



Full wwPDB EM Validation Report ⓘ

Jul 9, 2023 – 11:48 am BST

PDB ID : 8BPO
EMDB ID : EMD-16155
Title : Structure of rabbit 80S ribosome translating beta-tubulin in complex with tetratricopeptide protein 5 (TTC5) and S-phase Cyclin A Associated Protein residing in the ER (SCAPER)
Authors : Hopfler, M.; Absmeier, E.; Passmore, L.A.; Hegde, R.S.
Deposited on : 2022-11-17
Resolution : 2.80 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev50
MolProbity : 4.02b-467
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) : 2.34

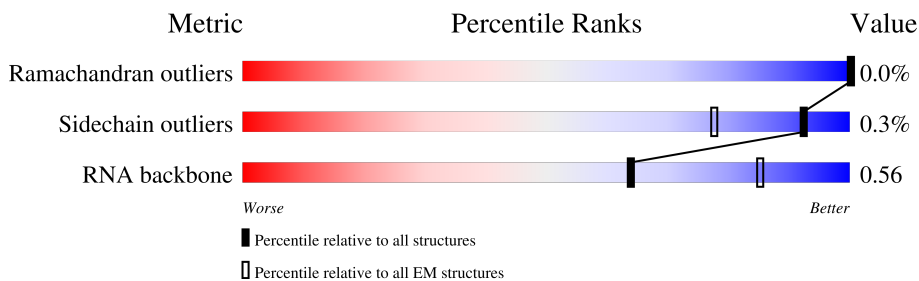
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A1	4380	 7% 61% 18% 19%
2	B1	120	 88% 12%
3	C1	156	 5% 78% 19%
4	D1	29	 69% 100%
5	A2	257	 96%
6	B2	403	 97%
7	C2	425	 85% 15%
8	D2	297	 99%

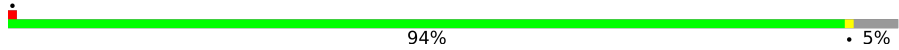
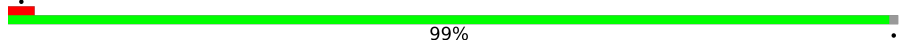
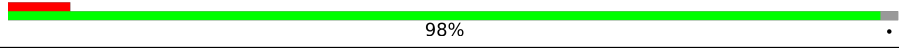
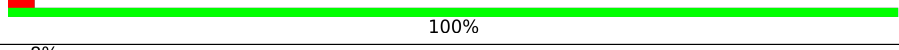
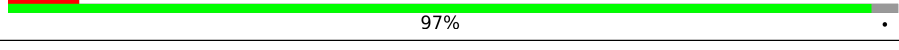

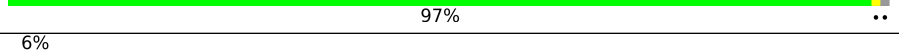
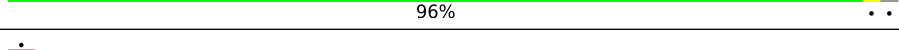
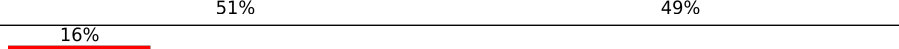
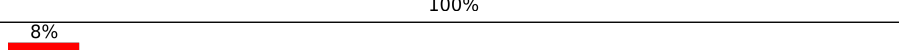
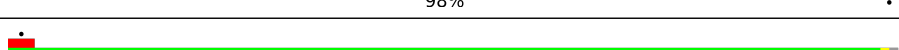
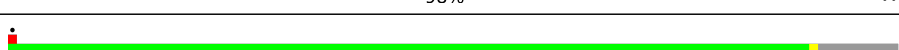

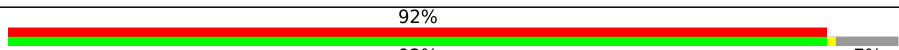




Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	E2	291	74% 26%
10	F2	247	91% 9%
11	G2	319	10% 72% 27%
12	H2	192	5% 99%
13	I2	214	96%
14	J2	178	9% 96%
15	K2	211	7% 99%
16	L2	218	63% 37%
17	M2	204	98%
18	N2	203	98%
19	O2	184	83% 17%
20	P2	187	99%
21	Q2	196	79% 21%
22	R2	176	100%
23	S2	160	6% 99%
24	T2	128	23% 79% 20%
25	U2	140	94% 6%
26	V2	157	40% 60%
27	W2	156	75% 24%
28	X2	145	92% 8%
29	Y2	136	99%
30	Z2	148	99%
31	a2	226	9% 46% 54%
32	b2	115	8% 85% 15%
33	c2	125	6% 86% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	d2	135	 94% . 5%
35	e2	110	 99% .
36	f2	116	 98% .
37	g2	122	 100%
38	h2	105	 97% .
39	i2	97	 88% . 11%
40	j2	70	 97% ..
41	k2	51	 96% ..
42	l2	102	 51% 49%
43	m2	25	 100%
44	n2	106	 98% .
45	o2	92	 98% ..
46	p2	137	 90% . 9%
47	q2	318	 62% 38% 59%
48	r2	165	 92% . 7%
49	s2	1411	 28% 72% 27%
50	t2	489	 85% . 15% 56%
51	u2	64	 83% 17% 16%

2 Entry composition [i](#)

There are 53 unique types of molecules in this entry. The entry contains 143326 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 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A1	3543	75972	33833	13910	24686	3543	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B1	120	2558	1141	456	842	119	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C1	151	3208	1432	564	1062	150	0	0

- Molecule 4 is a protein called Nascent polypeptide-associated complex subunit alpha N-terminal region.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D1	29	150	92	29	29	0	0

- Molecule 5 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A2	248	1898	1189	389	314	6	0	0

- Molecule 6 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B2	394	3172	2020	597	542	13	0	0

- Molecule 7 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C2	362	2883	1812	577	480	14	0	0

- Molecule 8 is a protein called Ribosomal_L18_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D2	293	2391	1512	438	427	14	0	0

- Molecule 9 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E2	216	1729	1115	329	282	3	0	0

- Molecule 10 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F2	225	1875	1205	358	303	9	0	0

- Molecule 11 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G2	233	1879	1199	361	315	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G2	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 12 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H2	190	1516	954	284	272	6	0	0

- Molecule 13 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I2	205	1664	1056	321	274	13	0	0

- Molecule 14 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	J2	170	1362	861	254	241	6	0	0

- Molecule 15 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	K2	210	1702	1065	354	279	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K2	74	ARG	HIS	conflict	UNP G1TKB3
K2	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 16 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	L2	138	1137	727	221	182	7	0	0

- Molecule 17 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	M2	203	1701	1072	359	266	4	0	0

- Molecule 18 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	N2	199	1630	1051	319	255	5	0	0

- Molecule 19 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	O2	153	1242	777	241	215	9	0	0

- Molecule 20 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	P2	187	1514	946	315	249	4	0	0

- Molecule 21 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q2	155	1294	808	278	199	9	0	0

- Molecule 22 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R2	176	1462	930	285	236	11	0	0

- Molecule 23 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	S2	159	1298	823	252	217	6	0	0

- Molecule 24 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	T2	102	834	534	146	152	2	0	0

- Molecule 25 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	U2	131	979	618	184	172	5	0	0

- Molecule 26 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V2	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 27 is a protein called Ribosomal_L23eN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W2	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 28 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X2	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 29 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y2	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 30 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z2	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a2	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 32 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b2	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 33 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c2	107	888	560	171	155	2	0	0

- Molecule 34 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	d2	128	1053	667	216	165	5	0	0

- Molecule 35 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	e2	109	876	555	174	143	4	0	0

- Molecule 36 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	f2	114	906	566	187	147	6	0	0

- Molecule 37 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	g2	122	1013	640	204	168	1	0	0

- Molecule 38 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	h2	102	830	520	176	129	5	0	0

- Molecule 39 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	i2	86	705	434	155	111	5	0	0

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	j2	69	569	366	103	99	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j2	24	LYS	ASN	conflict	UNP G1U001

- Molecule 41 is a protein called 60S ribosomal protein L39-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	k2	50	447	286	96	64	1	0	0

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	l2	52	429	266	90	67	6	0	0

- Molecule 43 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	m2	25	239	145	64	27	3	0	0

- Molecule 44 is a protein called 60S ribosomal protein L36a-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	n2	104	851	533	174	138	6	0	0

- Molecule 45 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	o2	91	708	445	136	120	7	0	0

- Molecule 46 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	p2	124	994	616	205	167	6	0	0

- Molecule 47 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	q2	196	1507	959	263	276	9	0	0

- Molecule 48 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	r2	153	1160	722	218	217	3	0	0

- Molecule 49 is a protein called S phase cyclin A-associated protein in the endoplasmic reticulum.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	s2	395	3050	1943	525	557	25	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s2	-10	MET	-	initiating methionine	UNP Q9BY12
s2	-9	ASP	-	expression tag	UNP Q9BY12
s2	-8	TYR	-	expression tag	UNP Q9BY12
s2	-7	LYS	-	expression tag	UNP Q9BY12
s2	-6	ASP	-	expression tag	UNP Q9BY12
s2	-5	ASP	-	expression tag	UNP Q9BY12
s2	-4	ASP	-	expression tag	UNP Q9BY12
s2	-3	ASP	-	expression tag	UNP Q9BY12
s2	-2	LYS	-	expression tag	UNP Q9BY12
s2	-1	GLY	-	expression tag	UNP Q9BY12
s2	0	SER	-	expression tag	UNP Q9BY12

- Molecule 50 is a protein called Tetratricopeptide repeat protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	t2	418	3262	2050	573	626	13	0	0

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t2	-48	MET	-	initiating methionine	UNP Q8N0Z6
t2	-47	GLY	-	expression tag	UNP Q8N0Z6
t2	-46	HIS	-	expression tag	UNP Q8N0Z6
t2	-45	HIS	-	expression tag	UNP Q8N0Z6
t2	-44	HIS	-	expression tag	UNP Q8N0Z6
t2	-43	HIS	-	expression tag	UNP Q8N0Z6
t2	-42	HIS	-	expression tag	UNP Q8N0Z6
t2	-41	HIS	-	expression tag	UNP Q8N0Z6
t2	-40	GLU	-	expression tag	UNP Q8N0Z6
t2	-39	ASN	-	expression tag	UNP Q8N0Z6
t2	-38	LEU	-	expression tag	UNP Q8N0Z6
t2	-37	TYR	-	expression tag	UNP Q8N0Z6
t2	-36	PHE	-	expression tag	UNP Q8N0Z6
t2	-35	GLN	-	expression tag	UNP Q8N0Z6
t2	-34	GLY	-	expression tag	UNP Q8N0Z6
t2	-33	SER	-	expression tag	UNP Q8N0Z6
t2	-32	ALA	-	expression tag	UNP Q8N0Z6
t2	-31	TRP	-	expression tag	UNP Q8N0Z6
t2	-30	SER	-	expression tag	UNP Q8N0Z6
t2	-29	HIS	-	expression tag	UNP Q8N0Z6
t2	-28	PRO	-	expression tag	UNP Q8N0Z6
t2	-27	GLN	-	expression tag	UNP Q8N0Z6
t2	-26	PHE	-	expression tag	UNP Q8N0Z6
t2	-25	GLU	-	expression tag	UNP Q8N0Z6
t2	-24	LYS	-	expression tag	UNP Q8N0Z6
t2	-23	GLY	-	expression tag	UNP Q8N0Z6
t2	-22	GLY	-	expression tag	UNP Q8N0Z6
t2	-21	GLY	-	expression tag	UNP Q8N0Z6
t2	-20	SER	-	expression tag	UNP Q8N0Z6
t2	-19	GLY	-	expression tag	UNP Q8N0Z6
t2	-18	GLY	-	expression tag	UNP Q8N0Z6
t2	-17	GLY	-	expression tag	UNP Q8N0Z6
t2	-16	SER	-	expression tag	UNP Q8N0Z6
t2	-15	GLY	-	expression tag	UNP Q8N0Z6
t2	-14	GLY	-	expression tag	UNP Q8N0Z6
t2	-13	SER	-	expression tag	UNP Q8N0Z6
t2	-12	ALA	-	expression tag	UNP Q8N0Z6
t2	-11	TRP	-	expression tag	UNP Q8N0Z6
t2	-10	SER	-	expression tag	UNP Q8N0Z6
t2	-9	HIS	-	expression tag	UNP Q8N0Z6
t2	-8	PRO	-	expression tag	UNP Q8N0Z6
t2	-7	GLN	-	expression tag	UNP Q8N0Z6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
t2	-6	PHE	-	expression tag	UNP Q8N0Z6
t2	-5	GLU	-	expression tag	UNP Q8N0Z6
t2	-4	LYS	-	expression tag	UNP Q8N0Z6
t2	-3	GLY	-	expression tag	UNP Q8N0Z6
t2	-2	SER	-	expression tag	UNP Q8N0Z6
t2	-1	SER	-	expression tag	UNP Q8N0Z6
t2	0	GLY	-	expression tag	UNP Q8N0Z6

- Molecule 51 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	u2	11	82	50	18	13	1	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u2	61	MET	-	expression tag	UNP P07437
u2	62	LYS	-	expression tag	UNP P07437
u2	63	LEU	-	expression tag	UNP P07437
u2	64	VAL	-	expression tag	UNP P07437

- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
52	A1	194	194	194	0
52	B1	7	7	7	0
52	C1	6	6	6	0
52	B2	1	1	1	0
52	I2	1	1	1	0
52	O2	2	2	2	0
52	U2	1	1	1	0
52	Z2	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
52	f2	1	Total 1	Mg 1	0

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).


Mol	Chain	Residues	Atoms		AltConf
53	f2	1	Total 1	Zn 1	0
53	i2	1	Total 1	Zn 1	0
53	l2	1	Total 1	Zn 1	0
53	n2	1	Total 1	Zn 1	0
53	o2	1	Total 1	Zn 1	0

3 Residue-property plots

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


- Molecule 1: 28S ribosomal RNA

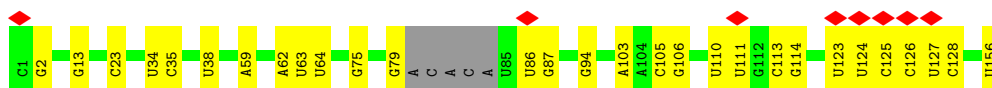


Chain B1:  88% 12%



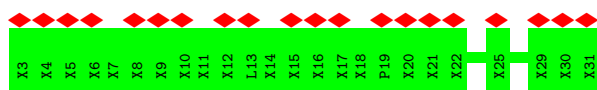
- Molecule 3: 5.8S ribosomal RNA

Chain C1:  5% 78% 19%



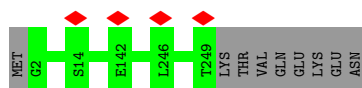
- Molecule 4: Nascent polypeptide-associated complex subunit alpha N-terminal region

Chain D1:  69% 100%



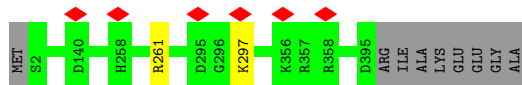
- Molecule 5: 60S ribosomal protein L8

Chain A2:  96%




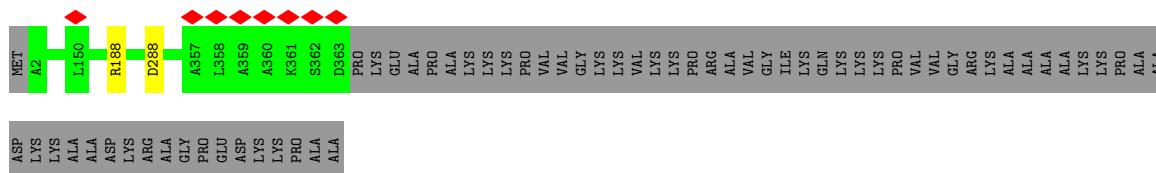
- Molecule 6: Ribosomal protein L3

Chain B2:  97%



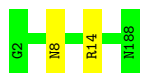
- Molecule 7: 60S ribosomal protein L4

Chain C2:  85% 15%

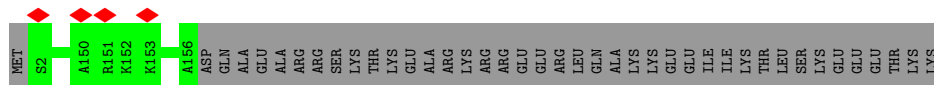
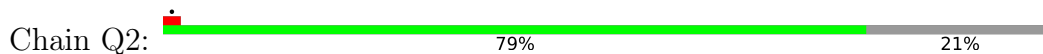


- Molecule 8: Ribosomal_L18_c domain-containing protein

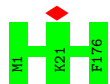
Chain D2:  99%



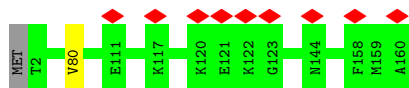
- Molecule 21: 60S ribosomal protein L19



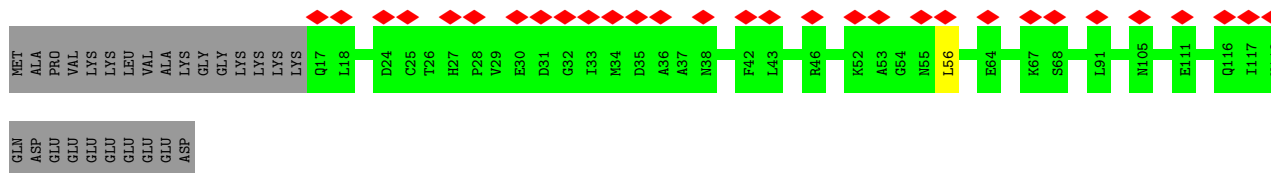
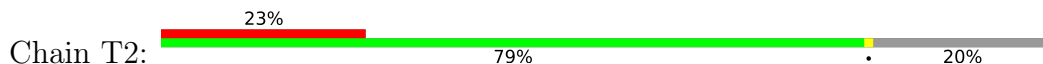
- Molecule 22: 60S ribosomal protein L18a



