



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 04:36 am GMT

PDB ID : 6Y7C
EMDB ID : EMD-10713
Title : Early cytoplasmic yeast pre-40S particle (purified with Tsr1 as bait)
Authors : Shayan, R.; Plassart, L.; Plisson-Chastang, C.
Deposited on : 2020-02-28
Resolution : 3.80 Å (reported)
Based on initial model : 6FAI

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:

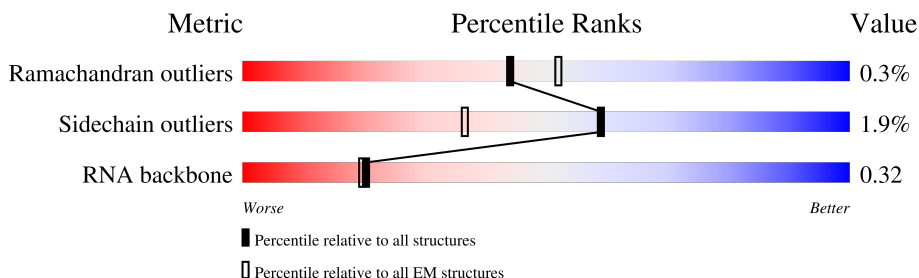
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1735	
2	A	252	
3	B	255	
4	C	254	
5	E	261	
6	F	225	
7	G	236	
8	H	190	

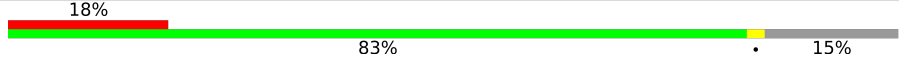
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Mol	Chain	Length	Quality of chain
9	I	200	9% 94% 6%
10	J	197	5% 87% 7% 6%
11	L	156	12% 97% ..
12	M	143	39% 85% . 13%
13	N	151	9% 96% ..
14	O	137	14% 90% . 7%
15	P	142	31% 82% 7% 11%
16	Q	143	24% 87% . 11%
17	R	136	40% 81% . 15%
18	S	146	38% 88% 5% 8%
19	T	144	12% 95% ..
20	U	121	42% 55% . 45%
21	V	87	6% 97% ..
22	W	130	. 95% ..
23	X	145	9% 94% 5% .
24	Y	135	13% 93% 6% .
25	Z	108	24% 57% . 42%
26	b	82	30% 94% 5% .
27	c	67	34% 94% 6%
28	d	56	23% 45% .. 52%
29	e	63	44% 83% 13% 5%
30	h	274	7% 62% . 35%
31	i	483	19% 50% .. 46%
32	j	463	7% 12% 88%
33	l	425	18% 65% . 33%

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Mol	Chain	Length	Quality of chain
34	t	788	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '18%', a large green segment in the middle labeled '83%', and a small grey segment on the right labeled '15%'. A small black dot is visible on the green segment near the right edge.</p>

2 Entry composition i

There are 34 unique types of molecules in this entry. The entry contains 79690 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 20S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1735	36965	16530	6537	12163	1735	0	0

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	206	1614	1039	284	289	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	PHE	ASP	conflict	UNP P32905

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	214	1709	1084	310	311	4	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	220	1662	1065	295	300	2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	260	2068	1316	389	360	3	0	0

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	206	1609	1007	300	299	3	0	0

- Molecule 7 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	226	1799	1129	346	321	3	0	0

- Molecule 8 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	H	168	1362	880	239	243	0	0

- Molecule 9 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	I	188	1489	925	298	264	2	0	0

- Molecule 10 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	J	185	1494	943	289	261	1	0	0

- Molecule 11 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	155	1213	774	230	206	3	0	0

- Molecule 12 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	125	941	591	166	182	2	0	0

- Molecule 13 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	150	Total	C	N	O	S	0	0
			1193	759	224	208	2		

- Molecule 14 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	128	Total	C	N	O	S	0	0
			950	582	188	177	3		

- Molecule 15 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	127	Total	C	N	O	S	0	0
			1001	637	186	171	7		

- Molecule 16 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	127	Total	C	N	O	0	0
			993	640	177	176		

- Molecule 17 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	115	Total	C	N	O	S	0	0
			924	575	173	174	2		

- Molecule 18 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	135	Total	C	N	O	S	0	0
			1110	696	215	197	2		

- Molecule 19 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 20 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
20	U	67	541	344	102	95	0	0

- Molecule 21 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V	87	685	420	125	138	2	0	0

- Molecule 22 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W	129	1019	650	188	178	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	51	VAL	GLU	conflict	UNP P0C0W1

- Molecule 23 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	144	1121	708	220	191	2	0	0

- Molecule 24 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	Y	134	1073	676	208	189	0	0

- Molecule 25 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	Z	63	512	328	94	90	0	0

- Molecule 26 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	81	Total	C	N	O	S	0	0
			611	382	110	114	5		

- Molecule 27 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 28 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	27	Total	C	N	O	S	0	0
			219	133	46	36	4		

- Molecule 29 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	e	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 30 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	179	Total	C	N	O	S	0	0
			1416	906	256	250	4		

- Molecule 31 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	261	Total	C	N	O	S	0	0
			2125	1384	363	375	3		

- Molecule 32 is a protein called Protein LTV1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	55	Total	C	N	O	S	0	0
			465	283	66	113	3		

- Molecule 33 is a protein called Serine/threonine-protein kinase RIO2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	l	286	2322	1464	410	430	18	0	0

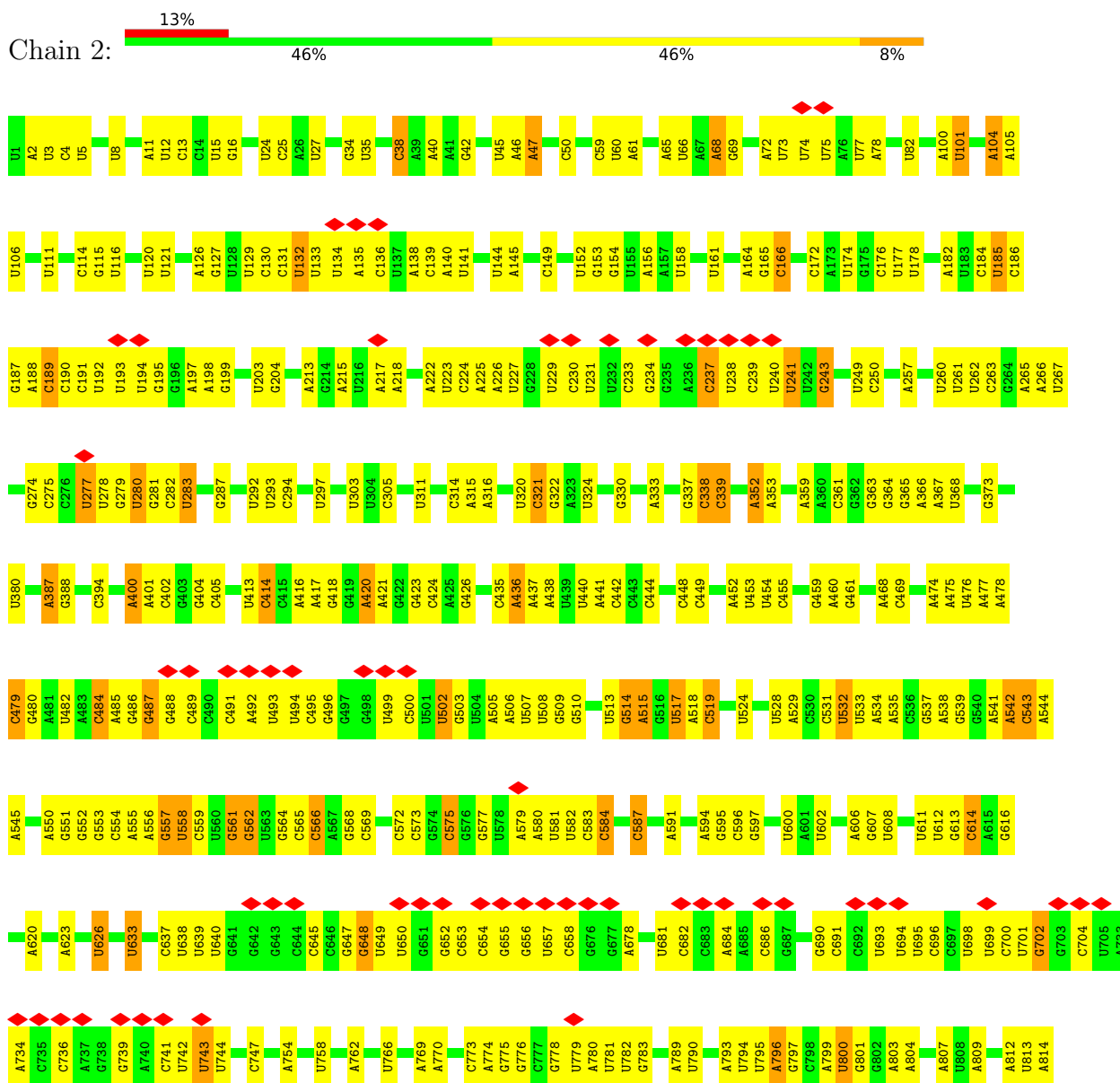
- Molecule 34 is a protein called Ribosome biogenesis protein TSR1.

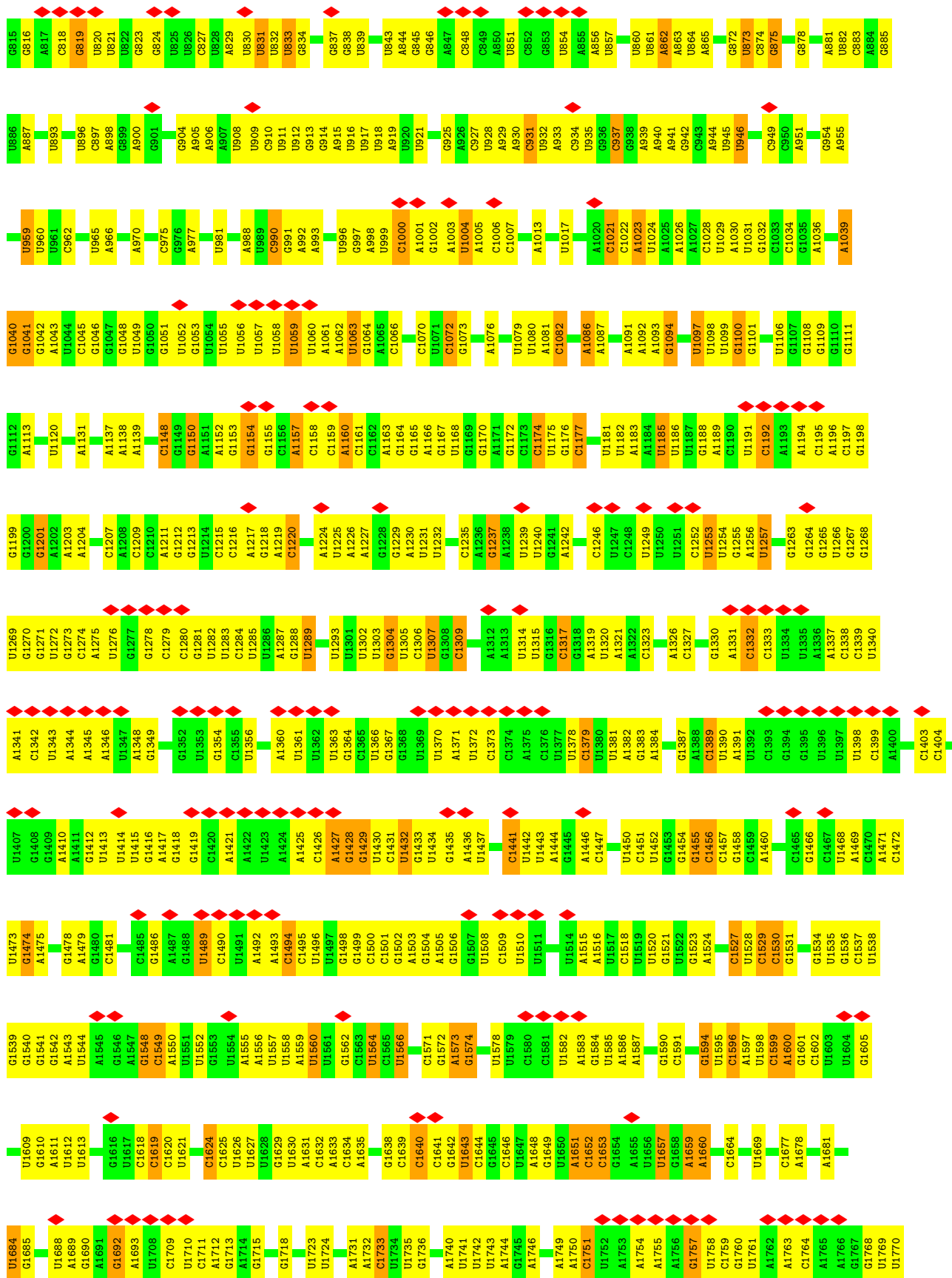
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	t	667	5401	3447	932	1008	14	0	0

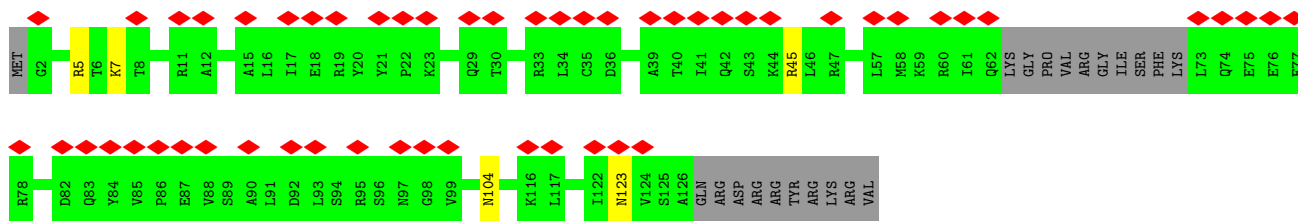
3 Residue-property plots [i](#)

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

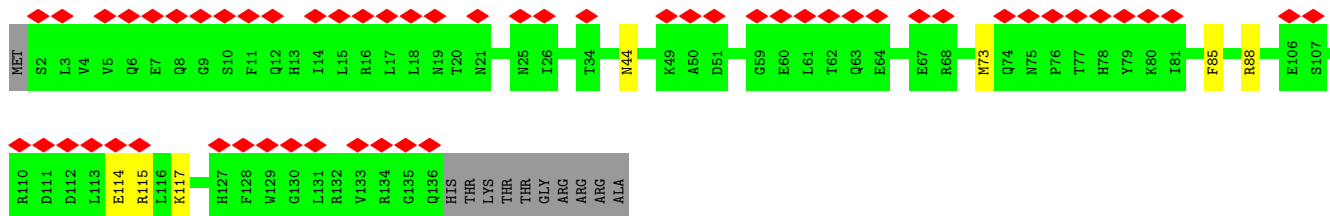
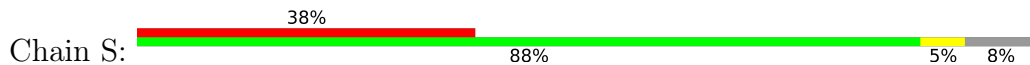
- Molecule 1: 20S ribosomal RNA



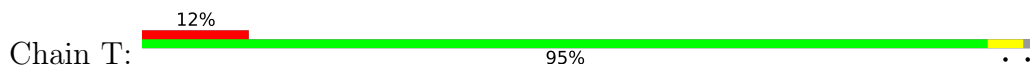




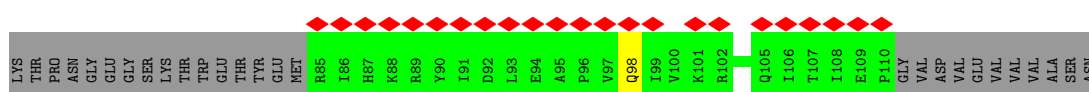
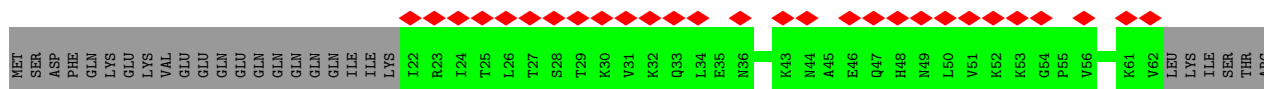
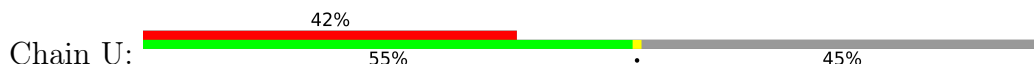
• Molecule 18: 40S ribosomal protein S18-A



• Molecule 19: 40S ribosomal protein S19-A



• Molecule 20: 40S ribosomal protein S20

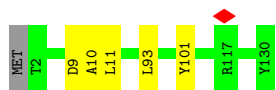


• Molecule 21: 40S ribosomal protein S21-A

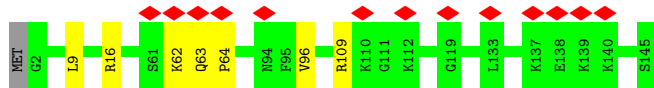


• Molecule 22: 40S ribosomal protein S22-A

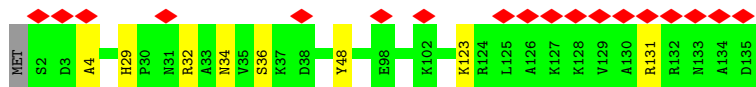
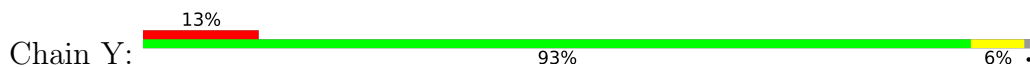




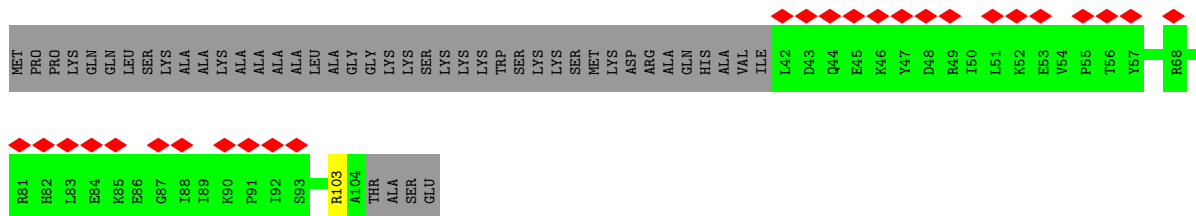
• Molecule 23: 40S ribosomal protein S23-A



