



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:37 am GMT

PDB ID : 6G5H
EMDB ID : EMD-4352
Title : Cryo-EM structure of a late human pre-40S ribosomal subunit - Mature
Authors : Ameismeier, M.; Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on : 2018-03-29
Resolution : 3.60 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:

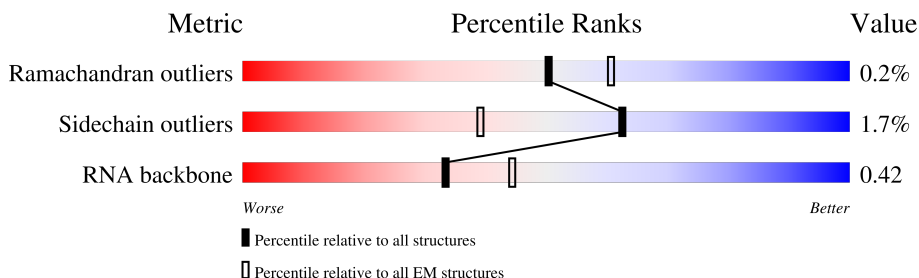
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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.



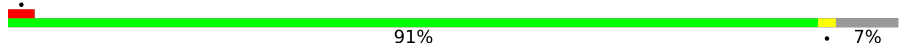

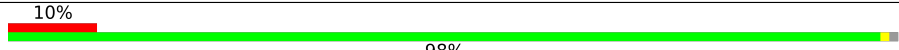
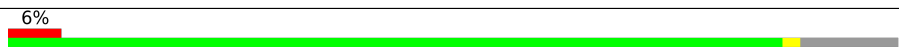

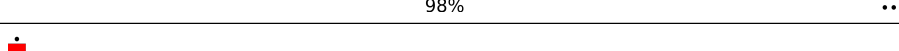
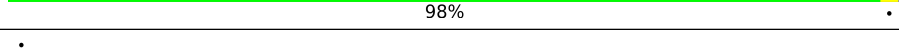
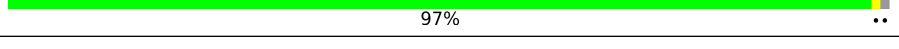
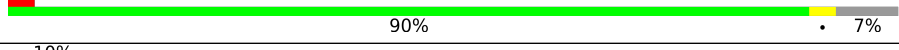

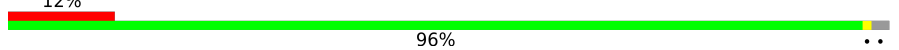
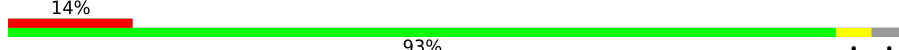
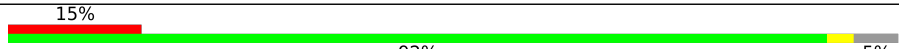


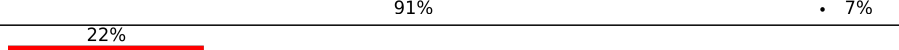


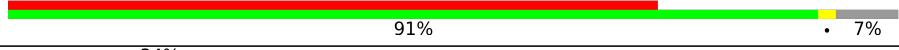

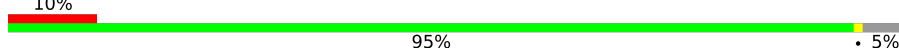
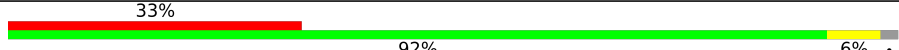

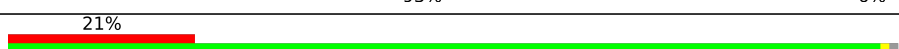
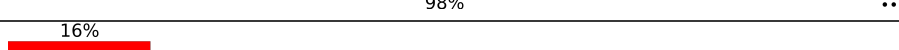
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	2	1868	
2	A	295	
3	B	264	
4	C	293	
5	E	263	
6	G	249	
7	H	194	
8	I	208	


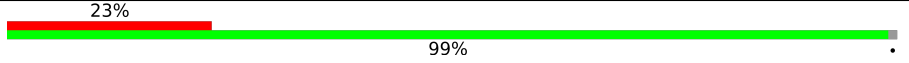
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Mol	Chain	Length	Quality of chain
9	J	194	 91% 7%
10	L	158	 13% 91% 5%
11	N	151	 10% 98% ..
12	O	151	 6% 87% 11%
13	V	83	 98% ..
14	W	130	 98% ..
15	X	143	 97% ..
16	Y	133	 90% 7%
17	a	115	 10% 85% 12%
18	b	84	 12% 96% ..
19	d	56	 14% 93% . .
20	e	59	 15% 92% 5%
21	h	25	 44% 88% 8%
22	D	243	 16% 91% 7%
23	F	204	 22% 89% 7%
24	K	165	 15% 55% 42%
25	M	132	 73% 91% 7%
26	P	145	 34% 82% 17%
27	Q	146	 10% 95% 5%
28	R	135	 33% 92% 6%
29	S	152	 45% 93% 6%
30	T	145	 21% 98% ..
31	U	119	 16% 81% 15%
32	Z	125	 30% 57% 42%
33	c	69	 29% 84% 12%

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Mol	Chain	Length	Quality of chain
34	f	156	
35	g	317	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 74342 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1665	35552	15869	6385	11633	1665	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	1772	C	G	conflict	GB 337376

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	206	1624	1035	287	294	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	213	1729	1098	309	308	14	0	0

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	218	1682	1090	289	293	10	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	262	2076	1324	386	358	8	0	0

- Molecule 6 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	230	1862	1164	371	320	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	H	186	1501	957	276	267	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	I	205	1682	1056	331	290	5	0	0

- Molecule 9 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	180	1499	955	300	242	2	0	0

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	151	1229	782	230	211	6	0	0

- Molecule 11 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	N	149	1202	770	228	203	1	0	0

- Molecule 12 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	O	135	1006	616	198	186	6	0	0

- Molecule 13 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	V	82	625	384	116	120	5	0	0

- Molecule 14 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	W	129	1034	659	193	176	6	0	0

- Molecule 15 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	X	141	1098	693	219	183	3	0	0

- Molecule 16 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Y	124	1014	641	198	170	5	0	0

- Molecule 17 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	a	101	814	507	170	132	5	0	0

- Molecule 18 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	b	82	640	402	118	113	7	0	0

- Molecule 19 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	d	54	455	284	93	73	5	0	0

- Molecule 20 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	e	56	Total	C	N	O	S	0	0
			442	273	96	72	1		

- Molecule 21 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	h	24	Total	C	N	O	S	0	0
			231	140	63	26	2		

- Molecule 22 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	225	Total	C	N	O	S	0	0
			1748	1115	315	311	7		

- Molecule 23 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 24 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	K	95	Total	C	N	O	S	0	0
			800	522	142	131	5		

- Molecule 25 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 26 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 27 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Q	139	1109	704	210	192	3	0	0

- Molecule 28 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	R	132	1066	669	199	194	4	0	0

- Molecule 29 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	S	143	1184	743	240	200	1	0	0

- Molecule 30 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	T	144	1122	703	217	199	3	0	0

- Molecule 31 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	U	101	803	504	153	142	4	0	0

- Molecule 32 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Z	72	574	368	104	101	1	0	0

- Molecule 33 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	61	479	292	95	90	2	0	0

- Molecule 34 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	72	Total	C	N	O	S	0	0
			585	366	114	97	8		

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	314	Total	C	N	O	S	0	0
			2440	1537	425	466	12		

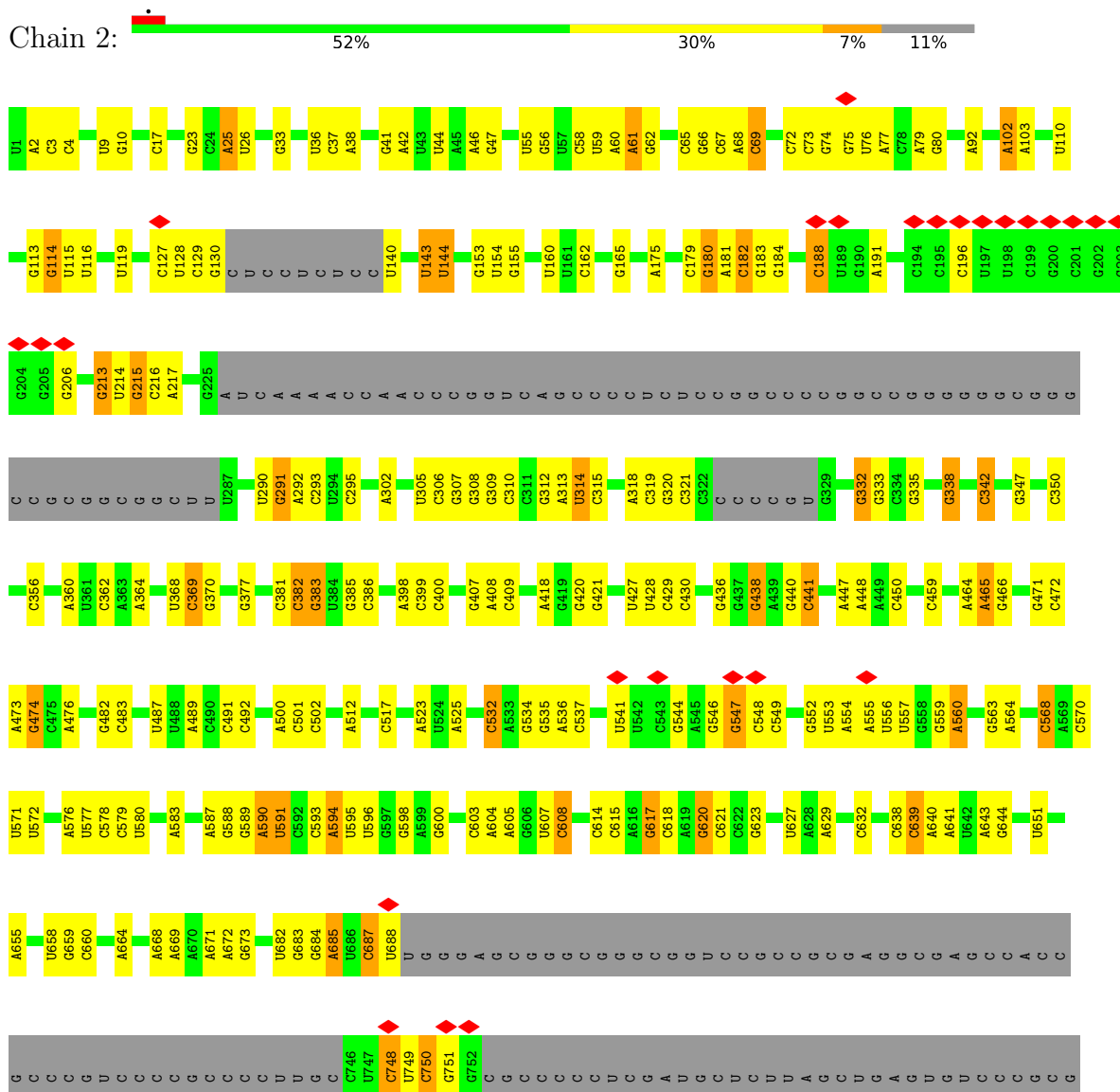
- Molecule 36 is ZINC ION (three-letter code: ZN) (formula: Zn).

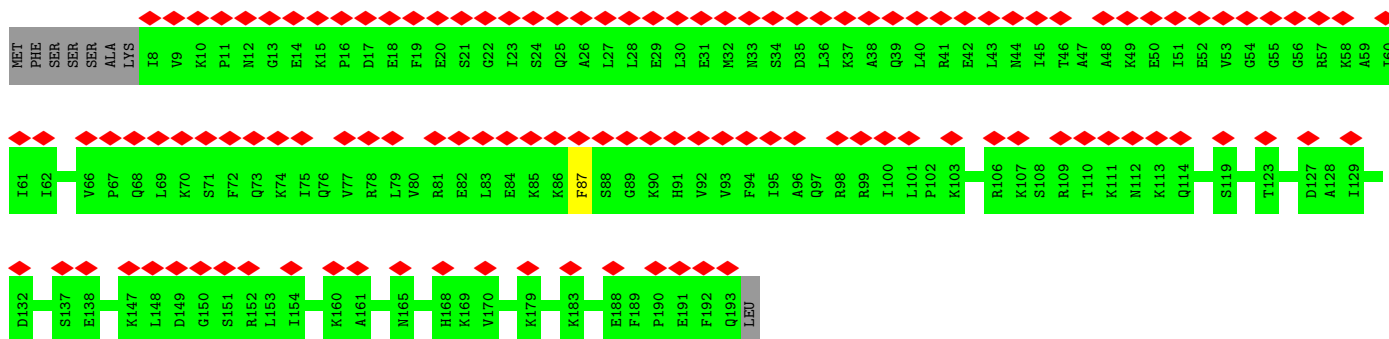
Mol	Chain	Residues	Atoms		AltConf
36	a	1	Total	Zn	0
			1	1	
36	d	1	Total	Zn	0
			1	1	
36	f	1	Total	Zn	0
			1	1	

3 Residue-property plots [i](#)

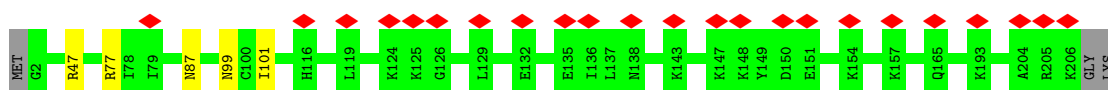
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 18S ribosomal RNA

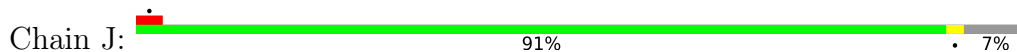




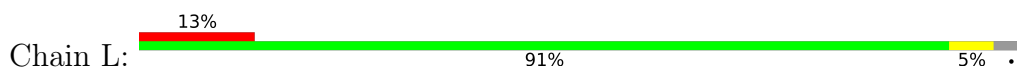
• Molecule 8: 40S ribosomal protein S8



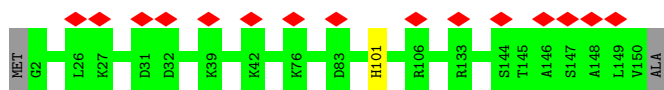
• Molecule 9: 40S ribosomal protein S9



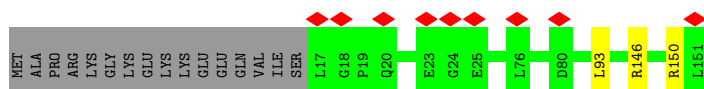
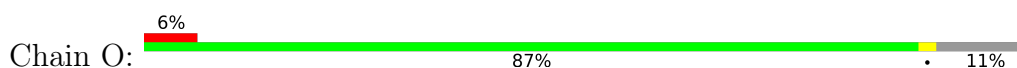
• Molecule 10: 40S ribosomal protein S11



• Molecule 11: 40S ribosomal protein S13

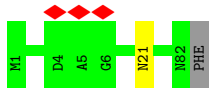


• Molecule 12: 40S ribosomal protein S14



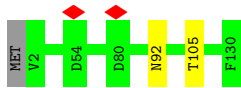
• Molecule 13: 40S ribosomal protein S21

Chain V:  98%



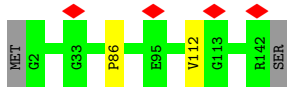
- Molecule 14: 40S ribosomal protein S15a

Chain W:  98%




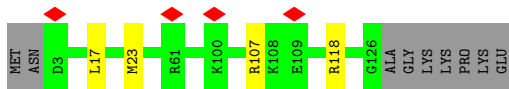
- Molecule 15: 40S ribosomal protein S23

