4	104	U	N3-C2-O2	-5.36	118.45	122.20
1	1	948	C	C6-N1-C2	-5.36	118.16	120.30
4	4	1541	G	C2-N3-C4	5.36	114.58	111.90
4	4	343	C	C6-N1-C2	-5.35	118.16	120.30
4	4	1514	U	C2-N1-C1'	5.35	124.12	117.70
4	4	1893	C	N3-C2-O2	-5.34	118.16	121.90
4	4	2294	C	N1-C2-O2	5.33	122.10	118.90
1	1	433	C	N1-C2-O2	5.33	122.10	118.90
1	1	624	C	N1-C2-O2	5.33	122.10	118.90
4	4	654(D)	G	N3-C4-C5	-5.32	125.94	128.60
4	4	1055	G	N3-C4-C5	-5.32	125.94	128.60
4	4	2715	C	C2-N1-C1'	5.32	124.65	118.80
4	4	719	C	N1-C2-O2	5.32	122.09	118.90
4	4	2559	C	N1-C2-O2	5.30	122.08	118.90
4	4	2556	C	N3-C2-O2	-5.30	118.19	121.90
4	4	2703	C	C6-N1-C2	-5.30	118.18	120.30
5	5	37	C	N3-C2-O2	-5.30	118.19	121.90
4	4	2284	C	C2-N1-C1'	5.30	124.63	118.80
38	e	11	CYS	CA-CB-SG	5.28	123.51	114.00
4	4	2099	U	C2-N1-C1'	5.28	124.03	117.70
1	1	936	C	N1-C2-O2	5.27	122.06	118.90
1	1	982	U	N1-C2-O2	5.26	126.48	122.80
4	4	243	U	N1-C2-O2	5.26	126.48	122.80
43	j	94	LEU	CA-CB-CG	5.26	127.40	115.30
4	4	1180	C	C6-N1-C2	-5.24	118.20	120.30
2	2	3	C	C6-N1-C2	-5.24	118.20	120.30
1	1	1282	C	C5-C6-N1	5.24	123.62	121.00
5	5	37	C	C2-N1-C1'	5.23	124.56	118.80
4	4	1722	A	C2-N3-C4	5.23	113.22	110.60
4	4	2681	C	C2-N1-C1'	5.21	124.53	118.80
1	1	1303	C	C2-N1-C1'	5.21	124.53	118.80
1	1	1492	A	C2-N3-C4	5.21	113.21	110.60
1	1	982	U	C2-N1-C1'	5.20	123.94	117.70
4	4	654(D)	G	N3-C4-N9	5.20	129.12	126.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	373	U	N3-C2-O2	-5.20	118.56	122.20
4	4	2720	U	N1-C2-O2	5.20	126.44	122.80
4	4	1294	U	C2-N1-C1'	5.19	123.93	117.70
4	4	275	G	C8-N9-C1'	-5.18	120.27	127.00
57	x	63	ASP	CB-CG-OD1	5.17	122.95	118.30
4	4	1982	C	N1-C2-O2	5.17	122.00	118.90
1	1	1127	G	C2-N3-C4	5.16	114.48	111.90
1	1	904	C	N1-C2-O2	5.16	122.00	118.90
1	1	764	C	C6-N1-C2	-5.15	118.24	120.30
4	4	373	U	N1-C2-O2	5.15	126.40	122.80
4	4	41	C	N1-C2-O2	5.15	121.99	118.90
7	7	84	GLY	C-N-CA	5.14	134.56	121.70
4	4	1092	C	N1-C2-O2	5.14	121.98	118.90
4	4	2681	C	N1-C2-O2	5.13	121.98	118.90
19	L	66	LEU	CA-CB-CG	5.13	127.11	115.30
1	1	948	C	N3-C2-O2	-5.13	118.31	121.90
1	1	563	A	C4-N9-C1'	5.12	135.52	126.30
1	1	936	C	C2-N1-C1'	5.12	124.44	118.80
5	5	30	C	N3-C2-O2	-5.12	118.32	121.90
4	4	543	C	C6-N1-C2	-5.11	118.25	120.30
43	j	86	MET	CA-CB-CG	5.11	121.99	113.30
41	h	60	ASN	C-N-CA	5.11	134.47	121.70
19	L	19	LEU	CA-CB-CG	5.10	127.04	115.30
4	4	924	C	N1-C2-O2	5.10	121.96	118.90
4	4	1313	U	C2-N1-C1'	5.10	123.81	117.70
28	U	457	LEU	CA-CB-CG	5.09	127.01	115.30
4	4	2769	C	C6-N1-C1'	-5.09	114.69	120.80
1	1	982	U	OP2-P-O3'	5.09	116.39	105.20
4	4	2421	G	N3-C4-C5	-5.09	126.06	128.60
1	1	365	U	N3-C2-O2	-5.08	118.64	122.20
1	1	863	U	N3-C2-O2	-5.08	118.64	122.20
4	4	1931	U	N3-C2-O2	-5.08	118.65	122.20
4	4	1512	U	C2-N1-C1'	5.07	123.79	117.70
4	4	1781	C	N1-C2-O2	5.07	121.94	118.90
4	4	2471	C	N1-C2-O2	5.07	121.94	118.90
4	4	1923	U	C2-N1-C1'	5.07	123.78	117.70
1	1	528	C	C2-N1-C1'	5.06	124.37	118.80
4	4	1370	C	C2-N1-C1'	5.06	124.37	118.80
8	A	149	LEU	CA-CB-CG	5.05	126.93	115.30
6	6	13	GLU	C-N-CA	5.05	134.32	121.70
4	4	2254	C	N3-C2-O2	-5.04	118.37	121.90
1	1	235	C	N3-C2-O2	-5.04	118.37	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4	343	C	N1-C2-O2	5.04	121.92	118.90
4	4	2871	C	N3-C2-O2	-5.03	118.38	121.90
1	1	1218	C	P-O3'-C3'	5.03	125.74	119.70
4	4	1075	C	C6-N1-C1'	-5.02	114.77	120.80
4	4	2871	C	N1-C2-O2	5.02	121.91	118.90
19	L	11	ARG	CA-CB-CG	5.02	124.44	113.40
4	4	749	C	N1-C2-O2	5.02	121.91	118.90
1	1	235	C	N1-C2-O2	5.00	121.90	118.90
1	1	1352	C	C6-N1-C2	-5.00	118.30	120.30
1	1	1026	G	C4-N9-C1'	5.00	133.00	126.50

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	6	123	ASP	Peptide
6	6	14	LYS	Peptide
6	6	142	SER	Peptide
7	7	133	HIS	Peptide
8	A	156	LYS	Peptide
8	A	157	ARG	Peptide
9	B	18	TRP	Peptide
13	F	121	ALA	Peptide
13	F	80	VAL	Peptide
14	G	81	HIS	Peptide
23	P	65	ILE	Peptide
28	U	183	MET	Peptide
28	U	352	VAL	Peptide
28	U	533	VAL	Peptide
29	V	71	ASP	Peptide
33	Z	40	HIS	Peptide
40	g	244	ARG	Peptide
40	g	245	PRO	Peptide
41	h	144	ARG	Peptide
41	h	51	PHE	Peptide
41	h	61	ARG	Peptide
43	j	141	PHE	Peptide
43	j	172	LEU	Peptide
44	k	20	ALA	Peptide
44	k	9	ILE	Peptide
45	l	55	UNK	Peptide
50	q	18	ARG	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
57	x	6	ILE	Peptide
58	y	6	ASP	Peptide
58	y	7	VAL	Peptide
59	z	55	TYR	Peptide
59	z	62	GLU	Peptide
59	z	81	LYS	Peptide
59	z	83	THR	Peptide
59	z	97	ARG	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
6	6	176/178 (99%)	134 (76%)	38 (22%)	4 (2%)	6 38
7	7	144/146 (99%)	124 (86%)	20 (14%)	0	100 100
8	A	233/235 (99%)	203 (87%)	29 (12%)	1 (0%)	34 70
9	B	205/207 (99%)	170 (83%)	35 (17%)	0	100 100
10	C	206/208 (99%)	190 (92%)	16 (8%)	0	100 100
11	D	149/151 (99%)	144 (97%)	5 (3%)	0	100 100
12	E	99/101 (98%)	93 (94%)	6 (6%)	0	100 100
13	F	153/155 (99%)	118 (77%)	34 (22%)	1 (1%)	22 60
14	G	136/138 (99%)	122 (90%)	14 (10%)	0	100 100
15	H	125/127 (98%)	109 (87%)	16 (13%)	0	100 100
16	I	97/99 (98%)	87 (90%)	10 (10%)	0	100 100
17	J	117/119 (98%)	100 (86%)	16 (14%)	1 (1%)	17 54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	K	123/125 (98%)	114 (93%)	9 (7%)	0	100	100
19	L	117/119 (98%)	101 (86%)	15 (13%)	1 (1%)	17	54
20	M	58/60 (97%)	47 (81%)	11 (19%)	0	100	100
21	N	86/88 (98%)	79 (92%)	7 (8%)	0	100	100
22	O	82/84 (98%)	73 (89%)	8 (10%)	1 (1%)	13	50
23	P	98/100 (98%)	93 (95%)	4 (4%)	1 (1%)	15	52
24	Q	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
25	R	86/88 (98%)	76 (88%)	10 (12%)	0	100	100
26	S	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
27	T	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
28	U	657/687 (96%)	555 (84%)	100 (15%)	2 (0%)	41	74
29	V	76/78 (97%)	68 (90%)	8 (10%)	0	100	100
30	W	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
31	X	69/71 (97%)	65 (94%)	4 (6%)	0	100	100
32	Y	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
33	Z	69/71 (97%)	40 (58%)	29 (42%)	0	100	100
34	a	57/59 (97%)	50 (88%)	7 (12%)	0	100	100
35	b	48/50 (96%)	36 (75%)	12 (25%)	0	100	100
36	c	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
37	d	62/64 (97%)	50 (81%)	12 (19%)	0	100	100
38	e	35/37 (95%)	30 (86%)	4 (11%)	1 (3%)	4	34
39	f	225/227 (99%)	189 (84%)	36 (16%)	0	100	100
40	g	273/275 (99%)	244 (89%)	28 (10%)	1 (0%)	34	70
41	h	203/205 (99%)	172 (85%)	31 (15%)	0	100	100
42	i	206/208 (99%)	187 (91%)	19 (9%)	0	100	100
43	j	177/179 (99%)	145 (82%)	31 (18%)	1 (1%)	25	62
44	k	174/176 (99%)	148 (85%)	25 (14%)	1 (1%)	25	62
45	l	1/130 (1%)	1 (100%)	0	0	100	100
48	o	137/139 (99%)	126 (92%)	11 (8%)	0	100	100
49	p	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
50	q	148/150 (99%)	120 (81%)	28 (19%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	r	139/141 (99%)	127 (91%)	12 (9%)	0	100	100
52	s	116/118 (98%)	104 (90%)	12 (10%)	0	100	100
53	t	97/99 (98%)	86 (89%)	11 (11%)	0	100	100
54	u	136/138 (99%)	121 (89%)	15 (11%)	0	100	100
55	v	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
56	w	99/101 (98%)	88 (89%)	11 (11%)	0	100	100
57	x	111/113 (98%)	102 (92%)	8 (7%)	1 (1%)	17	54
58	y	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	14	51
59	z	99/101 (98%)	72 (73%)	25 (25%)	2 (2%)	7	41
All	All	6614/6873 (96%)	5765 (87%)	829 (12%)	20 (0%)	44	74