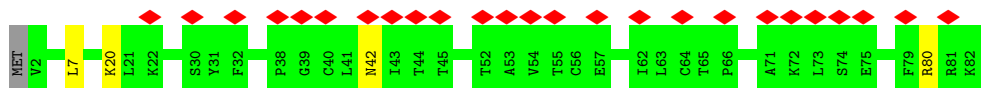
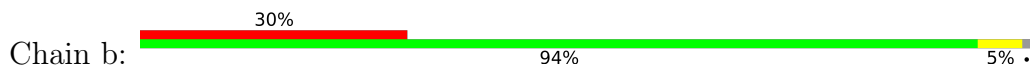
• Molecule 24: 40S ribosomal protein S24-A



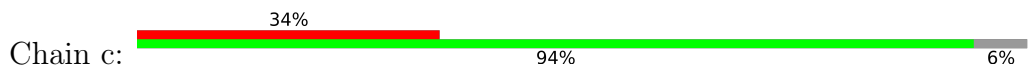
• Molecule 25: 40S ribosomal protein S25-A



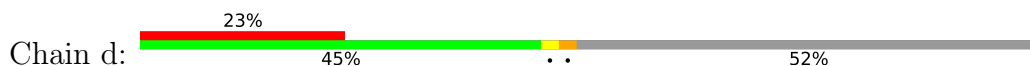
• Molecule 26: 40S ribosomal protein S27-A



• Molecule 27: 40S ribosomal protein S28-A



• Molecule 28: 40S ribosomal protein S29-A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19564	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 ($e^-/\text{\AA}^2$)	29.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.410	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	384.12003, 384.12003, 384.12003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	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: A2M

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	0.78	6/41219 (0.0%)	1.41	607/64175 (0.9%)
2	A	0.33	0/1656	0.63	1/2264 (0.0%)
3	B	0.31	0/1733	0.68	0/2329
4	C	0.32	0/1692	0.66	2/2296 (0.1%)
5	E	0.38	0/2109	0.72	1/2839 (0.0%)
6	F	0.29	0/1629	0.65	0/2202
7	G	0.33	0/1823	0.63	0/2439
8	H	0.32	0/1382	0.73	1/1857 (0.1%)
9	I	0.38	0/1514	0.65	0/2021
10	J	0.33	0/1519	0.72	1/2035 (0.0%)
11	L	0.43	0/1239	0.60	0/1673
12	M	0.31	0/942	0.70	0/1263
13	N	0.32	0/1216	0.66	0/1638
14	O	0.31	0/961	0.63	0/1290
15	P	0.37	0/1020	0.66	0/1367
16	Q	0.36	0/1011	0.78	0/1362
17	R	0.27	0/931	0.65	0/1249
18	S	0.30	0/1128	0.72	0/1518
19	T	0.31	0/1129	0.60	0/1514
20	U	0.27	0/545	0.59	0/733
21	V	0.33	0/693	0.66	0/932
22	W	0.35	0/1036	0.68	0/1393
23	X	0.36	0/1139	0.79	2/1518 (0.1%)
24	Y	0.40	0/1087	0.73	0/1449
25	Z	0.27	0/519	0.55	0/696
26	b	0.30	0/621	0.64	0/838
27	c	0.28	0/499	0.61	0/670
28	d	0.29	0/221	0.69	0/291
29	e	0.35	0/483	0.72	0/643
30	h	0.31	0/1441	0.69	0/1940
31	i	0.36	0/2179	0.76	1/2956 (0.0%)
32	j	0.29	0/470	0.64	0/632

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	l	0.32	0/2364	0.63	1/3169 (0.0%)
34	t	2.60	7/5520 (0.1%)	0.64	4/7456 (0.1%)
All	All	0.89	13/84670 (0.0%)	1.12	621/122647 (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
2	A	0	1
3	B	0	4
4	C	0	2
5	E	0	3
6	F	0	3
7	G	0	2
8	H	0	3
10	J	0	4
11	L	0	2
12	M	0	2
13	N	0	1
14	O	0	2
15	P	0	6
16	Q	0	1
17	R	0	1
18	S	0	6
19	T	0	5
20	U	0	1
21	V	0	1
22	W	0	2
23	X	0	2
24	Y	0	4
26	b	0	1
29	e	0	6
30	h	0	4
31	i	0	13
33	l	0	4
34	t	0	5
All	All	0	91

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	t	524	GLU	CB-CG	157.17	4.50	1.52
1	2	436	A2M	O3'-P	-83.60	0.60	1.61
1	2	420	A2M	O3'-P	-60.90	0.88	1.61
34	t	349	TYR	CD1-CE1	58.33	2.26	1.39
34	t	349	TYR	CD2-CE2	57.92	2.26	1.39
34	t	349	TYR	CE2-CZ	40.27	1.91	1.38
34	t	349	TYR	CE1-CZ	40.03	1.90	1.38
34	t	349	TYR	CG-CD1	32.41	1.81	1.39
34	t	349	TYR	CG-CD2	31.82	1.80	1.39
1	2	796	A2M	O3'-P	-29.45	1.25	1.61
1	2	100	A2M	O3'-P	-21.11	1.35	1.61
1	2	931	C	C5-C6	-5.91	1.29	1.34
1	2	47	A	N9-C4	5.83	1.41	1.37