Chain X:  97%




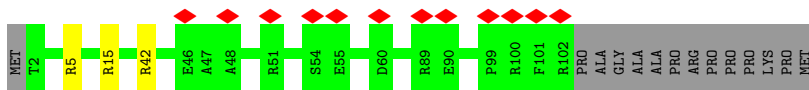
- Molecule 16: 40S ribosomal protein S24

Chain Y:  90%



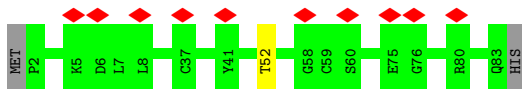
- Molecule 17: 40S ribosomal protein S26

Chain a:  10% 85% 12%

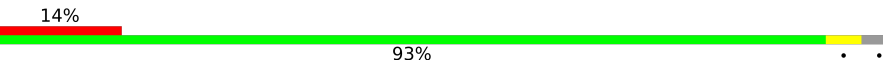


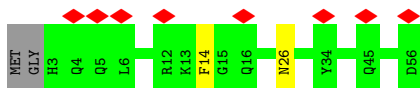
- Molecule 18: 40S ribosomal protein S27

Chain b:  12% 96%

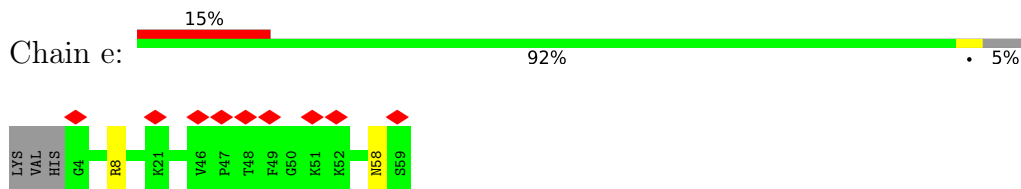


- Molecule 19: 40S ribosomal protein S29

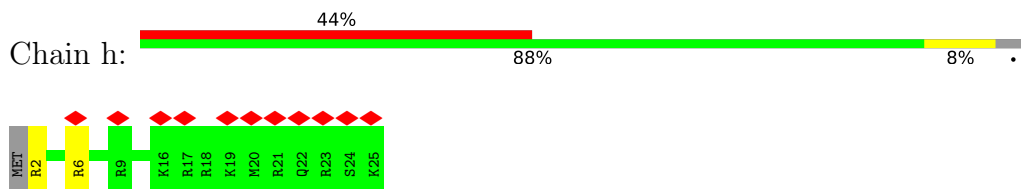
Chain d:  14% 93%



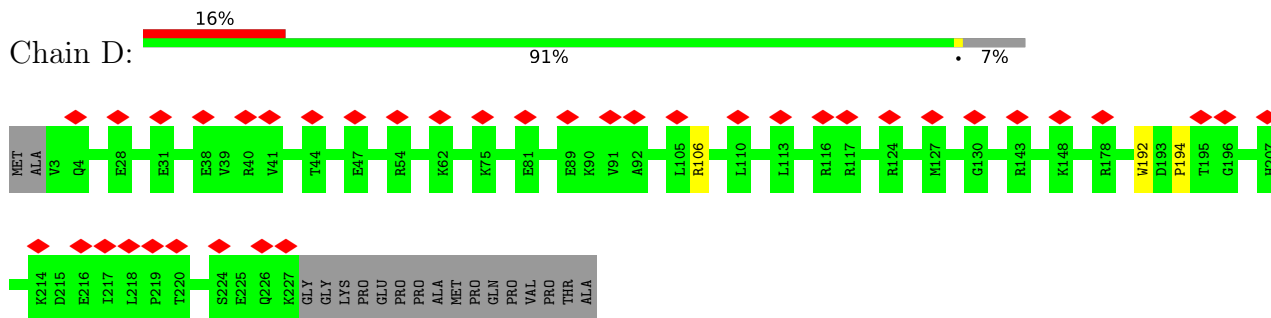
• Molecule 20: 40S ribosomal protein S30



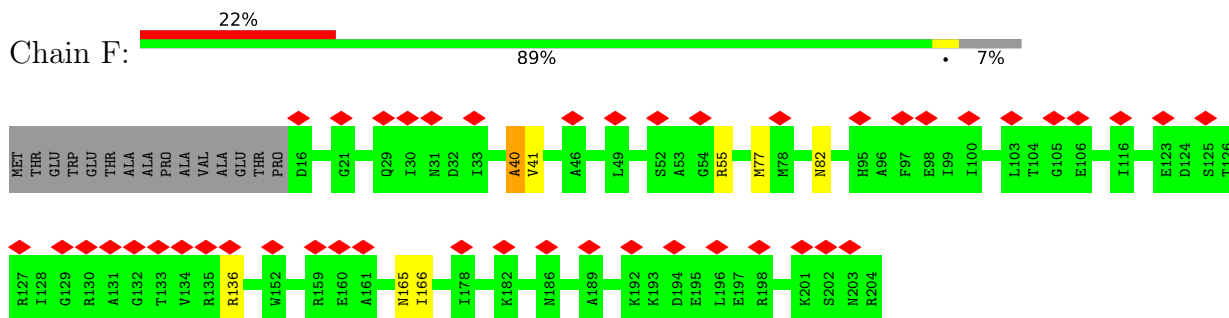
• Molecule 21: 60S ribosomal protein L41



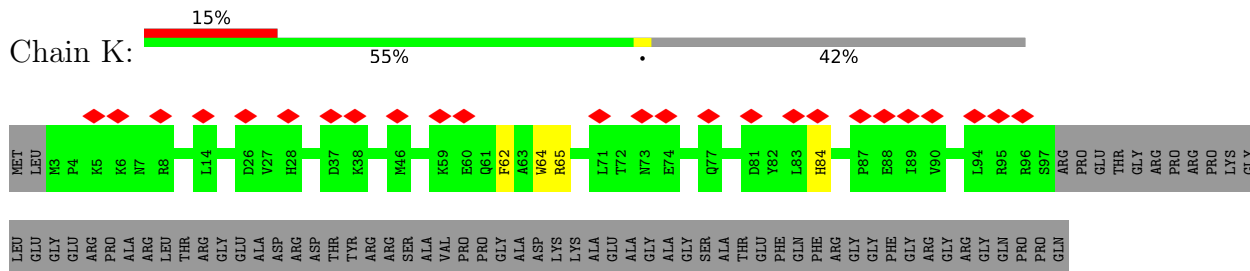
• Molecule 22: 40S ribosomal protein S3



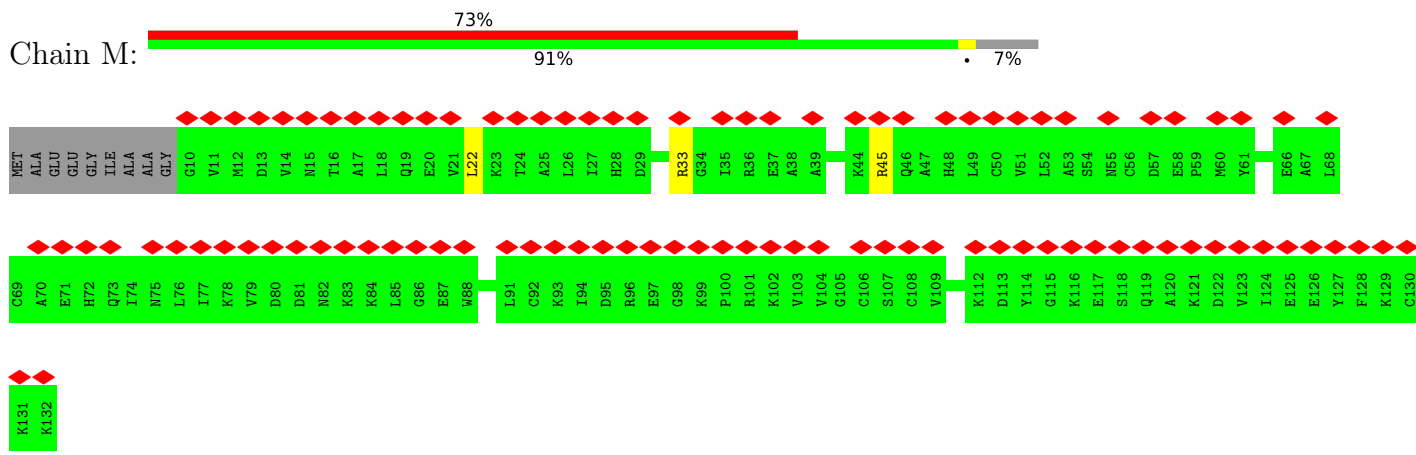
• Molecule 23: 40S ribosomal protein S5



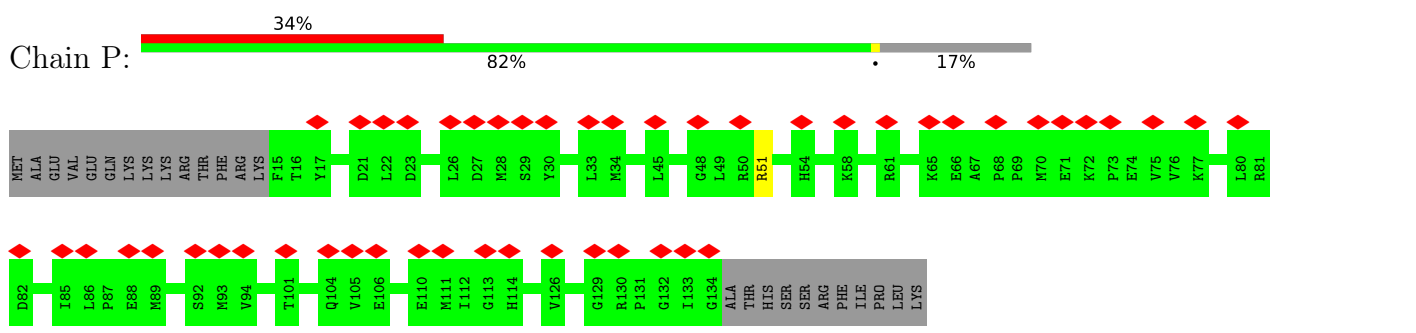
• Molecule 24: 40S ribosomal protein S10



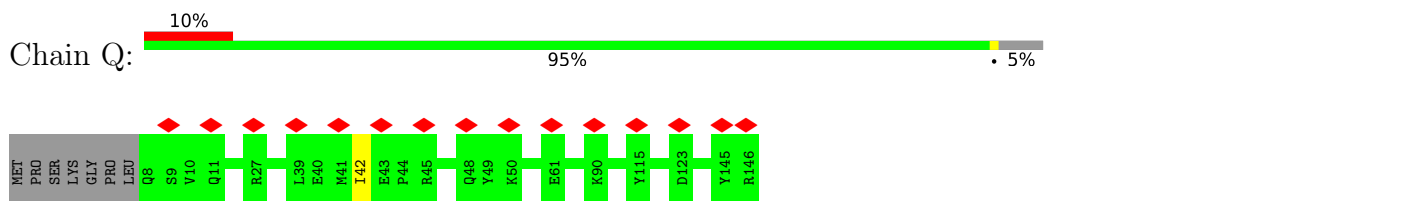
• Molecule 25: 40S ribosomal protein S12



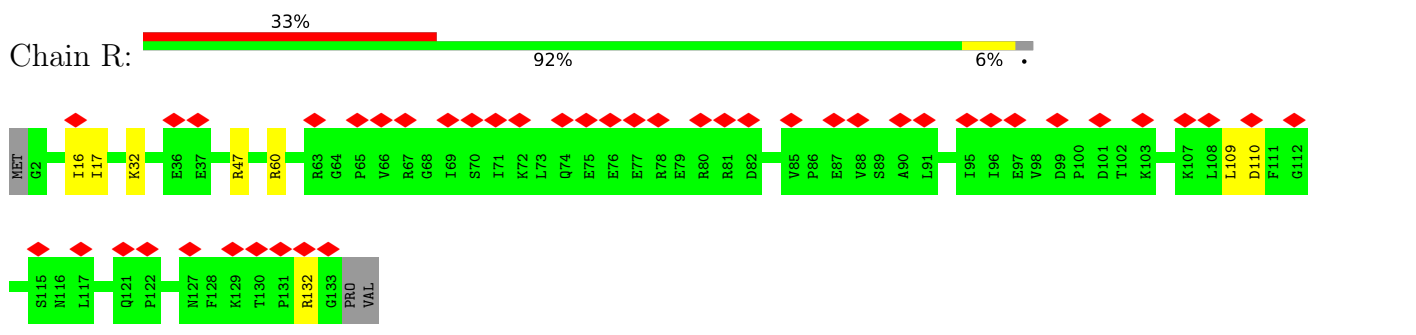
• Molecule 26: 40S ribosomal protein S15



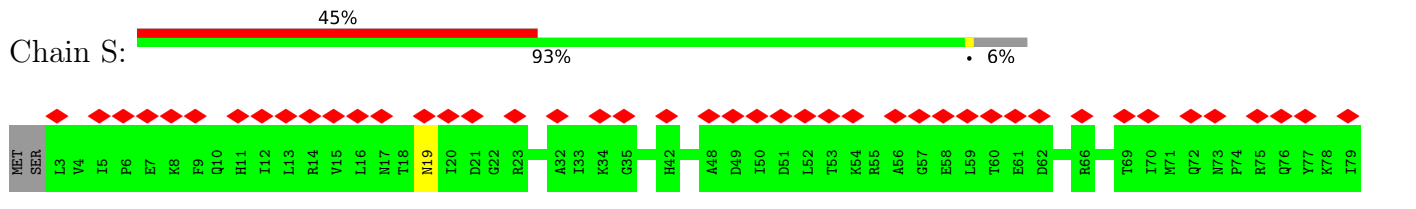
• Molecule 27: 40S ribosomal protein S16



• Molecule 28: 40S ribosomal protein S17

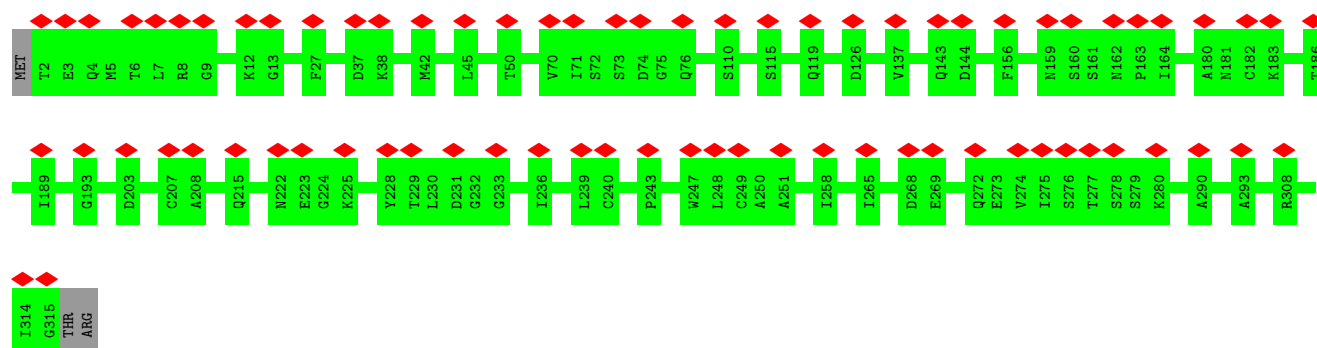


• Molecule 29: 40S ribosomal protein S18



● Molecule 35: Receptor of activated protein C kinase 1

Chain g:  23% 99%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70822	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 ($e^-/\text{\AA}^2$)	2.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.372	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	2	1.13	0/39755	1.39	545/61954 (0.9%)
2	A	0.56	0/1661	0.70	0/2259
3	B	0.54	0/1756	0.70	0/2350
4	C	0.65	0/1718	0.77	1/2322 (0.0%)
5	E	0.64	1/2118 (0.0%)	0.72	3/2849 (0.1%)
6	G	0.48	0/1885	0.67	0/2510
7	H	0.37	0/1524	0.64	0/2042
8	I	0.57	0/1711	0.70	0/2282
9	J	0.68	0/1524	0.75	0/2035
10	L	0.65	0/1250	0.67	0/1673
11	N	0.54	0/1226	0.69	0/1649
12	O	0.51	0/1019	0.74	1/1367 (0.1%)
13	V	0.54	0/631	0.68	0/844
14	W	0.61	0/1051	0.72	0/1406
15	X	0.65	0/1116	0.73	0/1490
16	Y	0.59	0/1031	0.71	0/1370
17	a	0.63	0/828	0.65	0/1109
18	b	0.48	0/653	0.67	0/876
19	d	0.53	0/466	0.74	0/618
20	e	0.50	0/447	0.64	0/587
21	h	0.40	0/232	0.71	0/295
22	D	0.45	0/1776	0.71	0/2392
23	F	0.42	0/1516	0.67	0/2037
24	K	0.45	0/824	0.74	1/1112 (0.1%)
25	M	0.33	0/963	0.67	1/1291 (0.1%)
26	P	0.40	0/1003	0.61	0/1341
27	Q	0.51	0/1126	0.71	0/1506
28	R	0.42	0/1080	0.73	2/1449 (0.1%)
29	S	0.35	0/1202	0.65	0/1610
30	T	0.44	0/1142	0.67	0/1530
31	U	0.43	0/813	0.70	0/1092
32	Z	0.36	0/580	0.68	0/780