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
59	z	98	VAL
19	L	106	ASN
22	O	83	GLU
28	U	146	LEU
38	e	12	ASP
40	g	245	PRO
28	U	353	ALA
6	6	79	ARG
8	A	240	GLN
13	F	151	TYR
23	P	66	SER
44	k	170	ARG
59	z	39	VAL
43	j	142	PRO
6	6	15	PRO
17	J	58	PRO
58	y	8	ILE
57	x	6	ILE
6	6	124	ILE
6	6	111	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	6	157/157 (100%)	155 (99%)	2 (1%)	69	82
7	7	122/122 (100%)	121 (99%)	1 (1%)	81	89
8	A	202/203 (100%)	195 (96%)	7 (4%)	36	64
9	B	160/161 (99%)	152 (95%)	8 (5%)	24	55
10	C	180/180 (100%)	176 (98%)	4 (2%)	52	72
11	D	115/116 (99%)	112 (97%)	3 (3%)	46	69
12	E	90/90 (100%)	86 (96%)	4 (4%)	28	57
13	F	126/126 (100%)	121 (96%)	5 (4%)	31	59
14	G	119/119 (100%)	115 (97%)	4 (3%)	37	64
15	H	98/98 (100%)	97 (99%)	1 (1%)	76	86
16	I	88/89 (99%)	87 (99%)	1 (1%)	73	85
17	J	90/90 (100%)	87 (97%)	3 (3%)	38	65
18	K	104/104 (100%)	100 (96%)	4 (4%)	33	61
19	L	94/95 (99%)	90 (96%)	4 (4%)	29	58
20	M	49/49 (100%)	48 (98%)	1 (2%)	55	75
21	N	79/79 (100%)	79 (100%)	0	100	100
22	O	72/72 (100%)	70 (97%)	2 (3%)	43	68
23	P	94/95 (99%)	94 (100%)	0	100	100
24	Q	61/61 (100%)	59 (97%)	2 (3%)	38	65
25	R	74/75 (99%)	71 (96%)	3 (4%)	30	59
26	S	76/76 (100%)	75 (99%)	1 (1%)	69	82
27	T	19/20 (95%)	18 (95%)	1 (5%)	22	54
28	U	558/579 (96%)	548 (98%)	10 (2%)	59	77
29	V	62/62 (100%)	60 (97%)	2 (3%)	39	65
30	W	78/79 (99%)	75 (96%)	3 (4%)	33	61
31	X	66/66 (100%)	62 (94%)	4 (6%)	18	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Y	51/52 (98%)	51 (100%)	0	100	100
33	Z	63/63 (100%)	60 (95%)	3 (5%)	25	56
34	a	51/51 (100%)	49 (96%)	2 (4%)	32	60
35	b	49/49 (100%)	48 (98%)	1 (2%)	55	75
36	c	41/41 (100%)	39 (95%)	2 (5%)	25	55
37	d	53/54 (98%)	51 (96%)	2 (4%)	33	61
38	e	34/34 (100%)	32 (94%)	2 (6%)	19	51
39	f	179/179 (100%)	178 (99%)	1 (1%)	86	92
40	g	217/217 (100%)	214 (99%)	3 (1%)	67	81
41	h	165/165 (100%)	164 (99%)	1 (1%)	86	92
42	i	165/165 (100%)	164 (99%)	1 (1%)	86	92
43	j	153/153 (100%)	146 (95%)	7 (5%)	27	56
44	k	146/146 (100%)	145 (99%)	1 (1%)	84	91
45	l	1/1 (100%)	1 (100%)	0	100	100
48	o	117/118 (99%)	117 (100%)	0	100	100
49	p	100/100 (100%)	100 (100%)	0	100	100
50	q	116/116 (100%)	112 (97%)	4 (3%)	37	64
51	r	111/111 (100%)	109 (98%)	2 (2%)	59	77
52	s	101/101 (100%)	98 (97%)	3 (3%)	41	66
53	t	77/77 (100%)	73 (95%)	4 (5%)	23	54
54	u	120/120 (100%)	114 (95%)	6 (5%)	24	55
55	v	92/93 (99%)	90 (98%)	2 (2%)	52	72
56	w	82/82 (100%)	81 (99%)	1 (1%)	71	84
57	x	91/92 (99%)	90 (99%)	1 (1%)	73	85
58	y	74/75 (99%)	73 (99%)	1 (1%)	67	81
59	z	84/85 (99%)	83 (99%)	1 (1%)	71	84
All	All	5566/5603 (99%)	5435 (98%)	131 (2%)	51	71

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	20	ARG
6	6	28	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	7	113	ARG
8	A	30	ARG
8	A	63	MET
8	A	83	MET
8	A	144	ARG
8	A	149	LEU
8	A	175	ARG
8	A	226	ARG
9	B	38	ARG
9	B	83	ARG
9	B	85	ARG
9	B	127	ARG
9	B	132	ARG
9	B	140	ARG
9	B	164	ARG
9	B	179	ARG
10	C	3	ARG
10	C	25	ARG
10	C	165	MET
10	C	187	ARG
11	D	10	MET
11	D	24	ARG
11	D	64	ARG
12	E	1	MET
12	E	2	ARG
12	E	67	MET
12	E	71	ARG
13	F	3	ARG
13	F	10	ARG
13	F	32	ARG
13	F	48	LYS
13	F	84	ASN
14	G	37	ARG
14	G	68	ARG
14	G	69	ARG
14	G	116	LYS
15	H	128	ARG
16	I	60	ARG
17	J	57	THR
17	J	117	ASN
17	J	120	ARG
18	K	20	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	K	41	ARG
18	K	89	ARG
18	K	114	LYS
19	L	11	ARG
19	L	80	ARG
19	L	96	LEU
19	L	104	ARG
20	M	45	ARG
22	O	5	ARG
22	O	8	ARG
24	Q	64	ARG
24	Q	87	ARG
25	R	36	ARG
25	R	37	ARG
25	R	65	ASN
26	S	34	LYS
27	T	10	ARG
28	U	11	ARG
28	U	38	ARG
28	U	132	ARG
28	U	141	LYS
28	U	160	ARG
28	U	183	MET
28	U	284	LEU
28	U	351	ARG
28	U	357	ARG
28	U	588	MET
29	V	14	ARG
29	V	74	ARG
30	W	26	ARG
30	W	40	ARG
30	W	92	LYS
31	X	26	ARG
31	X	53	LEU
31	X	65	ASN
31	X	69	ARG
33	Z	38	LYS
33	Z	58	ARG
33	Z	71	ARG
34	a	40	LYS
34	a	56	LYS
35	b	25	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	c	1	MET
36	c	10	ARG
37	d	47	LYS
37	d	59	LYS
38	e	18	ARG
38	e	22	ARG
39	f	7	ARG
40	g	35	LYS
40	g	43	ARG
40	g	203	ASN
41	h	57	LYS
42	i	38	ARG
43	j	22	ARG
43	j	51	ARG
43	j	83	ARG
43	j	86	MET
43	j	95	ARG
43	j	155	MET
43	j	170	ARG
44	k	97	ARG
50	q	7	ARG
50	q	49	ARG
50	q	67	MET
50	q	81	GLN
51	r	3	MET
51	r	133	ARG
52	s	2	ARG
52	s	86	ARG
52	s	105	ARG
53	t	13	ARG
53	t	23	ARG
53	t	25	ARG
53	t	97	ARG
54	u	39	ARG
54	u	51	ARG
54	u	54	ARG
54	u	99	LEU
54	u	108	ARG
54	u	111	ARG
55	v	3	ARG
55	v	95	LEU
56	w	100	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
57	x	40	ASN
58	y	76	ARG
59	z	101	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
7	7	17	GLN
7	7	28	ASN
12	E	7	ASN
13	F	97	GLN
20	M	49	HIS
23	P	26	GLN
23	P	94	ASN
28	U	165	GLN
28	U	362	HIS
28	U	625	ASN
28	U	664	GLN
29	V	29	GLN
40	g	96	HIS
40	g	203	ASN
41	h	129	HIS
41	h	132	HIS
41	h	143	ASN
43	j	132	ASN
48	o	56	ASN
48	o	128	HIS
49	p	82	ASN
50	q	81	GLN
51	r	12	GLN
51	r	123	HIS
51	r	141	GLN
54	u	58	ASN
59	z	6	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1506/1507 (99%)	395 (26%)	11 (0%)
2	2	75/76 (98%)	27 (36%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	3	9/15 (60%)	7 (77%)	1 (11%)
4	4	2900/2901 (99%)	544 (18%)	10 (0%)
5	5	118/119 (99%)	36 (30%)	4 (3%)
All	All	4608/4618 (99%)	1009 (21%)	26 (0%)