All (621) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	420	A2M	P-O3'-C3'	-62.56	44.63	119.70
1	2	796	A2M	OP2-P-O3'	-35.31	27.51	105.20
1	2	436	A2M	O3'-P-O5'	-31.29	44.55	104.00
1	2	420	A2M	OP1-P-O3'	-29.92	39.37	105.20
1	2	436	A2M	P-O3'-C3'	-29.56	84.23	119.70
1	2	100	A2M	OP2-P-O3'	26.71	163.95	105.20
1	2	100	A2M	OP1-P-O3'	-26.29	47.35	105.20
1	2	796	A2M	P-O3'-C3'	-25.24	89.41	119.70
1	2	100	A2M	P-O3'-C3'	-21.76	93.59	119.70
1	2	420	A2M	OP2-P-O3'	20.54	150.39	105.20
1	2	436	A2M	OP2-P-O3'	-18.33	64.87	105.20
1	2	100	A2M	O3'-P-O5'	-15.77	74.03	104.00
1	2	436	A2M	OP1-P-O3'	13.78	135.52	105.20
1	2	1640	C	N1-C2-O2	12.34	126.30	118.90
1	2	1389	C	C2-N1-C1'	11.82	131.80	118.80
1	2	1055	U	C2-N1-C1'	11.79	131.84	117.70
1	2	1620	C	N1-C2-O2	11.40	125.74	118.90
1	2	1004	U	C2-N1-C1'	11.38	131.35	117.70
1	2	1004	U	N1-C2-O2	10.94	130.46	122.80
1	2	1056	U	C2-N1-C1'	10.76	130.61	117.70
1	2	1185	U	C2-N1-C1'	10.73	130.57	117.70
1	2	12	U	N1-C2-O2	10.39	130.07	122.80
1	2	1640	C	C2-N1-C1'	10.35	130.19	118.80
1	2	1640	C	N3-C2-O2	-10.30	114.69	121.90
1	2	12	U	N3-C2-O2	-10.29	115.00	122.20
1	2	1627	U	C5-C4-O4	-10.27	119.74	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1596	C	C2-N1-C1'	10.14	129.95	118.80
1	2	959	U	C2-N1-C1'	10.06	129.78	117.70
1	2	1000	C	O4'-C1'-N1	9.96	116.17	108.20
1	2	1082	C	N1-C2-O2	9.85	124.81	118.90
1	2	1055	U	C5-C6-N1	9.77	127.59	122.70
1	2	1004	U	N3-C2-O2	-9.73	115.39	122.20
1	2	1246	C	N1-C2-O2	9.60	124.66	118.90
1	2	1602	C	N1-C2-O2	9.60	124.66	118.90
1	2	1627	U	N3-C4-O4	9.58	126.11	119.40
1	2	1612	U	N3-C2-O2	-9.57	115.50	122.20
1	2	1389	C	N1-C2-O2	9.54	124.62	118.90
1	2	1282	U	C5-C6-N1	9.45	127.43	122.70
1	2	1527	C	N3-C2-O2	-9.44	115.29	121.90
1	2	1021	C	C2-N1-C1'	9.38	129.12	118.80
1	2	1527	C	N1-C2-O2	9.38	124.53	118.90
1	2	1612	U	N1-C2-O2	9.36	129.35	122.80
1	2	1282	U	C2-N1-C1'	9.35	128.92	117.70
1	2	614	C	N1-C2-O2	9.34	124.50	118.90
1	2	1082	C	C2-N1-C1'	9.32	129.06	118.80
1	2	68	A	P-O3'-C3'	9.32	130.88	119.70
1	2	758	U	N1-C2-O2	9.30	129.31	122.80
1	2	1620	C	N3-C2-O2	-9.22	115.45	121.90
1	2	1006	C	C2-N1-C1'	9.21	128.93	118.80
1	2	1185	U	N1-C2-O2	9.19	129.23	122.80
1	2	758	U	C2-N1-C1'	9.16	128.69	117.70
1	2	418	G	N3-C4-N9	9.15	131.49	126.00
1	2	1389	C	C6-N1-C2	-9.05	116.68	120.30
1	2	758	U	N3-C2-O2	-9.04	115.87	122.20
1	2	1509	C	N1-C2-O2	8.98	124.29	118.90
1	2	575	C	N1-C2-O2	8.95	124.27	118.90
1	2	1185	U	N3-C2-O2	-8.94	115.94	122.20
1	2	453	U	N1-C2-O2	8.81	128.97	122.80
1	2	1055	U	C6-N1-C2	-8.80	115.72	121.00
1	2	1055	U	N3-C2-O2	-8.71	116.10	122.20
1	2	237	C	N1-C2-O2	8.65	124.09	118.90
1	2	1389	C	N3-C2-O2	-8.64	115.85	121.90
1	2	532	U	N3-C2-O2	-8.49	116.25	122.20
1	2	453	U	N3-C2-O2	-8.48	116.27	122.20
1	2	1612	U	C2-N1-C1'	8.47	127.87	117.70
1	2	1620	C	C2-N1-C1'	8.46	128.11	118.80
1	2	1220	C	C6-N1-C2	-8.41	116.93	120.30
1	2	229	U	C2-N1-C1'	8.40	127.78	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1733	C	C2-N1-C1'	8.40	128.03	118.80
1	2	1585	U	N3-C2-O2	-8.37	116.34	122.20
1	2	190	C	N3-C2-O2	-8.37	116.04	121.90
1	2	38	C	N1-C2-O2	8.31	123.89	118.90
1	2	959	U	N3-C2-O2	-8.26	116.42	122.20
1	2	1494	C	C2-N1-C1'	8.20	127.81	118.80
1	2	1006	C	N1-C2-O2	8.16	123.80	118.90
1	2	1585	U	N1-C2-O2	8.14	128.50	122.80
1	2	532	U	N1-C2-O2	8.12	128.48	122.80
1	2	1403	C	C2-N1-C1'	8.09	127.70	118.80
1	2	702	G	C6-C5-N7	-8.06	125.57	130.40
1	2	283	U	N3-C2-O2	-8.05	116.56	122.20
1	2	1494	C	N1-C2-O2	7.95	123.67	118.90
1	2	191	C	N1-C2-O2	7.94	123.67	118.90
1	2	1772	C	C2-N1-C1'	7.93	127.52	118.80
1	2	959	U	N1-C2-O2	7.86	128.31	122.80
1	2	1066	C	N3-C2-O2	-7.83	116.42	121.90
1	2	1246	C	N3-C2-O2	-7.82	116.42	121.90
1	2	185	U	N3-C2-O2	-7.81	116.73	122.20
1	2	931	C	C5-C4-N4	-7.80	114.74	120.20
1	2	229	U	N1-C2-O2	7.79	128.26	122.80
1	2	283	U	N1-C2-O2	7.79	128.25	122.80
1	2	1307	U	C2-N1-C1'	7.79	127.05	117.70
1	2	1489	U	C2-N1-C1'	7.79	127.05	117.70
1	2	1082	C	N3-C2-O2	-7.78	116.45	121.90
1	2	241	U	N1-C2-O2	7.76	128.23	122.80
1	2	189	C	N1-C2-O2	7.75	123.55	118.90
1	2	47	A	C2-N3-C4	7.73	114.47	110.60
1	2	1389	C	C6-N1-C1'	-7.73	111.52	120.80
1	2	1501	C	C5-C6-N1	7.68	124.84	121.00
1	2	1489	U	N1-C2-O2	7.67	128.17	122.80
1	2	1509	C	N3-C2-O2	-7.66	116.54	121.90
1	2	558	U	N3-C2-O2	-7.65	116.84	122.20
1	2	1055	U	N1-C2-O2	7.65	128.16	122.80
1	2	1004	U	C6-N1-C1'	-7.64	110.50	121.20
1	2	1246	C	C2-N1-C1'	7.62	127.18	118.80
1	2	1596	C	C5-C6-N1	7.62	124.81	121.00
1	2	1501	C	C6-N1-C2	-7.60	117.26	120.30
34	t	524	GLU	CA-CB-CG	7.58	130.09	113.40
1	2	1378	U	N3-C2-O2	-7.57	116.90	122.20
1	2	519	C	N1-C2-O2	7.55	123.43	118.90
1	2	277	U	N1-C2-O2	7.53	128.07	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	283	U	C2-N1-C1'	7.53	126.74	117.70
1	2	796	A2M	O3'-P-O5'	7.51	118.27	104.00
1	2	185	U	N1-C2-O2	7.51	128.06	122.80
1	2	558	U	N1-C2-O2	7.51	128.06	122.80
1	2	1317	C	N1-C2-O2	7.51	123.41	118.90
1	2	238	U	C2-N1-C1'	7.51	126.71	117.70
1	2	1530	C	N1-C2-O2	7.49	123.40	118.90
1	2	418	G	N3-C4-C5	-7.47	124.86	128.60
1	2	1332	C	N1-C2-O2	7.46	123.38	118.90
1	2	519	C	N3-C2-O2	-7.45	116.69	121.90
1	2	1596	C	C6-N1-C1'	-7.43	111.89	120.80
1	2	484	C	C2-N1-C1'	7.41	126.94	118.80
1	2	229	U	N3-C2-O2	-7.40	117.02	122.20
1	2	1530	C	C2-N1-C1'	7.38	126.91	118.80
1	2	1596	C	N1-C2-O2	7.37	123.32	118.90
1	2	418	G	C4-N9-C1'	7.37	136.08	126.50
1	2	1640	C	C6-N1-C2	-7.35	117.36	120.30
1	2	241	U	C2-N1-C1'	7.35	126.52	117.70
1	2	931	C	N3-C4-C5	7.34	124.84	121.90
1	2	12	U	C2-N1-C1'	7.30	126.46	117.70
1	2	1560	U	C2-N1-C1'	7.30	126.47	117.70
1	2	1646	C	N1-C2-O2	7.28	123.27	118.90
1	2	1021	C	C5-C6-N1	7.28	124.64	121.00
1	2	1153	G	C4-N9-C1'	7.27	135.95	126.50
1	2	1489	U	N3-C2-O2	-7.26	117.12	122.20
1	2	1378	U	C2-N1-C1'	7.25	126.41	117.70
1	2	566	C	C5-C6-N1	7.25	124.63	121.00
1	2	1378	U	N1-C2-O2	7.25	127.87	122.80
1	2	277	U	N3-C2-O2	-7.24	117.14	122.20
1	2	614	C	C2-N1-C1'	7.23	126.75	118.80
1	2	1056	U	C6-N1-C1'	-7.22	111.09	121.20
1	2	1246	C	C6-N1-C2	-7.22	117.41	120.30
1	2	1257	U	C2-N1-C1'	7.22	126.36	117.70
31	i	283	LEU	CA-CB-CG	7.22	131.90	115.30
1	2	614	C	N3-C2-O2	-7.21	116.85	121.90
1	2	237	C	N3-C2-O2	-7.19	116.86	121.90
1	2	873	U	N1-C2-O2	7.19	127.83	122.80
1	2	1148	C	N1-C2-O2	7.18	123.21	118.90
1	2	1021	C	C6-N1-C2	-7.17	117.43	120.30
1	2	101	U	N3-C2-O2	-7.15	117.19	122.20
1	2	1153	G	C6-C5-N7	-7.11	126.13	130.40
1	2	873	U	C2-N1-C1'	7.11	126.23	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1148	C	C2-N1-C1'	7.09	126.60	118.80
1	2	1220	C	C5-C6-N1	7.06	124.53	121.00
1	2	702	G	N3-C4-N9	7.05	130.23	126.00
1	2	339	C	C2-N1-C1'	7.05	126.56	118.80
1	2	68	A	OP1-P-O3'	7.04	120.69	105.20
1	2	682	C	N1-C2-O2	7.03	123.12	118.90
1	2	241	U	N3-C2-O2	-7.03	117.28	122.20
1	2	587	C	C2-N1-C1'	7.02	126.52	118.80
1	2	1253	U	N1-C2-O2	7.01	127.71	122.80
1	2	184	C	C2-N1-C1'	7.00	126.50	118.80
1	2	1669	U	N3-C2-O2	-6.99	117.31	122.20
1	2	1432	U	C2-N1-C1'	6.98	126.07	117.70
1	2	238	U	N1-C2-O2	6.97	127.68	122.80
1	2	1640	C	C6-N1-C1'	-6.96	112.45	120.80
10	J	93	LEU	CA-CB-CG	6.96	131.30	115.30
1	2	414	C	N1-C2-O2	6.95	123.07	118.90
1	2	1082	C	C6-N1-C1'	-6.95	112.47	120.80
1	2	1153	G	N3-C4-N9	6.93	130.16	126.00
1	2	558	U	C2-N1-C1'	6.92	126.01	117.70
1	2	297	U	N3-C2-O2	-6.91	117.36	122.20
1	2	35	U	C2-N1-C1'	6.90	125.98	117.70
1	2	418	G	C8-N9-C1'	-6.89	118.04	127.00
1	2	1498	G	N7-C8-N9	6.89	116.55	113.10
1	2	1659	A	O4'-C1'-N9	6.87	113.69	108.20
1	2	104	A	P-O3'-C3'	6.86	127.93	119.70
1	2	1185	U	C6-N1-C1'	-6.86	111.60	121.20
1	2	1733	C	N1-C2-O2	6.85	123.01	118.90
23	X	9	LEU	CA-CB-CG	6.84	131.04	115.30
1	2	1494	C	C6-N1-C2	-6.83	117.57	120.30
1	2	1560	U	N1-C2-O2	6.80	127.56	122.80
1	2	238	U	N3-C2-O2	-6.78	117.45	122.20
1	2	531	C	N1-C2-O2	6.75	122.95	118.90
1	2	1040	G	N3-C4-N9	-6.75	121.95	126.00
1	2	101	U	N1-C2-O2	6.75	127.52	122.80
1	2	1160	A	C6-N1-C2	-6.74	114.55	118.60
1	2	1620	C	C6-N1-C2	-6.74	117.61	120.30
1	2	575	C	N3-C2-O2	-6.73	117.19	121.90
1	2	633	U	N1-C2-O2	6.72	127.51	122.80
1	2	1455	G	C4-N9-C1'	6.72	135.24	126.50
1	2	1253	U	C2-N1-C1'	6.71	125.75	117.70
1	2	946	U	N1-C2-O2	6.71	127.50	122.80
1	2	1056	U	N1-C2-O2	6.71	127.50	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1327	C	N3-C2-O2	-6.70	117.21	121.90
1	2	1154	G	C4-N9-C1'	6.70	135.21	126.50
1	2	1148	C	C5-C6-N1	6.69	124.35	121.00
1	2	149	C	C2-N1-C1'	6.68	126.15	118.80
1	2	1201	G	C4-C5-N7	6.67	113.47	110.80
1	2	1100	G	N3-C4-N9	6.66	130.00	126.00
2	A	150	ASP	C-N-CA	6.66	138.35	121.70
1	2	1455	G	N3-C4-N9	6.66	130.00	126.00
1	2	543	C	O5'-P-OP1	-6.66	99.71	105.70
1	2	1039	A	O4'-C1'-N9	6.65	113.52	108.20
1	2	1573	A	P-O3'-C3'	6.65	127.67	119.70
1	2	1201	G	N1-C6-O6	6.62	123.88	119.90
1	2	82	U	N1-C2-O2	6.61	127.43	122.80
1	2	929	A	N7-C8-N9	6.60	117.10	113.80
1	2	831	U	N1-C2-O2	6.58	127.40	122.80
1	2	1257	U	N1-C2-O2	6.56	127.39	122.80
1	2	1427	A	P-O3'-C3'	6.55	127.57	119.70
1	2	633	U	N3-C2-O2	-6.54	117.62	122.20
1	2	1271	G	C4-N9-C1'	-6.54	118.00	126.50
1	2	1153	G	C8-N9-C1'	-6.52	118.53	127.00
1	2	1006	C	C6-N1-C1'	-6.51	112.99	120.80
1	2	1389	C	C5-C6-N1	6.50	124.25	121.00
1	2	400	A	P-O3'-C3'	6.50	127.50	119.70
1	2	584	C	C5-C6-N1	6.49	124.24	121.00
1	2	927	C	C6-N1-C2	-6.48	117.71	120.30
1	2	862	A	P-O3'-C3'	6.48	127.47	119.70
1	2	1403	C	N1-C2-O2	6.47	122.78	118.90
1	2	149	C	N1-C2-O2	6.46	122.78	118.90
1	2	1168	U	C5-C6-N1	6.46	125.93	122.70
1	2	1165	G	N7-C8-N9	6.46	116.33	113.10
1	2	1056	U	N3-C4-O4	6.45	123.92	119.40
1	2	502	U	C5-C6-N1	6.45	125.92	122.70
1	2	937	C	N1-C2-O2	6.44	122.77	118.90
1	2	1498	G	C4-C5-N7	6.44	113.38	110.80
1	2	120	U	N3-C2-O2	-6.44	117.69	122.20
1	2	873	U	N3-C2-O2	-6.43	117.70	122.20
1	2	1456	C	C2-N1-C1'	6.43	125.88	118.80
1	2	1432	U	N3-C2-O2	-6.43	117.70	122.20
1	2	1253	U	N3-C2-O2	-6.42	117.70	122.20
1	2	1154	G	N3-C4-N9	6.42	129.85	126.00
1	2	303	U	N1-C2-O2	6.39	127.28	122.80
1	2	1332	C	C2-N1-C1'	6.39	125.83	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1059	U	N1-C2-O2	6.39	127.27	122.80
1	2	1056	U	C5-C6-N1	6.38	125.89	122.70
1	2	1252	C	C6-N1-C2	-6.38	117.75	120.30
1	2	38	C	N3-C2-O2	-6.37	117.44	121.90
1	2	1757	G	N3-C4-N9	6.35	129.81	126.00
1	2	1282	U	N1-C2-O2	6.34	127.24	122.80
1	2	626	U	N1-C2-O2	6.33	127.23	122.80
1	2	1560	U	N3-C2-O2	-6.32	117.78	122.20
1	2	838	G	N3-C4-N9	6.32	129.79	126.00
1	2	277	U	C2-N1-C1'	6.31	125.27	117.70
1	2	1502	G	C6-C5-N7	-6.29	126.62	130.40
1	2	1055	U	C6-N1-C1'	-6.29	112.39	121.20
1	2	1657	U	N3-C2-O2	-6.28	117.80	122.20
1	2	1201	G	C5-C6-O6	-6.28	124.83	128.60
1	2	5	U	N3-C2-O2	-6.27	117.81	122.20
1	2	1271	G	N3-C4-N9	-6.27	122.24	126.00
1	2	1040	G	C6-C5-N7	6.26	134.16	130.40
1	2	1602	C	N3-C2-O2	-6.25	117.53	121.90
1	2	1021	C	C6-N1-C1'	-6.24	113.31	120.80
1	2	1040	G	C4-N9-C1'	-6.24	118.39	126.50
1	2	682	C	N3-C2-O2	-6.23	117.54	121.90
1	2	297	U	N1-C2-O2	6.23	127.16	122.80
1	2	1177	C	C6-N1-C2	-6.23	117.81	120.30
1	2	1066	C	N1-C2-O2	6.22	122.63	118.90
1	2	35	U	C5-C6-N1	6.22	125.81	122.70
1	2	1627	U	C5-C6-N1	6.20	125.80	122.70
1	2	626	U	C2-N1-C1'	6.20	125.14	117.70
1	2	550	A	N1-C2-N3	6.17	132.39	129.30
1	2	1257	U	N3-C2-O2	-6.17	117.88	122.20
1	2	1174	C	N1-C2-O2	6.16	122.60	118.90
1	2	1271	G	C8-N9-C1'	6.16	135.01	127.00
1	2	1021	C	N1-C2-O2	6.14	122.58	118.90
1	2	1600	A	P-O3'-C3'	6.14	127.07	119.70
1	2	965	U	N3-C2-O2	-6.14	117.90	122.20
1	2	1174	C	C5-C6-N1	6.14	124.07	121.00
1	2	476	U	C5-C6-N1	6.13	125.77	122.70
1	2	1566	U	C5-C6-N1	6.13	125.76	122.70
1	2	819	G	P-O3'-C3'	6.12	127.05	119.70
1	2	1006	C	N3-C2-O2	-6.12	117.61	121.90
1	2	1059	U	N3-C2-O2	-6.12	117.92	122.20
1	2	1237	G	C4-N9-C1'	6.12	134.45	126.50
1	2	517	U	N3-C2-O2	-6.11	117.92	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1427	A	OP2-P-O3'	6.11	118.64	105.20
1	2	297	U	C2-N1-C1'	6.10	125.02	117.70
1	2	1495	C	C6-N1-C2	-6.10	117.86	120.30
1	2	1733	C	C6-N1-C1'	-6.09	113.49	120.80
1	2	1040	G	C8-N9-C1'	6.09	134.92	127.00
1	2	557	G	N3-C4-C5	-6.08	125.56	128.60
1	2	1494	C	N3-C2-O2	-6.07	117.65	121.90
1	2	633	U	C2-N1-C1'	6.05	124.96	117.70
1	2	1398	U	N3-C2-O2	-6.05	117.96	122.20
1	2	1072	C	N3-C2-O2	-6.05	117.67	121.90
1	2	1398	U	C5-C6-N1	6.05	125.72	122.70
1	2	1646	C	N3-C2-O2	-6.04	117.67	121.90
1	2	1317	C	N3-C2-O2	-6.04	117.67	121.90
1	2	1669	U	N1-C2-O2	6.04	127.03	122.80
1	2	686	C	N1-C2-O2	6.04	122.52	118.90
1	2	1627	U	C2-N1-C1'	6.03	124.94	117.70
1	2	981	U	N3-C2-O2	-6.03	117.98	122.20
34	t	349	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	2	514	G	N9-C1'-C2'	-6.01	105.39	112.00
1	2	959	U	C6-N1-C1'	-6.01	112.79	121.20
1	2	1153	G	C4-C5-N7	6.01	113.20	110.80
1	2	339	C	C5-C6-N1	6.00	124.00	121.00
1	2	1185	U	C5-C6-N1	6.00	125.70	122.70
1	2	819	G	O4'-C1'-N9	6.00	113.00	108.20
1	2	1653	C	C6-N1-C2	-6.00	117.90	120.30
1	2	758	U	C5-C6-N1	5.99	125.69	122.70
1	2	469	C	N1-C2-O2	5.99	122.49	118.90
1	2	959	U	C6-N1-C2	-5.99	117.41	121.00
1	2	1056	U	N3-C2-O2	-5.99	118.01	122.20
1	2	519	C	C2-N1-C1'	5.98	125.38	118.80
1	2	303	U	N3-C2-O2	-5.98	118.01	122.20
1	2	1066	C	C6-N1-C2	-5.98	117.91	120.30
1	2	400	A	OP2-P-O3'	5.97	118.34	105.20
1	2	575	C	C2-N1-C1'	5.96	125.36	118.80
1	2	482	U	C5-C6-N1	5.96	125.68	122.70
1	2	1455	G	N3-C4-C5	-5.96	125.62	128.60
1	2	35	U	N1-C2-O2	5.94	126.96	122.80
1	2	1432	U	N1-C2-O2	5.94	126.96	122.80
1	2	1600	A	N1-C6-N6	5.94	122.16	118.60
1	2	517	U	N1-C2-O2	5.93	126.95	122.80
1	2	1086	A	P-O3'-C3'	5.92	126.80	119.70
1	2	144	U	C2-N1-C1'	5.91	124.80	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1428	G	O5'-P-OP2	-5.89	100.39	105.70
1	2	237	C	C6-N1-C2	-5.89	117.94	120.30
1	2	1455	G	C8-N9-C1'	-5.88	119.36	127.00
1	2	1625	C	C5-C6-N1	5.88	123.94	121.00
1	2	800	U	N1-C2-O2	5.87	126.91	122.80
1	2	743	U	C2-N1-C1'	5.87	124.74	117.70
1	2	387	A	P-O3'-C3'	5.86	126.74	119.70
1	2	1004	U	C5-C6-N1	5.86	125.63	122.70
1	2	1332	C	N3-C2-O2	-5.86	117.80	121.90
1	2	702	G	C4-N9-C1'	5.86	134.11	126.50
5	E	193	GLY	N-CA-C	5.85	127.73	113.10
1	2	1157	A	N1-C6-N6	-5.85	115.09	118.60
1	2	1309	C	N1-C2-O2	5.84	122.41	118.90
1	2	1529	C	C6-N1-C2	-5.84	117.96	120.30
1	2	1600	A	OP1-P-O3'	5.84	118.04	105.20
1	2	1063	U	C5-C4-O4	5.83	129.40	125.90
1	2	1100	G	N3-C4-C5	-5.82	125.69	128.60
1	2	515	A	N7-C8-N9	5.82	116.71	113.80
1	2	1772	C	C6-N1-C2	-5.81	117.98	120.30
1	2	1783	C	N1-C2-O2	5.81	122.38	118.90
1	2	1168	U	C2-N1-C1'	5.81	124.67	117.70
1	2	532	U	C2-N1-C1'	5.80	124.67	117.70
1	2	965	U	N1-C2-O2	5.80	126.86	122.80
1	2	1201	G	C6-C5-N7	-5.80	126.92	130.40
1	2	1160	A	O4'-C1'-N9	5.79	112.83	108.20
8	H	154	LEU	CA-CB-CG	5.79	128.62	115.30
1	2	305	C	C5-C6-N1	5.79	123.89	121.00
1	2	1270	G	N9-C4-C5	5.78	107.71	105.40
1	2	1403	C	C6-N1-C2	-5.78	117.99	120.30
1	2	166	C	N1-C2-O2	5.77	122.36	118.90
1	2	1398	U	N1-C2-O2	5.77	126.84	122.80
1	2	931	C	N1-C2-O2	5.76	122.36	118.90
34	t	646	LEU	CA-CB-CG	5.76	128.55	115.30
1	2	184	C	C5-C6-N1	5.76	123.88	121.00
1	2	453	U	C2-N1-C1'	5.75	124.60	117.70
23	X	63	GLN	C-N-CD	-5.75	107.96	120.60
1	2	484	C	C6-N1-C2	-5.74	118.01	120.30
1	2	1398	U	C6-N1-C2	-5.73	117.56	121.00
1	2	1751	C	N1-C2-O2	5.73	122.34	118.90
1	2	1332	C	C6-N1-C2	-5.73	118.01	120.30
1	2	542	A	OP1-P-O3'	5.73	117.80	105.20
1	2	1684	U	C2-N1-C1'	5.72	124.57	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	469	C	N3-C2-O2	-5.72	117.90	121.90
1	2	1006	C	C6-N1-C2	-5.71	118.01	120.30
1	2	1657	U	N1-C2-O2	5.71	126.80	122.80
1	2	561	G	C4-N9-C1'	5.71	133.93	126.50
1	2	1174	C	C2-N1-C1'	5.71	125.08	118.80
1	2	50	C	N1-C2-O2	5.70	122.32	118.90
1	2	190	C	C6-N1-C2	-5.70	118.02	120.30
1	2	1263	G	C4-C5-N7	5.70	113.08	110.80
1	2	1246	C	C5-C6-N1	5.70	123.85	121.00
1	2	1270	G	N3-C4-N9	-5.70	122.58	126.00
1	2	191	C	N3-C2-O2	-5.70	117.91	121.90
1	2	848	C	N3-C2-O2	-5.69	117.91	121.90
1	2	1474	G	C6-C5-N7	-5.69	126.98	130.40
1	2	1564	U	C2-N1-C1'	5.69	124.53	117.70
1	2	82	U	N3-C2-O2	-5.68	118.22	122.20
1	2	584	C	C2-N1-C1'	5.68	125.05	118.80
1	2	1070	C	O4'-C1'-N1	5.68	112.74	108.20
1	2	1643	U	N1-C2-O2	5.67	126.77	122.80
1	2	418	G	C2-N3-C4	5.67	114.74	111.90
1	2	990	C	C2-N1-C1'	5.67	125.04	118.80
1	2	1034	C	C6-N1-C2	-5.67	118.03	120.30
1	2	1282	U	C6-N1-C1'	-5.66	113.27	121.20
1	2	838	G	C4-N9-C1'	5.66	133.86	126.50
1	2	184	C	C6-N1-C2	-5.66	118.04	120.30
1	2	1494	C	C5-C6-N1	5.66	123.83	121.00
1	2	1548	G	C4-N9-C1'	5.66	133.86	126.50
1	2	484	C	N1-C2-O2	5.65	122.29	118.90
1	2	489	C	N1-C2-O2	5.64	122.28	118.90
1	2	1549	C	C6-N1-C2	-5.64	118.04	120.30
1	2	1723	U	C5-C6-N1	5.64	125.52	122.70
1	2	1646	C	C6-N1-C2	-5.64	118.04	120.30
1	2	1528	U	C5-C6-N1	5.63	125.52	122.70
1	2	1498	G	C5-N7-C8	-5.62	101.49	104.30
1	2	230	C	C6-N1-C2	-5.62	118.05	120.30
1	2	120	U	N1-C2-O2	5.61	126.73	122.80
1	2	1034	C	C5-C6-N1	5.60	123.80	121.00
1	2	758	U	C6-N1-C1'	-5.60	113.36	121.20
1	2	1153	G	N7-C8-N9	5.60	115.90	113.10
1	2	929	A	C4-N9-C1'	5.59	136.37	126.30
1	2	1059	U	C5-C6-N1	5.59	125.50	122.70
1	2	1154	G	C8-N9-C1'	-5.59	119.73	127.00
1	2	484	C	C5-C6-N1	5.58	123.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1452	U	C5-C6-N1	5.58	125.49	122.70
1	2	1307	U	N1-C2-O2	5.58	126.70	122.80
1	2	519	C	C6-N1-C2	-5.57	118.07	120.30
1	2	1366	U	C5-C6-N1	5.57	125.49	122.70
1	2	1474	G	N7-C8-N9	5.56	115.88	113.10
1	2	1529	C	C2-N1-C1'	5.56	124.92	118.80
1	2	1474	G	C4-N9-C1'	5.56	133.73	126.50
1	2	1040	G	N9-C4-C5	5.55	107.62	105.40
1	2	1403	C	C5-C6-N1	5.55	123.78	121.00
1	2	1282	U	C6-N1-C2	-5.55	117.67	121.00
1	2	796	A2M	OP1-P-O3'	-5.55	92.99	105.20
1	2	1006	C	C5-C6-N1	5.55	123.77	121.00
1	2	1100	G	C2-N3-C4	5.55	114.67	111.90
1	2	819	G	OP2-P-O3'	5.54	117.40	105.20
1	2	1153	G	N9-C4-C5	-5.54	103.18	105.40
1	2	1120	U	N1-C2-O2	5.54	126.68	122.80
1	2	120	U	C2-N1-C1'	5.54	124.34	117.70
1	2	1022	C	N1-C2-O2	5.53	122.22	118.90
1	2	1684	U	N3-C2-O2	-5.53	118.33	122.20
1	2	568	G	N3-C4-N9	5.53	129.32	126.00
1	2	1498	G	C8-N9-C4	-5.53	104.19	106.40
1	2	243	G	N7-C8-N9	5.52	115.86	113.10
1	2	1403	C	C6-N1-C1'	-5.52	114.17	120.80
1	2	1620	C	C6-N1-C1'	-5.52	114.17	120.80
1	2	280	U	P-O3'-C3'	5.52	126.33	119.70
1	2	230	C	C5-C6-N1	5.52	123.76	121.00
1	2	561	G	C8-N9-C1'	-5.52	119.83	127.00
1	2	1772	C	C5-C6-N1	5.51	123.75	121.00
1	2	1063	U	N3-C2-O2	-5.50	118.35	122.20
1	2	587	C	N1-C2-O2	5.50	122.20	118.90
1	2	1591	C	C5-C6-N1	5.50	123.75	121.00
1	2	596	C	C5-C6-N1	5.49	123.75	121.00
1	2	1307	U	C6-N1-C1'	-5.49	113.51	121.20
1	2	555	A	C4-N9-C1'	5.48	136.17	126.30
1	2	831	U	N3-C2-O2	-5.48	118.37	122.20
1	2	174	U	N3-C2-O2	-5.47	118.37	122.20
1	2	1063	U	N3-C4-O4	-5.47	115.57	119.40
1	2	799	A	C2-N3-C4	5.47	113.33	110.60
1	2	172	C	N1-C2-O2	5.46	122.18	118.90
1	2	1289	U	N3-C2-O2	-5.46	118.38	122.20
1	2	1252	C	C2-N1-C1'	5.46	124.80	118.80
1	2	1041	G	N3-C4-N9	-5.45	122.73	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1022	C	C2-N1-C1'	5.45	124.79	118.80
1	2	875	G	O4'-C1'-N9	5.45	112.56	108.20
1	2	946	U	N3-C2-O2	-5.44	118.39	122.20
1	2	1070	C	C2-N1-C1'	-5.44	112.82	118.80
1	2	1596	C	C6-N1-C2	-5.43	118.13	120.30
1	2	1787	C	C6-N1-C2	-5.43	118.13	120.30
1	2	885	G	C8-N9-C4	-5.43	104.23	106.40
1	2	149	C	C6-N1-C2	-5.43	118.13	120.30
1	2	321	C	OP1-P-O3'	5.42	117.13	105.20
1	2	702	G	N9-C4-C5	-5.42	103.23	105.40
1	2	686	C	N3-C2-O2	-5.42	118.11	121.90
4	C	240	LEU	CA-CB-CG	5.42	127.76	115.30
1	2	132	U	O4'-C1'-N1	5.42	112.53	108.20
1	2	1398	U	C2-N1-C1'	5.42	124.20	117.70
1	2	106	U	N3-C2-O2	-5.41	118.41	122.20
1	2	303	U	C2-N1-C1'	5.41	124.19	117.70
1	2	267	U	N3-C2-O2	-5.40	118.42	122.20
1	2	1684	U	N1-C2-O2	5.40	126.58	122.80
1	2	106	U	N1-C2-O2	5.40	126.58	122.80
1	2	1612	U	C6-N1-C2	-5.39	117.76	121.00
1	2	514	G	C3'-C2'-C1'	5.39	105.81	101.50
1	2	394	C	C6-N1-C2	-5.39	118.14	120.30
1	2	1154	G	C6-C5-N7	-5.38	127.17	130.40
1	2	1498	G	C6-C5-N7	-5.38	127.17	130.40
1	2	440	U	C2-N3-C4	-5.38	123.77	127.00
1	2	387	A	OP2-P-O3'	5.37	117.01	105.20
1	2	1070	C	C6-N1-C1'	5.37	127.24	120.80
1	2	1148	C	C6-N1-C2	-5.37	118.15	120.30
1	2	1640	C	C5-C6-N1	5.37	123.68	121.00
1	2	1309	C	N3-C2-O2	-5.36	118.15	121.90
1	2	1757	G	C8-N9-C1'	-5.36	120.03	127.00
1	2	1772	C	C6-N1-C1'	-5.36	114.37	120.80
1	2	702	G	C8-N9-C1'	-5.36	120.04	127.00
1	2	1023	A	O4'-C1'-N9	5.36	112.48	108.20
1	2	1150	G	N3-C4-N9	5.35	129.21	126.00
1	2	1502	G	N7-C8-N9	5.35	115.78	113.10
1	2	1548	G	N3-C4-C5	-5.35	125.92	128.60
1	2	1040	G	C4-C5-N7	-5.35	108.66	110.80
1	2	743	U	C5-C6-N1	5.35	125.37	122.70
1	2	1304	G	N3-C4-N9	5.35	129.21	126.00
34	t	349	TYR	CD1-CG-CD2	5.35	123.78	117.90
1	2	174	U	C2-N1-C1'	5.34	124.11	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1309	C	C2-N1-C1'	5.34	124.68	118.80
1	2	1644	C	C5-C6-N1	5.34	123.67	121.00
1	2	294	C	C6-N1-C2	-5.34	118.16	120.30
1	2	1441	C	C6-N1-C2	-5.33	118.17	120.30
1	2	1192	C	N1-C2-O2	5.33	122.10	118.90
1	2	1024	U	C2-N1-C1'	5.33	124.09	117.70
1	2	339	C	C6-N1-C2	-5.33	118.17	120.30
1	2	185	U	C2-N1-C1'	5.32	124.08	117.70
1	2	38	C	C2-N1-C1'	5.32	124.65	118.80
1	2	965	U	C2-N1-C1'	5.32	124.08	117.70
1	2	614	C	C5-C6-N1	5.31	123.66	121.00
1	2	1185	U	C6-N1-C2	-5.31	117.81	121.00
1	2	1317	C	C2-N1-C1'	5.31	124.64	118.80
1	2	1625	C	N1-C2-O2	5.31	122.09	118.90
1	2	555	A	C8-N9-C1'	-5.31	118.14	127.70
1	2	47	A	N3-C4-C5	-5.30	123.09	126.80
1	2	1772	C	N1-C2-O2	5.30	122.08	118.90
1	2	1263	G	N9-C4-C5	-5.30	103.28	105.40
1	2	885	G	N1-C6-O6	-5.30	116.72	119.90
1	2	1433	G	C4-N9-C1'	5.30	133.39	126.50
1	2	614	C	C6-N1-C2	-5.30	118.18	120.30
1	2	1154	G	N3-C4-C5	-5.29	125.95	128.60
1	2	1174	C	C6-N1-C2	-5.29	118.18	120.30
1	2	440	U	N1-C2-N3	5.29	118.07	114.90
1	2	883	C	N1-C2-O2	5.29	122.07	118.90
1	2	1165	G	C4-N9-C1'	5.29	133.38	126.50
1	2	5	U	N1-C2-O2	5.29	126.50	122.80
1	2	487	G	N7-C8-N9	5.27	115.74	113.10
1	2	449	C	C6-N1-C2	-5.26	118.19	120.30
1	2	1474	G	N3-C4-N9	5.26	129.16	126.00
1	2	800	U	N3-C2-O2	-5.26	118.52	122.20
1	2	959	U	C5-C6-N1	5.25	125.33	122.70
1	2	47	A	N3-C4-N9	5.25	131.60	127.40
1	2	229	U	C5-C6-N1	5.25	125.33	122.70
1	2	1094	G	C8-N9-C1'	-5.25	120.17	127.00
1	2	682	C	C6-N1-C2	-5.24	118.20	120.30
1	2	1150	G	N3-C4-C5	-5.24	125.98	128.60
1	2	1379	C	C5-C6-N1	5.24	123.62	121.00
1	2	626	U	N3-C2-O2	-5.23	118.54	122.20
1	2	1094	G	N3-C4-N9	5.23	129.14	126.00
1	2	1304	G	N3-C4-C5	-5.23	125.98	128.60
1	2	1304	G	C4-N9-C1'	5.23	133.30	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1041	G	P-O3'-C3'	5.23	125.98	119.70
1	2	189	C	N3-C2-O2	-5.23	118.24	121.90
1	2	405	C	N3-C2-O2	-5.23	118.24	121.90
1	2	557	G	C4-N9-C1'	5.22	133.29	126.50
1	2	1660	A	N9-C4-C5	5.22	107.89	105.80
1	2	1530	C	C6-N1-C1'	-5.22	114.54	120.80
1	2	1056	U	C6-N1-C2	-5.22	117.87	121.00
1	2	561	G	N3-C4-N9	5.21	129.13	126.00
1	2	1757	G	C4-N9-C1'	5.21	133.28	126.50
1	2	1176	G	O4'-C1'-N9	5.21	112.37	108.20
33	1	295	LEU	CA-CB-CG	5.21	127.29	115.30
1	2	1201	G	N7-C8-N9	5.21	115.70	113.10
1	2	1494	C	C6-N1-C1'	-5.21	114.55	120.80
1	2	1354	G	C4-N9-C1'	5.20	133.26	126.50
1	2	1354	G	N3-C4-N9	5.20	129.12	126.00
1	2	1619	C	O5'-P-OP1	-5.20	101.02	105.70
1	2	352	A	P-O3'-C3'	5.20	125.94	119.70
4	C	58	LEU	CA-CB-CG	5.19	127.25	115.30
1	2	1528	U	C2-N1-C1'	5.19	123.93	117.70
1	2	1051	G	C4-N9-C1'	5.19	133.24	126.50
1	2	1600	A	C5-C6-N6	-5.18	119.55	123.70
1	2	262	U	N1-C2-O2	5.18	126.42	122.80
1	2	758	U	C6-N1-C2	-5.17	117.90	121.00
1	2	557	G	N3-C4-N9	5.17	129.10	126.00
1	2	562	G	N3-C4-N9	5.17	129.10	126.00
1	2	1625	C	C6-N1-C2	-5.17	118.23	120.30
1	2	1024	U	N3-C2-O2	-5.17	118.58	122.20
1	2	230	C	C2-N1-C1'	5.16	124.48	118.80
1	2	1612	U	C5-C6-N1	5.16	125.28	122.70
1	2	237	C	C2-N1-C1'	5.15	124.47	118.80
1	2	1059	U	C2-N1-C1'	5.15	123.88	117.70
1	2	1574	G	C8-N9-C1'	5.15	133.69	127.00
1	2	1643	U	N3-C2-O2	-5.15	118.60	122.20
1	2	587	C	C6-N1-C2	-5.14	118.24	120.30
1	2	338	C	C2-N1-C1'	5.14	124.45	118.80
1	2	1429	G	O4'-C1'-N9	5.14	112.31	108.20
1	2	833	U	C5-C4-O4	5.14	128.98	125.90
1	2	838	G	N3-C4-C5	-5.14	126.03	128.60
1	2	1048	G	N3-C4-N9	-5.14	122.92	126.00
1	2	177	U	O5'-P-OP2	-5.13	101.08	105.70
1	2	1502	G	C8-N9-C4	-5.13	104.35	106.40
1	2	1624	C	C5-C6-N1	5.13	123.57	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	962	C	C6-N1-C2	-5.12	118.25	120.30
1	2	479	C	C5-C6-N1	5.12	123.56	121.00
1	2	1237	G	C8-N9-C1'	-5.12	120.35	127.00
1	2	1599	C	N1-C2-O2	5.12	121.97	118.90
1	2	1652	C	P-O3'-C3'	5.12	125.84	119.70
1	2	736	C	C5-C6-N1	5.12	123.56	121.00
1	2	747	C	N1-C2-O2	5.12	121.97	118.90
1	2	1051	G	C6-C5-N7	-5.11	127.33	130.40
1	2	229	U	C6-N1-C1'	-5.11	114.05	121.20
1	2	1097	U	N1-C2-O2	5.10	126.37	122.80
1	2	937	C	C5-C6-N1	5.10	123.55	121.00
1	2	1548	G	N7-C8-N9	5.09	115.65	113.10
1	2	1165	G	C6-C5-N7	-5.09	127.34	130.40
1	2	949	C	C6-N1-C2	-5.09	118.27	120.30
1	2	1495	C	C5-C6-N1	5.09	123.54	121.00
1	2	1548	G	C8-N9-C4	-5.08	104.37	106.40
1	2	1263	G	C6-C5-N7	-5.08	127.35	130.40
1	2	1327	C	N1-C2-O2	5.08	121.95	118.90
1	2	262	U	N3-C2-O2	-5.08	118.64	122.20
1	2	237	C	C5-C6-N1	5.08	123.54	121.00
1	2	243	G	C4-C5-N7	5.08	112.83	110.80
1	2	566	C	C6-N1-C2	-5.08	118.27	120.30
1	2	1332	C	C5-C6-N1	5.08	123.54	121.00
1	2	1017	U	N1-C2-O2	5.08	126.35	122.80
1	2	882	U	N1-C2-O2	5.07	126.35	122.80
1	2	1651	A	C2-N3-C4	5.07	113.14	110.60
1	2	975	C	C6-N1-C2	-5.07	118.27	120.30
1	2	324	U	N3-C2-O2	-5.07	118.65	122.20
1	2	833	U	N3-C4-O4	-5.07	115.85	119.40
1	2	1733	C	C5-C6-N1	5.06	123.53	121.00
1	2	1783	C	C2-N1-C1'	5.06	124.36	118.80
1	2	1176	G	C8-N9-C1'	5.05	133.57	127.00
1	2	990	C	N1-C2-O2	5.05	121.93	118.90
1	2	1660	A	C8-N9-C4	-5.05	103.78	105.80
1	2	553	G	N1-C6-O6	-5.03	116.88	119.90
1	2	1307	U	N3-C2-O2	-5.03	118.68	122.20
1	2	1692	G	C4-N9-C1'	5.03	133.04	126.50
1	2	1309	C	C6-N1-C2	-5.03	118.29	120.30
1	2	1024	U	N1-C2-O2	5.03	126.32	122.80
1	2	311	U	O5'-P-OP2	-5.02	101.18	105.70
1	2	1590	G	C4-N9-C1'	5.02	133.03	126.50
1	2	1594	G	N3-C2-N2	5.02	123.42	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1271	G	C6-C5-N7	5.02	133.41	130.40
1	2	1562	G	C8-N9-C4	-5.01	104.39	106.40
1	2	893	U	N3-C2-O2	-5.01	118.69	122.20
1	2	243	G	C6-C5-N7	-5.00	127.40	130.40
1	2	600	U	C5-C6-N1	5.00	125.20	122.70
1	2	648	G	C6-C5-N7	-5.00	127.40	130.40
1	2	1039	A	C4-N9-C1'	5.00	135.30	126.30