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.42	0/481	0.83	2/643 (0.3%)
34	f	0.37	0/595	0.58	0/785
35	g	0.40	0/2497	0.65	0/3399
All	All	0.88	1/79200 (0.0%)	1.13	556/114854 (0.5%)

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
8	I	0	1
11	N	0	1
12	O	0	1
15	X	0	1
16	Y	0	1
18	b	0	1
22	D	0	1
23	F	0	4
27	Q	0	1
30	T	0	1
34	f	0	1
All	All	0	14

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	237	SER	C-N	-5.30	1.21	1.34

All (556) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1016	U	N1-C2-O2	12.00	131.20	122.80
1	2	1016	U	C2-N1-C1'	11.61	131.63	117.70
1	2	1751	C	N1-C2-O2	11.22	125.63	118.90
1	2	1016	U	N3-C2-O2	-11.05	114.46	122.20
1	2	1751	C	C2-N1-C1'	10.65	130.51	118.80
1	2	1688	C	C6-N1-C2	-10.56	116.08	120.30
1	2	1416	C	C5-C6-N1	10.38	126.19	121.00
1	2	1389	C	C2-N1-C1'	10.31	130.15	118.80
1	2	853	C	N3-C2-O2	-10.18	114.77	121.90
1	2	1688	C	N3-C2-O2	-10.13	114.81	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	37	ASP	CB-CG-OD1	9.95	127.25	118.30
1	2	1453	C	N1-C2-O2	9.91	124.85	118.90
1	2	750	C	C6-N1-C2	-9.88	116.35	120.30
1	2	1453	C	C2-N1-C1'	9.88	129.67	118.80
1	2	1389	C	C6-N1-C2	-9.84	116.36	120.30
1	2	1703	C	C6-N1-C2	-9.72	116.41	120.30
1	2	356	C	C2-N1-C1'	9.65	129.41	118.80
1	2	853	C	N1-C2-O2	9.61	124.66	118.90
1	2	36	U	N1-C1'-C2'	-9.60	101.44	112.00
1	2	853	C	C2-N1-C1'	9.32	129.06	118.80
1	2	591	U	O4'-C1'-N1	9.31	115.65	108.20
1	2	1551	U	C2-N1-C1'	9.01	128.51	117.70
1	2	37	C	N1-C1'-C2'	-8.90	102.21	112.00
28	R	110	ASP	CB-CG-OD1	8.89	126.31	118.30
1	2	356	C	C6-N1-C1'	-8.82	110.22	120.80
1	2	1416	C	C6-N1-C2	-8.82	116.77	120.30
1	2	1750	C	C5-C6-N1	8.73	125.37	121.00
1	2	38	A	N9-C1'-C2'	-8.71	102.42	112.00
1	2	1621	U	N3-C2-O2	-8.57	116.20	122.20
1	2	1265	A	C8-N9-C4	-8.54	102.39	105.80
1	2	1840	U	C5-C6-N1	8.54	126.97	122.70
1	2	1153	C	N1-C2-O2	8.38	123.93	118.90
1	2	750	C	C2-N1-C1'	8.34	127.97	118.80
1	2	1520	G	C4-N9-C1'	8.29	137.28	126.50
1	2	1440	C	C6-N1-C2	-8.26	117.00	120.30
1	2	1019	C	N3-C2-O2	-8.26	116.12	121.90
1	2	1774	C	C5-C6-N1	8.24	125.12	121.00
1	2	1311	C	N1-C2-O2	8.22	123.83	118.90
1	2	1016	U	C6-N1-C1'	-8.21	109.71	121.20
1	2	853	C	C6-N1-C2	-8.17	117.03	120.30
1	2	750	C	N1-C2-O2	8.13	123.78	118.90
1	2	842	C	C5-C6-N1	8.13	125.07	121.00
1	2	1624	U	C2-N1-C1'	8.13	127.46	117.70
1	2	823	U	N3-C2-O2	-8.06	116.56	122.20
1	2	1416	C	N1-C2-O2	7.97	123.68	118.90
1	2	1323	U	N1-C2-O2	7.95	128.37	122.80
1	2	1621	U	N1-C2-O2	7.95	128.37	122.80
1	2	532	C	C2-N1-C1'	7.94	127.54	118.80
1	2	1538	C	C6-N1-C2	-7.92	117.13	120.30
1	2	1234	C	N1-C2-O2	7.91	123.65	118.90
1	2	931	C	C6-N1-C2	-7.88	117.15	120.30
1	2	1416	C	C2-N1-C1'	7.85	127.44	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	501	C	C2-N1-C1'	7.83	127.41	118.80
1	2	1139	C	N1-C2-O2	7.83	123.60	118.90
1	2	1153	C	C2-N1-C1'	7.82	127.40	118.80
1	2	1751	C	C6-N1-C1'	-7.81	111.43	120.80
1	2	1684	C	C6-N1-C2	-7.76	117.20	120.30
1	2	608	C	C2-N1-C1'	7.75	127.33	118.80
1	2	130	G	C4-N9-C1'	7.75	136.57	126.50
1	2	1453	C	C6-N1-C1'	-7.73	111.52	120.80
1	2	750	C	C5-C6-N1	7.73	124.86	121.00
1	2	918	U	N3-C4-O4	-7.72	114.00	119.40
1	2	369	C	C2-N1-C1'	7.71	127.28	118.80
1	2	918	U	C5-C4-O4	7.71	130.53	125.90
1	2	1202	U	N3-C2-O2	-7.69	116.82	122.20
1	2	632	C	C2-N1-C1'	7.68	127.25	118.80
1	2	1624	U	N1-C2-O2	7.68	128.17	122.80
1	2	1123	C	N1-C2-O2	7.63	123.48	118.90
1	2	1774	C	C6-N1-C2	-7.62	117.25	120.30
1	2	1565	C	P-O3'-C3'	7.61	128.83	119.70
1	2	1060	A	O4'-C1'-N9	7.50	114.20	108.20
1	2	842	C	C6-N1-C2	-7.48	117.31	120.30
1	2	973	C	C6-N1-C2	-7.48	117.31	120.30
1	2	1708	C	C5-C6-N1	7.47	124.73	121.00
1	2	1403	C	P-O3'-C3'	7.46	128.65	119.70
1	2	632	C	C5-C6-N1	7.46	124.73	121.00
1	2	1230	C	C6-N1-C2	-7.45	117.32	120.30
1	2	182	C	C2-N1-C1'	7.45	126.99	118.80
1	2	958	G	C4-N9-C1'	7.43	136.16	126.50
1	2	750	C	N3-C2-O2	-7.43	116.70	121.90
1	2	1205	C	C6-N1-C2	-7.41	117.34	120.30
1	2	1591	C	N1-C2-O2	7.40	123.34	118.90
1	2	1751	C	C5-C6-N1	7.40	124.70	121.00
1	2	1778	C	C2-N1-C1'	7.38	126.91	118.80
1	2	1600	G	N3-C4-C5	-7.31	124.94	128.60
1	2	1738	C	C6-N1-C2	-7.30	117.38	120.30
1	2	1081	U	N3-C2-O2	-7.24	117.13	122.20
1	2	1600	G	C4-N9-C1'	7.24	135.91	126.50
1	2	532	C	C6-N1-C1'	-7.24	112.11	120.80
1	2	1751	C	N3-C2-O2	-7.23	116.84	121.90
1	2	1153	C	N3-C2-O2	-7.21	116.86	121.90
1	2	1527	C	C6-N1-C2	-7.20	117.42	120.30
1	2	1728	U	C2-N1-C1'	7.18	126.32	117.70
1	2	958	G	O4'-C1'-N9	7.17	113.94	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1714	U	C2-N1-C1'	7.17	126.30	117.70
1	2	1624	U	N3-C2-O2	-7.14	117.20	122.20
1	2	1728	U	N1-C2-O2	7.14	127.80	122.80
1	2	1574	C	C5-C6-N1	7.12	124.56	121.00
1	2	1590	C	N1-C2-O2	7.11	123.17	118.90
1	2	547	G	P-O3'-C3'	7.11	128.23	119.70
1	2	1323	U	N3-C2-O2	-7.10	117.23	122.20
1	2	501	C	C6-N1-C1'	-7.08	112.30	120.80
1	2	1330	G	P-O3'-C3'	7.07	128.19	119.70
1	2	1090	C	C6-N1-C2	-7.07	117.47	120.30
1	2	1265	A	N7-C8-N9	7.07	117.33	113.80
1	2	1017	U	N3-C2-O2	-7.05	117.26	122.20
1	2	1172	U	N3-C2-O2	-7.05	117.26	122.20
1	2	1303	C	N1-C2-O2	7.02	123.11	118.90
1	2	1684	C	C5-C6-N1	7.01	124.50	121.00
1	2	369	C	C6-N1-C1'	-6.99	112.41	120.80
1	2	856	C	N1-C2-O2	6.96	123.08	118.90
1	2	1585	U	P-O3'-C3'	6.96	128.05	119.70
1	2	1729	U	C2-N1-C1'	6.93	126.02	117.70
1	2	632	C	C6-N1-C2	-6.92	117.53	120.30
1	2	905	C	N1-C2-O2	6.91	123.05	118.90
1	2	1308	U	P-O3'-C3'	6.89	127.96	119.70
1	2	1572	C	N1-C2-O2	6.88	123.03	118.90
1	2	608	C	N1-C2-O2	6.85	123.01	118.90
1	2	1384	C	N1-C2-O2	6.85	123.01	118.90
1	2	1524	G	N3-C4-N9	6.85	130.11	126.00
1	2	182	C	C6-N1-C1'	-6.82	112.61	120.80
1	2	618	C	O5'-P-OP1	-6.82	99.56	105.70
1	2	1288	U	N1-C2-O2	6.80	127.56	122.80
1	2	905	C	N3-C2-O2	-6.79	117.14	121.90
1	2	1017	U	N1-C2-O2	6.78	127.55	122.80
1	2	1314	U	N1-C2-O2	6.78	127.54	122.80
1	2	608	C	C5-C6-N1	6.76	124.38	121.00
1	2	685	A	N1-C6-N6	-6.76	114.55	118.60
1	2	1000	C	N3-C2-O2	-6.74	117.18	121.90
1	2	61	A	N9-C1'-C2'	-6.72	104.61	112.00
1	2	1231	C	C6-N1-C2	-6.72	117.61	120.30
1	2	1362	U	N1-C2-O2	6.72	127.50	122.80
1	2	1112	U	N3-C2-O2	-6.71	117.50	122.20
1	2	958	G	C6-C5-N7	-6.71	126.38	130.40
1	2	37	C	C4'-C3'-O3'	6.70	126.41	113.00
1	2	383	G	C8-N9-C1'	6.70	135.71	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1551	U	N3-C2-O2	-6.70	117.51	122.20
1	2	973	C	N1-C2-O2	6.69	122.92	118.90
1	2	814	U	N3-C2-O2	-6.67	117.53	122.20
1	2	1865	C	C6-N1-C2	-6.67	117.63	120.30
1	2	1111	U	N1-C2-O2	6.66	127.47	122.80
1	2	931	C	C5-C6-N1	6.66	124.33	121.00
1	2	1362	U	N3-C2-O2	-6.66	117.54	122.20
1	2	1527	C	C5-C6-N1	6.65	124.33	121.00
1	2	659	G	C4-N9-C1'	6.65	135.14	126.50
1	2	1527	C	N1-C2-O2	6.65	122.89	118.90
1	2	571	U	N3-C2-O2	-6.65	117.55	122.20
1	2	1520	G	P-O3'-C3'	6.64	127.67	119.70
1	2	441	C	C2-N1-C1'	6.64	126.10	118.80
1	2	1302	G	P-O3'-C3'	6.63	127.66	119.70
1	2	685	A	C8-N9-C4	-6.62	103.15	105.80
1	2	1081	U	C2-N1-C1'	6.62	125.64	117.70
1	2	1123	C	N3-C2-O2	-6.61	117.27	121.90
1	2	1520	G	C8-N9-C1'	-6.61	118.41	127.00
1	2	1494	U	P-O3'-C3'	6.59	127.61	119.70
1	2	1006	C	C5-C6-N1	6.59	124.29	121.00
1	2	1111	U	N3-C2-O2	-6.59	117.59	122.20
1	2	215	G	C4-N9-C1'	6.57	135.04	126.50
1	2	1750	C	C6-N1-C2	-6.57	117.67	120.30
1	2	213	G	C4-N9-C1'	6.57	135.04	126.50
1	2	1235	G	C8-N9-C1'	-6.55	118.48	127.00
1	2	842	C	N1-C2-O2	6.55	122.83	118.90
1	2	1615	U	N1-C2-O2	6.54	127.38	122.80
1	2	639	C	C6-N1-C2	-6.54	117.69	120.30
1	2	856	C	N3-C2-O2	-6.53	117.33	121.90
1	2	430	C	C2-N1-C1'	6.53	125.98	118.80
1	2	1053	C	C2-N1-C1'	6.53	125.98	118.80
1	2	130	G	C8-N9-C1'	-6.52	118.53	127.00
1	2	1019	C	C6-N1-C2	-6.50	117.70	120.30
1	2	1112	U	N1-C2-O2	6.48	127.34	122.80
1	2	967	C	C6-N1-C2	-6.48	117.71	120.30
1	2	1714	U	C5-C6-N1	6.47	125.93	122.70
1	2	1389	C	C5-C6-N1	6.46	124.23	121.00
1	2	1172	U	N1-C2-O2	6.45	127.32	122.80
1	2	1600	G	N3-C4-N9	6.45	129.87	126.00
1	2	1648	G	P-O3'-C3'	6.42	127.41	119.70
1	2	102	A	P-O3'-C3'	6.42	127.40	119.70
1	2	809	A	N7-C8-N9	6.40	117.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1629	C	C5-C6-N1	6.40	124.20	121.00
1	2	1019	C	N1-C2-O2	6.39	122.73	118.90
1	2	143	U	P-O3'-C3'	6.36	127.33	119.70
1	2	809	A	C8-N9-C4	-6.35	103.26	105.80
1	2	293	C	C2-N1-C1'	6.35	125.78	118.80
1	2	967	C	C5-C6-N1	6.35	124.17	121.00
1	2	1840	U	C6-N1-C2	-6.34	117.20	121.00
1	2	1233	G	N3-C4-N9	6.34	129.80	126.00
1	2	1233	G	C8-N9-C1'	-6.33	118.77	127.00
1	2	1078	C	C6-N1-C2	-6.33	117.77	120.30
1	2	1314	U	N3-C2-O2	-6.32	117.78	122.20
1	2	1464	C	O4'-C1'-N1	6.32	113.25	108.20
1	2	1233	G	C4-N9-C1'	6.31	134.71	126.50
1	2	180	G	C4-N9-C1'	6.31	134.70	126.50
1	2	459	C	C2-N1-C1'	6.30	125.73	118.80
1	2	1512	C	C6-N1-C2	-6.30	117.78	120.30
1	2	1111	U	C2-N1-C1'	6.29	125.25	117.70
1	2	1717	C	C5-C6-N1	6.29	124.14	121.00
1	2	632	C	N1-C2-O2	6.29	122.67	118.90
1	2	842	C	C2-N1-C1'	6.27	125.70	118.80
1	2	1536	G	C8-N9-C4	-6.27	103.89	106.40
1	2	338	G	C4-N9-C1'	6.27	134.65	126.50
1	2	1688	C	N1-C2-N3	6.26	123.59	119.20
1	2	1235	G	C4-N9-C1'	6.26	134.64	126.50
1	2	1708	C	C6-N1-C2	-6.26	117.80	120.30
1	2	1523	C	N1-C2-O2	6.26	122.66	118.90
1	2	623	G	C4-C5-N7	6.26	113.30	110.80
1	2	1242	U	N1-C2-O2	6.25	127.18	122.80
1	2	1389	C	C6-N1-C1'	-6.25	113.29	120.80
1	2	926	A	C4-N9-C1'	6.25	137.56	126.30
1	2	1838	U	P-O3'-C3'	6.25	127.20	119.70
1	2	1288	U	N3-C2-O2	-6.25	117.83	122.20
1	2	474	G	C4-N9-C1'	6.25	134.62	126.50
1	2	1139	C	C2-N1-C1'	6.25	125.67	118.80
1	2	1558	C	P-O3'-C3'	6.24	127.19	119.70
1	2	844	U	N3-C2-O2	-6.23	117.84	122.20
1	2	620	G	P-O3'-C3'	6.22	127.17	119.70
1	2	1230	C	C2-N1-C1'	6.21	125.63	118.80
1	2	1438	A	P-O3'-C3'	6.20	127.14	119.70
1	2	1453	C	N3-C2-O2	-6.20	117.56	121.90
1	2	1348	G	C4-C5-N7	6.20	113.28	110.80
1	2	1601	A	P-O3'-C3'	6.20	127.14	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	811	A	P-O3'-C3'	6.20	127.14	119.70
1	2	1095	C	C6-N1-C2	-6.19	117.83	120.30
1	2	1807	C	C2-N1-C1'	6.19	125.61	118.80
1	2	1807	C	C5-C6-N1	6.18	124.09	121.00
1	2	188	C	C2-N1-C1'	6.17	125.59	118.80
1	2	748	C	C5-C6-N1	6.17	124.08	121.00
1	2	1729	U	C5-C6-N1	6.17	125.78	122.70
1	2	590	A	C4-N9-C1'	6.16	137.39	126.30
1	2	570	C	N3-C2-O2	-6.15	117.60	121.90
1	2	114	G	P-O3'-C3'	6.13	127.06	119.70
1	2	1807	C	C6-N1-C2	-6.13	117.85	120.30
1	2	568	C	N1-C2-O2	6.13	122.58	118.90
1	2	974	C	C2-N1-C1'	6.12	125.53	118.80
1	2	1233	G	C6-C5-N7	-6.12	126.73	130.40
1	2	179	C	C2-N1-C1'	6.11	125.52	118.80
1	2	1139	C	N3-C2-O2	-6.11	117.62	121.90
1	2	491	C	C2-N1-C1'	6.11	125.52	118.80
1	2	1243	U	N1-C2-O2	6.11	127.08	122.80
1	2	25	A	O4'-C1'-N9	6.10	113.08	108.20
1	2	578	C	C6-N1-C2	-6.09	117.86	120.30
1	2	1342	U	P-O3'-C3'	6.07	126.98	119.70
1	2	1649	U	N1-C2-O2	6.07	127.05	122.80
1	2	309	G	O4'-C1'-N9	6.07	113.05	108.20
1	2	1563	G	C6-C5-N7	-6.06	126.77	130.40
1	2	590	A	C8-N9-C1'	-6.06	116.80	127.70
1	2	1425	G	P-O3'-C3'	6.05	126.96	119.70
1	2	1649	U	N3-C2-O2	-6.05	117.97	122.20
1	2	441	C	C6-N1-C1'	-6.03	113.56	120.80
1	2	1600	G	C8-N9-C1'	-6.03	119.16	127.00
1	2	80	G	C4-N9-C1'	6.02	134.33	126.50
1	2	1738	C	C5-C6-N1	6.02	124.01	121.00
1	2	1202	U	C2-N1-C1'	6.01	124.91	117.70
1	2	1311	C	N3-C2-O2	-6.00	117.70	121.90
1	2	881	G	N3-C4-N9	5.99	129.60	126.00
1	2	973	C	N3-C2-O2	-5.97	117.72	121.90
1	2	1259	A	C2-N3-C4	5.97	113.59	110.60
1	2	809	A	O4'-C1'-N9	5.97	112.98	108.20
1	2	1006	C	C6-N1-C2	-5.97	117.91	120.30
1	2	1234	C	N3-C2-O2	-5.96	117.73	121.90
1	2	958	G	C8-N9-C1'	-5.95	119.27	127.00
1	2	1687	C	N1-C2-O2	5.94	122.47	118.90
1	2	165	G	C4-N9-C1'	5.94	134.22	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1590	C	N3-C2-O2	-5.93	117.75	121.90
1	2	1047	C	C5-C6-N1	5.93	123.97	121.00
1	2	856	C	C2-N1-C1'	5.92	125.32	118.80
1	2	140	U	C2-N1-C1'	5.92	124.80	117.70
1	2	856	C	C6-N1-C2	-5.91	117.94	120.30
1	2	1153	C	C6-N1-C2	-5.91	117.94	120.30
1	2	1078	C	C2-N1-C1'	5.90	125.29	118.80
1	2	430	C	C6-N1-C1'	-5.90	113.72	120.80
1	2	804	U	C5-C6-N1	5.90	125.65	122.70
1	2	465	A	P-O3'-C3'	5.89	126.77	119.70