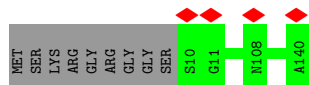
- Molecule 23: 60S ribosomal protein L21



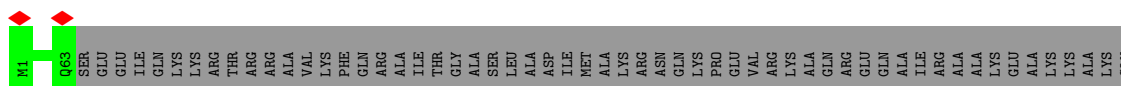
- Molecule 24: 60S ribosomal protein L22

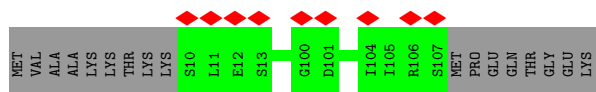


- Molecule 25: 60S ribosomal protein L23

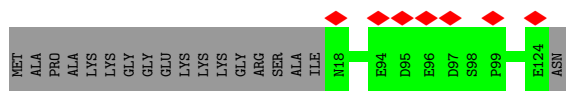
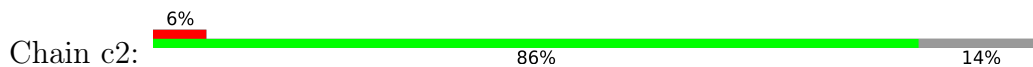


- Molecule 26: Ribosomal protein L24

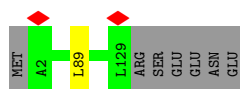




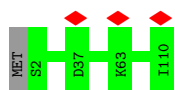
- Molecule 33: 60S ribosomal protein L31



- Molecule 34: Ribosomal protein L32



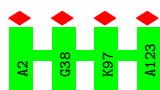
- Molecule 35: 60S ribosomal protein L35a



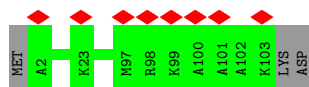
- Molecule 36: 60S ribosomal protein L34



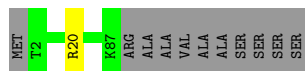
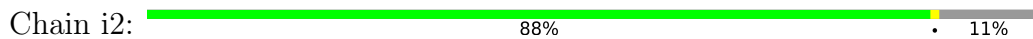
- Molecule 37: 60S ribosomal protein L35



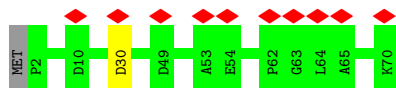
- Molecule 38: 60S ribosomal protein L36



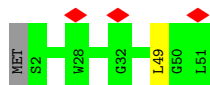
- Molecule 39: Ribosomal protein L37



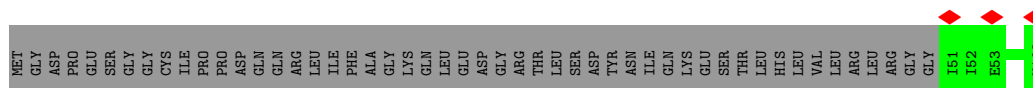
- Molecule 40: 60S ribosomal protein L38



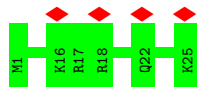
- Molecule 41: 60S ribosomal protein L39-like



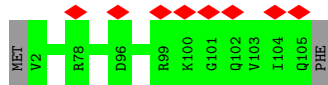
- Molecule 42: Ubiquitin-60S ribosomal protein L40



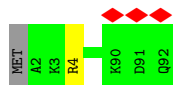
- Molecule 43: 60S ribosomal protein L41



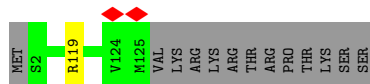
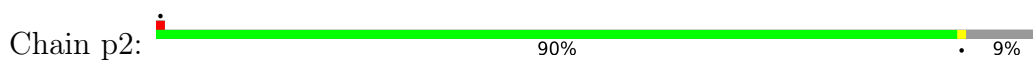
- Molecule 44: 60S ribosomal protein L36a-like



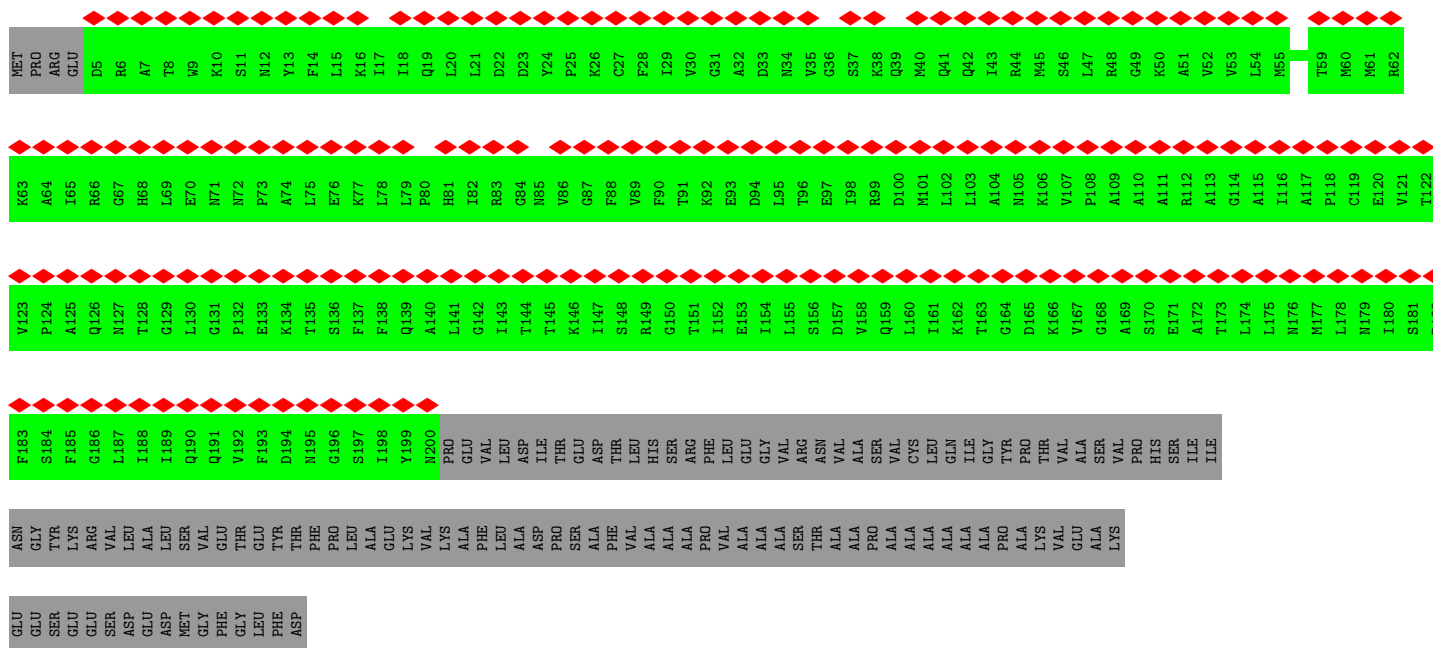
- Molecule 45: 60S ribosomal protein L37a



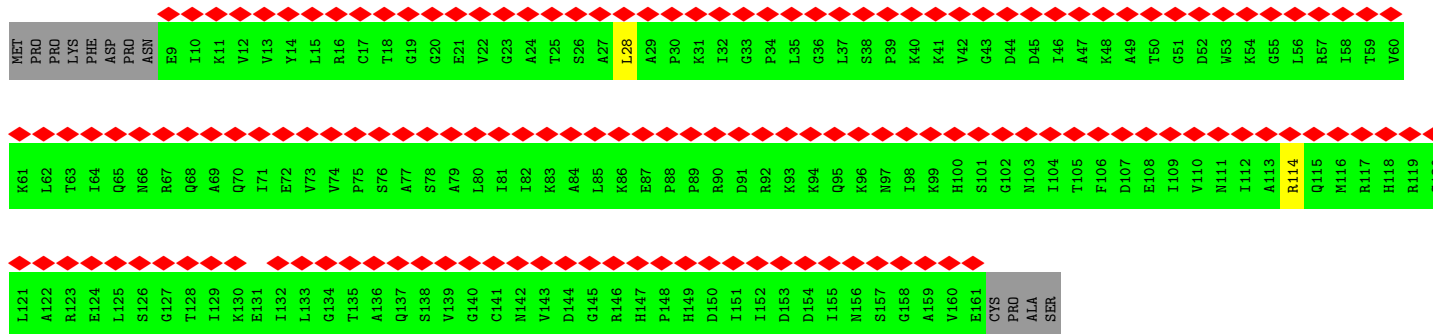
Molecule 46: 60S ribosomal protein L28



Molecule 47: 60S acidic ribosomal protein P0



Molecule 48: 60S ribosomal protein L12



Molecule 49: S phase cyclin A-associated protein in the endoplasmic reticulum



PRO	LYS	ILE	PRO	THR	ALA	GLN	GLU	MET	LYS	LYS	PRO	GLN	GLY	D1093	P1094	F1095	M1096	N1097	R1098	V1099	Q1100	D1101	L1102	I1103	S1104	Y1105	V1106	I1107	N1108	M1109	G1110	L1111	I1112	D1113	K1114	L1115	C1116	A1117	C1118	F1119	L1120	S1121	V1122	GLN	GLY	PRO	VAL	ASP	GLU	M1129	P1130	K1131	M1132	A1133	I1134	F1135	L1136	Q1137
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------

H1138	A1139	A1140	G1141	L1142	L1143	H1144	A1145	M1146	T1147	T1148	L1149	PHE	ALA	VAL	THR	GLY	ARG	SER	SER	TYR	SER	ILE	PHE	ASP	ASN	ASN	ARG	GLN	ASP	PRO	THR	G1170	L1171	T1172	D1173	A1174	L1175	Q1176	A1177	T1178	D1179	L1180	A1181	G1182	V1183	L1184	H1185	M1186	L1187	Y1188	C1189	V1190	L1191	F1192	H1193	GLY	THR	ILE	LEU
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----

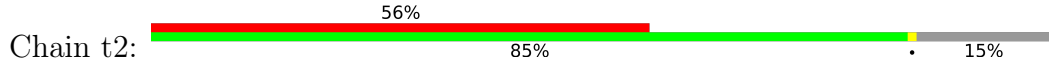
ASP	PRO	THR	ALA	SER	PRO	LYS	ASN	TYR	THR	Q1210	M1211	T1212	I1213	Q1214	V1215	A1216	I1217	Q1218	S1219	L1220	R1221	F1222	F1223	M1224	S1225	F1226	A1227	A1228	L1229	H1230	L1231	P1232	A1233	F1234	Q1235	S1236	I1237	V1238	G1239	A1240	E1241	G1242	S1244	L1245	A1246	F1247	R1249	M1250	M1251	S1252	S1253	L1254	L1255	G1256	H1257
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

C1258	S1259	Q1260	V1261	C1263	E1264	S1265	L1266	L1267	H1268	E1269	I1270	I1271	V1272	C1273	G1274	Y1275	Y1276	F1277	T1278	V1279	M1280	H1281	P1282	D1283	M1284	Q1285	V1286	I1287	V1288	Q1289	S1290	ARG	HIS	PRO	T1295	V1296	L1297	Q1298	K1299	L1300	L1301	Q1302	L1303	F1304	F1305	Q1306	Y1307	F1308	S1309	D1310	P1311	R1312	L1313	I1314	K1315	V1316	L1317
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

F1318	P1319	S1320	L1321	I1322	A1323	A1324	C1325	N1326	M1327	M1328	H1329	Q1330	M1331	K1332	I1333	I1334	L1335	E1336	Q1337	I1338	M1339	S1340	C1341	V1342	L1343	L1344	T1345	I1346	I1348	Q1349	D1350	L1351	A1352	Q1353	T1354	P1355	G1356	Q1357	ALA	ASN	GLN	TYR	PRO	PRO	LYS	GLY	GLN	ASP	TYR	LEU	LEU	GLU
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LEU	ALA	ASN	ARG	PHE	HIS	HIS	HIS	GLN	GLN	ALA	TRP	LEU	GLU	THR	ALA	ARG	GLN	GLY	PHE	PRO	ALA	TRP	SER	HIS	LEU	LYS	GLU	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 50: Tetratricopeptide repeat protein 5



MET	GLY	HIS	HIS	HIS	HIS	HIS	GLU	ASN	LEU	TYR	PHE	GLN	GLY	TRP	ALA	SER	HIS	LEU	LYS	GLU	LYS	GLY	SER	GLY	GLY	GLY	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	SER	GLY	GLY	MET	MET	PRO
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

I12	L13	Q14	K15	L16	Q17	E18	L19	V20	D21	Q22	L23	Y24	S25	F26	R27	D28	C29	Y30	F31	E32	T33	H34	S35	V36	E37	D38	A39	G40	R41	K42	Q43	Q44	D45	V46	Q47	K48	E49	M50	E51	K52	T53	Q54	Q55	Q56	M57	E58	E59	V60	V61	G62	S63	V64	Q65	G66	K67	A68	Q69	L71
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

M72	L73	T74	G75	K76	A77	L78	VAL	THR	PRO	ASP	TYR	SER	PRO	LYS	A88	E89	E90	L91	L92	S93	K94	V96	K97	L98	E99	P100	E101	L102	V103	E104	A105	V106	N107	Q108	L109	G110	E111	V112	Y113	W114	K115	K116	G117	L118	V119	A120	A121	A122	H123	T124	C125	F126	S127	G128	A129	L130	T131
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

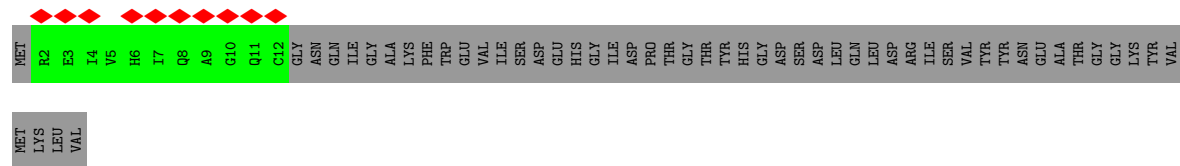
H132	C133	R134	M135	K136	V137	S138	L139	Q140	N141	L142	S143	M144	V145	L146	R147	Q148	L149	R150	T151	D152	T153	E154	D155	E156	H157	H160	V161	M162	D163	S164	V165	R166	Q167	A168	K169	L170	A171	V172	Q173	M174	D175	V176	H177	D178	G179	R180	S181	H182	Y183	I184	L185	S188	Y189	L190	S191	L192	Y193
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

F194	S195	T196	G197	Q198	N199	P200	K201	I202	S203	L207	S208	A209	Y210	A211	A213	E214	K215	V216	D217	R218	K219	A220	S221	S222	N223	P224	D225	L228	M229	R230	A231	T232	L233	H234	E237	E238	S239	E242	E245	G246	F247	S248	R249	A252	L253	A256	M257	P258	E259	Q262
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

R263	E264	Q265	L267	L268	R273	E279	S280	K285	T286	K287	K288	S291	M292	L293	G294	S295	L296	R297	H300	L301	G302	F303	C304	S305	D306	G307	H308	Y309	Q310	S311	A312	S313	G314	Q315	K316	V317	T318	L319	E320	L321	L324	S325	T326	L327	P329	G330	V331	N332	S333	G334	A335
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

L338	T347	E348	E349	D359	S360	D361	T365	Q374	L386	N390	Q397	G400	K401	D402	M419	G420	S425	S426	A431	T432	V433	A434	S435	R436	P437	GLN	CYS	GLU
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----

• Molecule 51: Tubulin beta chain



MET
LYS
LEU
VAL

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18949	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44.7	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	431.08, 431.08, 431.08	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.829, 0.829, 0.829	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	A1	0.32	0/84976	1.06	399/132520 (0.3%)
2	B1	0.29	0/2858	1.01	11/4455 (0.2%)
3	C1	0.30	0/3581	1.00	2/5577 (0.0%)
4	D1	0.31	0/14	0.52	0/16
5	A2	0.29	0/1936	0.63	0/2596
6	B2	0.28	0/3240	0.60	0/4339
7	C2	0.28	0/2937	0.65	1/3946 (0.0%)
8	D2	0.28	0/2437	0.56	0/3264
9	E2	0.27	0/1762	0.62	0/2362
10	F2	0.28	0/1911	0.59	0/2549
11	G2	0.28	0/1910	0.59	0/2569
12	H2	0.29	0/1535	0.64	0/2063
13	I2	0.27	0/1702	0.58	0/2272
14	J2	0.30	0/1385	0.68	0/1852
15	K2	0.28	0/1733	0.64	0/2316
16	L2	0.28	0/1158	0.62	0/1547
17	M2	0.28	0/1746	0.66	1/2338 (0.0%)
18	N2	0.30	0/1662	0.64	0/2222
19	O2	0.29	0/1268	0.59	0/1700
20	P2	0.27	0/1538	0.66	0/2054
21	Q2	0.32	0/1310	0.70	0/1734
22	R2	0.29	0/1501	0.65	0/2012
23	S2	0.27	0/1326	0.58	0/1770
24	T2	0.32	0/848	0.72	1/1138 (0.1%)
25	U2	0.29	0/993	0.61	0/1332
26	V2	0.29	0/541	0.60	0/720
27	W2	0.27	0/984	0.62	0/1323
28	X2	0.27	0/1132	0.63	0/1504
29	Y2	0.29	0/1130	0.63	0/1507
30	Z2	0.28	0/1191	0.60	0/1590
31	a2	0.24	0/861	0.59	0/1138
32	b2	0.32	0/771	0.63	0/1034

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c2	0.28	0/903	0.63	0/1216
34	d2	0.27	0/1071	0.62	1/1429 (0.1%)
35	e2	0.29	0/895	0.63	0/1198
36	f2	0.27	0/916	0.64	0/1220
37	g2	0.27	0/1021	0.64	0/1348
38	h2	0.29	0/841	0.67	0/1112
39	i2	0.26	0/720	0.64	0/952
40	j2	0.30	0/575	0.71	1/761 (0.1%)
41	k2	0.26	0/459	0.68	1/608 (0.2%)
42	l2	0.26	0/435	0.61	0/575
43	m2	0.31	0/240	0.82	0/305
44	n2	0.27	0/864	0.57	0/1140
45	o2	0.26	0/718	0.59	0/953
46	p2	0.27	0/1010	0.69	0/1354
47	q2	0.27	0/1530	0.61	0/2064
48	r2	0.28	0/1174	0.70	1/1582 (0.1%)
49	s2	0.34	0/3090	0.69	2/4169 (0.0%)
50	t2	0.30	0/3323	0.65	3/4494 (0.1%)
51	u2	0.22	0/82	0.62	0/109
All	All	0.31	0/153744	0.92	424/225948 (0.2%)

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
15	K2	0	1
17	M2	0	2
23	S2	0	1
All	All	0	4

There are no bond length outliers.

