



Full wwPDB EM Validation Report ⓘ

Dec 17, 2022 – 09:59 pm GMT

PDB ID : 6ZU9
EMDB ID : EMD-11439
Title : Structure of a yeast ABCE1-bound 48S initiation complex
Authors : Kratzat, H.; Mackens-Kiani, T.; Cheng, J.; Berninghausen, O.; Becker, T.; Beckmann, R.
Deposited on : 2020-07-22
Resolution : 6.20 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
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

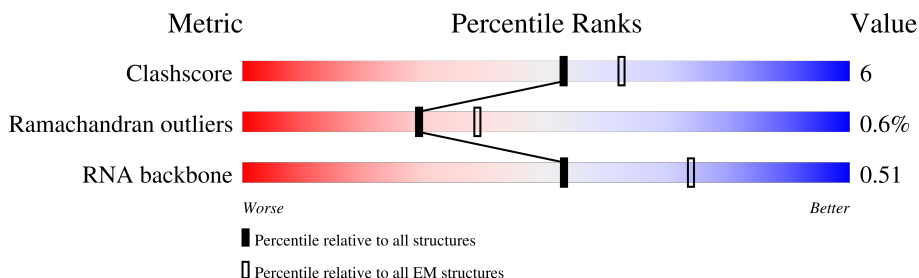
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 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.





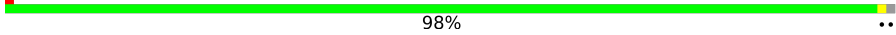
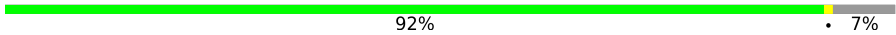
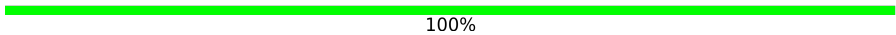
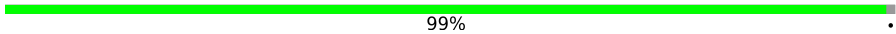
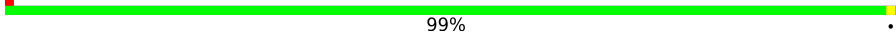
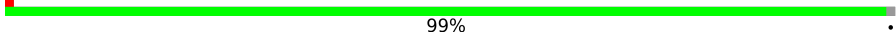

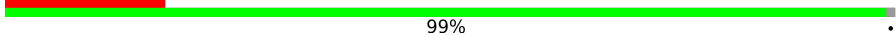



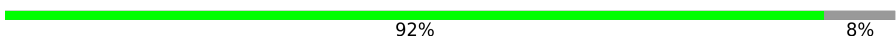


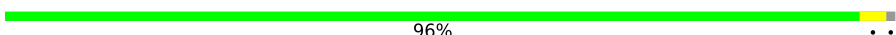

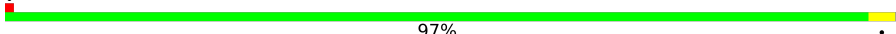
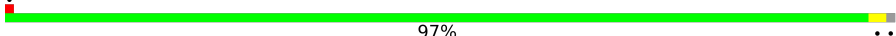


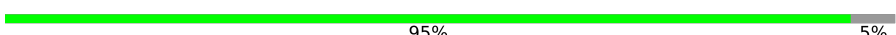

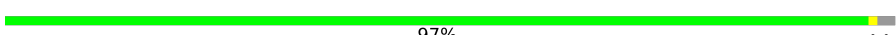
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
RNA backbone	4643	859

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	1800	
2	P	252	
3	Q	255	
4	R	254	
5	S	261	
6	T	236	
7	U	190	
8	V	200	



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Mol	Chain	Length	Quality of chain
9	W	197	
10	X	155	
11	Y	151	
12	Z	136	
13	a	87	
14	b	130	
15	c	145	
16	d	135	
17	e	119	
18	f	82	
19	g	63	
20	E	141	
21	B	240	
22	C	225	
23	D	105	
24	F	143	
25	H	143	
26	I	136	
27	J	146	
28	K	144	
29	L	121	
30	M	108	
31	N	56	
32	O	152	
33	h	319	

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Mol	Chain	Length	Quality of chain
34	i	67	 94% 6%
35	l	347	 84% 95% 5%
36	r	135	 38% 39% 61%
37	1	75	 7% 51% 31% 16%
38	m	405	 13% 36% 64%
39	o	964	 54% 45%
40	p	763	 22% 83% 15%
41	q	812	 77% 22%
42	3	8	 12% 38% 38% 12% 12%
43	A	153	 61% 5% 34%
44	k	608	 8% 94% 5%

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 78384 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
1	2	1771	Total	C	N	O	P	0	0
			37739	16872	6683	12413	1771		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
2	P	206	Total	C	N	O	0	0
			1020	608	206	206		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Q	226	Total	C	N	O	0	0
			1119	667	226	226		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	R	216	Total	C	N	O	0	0
			1058	626	216	216		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	S	258	Total	C	N	O	0	0
			1267	751	258	258		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	T	228	Total	C	N	O	0	0
			1123	667	228	228		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	U	184	Total	C	N	O	0	0
			913	545	184	184		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	V	187	Total	C	N	O	0	0
			919	545	187	187		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	W	184	Total	C	N	O	0	0
			910	542	184	184		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	X	142	Total	C	N	O	0	0
			702	418	142	142		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	147	ALA	GLY	conflict	UNP P0CX47

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	Y	150	Total	C	N	O	0	0
			742	442	150	150		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Z	127	Total	C	N	O	0	0
			620	366	127	127		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	a	87	Total	C	N	O	0	0
			429	255	87	87		

- Molecule 14 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	b	129	Total	C	N	O	0	0
			634	376	129	129		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	c	144	Total	C	N	O	0	0
			704	416	144	144		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	d	134	Total	C	N	O	0	0
			661	393	134	134		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	e	97	Total	C	N	O	0	0
			482	288	97	97		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	f	81	Total	C	N	O	0	0
			400	238	81	81		

- Molecule 19 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	g	53	Total	C	N	O	0	0
			261	155	53	53		

- Molecule 20 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	E	117	Total	C	N	O	0	0
			576	342	117	117		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	137	SER	ARG	conflict	UNP Q01855

- Molecule 21 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	B	222	Total	C	N	O	0	0
			1093	649	222	222		

- Molecule 22 is a protein called Rps5p.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	C	206	Total	C	N	O	0	0
			1020	608	206	206		

- Molecule 23 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	D	92	Total	C	N	O	0	0
			456	272	92	92		

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	F	121	Total	C	N	O	0	0
			595	353	121	121		

- Molecule 25 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	H	141	Total	C	N	O	0	0
			693	411	141	141		

- Molecule 26 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	I	121	Total	C	N	O	0	0
			600	358	121	121		

- Molecule 27 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	J	145	Total	C	N	O	0	0
			715	425	145	145		

- Molecule 28 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	K	143	Total	C	N	O	0	0
			700	414	143	143		

- Molecule 29 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	L	100	Total	C	N	O	0	0
			496	296	100	100		

- Molecule 30 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	M	82	Total	C	N	O	0	0
			407	243	82	82		

- Molecule 31 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	N	53	Total	C	N	O	0	0
			260	154	53	53		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	O	73	Total	C	N	O	0	0
			361	215	73	73		

- Molecule 33 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	h	312	Total	C	N	O	0	0
			1538	914	312	312		

- Molecule 34 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	i	63	Total	C	N	O	0	0
			310	184	63	63		

- Molecule 35 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	l	330	Total	C	N	O	0	0
			1624	964	330	330		

- Molecule 36 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	r	53	Total	C	N	O	0	0
			261	155	53	53		

- Molecule 37 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1	75	Total	C	N	O	P	0	0
			1639	734	298	531	76		

- Molecule 38 is a protein called Eukaryotic translation initiation factor 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	147	Total	C	N	O	0	0
			726	432	147	147		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	183	LEU	PRO	conflict	UNP P38431

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	o	529	Total	C	N	O	0	0
			2632	1574	529	529		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	p	646	Total	C	N	O	0	0
			3201	1909	646	646		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	q	636	Total	C	N	O	0	0
			3169	1897	636	636		

- Molecule 42 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3	8	Total	C	N	O	P	0	0
			171	77	32	54	8		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 1A.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	A	101	Total	C	N	O	0	0
			497	295	101	101		

- Molecule 44 is a protein called Translation initiation factor RLI1.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	k	579	Total	C	N	O	0	0
			2860	1702	579	579		

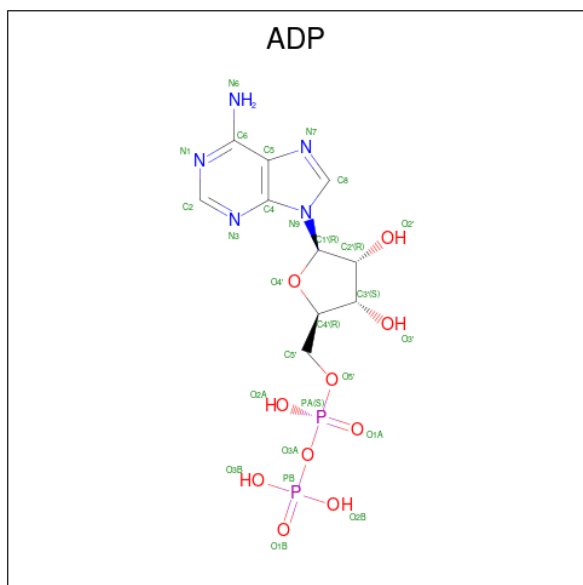
- Molecule 45 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	2	2	Total	Mg	0
			2	2	
45	k	2	Total	Mg	0
			2	2	

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

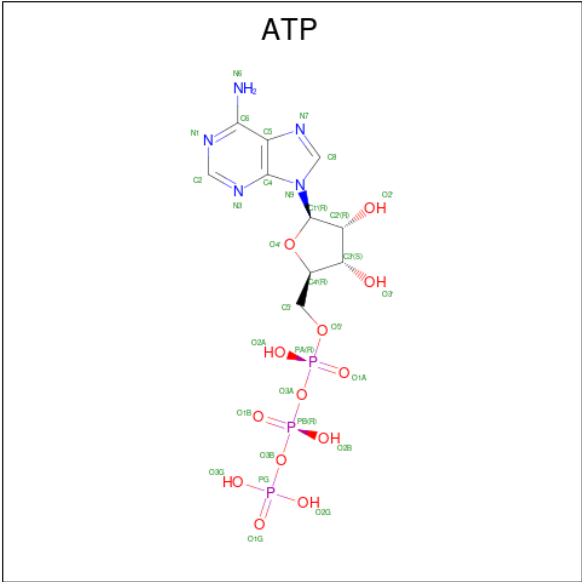
Mol	Chain	Residues	Atoms	AltConf
46	N	1	Total Zn 1 1	0
46	O	1	Total Zn 1 1	0
46	m	1	Total Zn 1 1	0

- Molecule 47 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).



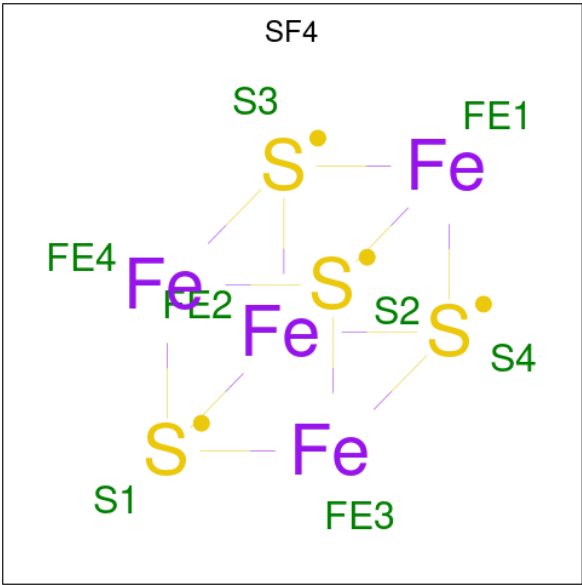
Mol	Chain	Residues	Atoms					AltConf
47	k	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 48 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					AltConf
48	k	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 49 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