1	2	1564	C	C2-N1-C1'	5.88	125.27	118.80
1	2	1235	G	N3-C4-N9	5.88	129.53	126.00
1	2	1629	C	N1-C2-O2	5.88	122.43	118.90
1	2	1658	G	N3-C4-N9	5.88	129.53	126.00
1	2	608	C	C6-N1-C2	-5.88	117.95	120.30
1	2	1310	U	N3-C2-O2	-5.88	118.08	122.20
1	2	1180	C	N1-C2-O2	5.87	122.42	118.90
1	2	803	C	C6-N1-C2	-5.87	117.95	120.30
1	2	617	G	N3-C4-N9	5.87	129.52	126.00
1	2	1261	C	N3-C2-O2	-5.86	117.80	121.90
1	2	1703	C	C5-C6-N1	5.86	123.93	121.00
1	2	1591	C	C2-N1-C1'	5.85	125.23	118.80
1	2	1177	U	C6-N1-C2	-5.85	117.49	121.00
1	2	579	C	C6-N1-C2	-5.84	117.96	120.30
1	2	37	C	C1'-C2'-O2'	-5.83	93.10	110.60
1	2	1172	U	C2-N1-C1'	5.83	124.70	117.70
1	2	1535	U	O5'-P-OP1	-5.82	100.47	105.70
1	2	1538	C	C5-C6-N1	5.81	123.90	121.00
1	2	651	U	N3-C2-O2	-5.80	118.14	122.20
1	2	1629	C	C6-N1-C2	-5.80	117.98	120.30
5	E	42	LEU	CA-CB-CG	5.80	128.65	115.30
1	2	1015	U	C2-N3-C4	-5.80	123.52	127.00
1	2	1565	C	OP1-P-O3'	5.79	117.94	105.20
1	2	140	U	C6-N1-C1'	-5.79	113.10	121.20
1	2	1389	C	N3-C2-O2	-5.78	117.86	121.90
1	2	1551	U	O4'-C1'-N1	5.78	112.82	108.20
1	2	427	U	O4'-C1'-N1	5.78	112.82	108.20
1	2	844	U	C2-N3-C4	-5.78	123.53	127.00
1	2	571	U	N1-C2-O2	5.77	126.84	122.80
1	2	1081	U	C6-N1-C2	-5.77	117.53	121.00
1	2	1865	C	N3-C2-O2	-5.76	117.86	121.90
1	2	1757	G	N3-C4-N9	5.76	129.46	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1234	C	C2-N1-C1'	5.76	125.14	118.80
1	2	1751	C	C6-N1-C2	-5.76	118.00	120.30
1	2	926	A	C8-N9-C1'	-5.75	117.35	127.70
1	2	1524	G	C6-C5-N7	-5.75	126.95	130.40
5	E	101	LEU	CA-CB-CG	-5.75	102.08	115.30
1	2	293	C	C6-N1-C1'	-5.75	113.90	120.80
1	2	853	C	C6-N1-C1'	-5.74	113.91	120.80
1	2	1286	G	N3-C4-N9	5.74	129.44	126.00
1	2	1551	U	C6-N1-C1'	-5.74	113.16	121.20
1	2	1218	C	N1-C2-O2	5.74	122.34	118.90
1	2	1025	U	C5-C6-N1	5.73	125.56	122.70
1	2	1467	C	C5-C6-N1	5.73	123.86	121.00
1	2	1774	C	C2-N1-C1'	5.73	125.10	118.80
1	2	881	G	N9-C4-C5	-5.72	103.11	105.40
1	2	36	U	C4'-C3'-O3'	5.71	124.43	113.00
1	2	1094	C	C5-C6-N1	5.71	123.86	121.00
1	2	1205	C	C5-C6-N1	5.71	123.86	121.00
1	2	570	C	N1-C2-O2	5.71	122.32	118.90
1	2	1621	U	C2-N1-C1'	5.71	124.55	117.70
1	2	1590	C	C2-N1-C1'	5.70	125.07	118.80
1	2	438	G	C4-N9-C1'	5.70	133.91	126.50
1	2	459	C	C6-N1-C1'	-5.70	113.97	120.80
1	2	1192	U	C6-N1-C2	-5.67	117.60	121.00
1	2	877	C	C5-C6-N1	5.66	123.83	121.00
1	2	1589	A	N7-C8-N9	5.64	116.62	113.80
1	2	815	U	C2-N1-C1'	5.64	124.47	117.70
1	2	1047	C	C6-N1-C2	-5.64	118.04	120.30
1	2	1574	C	N1-C2-O2	5.62	122.28	118.90
1	2	814	U	N1-C2-O2	5.62	126.73	122.80
1	2	1362	U	C2-N1-C1'	5.61	124.43	117.70
1	2	1591	C	N3-C2-O2	-5.61	117.97	121.90
1	2	803	C	C2-N1-C1'	5.61	124.97	118.80
1	2	1311	C	C5-C6-N1	5.61	123.80	121.00
1	2	884	C	C5-C6-N1	5.60	123.80	121.00
1	2	1840	U	C2-N1-C1'	5.59	124.41	117.70
1	2	188	C	C6-N1-C1'	-5.59	114.09	120.80
1	2	1094	C	C6-N1-C2	-5.58	118.07	120.30
1	2	1696	C	C6-N1-C2	-5.58	118.07	120.30
1	2	617	G	C4-C5-N7	5.58	113.03	110.80
1	2	1778	C	C6-N1-C1'	-5.57	114.11	120.80
1	2	1560	U	N1-C2-O2	5.57	126.70	122.80
1	2	1574	C	C6-N1-C2	-5.57	118.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1261	C	N1-C2-O2	5.57	122.24	118.90
1	2	535	G	C4-N9-C1'	5.56	133.73	126.50
1	2	1551	U	N1-C2-O2	5.56	126.69	122.80
1	2	491	C	C6-N1-C1'	-5.56	114.13	120.80
1	2	383	G	C4-N9-C1'	-5.56	119.28	126.50
1	2	966	U	N3-C2-O2	-5.56	118.31	122.20
1	2	1520	G	C6-C5-N7	-5.56	127.07	130.40
1	2	1431	G	P-O3'-C3'	5.55	126.36	119.70
1	2	1624	U	C6-N1-C1'	-5.55	113.43	121.20
1	2	823	U	N1-C2-O2	5.55	126.68	122.80
1	2	1314	U	C2-N1-C1'	5.55	124.36	117.70
1	2	1427	C	C6-N1-C2	-5.55	118.08	120.30
1	2	639	C	C5-C6-N1	5.54	123.77	121.00
1	2	179	C	C6-N1-C1'	-5.54	114.15	120.80
1	2	1060	A	C5-N7-C8	-5.54	101.13	103.90
1	2	1186	U	N3-C2-O2	-5.53	118.33	122.20
1	2	1862	G	OP1-P-O3'	5.53	117.37	105.20
1	2	1794	C	N1-C2-O2	5.53	122.22	118.90
1	2	926	A	C6-C5-N7	-5.51	128.44	132.30
1	2	1137	U	C5-C6-N1	5.50	125.45	122.70
1	2	1844	U	N3-C2-O2	-5.50	118.35	122.20
1	2	1286	G	N3-C4-C5	-5.50	125.85	128.60
1	2	1616	U	N3-C2-O2	-5.50	118.35	122.20
1	2	23	G	C4-N9-C1'	5.49	133.63	126.50
1	2	580	U	N3-C2-O2	-5.49	118.36	122.20
1	2	55	U	C2-N1-C1'	-5.48	111.12	117.70
1	2	332	G	P-O3'-C3'	5.48	126.28	119.70
1	2	1053	C	C6-N1-C2	-5.48	118.11	120.30
1	2	1097	G	C6-C5-N7	-5.47	127.12	130.40
1	2	577	U	N1-C2-O2	5.47	126.63	122.80
1	2	891	G	C4-N9-C1'	5.47	133.62	126.50
1	2	1316	C	P-O3'-C3'	5.47	126.27	119.70
1	2	1464	C	P-O3'-C3'	5.47	126.27	119.70
1	2	560	A	N7-C8-N9	5.47	116.53	113.80
1	2	791	C	C5-C6-N1	5.47	123.73	121.00
1	2	1572	C	C5-C6-N1	5.46	123.73	121.00
1	2	1520	G	N3-C4-C5	-5.46	125.87	128.60
1	2	1256	G	C8-N9-C4	5.46	108.58	106.40
1	2	1538	C	N3-C2-O2	-5.46	118.08	121.90
1	2	1081	U	N1-C2-O2	5.46	126.62	122.80
1	2	1754	G	C6-C5-N7	-5.45	127.13	130.40
1	2	1242	U	N3-C2-O2	-5.45	118.39	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1060	A	N7-C8-N9	5.45	116.52	113.80
1	2	1366	G	C4-N9-C1'	5.45	133.58	126.50
1	2	1333	U	N1-C2-O2	5.44	126.61	122.80
1	2	1714	U	C6-N1-C2	-5.44	117.74	121.00
1	2	659	G	C8-N9-C1'	-5.44	119.93	127.00
1	2	926	A	N3-C4-N9	5.43	131.75	127.40
1	2	1212	G	C5-C6-O6	5.43	131.86	128.60
1	2	1453	C	C5-C6-N1	5.43	123.72	121.00
1	2	180	G	P-O3'-C3'	5.43	126.21	119.70
1	2	570	C	C6-N1-C2	-5.43	118.13	120.30
1	2	877	C	C2-N1-C1'	5.42	124.77	118.80
1	2	617	G	C6-C5-N7	-5.41	127.16	130.40
1	2	1366	G	N3-C4-N9	5.40	129.24	126.00
1	2	1625	U	N3-C2-O2	-5.40	118.42	122.20
1	2	973	C	C2-N1-C1'	5.39	124.73	118.80
1	2	1407	U	C5-C4-O4	-5.39	122.66	125.90
1	2	824	C	N3-C2-O2	-5.39	118.13	121.90
1	2	578	C	N3-C2-O2	-5.38	118.13	121.90
4	C	233	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	2	1643	U	N3-C2-O2	-5.37	118.44	122.20
1	2	594	A	P-O3'-C3'	5.37	126.14	119.70
1	2	685	A	N7-C8-N9	5.36	116.48	113.80
1	2	1242	U	C2-N1-C1'	5.36	124.14	117.70
1	2	215	G	C8-N9-C1'	-5.36	120.03	127.00
1	2	213	G	C8-N9-C1'	-5.36	120.03	127.00
1	2	1140	G	C4-C5-N7	5.36	112.94	110.80
1	2	617	G	N9-C4-C5	-5.36	103.26	105.40
1	2	1754	G	N7-C8-N9	5.35	115.78	113.10
1	2	945	U	C5-C6-N1	5.35	125.38	122.70
24	K	84	HIS	C-N-CA	-5.35	108.32	121.70
1	2	823	U	C2-N1-C1'	5.35	124.12	117.70
1	2	557	U	C5-C4-O4	-5.35	122.69	125.90
1	2	1430	C	C5-C6-N1	5.35	123.67	121.00
1	2	1563	G	N3-C4-N9	5.35	129.21	126.00
1	2	25	A	N9-C1'-C2'	5.34	120.95	114.00
1	2	1123	C	C6-N1-C2	-5.33	118.17	120.30
1	2	1592	C	C6-N1-C2	-5.33	118.17	120.30
1	2	541	U	C6-N1-C1'	-5.32	113.75	121.20
1	2	1440	C	C5-C6-N1	5.32	123.66	121.00
1	2	1683	C	N1-C2-O2	5.32	122.09	118.90
1	2	1625	U	C2-N1-C1'	5.32	124.08	117.70
1	2	1160	U	C5-C6-N1	5.32	125.36	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	160	ILE	CG1-CB-CG2	-5.31	99.71	111.40
1	2	967	C	N1-C2-O2	5.31	122.08	118.90
1	2	1666	C	N1-C2-O2	5.31	122.08	118.90
1	2	1329	U	C2-N1-C1'	5.30	124.07	117.70
1	2	1277	C	C2-N1-C1'	5.30	124.63	118.80
1	2	1123	C	C2-N1-C1'	5.30	124.63	118.80
1	2	1289	U	N3-C2-O2	-5.30	118.49	122.20
1	2	1429	G	O5'-P-OP2	5.29	117.05	110.70
25	M	22	LEU	CA-CB-CG	-5.29	103.12	115.30
1	2	1589	A	C5-N7-C8	-5.29	101.25	103.90
1	2	1053	C	C5-C6-N1	5.29	123.65	121.00
1	2	1520	G	C8-N9-C4	-5.29	104.28	106.40
1	2	1753	C	C2-N1-C1'	5.29	124.61	118.80
1	2	1233	G	C4-C5-N7	5.28	112.91	110.80
1	2	1601	A	OP2-P-O3'	5.28	116.82	105.20
1	2	1311	C	C6-N1-C2	-5.28	118.19	120.30
1	2	1510	G	C8-N9-C4	-5.26	104.30	106.40
1	2	973	C	C5-C6-N1	5.26	123.63	121.00
1	2	1524	G	C4-C5-N7	5.26	112.90	110.80
1	2	143	U	OP2-P-O3'	5.25	116.75	105.20
1	2	958	G	N7-C8-N9	5.25	115.72	113.10
1	2	1524	G	C4-N9-C1'	5.25	133.33	126.50
1	2	541	U	C2-N1-C1'	5.25	124.00	117.70
1	2	1511	U	P-O3'-C3'	5.25	126.00	119.70
1	2	577	U	N3-C2-O2	-5.24	118.53	122.20
1	2	909	G	N3-C4-N9	5.24	129.15	126.00
1	2	1842	C	C6-N1-C2	-5.24	118.20	120.30
1	2	1430	C	P-O3'-C3'	5.24	125.98	119.70
1	2	342	C	C2-N1-C1'	5.24	124.56	118.80
1	2	1629	C	N3-C2-O2	-5.24	118.23	121.90
1	2	1844	U	C2-N1-C1'	5.24	123.98	117.70
1	2	898	U	N3-C2-O2	-5.23	118.54	122.20
1	2	1191	C	C6-N1-C2	-5.23	118.21	120.30
1	2	1728	U	N3-C2-O2	-5.23	118.54	122.20
1	2	1230	C	C5-C6-N1	5.23	123.61	121.00
1	2	180	G	C8-N9-C1'	-5.23	120.21	127.00
1	2	1703	C	C6-N1-C1'	5.23	127.07	120.80
1	2	1440	C	P-O3'-C3'	5.22	125.96	119.70
1	2	1696	C	N3-C2-O2	-5.22	118.25	121.90
1	2	144	U	O5'-P-OP2	-5.21	101.01	105.70
1	2	1243	U	N3-C2-O2	-5.21	118.55	122.20
1	2	833	C	N1-C2-O2	5.21	122.03	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1867	U	C2-N1-C1'	5.21	123.95	117.70
1	2	879	C	C2-N1-C1'	5.21	124.53	118.80
1	2	1202	U	C6-N1-C2	-5.21	117.88	121.00
1	2	877	C	N1-C2-O2	5.21	122.02	118.90
1	2	1140	G	N9-C4-C5	-5.20	103.32	105.40
1	2	1774	C	N1-C2-O2	5.20	122.02	118.90
1	2	1186	U	N1-C2-O2	5.20	126.44	122.80
1	2	1654	G	C6-C5-N7	-5.20	127.28	130.40
1	2	1666	C	C5-C6-N1	5.20	123.60	121.00
1	2	594	A	OP1-P-O3'	5.20	116.63	105.20
1	2	1277	C	N1-C2-O2	5.20	122.02	118.90
1	2	1041	G	C4-N9-C1'	5.19	133.25	126.50
1	2	1090	C	C5-C6-N1	5.19	123.59	121.00
1	2	687	C	N1-C2-O2	5.18	122.01	118.90
1	2	1525	C	C6-N1-C2	-5.18	118.23	120.30
1	2	687	C	C2-N1-C1'	5.18	124.50	118.80
1	2	1154	U	C5-C6-N1	5.18	125.29	122.70
1	2	687	C	N3-C2-O2	-5.18	118.28	121.90
12	O	146	ARG	CG-CD-NE	-5.17	100.93	111.80
1	2	804	U	C2-N1-C1'	5.17	123.90	117.70
1	2	793	G	P-O3'-C3'	5.16	125.89	119.70
1	2	750	C	P-O3'-C3'	5.16	125.89	119.70
33	c	36	ASP	C-N-CA	5.16	134.59	121.70
1	2	162	C	C2-N1-C1'	-5.15	113.14	118.80
1	2	870	A	P-O3'-C3'	5.15	125.88	119.70
1	2	824	C	C6-N1-C2	-5.14	118.24	120.30
1	2	571	U	C2-N1-C1'	5.14	123.87	117.70
1	2	314	U	P-O3'-C3'	5.14	125.87	119.70
1	2	572	U	N1-C2-O2	5.14	126.40	122.80
1	2	1472	C	C5-C6-N1	5.13	123.57	121.00
1	2	1534	C	P-O3'-C3'	5.13	125.86	119.70
1	2	930	C	C5-C6-N1	5.13	123.56	121.00
1	2	92	A	OP2-P-O3'	5.13	116.48	105.20
1	2	291	G	P-O3'-C3'	5.13	125.86	119.70
1	2	682	U	N3-C2-O2	-5.13	118.61	122.20
1	2	1844	U	N1-C2-O2	5.13	126.39	122.80
1	2	877	C	C6-N1-C2	-5.13	118.25	120.30
1	2	382	C	P-O3'-C3'	5.12	125.84	119.70
1	2	1658	G	N3-C4-C5	-5.12	126.04	128.60
1	2	1259	A	C4-C5-N7	5.12	113.26	110.70
1	2	1153	C	C6-N1-C1'	-5.11	114.66	120.80
1	2	1527	C	N3-C2-O2	-5.11	118.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	608	C	C6-N1-C1'	-5.11	114.67	120.80
1	2	1510	G	N7-C8-N9	5.11	115.65	113.10
1	2	1615	U	N3-C2-O2	-5.11	118.63	122.20
1	2	1666	C	C2-N1-C1'	5.11	124.42	118.80
1	2	1494	U	OP2-P-O3'	5.10	116.43	105.20
1	2	824	C	N1-C2-O2	5.10	121.96	118.90
1	2	1123	C	C5-C6-N1	5.09	123.55	121.00
1	2	1714	U	N3-C4-O4	5.09	122.97	119.40
1	2	1139	C	C6-N1-C1'	-5.09	114.69	120.80
1	2	815	U	N3-C2-O2	-5.09	118.64	122.20
1	2	1844	U	C5-C6-N1	5.09	125.24	122.70
1	2	1022	U	C2-N1-C1'	5.08	123.80	117.70
1	2	984	C	C6-N1-C2	-5.08	118.27	120.30
1	2	474	G	C8-N9-C1'	-5.08	120.40	127.00
1	2	1503	C	N1-C2-O2	5.07	121.94	118.90
1	2	1839	U	C5-C6-N1	5.07	125.23	122.70
1	2	1520	G	N3-C4-N9	5.07	129.04	126.00
1	2	338	G	C8-N9-C1'	-5.06	120.43	127.00
1	2	967	C	C2-N1-C1'	5.06	124.36	118.80
1	2	1416	C	N3-C2-O2	-5.06	118.36	121.90
1	2	1590	C	C6-N1-C2	-5.05	118.28	120.30
1	2	1192	U	C5-C6-N1	5.05	125.23	122.70
1	2	69	C	C2-N1-C1'	5.05	124.35	118.80
1	2	1118	C	N1-C2-O2	5.05	121.93	118.90
1	2	814	U	C2-N1-C1'	5.04	123.75	117.70
1	2	641	A	C5-C6-N6	-5.04	119.67	123.70
1	2	1286	G	C4-N9-C1'	5.04	133.06	126.50
1	2	1425	G	C2'-C3'-O3'	5.04	121.77	113.70
1	2	1303	C	C2-N1-C1'	5.04	124.34	118.80
1	2	1233	G	N9-C4-C5	-5.03	103.39	105.40
1	2	1106	C	C6-N1-C2	-5.03	118.29	120.30
1	2	1761	U	C5-C6-N1	5.03	125.22	122.70
1	2	1425	G	C4-N9-C1'	5.03	133.04	126.50
1	2	898	U	N1-C2-O2	5.03	126.32	122.80
1	2	1794	C	N3-C2-O2	-5.03	118.38	121.90
1	2	1366	G	N3-C4-C5	-5.02	126.09	128.60
28	R	109	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	2	881	G	C4-C5-N7	5.02	112.81	110.80
1	2	1840	U	C5-C4-O4	-5.02	122.89	125.90
1	2	102	A	OP2-P-O3'	5.02	116.23	105.20
1	2	1855	G	C8-N9-C1'	-5.02	120.48	127.00
1	2	1729	U	N1-C2-O2	5.01	126.31	122.80