All (424) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	2258	C	N1-C2-O2	13.81	127.18	118.90
1	A1	2258	C	C2-N1-C1'	13.16	133.28	118.80
1	A1	2258	C	N3-C2-O2	-11.55	113.82	121.90
1	A1	2505	C	C6-N1-C2	-10.26	116.20	120.30
1	A1	2258	C	C6-N1-C2	-9.90	116.34	120.30
1	A1	100	C	C2-N1-C1'	9.62	129.38	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	4948	C	N1-C2-O2	9.54	124.63	118.90
1	A1	2627	C	N1-C2-O2	9.44	124.56	118.90
1	A1	2505	C	N1-C2-O2	9.33	124.50	118.90
2	B1	29	C	N1-C2-O2	9.04	124.32	118.90
1	A1	2505	C	N3-C2-O2	-8.96	115.63	121.90
1	A1	4759	C	N1-C2-O2	8.92	124.25	118.90
1	A1	4948	C	C2-N1-C1'	8.90	128.59	118.80
1	A1	2867	C	N3-C2-O2	-8.80	115.74	121.90
1	A1	2258	C	C6-N1-C1'	-8.76	110.29	120.80
1	A1	100	C	N1-C2-O2	8.62	124.07	118.90
1	A1	4413	C	C2-N1-C1'	8.60	128.25	118.80
1	A1	4948	C	N3-C2-O2	-8.41	116.01	121.90
1	A1	2627	C	C2-N1-C1'	8.33	127.96	118.80
1	A1	1639	U	C2-N1-C1'	8.24	127.59	117.70
1	A1	4759	C	C2-N1-C1'	8.05	127.66	118.80
1	A1	3739	C	C2-N1-C1'	8.04	127.65	118.80
1	A1	4880	C	C2-N1-C1'	7.99	127.59	118.80
1	A1	4354	U	C2-N1-C1'	7.99	127.28	117.70
1	A1	1612	G	N3-C4-N9	7.97	130.78	126.00
2	B1	29	C	C2-N1-C1'	7.97	127.57	118.80
1	A1	4413	C	N1-C2-O2	7.97	123.68	118.90
1	A1	3909	C	N1-C2-O2	7.91	123.65	118.90
1	A1	271	C	N1-C2-O2	7.90	123.64	118.90
1	A1	4758	U	C2-N1-C1'	7.89	127.17	117.70
1	A1	4423	U	C2-N1-C1'	7.85	127.12	117.70
1	A1	2627	C	N3-C2-O2	-7.82	116.42	121.90
1	A1	4148	C	N1-C2-O2	7.81	123.59	118.90
1	A1	2410	C	C2-N1-C1'	7.81	127.39	118.80
1	A1	1639	U	N1-C2-O2	7.75	128.22	122.80
1	A1	1081	C	N3-C2-O2	-7.75	116.48	121.90
1	A1	4303	C	C2-N1-C1'	7.73	127.30	118.80
2	B1	29	C	N3-C2-O2	-7.70	116.51	121.90
1	A1	1993	C	N1-C2-O2	7.63	123.48	118.90
1	A1	1381	U	C2-N1-C1'	7.57	126.78	117.70
1	A1	4413	C	N3-C2-O2	-7.56	116.61	121.90
1	A1	1484	G	N3-C4-C5	-7.55	124.82	128.60
1	A1	219	G	C4-N9-C1'	7.54	136.30	126.50
1	A1	2820	C	N1-C2-O2	7.52	123.41	118.90
1	A1	100	C	N3-C2-O2	-7.51	116.64	121.90
1	A1	219	G	N3-C4-C5	-7.51	124.85	128.60
1	A1	141	C	C2-N1-C1'	7.47	127.01	118.80
50	t2	21	ASP	CB-CG-OD1	7.46	125.01	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	2258	C	C5-C6-N1	7.42	124.71	121.00
1	A1	1484	G	N3-C4-N9	7.42	130.45	126.00
1	A1	1484	G	C4-N9-C1'	7.39	136.11	126.50
1	A1	4758	U	N1-C2-O2	7.39	127.97	122.80
1	A1	4444	C	N1-C2-O2	7.33	123.30	118.90
1	A1	4241	C	N1-C2-O2	7.32	123.29	118.90
1	A1	1481	C	C2-N1-C1'	7.31	126.84	118.80
1	A1	4420	U	C2-N1-C1'	7.30	126.46	117.70
1	A1	4759	C	N3-C2-O2	-7.24	116.83	121.90
1	A1	4354	U	N1-C2-O2	7.24	127.86	122.80
1	A1	1612	G	C4-N9-C1'	7.22	135.88	126.50
1	A1	4880	C	N1-C2-O2	7.20	123.22	118.90
1	A1	2016	C	N1-C2-O2	7.17	123.20	118.90
1	A1	1381	U	N3-C2-O2	-7.16	117.19	122.20
1	A1	3909	C	C2-N1-C1'	7.14	126.65	118.80
1	A1	4305	G	C4-N9-C1'	7.12	135.75	126.50
1	A1	4420	U	N1-C2-O2	7.08	127.76	122.80
1	A1	2528	G	C4-N9-C1'	7.07	135.69	126.50
1	A1	3741	C	N3-C2-O2	-7.06	116.96	121.90
1	A1	3909	C	N3-C2-O2	-7.04	116.97	121.90
1	A1	4709	U	N1-C2-O2	7.04	127.73	122.80
1	A1	2803	U	N3-C2-O2	-7.00	117.30	122.20
1	A1	4423	U	N1-C2-O2	7.00	127.70	122.80
1	A1	2046	G	P-O3'-C3'	7.00	128.10	119.70
1	A1	2695	A	P-O3'-C3'	6.98	128.08	119.70
1	A1	1598	C	N1-C2-O2	6.97	123.08	118.90
1	A1	112	C	C2-N1-C1'	6.96	126.46	118.80
1	A1	1639	U	N3-C2-O2	-6.95	117.34	122.20
1	A1	4423	U	N3-C2-O2	-6.94	117.34	122.20
49	s2	1136	LEU	CA-CB-CG	6.94	131.26	115.30
2	B1	29	C	C6-N1-C2	-6.92	117.53	120.30
1	A1	4612	C	N1-C2-O2	6.91	123.05	118.90
1	A1	2627	C	C6-N1-C2	-6.89	117.55	120.30
1	A1	1381	U	N1-C2-O2	6.88	127.62	122.80
1	A1	3909	C	C6-N1-C2	-6.87	117.55	120.30
1	A1	685	C	P-O3'-C3'	6.86	127.93	119.70
1	A1	472	C	N1-C2-O2	6.82	122.99	118.90
1	A1	4758	U	N3-C2-O2	-6.80	117.44	122.20
1	A1	2505	C	C5-C6-N1	6.79	124.39	121.00
1	A1	4420	U	N3-C2-O2	-6.76	117.47	122.20
1	A1	220	C	C2-N1-C1'	6.75	126.23	118.80
1	A1	130	C	N3-C2-O2	-6.74	117.18	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	3636	C	C6-N1-C2	-6.74	117.60	120.30
1	A1	4709	U	N3-C2-O2	-6.71	117.50	122.20
1	A1	2528	G	N3-C4-C5	-6.70	125.25	128.60
1	A1	219	G	N3-C4-N9	6.70	130.02	126.00
1	A1	100	C	C6-N1-C1'	-6.70	112.76	120.80
1	A1	2568	C	N1-C2-O2	6.68	122.91	118.90
1	A1	4303	C	N1-C2-O2	6.66	122.89	118.90
1	A1	4354	U	N3-C2-O2	-6.65	117.54	122.20
1	A1	282	C	N1-C2-O2	6.65	122.89	118.90
1	A1	1777	C	N1-C2-O2	6.63	122.88	118.90
1	A1	4958	C	N1-C2-O2	6.61	122.87	118.90
1	A1	1072	C	P-O3'-C3'	6.60	127.62	119.70
1	A1	1612	G	C8-N9-C1'	-6.56	118.47	127.00
1	A1	4880	C	N3-C2-O2	-6.55	117.31	121.90
1	A1	2351	C	C2-N1-C1'	6.55	126.00	118.80
1	A1	1612	G	N3-C4-C5	-6.53	125.33	128.60
1	A1	4303	C	C6-N1-C2	-6.53	117.69	120.30
3	C1	64	U	N3-C2-O2	-6.52	117.64	122.20
1	A1	1735	U	N1-C2-O2	6.51	127.36	122.80
1	A1	4444	C	N3-C2-O2	-6.51	117.34	121.90
1	A1	2803	U	N1-C2-O2	6.51	127.36	122.80
1	A1	4413	C	C6-N1-C2	-6.50	117.70	120.30
1	A1	2704	C	C2-N1-C1'	6.48	125.93	118.80
7	C2	288	ASP	CB-CG-OD1	6.47	124.13	118.30
1	A1	1671	U	N3-C2-O2	-6.47	117.67	122.20
1	A1	4314	C	N1-C2-O2	6.46	122.78	118.90
1	A1	2089	G	P-O3'-C3'	6.46	127.45	119.70
40	j2	30	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A1	74	G	C4-N9-C1'	6.43	134.86	126.50
1	A1	74	G	C8-N9-C1'	-6.42	118.66	127.00
1	A1	271	C	N3-C2-O2	-6.40	117.42	121.90
1	A1	1247	U	N1-C2-O2	6.38	127.26	122.80
1	A1	2806	A	O4'-C1'-N9	6.38	113.30	108.20
1	A1	3657	U	N3-C2-O2	-6.32	117.78	122.20
1	A1	2528	G	N3-C4-N9	6.28	129.77	126.00
1	A1	2008	U	C2-N1-C1'	6.27	125.22	117.70
1	A1	2410	C	C5-C6-N1	6.26	124.13	121.00
1	A1	4303	C	N3-C2-O2	-6.26	117.52	121.90
1	A1	1210	C	C2-N1-C1'	6.25	125.67	118.80
1	A1	4266	G	N3-C4-C5	-6.24	125.48	128.60
1	A1	1993	C	N3-C2-O2	-6.24	117.53	121.90
1	A1	3876	A	P-O3'-C3'	6.21	127.16	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	1484	G	C8-N9-C1'	-6.20	118.95	127.00
1	A1	4682	U	N3-C2-O2	-6.18	117.88	122.20
1	A1	50	C	N1-C2-O2	6.18	122.61	118.90
1	A1	1081	C	N1-C2-O2	6.17	122.60	118.90
1	A1	271	C	C2-N1-C1'	6.17	125.59	118.80
1	A1	4869	U	C2-N1-C1'	6.17	125.10	117.70
1	A1	4171	C	N1-C2-O2	6.17	122.60	118.90
1	A1	1777	C	C2-N1-C1'	6.16	125.58	118.80
1	A1	4948	C	C6-N1-C1'	-6.16	113.41	120.80
1	A1	1210	C	N1-C2-O2	6.14	122.58	118.90
1	A1	2860	C	N1-C2-O2	6.14	122.58	118.90
1	A1	100	C	C6-N1-C2	-6.13	117.85	120.30
1	A1	115	C	C2-N1-C1'	6.12	125.54	118.80
1	A1	219	G	C8-N9-C1'	-6.12	119.04	127.00
1	A1	4241	C	C2-N1-C1'	6.12	125.53	118.80
1	A1	2410	C	C6-N1-C2	-6.12	117.85	120.30
1	A1	219	G	C2-N3-C4	6.11	114.96	111.90
1	A1	3657	U	N1-C2-O2	6.11	127.08	122.80
1	A1	978	G	N3-C4-N9	-6.10	122.34	126.00
1	A1	2016	C	N3-C2-O2	-6.09	117.64	121.90
1	A1	2820	C	N3-C2-O2	-6.08	117.64	121.90
1	A1	4148	C	N3-C2-O2	-6.08	117.65	121.90
41	k2	49	LEU	CA-CB-CG	6.07	129.27	115.30
1	A1	1993	C	C2-N1-C1'	6.07	125.48	118.80
1	A1	661	C	C2-N1-C1'	6.06	125.47	118.80
1	A1	1792	U	C2-N1-C1'	6.06	124.97	117.70
1	A1	3741	C	N1-C2-O2	6.06	122.53	118.90
1	A1	4871	C	N1-C2-O2	6.05	122.53	118.90
1	A1	1800	U	N3-C2-O2	-6.03	117.98	122.20
1	A1	4444	C	C6-N1-C2	-6.03	117.89	120.30
1	A1	4232	U	P-O3'-C3'	6.03	126.93	119.70
1	A1	4747	C	C2-N1-C1'	6.02	125.42	118.80
1	A1	2867	C	C6-N1-C2	-6.01	117.90	120.30
1	A1	1632	A	C2-N3-C4	6.00	113.60	110.60
1	A1	1735	U	N3-C2-O2	-6.00	118.00	122.20
1	A1	2008	U	N1-C2-O2	6.00	127.00	122.80
2	B1	102	U	N1-C2-O2	5.99	126.99	122.80
1	A1	1340	C	C5-C6-N1	5.97	123.98	121.00
1	A1	1458	C	N1-C2-O2	5.97	122.48	118.90
1	A1	4241	C	N3-C2-O2	-5.96	117.73	121.90
1	A1	4682	U	N1-C2-O2	5.95	126.96	122.80
1	A1	3739	C	C6-N1-C2	-5.94	117.92	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	1440	U	P-O3'-C3'	5.93	126.82	119.70
1	A1	4476	C	C2-N1-C1'	5.93	125.33	118.80
1	A1	4148	C	C2-N1-C1'	5.93	125.32	118.80
1	A1	4759	C	C6-N1-C2	-5.92	117.93	120.30
1	A1	1514	U	N1-C2-O2	5.92	126.94	122.80
1	A1	2011	C	N1-C2-O2	5.91	122.45	118.90
1	A1	4199	C	N1-C2-O2	5.91	122.45	118.90
1	A1	1370	G	P-O3'-C3'	5.91	126.79	119.70
1	A1	2266	C	P-O3'-C3'	5.91	126.79	119.70
1	A1	4266	G	C4-N9-C1'	5.90	134.17	126.50
1	A1	4714	C	N1-C2-O2	5.90	122.44	118.90
1	A1	1671	U	N1-C2-O2	5.89	126.92	122.80
1	A1	658	C	N1-C2-O2	5.89	122.43	118.90
1	A1	3888	G	P-O3'-C3'	5.89	126.77	119.70
1	A1	4266	G	N3-C4-N9	5.88	129.53	126.00
1	A1	4880	C	C6-N1-C2	-5.88	117.95	120.30
2	B1	28	C	N1-C2-O2	5.88	122.42	118.90
1	A1	406	C	P-O3'-C3'	5.87	126.75	119.70
1	A1	2560	C	C2-N1-C1'	5.87	125.25	118.80
1	A1	696	C	P-O3'-C3'	5.86	126.74	119.70
1	A1	2008	U	N3-C2-O2	-5.84	118.11	122.20
17	M2	44	ARG	CG-CD-NE	5.83	124.04	111.80
1	A1	2528	G	C8-N9-C1'	-5.82	119.44	127.00
1	A1	1847	C	C2-N1-C1'	5.81	125.19	118.80
1	A1	134	G	P-O3'-C3'	5.81	126.67	119.70
1	A1	265	C	P-O3'-C3'	5.80	126.66	119.70
1	A1	2502	A	OP1-P-O3'	5.80	117.95	105.20
1	A1	2281	U	N1-C2-O2	5.79	126.86	122.80
1	A1	1247	U	N3-C2-O2	-5.79	118.14	122.20
1	A1	3693	U	N1-C2-O2	5.79	126.85	122.80
1	A1	155	C	N3-C2-O2	-5.79	117.85	121.90
1	A1	1215	C	N1-C2-O2	5.78	122.37	118.90
34	d2	89	LEU	CA-CB-CG	5.78	128.60	115.30
1	A1	112	C	C6-N1-C2	-5.78	117.99	120.30
1	A1	4354	U	C5-C6-N1	5.78	125.59	122.70
1	A1	4948	C	C6-N1-C2	-5.78	117.99	120.30
1	A1	2505	C	C2-N1-C1'	5.76	125.14	118.80
1	A1	2410	C	N1-C2-O2	5.76	122.35	118.90
1	A1	4413	C	O4'-C1'-N1	5.76	112.81	108.20
1	A1	449	C	P-O3'-C3'	5.75	126.60	119.70
1	A1	220	C	C6-N1-C2	-5.74	118.00	120.30
50	t2	92	LEU	CB-CG-CD2	5.73	120.74	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	4413	C	C6-N1-C1'	-5.72	113.93	120.80
1	A1	3870	C	C2-N1-C1'	5.72	125.09	118.80
1	A1	1237	C	N1-C2-O2	5.71	122.33	118.90
24	T2	56	LEU	CA-CB-CG	5.71	128.44	115.30
1	A1	1731	C	C2-N1-C1'	5.71	125.08	118.80
1	A1	4170	A	P-O3'-C3'	5.70	126.55	119.70
1	A1	4766	C	C2-N1-C1'	5.70	125.07	118.80
1	A1	4146	G	N3-C4-N9	5.70	129.42	126.00
1	A1	263	G	C4-N9-C1'	5.68	133.88	126.50
1	A1	4612	C	N3-C2-O2	-5.68	117.93	121.90
1	A1	1577	G	N3-C2-N2	-5.67	115.93	119.90
1	A1	4243	C	C6-N1-C2	-5.67	118.03	120.30
1	A1	4752	U	N1-C2-O2	5.66	126.76	122.80
1	A1	4709	U	C2-N1-C1'	5.66	124.49	117.70
1	A1	2803	U	C2-N1-C1'	5.65	124.48	117.70
1	A1	4613	C	N1-C2-O2	5.64	122.29	118.90
1	A1	115	C	N1-C2-O2	5.64	122.28	118.90
1	A1	1485	C	N1-C2-O2	5.64	122.28	118.90
1	A1	2568	C	N3-C2-O2	-5.63	117.96	121.90
1	A1	1483	C	N1-C2-O2	5.63	122.28	118.90
1	A1	2016	C	C6-N1-C2	-5.62	118.05	120.30
1	A1	3693	U	N3-C2-O2	-5.61	118.27	122.20
1	A1	1481	C	N1-C2-O2	5.60	122.26	118.90
1	A1	1477	C	P-O3'-C3'	5.59	126.41	119.70
1	A1	4194	U	N3-C2-O2	-5.59	118.28	122.20
1	A1	2532	C	C2-N1-C1'	5.59	124.95	118.80
1	A1	3622	C	N1-C2-O2	5.59	122.25	118.90
1	A1	282	C	N3-C2-O2	-5.59	117.99	121.90
1	A1	1598	C	N3-C2-O2	-5.59	117.99	121.90
1	A1	202	C	C2-N1-C1'	5.58	124.94	118.80
1	A1	3876	A	OP2-P-O3'	5.57	117.46	105.20
1	A1	4215	C	N1-C2-O2	5.57	122.24	118.90
1	A1	4206	C	C2-N1-C1'	5.56	124.92	118.80
1	A1	217	C	C2-N1-C1'	5.56	124.91	118.80
1	A1	3778	U	N1-C2-O2	5.56	126.69	122.80
1	A1	1514	U	N3-C2-O2	-5.55	118.31	122.20
1	A1	974	C	N1-C2-O2	5.55	122.23	118.90
1	A1	1325	C	N1-C2-O2	5.54	122.23	118.90
1	A1	2856	C	N1-C2-O2	5.54	122.23	118.90
1	A1	2667	C	N1-C2-O2	5.54	122.22	118.90
1	A1	131	C	N1-C2-O2	5.53	122.22	118.90
1	A1	472	C	N3-C2-O2	-5.53	118.03	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	4146	G	C4-N9-C1'	5.53	133.68	126.50
1	A1	1485	C	C2-N1-C1'	5.52	124.88	118.80
1	A1	1929	A	C4-N9-C1'	5.51	136.22	126.30
1	A1	1309	C	C5-C6-N1	5.51	123.75	121.00
1	A1	1639	U	C6-N1-C1'	-5.50	113.49	121.20
2	B1	102	U	N3-C2-O2	-5.50	118.35	122.20
1	A1	1633	G	P-O3'-C3'	5.50	126.30	119.70
1	A1	4958	C	N3-C2-O2	-5.50	118.05	121.90
48	r2	28	LEU	CA-CB-CG	5.50	127.95	115.30
1	A1	3709	U	C2-N1-C1'	5.47	124.27	117.70