All (1009) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	8	A
1	1	9	G
1	1	32	A
1	1	39	G
1	1	41	G
1	1	47	C
1	1	48	C
1	1	50	A
1	1	51	A
1	1	65	U
1	1	66	G
1	1	80	G
1	1	81	U
1	1	83	U
1	1	84	U
1	1	88	A
1	1	89	C
1	1	90	U
1	1	91	C
1	1	97	G
1	1	110	C
1	1	121	C
1	1	129(A)	G
1	1	131	C
1	1	134	A
1	1	135	C
1	1	139	G
1	1	145	G
1	1	152	A
1	1	173	U
1	1	189(C)	C
1	1	189(E)	U
1	1	189(F)	U
1	1	189(G)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	189(H)	G
1	1	189(I)	G
1	1	195	A
1	1	197	A
1	1	198	G
1	1	204	U
1	1	216	G
1	1	217	C
1	1	236	G
1	1	247	G
1	1	251	G
1	1	266	G
1	1	267	C
1	1	274	A
1	1	280	C
1	1	289	G
1	1	306	G
1	1	321	A
1	1	328	C
1	1	332	G
1	1	344	A
1	1	345	C
1	1	346	G
1	1	350	G
1	1	351	G
1	1	352	C
1	1	354	G
1	1	365	U
1	1	368	U
1	1	372	C
1	1	373	A
1	1	388	G
1	1	390	C
1	1	393	A
1	1	397	A
1	1	398	C
1	1	409	G
1	1	411	A
1	1	414	A
1	1	421	U
1	1	422	C
1	1	423	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	424	G
1	1	428	G
1	1	429	U
1	1	433	C
1	1	438	G
1	1	439	A
1	1	452	A
1	1	455	C
1	1	470	C
1	1	472	A
1	1	484	G
1	1	491	G
1	1	497	A
1	1	498	U
1	1	499	A
1	1	510	A
1	1	511	C
1	1	512	U
1	1	521	G
1	1	524	G
1	1	527	G
1	1	531	U
1	1	547	A
1	1	559	A
1	1	564	C
1	1	572	A
1	1	573	A
1	1	574	A
1	1	575	G
1	1	576	G
1	1	577	G
1	1	586	C
1	1	588	G
1	1	633	G
1	1	650	G
1	1	653	A
1	1	661	G
1	1	662	G
1	1	665	A
1	1	673	G
1	1	679	C
1	1	681	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	682	G
1	1	695	A
1	1	700	G
1	1	701	C
1	1	703	G
1	1	704	A
1	1	707	C
1	1	712	A
1	1	713	G
1	1	717	C
1	1	718	G
1	1	720	C
1	1	722	A
1	1	723	U
1	1	724	G
1	1	750	G
1	1	753	A
1	1	755	G
1	1	758	G
1	1	777	A
1	1	781	A
1	1	792	A
1	1	793	U
1	1	794	A
1	1	799	G
1	1	802	A
1	1	810	C
1	1	812	C
1	1	813	U
1	1	817	C
1	1	818	G
1	1	828	A
1	1	840	C
1	1	841	U
1	1	848	C
1	1	872	A
1	1	873	A
1	1	876	G
1	1	889	A
1	1	902	G
1	1	907	A
1	1	916	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	934	C
1	1	935	A
1	1	937	A
1	1	938	A
1	1	941	G
1	1	944	G
1	1	945	G
1	1	948	C
1	1	951	G
1	1	954	G
1	1	956	U
1	1	957	U
1	1	958	A
1	1	960	U
1	1	961	U
1	1	962	C
1	1	969	A
1	1	971	G
1	1	972	C
1	1	974	A
1	1	975	A
1	1	976	G
1	1	977	A
1	1	978	A
1	1	979	C
1	1	980	C
1	1	981	U
1	1	983	A
1	1	984	C
1	1	985	C
1	1	987	G
1	1	990	C
1	1	991	U
1	1	992	U
1	1	993	G
1	1	994	A
1	1	995	C
1	1	996	A
1	1	998	G
1	1	1000	U
1	1	1001	A
1	1	1001(A)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1003	G
1	1	1004	A
1	1	1005	A
1	1	1007	C
1	1	1008	C
1	1	1009	G
1	1	1010	G
1	1	1011	G
1	1	1013	G
1	1	1014	A
1	1	1016	A
1	1	1018	C
1	1	1022	G
1	1	1023	G
1	1	1024	G
1	1	1027	C
1	1	1028	C
1	1	1030	C
1	1	1030(C)	G
1	1	1030(D)	A
1	1	1033	G
1	1	1034	G
1	1	1036	G
1	1	1039	C
1	1	1043	C
1	1	1054	C
1	1	1055	A
1	1	1057	G
1	1	1059	C
1	1	1065	U
1	1	1081	G
1	1	1084	G
1	1	1094	G
1	1	1095	U
1	1	1101	A
1	1	1104	G
1	1	1113	C
1	1	1114	C
1	1	1115	C
1	1	1122	U
1	1	1123	A
1	1	1125	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1126	U
1	1	1127	G
1	1	1128	C
1	1	1129	C
1	1	1130	A
1	1	1131	G
1	1	1132	C
1	1	1133	G
1	1	1134	G
1	1	1136	U
1	1	1138	G
1	1	1139	G
1	1	1140	C
1	1	1142	G
1	1	1145	C
1	1	1146	A
1	1	1149	C
1	1	1151	A
1	1	1156	G
1	1	1157	A
1	1	1158	C
1	1	1159	U
1	1	1170	A
1	1	1171	G
1	1	1172	C
1	1	1174	G
1	1	1181	G
1	1	1184	G
1	1	1190	G
1	1	1196	U
1	1	1197	G
1	1	1200	C
1	1	1201	A
1	1	1202	G
1	1	1211	U
1	1	1212	U
1	1	1214	C
1	1	1217	C
1	1	1218	C
1	1	1219	U
1	1	1220	G
1	1	1224	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1225	A
1	1	1228	C
1	1	1229	A
1	1	1230	C
1	1	1232	U
1	1	1233	G
1	1	1234	C
1	1	1236	A
1	1	1238	A
1	1	1239	A
1	1	1240	U
1	1	1241	G
1	1	1243	C
1	1	1244	C
1	1	1245	A
1	1	1250	A
1	1	1252	A
1	1	1255	G
1	1	1257	U
1	1	1258	G
1	1	1263	C
1	1	1265	G
1	1	1266	G
1	1	1267	C
1	1	1268	A
1	1	1269	A
1	1	1273	G
1	1	1276	G
1	1	1278	U
1	1	1279	A
1	1	1280	A
1	1	1284	C
1	1	1285	A
1	1	1286	A
1	1	1287	A
1	1	1288	A
1	1	1290	G
1	1	1291	G
1	1	1292	U
1	1	1293	G
1	1	1295	G
1	1	1297	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1298	C
1	1	1299	A
1	1	1300	G
1	1	1301	U
1	1	1302	U
1	1	1303	C
1	1	1310	G
1	1	1314	C
1	1	1315	U
1	1	1317	C
1	1	1318	A
1	1	1319	A
1	1	1321	C
1	1	1322	C
1	1	1323	G
1	1	1325	C
1	1	1326	C
1	1	1328	C
1	1	1329	A
1	1	1331	G
1	1	1334	G
1	1	1337	G
1	1	1339	A
1	1	1341	U
1	1	1342	C
1	1	1343	G
1	1	1346	A
1	1	1351	U
1	1	1356	G
1	1	1357	A
1	1	1358	U
1	1	1359	C
1	1	1362	C
1	1	1363(A)	A
1	1	1364	U
1	1	1368	G
1	1	1370	G
1	1	1371	G
1	1	1374	A
1	1	1375	A
1	1	1376	U
1	1	1381	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1382	C
1	1	1384	C
1	1	1385	G
1	1	1398	A
1	1	1419	G
1	1	1441	G
1	1	1444	C
1	1	1446	U
1	1	1452	C
1	1	1456	G
1	1	1457	G
1	1	1492	A
1	1	1493	A
1	1	1494	G
1	1	1502	A
1	1	1503	A
1	1	1504	G
1	1	1506	U
1	1	1517	G
1	1	1529	G
1	1	1530	G
1	1	1531	A
1	1	1532	U
1	1	1533	C
1	1	1534	A
2	2	6	G
2	2	8	U
2	2	9	A
2	2	10	G
2	2	12	U
2	2	14	A
2	2	15	G
2	2	17	C
2	2	18	G
2	2	19	G
2	2	20	U
2	2	21	A
2	2	25	C
2	2	29	G
2	2	32	U
2	2	36	A
2	2	37	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	2	40	C
2	2	44	G
2	2	46	G
2	2	54	U
2	2	55	U
2	2	56	C
2	2	60	U
2	2	64	A
2	2	65	G
2	2	75	C
3	3	7	U
3	3	9	A
3	3	11	G
3	3	12	U
3	3	13	U
3	3	14	U
3	3	15	U
4	4	10	G
4	4	11	G
4	4	13	A
4	4	14	A
4	4	27	G
4	4	32	C
4	4	34	C
4	4	41	C
4	4	45	C
4	4	55	G
4	4	64	A
4	4	71	A
4	4	74	A
4	4	75	G
4	4	84	A
4	4	88	G
4	4	92	A
4	4	110	G
4	4	114	U
4	4	118	A
4	4	120	U
4	4	122	G
4	4	125	G
4	4	128	C
4	4	131	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	139(A)	G
4	4	141	A
4	4	156	U
4	4	158	U
4	4	196	A
4	4	197	A
4	4	199	A
4	4	200	U
4	4	205	G
4	4	215	G
4	4	216	A
4	4	222	A
4	4	227	A
4	4	228	A
4	4	229	A
4	4	245	G
4	4	248	G
4	4	252	G
4	4	265	A
4	4	267	C
4	4	271(B)	C
4	4	271(L)	U
4	4	271(M)	G
4	4	271(N)	U
4	4	271(X)	G
4	4	271(Y)	U
4	4	276	A
4	4	277	C
4	4	278	A
4	4	283	A
4	4	295	G
4	4	302	C
4	4	311	A
4	4	317	G
4	4	323	G
4	4	329	G
4	4	330	A
4	4	339	U
4	4	345	A
4	4	346	A
4	4	352	G
4	4	353	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	362	U
4	4	363	G
4	4	371	A
4	4	372	G
4	4	380	U
4	4	386	G
4	4	387	U
4	4	396	G
4	4	404	C
4	4	405	U
4	4	411	G
4	4	412	A
4	4	422	A
4	4	428	A
4	4	437	G
4	4	446	G