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	D	194	PRO	Peptide
23	F	165	ASN	Peptide
23	F	40	ALA	Peptide
23	F	77	MET	Peptide
23	F	82	ASN	Peptide
8	I	101	ILE	Peptide
11	N	101	HIS	Peptide
12	O	93	LEU	Peptide
27	Q	42	ILE	Peptide
30	T	36	THR	Peptide
15	X	112	VAL	Peptide
16	Y	118	ARG	Peptide
18	b	52	THR	Peptide
34	f	87	THR	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	
2	A	204/295 (69%)	190 (93%)	14 (7%)	0	100	100
3	B	211/264 (80%)	187 (89%)	24 (11%)	0	100	100
4	C	216/293 (74%)	195 (90%)	20 (9%)	1 (0%)	29	68
5	E	260/263 (99%)	230 (88%)	30 (12%)	0	100	100
6	G	228/249 (92%)	213 (93%)	15 (7%)	0	100	100
7	H	184/194 (95%)	171 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	I	203/208 (98%)	189 (93%)	14 (7%)	0	100	100
9	J	178/194 (92%)	163 (92%)	14 (8%)	1 (1%)	25	64
10	L	149/158 (94%)	133 (89%)	16 (11%)	0	100	100
11	N	147/151 (97%)	135 (92%)	12 (8%)	0	100	100
12	O	133/151 (88%)	123 (92%)	10 (8%)	0	100	100
13	V	80/83 (96%)	74 (92%)	6 (8%)	0	100	100
14	W	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
15	X	139/143 (97%)	127 (91%)	11 (8%)	1 (1%)	22	61
16	Y	122/133 (92%)	111 (91%)	11 (9%)	0	100	100
17	a	99/115 (86%)	91 (92%)	8 (8%)	0	100	100
18	b	80/84 (95%)	69 (86%)	11 (14%)	0	100	100
19	d	52/56 (93%)	49 (94%)	2 (4%)	1 (2%)	8	42
20	e	54/59 (92%)	47 (87%)	7 (13%)	0	100	100
21	h	22/25 (88%)	22 (100%)	0	0	100	100
22	D	223/243 (92%)	201 (90%)	21 (9%)	1 (0%)	34	71
23	F	187/204 (92%)	172 (92%)	12 (6%)	3 (2%)	9	46
24	K	93/165 (56%)	86 (92%)	7 (8%)	0	100	100
25	M	121/132 (92%)	114 (94%)	7 (6%)	0	100	100
26	P	118/145 (81%)	115 (98%)	3 (2%)	0	100	100
27	Q	137/146 (94%)	122 (89%)	15 (11%)	0	100	100
28	R	130/135 (96%)	113 (87%)	17 (13%)	0	100	100
29	S	141/152 (93%)	130 (92%)	11 (8%)	0	100	100
30	T	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
31	U	99/119 (83%)	90 (91%)	9 (9%)	0	100	100
32	Z	70/125 (56%)	68 (97%)	2 (3%)	0	100	100
33	c	59/69 (86%)	52 (88%)	7 (12%)	0	100	100
34	f	70/156 (45%)	60 (86%)	10 (14%)	0	100	100
35	g	312/317 (98%)	277 (89%)	35 (11%)	0	100	100
All	All	4790/5501 (87%)	4369 (91%)	413 (9%)	8 (0%)	50	79

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	D	192	TRP
23	F	166	ILE
9	J	161	LEU
19	d	14	PHE
4	C	135	GLY
15	X	86	PRO
23	F	40	ALA
23	F	41	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	172/243 (71%)	168 (98%)	4 (2%)	50	76
3	B	194/231 (84%)	193 (100%)	1 (0%)	88	95
4	C	182/225 (81%)	173 (95%)	9 (5%)	25	59
5	E	224/225 (100%)	224 (100%)	0	100	100
6	G	200/218 (92%)	197 (98%)	3 (2%)	65	84
7	H	167/174 (96%)	166 (99%)	1 (1%)	86	94
8	I	178/180 (99%)	174 (98%)	4 (2%)	52	77
9	J	160/168 (95%)	157 (98%)	3 (2%)	57	80
10	L	135/142 (95%)	127 (94%)	8 (6%)	19	55
11	N	130/131 (99%)	130 (100%)	0	100	100
12	O	104/119 (87%)	103 (99%)	1 (1%)	76	88
13	V	66/67 (98%)	65 (98%)	1 (2%)	65	84
14	W	112/113 (99%)	110 (98%)	2 (2%)	59	81
15	X	113/115 (98%)	113 (100%)	0	100	100
16	Y	108/115 (94%)	105 (97%)	3 (3%)	43	72
17	a	88/98 (90%)	85 (97%)	3 (3%)	37	69
18	b	74/76 (97%)	74 (100%)	0	100	100
19	d	48/49 (98%)	47 (98%)	1 (2%)	53	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	e	45/48 (94%)	43 (96%)	2 (4%)	28	63
21	h	23/24 (96%)	21 (91%)	2 (9%)	10	41
22	D	188/202 (93%)	187 (100%)	1 (0%)	88	95
23	F	159/170 (94%)	157 (99%)	2 (1%)	69	86
24	K	86/136 (63%)	83 (96%)	3 (4%)	36	68
25	M	104/108 (96%)	102 (98%)	2 (2%)	57	80
26	P	107/130 (82%)	106 (99%)	1 (1%)	78	90
27	Q	115/121 (95%)	115 (100%)	0	100	100
28	R	118/122 (97%)	112 (95%)	6 (5%)	24	58
29	S	124/132 (94%)	123 (99%)	1 (1%)	81	91
30	T	114/115 (99%)	113 (99%)	1 (1%)	78	90
31	U	93/107 (87%)	88 (95%)	5 (5%)	22	57
32	Z	64/103 (62%)	63 (98%)	1 (2%)	62	83
33	c	54/62 (87%)	53 (98%)	1 (2%)	57	80
34	f	65/140 (46%)	65 (100%)	0	100	100
35	g	272/275 (99%)	272 (100%)	0	100	100
All	All	4186/4684 (89%)	4114 (98%)	72 (2%)	62	82