1	A1	496	G	N3-C4-N9	5.47	129.28	126.00
1	A1	126	C	C2-N1-C1'	5.47	124.81	118.80
1	A1	704	C	C2-N1-C1'	5.46	124.81	118.80
1	A1	4305	G	C8-N9-C1'	-5.46	119.89	127.00
1	A1	118	C	N1-C2-O2	5.46	122.18	118.90
1	A1	2351	C	C6-N1-C2	-5.46	118.12	120.30
1	A1	978	G	C4-N9-C1'	-5.46	119.41	126.50
1	A1	141	C	C6-N1-C1'	-5.45	114.26	120.80
1	A1	934	C	N1-C2-O2	5.45	122.17	118.90
1	A1	975	C	C6-N1-C2	-5.44	118.12	120.30
1	A1	4869	U	N3-C2-O2	-5.43	118.40	122.20
49	s2	967	LEU	CA-CB-CG	5.43	127.79	115.30
1	A1	1993	C	C6-N1-C2	-5.43	118.13	120.30
1	A1	2705	G	N3-C4-N9	5.42	129.25	126.00
1	A1	3657	U	C2-N1-C1'	5.42	124.21	117.70
1	A1	1514	U	C2-N1-C1'	5.42	124.21	117.70
1	A1	4482	U	N3-C2-O2	-5.42	118.41	122.20
1	A1	1853	G	C4-N9-C1'	5.41	133.53	126.50
1	A1	3739	C	C5-C6-N1	5.41	123.70	121.00
1	A1	4243	C	C2-N1-C1'	5.41	124.75	118.80
1	A1	2470	C	N1-C2-O2	5.40	122.14	118.90
1	A1	1929	A	C2-N3-C4	5.39	113.30	110.60
1	A1	3739	C	C6-N1-C1'	-5.38	114.34	120.80
1	A1	469	C	N1-C2-O2	5.37	122.12	118.90
1	A1	4759	C	C6-N1-C1'	-5.37	114.36	120.80
1	A1	1477	C	C6-N1-C2	-5.37	118.15	120.30
1	A1	4254	G	N3-C4-C5	-5.36	125.92	128.60
2	B1	28	C	C6-N1-C2	-5.33	118.17	120.30
1	A1	4360	U	N3-C2-O2	-5.33	118.47	122.20
1	A1	271	C	C6-N1-C2	-5.33	118.17	120.30
1	A1	4561	C	N1-C2-O2	5.33	122.10	118.90
1	A1	922(B)	C	P-O3'-C3'	5.33	126.09	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	1482	G	O4'-C1'-N9	5.32	112.46	108.20
1	A1	1308	C	C6-N1-C2	-5.32	118.17	120.30
1	A1	1292	C	C2-N1-C1'	5.32	124.65	118.80
1	A1	1726	U	N3-C2-O2	-5.31	118.48	122.20
1	A1	1236	C	C6-N1-C2	-5.31	118.17	120.30
1	A1	3761	C	N1-C2-O2	5.31	122.09	118.90
1	A1	4880	C	C6-N1-C1'	-5.31	114.43	120.80
1	A1	472	C	C2-N1-C1'	5.31	124.64	118.80
1	A1	495	C	C2-N1-C1'	5.31	124.64	118.80
1	A1	1238	A	P-O3'-C3'	5.31	126.07	119.70
1	A1	2627	C	C6-N1-C1'	-5.30	114.44	120.80
50	t2	185	LEU	CA-CB-CG	5.30	127.49	115.30
1	A1	4560	C	N1-C2-O2	5.29	122.08	118.90
1	A1	4752	U	N3-C2-O2	-5.29	118.50	122.20
1	A1	390	C	C6-N1-C2	-5.29	118.19	120.30
1	A1	450	G	O5'-P-OP2	-5.29	100.94	105.70
1	A1	1327	C	C5-C6-N1	5.28	123.64	121.00
1	A1	2704	C	N1-C2-O2	5.28	122.07	118.90
1	A1	5050	C	C2-N1-C1'	5.28	124.60	118.80
1	A1	50	C	N3-C2-O2	-5.27	118.21	121.90
1	A1	1577	G	C2-N3-C4	5.27	114.54	111.90
1	A1	4119	C	P-O3'-C3'	5.27	126.02	119.70
1	A1	3911	C	C5-C6-N1	5.26	123.63	121.00
1	A1	1720	C	N1-C2-O2	5.26	122.06	118.90
1	A1	2860	C	N3-C2-O2	-5.26	118.22	121.90
1	A1	4305	G	N3-C4-C5	-5.26	125.97	128.60
1	A1	30	C	C2-N1-C1'	5.26	124.58	118.80
1	A1	1482	G	C4-N9-C1'	5.25	133.33	126.50
1	A1	4194	U	C2-N1-C1'	5.25	124.00	117.70
2	B1	94	C	N1-C2-O2	5.25	122.05	118.90
1	A1	1628	C	C5-C6-N1	5.25	123.62	121.00
1	A1	4314	C	N3-C2-O2	-5.24	118.23	121.90
3	C1	64	U	N1-C2-O2	5.24	126.47	122.80
1	A1	4601	U	N1-C2-O2	5.23	126.46	122.80
1	A1	275	C	P-O3'-C3'	5.23	125.98	119.70
1	A1	1800	U	N1-C2-O2	5.23	126.46	122.80
1	A1	1792	U	N1-C2-O2	5.23	126.46	122.80
1	A1	2787	A	C2-N3-C4	5.22	113.21	110.60
1	A1	4254	G	C4-N9-C1'	5.22	133.29	126.50
1	A1	1915	C	N1-C2-O2	5.21	122.03	118.90
1	A1	1211	G	P-O3'-C3'	5.21	125.95	119.70
1	A1	4869	U	N1-C2-O2	5.21	126.45	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	263	G	N3-C4-N9	5.21	129.12	126.00
1	A1	220	C	C5-C6-N1	5.21	123.60	121.00
2	B1	28	C	N3-C2-O2	-5.21	118.25	121.90
1	A1	4293	U	N3-C2-O2	-5.20	118.56	122.20
1	A1	922(B)	C	OP1-P-O3'	5.19	116.62	105.20
1	A1	2362	U	N3-C2-O2	-5.19	118.57	122.20
1	A1	661	C	C6-N1-C2	-5.18	118.23	120.30
1	A1	4308	C	N1-C2-O2	5.18	122.01	118.90
1	A1	100	C	O4'-C1'-N1	5.18	112.34	108.20
1	A1	112	C	N1-C2-O2	5.18	122.01	118.90
1	A1	2281	U	N3-C2-O2	-5.18	118.58	122.20
1	A1	2705	G	C4-N9-C1'	5.18	133.23	126.50
1	A1	1309	C	C6-N1-C2	-5.17	118.23	120.30
1	A1	1247	U	C2-N1-C1'	5.17	123.90	117.70
1	A1	472	C	C6-N1-C2	-5.17	118.23	120.30
1	A1	2787	A	C4-N9-C1'	5.17	135.60	126.30
1	A1	3739	C	N1-C2-O2	5.17	122.00	118.90
1	A1	126	C	C6-N1-C2	-5.16	118.23	120.30
1	A1	1325	C	N3-C2-O2	-5.16	118.29	121.90
1	A1	3625	G	P-O3'-C3'	5.16	125.89	119.70
1	A1	2627	C	C5-C6-N1	5.15	123.58	121.00
1	A1	4758	U	C6-N1-C1'	-5.15	113.99	121.20
1	A1	504	G	P-O3'-C3'	5.15	125.88	119.70
1	A1	4305	G	C8-N9-C4	-5.15	104.34	106.40
1	A1	112	C	C5-C6-N1	5.14	123.57	121.00
1	A1	3882	C	C2-N1-C1'	5.14	124.46	118.80
1	A1	4303	C	O4'-C1'-N1	5.14	112.31	108.20
1	A1	4171	C	N3-C2-O2	-5.14	118.30	121.90
2	B1	29	C	C5-C6-N1	5.13	123.57	121.00
1	A1	685	C	O5'-P-OP2	-5.13	101.08	105.70
1	A1	2860	C	C6-N1-C2	-5.13	118.25	120.30
1	A1	217	C	N1-C2-O2	5.13	121.98	118.90
1	A1	118	C	C2-N1-C1'	5.12	124.44	118.80
1	A1	263	G	C8-N9-C1'	-5.12	120.34	127.00
1	A1	4162	C	N1-C2-O2	5.12	121.97	118.90
1	A1	4482	U	N1-C2-O2	5.12	126.38	122.80
1	A1	96	U	N3-C2-O2	-5.11	118.62	122.20
1	A1	2410	C	C6-N1-C1'	-5.10	114.67	120.80
1	A1	495	C	C6-N1-C2	-5.10	118.26	120.30
1	A1	916	C	N1-C2-O2	5.10	121.96	118.90
1	A1	4254	G	N3-C4-N9	5.10	129.06	126.00
1	A1	1179	U	C2-N1-C1'	5.10	123.81	117.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A1	496	G	N3-C4-C5	-5.09	126.05	128.60
1	A1	4444	C	C2-N1-C1'	5.09	124.40	118.80
1	A1	1792	U	N3-C2-O2	-5.09	118.64	122.20
1	A1	155	C	N1-C2-O2	5.09	121.95	118.90
1	A1	2553	A	O4'-C1'-N9	5.08	112.26	108.20
1	A1	4642	U	N3-C2-O2	-5.08	118.65	122.20
1	A1	1210	C	N3-C2-O2	-5.08	118.35	121.90
1	A1	118	C	C6-N1-C2	-5.07	118.27	120.30
1	A1	4906	C	C2-N1-C1'	5.07	124.38	118.80
1	A1	1088	C	C6-N1-C2	-5.07	118.27	120.30
1	A1	3650	C	C6-N1-C2	-5.06	118.28	120.30
1	A1	125	C	P-O3'-C3'	5.06	125.77	119.70
1	A1	3603	G	P-O3'-C3'	5.05	125.77	119.70
1	A1	4412	C	C2-N1-C1'	5.05	124.36	118.80
1	A1	2502	A	P-O3'-C3'	5.05	125.76	119.70
1	A1	959	G	P-O3'-C3'	5.05	125.76	119.70
1	A1	1484	G	C2-N3-C4	5.04	114.42	111.90
1	A1	2767	U	N3-C2-O2	-5.04	118.67	122.20
1	A1	4243	C	N1-C2-O2	5.04	121.92	118.90
1	A1	4423	U	C6-N1-C1'	-5.04	114.15	121.20
1	A1	5047	C	N1-C2-O2	5.04	121.92	118.90
1	A1	4942	C	C2-N1-C1'	5.03	124.34	118.80
1	A1	4957	C	N1-C2-O2	5.03	121.92	118.90
1	A1	1481	C	C6-N1-C1'	-5.03	114.76	120.80
1	A1	141	C	N1-C2-O2	5.03	121.92	118.90
1	A1	1607	C	N3-C2-O2	-5.03	118.38	121.90
1	A1	4398	C	C6-N1-C2	-5.03	118.29	120.30
1	A1	4560	C	C2-N1-C1'	5.03	124.33	118.80
1	A1	1469	C	C6-N1-C2	-5.03	118.29	120.30
1	A1	390	C	C5-C6-N1	5.03	123.51	121.00
1	A1	4601	U	N3-C2-O2	-5.03	118.68	122.20
1	A1	274	C	C2-N1-C1'	5.03	124.33	118.80
1	A1	2439	G	C4-N9-C1'	5.03	133.03	126.50
1	A1	2362	U	N1-C2-O2	5.02	126.31	122.80
1	A1	4199	C	N3-C2-O2	-5.01	118.39	121.90
1	A1	4206	C	C6-N1-C2	-5.01	118.30	120.30
1	A1	1411(B)	C	N1-C2-O2	5.01	121.91	118.90
1	A1	2726	G	C4-N9-C1'	5.01	133.01	126.50
1	A1	658	C	N3-C2-O2	-5.01	118.39	121.90
1	A1	1777	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	K2	63	THR	Peptide
17	M2	76	PRO	Peptide
17	M2	78	GLY	Peptide
23	S2	80	VAL	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	
4	D1	2/29 (7%)	1 (50%)	1 (50%)	0	100	100
5	A2	246/257 (96%)	234 (95%)	12 (5%)	0	100	100
6	B2	392/403 (97%)	384 (98%)	8 (2%)	0	100	100
7	C2	360/425 (85%)	343 (95%)	17 (5%)	0	100	100
8	D2	291/297 (98%)	283 (97%)	8 (3%)	0	100	100
9	E2	208/291 (72%)	201 (97%)	7 (3%)	0	100	100
10	F2	223/247 (90%)	215 (96%)	8 (4%)	0	100	100
11	G2	229/319 (72%)	223 (97%)	6 (3%)	0	100	100
12	H2	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
13	I2	201/214 (94%)	196 (98%)	5 (2%)	0	100	100
14	J2	168/178 (94%)	166 (99%)	2 (1%)	0	100	100
15	K2	208/211 (99%)	197 (95%)	10 (5%)	1 (0%)	29	61
16	L2	136/218 (62%)	131 (96%)	5 (4%)	0	100	100
17	M2	201/204 (98%)	194 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	N2	197/203 (97%)	192 (98%)	5 (2%)	0	100	100
19	O2	151/184 (82%)	149 (99%)	2 (1%)	0	100	100
20	P2	185/187 (99%)	177 (96%)	8 (4%)	0	100	100
21	Q2	153/196 (78%)	148 (97%)	5 (3%)	0	100	100
22	R2	174/176 (99%)	166 (95%)	8 (5%)	0	100	100
23	S2	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
24	T2	100/128 (78%)	96 (96%)	4 (4%)	0	100	100
25	U2	129/140 (92%)	125 (97%)	4 (3%)	0	100	100
26	V2	61/157 (39%)	57 (93%)	4 (7%)	0	100	100
27	W2	116/156 (74%)	114 (98%)	2 (2%)	0	100	100
28	X2	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
29	Y2	133/136 (98%)	125 (94%)	7 (5%)	1 (1%)	19	49
30	Z2	145/148 (98%)	136 (94%)	9 (6%)	0	100	100
31	a2	100/226 (44%)	99 (99%)	1 (1%)	0	100	100
32	b2	96/115 (84%)	96 (100%)	0	0	100	100
33	c2	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
34	d2	126/135 (93%)	123 (98%)	3 (2%)	0	100	100
35	e2	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
36	f2	112/116 (97%)	110 (98%)	2 (2%)	0	100	100
37	g2	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
38	h2	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
39	i2	84/97 (87%)	83 (99%)	1 (1%)	0	100	100
40	j2	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
41	k2	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
42	l2	50/102 (49%)	49 (98%)	1 (2%)	0	100	100
43	m2	23/25 (92%)	23 (100%)	0	0	100	100
44	n2	102/106 (96%)	98 (96%)	4 (4%)	0	100	100
45	o2	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
46	p2	122/137 (89%)	117 (96%)	5 (4%)	0	100	100
47	q2	194/318 (61%)	185 (95%)	9 (5%)	0	100	100
48	r2	151/165 (92%)	133 (88%)	18 (12%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	s2	377/1411 (27%)	368 (98%)	9 (2%)	0	100	100
50	t2	414/489 (85%)	402 (97%)	12 (3%)	0	100	100
51	u2	9/64 (14%)	9 (100%)	0	0	100	100
All	All	7482/9782 (76%)	7227 (97%)	253 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	K2	64	VAL
29	Y2	90	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D1	2/2 (100%)	2 (100%)	0	100	100
5	A2	190/199 (96%)	190 (100%)	0	100	100
6	B2	342/348 (98%)	340 (99%)	2 (1%)	86	96
7	C2	302/347 (87%)	301 (100%)	1 (0%)	92	98
8	D2	247/250 (99%)	247 (100%)	0	100	100
9	E2	190/251 (76%)	189 (100%)	1 (0%)	88	96
10	F2	196/215 (91%)	196 (100%)	0	100	100
11	G2	200/272 (74%)	197 (98%)	3 (2%)	65	89
12	H2	169/171 (99%)	169 (100%)	0	100	100
13	I2	175/181 (97%)	175 (100%)	0	100	100
14	J2	143/149 (96%)	143 (100%)	0	100	100
15	K2	175/176 (99%)	175 (100%)	0	100	100
16	L2	117/161 (73%)	116 (99%)	1 (1%)	78	94
17	M2	171/172 (99%)	171 (100%)	0	100	100
18	N2	171/173 (99%)	171 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	O2	134/163 (82%)	134 (100%)	0	100	100
20	P2	164/164 (100%)	162 (99%)	2 (1%)	71	92
21	Q2	138/175 (79%)	138 (100%)	0	100	100
22	R2	157/157 (100%)	157 (100%)	0	100	100
23	S2	139/140 (99%)	139 (100%)	0	100	100
24	T2	92/114 (81%)	92 (100%)	0	100	100
25	U2	101/107 (94%)	101 (100%)	0	100	100
26	V2	55/126 (44%)	55 (100%)	0	100	100
27	W2	106/134 (79%)	105 (99%)	1 (1%)	78	94
28	X2	124/135 (92%)	124 (100%)	0	100	100
29	Y2	117/118 (99%)	117 (100%)	0	100	100
30	Z2	119/120 (99%)	119 (100%)	0	100	100
31	a2	84/172 (49%)	83 (99%)	1 (1%)	71	92
32	b2	84/98 (86%)	84 (100%)	0	100	100
33	c2	98/110 (89%)	98 (100%)	0	100	100
34	d2	114/121 (94%)	114 (100%)	0	100	100
35	e2	88/89 (99%)	88 (100%)	0	100	100
36	f2	98/99 (99%)	98 (100%)	0	100	100
37	g2	109/109 (100%)	109 (100%)	0	100	100
38	h2	86/89 (97%)	86 (100%)	0	100	100
39	i2	73/80 (91%)	72 (99%)	1 (1%)	67	90
40	j2	64/65 (98%)	64 (100%)	0	100	100
41	k2	47/48 (98%)	47 (100%)	0	100	100
42	l2	48/90 (53%)	48 (100%)	0	100	100
43	m2	24/24 (100%)	24 (100%)	0	100	100
44	n2	92/94 (98%)	92 (100%)	0	100	100
45	o2	74/75 (99%)	73 (99%)	1 (1%)	67	90
46	p2	108/121 (89%)	107 (99%)	1 (1%)	78	94
47	q2	164/258 (64%)	164 (100%)	0	100	100
48	r2	126/137 (92%)	125 (99%)	1 (1%)	81	94
49	s2	342/1239 (28%)	342 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	t2	360/416 (86%)	359 (100%)	1 (0%)	92	98
51	u2	8/53 (15%)	8 (100%)	0	100	100
All	All	6527/8307 (79%)	6510 (100%)	17 (0%)	92	98