There are no chirality outliers.

All (91) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	34	GLU	Peptide
3	B	129	THR	Peptide
3	B	157	GLN	Peptide
3	B	79	HIS	Peptide
3	B	80	SER	Peptide
4	C	36	VAL	Peptide
4	C	65	GLU	Peptide
5	E	206	ASP	Peptide
5	E	207	LEU	Peptide
5	E	94	ALA	Peptide
6	F	105	GLY	Peptide
6	F	39	GLU	Peptide
6	F	59	VAL	Peptide
7	G	169	TYR	Peptide
7	G	21	GLU	Peptide
8	H	182	VAL	Peptide
8	H	5	GLN	Peptide
8	H	7	LYS	Peptide
10	J	167	ALA	Peptide
10	J	168	ARG	Peptide
10	J	174	ARG	Peptide
10	J	64	GLU	Peptide
11	L	5	LEU	Peptide
11	L	6	THR	Peptide
12	M	100	TRP	Peptide
12	M	47	GLU	Peptide
13	N	84	ILE	Peptide
14	O	121	VAL	Peptide
14	O	72	LYS	Peptide
15	P	124	THR	Peptide

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Mol	Chain	Res	Type	Group
15	P	139	ILE	Peptide
15	P	31	GLU	Peptide
15	P	39	ALA	Peptide
15	P	68	PRO	Peptide
15	P	88	GLU	Peptide
16	Q	99	GLU	Peptide
17	R	123	ASN	Peptide
18	S	114	GLU	Peptide
18	S	115	ARG	Peptide
18	S	117	LYS	Peptide
18	S	73	MET	Peptide
18	S	85	PHE	Peptide
18	S	88	ARG	Peptide
19	T	100	ILE	Peptide
19	T	137	ALA	Peptide
19	T	33	TYR	Peptide
19	T	65	ILE	Peptide
19	T	70	GLN	Peptide
20	U	98	GLN	Peptide
21	V	27	ASP	Peptide
22	W	101	TYR	Peptide
22	W	9	ASP	Peptide
23	X	109	ARG	Peptide
23	X	62	LYS	Peptide
24	Y	29	HIS	Peptide
24	Y	34	ASN	Peptide
24	Y	4	ALA	Peptide
24	Y	48	TYR	Peptide
26	b	7	LEU	Peptide
29	e	15	LYS	Peptide
29	e	46	ASN	Peptide
29	e	50	VAL	Peptide
29	e	55	ARG	Peptide
29	e	56	MET	Peptide
29	e	57	ASN	Peptide
30	h	121	VAL	Peptide
30	h	145	PHE	Peptide
30	h	236	GLY	Peptide
30	h	96	SER	Peptide
31	i	242	TRP	Peptide
31	i	258	VAL	Peptide
31	i	261	GLU	Peptide