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	50	ASN
2	A	80	ARG
2	A	178	LEU
2	A	182	VAL
3	B	212	VAL
4	C	83	LEU
4	C	98	LEU
4	C	117	ARG
4	C	132	ASP
4	C	134	ASN
4	C	136	HIS
4	C	192	LEU
4	C	194	ARG
4	C	223	TYR
6	G	85	ARG

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Mol	Chain	Res	Type
6	G	105	ASN
6	G	189	ARG
7	H	87	PHE
8	I	47	ARG
8	I	77	ARG
8	I	87	ASN
8	I	99	ASN
9	J	136	ARG
9	J	144	ILE
9	J	159	PHE
10	L	22	ARG
10	L	39	ASN
10	L	65	ASN
10	L	69	ARG
10	L	89	ARG
10	L	118	ARG
10	L	132	ARG
10	L	144	LYS
12	O	150	ARG
13	V	21	ASN
14	W	92	ASN
14	W	105	THR
16	Y	17	LEU
16	Y	23	MET
16	Y	107	ARG
17	a	5	ARG
17	a	15	ARG
17	a	42	ARG
19	d	26	ASN
20	e	8	ARG
20	e	58	ASN
21	h	2	ARG
21	h	6	ARG
22	D	106	ARG
23	F	55	ARG
23	F	136	ARG
24	K	62	PHE
24	K	64	TRP
24	K	65	ARG
25	M	33	ARG
25	M	45	ARG
26	P	51	ARG

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Mol	Chain	Res	Type
28	R	16	ILE
28	R	17	ILE
28	R	32	LYS
28	R	47	ARG
28	R	60	ARG
28	R	132	ARG
29	S	19	ASN
30	T	27	LYS
31	U	27	ARG
31	U	34	LYS
31	U	36	CYS
31	U	47	ASN
31	U	79	ARG
32	Z	111	ARG
33	c	34	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	50	ASN
2	A	113	GLN
2	A	141	ASN
3	B	92	GLN
3	B	95	ASN
3	B	208	HIS
4	C	134	ASN
4	C	178	HIS
4	C	272	HIS
5	E	8	HIS
5	E	179	ASN
5	E	201	HIS
6	G	65	GLN
6	G	105	ASN
7	H	73	GLN
8	I	87	ASN
8	I	99	ASN
8	I	116	HIS
9	J	125	HIS
9	J	132	GLN
9	J	177	ASN
10	L	39	ASN
10	L	65	ASN

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Mol	Chain	Res	Type
10	L	100	ASN
11	N	58	HIS
11	N	105	ASN
13	V	21	ASN
14	W	92	ASN
15	X	61	GLN
17	a	43	ASN
22	D	22	ASN
22	D	226	GLN
23	F	179	ASN
24	K	61	GLN
24	K	77	GLN
27	Q	77	HIS
29	S	19	ASN
29	S	125	HIS
31	U	47	ASN
32	Z	103	HIS
33	c	26	GLN
34	f	139	HIS
35	g	64	HIS
35	g	133	ASN
35	g	181	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1656/1868 (88%)	529 (31%)	56 (3%)

All (529) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	C
1	2	4	C
1	2	9	U
1	2	10	G
1	2	17	C
1	2	25	A
1	2	26	U
1	2	33	G
1	2	41	G

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Mol	Chain	Res	Type
1	2	42	A
1	2	44	U
1	2	46	A
1	2	47	G
1	2	56	G
1	2	58	C
1	2	59	U
1	2	60	A
1	2	61	A
1	2	62	G
1	2	65	C
1	2	66	G
1	2	67	C
1	2	68	A
1	2	69	C
1	2	72	C
1	2	73	C
1	2	74	G
1	2	75	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	103	A
1	2	110	U
1	2	113	G
1	2	114	G
1	2	115	U
1	2	116	U
1	2	119	U
1	2	127	C
1	2	128	U
1	2	129	C
1	2	143	U
1	2	144	U
1	2	153	G
1	2	154	U
1	2	155	G
1	2	160	U
1	2	175	A
1	2	181	A
1	2	182	C
1	2	183	G

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Mol	Chain	Res	Type
1	2	184	G
1	2	188	C
1	2	191	A
1	2	196	C
1	2	206	G
1	2	213	G
1	2	214	U
1	2	215	G
1	2	216	C
1	2	217	A
1	2	290	U
1	2	291	G
1	2	292	A
1	2	295	C
1	2	302	A
1	2	305	U
1	2	306	C
1	2	307	G
1	2	308	G
1	2	310	C
1	2	312	G
1	2	313	A
1	2	315	C
1	2	318	A
1	2	319	C
1	2	320	G
1	2	321	C
1	2	332	G
1	2	333	G
1	2	335	G
1	2	338	G
1	2	342	C
1	2	347	G
1	2	350	C
1	2	360	A
1	2	362	C
1	2	364	A
1	2	368	U
1	2	369	C
1	2	370	G
1	2	377	G
1	2	381	C

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Mol	Chain	Res	Type
1	2	382	C
1	2	383	G
1	2	385	G
1	2	386	C
1	2	398	A
1	2	399	C
1	2	400	C
1	2	407	G
1	2	408	A
1	2	409	C
1	2	418	A
1	2	420	G
1	2	421	G
1	2	428	U
1	2	429	C
1	2	436	G
1	2	438	G
1	2	441	C
1	2	447	A
1	2	448	A
1	2	450	C
1	2	464	A
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	476	A
1	2	482	G
1	2	483	C
1	2	487	U
1	2	489	A
1	2	492	C
1	2	500	A
1	2	502	C
1	2	512	A
1	2	517	C
1	2	523	A
1	2	525	A
1	2	532	C
1	2	534	G

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Mol	Chain	Res	Type
1	2	536	A
1	2	537	C
1	2	544	G
1	2	546	G
1	2	548	C
1	2	549	C
1	2	552	G
1	2	553	U
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	563	G
1	2	564	A
1	2	568	C
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	593	C
1	2	594	A
1	2	595	U
1	2	596	U
1	2	598	G
1	2	600	G
1	2	603	C
1	2	604	A
1	2	605	A
1	2	607	U
1	2	608	C
1	2	614	C
1	2	615	C
1	2	617	G
1	2	621	C
1	2	627	U
1	2	629	A
1	2	638	C
1	2	639	C

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Mol	Chain	Res	Type
1	2	640	A
1	2	643	A
1	2	644	G
1	2	655	A
1	2	658	U
1	2	660	C
1	2	664	A
1	2	668	A
1	2	669	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	683	G
1	2	684	G
1	2	685	A
1	2	687	C
1	2	688	U
1	2	748	C
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C
1	2	793	G
1	2	794	A
1	2	797	C
1	2	798	G
1	2	801	U
1	2	809	A
1	2	810	A
1	2	812	A
1	2	821	G
1	2	822	U
1	2	823	U
1	2	824	C
1	2	827	A
1	2	830	A
1	2	834	C
1	2	844	U
1	2	847	A
1	2	852	G
1	2	856	C
1	2	859	G

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Mol	Chain	Res	Type
1	2	869	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	879	C
1	2	880	G
1	2	882	U
1	2	887	U
1	2	888	U
1	2	890	U
1	2	894	G
1	2	898	U
1	2	903	A
1	2	909	G
1	2	912	C
1	2	913	A
1	2	914	U
1	2	915	G
1	2	917	U
1	2	918	U
1	2	919	A
1	2	920	A
1	2	921	G
1	2	926	A
1	2	933	G
1	2	934	G
1	2	938	A
1	2	943	U
1	2	952	G
1	2	954	U
1	2	959	G
1	2	962	A
1	2	963	A
1	2	967	C
1	2	969	U
1	2	970	G
1	2	971	G
1	2	973	C
1	2	978	G
1	2	981	A

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Mol	Chain	Res	Type
1	2	982	G
1	2	988	C
1	2	989	C
1	2	990	A
1	2	992	A
1	2	999	G
1	2	1001	A
1	2	1002	U
1	2	1017	U
1	2	1023	A
1	2	1027	A
1	2	1029	G
1	2	1030	A
1	2	1040	G
1	2	1041	G
1	2	1042	A
1	2	1045	U
1	2	1049	A
1	2	1050	A
1	2	1053	C
1	2	1060	A
1	2	1067	C
1	2	1081	U
1	2	1083	A
1	2	1085	C
1	2	1088	U
1	2	1096	G
1	2	1114	U
1	2	1115	U
1	2	1116	C
1	2	1118	C
1	2	1119	A
1	2	1120	U
1	2	1121	G
1	2	1123	C
1	2	1133	A
1	2	1137	U
1	2	1138	C
1	2	1139	C
1	2	1143	A
1	2	1148	A
1	2	1149	A

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Mol	Chain	Res	Type
1	2	1153	C
1	2	1154	U
1	2	1156	U
1	2	1157	G
1	2	1166	G
1	2	1168	G
1	2	1170	A
1	2	1171	G
1	2	1195	A
1	2	1198	G
1	2	1207	G
1	2	1208	A
1	2	1211	G
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1232	U
1	2	1235	G
1	2	1236	G
1	2	1238	U
1	2	1242	U
1	2	1243	U
1	2	1245	G
1	2	1251	A
1	2	1253	A
1	2	1254	C
1	2	1257	G
1	2	1259	A
1	2	1260	A
1	2	1261	C
1	2	1270	G
1	2	1274	G
1	2	1275	G
1	2	1283	C
1	2	1284	A
1	2	1286	G
1	2	1288	U
1	2	1294	G
1	2	1298	G
1	2	1301	A

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Mol	Chain	Res	Type
1	2	1302	G
1	2	1303	C
1	2	1304	U
1	2	1308	U
1	2	1309	C
1	2	1313	A
1	2	1314	U
1	2	1315	U
1	2	1317	C
1	2	1320	G
1	2	1321	G
1	2	1322	G
1	2	1323	U
1	2	1327	G
1	2	1329	U
1	2	1330	G
1	2	1331	C
1	2	1343	U
1	2	1344	A
1	2	1348	G
1	2	1354	G
1	2	1358	U
1	2	1363	C
1	2	1364	U
1	2	1366	G
1	2	1369	A
1	2	1371	U
1	2	1373	C
1	2	1377	U
1	2	1378	A
1	2	1380	C
1	2	1382	A
1	2	1401	A
1	2	1402	A
1	2	1403	C
1	2	1404	U
1	2	1405	A
1	2	1406	G
1	2	1411	G
1	2	1414	A
1	2	1415	C
1	2	1416	C

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Mol	Chain	Res	Type
1	2	1426	U
1	2	1428	G
1	2	1429	G
1	2	1430	C
1	2	1431	G
1	2	1432	U
1	2	1439	A
1	2	1441	U
1	2	1442	U
1	2	1444	U
1	2	1446	A
1	2	1452	A
1	2	1454	A
1	2	1462	U
1	2	1463	U
1	2	1465	A
1	2	1466	G
1	2	1474	A
1	2	1476	A
1	2	1477	U
1	2	1478	U
1	2	1486	A
1	2	1487	A
1	2	1489	A
1	2	1494	U
1	2	1495	G
1	2	1498	A
1	2	1500	G
1	2	1505	U
1	2	1506	A
1	2	1507	G
1	2	1510	G
1	2	1512	C
1	2	1516	G
1	2	1517	G
1	2	1518	C
1	2	1519	U
1	2	1520	G
1	2	1521	C
1	2	1522	A
1	2	1523	C
1	2	1524	G

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Mol	Chain	Res	Type
1	2	1526	G
1	2	1531	A
1	2	1533	A
1	2	1534	C
1	2	1535	U
1	2	1536	G
1	2	1544	C
1	2	1548	G
1	2	1559	C
1	2	1560	U
1	2	1566	G
1	2	1567	G
1	2	1570	G
1	2	1572	C
1	2	1573	G
1	2	1574	C
1	2	1579	A
1	2	1580	A
1	2	1581	C
1	2	1582	C
1	2	1585	U
1	2	1586	U
1	2	1587	G
1	2	1588	A
1	2	1598	G
1	2	1599	U
1	2	1600	G
1	2	1601	A
1	2	1602	U
1	2	1603	G
1	2	1606	G
1	2	1607	A
1	2	1612	G
1	2	1615	U
1	2	1617	G
1	2	1618	C
1	2	1619	A
1	2	1621	U
1	2	1623	A
1	2	1630	A
1	2	1631	U
1	2	1632	G

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Mol	Chain	Res	Type
1	2	1635	C
1	2	1648	G
1	2	1649	U
1	2	1650	A
1	2	1654	G
1	2	1660	C
1	2	1663	A
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1678	A
1	2	1683	C
1	2	1695	A
1	2	1698	C
1	2	1699	A
1	2	1701	C
1	2	1704	C
1	2	1719	A
1	2	1721	U
1	2	1722	G
1	2	1725	U
1	2	1728	U
1	2	1729	U
1	2	1730	U
1	2	1748	G
1	2	1757	G
1	2	1761	U
1	2	1778	C
1	2	1783	C
1	2	1784	G
1	2	1785	C
1	2	1786	U
1	2	1799	G
1	2	1807	C
1	2	1813	A
1	2	1824	A
1	2	1825	A
1	2	1829	G
1	2	1831	A
1	2	1835	A
1	2	1836	G
1	2	1838	U

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Mol	Chain	Res	Type
1	2	1839	U
1	2	1840	U
1	2	1849	G
1	2	1850	A
1	2	1852	C
1	2	1856	C
1	2	1859	A
1	2	1860	A
1	2	1861	G
1	2	1862	G
1	2	1863	A
1	2	1865	C
1	2	1866	A
1	2	1868	U
1	2	1869	A

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	59	U
1	2	60	A
1	2	65	C
1	2	102	A
1	2	114	G
1	2	143	U
1	2	180	G
1	2	181	A
1	2	291	G
1	2	314	U
1	2	332	G
1	2	368	U
1	2	382	C
1	2	440	G
1	2	465	A
1	2	547	G
1	2	554	A
1	2	594	A
1	2	604	A
1	2	620	G
1	2	750	C
1	2	793	G
1	2	797	C

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Mol	Chain	Res	Type
1	2	811	A
1	2	870	A
1	2	958	G
1	2	980	A
1	2	1137	U
1	2	1231	C
1	2	1302	G
1	2	1308	U
1	2	1316	C
1	2	1330	G
1	2	1342	U
1	2	1403	C
1	2	1415	C
1	2	1425	G
1	2	1430	C
1	2	1431	G
1	2	1438	A
1	2	1440	C
1	2	1464	C
1	2	1494	U
1	2	1511	U
1	2	1520	G
1	2	1534	C
1	2	1558	C
1	2	1565	C
1	2	1585	U
1	2	1587	G
1	2	1601	A
1	2	1648	G
1	2	1649	U
1	2	1783	C
1	2	1838	U
1	2	1862	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