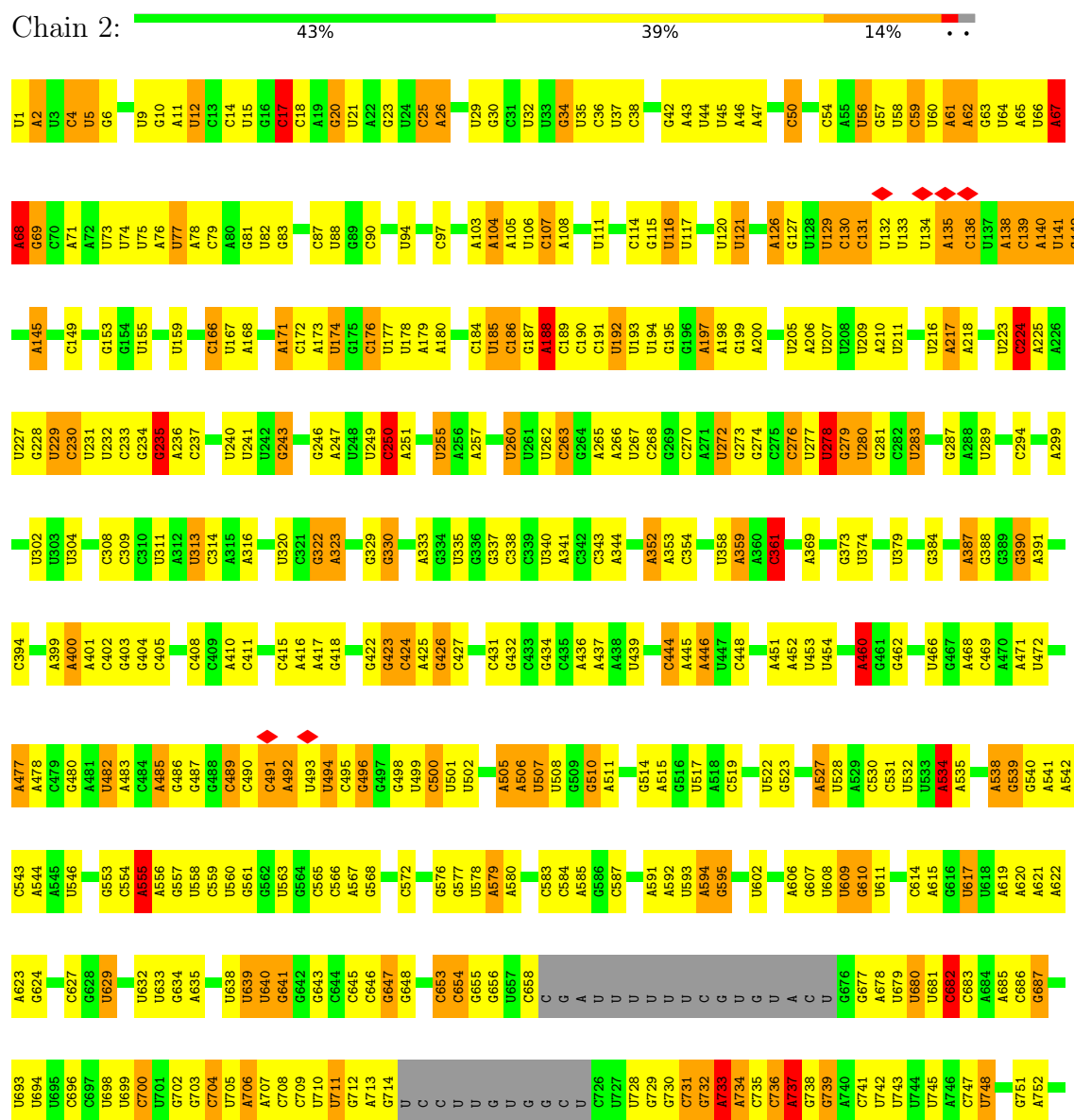


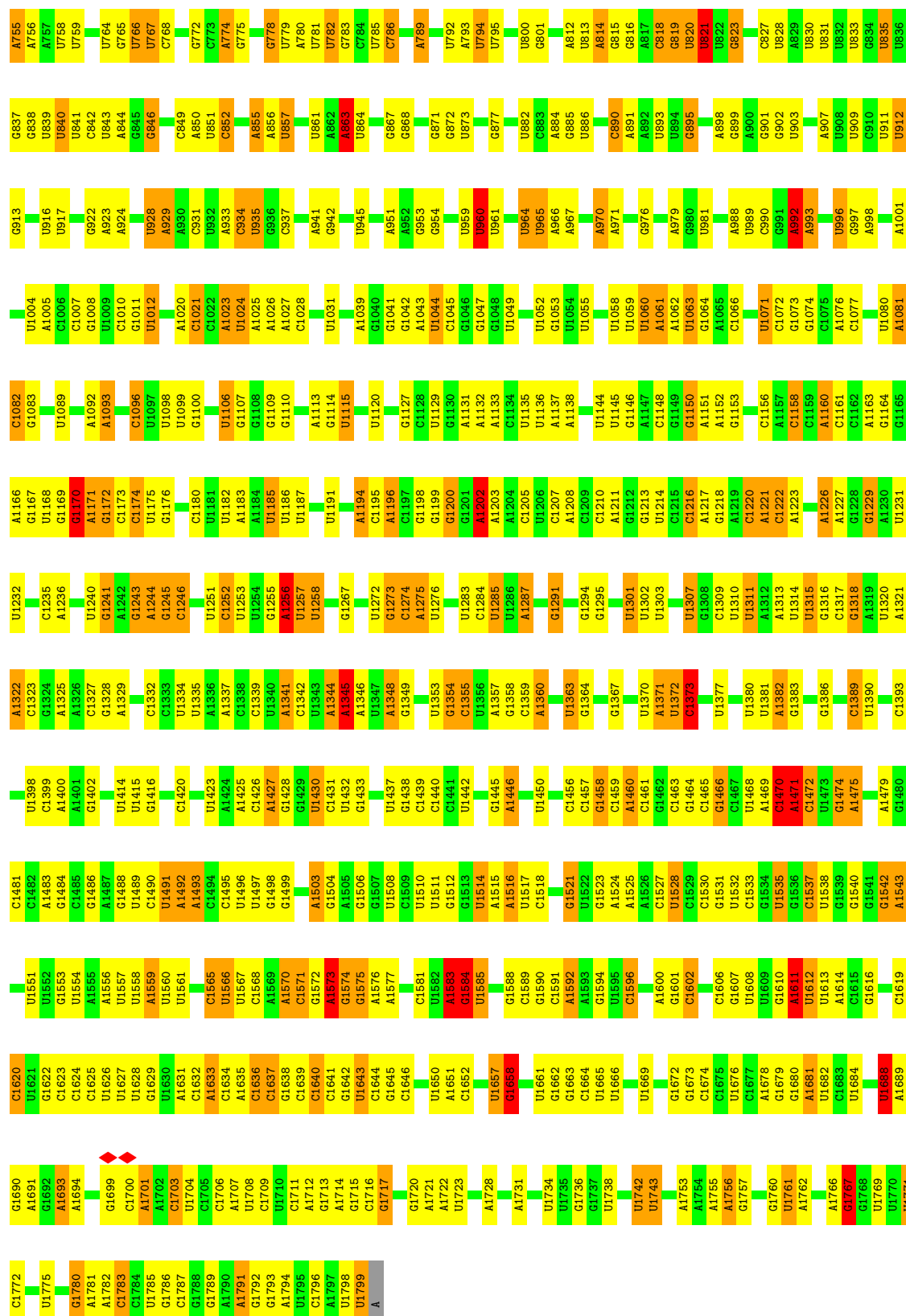
Mol	Chain	Residues	Atoms			AltConf
49	k	1	Total	Fe	S	0
			16	8	8	
49	k	1	Total	Fe	S	0
			16	8	8	

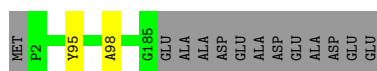
3 Residue-property plots

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

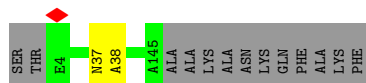
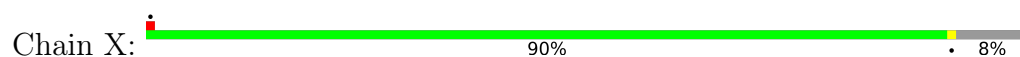
• Molecule 1: 18S ribosomal RNA







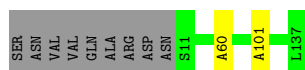
- Molecule 10: 40S ribosomal protein S11-A



- Molecule 11: 40S ribosomal protein S13



- Molecule 12: 40S ribosomal protein S14-A



- Molecule 13: 40S ribosomal protein S21-A



There are no outlier residues recorded for this chain.

- Molecule 14: 40S ribosomal protein S22-A

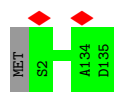


- Molecule 15: 40S ribosomal protein S23-A

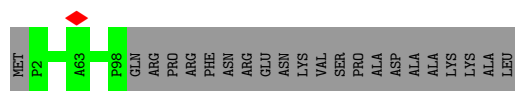
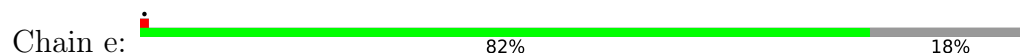


- Molecule 16: 40S ribosomal protein S24-A

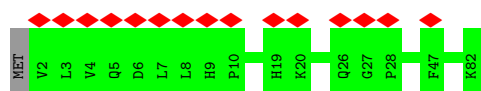




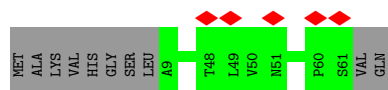
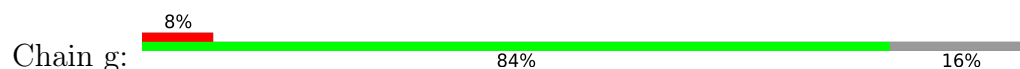
- Molecule 17: 40S ribosomal protein S26-A



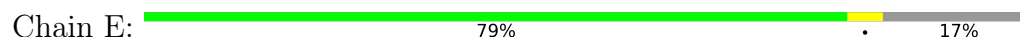
- Molecule 18: 40S ribosomal protein S27-A



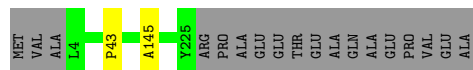
- Molecule 19: 40S ribosomal protein S30-A



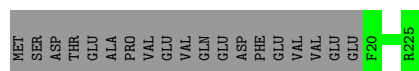
- Molecule 20: 40S ribosomal protein S15



- Molecule 21: 40S ribosomal protein S3

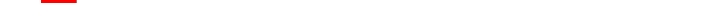


- Molecule 22: Rps5p



- Molecule 23: 40S ribosomal protein S10-A

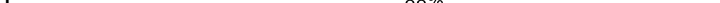
M1 V55 L68 I92 GLN GLU ARG ASN PRO THR GLN ARG PRO GLN ARG ARG TYR

- Chain F:  81% 15%

MET
 SER
 ASP
 VAL
 GLU
 GLU
 VAL
 VAL
 GLU
 VAL
 GLN
 GLU
 GLU
 THR
 VAL
 VAL
 GLU
 GLN
 THR
 ALA
 GLU
 GLU
 T23
 T2
 P82
 E83
 N84
 K85
 R108
 E109
 G110
 M111
 A112
 W126
 Q143

- Chain H:  96%

MET
SER
A3
V39
E40
E125
R143

- Chain I:  88% • 11%

MET	G2	R95	SER	ASN	GLY	VAL	L100	A126	GLN	ARG	ASP	ARG	ARG	TYR	ARG	LYS	ARG	VAL
-----	----	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain J: 97%

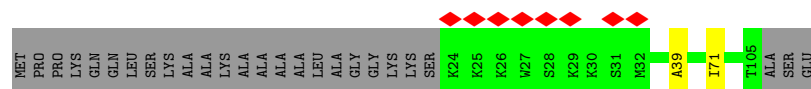
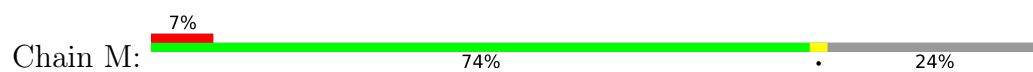
- Chain K:  97%

Diagram illustrating the protein structure with residues MET, P2, G72, G98, and E144. A red diamond is positioned above the E144 residue.

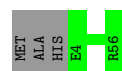
- Chain L: 83% 17%

MET	SER	ASP	PHE	GLN	LYS	GLU	LYS	VAL	GLU	GLU	GLN	GLU	GLN	GLN	GLN	GLN	ILE	I 20	A 119	SER	ASN
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-------	-----	-----

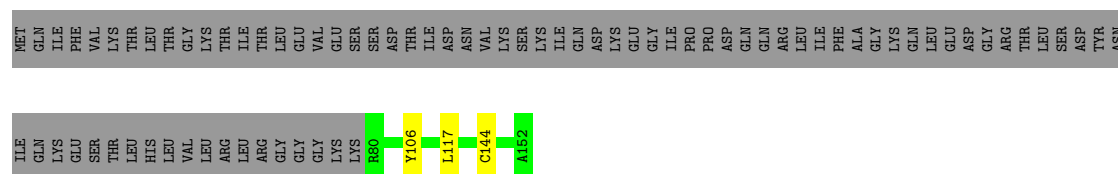
- 



- Molecule 31: 40S ribosomal protein S29-A



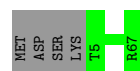
- Molecule 32: Ubiquitin-40S ribosomal protein S31



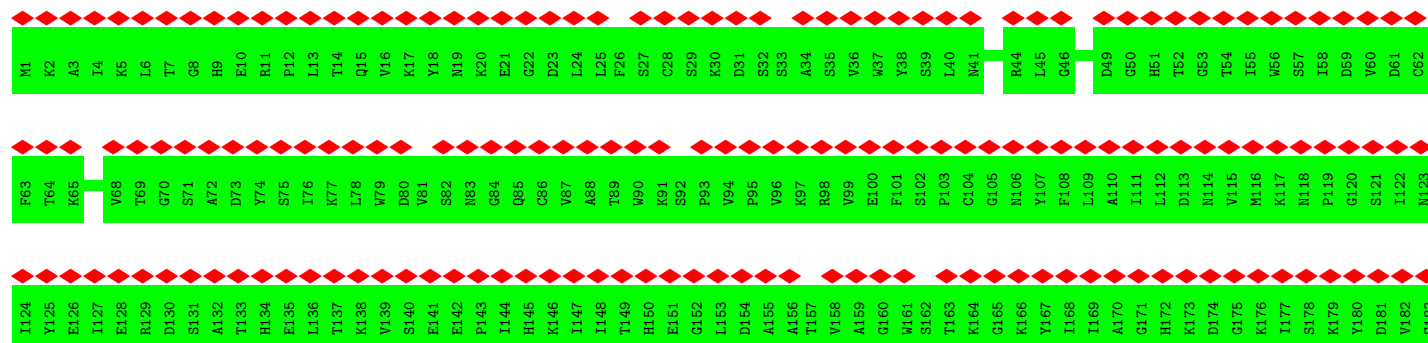
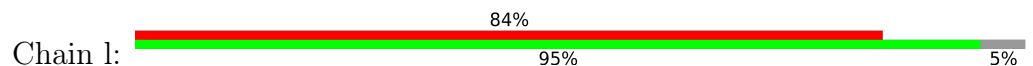
- Molecule 33: Guanine nucleotide-binding protein subunit beta-like protein