4	4	451	C
4	4	457	A
4	4	458	G
4	4	467	G
4	4	479	A
4	4	481	G
4	4	494	G
4	4	496	G
4	4	505	A
4	4	508	G
4	4	509	C
4	4	512	G
4	4	518	G
4	4	525	U
4	4	531	C
4	4	532	A
4	4	533	G
4	4	556	G
4	4	563	G
4	4	568	U
4	4	571	A
4	4	573	G
4	4	575	A
4	4	588	U
4	4	603	A
4	4	614(B)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	614(C)	A
4	4	615	G
4	4	620	G
4	4	622	G
4	4	637	A
4	4	645	C
4	4	650	C
4	4	651	G
4	4	654	A
4	4	654(A)	G
4	4	654(B)	C
4	4	654(C)	G
4	4	654(D)	G
4	4	654(E)	G
4	4	654(F)	C
4	4	654(G)	C
4	4	654(I)	C
4	4	654(J)	A
4	4	654(L)	G
4	4	654(M)	C
4	4	654(Q)	C
4	4	654(R)	C
4	4	654(T)	C
4	4	655	A
4	4	670	A
4	4	686	G
4	4	726	G
4	4	729	G
4	4	730	C
4	4	740	U
4	4	748	G
4	4	753	C
4	4	764	A
4	4	765	G
4	4	774	A
4	4	775	G
4	4	776	G
4	4	782	A
4	4	784	A
4	4	785	G
4	4	790	C
4	4	792	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	800	A
4	4	805	G
4	4	806	C
4	4	812	C
4	4	819	A
4	4	826	U
4	4	827	U
4	4	828	U
4	4	830	G
4	4	855	G
4	4	857	C
4	4	859	G
4	4	866	A
4	4	873	G
4	4	881	G
4	4	882	G
4	4	884	C
4	4	885	C
4	4	887	A
4	4	888	C
4	4	889	C
4	4	890	A
4	4	892	G
4	4	893	C
4	4	896	A
4	4	897	C
4	4	906	G
4	4	910	A
4	4	915	C
4	4	932	G
4	4	945	A
4	4	946	G
4	4	953	A
4	4	957	A
4	4	961	C
4	4	973	A
4	4	974	G
4	4	975	C
4	4	980	A
4	4	983	A
4	4	985	C
4	4	989	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	996	A
4	4	1009	A
4	4	1011	G
4	4	1013	C
4	4	1015	G
4	4	1022	G
4	4	1025	G
4	4	1026	U
4	4	1027	A
4	4	1033	U
4	4	1045	A
4	4	1046	A
4	4	1051	G
4	4	1055	G
4	4	1059	G
4	4	1060	U
4	4	1061	U
4	4	1064	C
4	4	1065	U
4	4	1066	U
4	4	1068	G
4	4	1070	A
4	4	1071	G
4	4	1077	A
4	4	1078	U
4	4	1080	C
4	4	1084	A
4	4	1085	A
4	4	1087	G
4	4	1088	A
4	4	1090	U
4	4	1092	C
4	4	1094	U
4	4	1097	U
4	4	1102	C
4	4	1103	A
4	4	1106	G
4	4	1116	C
4	4	1122	G
4	4	1127	A
4	4	1128	A
4	4	1130	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	1135	C
4	4	1136	G
4	4	1142(A)	A
4	4	1144	G
4	4	1148	A
4	4	1157	G
4	4	1173	G
4	4	1174	A
4	4	1175	U
4	4	1177	A
4	4	1186	G
4	4	1206	G
4	4	1210	A
4	4	1211	U
4	4	1212	G
4	4	1220	A
4	4	1225	G
4	4	1236	G
4	4	1247	A
4	4	1252	G
4	4	1253	A
4	4	1256	G
4	4	1265	A
4	4	1272	A
4	4	1273	U
4	4	1300	U
4	4	1301	A
4	4	1306	C
4	4	1314	C
4	4	1325	G
4	4	1329	U
4	4	1332	G
4	4	1333	C
4	4	1350	C
4	4	1359	A
4	4	1365	A
4	4	1368	G
4	4	1378	A
4	4	1384	A
4	4	1385	G
4	4	1395	A
4	4	1396	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	1398	C
4	4	1416	G
4	4	1417	C
4	4	1420	U
4	4	1427	A
4	4	1428	C
4	4	1445	A
4	4	1452	A
4	4	1455	G
4	4	1458	C
4	4	1460	A
4	4	1467	C
4	4	1478	G
4	4	1482	G
4	4	1490	A
4	4	1494	A
4	4	1504	C
4	4	1509	C
4	4	1509(A)	A
4	4	1531	C
4	4	1533	G
4	4	1537	G
4	4	1539	G
4	4	1540	U
4	4	1541	G
4	4	1547	C
4	4	1558	A
4	4	1566	A
4	4	1569	A
4	4	1584	C
4	4	1586	A
4	4	1607	C
4	4	1616	A
4	4	1640	C
4	4	1643	G
4	4	1648	C
4	4	1674	G
4	4	1694	C
4	4	1696	G
4	4	1703	G
4	4	1722	A
4	4	1739	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	1740	G
4	4	1741	A
4	4	1744	C
4	4	1746	G
4	4	1750	G
4	4	1762	A
4	4	1763	G
4	4	1764	G
4	4	1769	G
4	4	1773	A
4	4	1781	C
4	4	1799	G
4	4	1800	C
4	4	1801	G
4	4	1802	A
4	4	1815	A
4	4	1816	G
4	4	1828	G
4	4	1835	G
4	4	1847	A
4	4	1882	C
4	4	1885	A
4	4	1889	A
4	4	1899	G
4	4	1906	G
4	4	1913	A
4	4	1914	C
4	4	1917	U
4	4	1918	A
4	4	1919	A
4	4	1920	C
4	4	1925	C
4	4	1926	U
4	4	1929	G
4	4	1930	G
4	4	1931	U
4	4	1937	A
4	4	1938	A
4	4	1939	U
4	4	1940	U
4	4	1944	U
4	4	1955	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	1966	A
4	4	1967	C
4	4	1970	A
4	4	1971	A
4	4	1972	A
4	4	1981	A
4	4	1982	C
4	4	1991	U
4	4	1993	U
4	4	2013	A
4	4	2020	A
4	4	2021	C
4	4	2031	A
4	4	2032	G
4	4	2033	A
4	4	2035	G
4	4	2046	G
4	4	2052	G
4	4	2055	C
4	4	2056	G
4	4	2059	A
4	4	2060	A
4	4	2061	G
4	4	2062	A
4	4	2068	U
4	4	2069	G
4	4	2077	A
4	4	2093	G
4	4	2095	C
4	4	2102	U
4	4	2104	G
4	4	2109	U
4	4	2110	G
4	4	2113	U
4	4	2117	A
4	4	2119	A
4	4	2123	G
4	4	2125	G
4	4	2129	C
4	4	2130	U
4	4	2131	G
4	4	2133	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	2134	A
4	4	2135	A
4	4	2137	C
4	4	2139	C
4	4	2141	G
4	4	2145	C
4	4	2147	G
4	4	2153	G
4	4	2155	G
4	4	2158	A
4	4	2169	A
4	4	2170	A
4	4	2173	A
4	4	2174	C
4	4	2176	A
4	4	2180	U
4	4	2183	C
4	4	2184	G
4	4	2186	G
4	4	2187	G
4	4	2189	U
4	4	2190	G
4	4	2198	A
4	4	2206	G
4	4	2208	A
4	4	2218	U
4	4	2219	G
4	4	2225	A
4	4	2238	G
4	4	2239	G
4	4	2250	G
4	4	2266	A
4	4	2268	A
4	4	2279	G
4	4	2283	C
4	4	2285	C
4	4	2286	A
4	4	2287	A
4	4	2288	A
4	4	2305	A
4	4	2307	G
4	4	2308	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	2309	A
4	4	2319	G
4	4	2320	A
4	4	2325	G
4	4	2334	G
4	4	2335	A
4	4	2347	C
4	4	2350	C
4	4	2383	G
4	4	2385	C
4	4	2391	G
4	4	2406	U
4	4	2419	U
4	4	2421	G
4	4	2423	U
4	4	2425	A
4	4	2427	C
4	4	2428	G
4	4	2430	A
4	4	2432	A
4	4	2441	C
4	4	2445	G
4	4	2447	G
4	4	2448	A
4	4	2476	A
4	4	2478	A
4	4	2480	C
4	4	2494	G
4	4	2498	C
4	4	2503	A
4	4	2504	U
4	4	2505	G
4	4	2518	A
4	4	2520	C
4	4	2529	G
4	4	2535	G
4	4	2564	A
4	4	2566	A
4	4	2567	G
4	4	2572	A
4	4	2578	G
4	4	2602	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	2610	C
4	4	2611	U
4	4	2612	C
4	4	2630	G
4	4	2645	G
4	4	2646	C
4	4	2654	A
4	4	2682	U
4	4	2689	U
4	4	2690	C
4	4	2691	C
4	4	2702	U
4	4	2703	C
4	4	2712(A)	A
4	4	2713	A
4	4	2714	G
4	4	2715	C
4	4	2726	U
4	4	2727	G
4	4	2732	G
4	4	2733	A
4	4	2739	U
4	4	2744	G
4	4	2748	A
4	4	2752	C
4	4	2757	A
4	4	2761	G
4	4	2764	A
4	4	2765	A
4	4	2766	G
4	4	2769	C
4	4	2773	C
4	4	2778	A
4	4	2779	U
4	4	2780	G
4	4	2790	A
4	4	2791	C
4	4	2792	G
4	4	2794	C
4	4	2799	C
4	4	2801	A
4	4	2801(A)	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4	2802	G
4	4	2803	C
4	4	2818	G
4	4	2820	A
4	4	2821	A
4	4	2835	A
4	4	2836	U
4	4	2849	U
4	4	2850	A
4	4	2871	C
4	4	2872	G
4	4	2884	U
4	4	2886	G
4	4	2894	G
4	4	2895	U
5	5	3	C
5	5	9	G
5	5	12	C
5	5	13	A
5	5	15	A
5	5	21	G
5	5	24	G
5	5	25	A
5	5	26	A
5	5	27	C
5	5	32	C
5	5	35	U
5	5	38	C
5	5	41	U
5	5	42	C
5	5	43	C
5	5	44	G
5	5	45	A
5	5	46	A
5	5	50	G
5	5	51	G
5	5	52	A
5	5	53	A
5	5	54	G
5	5	57	A
5	5	66	A
5	5	67	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	5	68	C
5	5	73	A
5	5	77	U
5	5	81	G
5	5	89	G
5	5	97	G
5	5	109	C
5	5	110	G
5	5	113	G