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Mol	Chain	Res	Type	Group
31	i	276	GLN	Peptide
31	i	277	LYS	Peptide
31	i	278	PHE	Peptide
31	i	279	ILE	Peptide
31	i	280	ASN	Peptide
31	i	319	LYS	Peptide
31	i	322	LEU	Peptide
31	i	323	PHE	Peptide
31	i	380	TYR	Peptide
31	i	456	ILE	Peptide
33	l	228	CYS	Peptide
33	l	289	LYS	Peptide
33	l	98	GLY	Peptide
33	l	99	ASN	Peptide
34	t	379	PHE	Peptide
34	t	499	LYS	Peptide
34	t	528	LEU	Peptide
34	t	54	ARG	Peptide
34	t	95	LEU	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	204/252 (81%)	184 (90%)	20 (10%)	0	100	100
3	B	208/255 (82%)	174 (84%)	33 (16%)	1 (0%)	29	66
4	C	218/254 (86%)	191 (88%)	27 (12%)	0	100	100
5	E	258/261 (99%)	218 (84%)	38 (15%)	2 (1%)	19	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	204/225 (91%)	168 (82%)	36 (18%)	0	100	100
7	G	224/236 (95%)	200 (89%)	22 (10%)	2 (1%)	17	54
8	H	160/190 (84%)	130 (81%)	30 (19%)	0	100	100
9	I	184/200 (92%)	167 (91%)	17 (9%)	0	100	100
10	J	183/197 (93%)	149 (81%)	33 (18%)	1 (0%)	29	66
11	L	153/156 (98%)	126 (82%)	27 (18%)	0	100	100
12	M	111/143 (78%)	83 (75%)	28 (25%)	0	100	100
13	N	148/151 (98%)	133 (90%)	13 (9%)	2 (1%)	11	46
14	O	126/137 (92%)	108 (86%)	18 (14%)	0	100	100
15	P	121/142 (85%)	96 (79%)	25 (21%)	0	100	100
16	Q	125/143 (87%)	93 (74%)	32 (26%)	0	100	100
17	R	111/136 (82%)	98 (88%)	13 (12%)	0	100	100
18	S	133/146 (91%)	112 (84%)	21 (16%)	0	100	100
19	T	139/144 (96%)	126 (91%)	13 (9%)	0	100	100
20	U	61/121 (50%)	56 (92%)	5 (8%)	0	100	100
21	V	83/87 (95%)	66 (80%)	16 (19%)	1 (1%)	13	50
22	W	127/130 (98%)	112 (88%)	13 (10%)	2 (2%)	9	44
23	X	142/145 (98%)	123 (87%)	18 (13%)	1 (1%)	22	60
24	Y	132/135 (98%)	107 (81%)	24 (18%)	1 (1%)	19	57
25	Z	61/108 (56%)	55 (90%)	6 (10%)	0	100	100
26	b	79/82 (96%)	70 (89%)	8 (10%)	1 (1%)	12	48
27	c	61/67 (91%)	52 (85%)	9 (15%)	0	100	100
28	d	25/56 (45%)	23 (92%)	1 (4%)	1 (4%)	3	28
29	e	58/63 (92%)	41 (71%)	17 (29%)	0	100	100
30	h	176/274 (64%)	157 (89%)	19 (11%)	0	100	100
31	i	257/483 (53%)	200 (78%)	55 (21%)	2 (1%)	19	57
32	j	51/463 (11%)	42 (82%)	9 (18%)	0	100	100
33	l	274/425 (64%)	241 (88%)	33 (12%)	0	100	100
34	t	649/788 (82%)	577 (89%)	72 (11%)	0	100	100
All	All	5246/6795 (77%)	4478 (85%)	751 (14%)	17 (0%)	44	74

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	207	LEU
5	E	208	VAL
22	W	11	LEU
31	i	279	ILE
3	B	80	SER
24	Y	36	SER
26	b	20	LYS
21	V	11	LEU
22	W	10	ALA
28	d	22	ARG
7	G	70	PRO
10	J	120	LYS
13	N	85	PRO
31	i	256	PRO
7	G	69	LEU
13	N	23	PRO
23	X	64	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	
2	A	172/210 (82%)	166 (96%)	6 (4%)	36	64
3	B	191/224 (85%)	188 (98%)	3 (2%)	62	79
4	C	179/205 (87%)	176 (98%)	3 (2%)	60	78
5	E	221/222 (100%)	221 (100%)	0	100	100
6	F	173/191 (91%)	168 (97%)	5 (3%)	42	67
7	G	188/201 (94%)	186 (99%)	2 (1%)	73	85
8	H	151/170 (89%)	149 (99%)	2 (1%)	69	82
9	I	150/161 (93%)	150 (100%)	0	100	100
10	J	158/166 (95%)	151 (96%)	7 (4%)	28	57
11	L	129/137 (94%)	128 (99%)	1 (1%)	81	89
12	M	101/119 (85%)	99 (98%)	2 (2%)	55	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	N	127/128 (99%)	125 (98%)	2 (2%)	62	79
14	O	97/105 (92%)	94 (97%)	3 (3%)	40	65
15	P	105/118 (89%)	101 (96%)	4 (4%)	33	61
16	Q	107/119 (90%)	106 (99%)	1 (1%)	78	88
17	R	105/124 (85%)	101 (96%)	4 (4%)	33	61
18	S	120/129 (93%)	119 (99%)	1 (1%)	81	89
19	T	115/116 (99%)	114 (99%)	1 (1%)	78	88
20	U	64/114 (56%)	64 (100%)	0	100	100
21	V	74/74 (100%)	72 (97%)	2 (3%)	44	69
22	W	110/111 (99%)	109 (99%)	1 (1%)	78	88
23	X	119/120 (99%)	117 (98%)	2 (2%)	60	78
24	Y	112/113 (99%)	109 (97%)	3 (3%)	44	69
25	Z	56/89 (63%)	55 (98%)	1 (2%)	59	77
26	b	70/71 (99%)	68 (97%)	2 (3%)	42	67
27	c	56/60 (93%)	56 (100%)	0	100	100
28	d	25/49 (51%)	23 (92%)	2 (8%)	12	42
29	e	51/54 (94%)	49 (96%)	2 (4%)	32	60
30	h	156/238 (66%)	151 (97%)	5 (3%)	39	65
31	i	233/424 (55%)	225 (97%)	8 (3%)	37	64
32	j	53/419 (13%)	52 (98%)	1 (2%)	57	76
33	l	260/384 (68%)	253 (97%)	7 (3%)	44	69
34	t	582/703 (83%)	577 (99%)	5 (1%)	78	88
All	All	4610/5868 (79%)	4522 (98%)	88 (2%)	59	76

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	39	ASN
2	A	59	LEU
2	A	69	ASN
2	A	127	ARG
2	A	163	ASN
2	A	180	GLU
3	B	26	ARG

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Mol	Chain	Res	Type
3	B	148	ASN
3	B	209	ASN
4	C	119	LYS
4	C	121	VAL
4	C	148	LEU
6	F	84	LYS
6	F	148	ARG
6	F	157	ARG
6	F	186	ASN
6	F	194	LEU
7	G	102	VAL
7	G	159	ARG
8	H	9	LEU
8	H	79	ARG
10	J	3	ARG
10	J	52	ILE
10	J	53	ARG
10	J	57	ARG
10	J	115	LYS
10	J	129	ILE
10	J	142	ASN
11	L	129	ARG
12	M	103	LEU
12	M	105	LYS
13	N	42	ARG
13	N	127	ARG
14	O	42	VAL
14	O	52	ARG
14	O	136	ARG
15	P	57	MET
15	P	61	ARG
15	P	77	ARG
15	P	130	ARG
16	Q	53	LEU
17	R	5	ARG
17	R	7	LYS
17	R	45	ARG
17	R	104	ASN
18	S	44	ASN
19	T	127	ASN
21	V	11	LEU
21	V	21	ASN

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Mol	Chain	Res	Type
22	W	93	LEU
23	X	16	ARG
23	X	96	VAL
24	Y	32	ARG
24	Y	123	LYS
24	Y	131	ARG
25	Z	103	ARG
26	b	42	ASN
26	b	80	ARG
28	d	22	ARG
28	d	33	LYS
29	e	37	ARG
29	e	54	ARG
30	h	110	ARG
30	h	133	LYS
30	h	140	ARG
30	h	269	ARG
30	h	271	LYS
31	i	240	ARG
31	i	259	VAL
31	i	280	ASN
31	i	283	LEU
31	i	300	ASN
31	i	396	ARG
31	i	458	ARG
31	i	466	ARG
32	j	357	LEU
33	l	9	ARG
33	l	74	ARG
33	l	90	ASN
33	l	99	ASN
33	l	198	ARG
33	l	214	MET
33	l	278	ARG
34	t	225	ARG
34	t	232	ASN
34	t	248	ARG
34	t	634	ASN
34	t	638	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	23	HIS
2	A	39	ASN
2	A	69	ASN
2	A	131	GLN
2	A	163	ASN
3	B	148	ASN
3	B	157	GLN
3	B	209	ASN
4	C	59	HIS
4	C	87	GLN
4	C	209	ASN
4	C	220	ASN
6	F	44	ASN
6	F	186	ASN
7	G	65	GLN
8	H	29	ASN
9	I	116	HIS
10	J	176	ASN
13	N	101	HIS
13	N	105	ASN
16	Q	83	GLN
17	R	29	GLN
17	R	74	GLN
17	R	104	ASN
18	S	6	GLN
18	S	44	ASN
18	S	78	HIS
18	S	87	ASN
18	S	127	HIS
19	T	64	HIS
19	T	127	ASN
20	U	48	HIS
21	V	21	ASN
21	V	74	GLN
22	W	44	HIS
22	W	56	HIS
22	W	120	HIS
24	Y	29	HIS
24	Y	34	ASN
26	b	42	ASN
26	b	51	GLN
30	h	142	ASN
30	h	262	ASN

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Mol	Chain	Res	Type
31	i	280	ASN
31	i	300	ASN
33	l	38	HIS
33	l	90	ASN
33	l	99	ASN
33	l	160	ASN
33	l	182	ASN
33	l	185	HIS
33	l	256	GLN
34	t	56	ASN
34	t	116	GLN
34	t	127	HIS
34	t	144	ASN
34	t	232	ASN
34	t	237	ASN
34	t	255	ASN
34	t	290	ASN
34	t	634	ASN
34	t	638	ASN
34	t	647	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1711/1735 (98%)	821 (47%)	28 (1%)

All (821) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	8	U
1	2	11	A
1	2	13	C
1	2	15	U
1	2	16	G
1	2	24	U
1	2	25	C
1	2	27	U
1	2	34	G

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Mol	Chain	Res	Type
1	2	38	C
1	2	40	A
1	2	42	G
1	2	45	U
1	2	46	A
1	2	47	A
1	2	59	C
1	2	60	U
1	2	61	A
1	2	65	A
1	2	66	U
1	2	68	A
1	2	69	G
1	2	72	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	77	U
1	2	78	A
1	2	101	U
1	2	104	A
1	2	105	A
1	2	111	U
1	2	114	C
1	2	115	G
1	2	116	U
1	2	121	U
1	2	126	A
1	2	127	G
1	2	129	U
1	2	130	C
1	2	131	C
1	2	132	U
1	2	133	U
1	2	134	U
1	2	135	A
1	2	136	C
1	2	138	A
1	2	139	C
1	2	140	A
1	2	141	U
1	2	145	A

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Mol	Chain	Res	Type
1	2	152	U
1	2	153	G
1	2	154	G
1	2	156	A
1	2	158	U
1	2	161	U
1	2	164	A
1	2	165	G
1	2	166	C
1	2	176	C
1	2	178	U
1	2	182	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	189	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	197	A
1	2	198	A
1	2	199	G
1	2	203	U
1	2	204	G
1	2	213	A
1	2	215	A
1	2	217	A
1	2	218	A
1	2	222	A
1	2	223	U
1	2	224	C
1	2	225	A
1	2	226	A
1	2	227	U
1	2	231	U
1	2	233	C
1	2	234	G
1	2	237	C
1	2	239	C
1	2	240	U

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Mol	Chain	Res	Type
1	2	241	U
1	2	243	G
1	2	249	U
1	2	250	C
1	2	257	A
1	2	260	U
1	2	261	U
1	2	263	C
1	2	265	A
1	2	266	A
1	2	274	G
1	2	275	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	282	C
1	2	283	U
1	2	287	G
1	2	292	U
1	2	293	U
1	2	314	C
1	2	315	A
1	2	316	A
1	2	320	U
1	2	321	C
1	2	322	G
1	2	330	G
1	2	333	A
1	2	337	G
1	2	338	C
1	2	339	C
1	2	352	A
1	2	353	A
1	2	359	A
1	2	361	C
1	2	363	G
1	2	364	G
1	2	365	G
1	2	366	A
1	2	367	A

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Mol	Chain	Res	Type
1	2	368	U
1	2	373	G
1	2	380	U
1	2	388	G
1	2	400	A
1	2	401	A
1	2	402	C
1	2	404	G
1	2	413	U
1	2	414	C
1	2	416	A
1	2	417	A
1	2	420	A2M
1	2	421	A
1	2	423	G
1	2	424	C
1	2	426	G
1	2	435	C
1	2	436	A2M
1	2	437	A
1	2	438	A
1	2	441	A
1	2	442	C
1	2	444	C
1	2	448	C
1	2	452	A
1	2	454	U
1	2	455	C
1	2	459	G
1	2	460	A
1	2	461	G
1	2	468	A
1	2	474	A
1	2	475	A
1	2	477	A
1	2	478	A
1	2	479	C
1	2	480	G
1	2	484	C
1	2	485	A
1	2	486	G
1	2	487	G

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Mol	Chain	Res	Type
1	2	488	G
1	2	491	C
1	2	492	A
1	2	493	U
1	2	494	U
1	2	495	C
1	2	496	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	503	G
1	2	505	A
1	2	506	A
1	2	507	U
1	2	508	U
1	2	509	G
1	2	510	G
1	2	513	U
1	2	514	G
1	2	515	A
1	2	517	U
1	2	518	A
1	2	519	C
1	2	524	U
1	2	528	U
1	2	529	A
1	2	532	U
1	2	533	U
1	2	534	A
1	2	535	A
1	2	537	G
1	2	538	A
1	2	539	G
1	2	541	A
1	2	542	A
1	2	543	C
1	2	544	A
1	2	545	A
1	2	551	G
1	2	552	G
1	2	554	C
1	2	556	A

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Mol	Chain	Res	Type
1	2	557	G
1	2	558	U
1	2	559	C
1	2	561	G
1	2	562	G
1	2	564	G
1	2	565	C
1	2	566	C
1	2	569	C
1	2	572	C
1	2	573	C
1	2	575	C
1	2	577	G
1	2	579	A
1	2	580	A
1	2	581	U
1	2	582	U
1	2	583	C
1	2	584	C
1	2	587	C
1	2	591	A
1	2	594	A
1	2	595	G
1	2	597	G
1	2	602	U
1	2	606	A
1	2	607	G
1	2	608	U
1	2	611	U
1	2	612	U
1	2	613	G
1	2	614	C
1	2	616	G
1	2	620	A
1	2	623	A
1	2	626	U
1	2	633	U
1	2	637	C
1	2	638	U
1	2	639	U
1	2	640	U
1	2	645	C

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Mol	Chain	Res	Type
1	2	647	G
1	2	648	G
1	2	650	U
1	2	652	G
1	2	653	C
1	2	654	C
1	2	655	G
1	2	656	G
1	2	657	U
1	2	658	C
1	2	678	A
1	2	681	U
1	2	684	A
1	2	690	G
1	2	691	C
1	2	693	U
1	2	694	U
1	2	695	U
1	2	696	C
1	2	698	U
1	2	699	U
1	2	700	C
1	2	701	U
1	2	702	G
1	2	704	C
1	2	734	A
1	2	739	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	744	U
1	2	754	A
1	2	762	A
1	2	766	U
1	2	769	A
1	2	770	A
1	2	773	C
1	2	774	A
1	2	775	G
1	2	776	G
1	2	778	G
1	2	779	U

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Mol	Chain	Res	Type
1	2	780	A
1	2	781	U
1	2	782	U
1	2	783	G
1	2	789	A
1	2	790	U
1	2	793	A
1	2	794	U
1	2	795	U
1	2	796	A2M
1	2	797	G
1	2	800	U
1	2	801	G
1	2	803	A
1	2	804	A
1	2	807	A
1	2	809	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	816	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	823	G
1	2	824	G
1	2	827	C
1	2	829	A
1	2	830	U
1	2	831	U
1	2	832	U
1	2	833	U
1	2	834	G
1	2	837	G
1	2	839	U
1	2	843	U
1	2	844	A
1	2	845	G
1	2	846	G
1	2	851	U
1	2	854	U

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Mol	Chain	Res	Type
1	2	856	A
1	2	857	U
1	2	860	U
1	2	861	U
1	2	862	A
1	2	863	A
1	2	864	U
1	2	865	A
1	2	872	G
1	2	873	U
1	2	874	C
1	2	875	G
1	2	878	G
1	2	881	A
1	2	887	A
1	2	896	U
1	2	897	C
1	2	898	A
1	2	900	A
1	2	904	G
1	2	905	A
1	2	906	A
1	2	908	U
1	2	909	U
1	2	910	C
1	2	911	U
1	2	912	U
1	2	913	G
1	2	914	G
1	2	915	A
1	2	916	U
1	2	917	U
1	2	918	U
1	2	919	A
1	2	921	U
1	2	925	G
1	2	928	U
1	2	930	A
1	2	931	C
1	2	932	U
1	2	933	A
1	2	934	C

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Mol	Chain	Res	Type
1	2	935	U
1	2	937	C
1	2	939	A
1	2	940	A
1	2	941	A
1	2	942	G
1	2	944	A
1	2	945	U
1	2	946	U
1	2	951	A
1	2	954	G
1	2	955	A
1	2	959	U
1	2	960	U
1	2	966	A
1	2	970	A
1	2	977	A
1	2	988	A
1	2	990	C
1	2	991	G
1	2	992	A
1	2	993	A
1	2	996	U
1	2	997	G
1	2	998	A
1	2	999	U
1	2	1000	C
1	2	1001	A
1	2	1002	G
1	2	1003	A
1	2	1004	U
1	2	1005	A
1	2	1007	C
1	2	1013	A
1	2	1021	C
1	2	1023	A
1	2	1026	A
1	2	1028	C
1	2	1029	U
1	2	1030	A
1	2	1031	U
1	2	1032	G

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Mol	Chain	Res	Type
1	2	1036	A
1	2	1039	A
1	2	1040	G
1	2	1042	G
1	2	1043	A
1	2	1045	C
1	2	1046	G
1	2	1049	U
1	2	1052	U
1	2	1053	G
1	2	1057	U
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1062	A
1	2	1063	U
1	2	1064	G
1	2	1072	C
1	2	1073	G
1	2	1076	A
1	2	1079	U
1	2	1080	U
1	2	1081	A
1	2	1082	C
1	2	1086	A
1	2	1087	A
1	2	1091	A
1	2	1092	A
1	2	1093	A
1	2	1094	G
1	2	1097	U
1	2	1098	U
1	2	1099	U
1	2	1100	G
1	2	1101	G
1	2	1106	U
1	2	1108	G
1	2	1109	G
1	2	1111	G
1	2	1113	A
1	2	1131	A