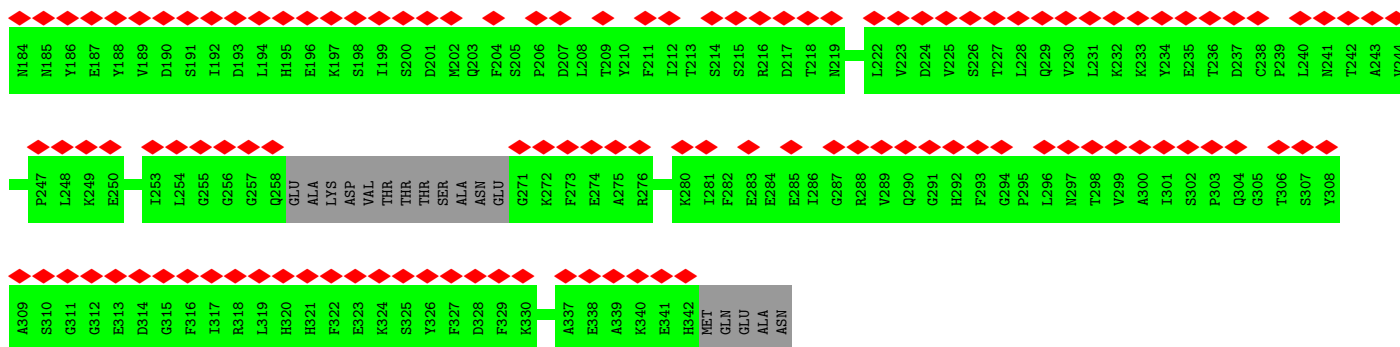


- Molecule 34: 40S ribosomal protein S28-B

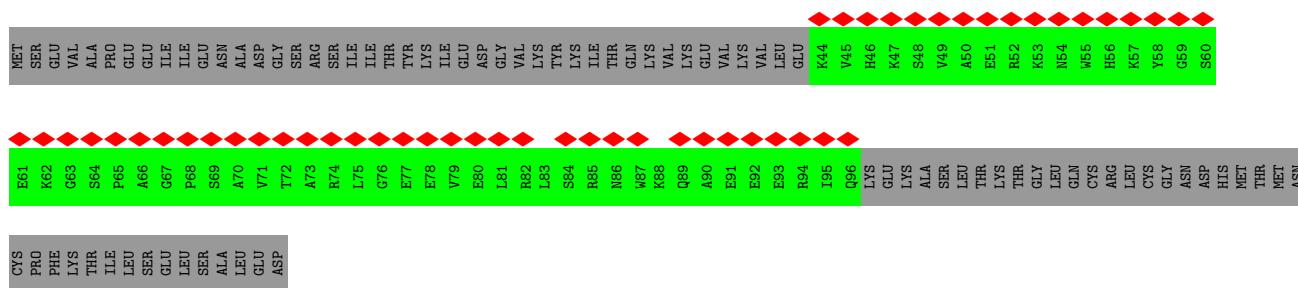


- Molecule 35: Eukaryotic translation initiation factor 3 subunit I





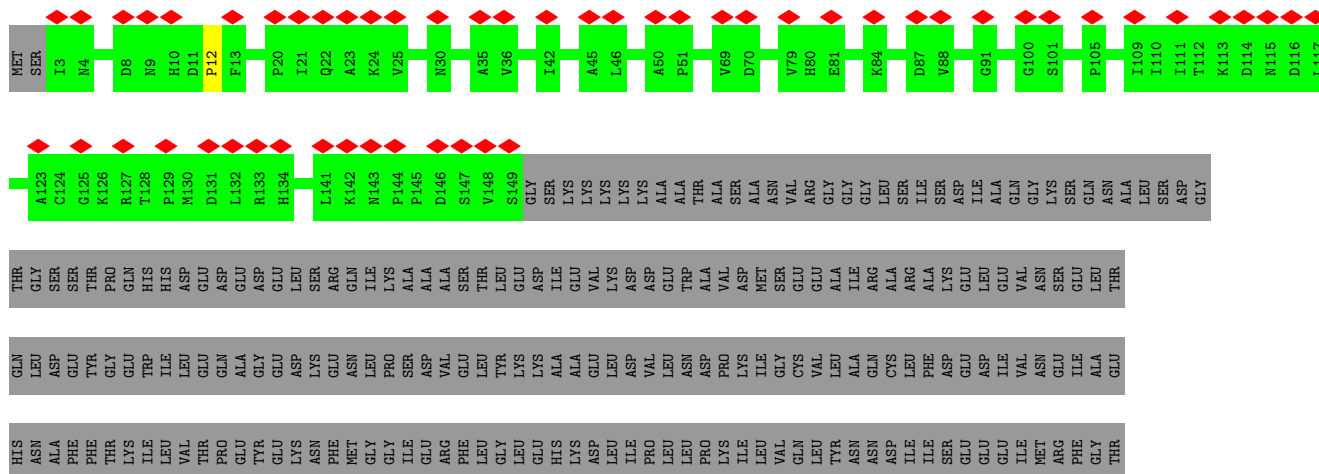
- Molecule 36: Eukaryotic translation initiation factor 3 subunit G



- Molecule 37: tRNA

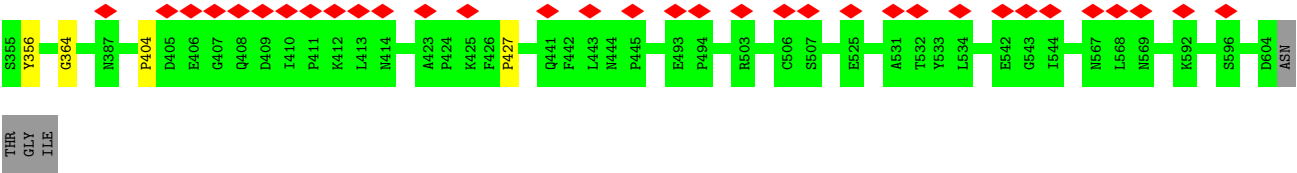


- Molecule 38: Eukaryotic translation initiation factor 5



Chain o:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12937	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	0.059	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.009	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, 2MG, ZN, M2G, 1MA, H2U, MG, 1MG, ADP, 5MC, RIA, G7M, T6A, ATP

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	0.66	2/42211 (0.0%)	1.50	865/65773 (1.3%)
2	P	0.32	0/1019	0.63	0/1419
3	Q	0.34	0/1117	0.73	1/1554 (0.1%)
4	R	0.33	0/1057	0.67	0/1465
5	S	0.35	0/1266	0.72	1/1757 (0.1%)
6	T	0.33	0/1122	0.62	0/1559
7	U	0.35	0/912	0.69	0/1271
8	V	0.33	0/917	0.62	0/1271
9	W	0.33	0/909	0.68	0/1265
10	X	0.34	0/701	0.69	0/975
11	Y	0.33	0/741	0.64	1/1031 (0.1%)
12	Z	0.34	0/619	0.72	0/856
13	a	0.35	0/428	0.71	0/594
14	b	0.32	0/633	0.69	0/878
15	c	0.36	0/703	0.67	0/973
16	d	0.34	0/660	0.63	0/917
17	e	0.32	0/481	0.69	0/670
18	f	0.40	0/399	0.95	0/554
19	g	0.36	0/260	0.76	0/360
20	E	0.34	0/575	0.66	0/798
21	B	0.35	0/1092	0.71	1/1517 (0.1%)
22	C	0.31	0/1019	0.64	0/1419
23	D	0.33	0/455	0.73	0/633
24	F	0.34	0/594	0.82	0/824
25	H	0.35	0/692	0.66	1/960 (0.1%)
26	I	0.30	0/598	0.58	0/831
27	J	0.34	0/714	0.65	0/992
28	K	0.35	0/699	0.64	0/968
29	L	0.34	0/495	0.62	0/689
30	M	0.33	0/406	0.74	0/565
31	N	0.34	0/259	0.68	0/358
32	O	0.37	0/360	0.87	0/500

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.34	0/1537	0.70	0/2137
34	i	0.36	0/309	0.77	0/428
35	l	0.31	0/1622	0.52	0/2252
36	r	0.26	0/260	0.47	0/360
37	1	0.35	1/1529 (0.1%)	0.67	0/2376
38	m	0.38	0/725	0.56	0/1008
39	o	0.40	0/2627	0.57	1/3662 (0.0%)
40	p	0.40	0/3197	0.57	0/4452
41	q	0.50	0/3163	0.58	0/4412
42	3	0.57	1/191 (0.5%)	1.13	2/295 (0.7%)
43	A	0.35	0/495	0.63	0/685
44	k	0.57	0/2858	0.98	0/3977
All	All	0.54	4/82626 (0.0%)	1.19	873/122240 (0.7%)

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
7	U	0	1
24	F	0	2
25	H	0	1
32	O	0	1
33	h	0	2
40	p	0	2
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1	1	A	OP3-P	-10.01	1.49	1.61
42	3	28	A	O3'-P	6.59	1.69	1.61
1	2	1360	A	N9-C4	-5.79	1.34	1.37
1	2	1113	A	N9-C4	-5.39	1.34	1.37