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B2	261	ARG
6	B2	297	LYS
7	C2	188	ARG
9	E2	58	ARG
11	G2	142	ARG
11	G2	143	GLN
11	G2	228	ARG
16	L2	79	LYS
20	P2	8	ASN
20	P2	14	ARG
27	W2	152	LYS
31	a2	117	ARG
39	i2	20	ARG
45	o2	4	ARG
46	p2	119	ARG
48	r2	114	ARG
50	t2	266	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
20	P2	8	ASN
22	R2	125	GLN
23	S2	69	GLN
33	c2	28	ASN
49	s2	1218	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	3516/4380 (80%)	723 (20%)	45 (1%)
2	B1	119/120 (99%)	11 (9%)	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C1	149/156 (95%)	28 (18%)	1 (0%)
All	All	3784/4656 (81%)	762 (20%)	46 (1%)

All (762) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	12	A
1	A1	13	U
1	A1	17	A
1	A1	25	A
1	A1	30	C
1	A1	35	U
1	A1	39	A
1	A1	42	A
1	A1	56	A
1	A1	58	G
1	A1	59	A
1	A1	64	A
1	A1	65	A
1	A1	73	A
1	A1	84	A
1	A1	91	G
1	A1	104	G
1	A1	108	A
1	A1	109	G
1	A1	110	C
1	A1	119	G
1	A1	126	C
1	A1	134	G
1	A1	135	G
1	A1	136	C
1	A1	141	C
1	A1	142	G
1	A1	146	G
1	A1	157	U
1	A1	159	C
1	A1	172	C
1	A1	177	G
1	A1	182	G
1	A1	200	U
1	A1	201	C
1	A1	202	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	209	U
1	A1	210	C
1	A1	216	C
1	A1	217	C
1	A1	219	G
1	A1	224	U
1	A1	233	U
1	A1	234	G
1	A1	246	G
1	A1	265	C
1	A1	266	C
1	A1	267	G
1	A1	271	C
1	A1	276	C
1	A1	278	G
1	A1	280	G
1	A1	297	U
1	A1	306	A
1	A1	309	C
1	A1	315	G
1	A1	316	U
1	A1	322	C
1	A1	334	A
1	A1	340	C
1	A1	350	C
1	A1	363	A
1	A1	387	G
1	A1	407	A
1	A1	410	A
1	A1	412	G
1	A1	413	G
1	A1	440	U
1	A1	449	C
1	A1	450	G
1	A1	452	A
1	A1	453	G
1	A1	454	U
1	A1	455	C
1	A1	467	U
1	A1	468	U
1	A1	481	G
1	A1	481(A)	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	482	G
1	A1	483	G
1	A1	486	C
1	A1	492	U
1	A1	493	G
1	A1	495	C
1	A1	496	G
1	A1	497	G
1	A1	498	C
1	A1	499	G
1	A1	505	G
1	A1	506	C
1	A1	510	U
1	A1	644	G
1	A1	647	G
1	A1	658	C
1	A1	659	G
1	A1	661	C
1	A1	666	G
1	A1	669	C
1	A1	670	G
1	A1	672	C
1	A1	685	C
1	A1	686	A
1	A1	687	U
1	A1	688	U
1	A1	696	C
1	A1	697	G
1	A1	704	C
1	A1	705	G
1	A1	708	G
1	A1	731	G
1	A1	738	C
1	A1	738(A)	C
1	A1	739	G
1	A1	746	A
1	A1	747	A
1	A1	749	G
1	A1	756	G
1	A1	758	G
1	A1	913	U
1	A1	914	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	917	A
1	A1	918	G
1	A1	923	C
1	A1	925	C
1	A1	926	G
1	A1	929	A
1	A1	932	A
1	A1	933	G
1	A1	934	C
1	A1	935	A
1	A1	935(A)	G
1	A1	936	C
1	A1	938	C
1	A1	939	G
1	A1	943	A
1	A1	944	A
1	A1	945	U
1	A1	956	A
1	A1	959	G
1	A1	960	A
1	A1	961	G
1	A1	964	A
1	A1	965	G
1	A1	966	A
1	A1	967	C
1	A1	968	C
1	A1	969	C
1	A1	972	C
1	A1	979	C
1	A1	983	C
1	A1	990	C
1	A1	1072	C
1	A1	1073	G
1	A1	1078	A
1	A1	1081	C
1	A1	1082	C
1	A1	1175	A
1	A1	1179	U
1	A1	1198	G
1	A1	1210	C
1	A1	1211	G
1	A1	1212	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	1215	C
1	A1	1234	G
1	A1	1235	G
1	A1	1236	C
1	A1	1237	C
1	A1	1238	A
1	A1	1239	C
1	A1	1272	C
1	A1	1273	G
1	A1	1274	A
1	A1	1275	G
1	A1	1277	G
1	A1	1284	G
1	A1	1287	G
1	A1	1292	C
1	A1	1293	G
1	A1	1296	G
1	A1	1301	C
1	A1	1303	A
1	A1	1304	C
1	A1	1313	C
1	A1	1326	A
1	A1	1330	A
1	A1	1337	A
1	A1	1354	A
1	A1	1358	G
1	A1	1359	G
1	A1	1371	A
1	A1	1377	G
1	A1	1379	C
1	A1	1387	A
1	A1	1394	G
1	A1	1397	A
1	A1	1398	A
1	A1	1419	G
1	A1	1420	A
1	A1	1421	G
1	A1	1433	A
1	A1	1435	G
1	A1	1436	C
1	A1	1437	C
1	A1	1438	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	1440	U
1	A1	1441	C
1	A1	1445	U
1	A1	1446	C
1	A1	1448	G
1	A1	1456	C
1	A1	1457	G
1	A1	1475	G
1	A1	1478	C
1	A1	1482	G
1	A1	1483	C
1	A1	1484	G
1	A1	1489	G
1	A1	1493	G
1	A1	1497	A
1	A1	1498	G
1	A1	1502	G
1	A1	1514	U
1	A1	1516	G
1	A1	1523	A
1	A1	1534	A
1	A1	1547	A
1	A1	1563	A
1	A1	1564	A
1	A1	1566	C
1	A1	1578	U
1	A1	1591	U
1	A1	1596	U
1	A1	1597	G
1	A1	1602	U
1	A1	1612	G
1	A1	1613	A
1	A1	1624	G
1	A1	1625	G
1	A1	1631	A
1	A1	1633	G
1	A1	1634	A
1	A1	1638	A
1	A1	1640	C
1	A1	1641	G
1	A1	1650	A
1	A1	1654	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	1661	C
1	A1	1676	C
1	A1	1677	U
1	A1	1731	C
1	A1	1734	G
1	A1	1741	G
1	A1	1742	A
1	A1	1750	G
1	A1	1756	U
1	A1	1761	G
1	A1	1764	G
1	A1	1767	A
1	A1	1769	G
1	A1	1772	C
1	A1	1775	A
1	A1	1780	A
1	A1	1781	U
1	A1	1787	A
1	A1	1797	G
1	A1	1799	G
1	A1	1803	G
1	A1	1804	A
1	A1	1806	G
1	A1	1809	C
1	A1	1815	G
1	A1	1818	G
1	A1	1819	G
1	A1	1821	G
1	A1	1822	U
1	A1	1828	C
1	A1	1835	G
1	A1	1836	G
1	A1	1837	A
1	A1	1842	G
1	A1	1843	A
1	A1	1855	G
1	A1	1869	G
1	A1	1882	U
1	A1	1889	U
1	A1	1890	G
1	A1	1892	A
1	A1	1893	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	1897	A
1	A1	1898	C
1	A1	1910	G
1	A1	1918	U
1	A1	1920	C
1	A1	1921	C
1	A1	1922	G
1	A1	1930	U
1	A1	1931	C
1	A1	1932	A
1	A1	1935	C
1	A1	1938	C
1	A1	1945	G
1	A1	1957	U
1	A1	1958	A
1	A1	1960	A
1	A1	1961	G
1	A1	1962	A
1	A1	1964	A
1	A1	1965	G
1	A1	1967	A
1	A1	1971	U
1	A1	1974	U
1	A1	1975	G
1	A1	1976	G
1	A1	1977	C
1	A1	1978	C
1	A1	1979	A
1	A1	1980	U
1	A1	1984	A
1	A1	1985	G
1	A1	1987	C
1	A1	1988	G
1	A1	1991	A
1	A1	1992	U
1	A1	1997	U
1	A1	1999	A
1	A1	2001	G
1	A1	2002	A
1	A1	2003	G
1	A1	2004	U
1	A1	2011	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	2015	U
1	A1	2018	C
1	A1	2020	U
1	A1	2022	C
1	A1	2026	A
1	A1	2034	G
1	A1	2044	U
1	A1	2046	G
1	A1	2047	A
1	A1	2048	U
1	A1	2052	G
1	A1	2055	G
1	A1	2056	G
1	A1	2062	C
1	A1	2064	G
1	A1	2069	A
1	A1	2071	A
1	A1	2084	U
1	A1	2090	U
1	A1	2092	G
1	A1	2093	G
1	A1	2094	C
1	A1	2095	A
1	A1	2097	A
1	A1	2098	G
1	A1	2099	C
1	A1	2100	G
1	A1	2101	A
1	A1	2102	G
1	A1	2104	A
1	A1	2105	A
1	A1	2106	G
1	A1	2107	A
1	A1	2108	G
1	A1	2110	G
1	A1	2259	G
1	A1	2260	C
1	A1	2267	U
1	A1	2268	A
1	A1	2275	G
1	A1	2289	C
1	A1	2299	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	2300	A
1	A1	2301	G
1	A1	2306	G
1	A1	2313	A
1	A1	2314	G
1	A1	2316	G
1	A1	2333	G
1	A1	2348	G
1	A1	2351	C
1	A1	2360	A
1	A1	2395	A
1	A1	2396	A
1	A1	2398	U
1	A1	2417	A
1	A1	2422	C
1	A1	2424	G
1	A1	2425	U
1	A1	2433	G
1	A1	2441	C
1	A1	2450	G
1	A1	2453	A
1	A1	2475	G
1	A1	2487	G
1	A1	2488	C
1	A1	2489	C
1	A1	2490	U
1	A1	2491	C
1	A1	2492	C
1	A1	2503	G
1	A1	2504	C
1	A1	2505	C
1	A1	2506	G
1	A1	2512	A
1	A1	2513	A
1	A1	2514	G
1	A1	2529	A
1	A1	2530	U
1	A1	2537	A
1	A1	2546	G
1	A1	2547	G
1	A1	2553	A
1	A1	2554	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	2566	G
1	A1	2568	C
1	A1	2575	U
1	A1	2583	C
1	A1	2586	G
1	A1	2587	A
1	A1	2589	C
1	A1	2602	G
1	A1	2618	G
1	A1	2619	G
1	A1	2620	G
1	A1	2627	C
1	A1	2638	G
1	A1	2653	C
1	A1	2662	G
1	A1	2663	G
1	A1	2669	C
1	A1	2670	C
1	A1	2676	A
1	A1	2686	G
1	A1	2687	U
1	A1	2694	G
1	A1	2695	A
1	A1	2696	A
1	A1	2707	U
1	A1	2708	U
1	A1	2709	C
1	A1	2710	C
1	A1	2711	G
1	A1	2714	G
1	A1	2721	G
1	A1	2725	A
1	A1	2726	G
1	A1	2740	U
1	A1	2743	A
1	A1	2744	A
1	A1	2754	G
1	A1	2760	G
1	A1	2763	U
1	A1	2764	A
1	A1	2769	U
1	A1	2772	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	2787	A
1	A1	2788	U
1	A1	2790	U
1	A1	2794	C
1	A1	2798	A
1	A1	2803	U
1	A1	2806	A
1	A1	2807	A
1	A1	2814	C
1	A1	2826	U
1	A1	2827	G
1	A1	2828	U
1	A1	2842	G
1	A1	2855	G
1	A1	2867	C
1	A1	2875	C
1	A1	2884	G
1	A1	3598	C
1	A1	3604	A
1	A1	3605	C
1	A1	3615	G
1	A1	3625	G
1	A1	3626	G
1	A1	3635	A
1	A1	3646	A
1	A1	3648	A
1	A1	3657	U
1	A1	3662	A
1	A1	3664	G
1	A1	3672	G
1	A1	3673	C
1	A1	3680	U
1	A1	3696	C
1	A1	3711	A
1	A1	3729	U
1	A1	3740	G
1	A1	3748	A
1	A1	3753	G
1	A1	3760	A
1	A1	3767	C
1	A1	3773	U
1	A1	3776	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	3777	G
1	A1	3784	A
1	A1	3786	U
1	A1	3791	C
1	A1	3810	C
1	A1	3811	G
1	A1	3812	C
1	A1	3814	U
1	A1	3817	A
1	A1	3819	G
1	A1	3838	U
1	A1	3839	G
1	A1	3840	U
1	A1	3851	U
1	A1	3876	A
1	A1	3877	A
1	A1	3878	C
1	A1	3879	G
1	A1	3889	G
1	A1	3892	U
1	A1	3897	G
1	A1	3898	G
1	A1	3901	A
1	A1	3905	A
1	A1	3906	A
1	A1	3907	G
1	A1	3908	A
1	A1	3915	U
1	A1	3916	G
1	A1	3917	A
1	A1	3938	G
1	A1	3939	G
1	A1	3943	A
1	A1	3946	G
1	A1	4066	U
1	A1	4069	U
1	A1	4073	A
1	A1	4076	G
1	A1	4084	G
1	A1	4086	G
1	A1	4088	C
1	A1	4109	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	4116	C
1	A1	4118	U
1	A1	4119	C
1	A1	4120	U
1	A1	4121	G
1	A1	4122	G
1	A1	4127	A
1	A1	4136	G
1	A1	4158	C
1	A1	4162	C
1	A1	4163	U
1	A1	4166	G
1	A1	4170	A
1	A1	4171	C
1	A1	4183	G
1	A1	4184	G
1	A1	4191	G
1	A1	4203	A
1	A1	4212	A
1	A1	4225	G
1	A1	4228	G
1	A1	4229	U
1	A1	4233	A
1	A1	4251	A
1	A1	4254	G
1	A1	4255	A
1	A1	4257	A
1	A1	4265	U
1	A1	4266	G
1	A1	4268	A
1	A1	4271	A
1	A1	4273	A
1	A1	4281	A
1	A1	4282	A
1	A1	4291	G
1	A1	4296	U
1	A1	4297	G
1	A1	4304	A
1	A1	4305	G
1	A1	4306	U
1	A1	4314	C
1	A1	4317	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	4318	C
1	A1	4319	C
1	A1	4326	G
1	A1	4329	G
1	A1	4330	G
1	A1	4332	C
1	A1	4349	C
1	A1	4350	C
1	A1	4354	U
1	A1	4355	G
1	A1	4373	G
1	A1	4377	G
1	A1	4378	A
1	A1	4380	A
1	A1	4387	C
1	A1	4391	G
1	A1	4393	G
1	A1	4394	A
1	A1	4395	U
1	A1	4396	A
1	A1	4398	C
1	A1	4401	G
1	A1	4411	G
1	A1	4419	U
1	A1	4421	C
1	A1	4422	A
1	A1	4437	U
1	A1	4444	C
1	A1	4448	G
1	A1	4449	A
1	A1	4464	A
1	A1	4466	C
1	A1	4471	U
1	A1	4472	G
1	A1	4475	G
1	A1	4488	A
1	A1	4500	U
1	A1	4510	A
1	A1	4512	U
1	A1	4513	A
1	A1	4515	G
1	A1	4518	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	4519	C
1	A1	4522	G
1	A1	4524	G
1	A1	4548	A
1	A1	4549	G
1	A1	4560	C
1	A1	4567	G
1	A1	4570	G
1	A1	4573	G
1	A1	4574	U
1	A1	4575	G
1	A1	4587	G
1	A1	4590	A
1	A1	4635	A
1	A1	4636	U
1	A1	4637	G
1	A1	4639	G
1	A1	4652	G
1	A1	4656	A
1	A1	4657	U
1	A1	4670	C
1	A1	4672	A
1	A1	4677	U
1	A1	4687	A
1	A1	4700	A
1	A1	4709	U
1	A1	4720	C
1	A1	4736	C
1	A1	4744	A
1	A1	4745	G
1	A1	4751	G
1	A1	4752	U
1	A1	4754	G
1	A1	4757	C
1	A1	4759	C
1	A1	4761	G
1	A1	4764	A
1	A1	4765	G
1	A1	4771	C
1	A1	4772	C
1	A1	4776	G
1	A1	4868	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	4870	G
1	A1	4871	C
1	A1	4875	G
1	A1	4882	U
1	A1	4883	C
1	A1	4885	U
1	A1	4895	C
1	A1	4897	G
1	A1	4903	G
1	A1	4910	A
1	A1	4912	G
1	A1	4913	G
1	A1	4919	G
1	A1	4921	C
1	A1	4922	C
1	A1	4924	C
1	A1	4925	U
1	A1	4927	G
1	A1	4928	C
1	A1	4931	G
1	A1	4937	C
1	A1	4938	A
1	A1	4940	C
1	A1	4943	A
1	A1	4944	C
1	A1	4948	C
1	A1	4949	G
1	A1	4950	U
1	A1	4951	G
1	A1	4956	A
1	A1	4957	C
1	A1	4958	C
1	A1	4960	G
1	A1	4963	G
1	A1	4964	C
1	A1	4965	U
1	A1	4966	A
1	A1	4967	A
1	A1	4976	U
1	A1	4985	U
1	A1	4988	U
1	A1	4989	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	4990	C
1	A1	4993	G
1	A1	5006	U
1	A1	5007	A
1	A1	5014	A
1	A1	5017	G
1	A1	5022	U
1	A1	5041	G
1	A1	5047	C
1	A1	5050	C
1	A1	5053	U
1	A1	5054	C
1	A1	5056	A
1	A1	5061	A
1	A1	5062	G
2	B1	7	G
2	B1	22	A
2	B1	25	G
2	B1	53	U
2	B1	54	A
2	B1	64	G
2	B1	97	G
2	B1	100	A
2	B1	110	G
2	B1	111	C
2	B1	120	U
3	C1	2	G
3	C1	13	G
3	C1	23	C
3	C1	34	U
3	C1	35	C
3	C1	38	U
3	C1	59	A
3	C1	62	A
3	C1	63	U
3	C1	75	G
3	C1	79	G
3	C1	86	U
3	C1	87	G
3	C1	94	G
3	C1	103	A
3	C1	105	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C1	106	G
3	C1	110	U
3	C1	111	U
3	C1	113	C
3	C1	114	G
3	C1	123	U
3	C1	124	U
3	C1	125	C
3	C1	126	C
3	C1	127	U
3	C1	128	C
3	C1	156	U