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	65	U
1	1	134	A
1	1	575	G
1	1	982	U
1	1	1000	U
1	1	1013	G
1	1	1015	A
1	1	1127	G
1	1	1218	C
1	1	1239	A
1	1	1291	G
3	3	14	U
4	4	752	A
4	4	1054	A
4	4	1077	A
4	4	1300	U
4	4	1647	G
4	4	1799	G
4	4	1919	A
4	4	1992	G
4	4	2610	C
4	4	2756	U
5	5	24	G
5	5	34	U
5	5	44	G
5	5	66	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 466 ligands modelled in this entry, 465 are 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	$\#\|Z\| > 2$
62	GDP	U	702	60,28	24,30,30	0.95	1 (4%)	30,47,47	1.26	4 (13%)

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
62	GDP	U	702	60,28	-	7/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	U	702	GDP	C6-N1	-2.42	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	U	702	GDP	C3'-C2'-C1'	3.46	106.18	100.98
62	U	702	GDP	PA-O3A-PB	-2.78	123.29	132.83
62	U	702	GDP	C5-C6-N1	2.34	118.08	113.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	U	702	GDP	C8-N7-C5	2.33	107.43	102.99

There are no chirality outliers.

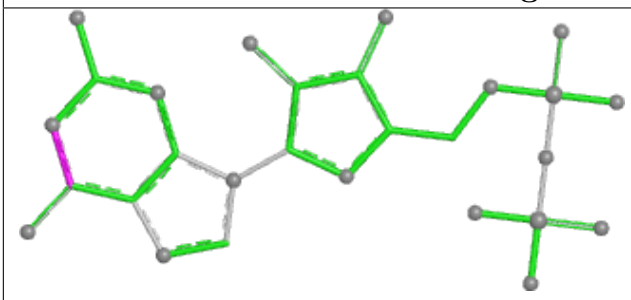
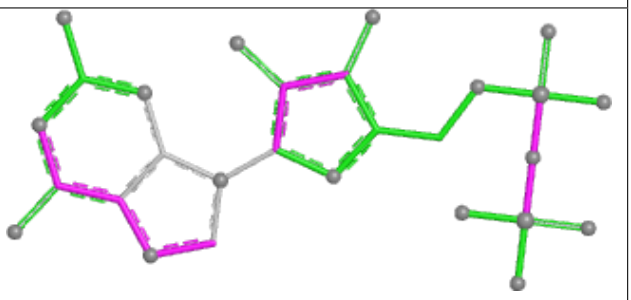
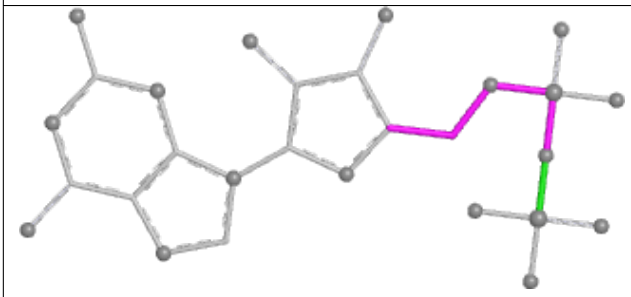
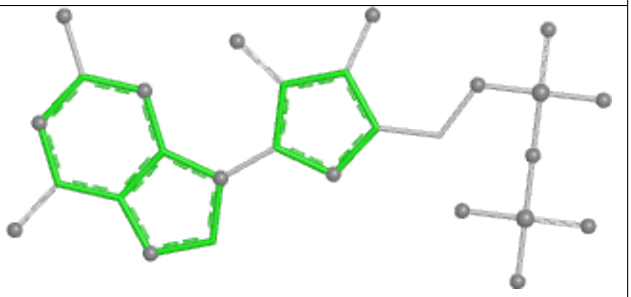
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	U	702	GDP	C5'-O5'-PA-O2A
62	U	702	GDP	C3'-C4'-C5'-O5'
62	U	702	GDP	O4'-C4'-C5'-O5'
62	U	702	GDP	PB-O3A-PA-O5'
62	U	702	GDP	C5'-O5'-PA-O1A
62	U	702	GDP	C5'-O5'-PA-O3A
62	U	702	GDP	C4'-C5'-O5'-PA

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 GDP U 702	
 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.

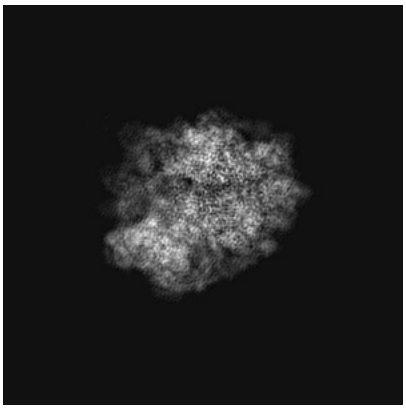
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3852. These allow visual inspection of the internal detail of the map and identification of artifacts.

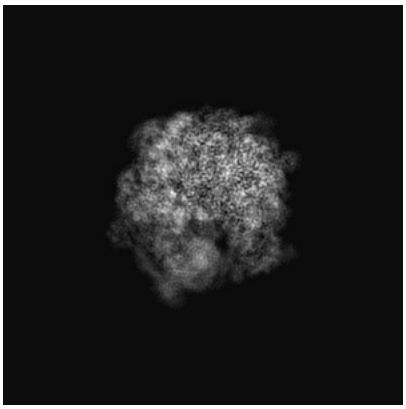
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

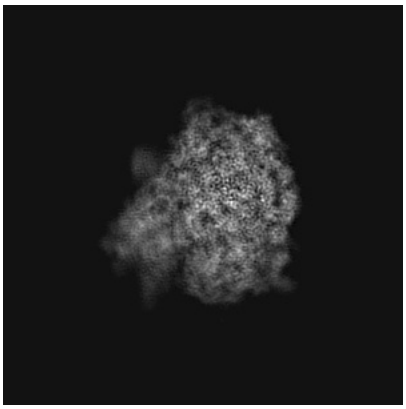
6.1.1 Primary map



X

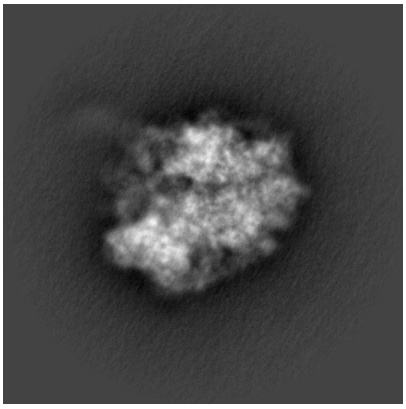


Y

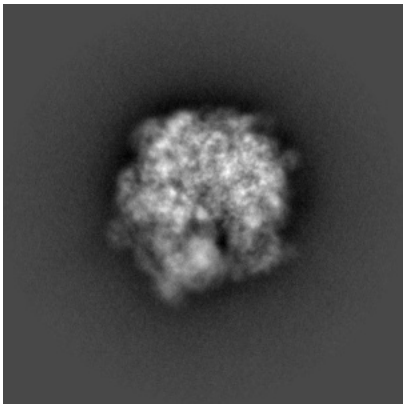


Z

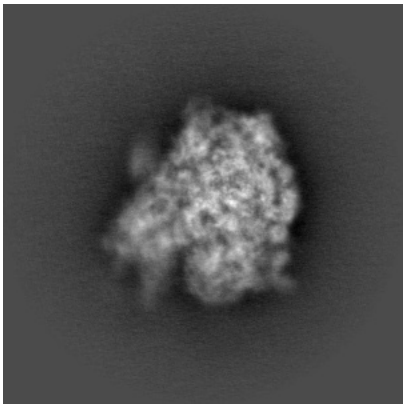
6.1.2 Raw map



X



Y

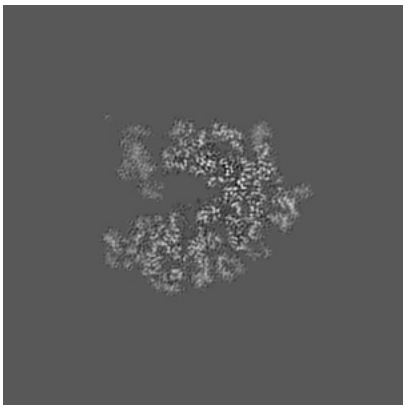


Z

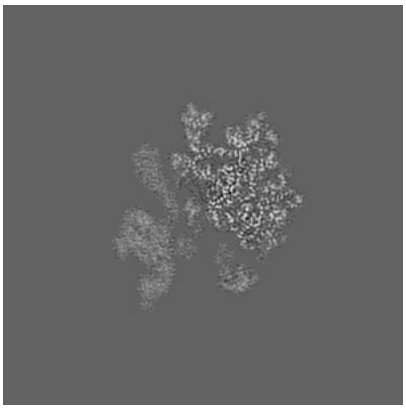
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