All (873) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1640	C	C5-C6-N1	14.40	128.20	121.00
1	2	1389	C	C2-N1-C1'	12.62	132.69	118.80
1	2	656	G	C8-N9-C1'	-12.23	111.09	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1072	C	C6-N1-C2	-11.75	115.60	120.30
1	2	1527	C	C2-N1-C1'	11.68	131.64	118.80
1	2	656	G	C4-N9-C1'	11.60	141.59	126.50
1	2	1640	C	C4-C5-C6	-11.14	111.83	117.40
1	2	1640	C	C2-N3-C4	10.92	125.36	119.90
1	2	1560	U	N1-C2-O2	10.79	130.35	122.80
1	2	583	C	C6-N1-C2	-10.51	116.10	120.30
1	2	782	U	N3-C2-O2	-10.50	114.85	122.20
1	2	517	U	N3-C2-O2	-10.49	114.85	122.20
1	2	653	C	N1-C2-O2	10.32	125.09	118.90
1	2	354	C	C5-C6-N1	10.30	126.15	121.00
1	2	1182	U	N1-C2-O2	10.25	129.98	122.80
1	2	1389	C	C5-C6-N1	10.17	126.09	121.00
42	3	28	A	P-O3'-C3'	10.16	131.89	119.70
1	2	1527	C	N1-C2-O2	10.14	124.98	118.90
1	2	140	A	O5'-P-OP2	10.13	122.86	110.70
1	2	517	U	N1-C2-O2	10.13	129.89	122.80
1	2	1560	U	N3-C2-O2	-10.07	115.15	122.20
1	2	1235	C	C6-N1-C2	-9.96	116.31	120.30
1	2	121	U	N3-C2-O2	-9.95	115.24	122.20
1	2	959	U	N3-C2-O2	-9.95	115.24	122.20
1	2	840	U	N3-C2-O2	-9.83	115.32	122.20
1	2	840	U	N1-C2-O2	9.82	129.68	122.80
1	2	1571	C	C5-C6-N1	9.80	125.90	121.00
1	2	121	U	N1-C2-O2	9.77	129.64	122.80
1	2	736	C	C6-N1-C2	-9.62	116.45	120.30
1	2	782	U	N1-C2-O2	9.51	129.46	122.80
1	2	1334	U	N3-C2-O2	-9.50	115.55	122.20
1	2	1458	G	N3-C4-C5	-9.50	123.85	128.60
1	2	1182	U	N3-C2-O2	-9.48	115.56	122.20
1	2	185	U	N3-C2-O2	-9.43	115.60	122.20
42	3	28	A	C2'-C3'-O3'	9.42	130.23	109.50
1	2	1307	U	N1-C2-O2	9.39	129.38	122.80
1	2	959	U	N1-C2-O2	9.39	129.37	122.80
1	2	453	U	C5-C6-N1	9.35	127.38	122.70
1	2	185	U	N1-C2-O2	9.34	129.34	122.80
1	2	583	C	C5-C6-N1	9.25	125.63	121.00
1	2	354	C	C6-N1-C2	-9.20	116.62	120.30
1	2	166	C	N1-C2-O2	9.20	124.42	118.90
1	2	224	C	C6-N1-C2	-9.17	116.63	120.30
1	2	14	C	C6-N1-C2	-9.12	116.65	120.30
1	2	1571	C	C6-N1-C2	-9.06	116.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	530	C	N1-C2-O2	9.04	124.33	118.90
1	2	1307	U	N3-C2-O2	-9.03	115.88	122.20
1	2	1222	C	C6-N1-C2	-8.96	116.71	120.30
1	2	1082	C	C2-N1-C1'	8.93	128.62	118.80
1	2	1389	C	N1-C2-O2	8.83	124.20	118.90
1	2	1389	C	C6-N1-C1'	-8.78	110.27	120.80
1	2	260	U	N3-C2-O2	-8.78	116.06	122.20
1	2	302	U	N3-C2-O2	-8.77	116.06	122.20
1	2	116	U	N3-C2-O2	-8.74	116.08	122.20
1	2	186	C	C2-N1-C1'	8.74	128.41	118.80
1	2	1332	C	C6-N1-C2	-8.73	116.81	120.30
1	2	50	C	N1-C2-O2	8.67	124.10	118.90
1	2	794	U	N1-C2-O2	8.65	128.86	122.80
1	2	121	U	C2-N1-C1'	8.65	128.08	117.70
1	2	224	C	N1-C2-O2	8.63	124.08	118.90
1	2	782	U	C2-N1-C1'	8.61	128.03	117.70
1	2	1145	U	C2-N1-C1'	8.58	127.99	117.70
1	2	1307	U	C2-N1-C1'	8.55	127.97	117.70
1	2	1458	G	N3-C4-N9	8.55	131.13	126.00
1	2	653	C	N3-C2-O2	-8.54	115.92	121.90
1	2	1560	U	C2-N1-C1'	8.53	127.94	117.70
1	2	1458	G	C4-N9-C1'	8.49	137.54	126.50
1	2	120	U	N3-C2-O2	-8.48	116.27	122.20
1	2	1528	U	N3-C2-O2	-8.43	116.30	122.20
1	2	1676	U	N1-C2-O2	8.43	128.70	122.80
1	2	1066	C	N1-C2-O2	8.41	123.94	118.90
1	2	736	C	C5-C6-N1	8.36	125.18	121.00
1	2	1214	U	N3-C2-O2	-8.36	116.35	122.20
1	2	1639	C	N1-C2-O2	8.34	123.90	118.90
1	2	1527	C	C5-C6-N1	8.31	125.16	121.00
1	2	322	G	P-O3'-C3'	8.31	129.68	119.70
1	2	1063	U	N1-C2-O2	8.29	128.60	122.80
1	2	1527	C	C6-N1-C1'	-8.23	110.93	120.80
1	2	1389	C	C6-N1-C2	-8.22	117.01	120.30
1	2	656	G	C6-C5-N7	-8.21	125.47	130.40
1	2	1528	U	N1-C2-O2	8.21	128.55	122.80
1	2	189	C	N1-C2-O2	8.21	123.83	118.90
1	2	224	C	N3-C2-O2	-8.16	116.19	121.90
1	2	1098	U	O5'-P-OP1	-8.14	98.37	105.70
1	2	453	U	N1-C2-O2	8.14	128.50	122.80
1	2	176	C	N1-C2-O2	8.13	123.78	118.90
1	2	794	U	N3-C2-O2	-8.12	116.52	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	530	C	N3-C2-O2	-8.09	116.23	121.90
1	2	267	U	N3-C2-O2	-8.08	116.55	122.20
1	2	584	C	C6-N1-C2	-8.08	117.07	120.30
1	2	1301	U	N3-C2-O2	-8.07	116.55	122.20
1	2	1220	C	C6-N1-C2	-8.05	117.08	120.30
1	2	283	U	N1-C2-O2	8.03	128.42	122.80
1	2	453	U	N3-C2-O2	-8.01	116.59	122.20
1	2	861	U	C2-N1-C1'	8.00	127.30	117.70
1	2	1472	C	O5'-P-OP2	-7.96	98.54	105.70
1	2	482	U	N3-C2-O2	-7.93	116.65	122.20
1	2	1007	C	C6-N1-C2	-7.92	117.13	120.30
1	2	1252	C	N1-C2-O2	7.91	123.64	118.90
1	2	283	U	N3-C2-O2	-7.90	116.67	122.20
1	2	482	U	N1-C2-O2	7.89	128.33	122.80
1	2	711	U	P-O3'-C3'	7.88	129.15	119.70
1	2	411	C	C5-C6-N1	7.87	124.94	121.00
1	2	736	C	C2-N1-C1'	7.86	127.45	118.80
1	2	77	U	P-O3'-C3'	7.85	129.12	119.70
1	2	959	U	C2-N1-C1'	7.85	127.12	117.70
1	2	176	C	N3-C2-O2	-7.85	116.41	121.90
1	2	1222	C	C5-C6-N1	7.82	124.91	121.00
1	2	1363	U	N1-C2-O2	7.82	128.27	122.80
1	2	1332	C	C5-C6-N1	7.81	124.90	121.00
1	2	1791	A	P-O3'-C3'	7.80	129.06	119.70
1	2	54	C	C5-C6-N1	7.78	124.89	121.00
1	2	1669	U	N3-C2-O2	-7.76	116.77	122.20
1	2	1252	C	C6-N1-C2	-7.76	117.20	120.30
1	2	1527	C	C6-N1-C2	-7.76	117.20	120.30
1	2	311	U	N1-C2-O2	7.75	128.23	122.80
1	2	1723	U	N3-C2-O2	-7.74	116.78	122.20
1	2	1258	U	N3-C2-O2	-7.72	116.80	122.20
1	2	120	U	N1-C2-O2	7.71	128.20	122.80
1	2	1458	G	C2-N3-C4	7.70	115.75	111.90
1	2	1258	U	N1-C2-O2	7.69	128.18	122.80
1	2	453	U	C2-N1-C1'	7.69	126.93	117.70
1	2	1182	U	C2-N1-C1'	7.68	126.92	117.70
1	2	1596	C	C2-N1-C1'	7.67	127.24	118.80
1	2	1072	C	C5-C6-N1	7.67	124.83	121.00
1	2	1620	C	C5-C6-N1	7.67	124.83	121.00
1	2	768	C	N1-C2-O2	7.66	123.50	118.90
1	2	405	C	N1-C2-O2	7.66	123.49	118.90
1	2	736	C	N1-C2-O2	7.65	123.49	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1381	U	N3-C2-O2	-7.65	116.85	122.20
1	2	1640	C	N1-C2-O2	7.65	123.49	118.90
1	2	190	C	C5-C6-N1	7.64	124.82	121.00
1	2	186	C	N1-C2-O2	7.61	123.46	118.90
1	2	1799	U	C2-N1-C1'	7.58	126.79	117.70
1	2	861	U	N3-C2-O2	-7.56	116.91	122.20
1	2	1256	A	P-O3'-C3'	7.56	128.77	119.70
1	2	107	C	C5-C6-N1	7.56	124.78	121.00
1	2	354	C	C2-N3-C4	7.55	123.68	119.90
1	2	1274	C	N1-C2-O2	7.53	123.42	118.90
1	2	1688	U	N1-C2-O2	7.53	128.07	122.80
1	2	35	U	N3-C2-O2	-7.51	116.94	122.20
1	2	864	U	C2-N1-C1'	7.51	126.72	117.70
1	2	990	C	C6-N1-C2	-7.51	117.30	120.30
1	2	36	C	N1-C2-O2	7.50	123.40	118.90
1	2	989	U	N3-C2-O2	-7.50	116.95	122.20
1	2	107	C	C6-N1-C2	-7.46	117.31	120.30
1	2	1566	U	N1-C2-O2	7.45	128.01	122.80
1	2	50	C	N3-C2-O2	-7.45	116.69	121.90
1	2	839	U	N3-C2-O2	-7.43	117.00	122.20
1	2	4	C	N1-C2-O2	7.42	123.35	118.90
1	2	302	U	N1-C2-O2	7.42	127.99	122.80
1	2	656	G	C5-C6-O6	-7.41	124.15	128.60
1	2	839	U	N1-C2-O2	7.41	127.99	122.80
1	2	1185	U	N1-C2-O2	7.41	127.99	122.80
1	2	387	A	OP2-P-O3'	7.40	121.48	105.20
1	2	1363	U	N3-C2-O2	-7.40	117.02	122.20
1	2	1619	C	N1-C2-O2	7.40	123.34	118.90
1	2	1063	U	N3-C2-O2	-7.39	117.02	122.20
1	2	12	U	N3-C2-O2	-7.39	117.03	122.20
1	2	432	G	C2-N3-C4	7.38	115.59	111.90
1	2	1258	U	C2-N1-C1'	7.38	126.56	117.70
1	2	610	G	C4-N9-C1'	7.37	136.08	126.50
1	2	928	U	P-O3'-C3'	7.37	128.54	119.70
1	2	1252	C	C2-N1-C1'	7.36	126.90	118.80
1	2	17	C	C6-N1-C2	-7.36	117.36	120.30
1	2	394	C	C5-C6-N1	7.35	124.67	121.00
1	2	1202	A	C2-N3-C4	7.34	114.27	110.60
1	2	861	U	N1-C2-O2	7.33	127.93	122.80
1	2	1214	U	N1-C2-O2	7.33	127.93	122.80
1	2	555	A	N7-C8-N9	7.32	117.46	113.80
1	2	682	C	C6-N1-C2	-7.31	117.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	819	G	P-O3'-C3'	7.31	128.48	119.70
1	2	1257	U	C2-N1-C1'	7.31	126.48	117.70
1	2	656	G	C4-C5-N7	7.30	113.72	110.80
1	2	54	C	C6-N1-C2	-7.30	117.38	120.30
1	2	176	C	C6-N1-C2	-7.28	117.39	120.30
1	2	1566	U	N3-C2-O2	-7.23	117.14	122.20
1	2	1584	G	C4-N9-C1'	-7.23	117.11	126.50
1	2	1689	A	N7-C8-N9	7.22	117.41	113.80
1	2	522	U	C5-C6-N1	7.21	126.31	122.70
1	2	1226	A	N7-C8-N9	7.21	117.40	113.80
1	2	311	U	N3-C2-O2	-7.20	117.16	122.20
1	2	1274	C	P-O3'-C3'	7.19	128.33	119.70
1	2	352	A	P-O3'-C3'	7.16	128.29	119.70
1	2	260	U	N1-C2-O2	7.16	127.81	122.80
1	2	1535	U	N3-C2-O2	-7.15	117.20	122.20
1	2	767	U	C2-N1-C1'	7.14	126.27	117.70
1	2	1535	U	N1-C2-O2	7.14	127.80	122.80
1	2	1461	C	C6-N1-C2	-7.13	117.45	120.30
1	2	1439	C	C6-N1-C2	-7.13	117.45	120.30
1	2	1561	U	N3-C2-O2	-7.12	117.21	122.20
1	2	1113	A	C4-C5-C6	-7.12	113.44	117.00
1	2	1676	U	N3-C2-O2	-7.12	117.22	122.20
1	2	411	C	C6-N1-C2	-7.12	117.45	120.30
1	2	1688	U	N3-C2-O2	-7.12	117.22	122.20
1	2	313	U	P-O3'-C3'	7.11	128.23	119.70
1	2	431	C	C2-N1-C1'	7.11	126.62	118.80
1	2	1420	C	N1-C2-O2	7.10	123.16	118.90
1	2	656	G	N7-C8-N9	7.10	116.65	113.10
1	2	989	U	N1-C2-O2	7.10	127.77	122.80
1	2	224	C	C2-N1-C1'	7.09	126.60	118.80
1	2	88	U	N3-C2-O2	-7.09	117.24	122.20
1	2	1214	U	C2-N1-C1'	7.08	126.19	117.70
1	2	87	C	C6-N1-C2	-7.07	117.47	120.30
1	2	1561	U	N1-C2-O2	7.05	127.74	122.80
1	2	94	U	C5-C6-N1	7.05	126.23	122.70
1	2	645	C	C6-N1-C2	-7.05	117.48	120.30
1	2	224	C	C5-C6-N1	7.04	124.52	121.00
1	2	656	G	N3-C4-N9	7.04	130.23	126.00
1	2	1573	A	P-O3'-C3'	7.04	128.14	119.70
1	2	116	U	N1-C2-O2	7.04	127.72	122.80
1	2	747	C	N1-C2-O2	7.04	123.12	118.90
1	2	54	C	C2-N1-C1'	7.03	126.53	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	645	C	C5-C6-N1	7.02	124.51	121.00
1	2	1639	C	N3-C2-O2	-7.02	116.99	121.90
1	2	1463	C	N1-C2-O2	7.01	123.11	118.90
1	2	758	U	N3-C2-O2	-6.99	117.31	122.20