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A1	125	C
1	A1	134	G
1	A1	245	C
1	A1	265	C
1	A1	275	C
1	A1	406	C
1	A1	449	C
1	A1	480	C
1	A1	485	C
1	A1	504	G
1	A1	684	G
1	A1	685	C
1	A1	696	C
1	A1	959	G
1	A1	971(A)	G
1	A1	1072	C
1	A1	1174	G
1	A1	1211	G
1	A1	1236	C
1	A1	1238	A
1	A1	1329	G
1	A1	1370	G
1	A1	1440	U
1	A1	1445	U
1	A1	1455	G
1	A1	1477	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	1633	G
1	A1	2046	G
1	A1	2089	G
1	A1	2266	C
1	A1	2502	A
1	A1	2546	G
1	A1	2695	A
1	A1	3603	G
1	A1	3625	G
1	A1	3876	A
1	A1	3888	G
1	A1	4119	C
1	A1	4170	A
1	A1	4232	U
1	A1	4448	G
1	A1	4699	U
1	A1	4719	G
1	A1	4884	G
1	A1	4989	U
3	C1	124	U

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 219 ligands modelled in this entry, 219 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A1	19

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A1	1252:C	O3'	1271:G	P	37.11
1	A1	1219:G	O3'	1233:G	P	19.96
1	A1	990:C	O3'	1064:G	P	18.26
1	A1	523:C	O3'	638:G	P	16.85
1	A1	1406(C):G	O3'	1411:C	P	16.23
1	A1	760:G	O3'	904:C	P	14.91
1	A1	1364:U	O3'	1368:A	P	14.23
1	A1	182:G	O3'	189:G	P	12.21
1	A1	1180:C	O3'	1183:C	P	9.84
1	A1	4729:A	O3'	4735:G	P	8.98
1	A1	1100:U	O3'	1168:G	P	7.94
1	A1	512:U	O3'	515:C	P	6.73
1	A1	500:G	O3'	504:G	P	6.06
1	A1	170:C	O3'	171:U	P	5.80
1	A1	1239:C	O3'	1244:G	P	5.07
1	A1	4740:G	O3'	4743:G	P	4.74
1	A1	751:G	O3'	752:G	P	3.37
1	A1	4899:G	O3'	4902:C	P	3.32
1	A1	5020:G	O3'	5021:C	P	3.29

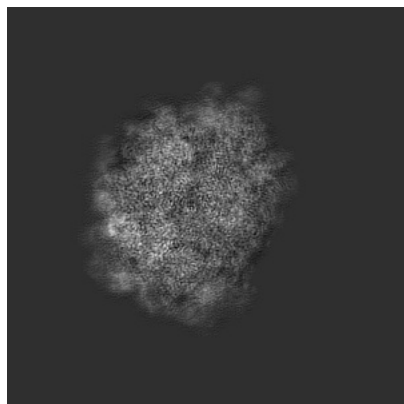
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16155. These allow visual inspection of the internal detail of the map and identification of artifacts.

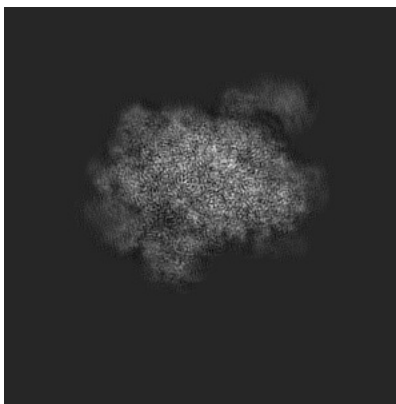
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

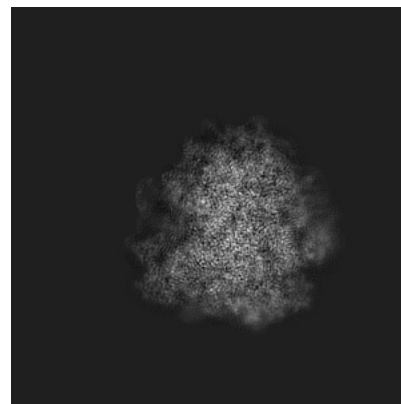
6.1.1 Primary map



X

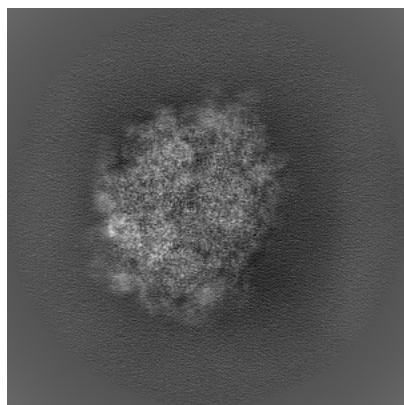


Y

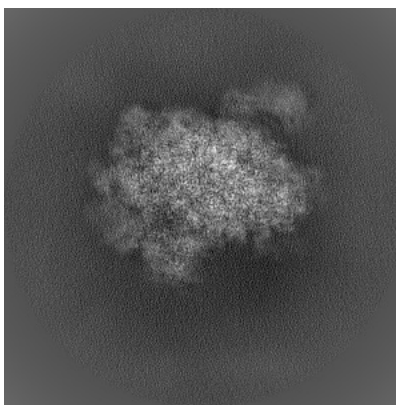


Z

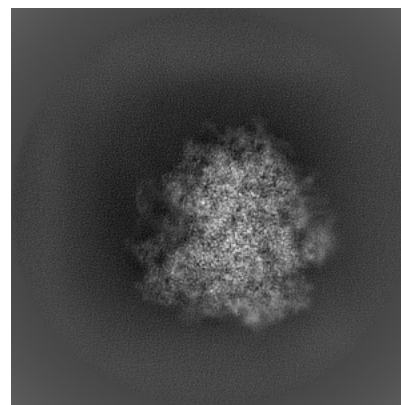
6.1.2 Raw map



X



Y

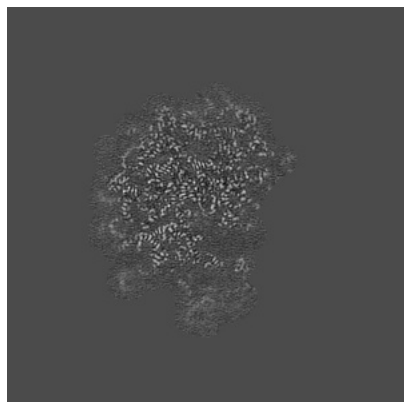


Z

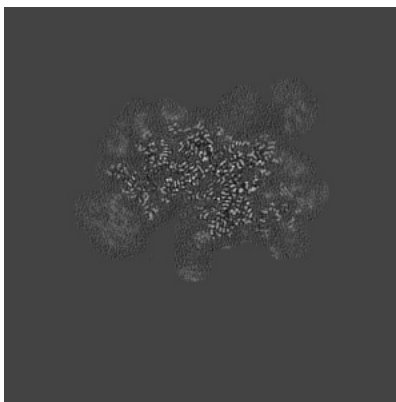
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

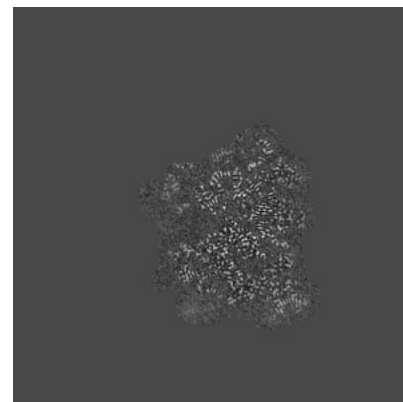
6.2.1 Primary map



X Index: 260

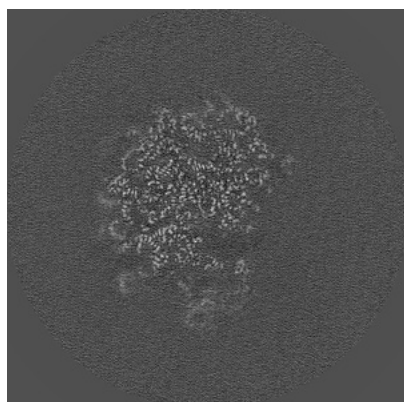


Y Index: 260

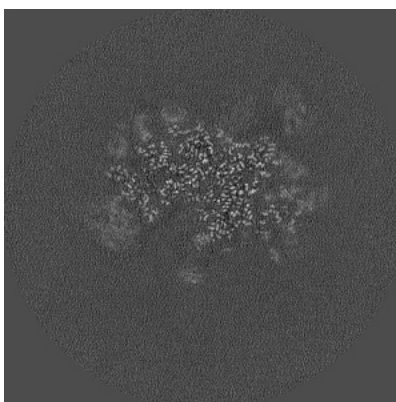


Z Index: 260

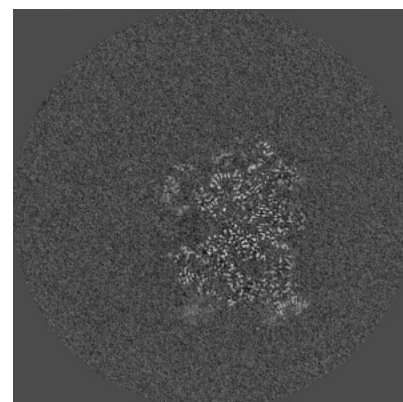
6.2.2 Raw map



X Index: 260



Y Index: 260

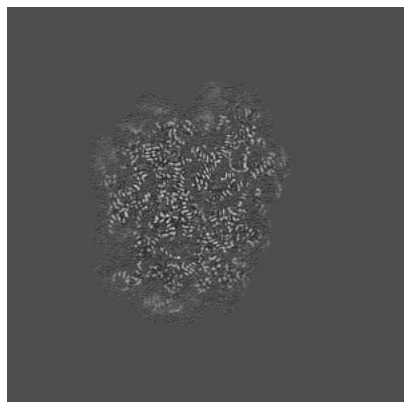


Z Index: 260

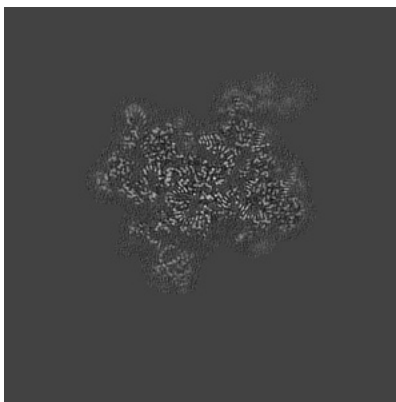
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