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Mol	Chain	Res	Type
1	2	1137	A
1	2	1138	A
1	2	1139	A
1	2	1148	C
1	2	1150	G
1	2	1152	A
1	2	1154	G
1	2	1155	G
1	2	1157	A
1	2	1158	C
1	2	1159	C
1	2	1160	A
1	2	1161	C
1	2	1163	A
1	2	1164	G
1	2	1166	A
1	2	1167	G
1	2	1170	G
1	2	1172	G
1	2	1174	C
1	2	1175	U
1	2	1177	C
1	2	1181	U
1	2	1182	U
1	2	1183	A
1	2	1185	U
1	2	1186	U
1	2	1188	G
1	2	1189	A
1	2	1191	U
1	2	1192	C
1	2	1194	A
1	2	1195	C
1	2	1196	A
1	2	1197	C
1	2	1198	G
1	2	1199	G
1	2	1201	G
1	2	1203	A
1	2	1204	A
1	2	1207	C
1	2	1209	C

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Mol	Chain	Res	Type
1	2	1211	A
1	2	1212	G
1	2	1213	G
1	2	1215	C
1	2	1216	C
1	2	1217	A
1	2	1218	G
1	2	1219	A
1	2	1220	C
1	2	1224	A
1	2	1225	U
1	2	1226	A
1	2	1227	A
1	2	1229	G
1	2	1230	A
1	2	1231	U
1	2	1232	U
1	2	1235	C
1	2	1237	G
1	2	1239	U
1	2	1240	U
1	2	1242	A
1	2	1249	U
1	2	1253	U
1	2	1254	U
1	2	1255	G
1	2	1256	A
1	2	1257	U
1	2	1264	G
1	2	1265	G
1	2	1266	U
1	2	1267	G
1	2	1268	G
1	2	1269	U
1	2	1272	U
1	2	1273	G
1	2	1274	C
1	2	1275	A
1	2	1276	U
1	2	1278	G
1	2	1279	C
1	2	1280	C

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Mol	Chain	Res	Type
1	2	1281	G
1	2	1283	U
1	2	1284	C
1	2	1285	U
1	2	1287	A
1	2	1288	G
1	2	1289	U
1	2	1293	U
1	2	1302	U
1	2	1303	U
1	2	1304	G
1	2	1305	U
1	2	1306	C
1	2	1307	U
1	2	1309	C
1	2	1314	U
1	2	1315	U
1	2	1317	C
1	2	1319	A
1	2	1320	U
1	2	1321	A
1	2	1323	C
1	2	1326	A
1	2	1330	G
1	2	1331	A
1	2	1332	C
1	2	1333	C
1	2	1337	A
1	2	1338	C
1	2	1339	C
1	2	1340	U
1	2	1341	A
1	2	1342	C
1	2	1343	U
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1348	A
1	2	1349	G
1	2	1356	U
1	2	1360	A
1	2	1361	U

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Mol	Chain	Res	Type
1	2	1363	U
1	2	1364	G
1	2	1367	G
1	2	1370	U
1	2	1371	A
1	2	1372	U
1	2	1373	C
1	2	1379	C
1	2	1381	U
1	2	1382	A
1	2	1383	G
1	2	1384	A
1	2	1387	G
1	2	1389	C
1	2	1390	U
1	2	1391	A
1	2	1399	C
1	2	1404	C
1	2	1410	A
1	2	1412	G
1	2	1413	U
1	2	1414	U
1	2	1415	U
1	2	1416	G
1	2	1417	A
1	2	1418	G
1	2	1419	G
1	2	1421	A
1	2	1425	A
1	2	1426	C
1	2	1428	G
1	2	1429	G
1	2	1430	U
1	2	1431	C
1	2	1432	U
1	2	1434	U
1	2	1435	G
1	2	1436	A
1	2	1437	U
1	2	1441	C
1	2	1442	U
1	2	1443	U

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Mol	Chain	Res	Type
1	2	1444	A
1	2	1446	A
1	2	1447	C
1	2	1450	U
1	2	1451	C
1	2	1454	G
1	2	1455	G
1	2	1456	C
1	2	1457	C
1	2	1458	G
1	2	1460	A
1	2	1466	G
1	2	1468	U
1	2	1469	A
1	2	1471	A
1	2	1472	C
1	2	1473	U
1	2	1474	G
1	2	1475	A
1	2	1478	G
1	2	1479	A
1	2	1481	C
1	2	1486	G
1	2	1489	U
1	2	1490	C
1	2	1492	A
1	2	1493	A
1	2	1494	C
1	2	1496	U
1	2	1499	G
1	2	1500	C
1	2	1503	A
1	2	1504	G
1	2	1505	A
1	2	1506	G
1	2	1508	U
1	2	1510	U
1	2	1515	A
1	2	1516	A
1	2	1518	C
1	2	1520	U
1	2	1521	G

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Mol	Chain	Res	Type
1	2	1523	G
1	2	1524	A
1	2	1527	C
1	2	1529	C
1	2	1530	C
1	2	1531	G
1	2	1534	G
1	2	1535	U
1	2	1536	G
1	2	1537	C
1	2	1538	U
1	2	1539	G
1	2	1540	G
1	2	1541	G
1	2	1542	G
1	2	1543	A
1	2	1544	U
1	2	1548	G
1	2	1549	C
1	2	1550	A
1	2	1552	U
1	2	1555	A
1	2	1556	A
1	2	1557	U
1	2	1558	U
1	2	1559	A
1	2	1560	U
1	2	1564	U
1	2	1566	U
1	2	1571	C
1	2	1572	G
1	2	1573	A
1	2	1574	G
1	2	1578	U
1	2	1582	U
1	2	1583	A
1	2	1584	G
1	2	1586	A
1	2	1587	A
1	2	1594	G
1	2	1595	U
1	2	1596	C

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Mol	Chain	Res	Type
1	2	1597	A
1	2	1598	U
1	2	1599	C
1	2	1600	A
1	2	1601	G
1	2	1605	G
1	2	1609	U
1	2	1610	G
1	2	1611	A
1	2	1613	U
1	2	1618	C
1	2	1619	C
1	2	1621	U
1	2	1624	C
1	2	1626	U
1	2	1629	G
1	2	1630	U
1	2	1631	A
1	2	1632	C
1	2	1633	A
1	2	1634	C
1	2	1635	A
1	2	1638	G
1	2	1639	C
1	2	1640	C
1	2	1641	C
1	2	1642	G
1	2	1643	U
1	2	1648	A
1	2	1649	G
1	2	1651	A
1	2	1652	C
1	2	1653	C
1	2	1657	U
1	2	1659	A
1	2	1660	A
1	2	1664	C
1	2	1677	C
1	2	1678	A
1	2	1681	A
1	2	1684	U
1	2	1685	G

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Mol	Chain	Res	Type
1	2	1688	U
1	2	1689	A
1	2	1690	G
1	2	1692	G
1	2	1693	A
1	2	1709	C
1	2	1710	U
1	2	1711	C
1	2	1712	A
1	2	1713	G
1	2	1715	G
1	2	1718	G
1	2	1724	U
1	2	1731	A
1	2	1732	A
1	2	1733	C
1	2	1735	U
1	2	1736	G
1	2	1740	A
1	2	1741	U
1	2	1742	U
1	2	1743	U
1	2	1744	A
1	2	1746	A
1	2	1749	A
1	2	1750	A
1	2	1751	C
1	2	1754	A
1	2	1755	A
1	2	1757	G
1	2	1758	U
1	2	1759	C
1	2	1760	G
1	2	1761	U
1	2	1763	A
1	2	1764	C
1	2	1768	G
1	2	1769	U
1	2	1770	U
1	2	1776	A
1	2	1779	U
1	2	1780	G

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Mol	Chain	Res	Type
1	2	1781	A
1	2	1782	A
1	2	1783	C
1	2	1787	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1795	U
1	2	1796	C
1	2	1797	A
1	2	1799	U

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	47	A
1	2	68	A
1	2	104	A
1	2	130	C
1	2	138	A
1	2	280	U
1	2	352	A
1	2	387	A
1	2	400	A
1	2	514	G
1	2	544	A
1	2	557	G
1	2	649	U
1	2	781	U
1	2	819	G
1	2	862	A
1	2	1041	G
1	2	1086	A
1	2	1196	A
1	2	1197	C
1	2	1226	A
1	2	1229	G
1	2	1427	A
1	2	1572	G
1	2	1573	A
1	2	1600	A
1	2	1618	C

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Mol	Chain	Res	Type
1	2	1652	C

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	2	796	1	18,25,26	1.79	4 (22%)	18,36,39	1.98	6 (33%)
1	A2M	2	420	1	18,25,26	1.25	3 (16%)	18,36,39	2.19	4 (22%)
1	A2M	2	100	1	18,25,26	1.65	5 (27%)	18,36,39	2.18	8 (44%)
1	A2M	2	436	1	18,25,26	1.47	4 (22%)	18,36,39	1.91	6 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	2	796	1	-	2/5/27/28	0/3/3/3
1	A2M	2	420	1	-	0/5/27/28	0/3/3/3
1	A2M	2	100	1	-	2/5/27/28	0/3/3/3
1	A2M	2	436	1	-	0/5/27/28	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	796	A2M	C5-C4	3.55	1.50	1.40
1	2	436	A2M	C5-C4	3.54	1.50	1.40
1	2	100	A2M	C5-C4	3.33	1.49	1.40
1	2	796	A2M	C2-N3	3.06	1.37	1.32
1	2	420	A2M	O4'-C1'	3.05	1.45	1.41
1	2	796	A2M	O3'-C3'	3.03	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	796	A2M	O4'-C1'	2.85	1.45	1.41
1	2	100	A2M	C2-N3	2.72	1.36	1.32
1	2	100	A2M	O4'-C1'	2.59	1.44	1.41
1	2	436	A2M	C2-N3	2.53	1.36	1.32
1	2	420	A2M	C2-N3	2.42	1.36	1.32
1	2	100	A2M	O3'-C3'	2.39	1.48	1.43
1	2	420	A2M	C5-C4	2.23	1.46	1.40
1	2	436	A2M	C6-C5	2.12	1.51	1.43
1	2	436	A2M	C2-N1	2.07	1.37	1.33
1	2	100	A2M	C3'-C2'	2.00	1.57	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	420	A2M	C5-C6-N6	-5.46	112.05	120.35
1	2	100	A2M	O5'-C5'-C4'	4.97	125.89	108.99
1	2	420	A2M	N6-C6-N1	4.70	128.33	118.57
1	2	420	A2M	N3-C2-N1	-4.28	121.99	128.68
1	2	436	A2M	N3-C2-N1	-4.01	122.41	128.68
1	2	436	A2M	C4-C5-N7	-3.53	105.72	109.40
1	2	100	A2M	O3'-C3'-C2'	3.41	120.84	111.17
1	2	100	A2M	N3-C2-N1	-3.36	123.42	128.68
1	2	796	A2M	N6-C6-N1	3.34	125.50	118.57
1	2	436	A2M	C2-N1-C6	3.32	124.43	118.75
1	2	796	A2M	O5'-C5'-C4'	3.03	119.30	108.99
1	2	796	A2M	O3'-C3'-C2'	2.96	119.57	111.17
1	2	796	A2M	O4'-C1'-C2'	-2.93	101.51	106.59
1	2	100	A2M	O4'-C1'-C2'	-2.78	101.77	106.59
1	2	100	A2M	N6-C6-N1	2.73	124.24	118.57
1	2	100	A2M	O4'-C4'-C5'	-2.52	101.09	109.37
1	2	796	A2M	N3-C2-N1	-2.48	124.81	128.68
1	2	436	A2M	C5-C6-N6	2.45	124.07	120.35
1	2	796	A2M	CM'-O2'-C2'	2.42	120.87	114.52
1	2	436	A2M	O2'-C2'-C1'	2.39	113.84	109.09
1	2	100	A2M	C2-N1-C6	2.15	122.42	118.75
1	2	100	A2M	O3'-C3'-C4'	2.11	117.16	111.05
1	2	420	A2M	O3'-C3'-C4'	2.10	117.12	111.05
1	2	436	A2M	C5-C6-N1	-2.02	115.77	120.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	100	A2M	O4'-C4'-C5'-O5'
1	2	100	A2M	C3'-C4'-C5'-O5'
1	2	796	A2M	O4'-C4'-C5'-O5'
1	2	796	A2M	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	2	28
12	M	7
34	t	6
33	l	4
32	j	2
15	P	2
3	B	2
30	h	1
19	T	1
20	U	1
21	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1293:U	O3'	1301:U	P	19.14
1	2	658:C	O3'	676:G	P	16.52
1	2	1693:A	O3'	1708:U	P	10.88
1	2	705:U	O3'	733:A	P	9.46
1	2	1508:U	O3'	1509:C	P	9.19
1	h	270:LEU	C	271:LYS	N	9.17
1	2	1257:U	O3'	1258:U	P	9.13
1	2	1250:U	O3'	1251:U	P	8.07
1	2	1437:U	O3'	1438:G	P	7.98
1	2	1448:G	O3'	1449:U	P	7.87
1	j	351:THR	C	352:GLU	N	7.87
1	l	75:LEU	C	76:THR	N	7.82
1	j	352:GLU	C	353:THR	N	7.11
1	T	51:GLU	C	52:GLY	N	7.03
1	M	67:THR	C	68:GLU	N	6.99
1	2	1377:U	O3'	1378:U	P	6.66
1	M	43:ARG	C	44:GLY	N	6.53
1	2	1421:A	O3'	1422:A	P	6.49
1	M	82:PRO	C	83:GLU	N	6.38
1	M	84:ASN	C	85:LYS	N	6.17
1	t	346:LEU	C	347:ASP	N	6.08
1	t	376:ASP	C	377:HIS	N	6.00
1	2	1501:C	O3'	1502:G	P	5.49
1	2	1145:U	O3'	1146:G	P	5.04
1	l	284:LEU	C	285:LYS	N	5.01
1	2	1438:G	O3'	1439:C	P	4.76
1	t	531:ILE	C	532:GLY	N	4.74
1	l	189:MET	C	190:GLU	N	4.73
1	t	752:HIS	C	753:GLY	N	4.73
1	P	48:GLY	C	49:MET	N	4.61
1	2	1242:A	O3'	1243:G	P	4.22
1	2	1560:U	O3'	1561:U	P	4.15
1	t	501:TYR	C	502:ARG	N	4.02
1	2	1486:G	O3'	1487:A	P	4.01
1	U	30:LYS	C	31:VAL	N	3.99
1	t	659:PRO	C	660:VAL	N	3.96
1	2	1497:U	O3'	1498:G	P	3.95
1	2	1285:U	O3'	1286:U	P	3.82
1	2	1260:U	O3'	1261:G	P	3.74
1	B	221:PRO	C	222:LYS	N	3.64
1	V	62:ARG	C	63:GLY	N	3.51
1	2	1324:G	O3'	1325:A	P	3.35
1	2	1244:A	O3'	1245:G	P	3.30

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	83:GLU	C	84:ASN	N	3.22
1	1	29:HIS	C	30:GLU	N	3.21
1	P	79:HIS	C	80:MET	N	3.19
1	M	125:ASN	C	126:TRP	N	3.17
1	B	81:PHE	C	82:ARG	N	3.11
1	M	23:THR	C	24:ILE	N	3.10
1	2	99:C	O3'	100:A2M	P	2.34
1	2	795:U	O3'	796:A2M	P	1.84
1	2	100:A2M	O3'	101:U	P	1.35
1	2	796:A2M	O3'	797:G	P	1.25
1	2	419:G	O3'	420:A2M	P	0.88
1	2	435:C	O3'	436:A2M	P	0.50

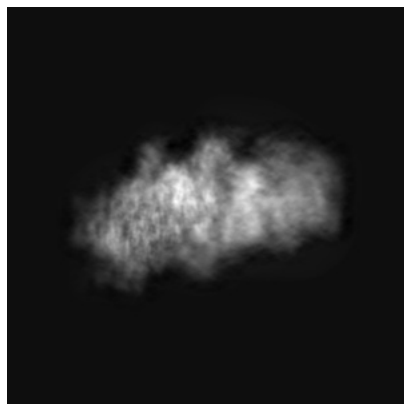
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10713. These allow visual inspection of the internal detail of the map and identification of artifacts.