1	2	755	A	P-O3'-C3'	6.98	128.08	119.70
1	2	733	A	C2-N3-C4	6.98	114.09	110.60
1	2	1458	G	C8-N9-C4	-6.98	103.61	106.40
1	2	530	C	C6-N1-C2	-6.98	117.51	120.30
1	2	490	C	C5-C6-N1	6.97	124.48	121.00
1	2	700	C	C5-C6-N1	6.97	124.48	121.00
1	2	934	C	N1-C2-O2	6.96	123.08	118.90
1	2	1145	U	C6-N1-C1'	-6.96	111.46	121.20
1	2	1393	C	C6-N1-C2	-6.96	117.52	120.30
1	2	1620	C	C6-N1-C2	-6.95	117.52	120.30
1	2	1489	U	C2-N1-C1'	6.94	126.03	117.70
1	2	54	C	N1-C2-O2	6.94	123.06	118.90
1	2	190	C	C6-N1-C2	-6.92	117.53	120.30
1	2	490	C	C6-N1-C2	-6.91	117.54	120.30
1	2	990	C	C5-C6-N1	6.91	124.45	121.00
1	2	639	U	P-O3'-C3'	6.88	127.95	119.70
1	2	141	U	P-O3'-C3'	6.86	127.93	119.70
1	2	1632	C	N1-C2-O2	6.86	123.02	118.90
1	2	90	C	C6-N1-C2	-6.85	117.56	120.30
1	2	583	C	C2-N1-C1'	6.85	126.33	118.80
1	2	1236	A	N7-C8-N9	6.85	117.22	113.80
1	2	1381	U	N1-C2-O2	6.84	127.58	122.80
1	2	494	U	C2-N1-C1'	6.83	125.90	117.70
1	2	186	C	C6-N1-C2	-6.82	117.57	120.30
1	2	1723	U	N1-C2-O2	6.79	127.55	122.80
1	2	758	U	N1-C2-O2	6.78	127.55	122.80
1	2	361	C	C6-N1-C2	-6.77	117.59	120.30
1	2	864	U	N1-C2-O2	6.77	127.54	122.80
1	2	4	C	N3-C2-O2	-6.76	117.17	121.90
1	2	1363	U	C2-N1-C1'	6.76	125.81	117.70
1	2	1023	A	P-O3'-C3'	6.75	127.80	119.70
1	2	174	U	N3-C2-O2	-6.75	117.47	122.20
1	2	873	U	N1-C2-O2	6.75	127.53	122.80
1	2	890	C	C6-N1-C2	-6.75	117.60	120.30
1	2	835	U	C5-C6-N1	6.74	126.07	122.70
1	2	686	C	C6-N1-C2	-6.73	117.61	120.30
1	2	1252	C	C5-C6-N1	6.73	124.37	121.00
1	2	967	A	O5'-P-OP1	-6.73	99.64	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	263	C	C6-N1-C2	-6.73	117.61	120.30
1	2	111	U	N3-C2-O2	-6.72	117.50	122.20
1	2	1220	C	C5-C6-N1	6.72	124.36	121.00
1	2	1235	C	N3-C2-O2	-6.72	117.20	121.90
1	2	172	C	N1-C2-O2	6.72	122.93	118.90
1	2	1707	A	C2-N3-C4	6.72	113.96	110.60
1	2	617	U	C2-N1-C1'	6.71	125.76	117.70
1	2	262	U	N3-C2-O2	-6.71	117.50	122.20
1	2	1640	C	C6-N1-C2	-6.69	117.62	120.30
1	2	94	U	N3-C2-O2	-6.69	117.52	122.20
1	2	11	A	N1-C2-N3	-6.68	125.96	129.30
1	2	1620	C	N1-C2-O2	6.68	122.91	118.90
1	2	1489	U	N1-C2-O2	6.68	127.47	122.80
1	2	1703	C	C6-N1-C2	-6.67	117.63	120.30
1	2	5	U	N3-C2-O2	-6.67	117.53	122.20
1	2	1489	U	N3-C2-O2	-6.67	117.53	122.20
1	2	1636	C	P-O3'-C3'	6.66	127.69	119.70
1	2	111	U	N1-C2-O2	6.66	127.46	122.80
1	2	174	U	N1-C2-O2	6.65	127.46	122.80
1	2	654	C	C6-N1-C2	-6.65	117.64	120.30
1	2	106	U	N1-C2-O2	6.64	127.45	122.80
1	2	1646	C	N1-C2-O2	6.64	122.89	118.90
1	2	1246	C	N1-C2-O2	6.64	122.88	118.90
1	2	1332	C	C2-N1-C1'	6.63	126.10	118.80
1	2	610	G	N3-C4-N9	6.63	129.98	126.00
1	2	1323	C	C5-C6-N1	6.63	124.31	121.00
1	2	1497	U	N1-C2-O2	6.62	127.44	122.80
1	2	394	C	C6-N1-C2	-6.61	117.66	120.30
1	2	935	U	N1-C2-O2	6.60	127.42	122.80
1	2	1148	C	C6-N1-C2	-6.59	117.66	120.30
1	2	1185	U	C2-N1-C1'	6.59	125.61	117.70
1	2	188	A	C2-N3-C4	6.58	113.89	110.60
1	2	431	C	C6-N1-C2	-6.57	117.67	120.30
1	2	1596	C	N1-C2-O2	6.56	122.84	118.90
1	2	453	U	C6-N1-C2	-6.56	117.06	121.00
1	2	184	C	C2-N1-C1'	6.55	126.01	118.80
1	2	494	U	N1-C2-O2	6.54	127.38	122.80
1	2	1783	C	N1-C2-O2	6.54	122.83	118.90
1	2	18	C	C6-N1-C2	-6.53	117.69	120.30
1	2	1393	C	C5-C6-N1	6.53	124.27	121.00
1	2	912	U	P-O3'-C3'	6.53	127.54	119.70
1	2	1255	G	N1-C6-O6	-6.53	115.98	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1235	C	C5-C6-N1	6.53	124.26	121.00
1	2	795	U	N3-C2-O2	-6.52	117.64	122.20
1	2	1082	C	C6-N1-C1'	-6.51	112.99	120.80
1	2	1742	U	P-O3'-C3'	6.51	127.51	119.70
1	2	767	U	N1-C2-O2	6.50	127.35	122.80
1	2	1551	U	N1-C2-O2	6.49	127.34	122.80
1	2	1273	G	P-O3'-C3'	6.48	127.48	119.70
1	2	792	U	N3-C2-O2	-6.48	117.66	122.20
1	2	491	C	C5-C6-N1	6.47	124.24	121.00
1	2	768	C	C6-N1-C2	-6.46	117.72	120.30
1	2	1185	U	N3-C2-O2	-6.46	117.68	122.20
1	2	88	U	N1-C2-O2	6.46	127.32	122.80
1	2	37	U	N3-C2-O2	-6.45	117.68	122.20
1	2	1584	G	C8-N9-C1'	6.45	135.39	127.00
1	2	166	C	N3-C2-O2	-6.45	117.39	121.90
1	2	276	C	N1-C2-O2	6.45	122.77	118.90
1	2	795	U	C5-C6-N1	6.44	125.92	122.70
1	2	1071	U	N3-C2-O2	-6.44	117.69	122.20
1	2	1245	G	OP2-P-O3'	6.43	119.34	105.20
1	2	1527	C	N3-C2-O2	-6.42	117.40	121.90
1	2	335	U	C5-C6-N1	6.42	125.91	122.70
1	2	1584	G	O4'-C1'-N9	6.42	113.33	108.20
1	2	609	U	P-O3'-C3'	6.42	127.40	119.70
1	2	387	A	P-O3'-C3'	6.41	127.39	119.70
1	2	1354	G	C4-N9-C1'	6.41	134.83	126.50
1	2	171	A	N9-C4-C5	-6.41	103.24	105.80
1	2	1420	C	N3-C2-O2	-6.40	117.42	121.90
1	2	68	A	P-O3'-C3'	6.40	127.38	119.70
1	2	745	U	N1-C2-O2	6.40	127.28	122.80
1	2	610	G	C8-N9-C1'	-6.38	118.70	127.00
1	2	278	U	P-O3'-C3'	6.38	127.36	119.70
1	2	818	C	C6-N1-C2	-6.38	117.75	120.30
1	2	1633	A	P-O3'-C3'	6.37	127.34	119.70
1	2	898	A	N1-C2-N3	-6.37	126.12	129.30
1	2	935	U	N3-C2-O2	-6.36	117.75	122.20
1	2	1021	C	N1-C2-O2	6.35	122.71	118.90
1	2	1560	U	C6-N1-C1'	-6.35	112.31	121.20
1	2	263	C	C5-C6-N1	6.35	124.17	121.00
1	2	400	A	P-O3'-C3'	6.34	127.30	119.70
1	2	627	C	C6-N1-C2	-6.34	117.77	120.30
1	2	555	A	C5-N7-C8	-6.33	100.73	103.90
1	2	1071	U	N1-C2-O2	6.32	127.22	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1458	G	C8-N9-C1'	-6.32	118.79	127.00
1	2	792	U	N1-C2-O2	6.31	127.22	122.80
1	2	857	U	N1-C2-O2	6.29	127.20	122.80
1	2	184	C	N1-C2-O2	6.29	122.67	118.90
1	2	759	U	N3-C2-O2	-6.28	117.80	122.20
1	2	617	U	N3-C2-O2	-6.28	117.81	122.20
1	2	489	C	C6-N1-C2	-6.27	117.79	120.30
1	2	1115	U	N1-C2-O2	6.26	127.18	122.80
1	2	1145	U	N1-C2-O2	6.26	127.18	122.80
1	2	1071	U	OP1-P-O3'	-6.26	91.43	105.20
1	2	828	U	N3-C2-O2	-6.25	117.82	122.20
1	2	646	C	C6-N1-C2	-6.25	117.80	120.30
1	2	1497	U	N3-C2-O2	-6.25	117.82	122.20
1	2	1010	C	N1-C2-O2	6.25	122.65	118.90
1	2	185	U	C2-N1-C1'	6.23	125.18	117.70
1	2	1428	G	O5'-P-OP2	-6.23	100.09	105.70
1	2	418	G	N3-C4-N9	6.23	129.74	126.00
1	2	640	U	P-O3'-C3'	6.23	127.17	119.70
1	2	517	U	C2-N1-C1'	6.22	125.17	117.70
1	2	1458	G	N7-C8-N9	6.22	116.21	113.10
1	2	768	C	N3-C2-O2	-6.20	117.56	121.90
1	2	90	C	C5-C6-N1	6.19	124.10	121.00
1	2	795	U	N1-C2-O2	6.19	127.13	122.80
1	2	1495	C	C5-C6-N1	6.19	124.09	121.00
1	2	782	U	C6-N1-C2	-6.18	117.29	121.00
1	2	494	U	N3-C2-O2	-6.17	117.88	122.20
1	2	1689	A	C8-N9-C4	-6.17	103.33	105.80
1	2	36	C	N3-C2-O2	-6.17	117.58	121.90
1	2	945	U	N1-C2-O2	6.17	127.12	122.80
1	2	945	U	N3-C2-O2	-6.16	117.89	122.20
1	2	1205	C	C5-C6-N1	6.16	124.08	121.00
1	2	1007	C	N3-C2-O2	-6.16	117.59	121.90
1	2	656	G	N9-C4-C5	-6.16	102.94	105.40
1	2	1742	U	C5-C6-N1	6.16	125.78	122.70
1	2	184	C	C5-C6-N1	6.15	124.07	121.00
1	2	531	C	N3-C2-O2	-6.15	117.60	121.90
1	2	90	C	N1-C2-O2	6.14	122.59	118.90
1	2	617	U	N1-C2-O2	6.14	127.10	122.80
1	2	1460	A	N7-C8-N9	6.14	116.87	113.80
1	2	653	C	C6-N1-C2	-6.13	117.85	120.30
1	2	280	U	P-O3'-C3'	6.13	127.06	119.70
1	2	1221	A	N7-C8-N9	6.13	116.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1651	A	N1-C2-N3	-6.12	126.24	129.30
1	2	1115	U	N3-C2-O2	-6.12	117.92	122.20
1	2	359	A	C2-N3-C4	6.12	113.66	110.60
1	2	992	A	O4'-C1'-N9	6.12	113.09	108.20
1	2	587	C	C5-C6-N1	6.11	124.06	121.00
1	2	94	U	C6-N1-C2	-6.11	117.34	121.00
1	2	1681	A	O5'-P-OP2	6.11	118.03	110.70
1	2	1180	C	C5-C6-N1	6.10	124.05	121.00
1	2	1174	C	N1-C2-O2	6.10	122.56	118.90
1	2	656	G	C5-N7-C8	-6.09	101.25	104.30
1	2	18	C	C5-C6-N1	6.09	124.05	121.00
1	2	1145	U	N3-C2-O2	-6.09	117.94	122.20
1	2	1530	C	N1-C2-O2	6.09	122.55	118.90
1	2	519	C	N1-C2-O2	6.09	122.55	118.90
1	2	1474	G	C2-N3-C4	6.09	114.94	111.90
1	2	1235	C	N1-C2-O2	6.09	122.55	118.90
1	2	294	C	C6-N1-C2	-6.08	117.87	120.30
1	2	629	U	C5-C6-N1	6.07	125.74	122.70
1	2	1148	C	C5-C6-N1	6.07	124.04	121.00
1	2	610	G	N3-C4-C5	-6.07	125.56	128.60
1	2	1301	U	N1-C2-O2	6.07	127.05	122.80
1	2	94	U	N1-C2-O2	6.07	127.05	122.80
1	2	237	C	N1-C2-O2	6.07	122.54	118.90
1	2	736	C	N3-C2-O2	-6.06	117.66	121.90
1	2	4	C	C6-N1-C2	-6.06	117.88	120.30
1	2	1389	C	C2-N3-C4	6.06	122.93	119.90
1	2	1236	A	C5-N7-C8	-6.06	100.87	103.90
1	2	172	C	C2-N1-C1'	6.05	125.46	118.80
1	2	207	U	N3-C2-O2	-6.05	117.96	122.20
1	2	873	U	N3-C2-O2	-6.05	117.97	122.20
1	2	1170	G	N3-C4-N9	6.05	129.63	126.00
1	2	1682	U	N1-C2-O2	6.05	127.03	122.80
1	2	67	A	N1-C2-N3	-6.04	126.28	129.30
1	2	189	C	C6-N1-C2	-6.04	117.88	120.30
1	2	1063	U	C5-C6-N1	6.04	125.72	122.70
1	2	745	U	N3-C2-O2	-6.03	117.98	122.20
1	2	270	C	N1-C2-O2	6.02	122.51	118.90
1	2	354	C	N1-C2-O2	6.02	122.51	118.90
1	2	608	U	N1-C2-O2	6.01	127.01	122.80
1	2	1742	U	N3-C2-O2	-6.01	117.99	122.20
1	2	1373	C	C6-N1-C2	-6.01	117.89	120.30
1	2	1415	U	N3-C2-O2	-6.01	117.99	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	140	A	O5'-P-OP1	-6.01	100.29	105.70
1	2	1602	C	C6-N1-C2	-6.01	117.90	120.30
1	2	1439	C	C5-C6-N1	6.01	124.00	121.00
1	2	12	U	N1-C2-O2	6.00	127.00	122.80
1	2	1232	U	N1-C2-O2	6.00	127.00	122.80
1	2	656	G	N3-C4-C5	-6.00	125.60	128.60
1	2	608	U	C2-N1-C1'	5.99	124.89	117.70
1	2	15	U	C5-C6-N1	5.99	125.69	122.70
1	2	1657	U	N3-C2-O2	-5.99	118.01	122.20
1	2	555	A	P-O3'-C3'	5.98	126.88	119.70
1	2	794	U	C2-N1-C1'	5.98	124.88	117.70
1	2	818	C	C5-C6-N1	5.98	123.99	121.00
1	2	17	C	C5-C6-N1	5.98	123.99	121.00
1	2	989	U	C2-N1-C1'	5.98	124.87	117.70
1	2	1113	A	N1-C2-N3	-5.98	126.31	129.30