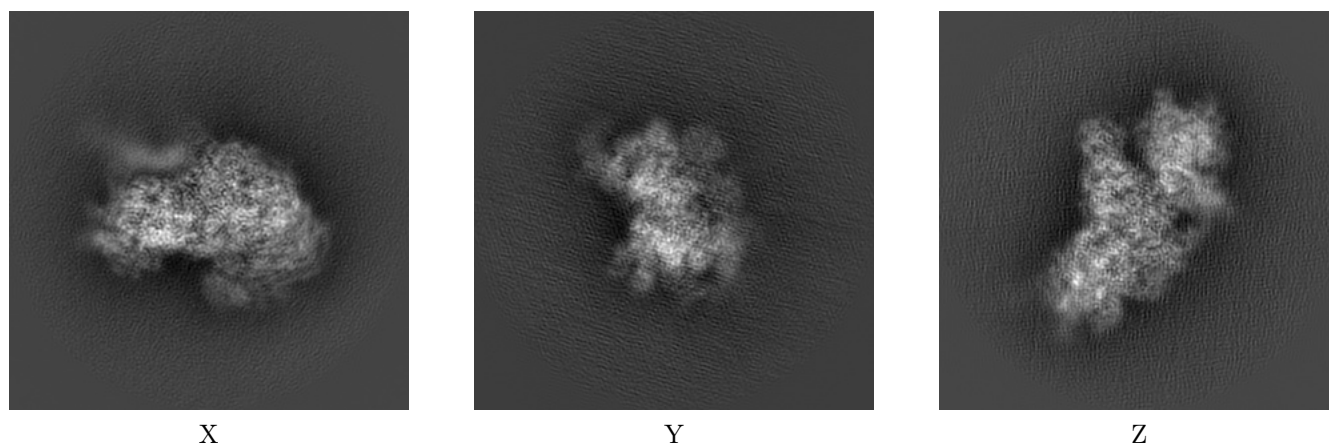
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4352. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

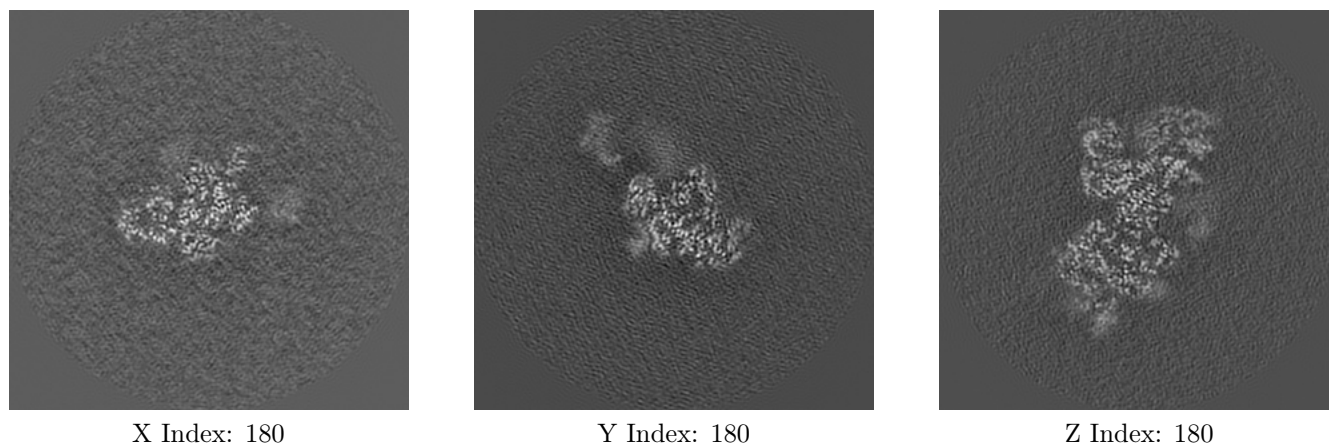
6.1.1 Primary map



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

6.2 Central slices [i](#)

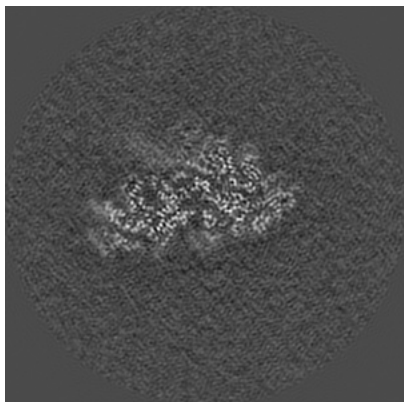
6.2.1 Primary map



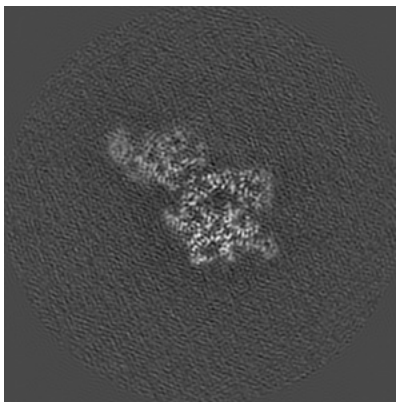
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

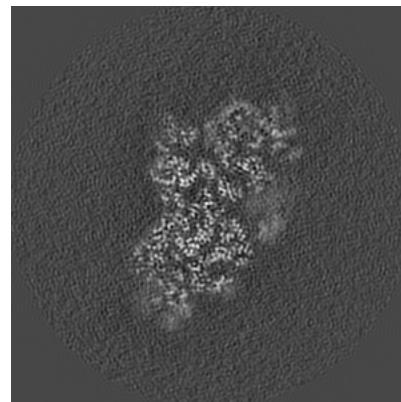
6.3.1 Primary map



X Index: 154



Y Index: 203



Z Index: 175

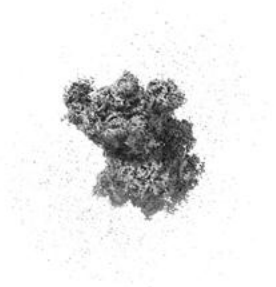
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

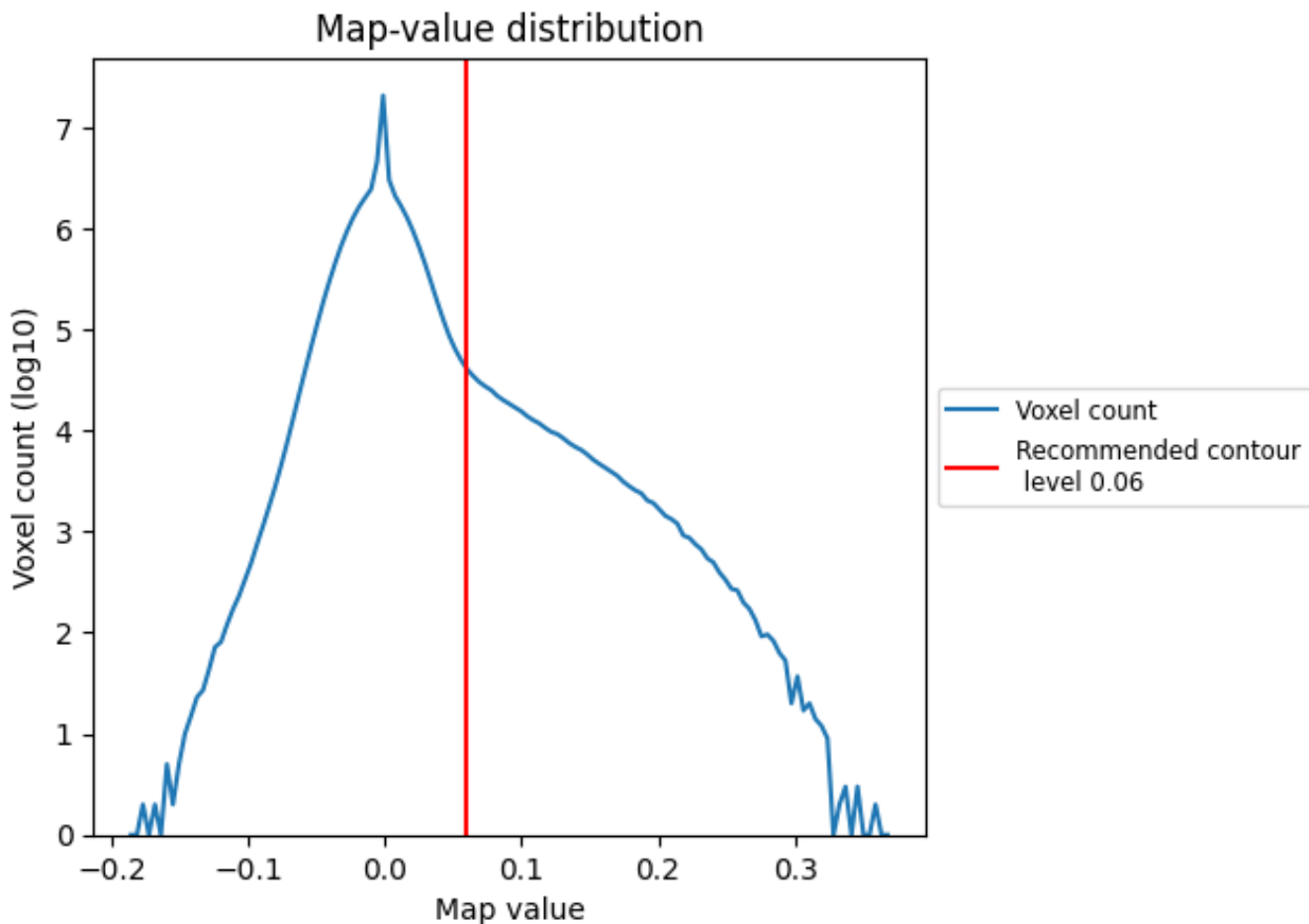
6.5 Mask visualisation

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

7 Map analysis [i](#)

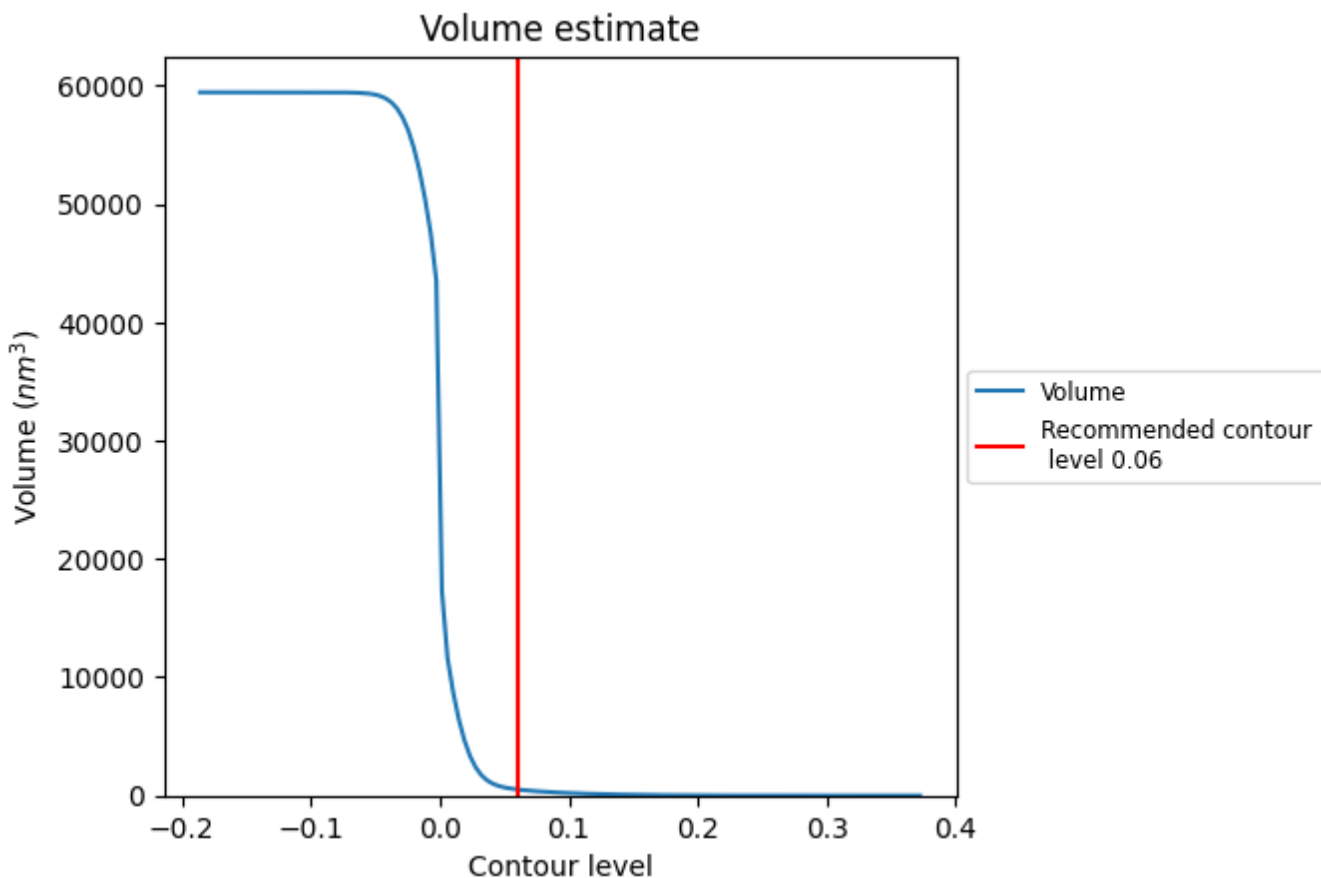
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

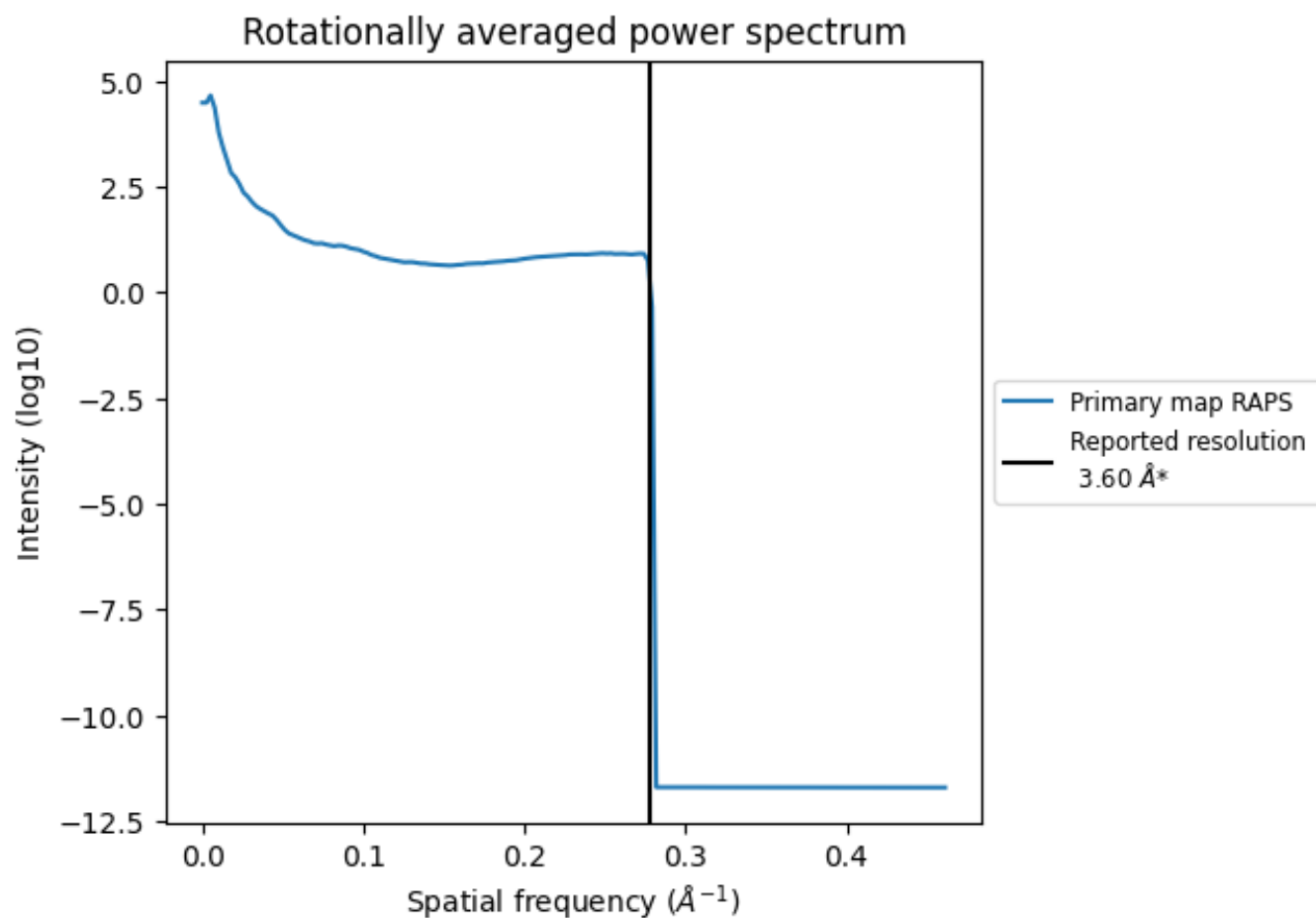
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 517 nm³; this corresponds to an approximate mass of 467 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