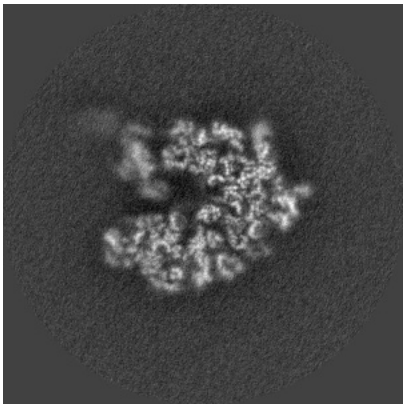
6.2.1 Primary map

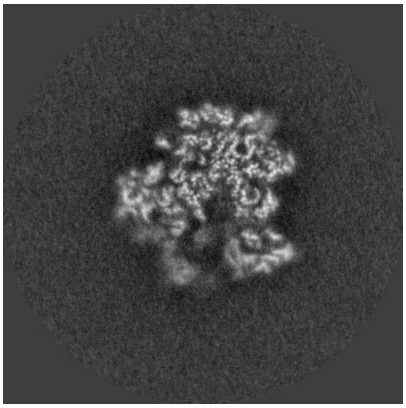

X Index: 210

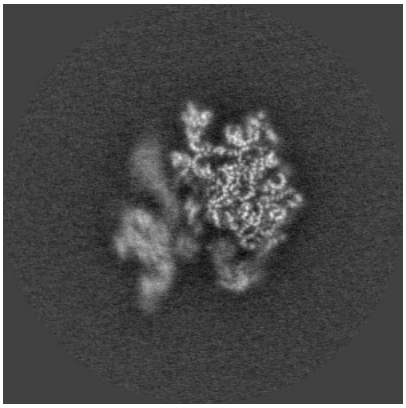
Y Index: 210


Z Index: 210

6.2.2 Raw map


X Index: 210

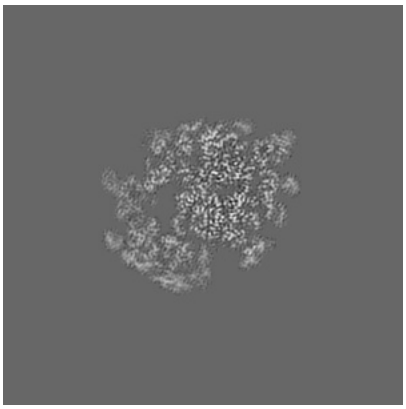

Y Index: 210


Z Index: 210

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

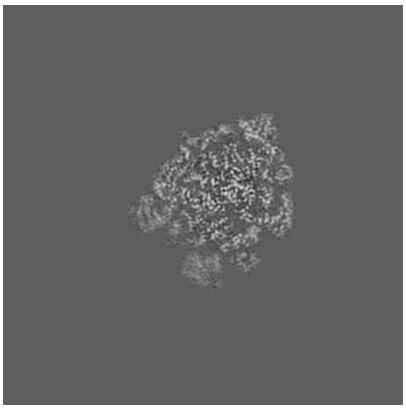
6.3 Largest variance slices (i)

6.3.1 Primary map



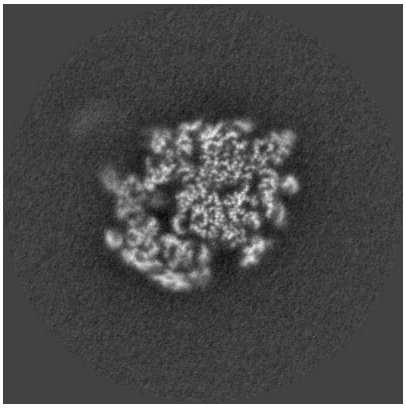
X Index: 239

Y Index: 218

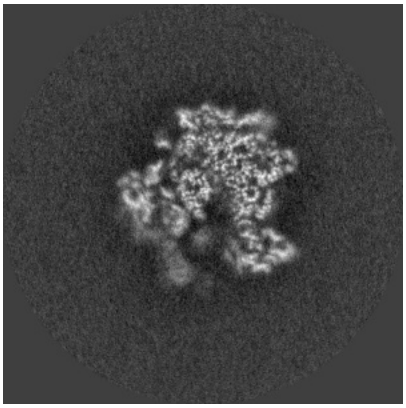


Z Index: 254

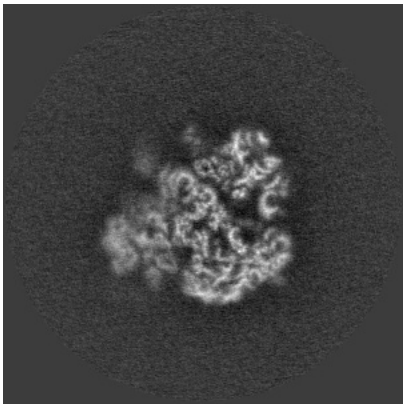
6.3.2 Raw map



X Index: 239



Y Index: 213

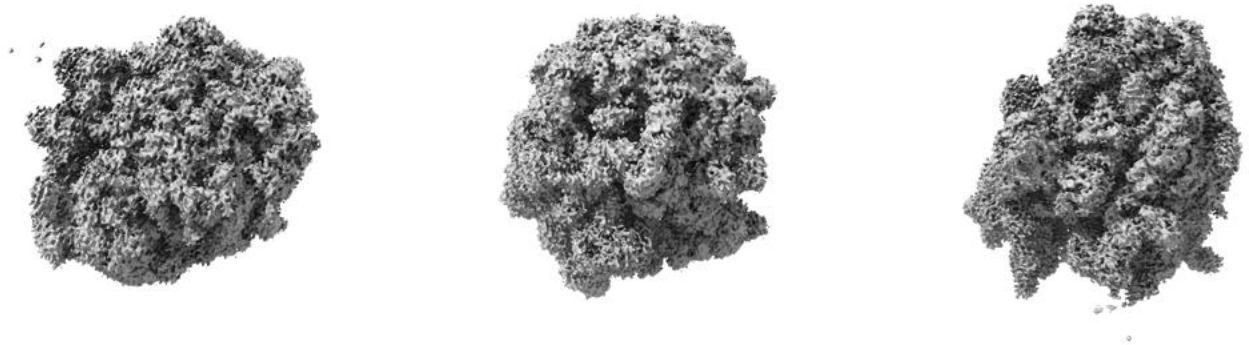


Z Index: 171

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

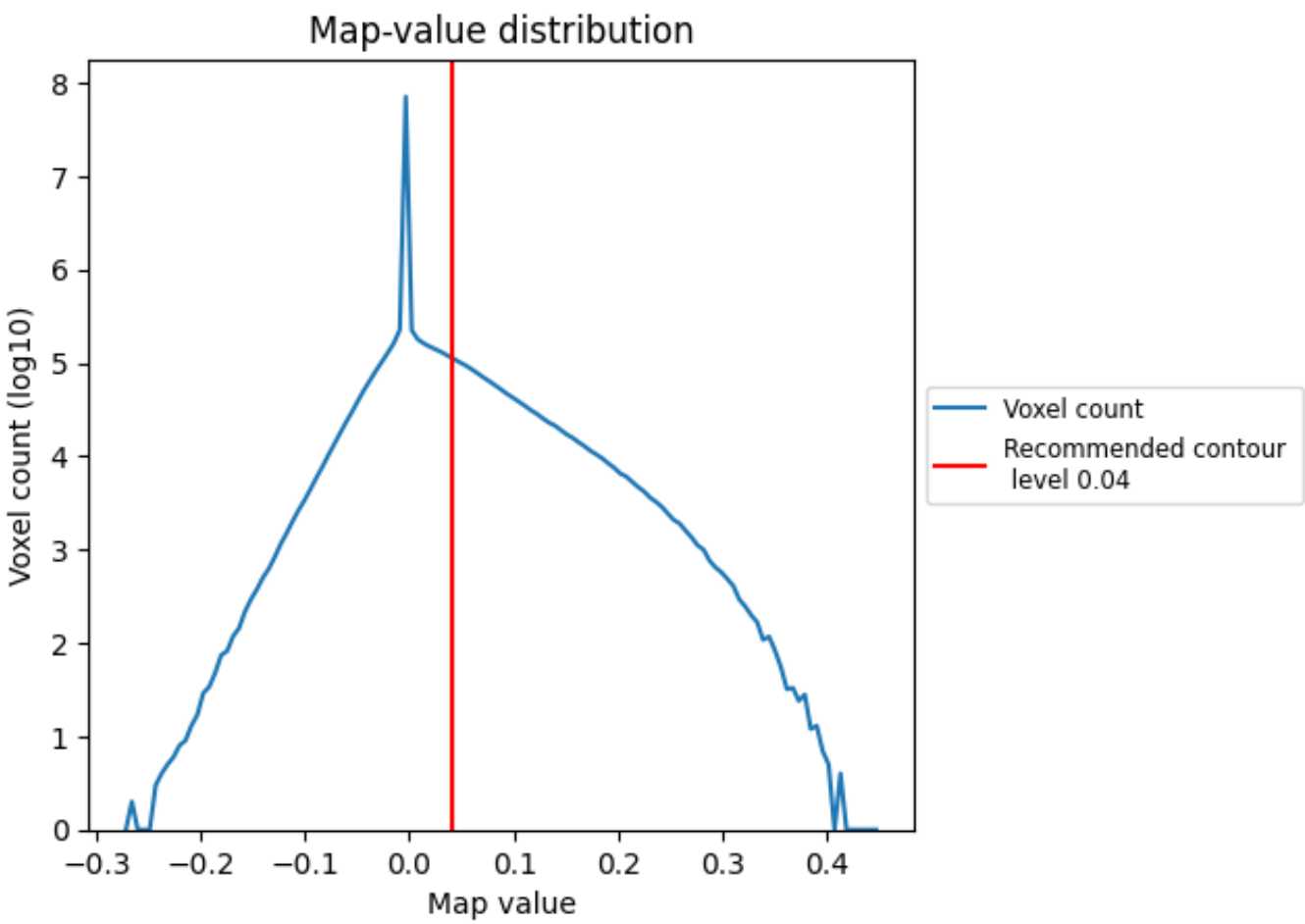
6.5 Mask visualisation (i)