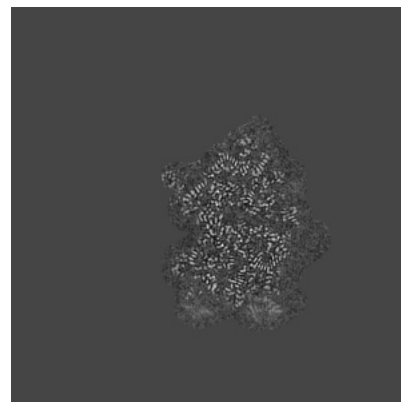
6.3.1 Primary map



X Index: 282

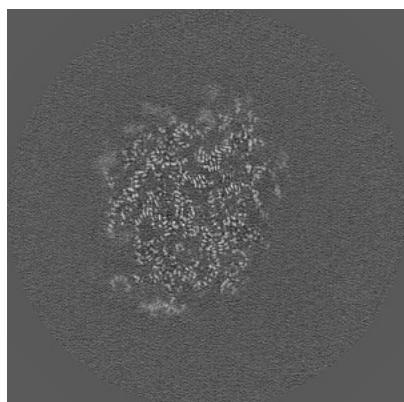


Y Index: 210

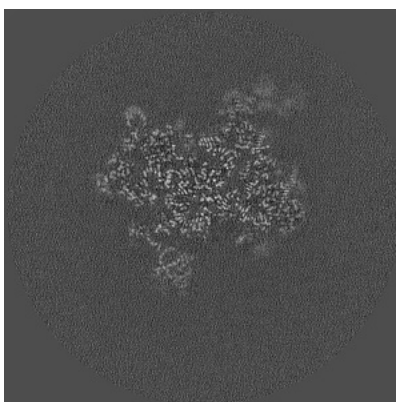


Z Index: 275

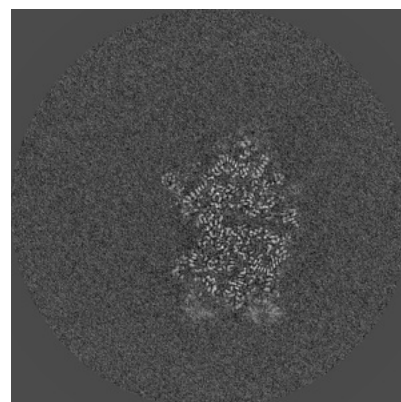
6.3.2 Raw map



X Index: 285



Y Index: 210

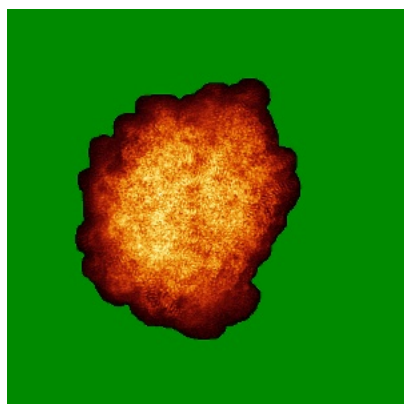


Z Index: 275

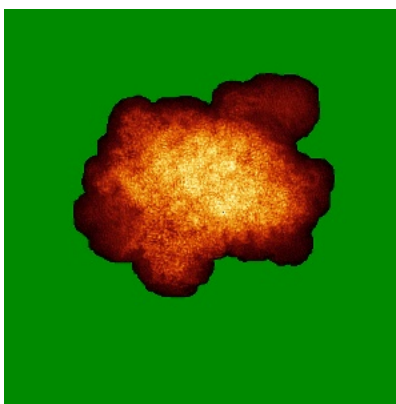
The images above show the largest variance slices of the map in three orthogonal directions.

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

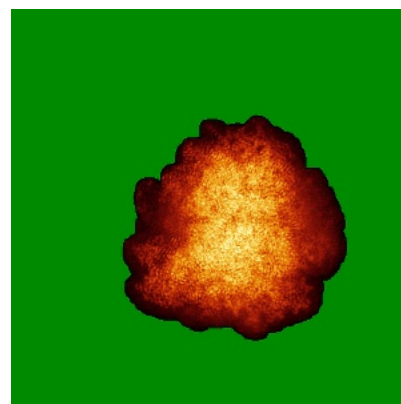
6.4.1 Primary map



X

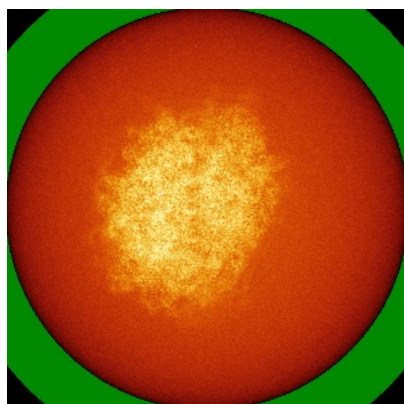


Y

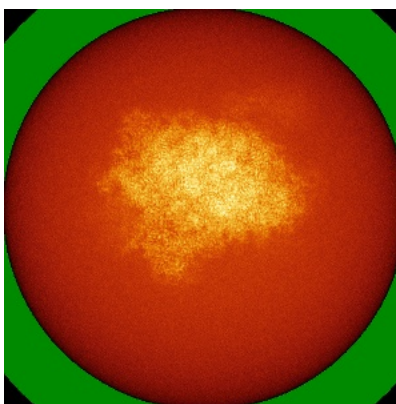


Z

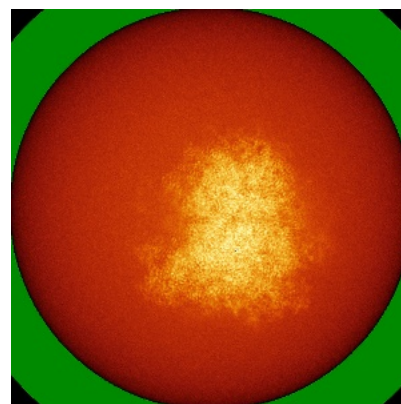
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



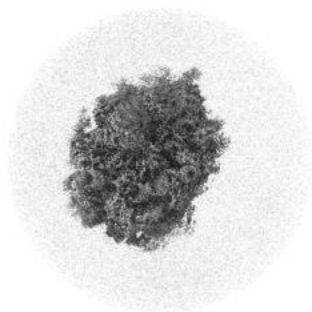
Y



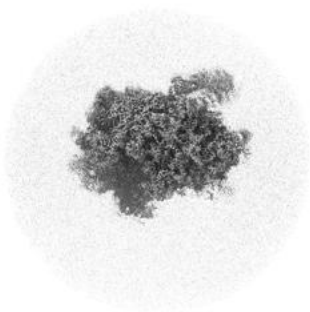
Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

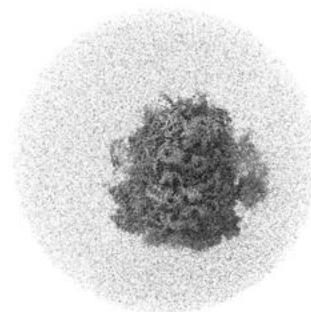
6.5.2 Raw map



X



Y



Z

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

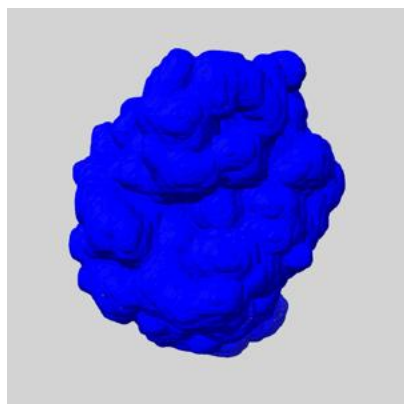
6.6 Mask visualisation [i](#)

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

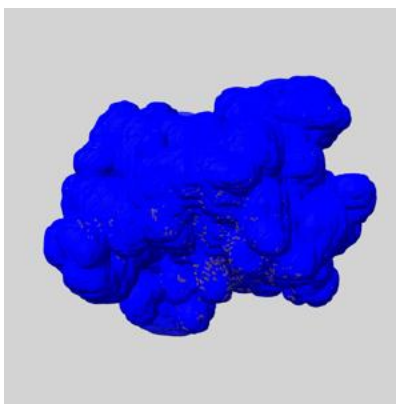
A mask typically either:

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

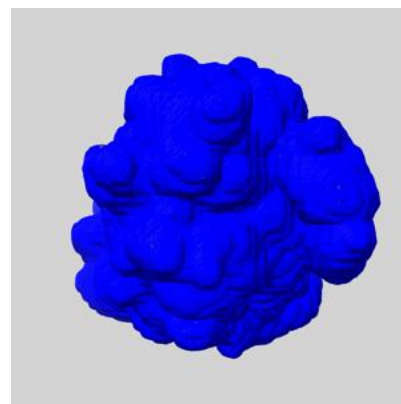
6.6.1 emd_16155_msk_1.map [i](#)



X



Y

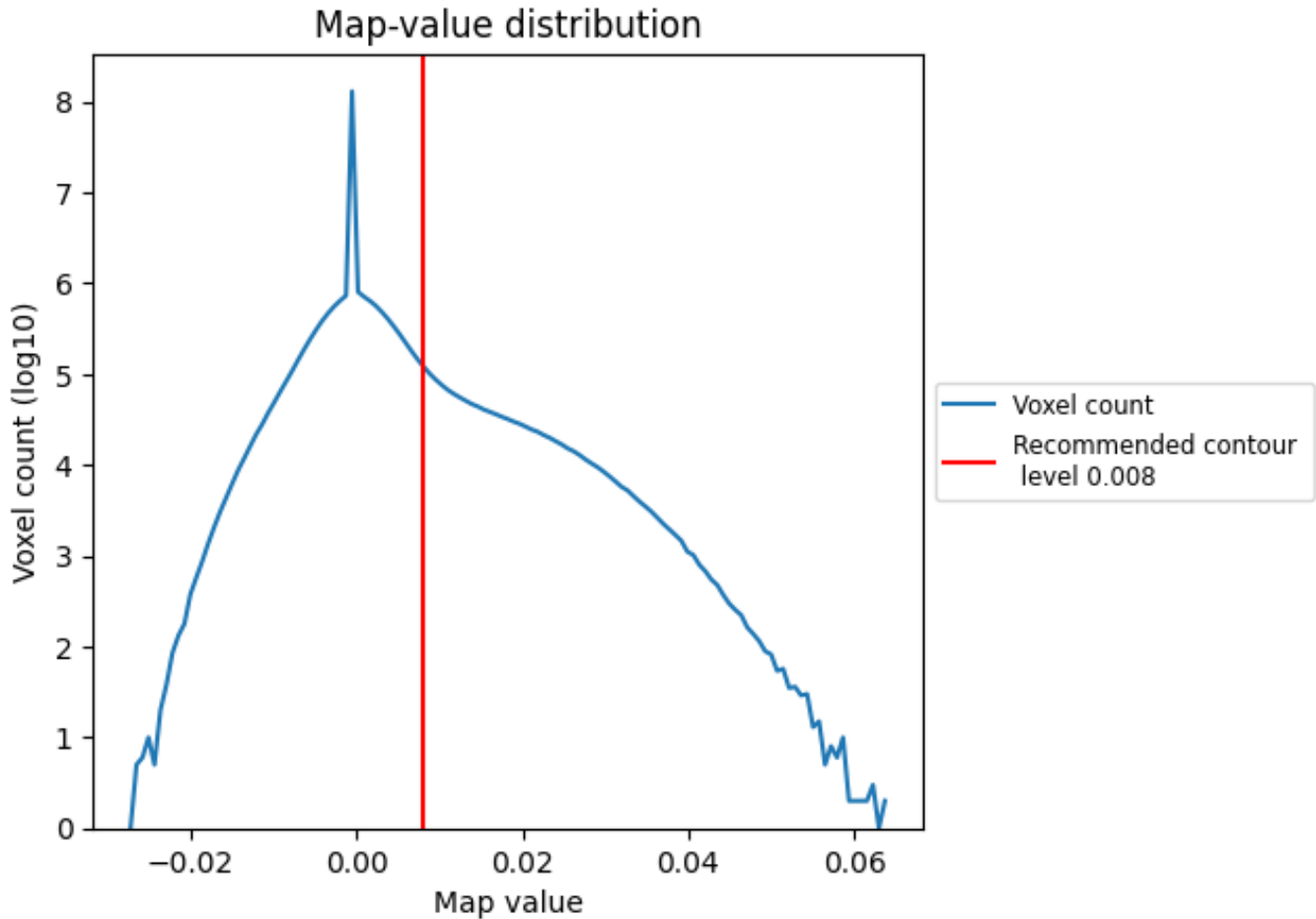


Z

7 Map analysis [i](#)

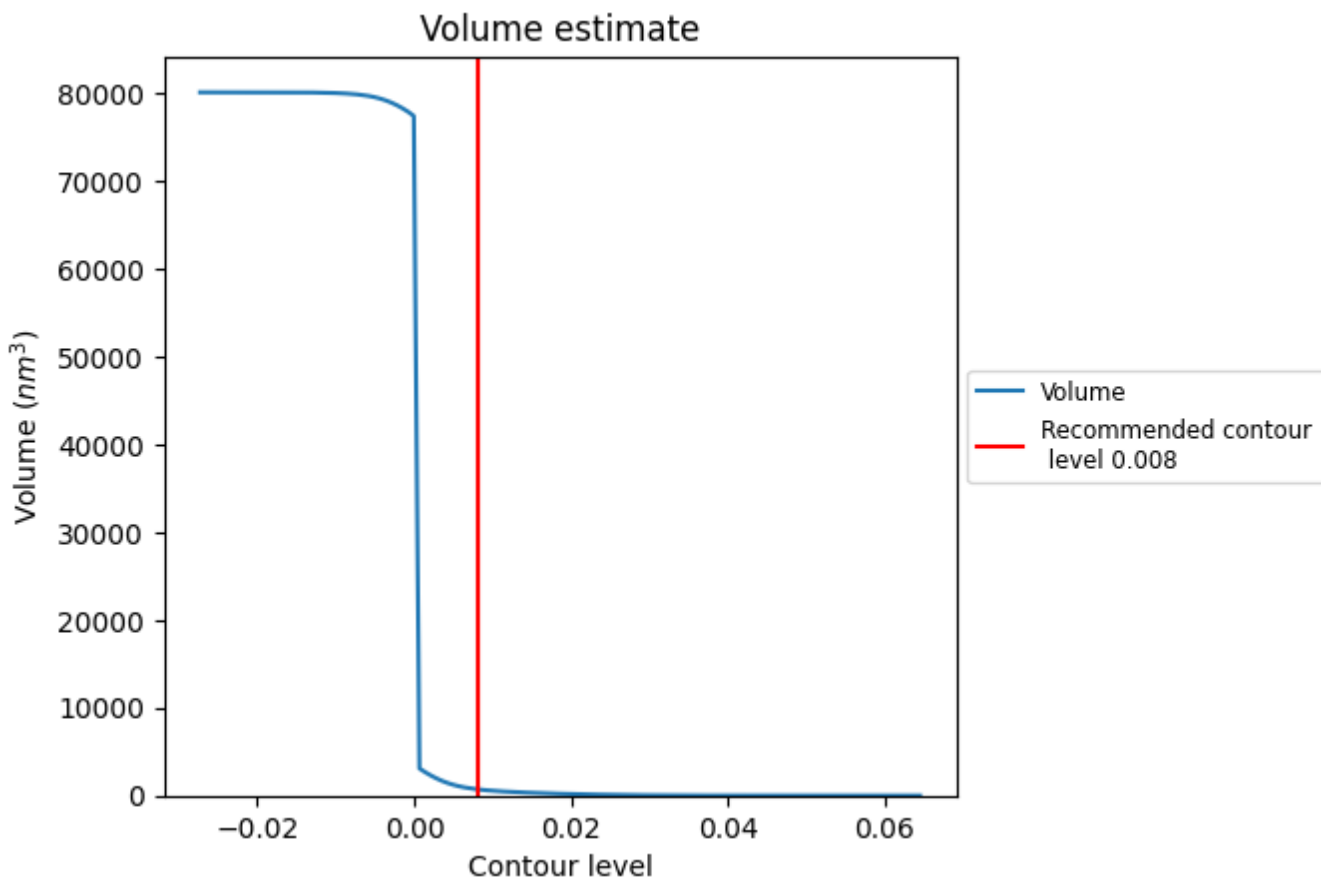
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