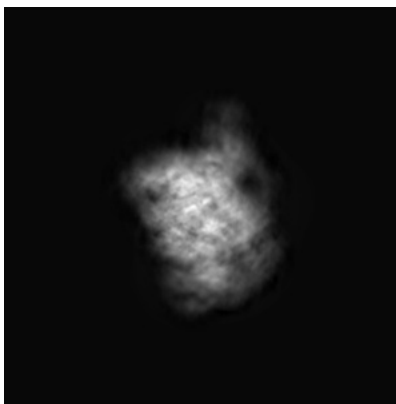
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

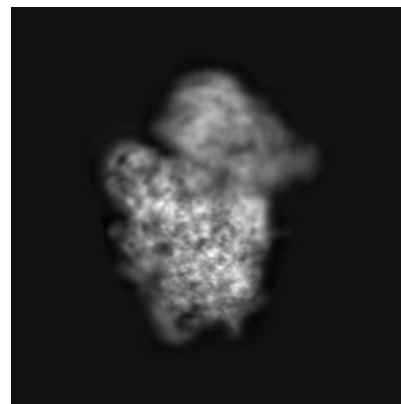
6.1.1 Primary map



X

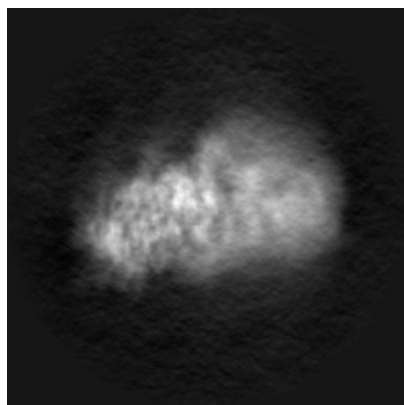


Y

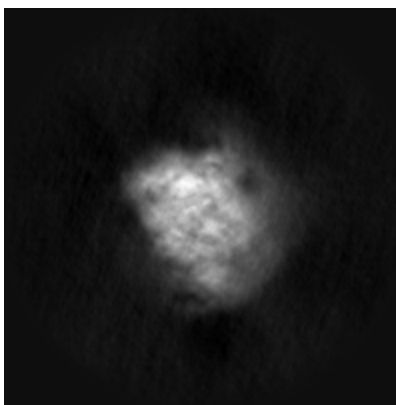


Z

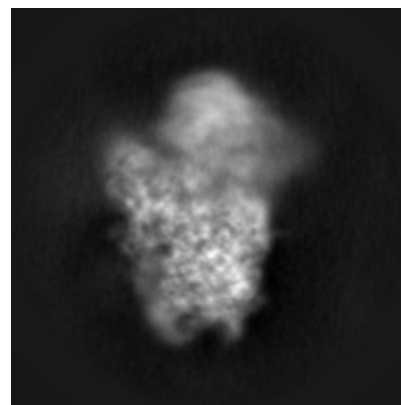
6.1.2 Raw map



X



Y

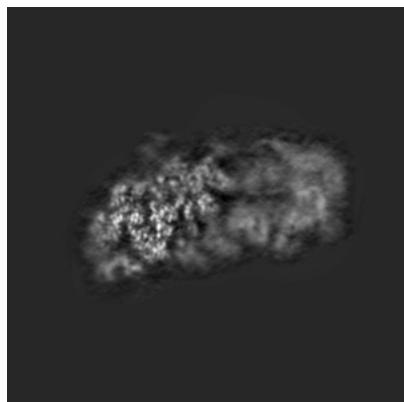


Z

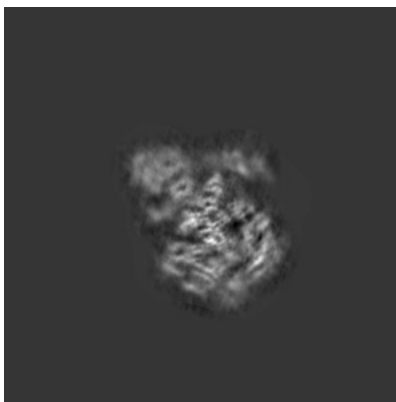
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

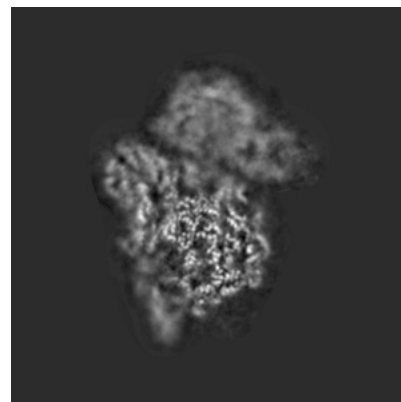
6.2.1 Primary map



X Index: 180

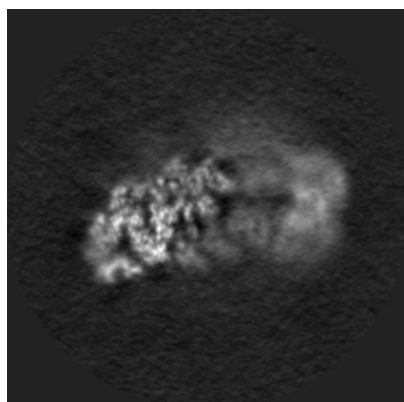


Y Index: 180

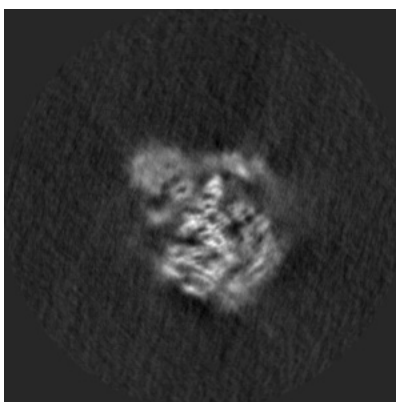


Z Index: 180

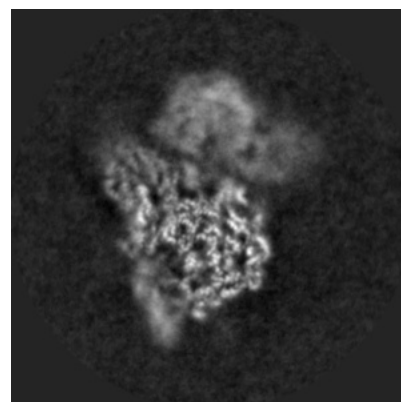
6.2.2 Raw map



X Index: 180



Y Index: 180

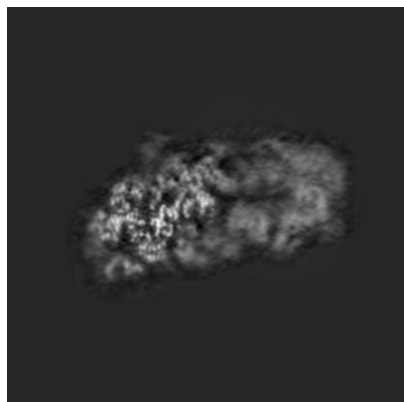


Z Index: 180

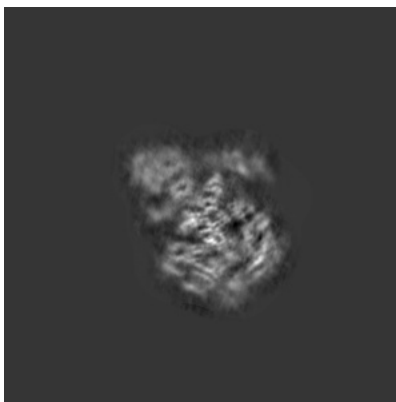
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

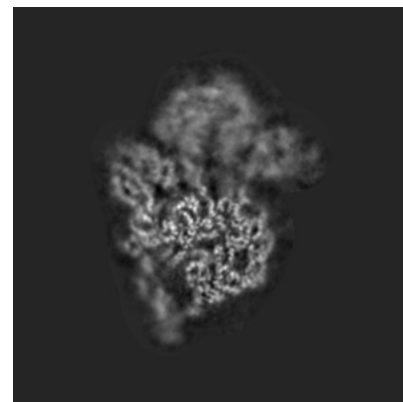
6.3.1 Primary map



X Index: 178

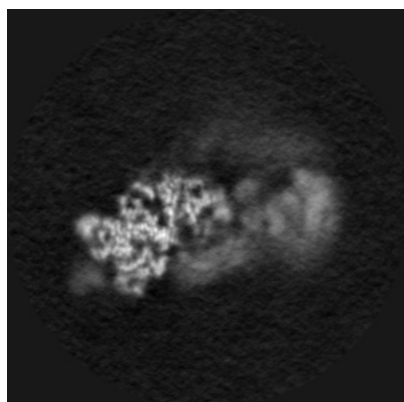


Y Index: 180

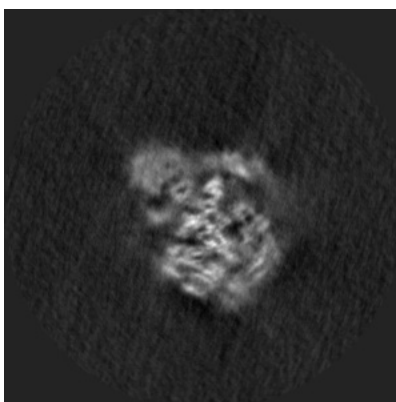


Z Index: 185

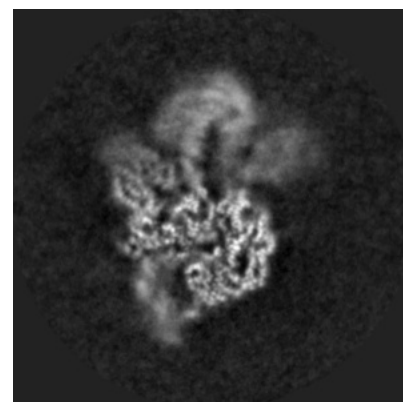
6.3.2 Raw map



X Index: 202



Y Index: 179

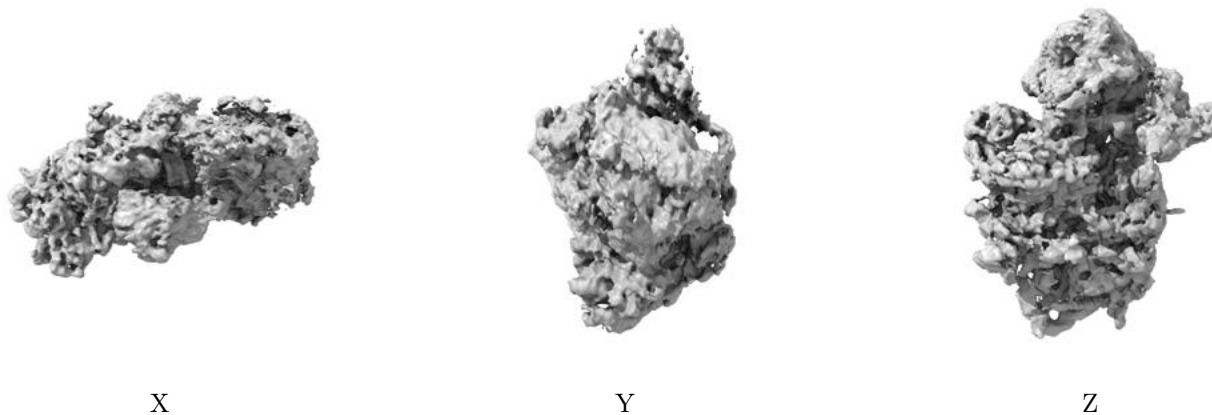


Z Index: 187

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

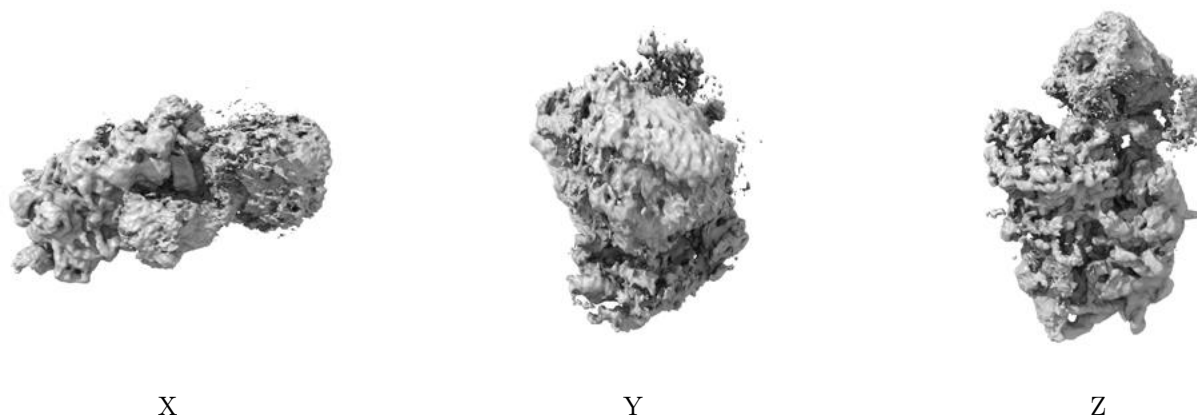
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

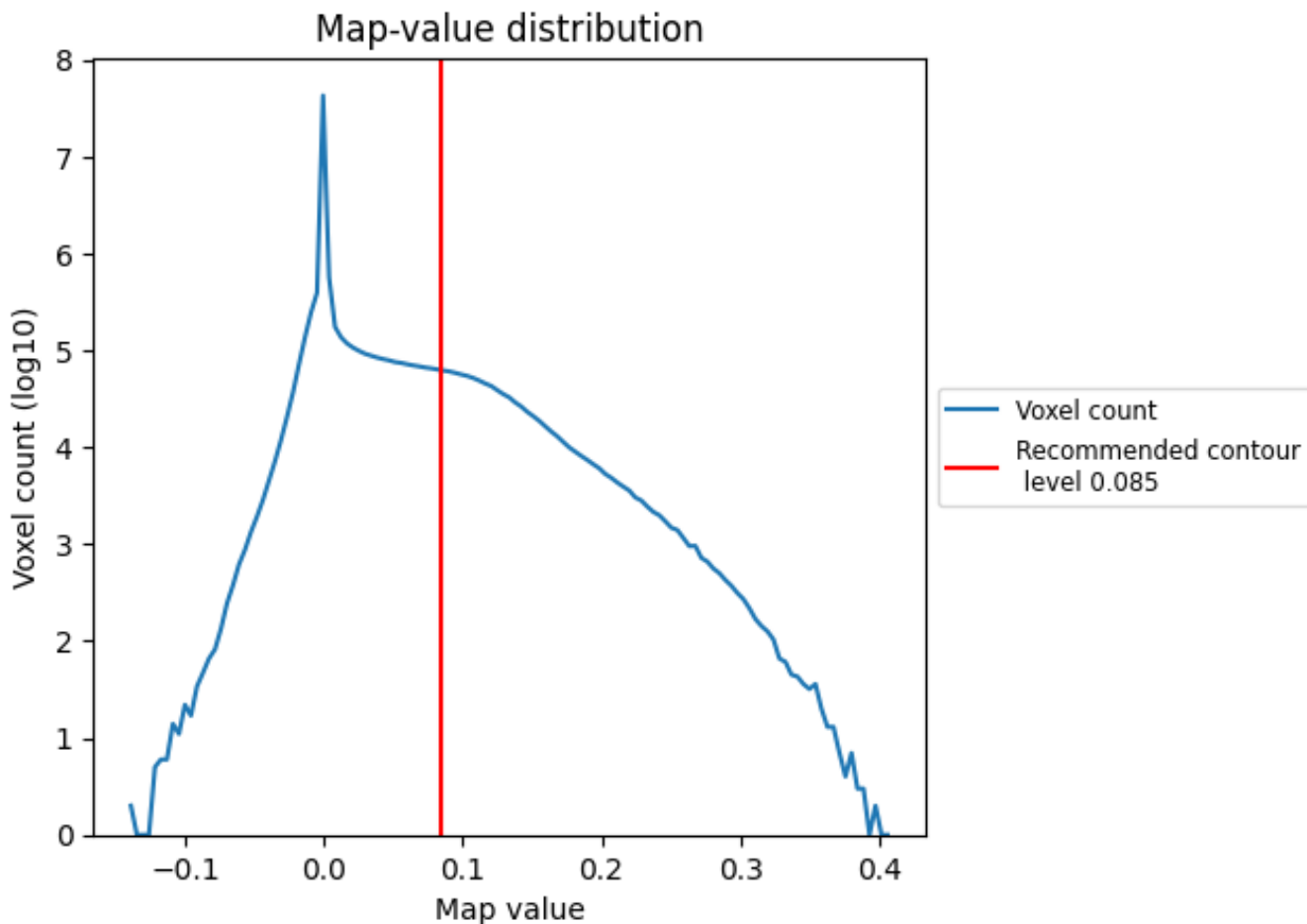
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

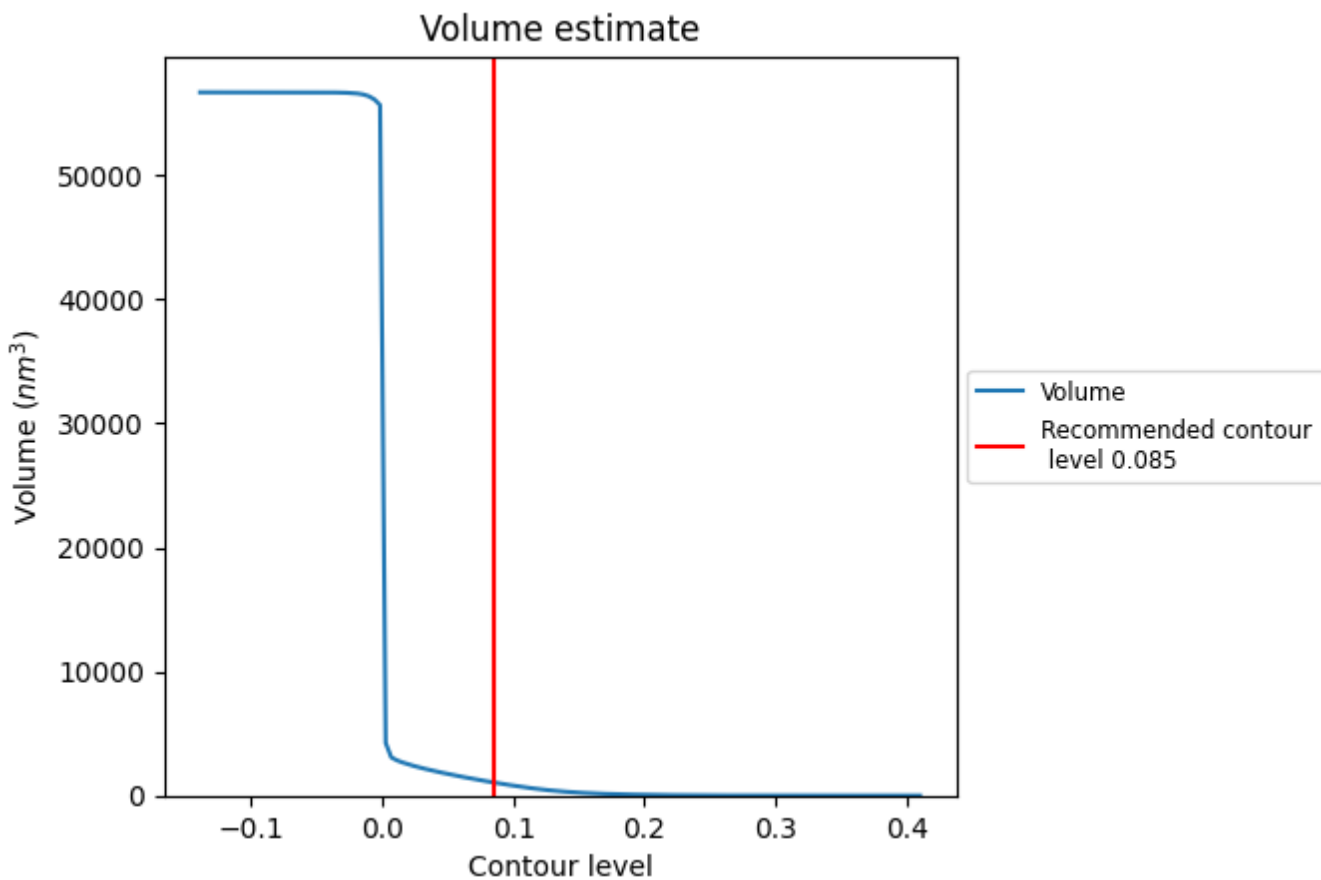
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