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

7 Map analysis (i)

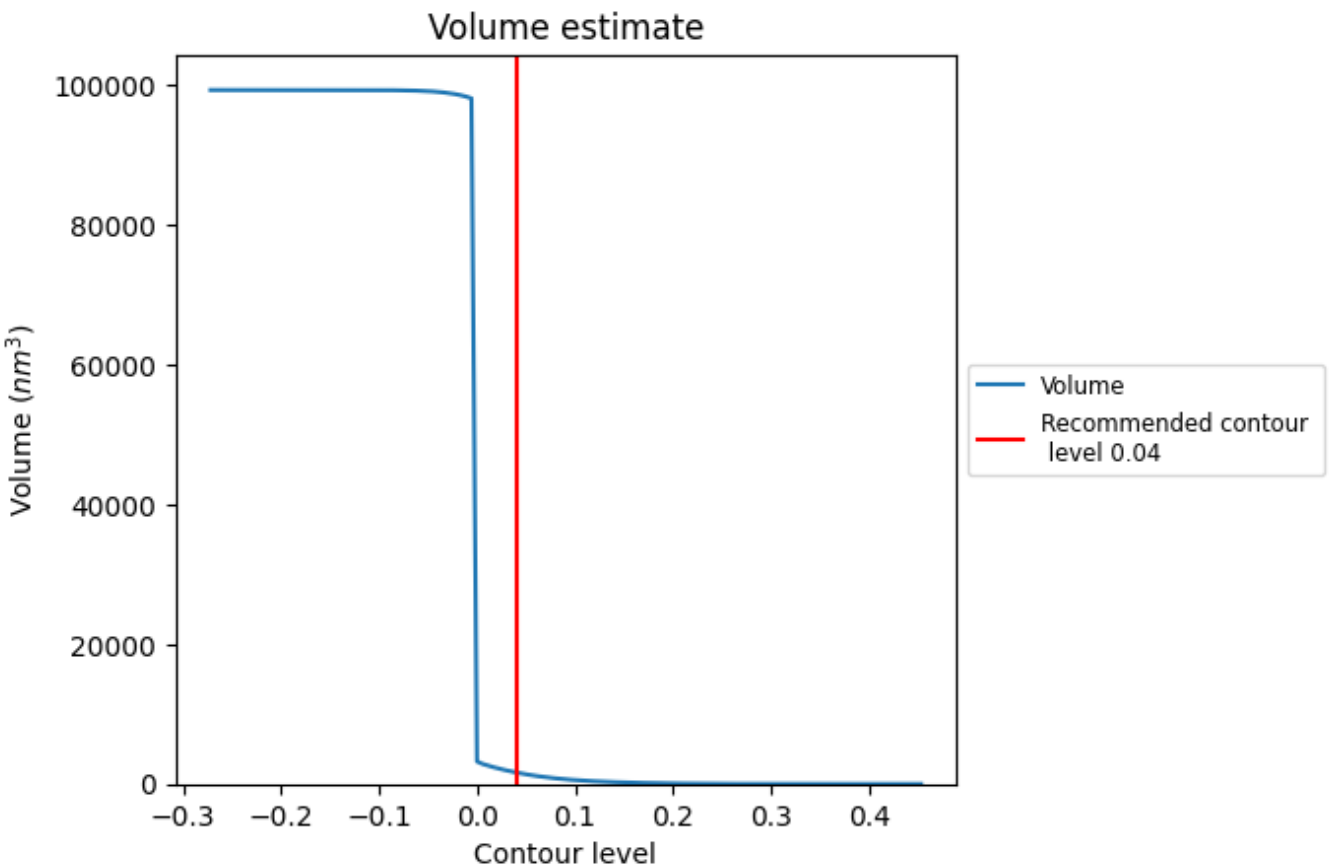
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

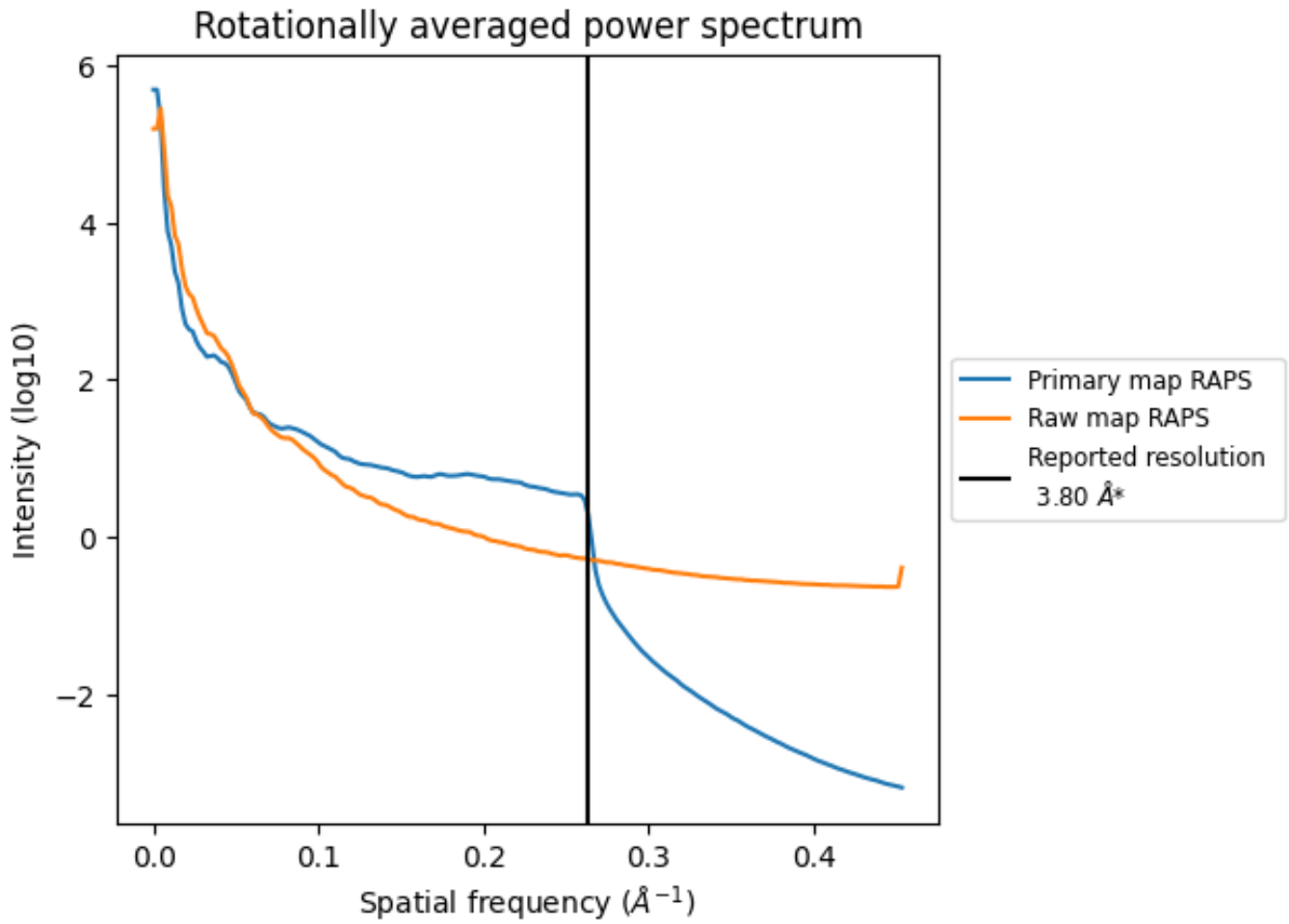
7.2 Volume estimate (i)



The volume at the recommended contour level is 1646 nm^3; this corresponds to an approximate mass of 1487 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)

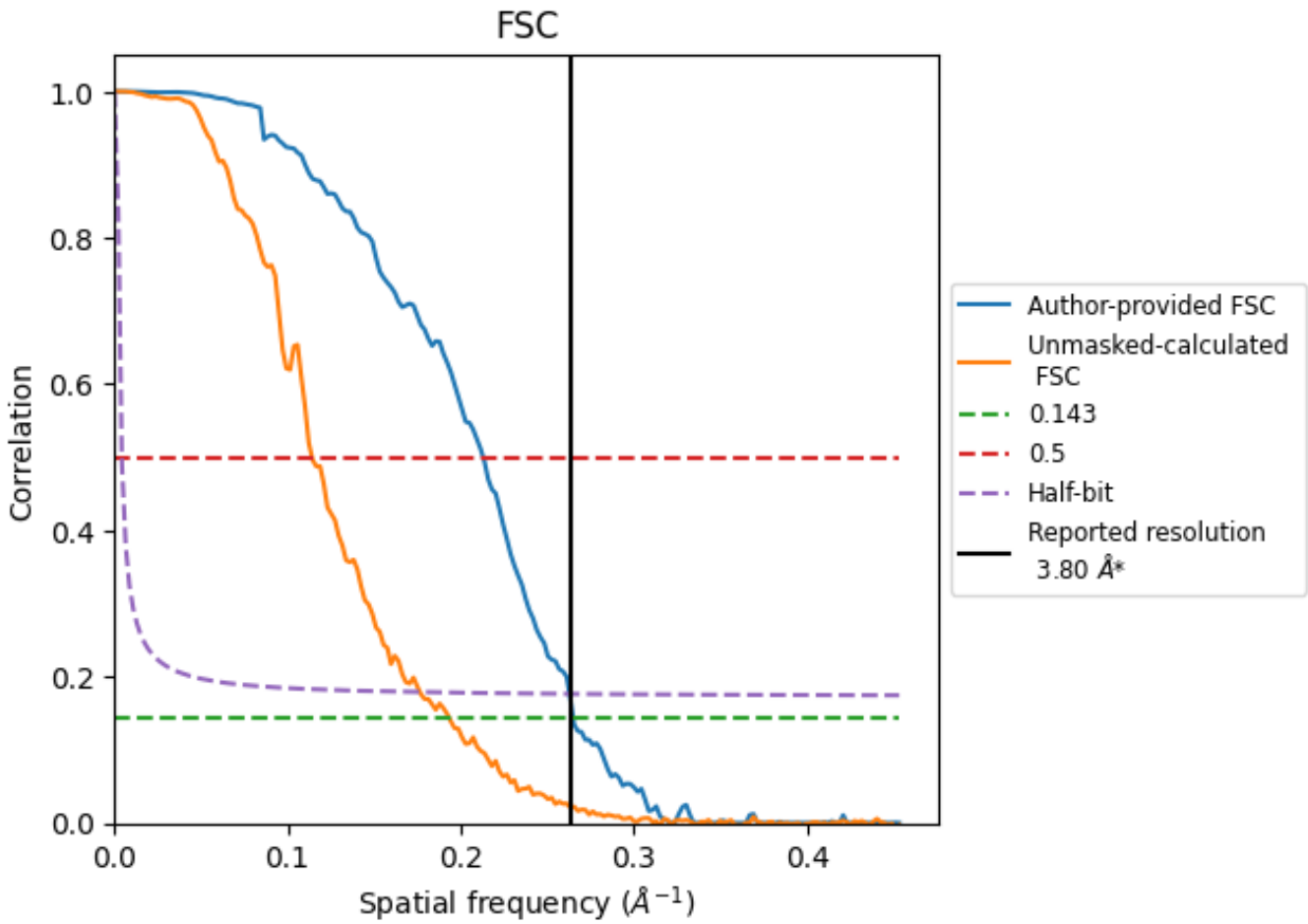


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

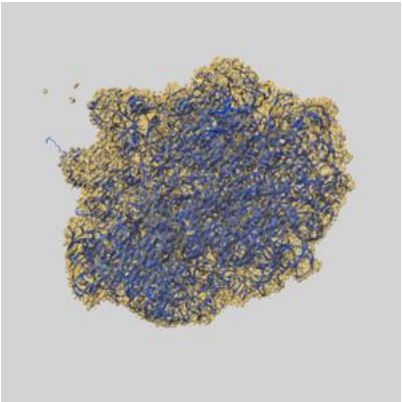
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.69	3.80
Unmasked-calculated*	5.17	8.76	5.67

*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 5.17 differs from the reported value 3.8 by more than 10 %

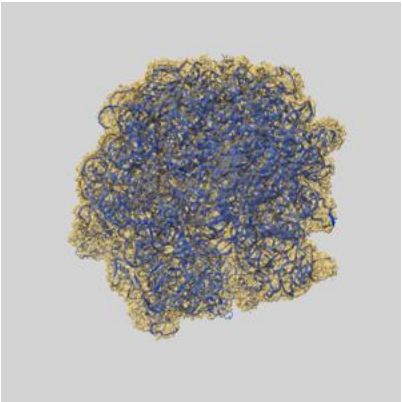
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3852 and PDB model 5OT7. Per-residue inclusion information can be found in section 3 on page 17.