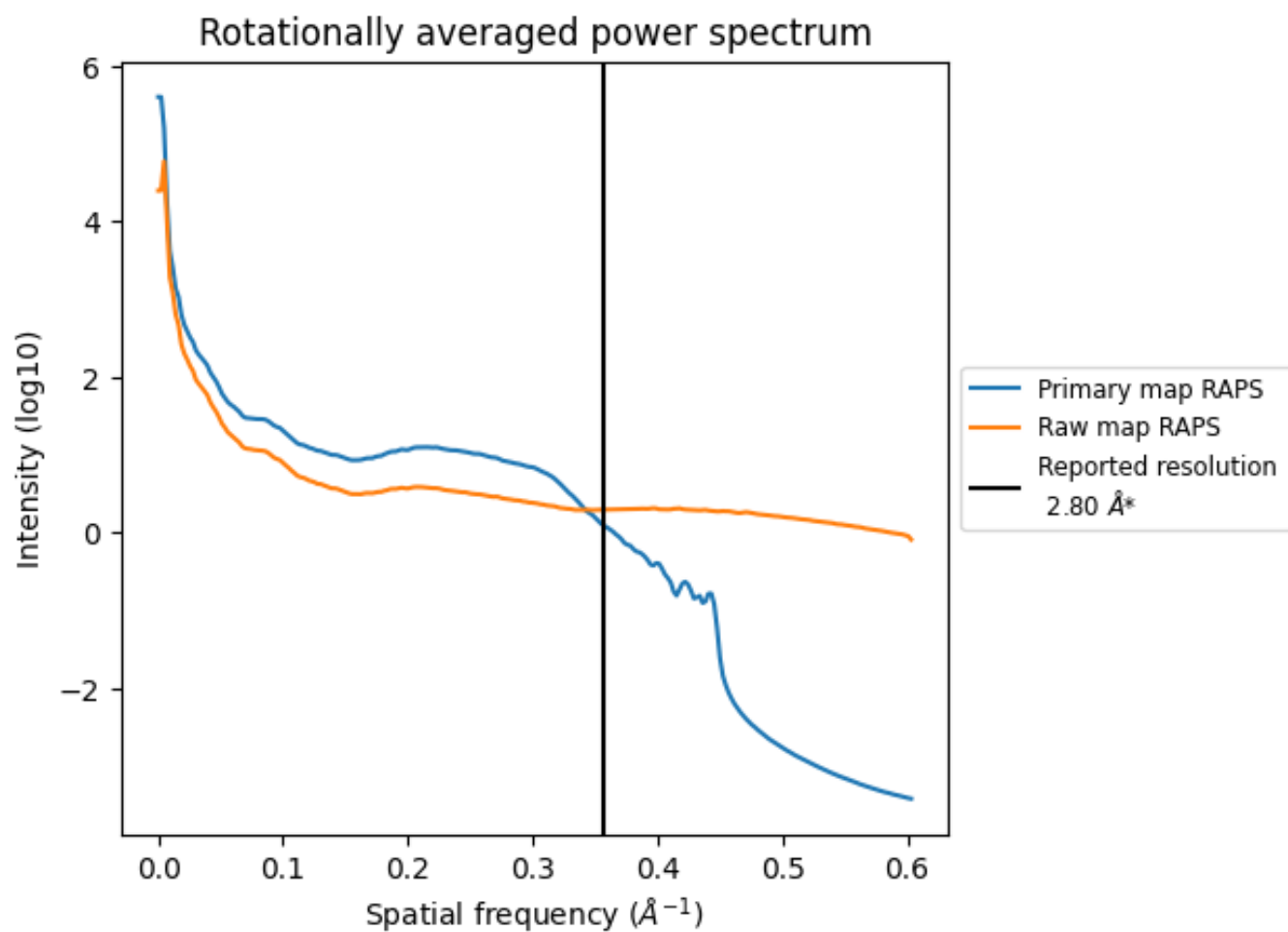
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 717 nm^3 ; this corresponds to an approximate mass of 648 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

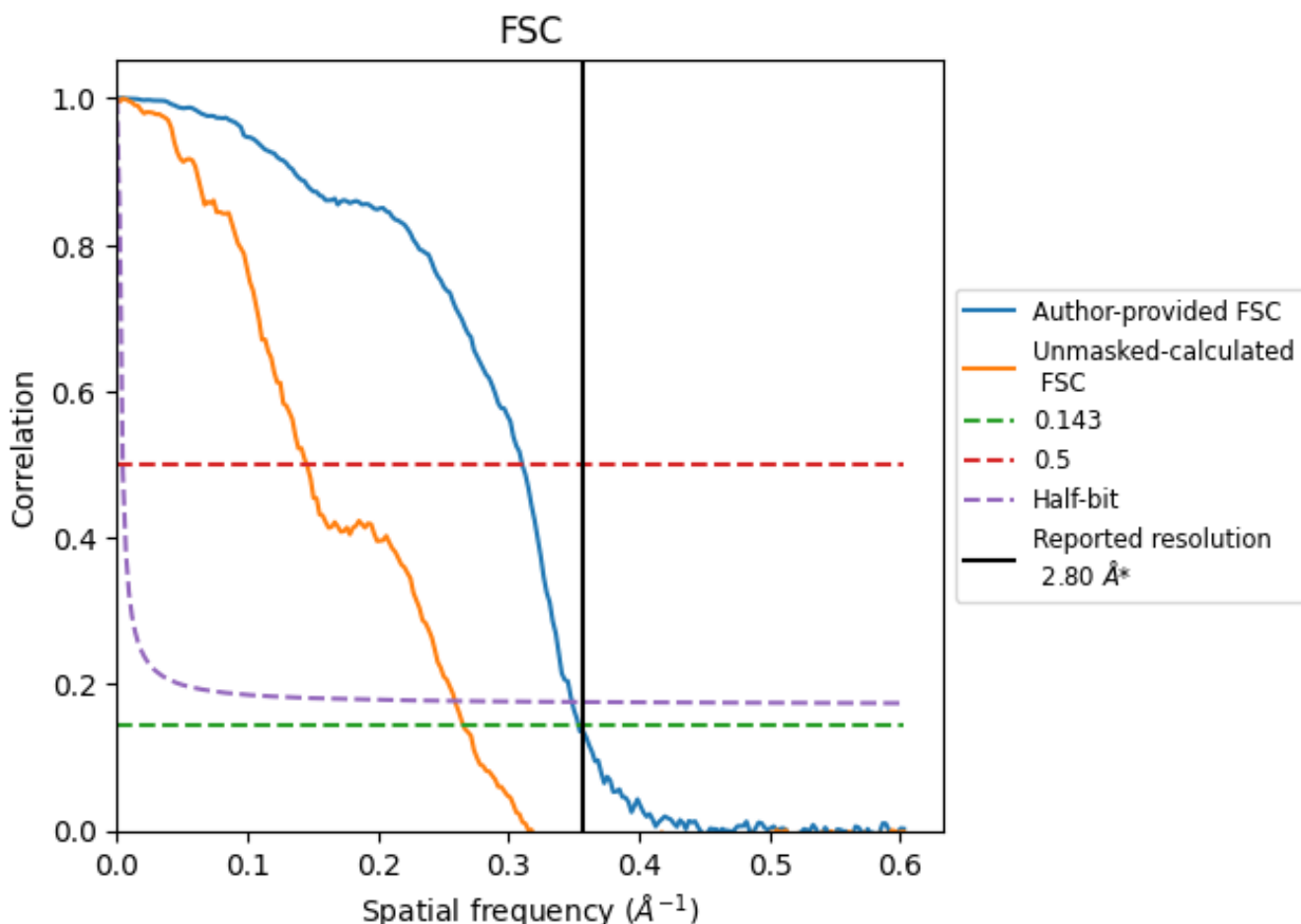


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

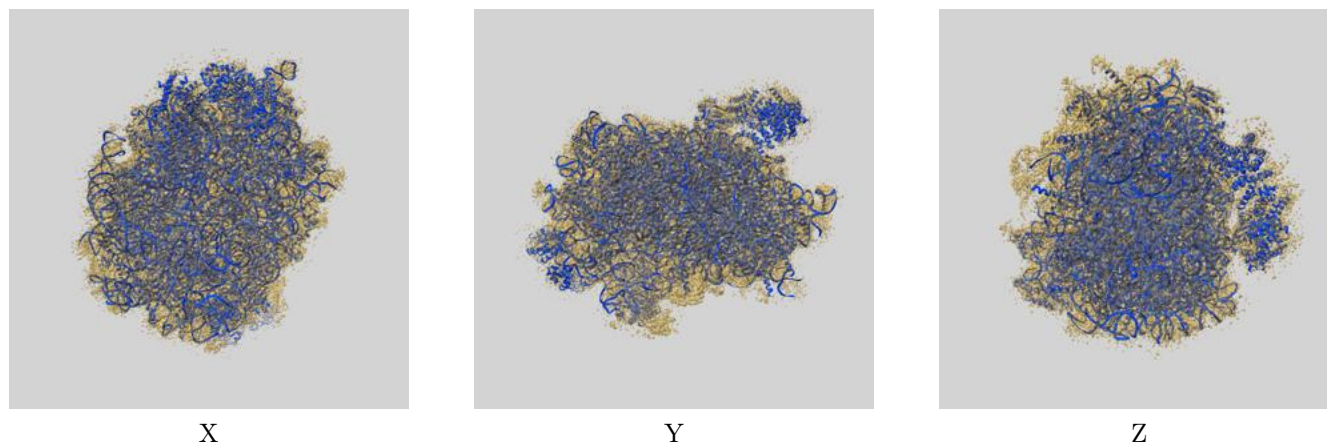
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.83	3.22	2.87
Unmasked-calculated*	3.76	6.87	3.86

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.76 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

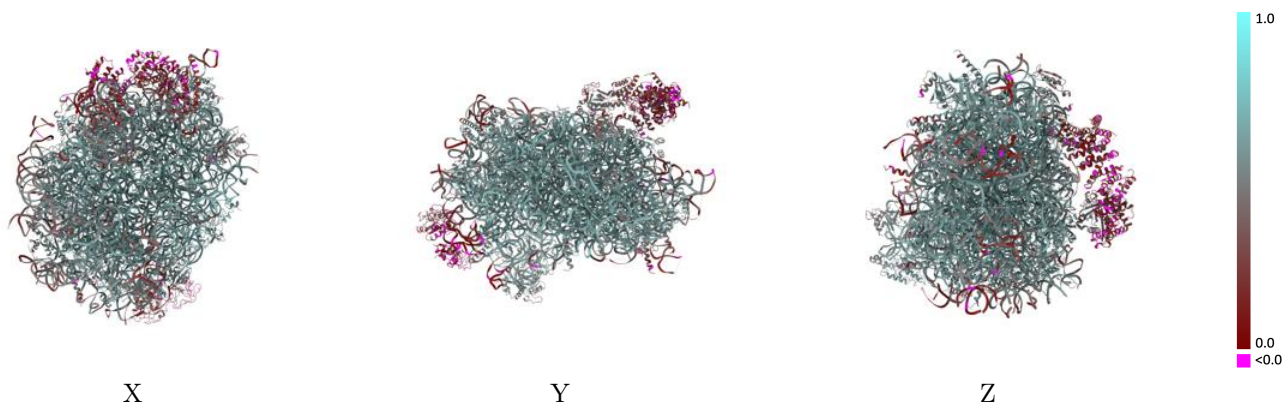
This section contains information regarding the fit between EMDB map EMD-16155 and PDB model 8BPO. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



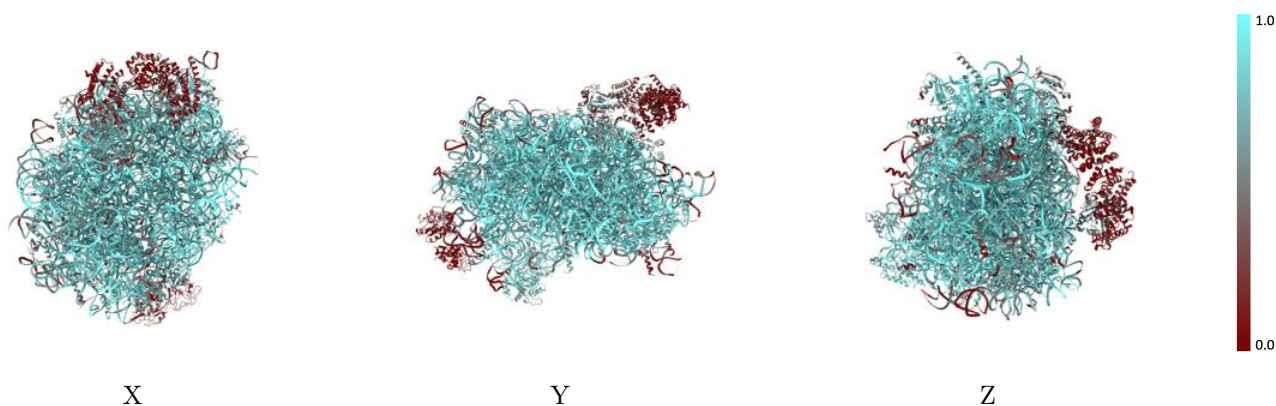
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



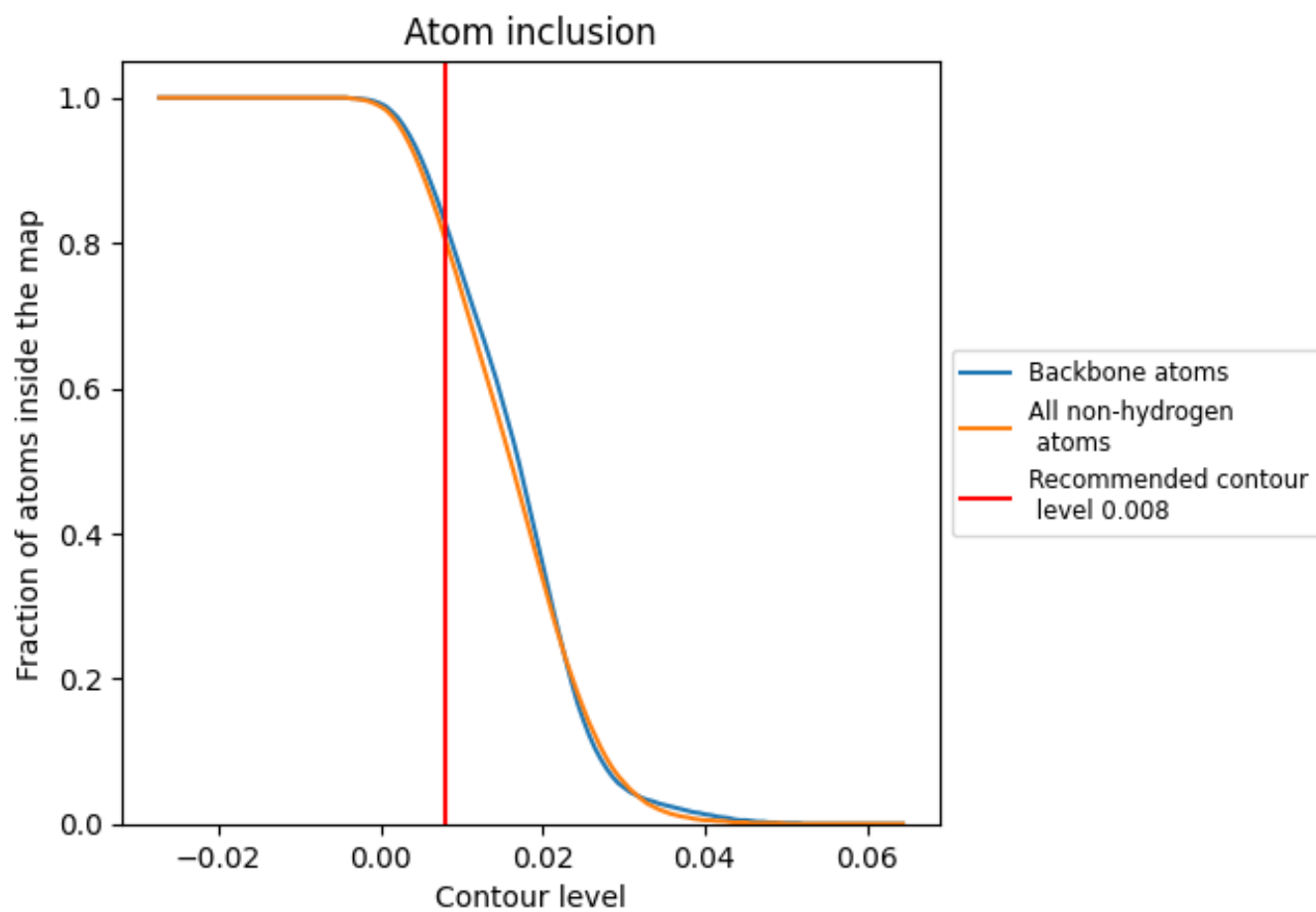
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary



































The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8040	 0.5490
A1	 0.8560	 0.5610
A2	 0.8830	 0.6230
B1	 0.9580	 0.6180
B2	 0.8650	 0.6080
C1	 0.8970	 0.5890
C2	 0.8700	 0.6000
D1	 0.3130	 0.3710
D2	 0.8190	 0.5710
E2	 0.7860	 0.5580
F2	 0.8760	 0.6160
G2	 0.7120	 0.5270
H2	 0.7650	 0.5660
I2	 0.8470	 0.6040
J2	 0.6960	 0.5040
K2	 0.8050	 0.5680
L2	 0.8270	 0.5780
M2	 0.9070	 0.6300
N2	 0.8680	 0.6050
O2	 0.8660	 0.6140
P2	 0.8900	 0.6180
Q2	 0.8310	 0.5890
R2	 0.8740	 0.6070
S2	 0.8140	 0.5760
T2	 0.5580	 0.4390
U2	 0.8390	 0.6030
V2	 0.8070	 0.6030
W2	 0.7950	 0.5720
X2	 0.8150	 0.5800
Y2	 0.8100	 0.5680
Z2	 0.9110	 0.6270
a2	 0.6750	 0.5250
b2	 0.7660	 0.5320
c2	 0.8060	 0.5720
d2	 0.8850	 0.6240



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e2	 0.8970	 0.6220
f2	 0.8260	 0.5860
g2	 0.7890	 0.5720
h2	 0.7650	 0.5490
i2	 0.9140	 0.6270
j2	 0.6500	 0.5190
k2	 0.8150	 0.5820
l2	 0.8150	 0.5860
m2	 0.6240	 0.4990
n2	 0.8150	 0.5990
o2	 0.8100	 0.5920
p2	 0.8740	 0.5970
q2	 0.1120	 0.1880
r2	 0.0370	 0.1160
s2	 0.1280	 0.1880
t2	 0.3250	 0.2750
u2	 0.2370	 0.2500