1	2	1430	U	P-O3'-C3'	5.98	126.87	119.70
1	2	1731	A	N1-C2-N3	-5.97	126.32	129.30
1	2	996	U	N3-C2-O2	-5.96	118.03	122.20
1	2	1650	U	C5-C6-N1	5.95	125.68	122.70
1	2	1012	U	C2-N3-C4	5.95	130.57	127.00
1	2	1145	U	O4'-C1'-N1	5.94	112.95	108.20
1	2	482	U	C2-N1-C1'	5.94	124.83	117.70
1	2	431	C	C5-C6-N1	5.94	123.97	121.00
1	2	1556	A	OP2-P-O3'	5.94	118.26	105.20
1	2	1771	U	N3-C2-O2	-5.93	118.05	122.20
1	2	838	G	N1-C6-O6	-5.92	116.35	119.90
1	2	830	U	C5-C6-N1	5.92	125.66	122.70
1	2	1567	U	N1-C2-O2	5.92	126.94	122.80
1	2	1253	U	N1-C2-O2	5.92	126.94	122.80
1	2	1007	C	N1-C2-O2	5.92	122.45	118.90
1	2	138	A	C2-N3-C4	5.91	113.56	110.60
1	2	531	C	C6-N1-C2	-5.91	117.94	120.30
1	2	1186	U	N3-C2-O2	-5.91	118.07	122.20
1	2	243	G	C4-C5-N7	5.90	113.16	110.80
1	2	1360	A	C5-N7-C8	-5.90	100.95	103.90
1	2	192	U	C6-N1-C2	-5.90	117.46	121.00
1	2	766	U	O5'-P-OP1	-5.90	100.39	105.70
1	2	262	U	C2-N1-C1'	5.90	124.78	117.70
1	2	1246	C	C5-C6-N1	5.90	123.95	121.00
1	2	255	U	N3-C2-O2	-5.89	118.07	122.20
1	2	1345	A	N1-C2-N3	-5.89	126.35	129.30
1	2	1	U	N3-C2-O2	-5.89	118.08	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	485	A	N7-C8-N9	5.88	116.74	113.80
1	2	1463	C	N3-C2-O2	-5.87	117.79	121.90
1	2	1252	C	N3-C2-O2	-5.87	117.79	121.90
1	2	646	C	C5-C6-N1	5.87	123.94	121.00
1	2	1066	C	C2-N1-C1'	5.87	125.25	118.80
1	2	405	C	N3-C2-O2	-5.86	117.80	121.90
1	2	768	C	C5-C6-N1	5.86	123.93	121.00
1	2	1045	C	C6-N1-C2	-5.86	117.96	120.30
1	2	1510	U	N1-C2-O2	5.86	126.90	122.80
1	2	846	G	N3-C4-N9	5.85	129.51	126.00
1	2	767	U	C6-N1-C1'	-5.85	113.01	121.20
1	2	138	A	C5-N7-C8	5.84	106.82	103.90
1	2	965	U	C2-N1-C1'	5.84	124.71	117.70
1	2	5	U	N1-C2-O2	5.84	126.89	122.80
1	2	117	U	N3-C2-O2	-5.84	118.11	122.20
1	2	609	U	OP2-P-O3'	5.84	118.04	105.20
1	2	768	C	C2-N1-C1'	5.83	125.22	118.80
1	2	374	U	C5-C6-N1	5.83	125.61	122.70
1	2	934	C	C2-N1-C1'	5.82	125.20	118.80
1	2	149	C	C6-N1-C2	-5.82	117.97	120.30
1	2	846	G	N3-C4-C5	-5.81	125.69	128.60
1	2	1129	U	N3-C2-O2	-5.81	118.13	122.20
1	2	823	G	N3-C4-C5	-5.80	125.70	128.60
1	2	1221	A	C8-N9-C4	-5.80	103.48	105.80
1	2	369	A	C2-N3-C4	5.80	113.50	110.60
1	2	786	C	C6-N1-C2	-5.80	117.98	120.30
1	2	243	G	N9-C4-C5	-5.80	103.08	105.40
1	2	262	U	N1-C2-O2	5.80	126.86	122.80
1	2	1205	C	C6-N1-C2	-5.80	117.98	120.30
1	2	1633	A	N1-C2-N3	-5.80	126.40	129.30
1	2	1323	C	C6-N1-C2	-5.79	117.98	120.30
1	2	843	U	C6-N1-C2	-5.79	117.53	121.00
1	2	1168	U	N3-C2-O2	-5.79	118.15	122.20
1	2	814	A	N1-C2-N3	-5.79	126.41	129.30
1	2	1658	G	C4-C5-N7	5.79	113.11	110.80
1	2	1658	G	N1-C6-O6	5.79	123.37	119.90
1	2	500	C	O4'-C1'-N1	5.78	112.83	108.20
1	2	1799	U	N3-C2-O2	-5.78	118.16	122.20
1	2	186	C	N3-C2-O2	-5.78	117.86	121.90
1	2	522	U	N1-C2-O2	5.78	126.84	122.80
1	2	608	U	N3-C2-O2	-5.77	118.16	122.20
1	2	1514	U	N1-C2-O2	5.77	126.84	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	827	C	C6-N1-C2	-5.76	118.00	120.30
1	2	149	C	N1-C2-O2	5.75	122.35	118.90
1	2	1063	U	C2-N1-C1'	5.75	124.60	117.70
1	2	1220	C	C2-N1-C1'	5.75	125.12	118.80
1	2	1327	C	N1-C2-O2	5.75	122.35	118.90
1	2	1632	C	N3-C2-O2	-5.75	117.88	121.90
1	2	130	C	C5-C6-N1	5.74	123.87	121.00
1	2	186	C	C6-N1-C1'	-5.74	113.91	120.80
1	2	466	U	N3-C2-O2	-5.74	118.18	122.20
1	2	1082	C	O4'-C1'-N1	5.74	112.79	108.20
1	2	863	A	C2-N3-C4	5.74	113.47	110.60
1	2	496	G	N1-C6-O6	5.74	123.34	119.90
1	2	1373	C	C5-C6-N1	5.74	123.87	121.00
1	2	1640	C	N1-C2-N3	-5.74	115.19	119.20
1	2	270	C	C2-N1-C1'	5.73	125.10	118.80
1	2	411	C	C2-N1-C1'	5.73	125.11	118.80
1	2	916	U	N3-C2-O2	-5.73	118.19	122.20
1	2	1551	U	N3-C2-O2	-5.72	118.20	122.20
1	2	911	U	N1-C2-O2	5.71	126.80	122.80
1	2	767	U	N3-C2-O2	-5.71	118.20	122.20
1	2	864	U	N3-C2-O2	-5.71	118.20	122.20
1	2	1565	C	C5-C6-N1	5.70	123.85	121.00
1	2	1600	A	C2-N3-C4	5.70	113.45	110.60
1	2	1460	A	C8-N9-C4	-5.69	103.52	105.80
1	2	1096	C	C6-N1-C2	-5.69	118.02	120.30
1	2	1245	G	N7-C8-N9	5.69	115.94	113.10
1	2	1644	C	C6-N1-C2	-5.69	118.02	120.30
1	2	1186	U	N1-C2-O2	5.69	126.78	122.80
1	2	38	C	C6-N1-C2	-5.68	118.03	120.30
1	2	1669	U	N1-C2-O2	5.68	126.78	122.80
1	2	1470	C	N1-C2-O2	5.68	122.31	118.90
1	2	1182	U	C6-N1-C1'	-5.68	113.25	121.20
1	2	64	U	N3-C2-O2	-5.67	118.23	122.20
1	2	1799	U	N1-C2-O2	5.67	126.77	122.80
1	2	1742	U	C6-N1-C2	-5.67	117.60	121.00
1	2	166	C	C2-N3-C4	5.67	122.73	119.90
1	2	840	U	C2-N1-C1'	5.66	124.50	117.70
1	2	120	U	C2-N1-C1'	5.66	124.49	117.70
1	2	1771	U	N1-C2-O2	5.66	126.76	122.80
1	2	1596	C	C6-N1-C1'	-5.66	114.01	120.80
1	2	640	U	N3-C2-O2	-5.65	118.24	122.20
1	2	1342	C	C6-N1-C2	-5.65	118.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	255	U	N1-C2-O2	5.65	126.75	122.80
1	2	472	U	N3-C2-O2	-5.65	118.24	122.20
1	2	522	U	N3-C2-O2	-5.64	118.25	122.20
1	2	14	C	C2-N1-C1'	5.63	125.00	118.80
1	2	1276	U	N3-C2-O2	-5.63	118.25	122.20
1	2	106	U	N3-C2-O2	-5.63	118.26	122.20
1	2	893	U	N3-C2-O2	-5.63	118.26	122.20
1	2	1666	U	N1-C2-O2	5.63	126.74	122.80
1	2	1	U	N1-C2-O2	5.63	126.74	122.80
1	2	965	U	N1-C2-O2	5.62	126.74	122.80
1	2	250	C	N1-C2-O2	5.62	122.27	118.90
1	2	587	C	C6-N1-C2	-5.61	118.05	120.30
1	2	748	U	N3-C2-O2	-5.61	118.27	122.20
1	2	87	C	C5-C6-N1	5.61	123.81	121.00
1	2	1742	U	N1-C2-O2	5.61	126.73	122.80
21	B	43	PRO	C-N-CA	5.61	135.73	121.70
1	2	361	C	C5-C6-N1	5.61	123.81	121.00
1	2	1291	G	N3-C4-C5	-5.61	125.80	128.60
1	2	1214	U	C6-N1-C2	-5.60	117.64	121.00
1	2	1171	A	N1-C2-N3	-5.60	126.50	129.30
1	2	1172	G	N7-C8-N9	5.60	115.90	113.10
1	2	1666	U	N3-C2-O2	-5.60	118.28	122.20
1	2	1688	U	C2-N1-C1'	5.60	124.42	117.70
1	2	189	C	C2-N1-C1'	5.60	124.96	118.80
1	2	446	A	C2-N3-C4	5.60	113.40	110.60
1	2	632	U	C5-C6-N1	5.60	125.50	122.70
1	2	35	U	N1-C2-O2	5.60	126.72	122.80
1	2	1072	C	OP1-P-OP2	5.60	128.00	119.60
1	2	1360	A	N7-C8-N9	5.60	116.60	113.80
1	2	1658	G	C6-C5-N7	-5.59	127.04	130.40
1	2	189	C	N3-C4-N4	5.59	121.92	118.00
1	2	842	C	C6-N1-C2	-5.59	118.06	120.30
1	2	1241	G	O4'-C1'-N9	5.59	112.67	108.20
1	2	97	C	N1-C2-O2	5.59	122.25	118.90
1	2	645	C	N1-C2-O2	5.59	122.25	118.90
1	2	748	U	N1-C2-O2	5.59	126.71	122.80
1	2	737	A	N1-C2-N3	-5.59	126.51	129.30
1	2	1317	C	C6-N1-C2	-5.59	118.06	120.30
1	2	1731	A	C5-C6-N6	-5.59	119.23	123.70
1	2	1657	U	N1-C2-O2	5.58	126.71	122.80
1	2	1619	C	N3-C2-O2	-5.58	118.00	121.90
1	2	795	U	C6-N1-C2	-5.57	117.66	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1543	A	N7-C8-N9	5.57	116.58	113.80
1	2	1731	A	C5-C6-N1	5.57	120.48	117.70
1	2	496	G	C6-C5-N7	-5.56	127.06	130.40
1	2	821	U	N1-C2-O2	5.56	126.69	122.80
1	2	835	U	OP1-P-OP2	-5.56	111.27	119.60
1	2	1232	U	N3-C2-O2	-5.56	118.31	122.20
1	2	1528	U	C2-N1-C1'	5.55	124.36	117.70
1	2	1706	C	C6-N1-C2	-5.55	118.08	120.30
1	2	861	U	C6-N1-C1'	-5.54	113.44	121.20
1	2	1049	U	N3-C2-O2	-5.54	118.32	122.20
1	2	1386	G	N3-C2-N2	-5.54	116.02	119.90
1	2	405	C	C2-N1-C1'	5.54	124.89	118.80
1	2	267	U	N1-C2-O2	5.54	126.67	122.80
1	2	1258	U	C5-C6-N1	5.53	125.47	122.70
1	2	1023	A	OP2-P-O3'	5.53	117.37	105.20
1	2	864	U	C6-N1-C1'	-5.53	113.46	121.20
1	2	1731	A	C2-N3-C4	5.53	113.36	110.60
1	2	839	U	C2-N1-C1'	5.52	124.33	117.70
1	2	260	U	C6-N1-C2	-5.52	117.69	121.00
1	2	633	U	N3-C2-O2	-5.52	118.34	122.20
1	2	1620	C	N3-C2-O2	-5.52	118.04	121.90
1	2	1341	A	N1-C2-N3	-5.51	126.54	129.30
1	2	1354	G	C8-N9-C1'	-5.51	119.84	127.00
1	2	1470	C	C6-N1-C2	-5.51	118.10	120.30
1	2	546	U	N3-C2-O2	-5.50	118.35	122.20
1	2	1062	A	N1-C2-N3	-5.50	126.55	129.30
1	2	491	C	C6-N1-C2	-5.50	118.10	120.30
1	2	530	C	C2-N1-C1'	5.50	124.85	118.80
1	2	895	G	N3-C2-N2	-5.50	116.05	119.90
1	2	1354	G	N3-C4-N9	5.50	129.30	126.00
1	2	171	A	N1-C2-N3	-5.50	126.55	129.30
1	2	656	G	N1-C6-O6	5.50	123.20	119.90
1	2	1382	A	OP1-P-O3'	5.50	117.30	105.20
1	2	184	C	C6-N1-C2	-5.49	118.10	120.30
1	2	1072	C	O5'-P-OP1	-5.49	100.76	105.70
1	2	270	C	C5-C6-N1	5.49	123.75	121.00
1	2	21	U	N3-C2-O2	-5.49	118.36	122.20
1	2	289	U	N3-C2-O2	-5.49	118.36	122.20
1	2	1491	U	C2-N1-C1'	5.48	124.28	117.70
1	2	996	U	N1-C2-O2	5.48	126.64	122.80
1	2	1734	U	N1-C2-O2	5.48	126.64	122.80
1	2	1643	U	N3-C2-O2	-5.48	118.36	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	821	U	N3-C2-O2	-5.47	118.37	122.20
1	2	1734	U	N3-C2-O2	-5.47	118.37	122.20
1	2	1514	U	C6-N1-C1'	-5.47	113.55	121.20
1	2	960	U	N3-C2-O2	-5.46	118.38	122.20
1	2	1161	C	C5-C6-N1	5.46	123.73	121.00
1	2	1672	G	N7-C8-N9	5.46	115.83	113.10
1	2	1704	U	N3-C2-O2	-5.45	118.38	122.20
1	2	1787	C	C5-C6-N1	5.45	123.73	121.00
1	2	823	G	C2-N3-C4	5.45	114.62	111.90
1	2	1355	C	C6-N1-C2	-5.45	118.12	120.30
1	2	1474	G	N9-C4-C5	5.45	107.58	105.40
1	2	1585	U	N1-C2-O2	5.45	126.62	122.80
1	2	1257	U	C6-N1-C1'	-5.45	113.57	121.20
1	2	1044	U	N1-C2-O2	5.44	126.61	122.80
5	S	193	GLY	N-CA-C	5.44	126.70	113.10
1	2	197	A	C2-N3-C4	5.44	113.32	110.60
1	2	1682	U	N3-C2-O2	-5.44	118.39	122.20
1	2	1226	A	C5-N7-C8	-5.44	101.18	103.90
1	2	472	U	N1-C2-O2	5.44	126.61	122.80
1	2	614	C	C6-N1-C2	-5.43	118.13	120.30
1	2	211	U	N3-C2-O2	-5.43	118.40	122.20
1	2	229	U	C2-N1-C1'	5.43	124.21	117.70
1	2	1612	U	N1-C2-O2	5.43	126.60	122.80
1	2	1664	C	C6-N1-C2	-5.42	118.13	120.30
1	2	130	C	C6-N1-C2	-5.42	118.13	120.30