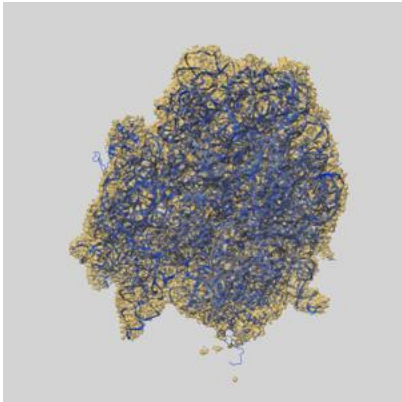
9.1 Map-model overlay (i)



X



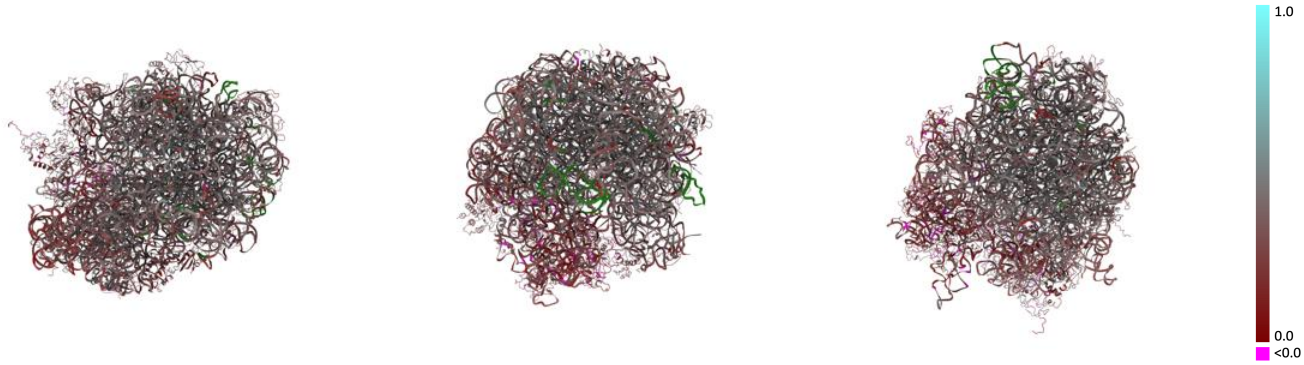
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

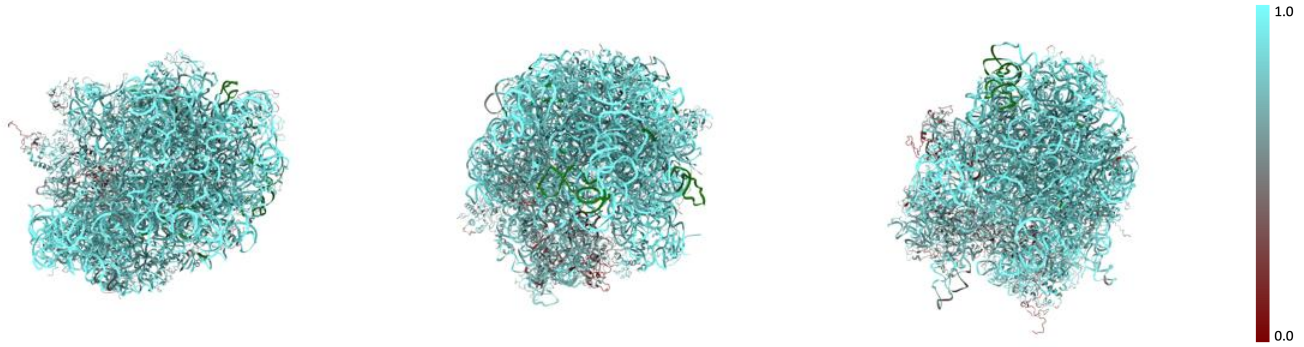
9.2 Q-score mapped to coordinate model (i)



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.

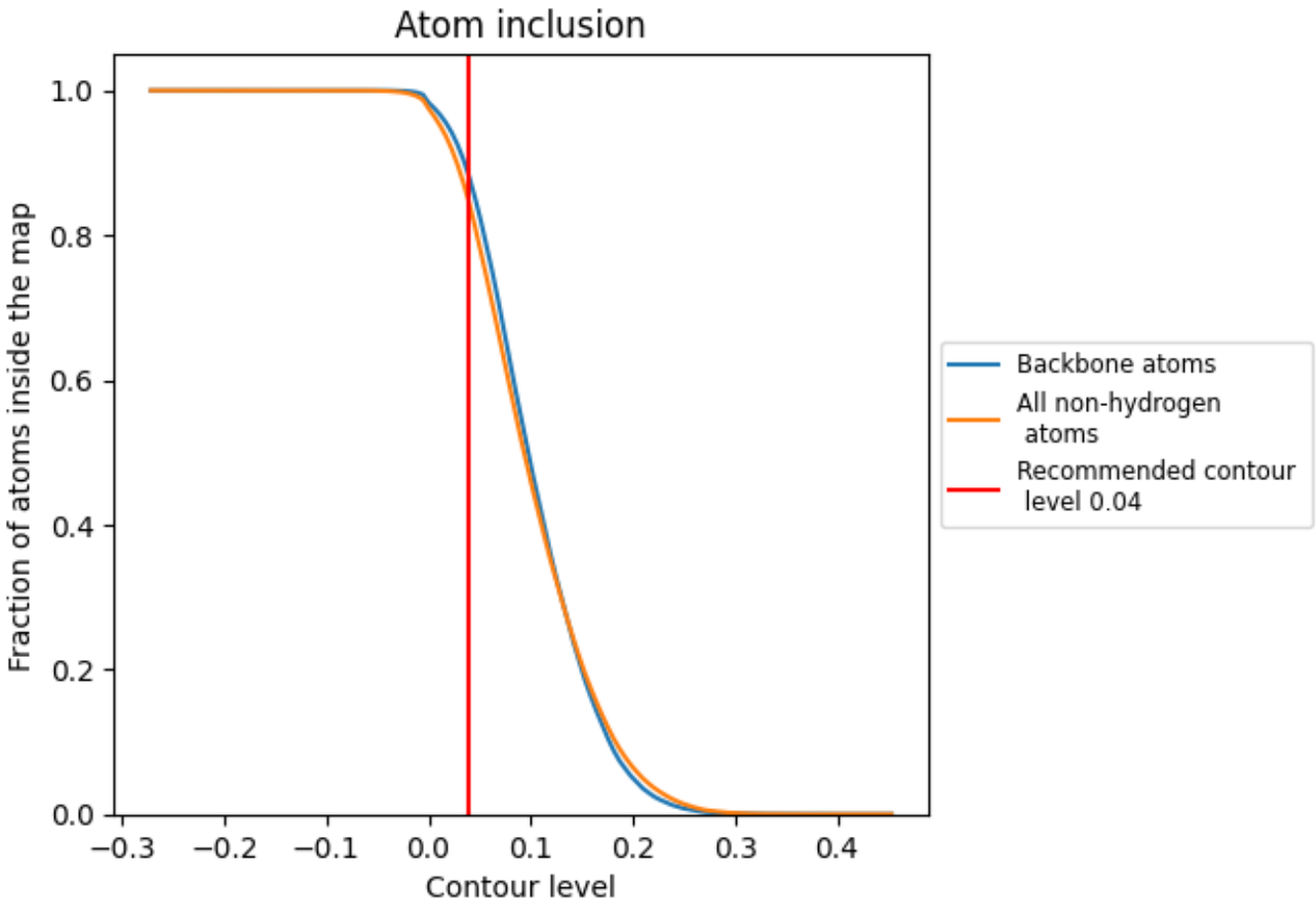
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8435	0.3440
1	0.8893	0.3010
2	0.5590	0.2480
3	0.6776	0.2650
4	0.9237	0.3940
5	0.9651	0.3580
6	0.7326	0.3180
7	0.4860	0.2470
A	0.6842	0.2650
B	0.6540	0.2580
C	0.8086	0.3130
D	0.8149	0.3780
E	0.7700	0.2750
F	0.5820	0.1940
G	0.8138	0.3510
H	0.7006	0.1920
I	0.6576	0.2290
J	0.6408	0.2150
K	0.7260	0.3820
L	0.5810	0.1840
M	0.5983	0.2100
N	0.7768	0.2670
O	0.8239	0.3540
P	0.7685	0.3500
Q	0.7215	0.2550
R	0.5870	0.1950
S	0.7811	0.3210
T	0.7760	0.1910
U	0.5982	0.2490
V	0.8319	0.4170
W	0.7915	0.3990
X	0.8270	0.3490
Y	0.8154	0.4020
Z	0.6214	0.1960
a	0.7964	0.3870

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	0.7404	0.2870
c	0.8359	0.4320
d	0.7702	0.3950
e	0.8108	0.4110
f	0.3722	0.1640
g	0.8036	0.4150
h	0.8256	0.4170
i	0.8170	0.3790
j	0.7358	0.2460
k	0.8162	0.3440
l	0.6636	0.3220
m	0.7233	0.3070
n	0.3792	0.2920
o	0.8374	0.4000
p	0.7607	0.4150
q	0.8117	0.3700
r	0.8120	0.4220
s	0.8317	0.4080
t	0.8432	0.3330
u	0.7778	0.3570
v	0.8581	0.4180
w	0.7913	0.3700
x	0.8275	0.4310
y	0.8467	0.4000
z	0.7931	0.2990