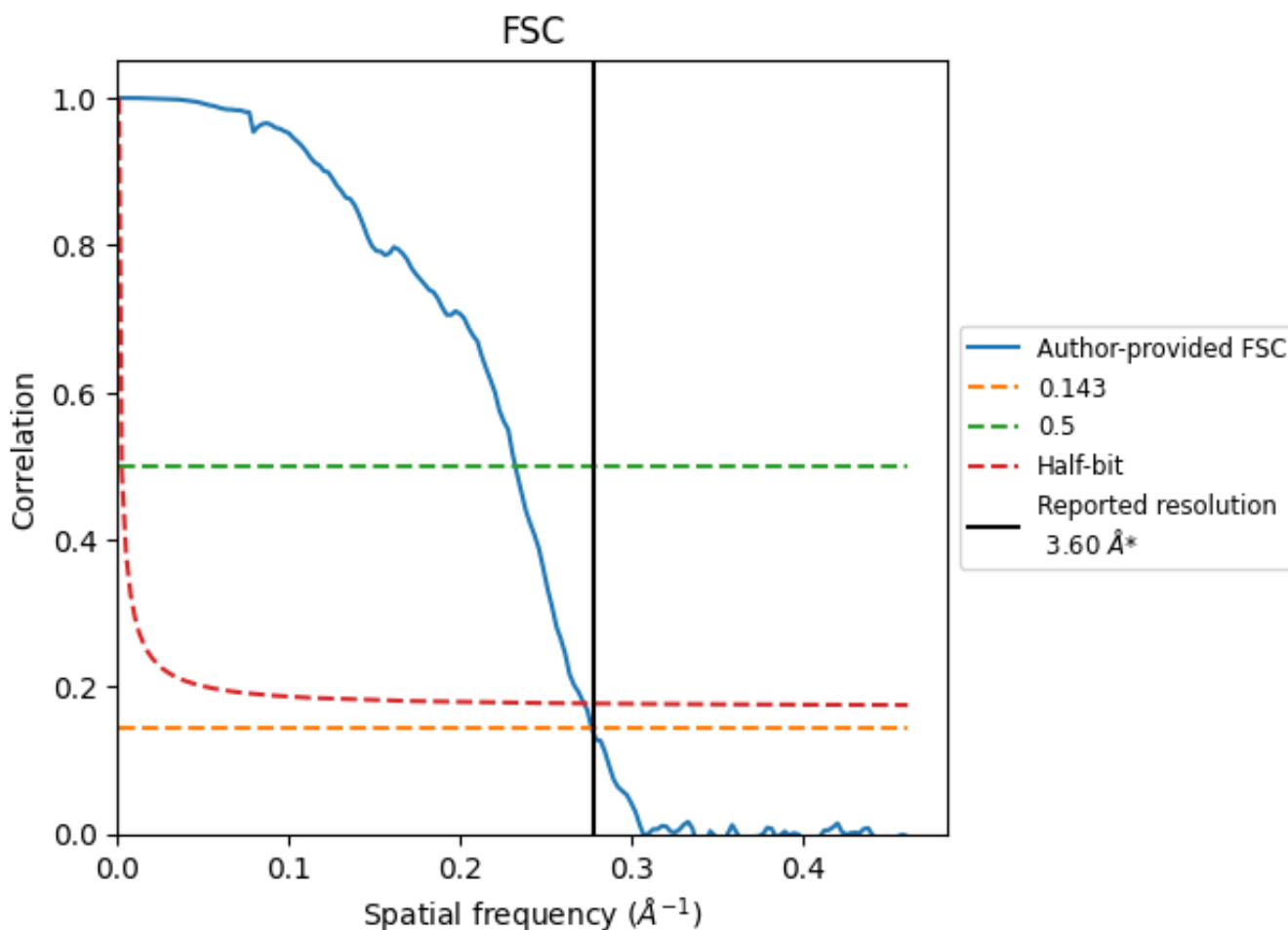


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

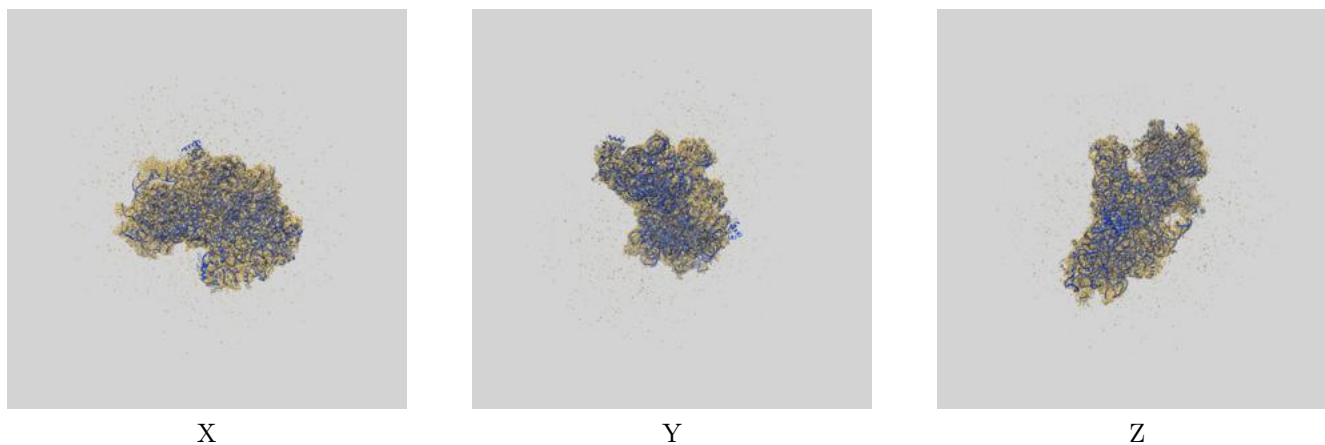
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.61	4.31	3.67
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

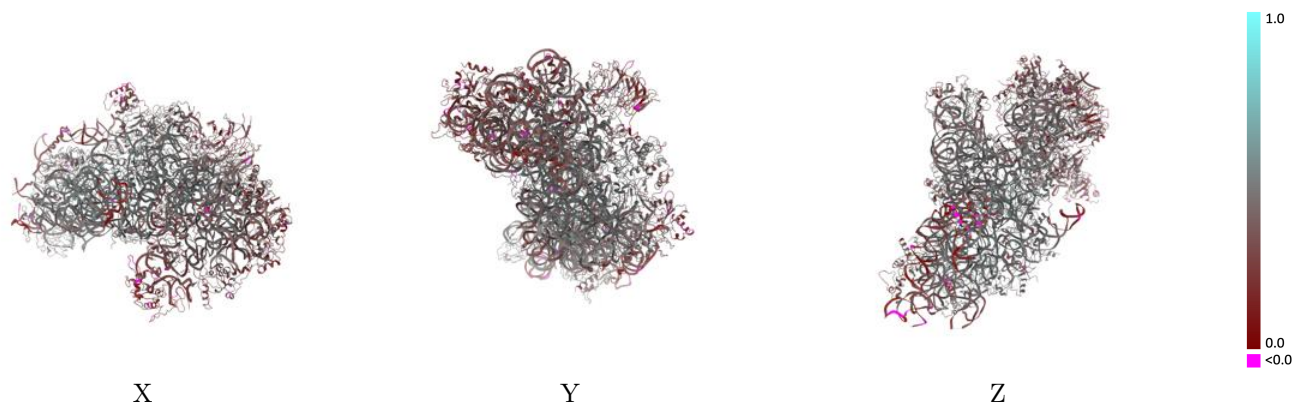
This section contains information regarding the fit between EMDB map EMD-4352 and PDB model 6G5H. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



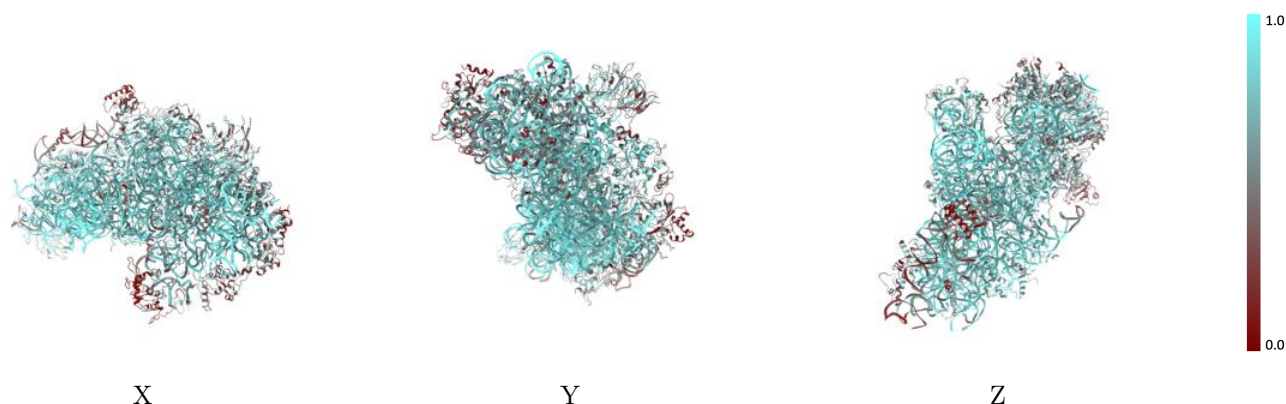
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



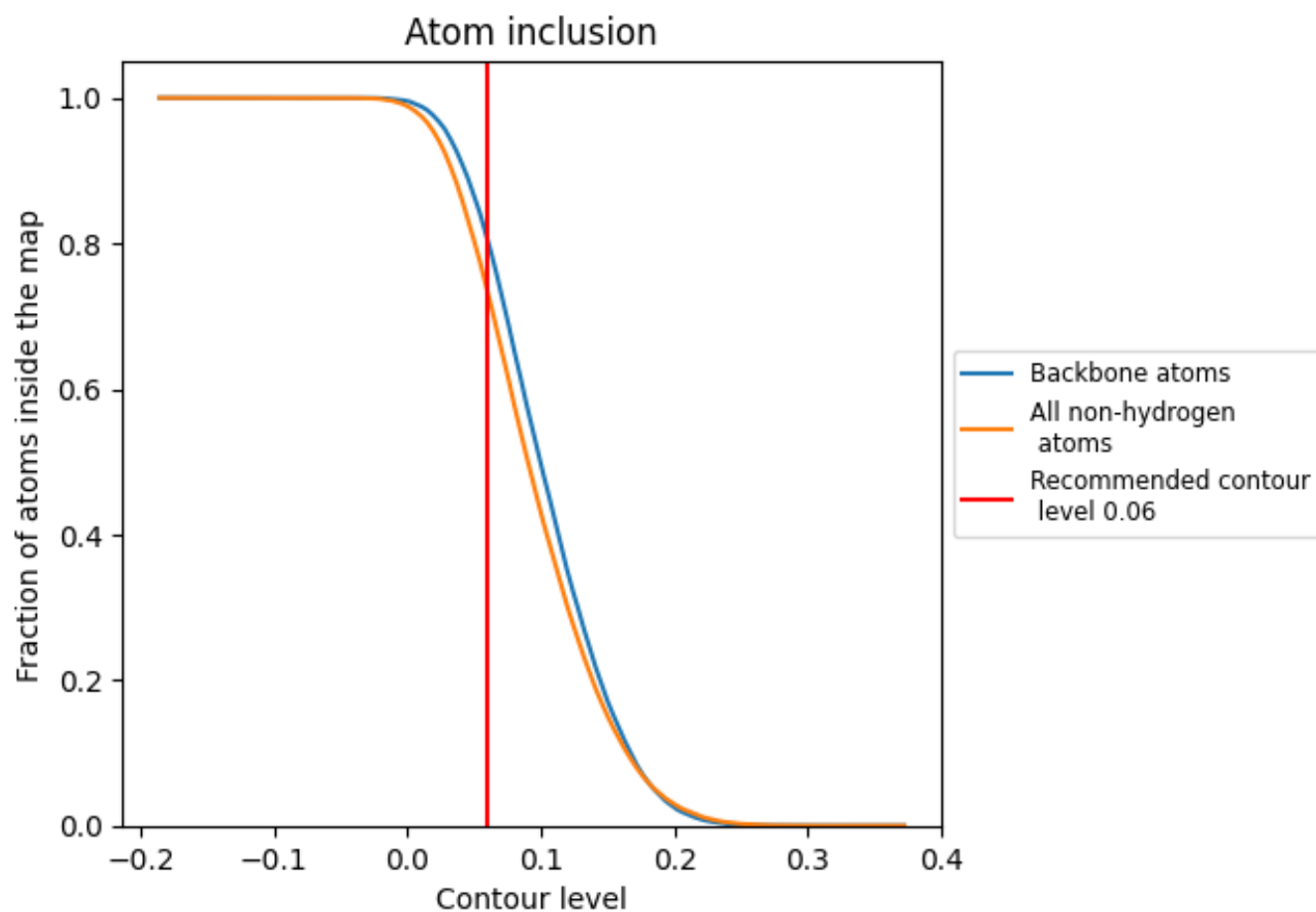
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).









































































9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 73% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7341	 0.4080
2	 0.8502	 0.4210
A	 0.7189	 0.4440
B	 0.6951	 0.4180
C	 0.7558	 0.4730
D	 0.6006	 0.3750
E	 0.7452	 0.4740
F	 0.5612	 0.3440
G	 0.7000	 0.4190
H	 0.3084	 0.2870
I	 0.6987	 0.4310
J	 0.7936	 0.4690
K	 0.5821	 0.3390
L	 0.7010	 0.4600
M	 0.2151	 0.2100
N	 0.7067	 0.4380
O	 0.7073	 0.4280
P	 0.4602	 0.3250
Q	 0.6291	 0.3780
R	 0.5241	 0.3770
S	 0.4442	 0.2990
T	 0.5659	 0.3400
U	 0.5882	 0.3890
V	 0.7398	 0.4640
W	 0.7614	 0.4890
X	 0.7675	 0.4900
Y	 0.7724	 0.4620
Z	 0.4011	 0.2570
a	 0.7110	 0.4550
b	 0.6146	 0.4260
c	 0.5054	 0.3770
d	 0.6370	 0.3480
e	 0.6698	 0.4400
f	 0.3088	 0.2460
g	 0.5754	 0.3320
h	 0.4429	 0.3470