1	2	323	A	N7-C8-N9	5.42	116.51	113.80
1	2	304	U	N3-C2-O2	-5.42	118.41	122.20
1	2	136	C	C6-N1-C2	-5.41	118.14	120.30
1	2	1674	C	C6-N1-C2	-5.41	118.13	120.30
1	2	1767	G	N3-C4-N9	-5.41	122.75	126.00
1	2	14	C	C5-C6-N1	5.41	123.70	121.00
1	2	531	C	N1-C2-O2	5.41	122.15	118.90
1	2	90	C	C2-N1-C1'	5.41	124.75	118.80
1	2	1652	C	N1-C2-O2	5.41	122.14	118.90
1	2	145	A	C2-N3-C4	5.40	113.30	110.60
1	2	469	C	C5-C6-N1	5.40	123.70	121.00
1	2	658	C	N1-C2-O2	5.40	122.14	118.90
1	2	1317	C	C5-C6-N1	5.40	123.70	121.00
1	2	384	G	N3-C4-N9	5.40	129.24	126.00
1	2	539	G	P-O3'-C3'	5.40	126.18	119.70
1	2	186	C	C5-C6-N1	5.40	123.70	121.00
1	2	1244	A	C2-N3-C4	5.40	113.30	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1475	A	N7-C8-N9	5.39	116.50	113.80
1	2	1470	C	C2-N1-C1'	5.39	124.73	118.80
1	2	585	A	N1-C2-N3	-5.39	126.61	129.30
1	2	627	C	C2-N1-C1'	5.39	124.73	118.80
1	2	1596	C	O4'-C1'-N1	5.38	112.50	108.20
1	2	270	C	C6-N1-C2	-5.38	118.15	120.30
1	2	909	U	N3-C2-O2	-5.38	118.44	122.20
1	2	1646	C	C5-C6-N1	5.38	123.69	121.00
1	2	1510	U	N3-C2-O2	-5.37	118.44	122.20
1	2	495	C	C6-N1-C2	-5.37	118.15	120.30
1	2	426	G	O5'-P-OP1	-5.37	100.87	105.70
1	2	1258	U	C6-N1-C2	-5.37	117.78	121.00
1	2	1307	U	C6-N1-C1'	-5.37	113.69	121.20
1	2	700	C	C6-N1-C2	-5.37	118.15	120.30
1	2	469	C	C6-N1-C2	-5.36	118.16	120.30
1	2	1532	U	N3-C2-O2	-5.36	118.45	122.20
1	2	857	U	N3-C2-O2	-5.36	118.45	122.20
1	2	886	U	N3-C2-O2	-5.36	118.45	122.20
1	2	519	C	C6-N1-C2	-5.35	118.16	120.30
1	2	1711	C	C6-N1-C2	-5.35	118.16	120.30
1	2	469	C	N1-C2-O2	5.35	122.11	118.90
1	2	1359	C	C5-C6-N1	5.34	123.67	121.00
1	2	1031	U	OP2-P-O3'	5.34	116.95	105.20
1	2	1468	U	N3-C2-O2	-5.34	118.46	122.20
11	Y	137	PRO	C-N-CA	5.34	135.05	121.70
1	2	794	U	C5-C6-N1	5.33	125.37	122.70
1	2	820	U	C5-C6-N1	5.33	125.37	122.70
1	2	1115	U	C5-C6-N1	5.33	125.36	122.70
1	2	1533	C	N3-C2-O2	-5.33	118.17	121.90
1	2	460	A	N1-C6-N6	-5.32	115.41	118.60
1	2	846	G	C2-N3-C4	5.31	114.56	111.90
1	2	1062	A	N9-C4-C5	-5.31	103.67	105.80
1	2	1226	A	C8-N9-C4	-5.31	103.67	105.80
1	2	614	C	N1-C2-O2	5.31	122.08	118.90
1	2	789	A	C2-N3-C4	5.31	113.25	110.60
1	2	1703	C	C5-C6-N1	5.31	123.66	121.00
1	2	224	C	P-O3'-C3'	5.31	126.07	119.70
1	2	1530	C	C2-N1-C1'	5.31	124.64	118.80
1	2	1173	C	C6-N1-C2	-5.30	118.18	120.30
1	2	1168	U	N1-C2-O2	5.30	126.51	122.80
1	2	1274	C	N3-C2-O2	-5.30	118.19	121.90
1	2	20	G	N1-C6-O6	-5.30	116.72	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	390	G	C4-N9-C1'	5.29	133.38	126.50
1	2	1537	C	O4'-C1'-N1	5.29	112.44	108.20
1	2	415	C	N1-C2-O2	5.29	122.08	118.90
1	2	639	U	N3-C2-O2	-5.29	118.50	122.20
1	2	1676	U	C2-N1-C1'	5.29	124.05	117.70
1	2	1703	C	N1-C2-O2	5.29	122.07	118.90
1	2	1253	U	N3-C2-O2	-5.28	118.50	122.20
1	2	685	A	N1-C2-N3	-5.28	126.66	129.30
1	2	50	C	C6-N1-C2	-5.28	118.19	120.30
1	2	782	U	C5-C6-N1	5.28	125.34	122.70
1	2	1742	U	C2-N1-C1'	5.28	124.03	117.70
1	2	627	C	C5-C6-N1	5.28	123.64	121.00
1	2	1493	A	O4'-C1'-N9	5.28	112.42	108.20
1	2	645	C	C2-N1-C1'	5.27	124.60	118.80
1	2	937	C	C6-N1-C2	-5.27	118.19	120.30
1	2	408	C	N1-C2-O2	5.27	122.06	118.90
1	2	485	A	C5-N7-C8	-5.27	101.27	103.90
1	2	1699	G	N3-C4-C5	-5.26	125.97	128.60
1	2	304	U	N1-C2-O2	5.26	126.48	122.80
1	2	1772	C	N1-C2-O2	5.26	122.05	118.90
1	2	873	U	C2-N1-C1'	5.25	124.00	117.70
1	2	1561	U	C2-N1-C1'	5.25	124.00	117.70
1	2	276	C	N3-C2-O2	-5.25	118.22	121.90
1	2	981	U	N1-C2-O2	5.25	126.48	122.80
1	2	1010	C	C6-N1-C2	-5.25	118.20	120.30
1	2	235	G	N3-C4-N9	-5.25	122.85	126.00
1	2	1334	U	N1-C2-O2	5.25	126.47	122.80
1	2	519	C	N3-C2-O2	-5.24	118.23	121.90
1	2	1471	A	P-O3'-C3'	5.24	125.99	119.70
1	2	172	C	C5-C6-N1	5.24	123.62	121.00
1	2	1481	C	C6-N1-C2	-5.24	118.21	120.30
1	2	1246	C	C6-N1-C2	-5.23	118.21	120.30
1	2	400	A	OP2-P-O3'	5.23	116.71	105.20
1	2	1514	U	C2-N1-C1'	5.23	123.98	117.70
1	2	1291	G	N3-C4-N9	5.23	129.14	126.00
1	2	1077	C	N1-C2-O2	5.22	122.03	118.90
1	2	830	U	N3-C4-O4	5.22	123.06	119.40
1	2	1574	G	C8-N9-C1'	5.22	133.78	127.00
1	2	432	G	N3-C4-C5	-5.22	125.99	128.60
1	2	639	U	OP2-P-O3'	5.21	116.67	105.20
1	2	1146	G	C2-N3-C4	5.21	114.50	111.90
1	2	1592	A	N1-C2-N3	-5.21	126.69	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	243	G	C5-C6-O6	-5.21	125.47	128.60
1	2	1021	C	C6-N1-C2	-5.20	118.22	120.30
1	2	1415	U	N1-C2-O2	5.20	126.44	122.80
1	2	262	U	C5-C6-N1	5.20	125.30	122.70
1	2	1636	C	OP2-P-O3'	5.20	116.63	105.20
1	2	496	G	C4-C5-N7	5.19	112.88	110.80
1	2	647	G	N3-C2-N2	-5.19	116.27	119.90
1	2	1761	U	N1-C2-O2	5.19	126.43	122.80
1	2	830	U	C6-N1-C2	-5.19	117.89	121.00
1	2	1106	U	N3-C2-O2	-5.19	118.57	122.20
1	2	1460	A	C5-N7-C8	-5.19	101.31	103.90
1	2	831	U	C5-C6-N1	5.18	125.29	122.70
1	2	890	C	C5-C6-N1	5.18	123.59	121.00
1	2	1106	U	N1-C2-O2	5.18	126.43	122.80
1	2	198	A	N1-C2-N3	-5.17	126.72	129.30
1	2	1731	A	N9-C4-C5	-5.17	103.73	105.80
1	2	1465	C	N1-C2-O2	5.17	122.00	118.90
1	2	1495	C	C6-N1-C2	-5.17	118.23	120.30
1	2	1560	U	O4'-C1'-N1	5.17	112.33	108.20
1	2	121	U	C6-N1-C2	-5.16	117.90	121.00
1	2	262	U	C6-N1-C2	-5.16	117.90	121.00
1	2	1503	A	O4'-C1'-N9	5.16	112.33	108.20
1	2	1583	A	O5'-P-OP1	5.16	116.90	110.70
1	2	1440	C	C6-N1-C2	-5.16	118.23	120.30
1	2	1533	C	N1-C2-O2	5.16	122.00	118.90
1	2	996	U	C2-N1-C1'	5.15	123.88	117.70
1	2	121	U	C6-N1-C1'	-5.15	113.99	121.20
1	2	506	A	C8-N9-C4	-5.15	103.74	105.80
1	2	1643	U	N1-C2-O2	5.15	126.40	122.80
1	2	431	C	N1-C2-O2	5.14	121.99	118.90
1	2	584	C	C5-C6-N1	5.14	123.57	121.00
1	2	1585	U	N3-C2-O2	-5.14	118.60	122.20
1	2	276	C	C6-N1-C2	-5.14	118.24	120.30
1	2	67	A	C4-C5-C6	-5.14	114.43	117.00
1	2	1423	U	N1-C2-O2	5.14	126.40	122.80
39	o	933	ALA	N-CA-CB	-5.14	102.91	110.10
1	2	909	U	N1-C2-O2	5.13	126.39	122.80
1	2	916	U	N1-C2-O2	5.13	126.39	122.80
1	2	1348	A	N1-C2-N3	-5.13	126.73	129.30
1	2	577	G	C8-N9-C4	-5.13	104.35	106.40
1	2	390	G	C8-N9-C1'	-5.13	120.34	127.00
1	2	500	C	N3-C2-O2	-5.13	118.31	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1066	C	N3-C2-O2	-5.13	118.31	121.90
1	2	411	C	N1-C2-O2	5.12	121.97	118.90
1	2	960	U	N1-C2-O2	5.12	126.38	122.80
1	2	1214	U	C5-C6-N1	5.12	125.26	122.70
1	2	1682	U	C2-N1-C1'	5.12	123.84	117.70
1	2	1021	C	C2-N1-C1'	5.12	124.43	118.80
3	Q	147	ALA	C-N-CA	5.12	134.49	121.70
1	2	1129	U	N1-C2-O2	5.11	126.38	122.80
1	2	1731	A	C4-C5-N7	5.11	113.26	110.70
1	2	863	A	N1-C2-N3	-5.11	126.74	129.30
1	2	615	A	N1-C2-N3	-5.11	126.74	129.30
1	2	1012	U	C5-C6-N1	5.11	125.25	122.70
1	2	1530	C	N3-C2-O2	-5.11	118.33	121.90
1	2	36	C	C6-N1-C2	-5.11	118.26	120.30
1	2	857	U	C5-C6-N1	5.11	125.25	122.70
1	2	934	C	N3-C2-O2	-5.10	118.33	121.90
1	2	1461	C	N1-C2-O2	5.10	121.96	118.90
1	2	243	G	N3-C4-N9	5.10	129.06	126.00
1	2	640	U	N1-C2-O2	5.10	126.37	122.80
1	2	758	U	C2-N1-C1'	5.10	123.82	117.70
1	2	679	U	N3-C2-O2	-5.10	118.63	122.20
1	2	1334	U	N1-C2-N3	5.09	117.96	114.90
1	2	391	A	N1-C2-N3	-5.09	126.75	129.30
1	2	534	A	C2-N3-C4	5.09	113.15	110.60
1	2	785	U	N1-C2-O2	5.09	126.36	122.80
1	2	1010	C	C2-N1-C1'	5.09	124.39	118.80
1	2	1311	U	N3-C2-O2	-5.09	118.64	122.20
1	2	1463	C	C6-N1-C2	-5.09	118.27	120.30
1	2	1761	U	C2-N1-C1'	5.09	123.81	117.70
1	2	189	C	N3-C2-O2	-5.08	118.34	121.90
1	2	466	U	N1-C2-O2	5.08	126.36	122.80
1	2	1082	C	N1-C2-O2	5.08	121.95	118.90
1	2	1113	A	N3-C4-C5	5.08	130.35	126.80
1	2	1291	G	C2-N3-C4	5.08	114.44	111.90
1	2	501	U	C5-C4-O4	5.07	128.94	125.90
1	2	959	U	C6-N1-C2	-5.07	117.96	121.00
1	2	405	C	C5-C6-N1	5.07	123.53	121.00
1	2	828	U	N1-C2-O2	5.07	126.35	122.80
1	2	149	C	C5-C6-N1	5.07	123.53	121.00
1	2	778	G	C8-N9-C4	-5.07	104.37	106.40
1	2	1309	C	C6-N1-C2	-5.06	118.28	120.30
25	H	39	VAL	C-N-CA	5.06	134.35	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	522	U	C6-N1-C2	-5.06	117.97	121.00
1	2	882	U	N1-C2-O2	5.06	126.34	122.80
1	2	1310	U	N1-C2-O2	5.06	126.34	122.80
1	2	959	U	C5-C6-N1	5.05	125.23	122.70
1	2	1437	U	N1-C2-O2	5.05	126.33	122.80
1	2	1701	A	O4'-C1'-N9	5.05	112.24	108.20
1	2	1664	C	C5-C6-N1	5.04	123.52	121.00
1	2	1235	C	C2-N1-C1'	5.04	124.35	118.80
1	2	1470	C	C5-C6-N1	5.04	123.52	121.00
1	2	1596	C	N3-C2-O2	-5.04	118.37	121.90
1	2	737	A	C2-N3-C4	5.04	113.12	110.60
1	2	1226	A	P-O3'-C3'	5.04	125.74	119.70
1	2	532	U	N1-C2-O2	5.03	126.32	122.80
1	2	189	C	C5-C6-N1	5.03	123.52	121.00
1	2	491	C	C2-N1-C1'	5.03	124.33	118.80
1	2	778	G	C4-N9-C1'	5.03	133.03	126.50
1	2	820	U	N3-C2-O2	-5.03	118.68	122.20
1	2	309	C	C6-N1-C2	-5.02	118.29	120.30
1	2	111	U	C2-N1-C1'	5.02	123.73	117.70
1	2	140	A	OP1-P-OP2	-5.02	112.07	119.60
1	2	1661	U	N3-C2-O2	-5.02	118.69	122.20
1	2	1344	A	P-O3'-C3'	5.02	125.72	119.70
1	2	117	U	N1-C2-O2	5.01	126.31	122.80
1	2	1226	A	OP1-P-O3'	5.01	116.23	105.20
1	2	1611	A	O4'-C1'-N9	5.01	112.21	108.20
1	2	654	C	C2-N1-C1'	5.01	124.31	118.80
1	2	492	A	O4'-C1'-N9	5.01	112.20	108.20
1	2	1245	G	P-O3'-C3'	5.00	125.70	119.70
1	2	1273	G	OP2-P-O3'	5.00	116.21	105.20
1	2	1174	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	F	110	GLY	Peptide
24	F	84	ASN	Peptide
25	H	40	GLU	Peptide
32	O	144	CYS	Peptide
7	U	64	VAL	Peptide
33	h	116	ASP	Peptide
33	h	117	LYS	Peptide