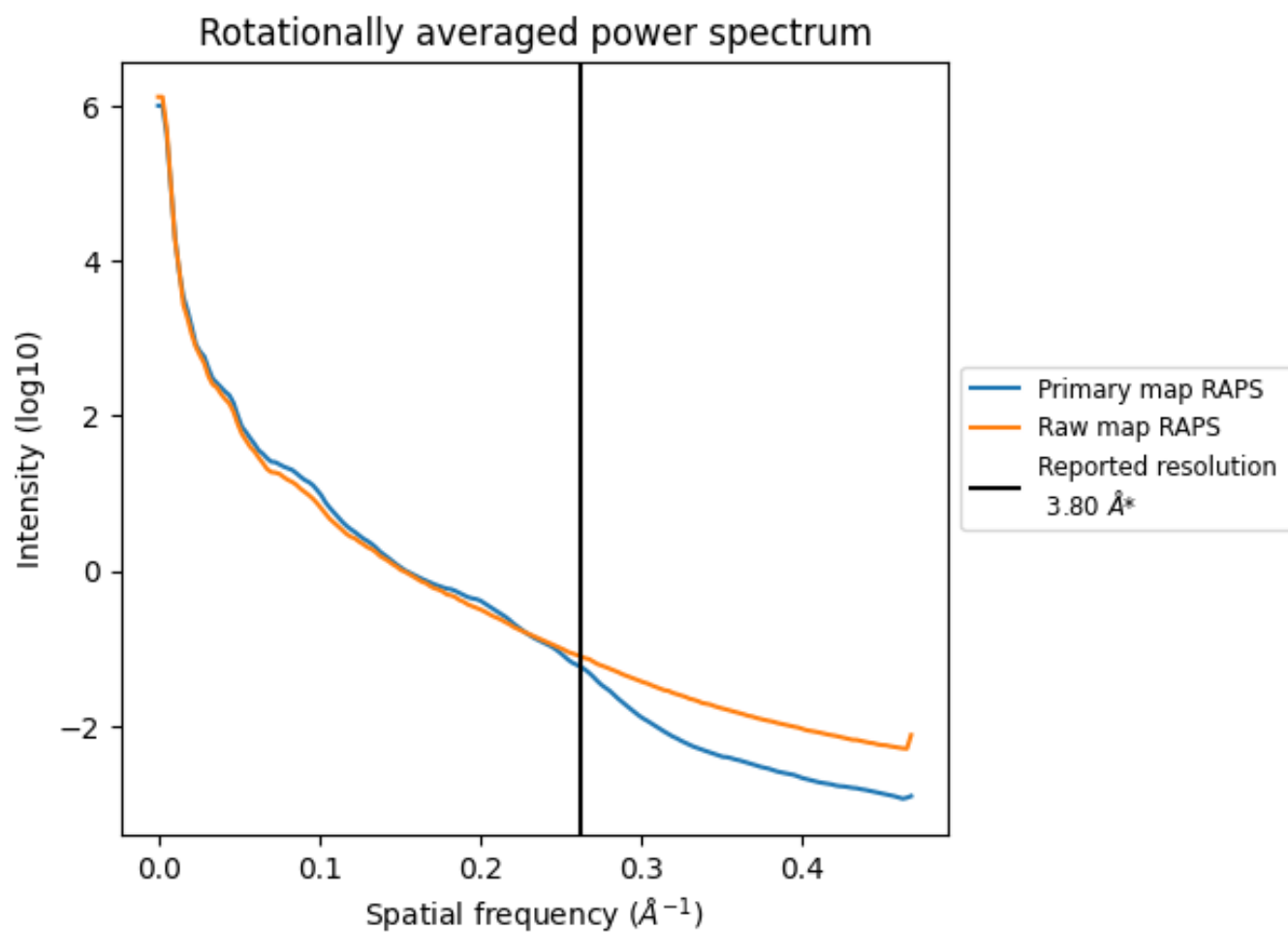
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1058 nm³; this corresponds to an approximate mass of 955 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

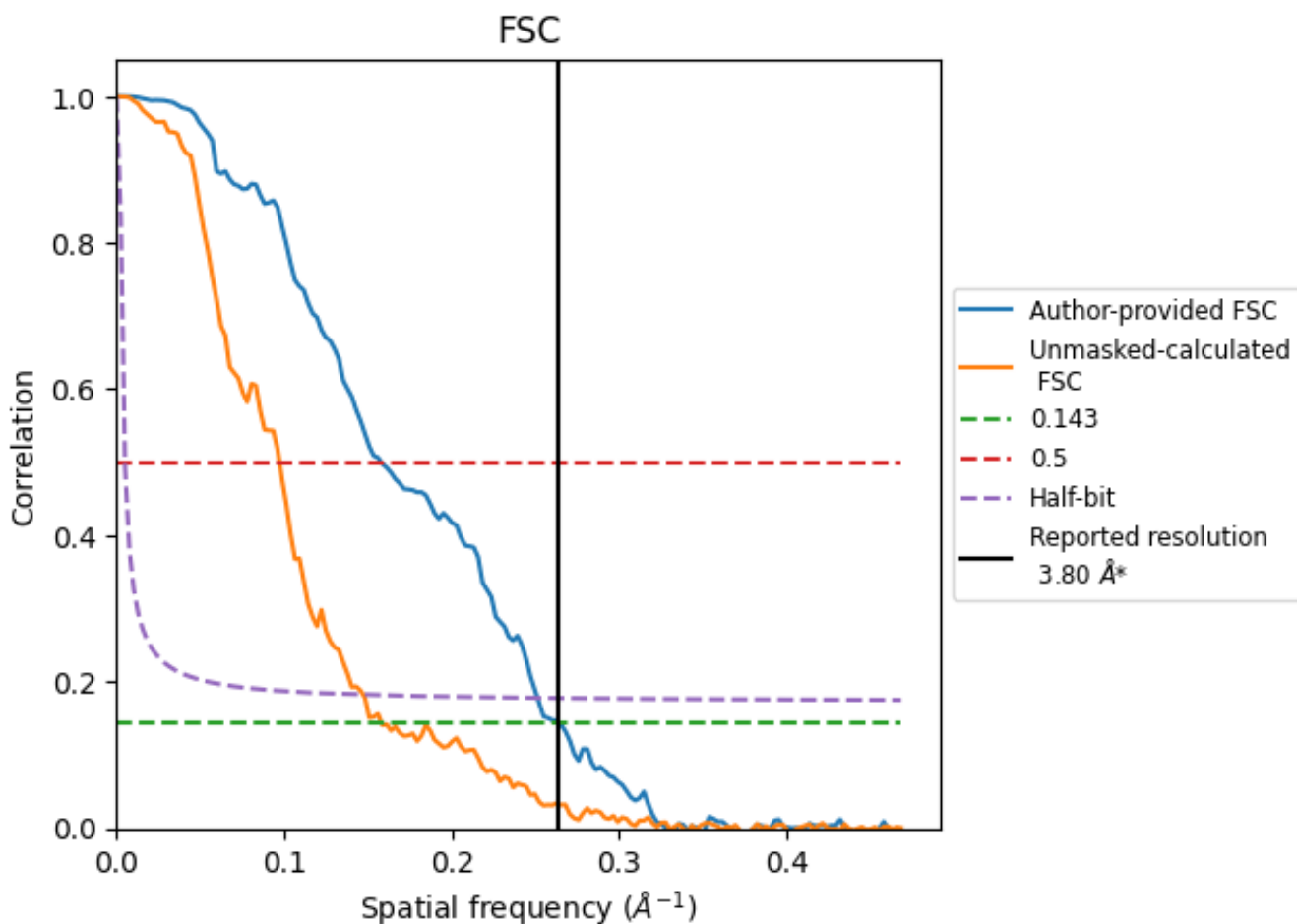


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

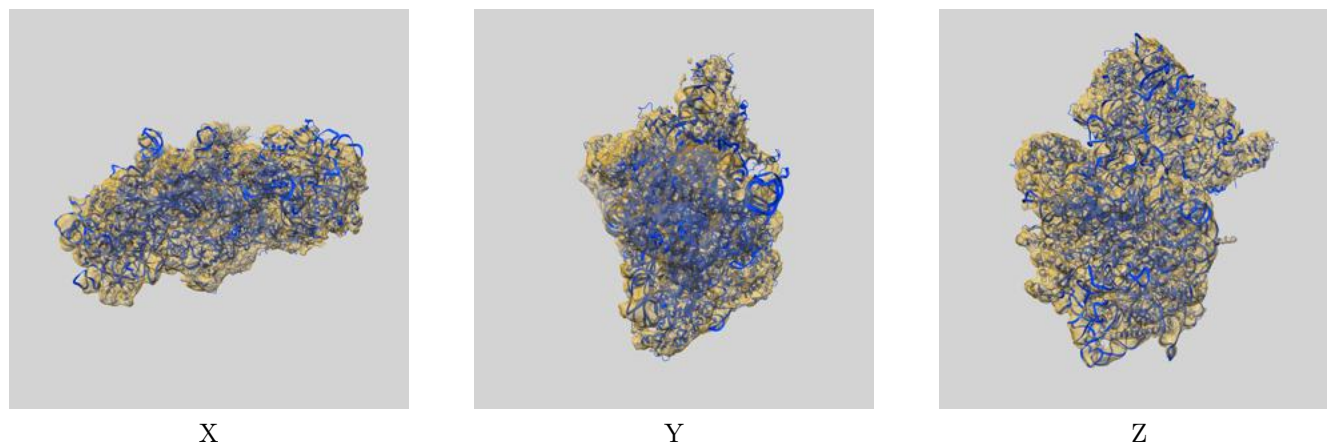
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	6.33	3.97
Unmasked-calculated*	6.31	10.27	6.78

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

9 Map-model fit [i](#)

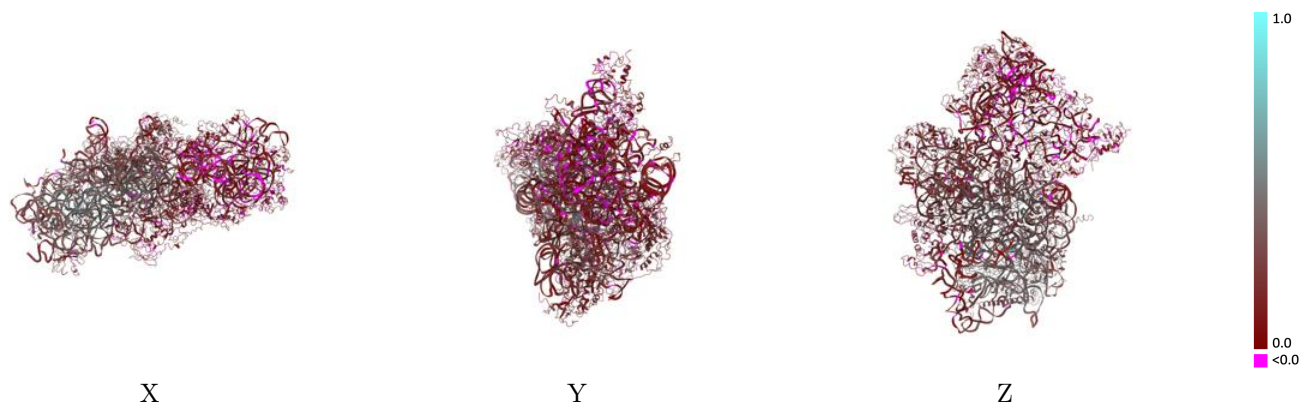
This section contains information regarding the fit between EMDB map EMD-10713 and PDB model 6Y7C. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)



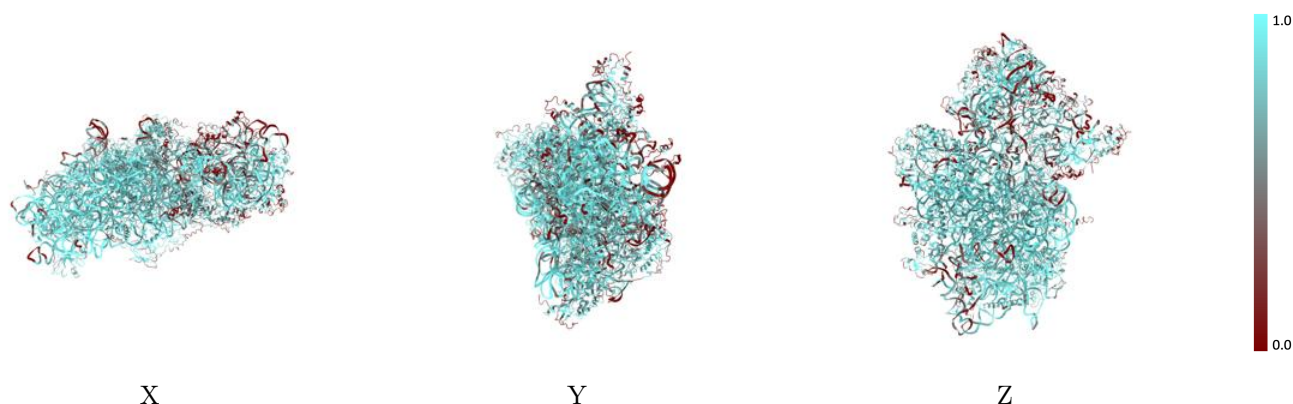
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



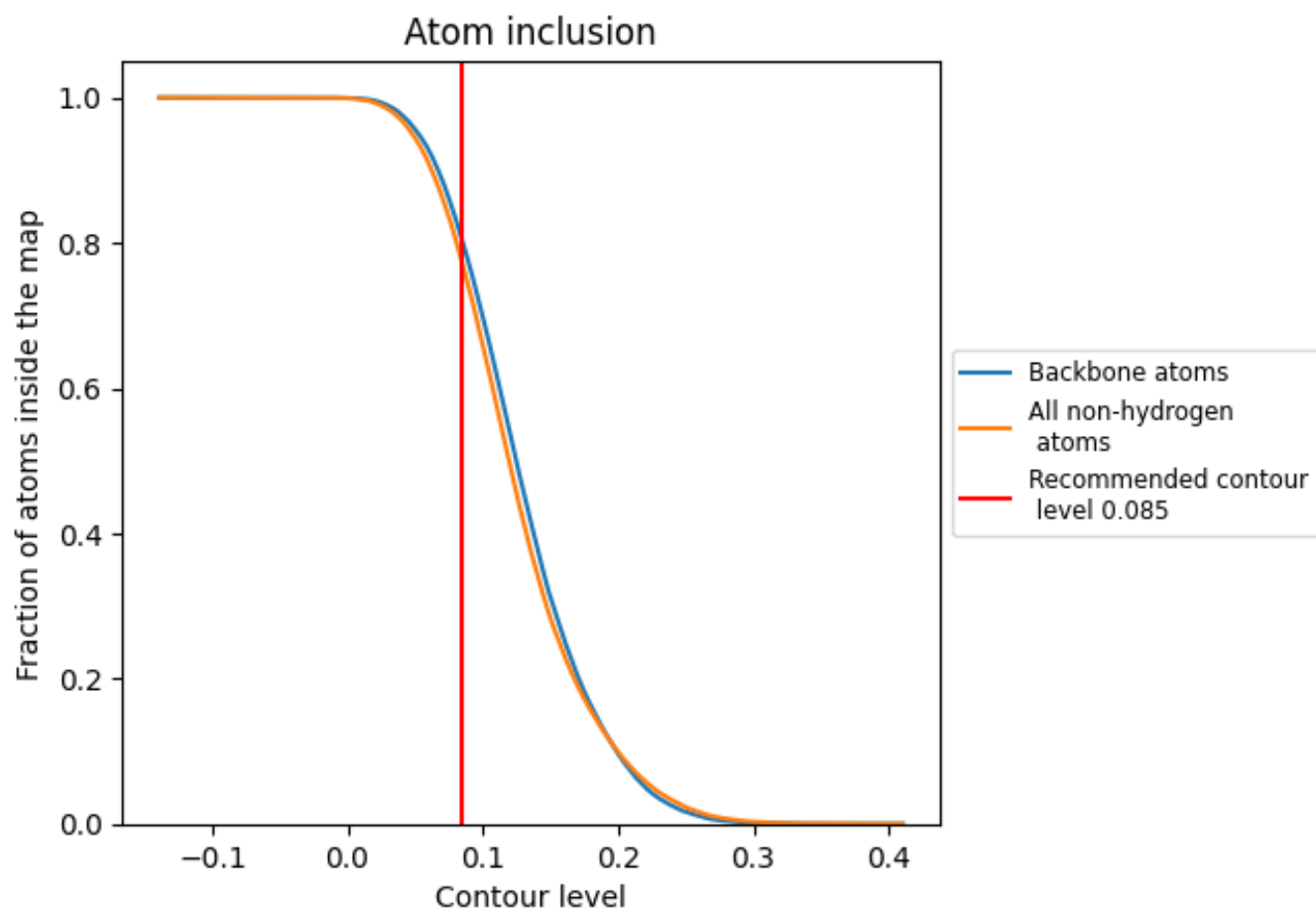
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.085).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 77% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7710	 0.2350
2	 0.8228	 0.2550
A	 0.8483	 0.2370
B	 0.7457	 0.2040
C	 0.8232	 0.2960
E	 0.9106	 0.3860
F	 0.7486	 0.1460
G	 0.8133	 0.2940
H	 0.7180	 0.1730
I	 0.8252	 0.3600
J	 0.8537	 0.3110
L	 0.8393	 0.4070
M	 0.4973	 0.1130
N	 0.7820	 0.2340
O	 0.7522	 0.1890
P	 0.6138	 0.1420
Q	 0.6622	 0.1260
R	 0.4555	 0.1930
S	 0.5677	 0.1420
T	 0.8085	 0.1350
U	 0.2226	 0.1450
V	 0.8677	 0.2430
W	 0.9217	 0.3060
X	 0.8172	 0.2890
Y	 0.7646	 0.3030
Z	 0.5242	 0.1520
b	 0.5963	 0.2230
c	 0.5702	 0.1390
d	 0.3286	 0.1210
e	 0.4641	 0.2070
h	 0.7637	 0.2230
i	 0.6182	 0.1120
j	 0.3290	 0.1540
l	 0.6651	 0.1440
t	 0.7203	 0.1630