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Mol	Chain	Res	Type	Group
40	p	336	TRP	Peptide
40	p	391	GLN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	37739	0	18984	347	0
2	P	1020	0	474	0	0
3	Q	1119	0	501	0	0
4	R	1058	0	497	1	0
5	S	1267	0	571	2	0
6	T	1123	0	514	7	0
7	U	913	0	400	1	0
8	V	919	0	450	3	0
9	W	910	0	420	1	0
10	X	702	0	304	2	0
11	Y	742	0	345	1	0
12	Z	620	0	311	1	0
13	a	429	0	201	0	0
14	b	634	0	289	0	0
15	c	704	0	324	0	0
16	d	661	0	312	0	0
17	e	482	0	223	0	0
18	f	400	0	177	0	0
19	g	261	0	113	0	0
20	E	576	0	264	3	0
21	B	1093	0	520	1	0
22	C	1020	0	482	0	0
23	D	456	0	196	1	0
24	F	595	0	288	0	0
25	H	693	0	323	2	0
26	I	600	0	259	1	0
27	J	715	0	318	4	0
28	K	700	0	334	3	0
29	L	496	0	207	0	0
30	M	407	0	182	1	0
31	N	260	0	112	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	O	361	0	162	1	0
33	h	1538	0	736	0	0
34	i	310	0	134	0	0
35	l	1624	0	727	0	0
36	r	261	0	122	0	0
37	1	1639	0	851	32	0
38	m	726	0	316	0	0
39	o	2632	0	1201	0	0
40	p	3201	0	1397	0	0
41	q	3169	0	1368	0	0
42	3	171	0	87	35	0
43	A	497	0	221	13	0
44	k	2860	0	1246	0	0
45	2	2	0	0	0	0
45	k	2	0	0	0	0
46	N	1	0	0	0	0
46	O	1	0	0	0	0
46	m	1	0	0	0	0
47	k	27	0	12	0	0
48	k	31	0	12	0	0
49	k	16	0	0	0	0
All	All	78384	0	37487	379	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (379) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1637:C:O4'	42:3:31:G:C6	1.66	1.48
1:2:1637:C:H4'	42:3:31:G:C5	1.82	1.13
1:2:1756:A:N1	43:A:67:LYS:HA	1.65	1.10
1:2:1637:C:C4'	42:3:31:G:C5	2.34	1.09
1:2:1637:C:C4	37:1:34:C:C2	2.42	1.07
1:2:1637:C:H4'	42:3:31:G:N7	1.72	1.02
1:2:1637:C:C4'	42:3:31:G:C6	2.44	1.00
1:2:1756:A:H2	43:A:67:LYS:CB	1.75	1.00
1:2:867:G:H1	1:2:961:U:H3	0.98	0.97
1:2:1640:C:N4	42:3:31:G:OP1	1.95	0.97
1:2:1055:U:H3	1:2:1064:G:H1	1.13	0.96
1:2:1679:G:N3	1:2:1722:A:N6	2.14	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1637:C:O4'	42:3:31:G:N1	2.00	0.94
1:2:1679:G:N2	1:2:1722:A:H62	1.64	0.94
1:2:1637:C:O2	42:3:31:G:N2	2.00	0.94
1:2:1658:G:N1	1:2:1743:U:O2	1.99	0.93
1:2:895:G:H1	1:2:917:U:H3	1.11	0.93
1:2:1588:G:H1	1:2:1608:U:H3	1.11	0.93
1:2:1637:C:N3	37:1:34:C:O2	2.02	0.92
1:2:1756:A:C2	43:A:67:LYS:CB	2.52	0.92
1:2:1637:C:O4'	42:3:31:G:C5	2.23	0.92
1:2:1680:G:N2	1:2:1721:A:N7	2.18	0.91
1:2:1637:C:N3	37:1:34:C:C2	2.37	0.91
1:2:1047:G:H1	1:2:1071:U:H3	1.15	0.91
1:2:1213:G:H1	1:2:1450:U:H3	1.09	0.91
1:2:1109:G:H1	1:2:1136:U:H3	1.19	0.91
1:2:69:G:H1	1:2:82:U:H3	0.96	0.89
1:2:1471:A:N6	1:2:1538:U:O2	2.07	0.87
1:2:1679:G:H21	1:2:1722:A:H62	1.18	0.87
1:2:480:G:H1	1:2:508:U:H3	1.22	0.85
1:2:699:U:H3	1:2:739:G:H1	0.85	0.84
1:2:1756:A:N1	43:A:67:LYS:CA	2.40	0.84
1:2:273:G:H1	1:2:283:U:H3	1.24	0.83
1:2:1044:U:H3	1:2:1074:G:H1	1.24	0.83
1:2:1663:G:H1	1:2:1738:U:H3	1.25	0.83
1:2:1187:U:H3	1:2:1198:G:H1	1.24	0.82
1:2:1637:C:H42	37:1:34:C:H1'	1.44	0.82
37:1:37:T6A:O14	42:3:28:A:H1'	1.80	0.81
1:2:1756:A:C2	43:A:67:LYS:HA	2.15	0.81
1:2:1756:A:C2	43:A:67:LYS:CA	2.62	0.81
1:2:1471:A:H62	1:2:1538:U:H3	1.27	0.80
1:2:1471:A:N6	1:2:1538:U:C2	2.52	0.77
1:2:1335:U:H3	1:2:1416:G:H1	1.29	0.77
37:1:37:T6A:C13	42:3:28:A:O4'	2.34	0.75
1:2:1756:A:N1	43:A:66:ARG:O	2.20	0.75
1:2:607:G:H1	1:2:1099:U:H3	1.30	0.74
1:2:1175:U:H3	1:2:1464:G:H1	1.34	0.73
1:2:1637:C:N4	37:1:34:C:C1'	2.52	0.72
1:2:1658:G:C6	1:2:1743:U:O2	2.43	0.71
1:2:868:G:H1	1:2:960:U:H3	1.37	0.71
37:1:37:T6A:C13	42:3:28:A:C1'	2.69	0.71
1:2:1637:C:C2	37:1:34:C:O2	2.44	0.70
1:2:1295:G:H1	1:2:1302:U:H3	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1637:C:N4	37:1:34:C:H1'	2.05	0.69
1:2:174:U:H3	1:2:266:A:H62	1.41	0.69
1:2:1001:A:H5'	37:1:39:C:OP1	1.93	0.69
1:2:1637:C:C1'	42:3:31:G:N1	2.55	0.69
1:2:1688:U:H3	1:2:1713:G:H1	1.41	0.68
1:2:1120:U:H3	1:2:1127:G:H1	1.41	0.67
1:2:1637:C:H1'	42:3:31:G:C2	2.30	0.67
1:2:1679:G:H21	1:2:1722:A:N6	1.90	0.67
1:2:188:A:H62	1:2:197:A:H8	1.43	0.66
1:2:1637:C:C4	37:1:34:C:N1	2.63	0.66
1:2:1229:G:H21	1:2:1256:A:H62	1.42	0.66
1:2:1638:G:OP1	42:3:31:G:H2'	1.96	0.66
1:2:1637:C:N4	37:1:34:C:N1	2.44	0.65
1:2:1637:C:C1'	42:3:31:G:C2	2.80	0.65
1:2:1566:U:H5''	27:J:39:GLY:H	1.62	0.64
1:2:1640:C:H42	42:3:31:G:P	2.20	0.64
1:2:1673:G:N1	1:2:1728:A:C2	2.64	0.63
1:2:1287:A:H8	1:2:1287:A:OP2	1.81	0.63
1:2:1775:U:H3	1:2:1786:G:H1	1.46	0.63
1:2:1673:G:C6	1:2:1728:A:N1	2.67	0.63
37:1:37:T6A:C13	42:3:28:A:H1'	2.30	0.62
1:2:1267:G:H1	1:2:1442:U:H3	1.46	0.62
1:2:1203:A:H61	1:2:1553:G:H1'	1.65	0.61
1:2:1684:U:H3	1:2:1717:G:H1	1.48	0.61
1:2:1756:A:N1	43:A:66:ARG:C	2.54	0.61
1:2:1756:A:N6	43:A:66:ARG:O	2.33	0.61
1:2:1637:C:C2	37:1:34:C:C2	2.88	0.61
1:2:1637:C:O4'	42:3:31:G:O6	2.14	0.60
1:2:1339:C:O2'	1:2:1341:A:N7	2.34	0.60
37:1:37:T6A:ODA	42:3:28:A:O4'	2.18	0.60
1:2:992:A:H2	1:2:1012:U:H3	1.49	0.60
37:1:13:C:H42	37:1:22:G:H1	1.49	0.60
1:2:1637:C:H42	37:1:34:C:C1'	2.12	0.60
1:2:1559:A:H5''	27:J:135:GLY:HA3	1.84	0.59
1:2:1588:G:N2	1:2:1608:U:O2	2.35	0.59
37:1:18:G:N3	37:1:18:G:H2'	2.16	0.59
1:2:895:G:N2	1:2:917:U:O2	2.31	0.59
1:2:647:G:H22	1:2:687:G:H1	1.50	0.59
1:2:1191:U:N3	37:1:34:C:H5'	2.17	0.59
1:2:1081:A:O2'	1:2:1083:G:N7	2.36	0.59
1:2:566:C:OP1	43:A:64:LYS:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:3:27:A:H2'	42:3:28:A:H8	1.68	0.58
1:2:748:U:H3	1:2:801:G:H1	1.52	0.57
1:2:1542:G:H1	1:2:1568:C:HO2'	1.50	0.57
1:2:246:G:N2	10:X:38:ALA:O	2.35	0.57
1:2:478:A:N1	1:2:510:G:O6	2.36	0.57
1:2:1585:U:H3	1:2:1611:A:H2	1.51	0.57
1:2:66:U:H5''	6:T:173:PRO:HA	1.86	0.57
37:1:15:G:H22	37:1:48:5MC:HM53	1.70	0.57
1:2:748:U:O2	1:2:801:G:N2	2.38	0.57
1:2:1176:G:N3	1:2:1195:C:O2'	2.37	0.57
1:2:704:C:H42	1:2:734:A:H61	1.52	0.57
1:2:1345:A:N6	1:2:1377:U:O2'	2.37	0.57
1:2:129:U:O2'	1:2:131:C:N4	2.38	0.57
1:2:1047:G:N2	1:2:1071:U:O2	2.36	0.57
1:2:1216:C:O2	1:2:1446:A:N6	2.38	0.56
37:1:37:T6A:ODB	42:3:28:A:H4'	2.05	0.56
1:2:67:A:N6	1:2:83:G:O2'	2.39	0.56
37:1:8:U:H3	37:1:13:C:H41	1.54	0.56
1:2:1673:G:O6	1:2:1728:A:N1	2.39	0.56
37:1:9:1MG:H4'	37:1:45:U:H2'	1.87	0.56
1:2:1380:U:O2'	1:2:1516:A:N1	2.36	0.56
1:2:231:U:O2	1:2:235:G:N2	2.38	0.56
1:2:278:U:OP2	1:2:279:G:N2	2.39	0.56
1:2:1294:G:H1	1:2:1303:U:H3	1.51	0.56
1:2:1229:G:H21	1:2:1256:A:N6	2.03	0.56
1:2:1785:U:H2'	1:2:1786:G:H8	1.71	0.55
1:2:25:C:H5'	1:2:26:A:H5'	1.87	0.55
1:2:1183:A:N3	1:2:1210:C:O2'	2.37	0.55
1:2:1187:U:O2	1:2:1198:G:N2	2.36	0.55
1:2:1158:C:H5	1:2:1581:C:H2'	1.72	0.55
1:2:1499:G:H1	1:2:1508:U:H3	1.52	0.55
1:2:10:G:H1	1:2:1144:U:H3	1.54	0.55
1:2:1174:C:O2'	1:2:1196:A:N6	2.39	0.55
1:2:1120:U:O2	1:2:1127:G:N2	2.36	0.55
1:2:1213:G:N2	1:2:1450:U:O2	2.35	0.55
1:2:1335:U:O2	1:2:1416:G:N2	2.33	0.55
1:2:1294:G:N2	1:2:1303:U:O2	2.41	0.54
1:2:1267:G:N2	1:2:1442:U:O2	2.38	0.54
1:2:1584:G:O2'	1:2:1610:G:N1	2.40	0.54
1:2:1583:A:N6	1:2:1612:U:OP2	2.41	0.54
1:2:1623:C:H2'	1:2:1624:C:H6	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1307:U:H3	1:2:1318:G:H21	1.56	0.54
1:2:1240:U:N3	1:2:1243:G:OP2	2.39	0.54
1:2:523:G:N2	1:2:528:U:OP2	2.41	0.54
1:2:976:G:N2	1:2:1024:U:OP2	2.41	0.54
1:2:167:U:H5''	6:T:135:PRO:HA	1.89	0.53
37:1:37:T6A:ODB	42:3:28:A:C4'	2.56	0.53
1:2:1637:C:C2	42:3:31:G:N2	2.76	0.53
1:2:1110:G:H1	1:2:1135:U:H3	1.55	0.53
1:2:1565:C:O2'	27:J:85:PHE:O	2.21	0.53
1:2:1275:A:O2'	21:B:145:ALA:O	2.27	0.53
1:2:979:A:N3	1:2:1775:U:O2'	2.40	0.53
1:2:1637:C:H5'	42:3:31:G:O6	2.09	0.53
1:2:205:U:H2'	1:2:206:A:H8	1.73	0.53
1:2:105:A:N6	1:2:308:C:O2	2.43	0.52
1:2:1202:A:N6	1:2:1457:C:O5'	2.42	0.52
1:2:1484:G:N2	1:2:1606:C:O2	2.42	0.52
1:2:44:U:OP2	1:2:437:A:N6	2.37	0.52
1:2:996:U:O2	1:2:1008:G:N2	2.39	0.52
1:2:56:U:OP1	1:2:403:G:N1	2.33	0.52
1:2:732:G:HO2'	1:2:735:C:N4	2.08	0.52
1:2:1471:A:N6	1:2:1538:U:H3	2.00	0.52
1:2:1756:A:C6	43:A:66:ARG:O	2.62	0.52
1:2:478:A:H2	1:2:510:G:H1	1.56	0.52
1:2:553:G:H3'	1:2:554:C:H2'	1.91	0.52
1:2:1624:C:H2'	1:2:1625:C:C6	2.45	0.52
1:2:607:G:N2	1:2:1099:U:O2	2.39	0.52
1:2:634:G:N2	1:2:965:U:OP2	2.43	0.52
1:2:941:A:O2'	1:2:1025:A:N6	2.43	0.52
1:2:142:G:H22	1:2:173:A:H2	1.58	0.52
1:2:1584:G:N2	1:2:1611:A:OP2	2.40	0.52
1:2:1681:A:N6	1:2:1720:G:O2'	2.42	0.51
1:2:732:G:O2'	1:2:735:C:N4	2.43	0.51
1:2:1623:C:H2'	1:2:1624:C:C6	2.45	0.51
1:2:793:A:H5''	1:2:794:U:H5'	1.92	0.51
1:2:929:A:OP1	1:2:931:C:N4	2.42	0.51
1:2:680:U:O4	1:2:682:C:N4	2.41	0.51
1:2:1483:A:OP2	1:2:1521:G:N2	2.42	0.51
1:2:224:C:N4	1:2:837:G:O6	2.44	0.51
1:2:1229:G:N2	1:2:1256:A:H62	2.08	0.51
1:2:1287:A:OP1	1:2:1313:A:H5'	2.11	0.51
1:2:1658:G:O6	1:2:1743:U:O2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:578:U:H4'	1:2:579:A:H5'	1.93	0.51
1:2:1499:G:N2	1:2:1508:U:O2	2.40	0.51
1:2:424:C:O2	1:2:427:C:N4	2.44	0.50
1:2:1109:G:N2	1:2:1136:U:O2	2.37	0.50
1:2:1115:U:O2	1:2:1131:A:N7	2.43	0.50
1:2:1295:G:N2	1:2:1302:U:O2	2.37	0.50
1:2:58:U:O2'	1:2:451:A:N3	2.43	0.50
1:2:1665:U:O2	1:2:1736:G:N2	2.41	0.50
1:2:273:G:N2	1:2:283:U:O2	2.40	0.50
1:2:821:U:O4	1:2:852:C:N3	2.44	0.50
1:2:1191:U:C2	37:1:34:C:C5'	2.95	0.50
1:2:126:A:N6	1:2:263:C:O2'	2.38	0.50
8:V:3:ILE:O	8:V:30:GLY:N	2.44	0.50
1:2:554:C:H1'	1:2:555:A:H2	1.77	0.50
1:2:567:A:H62	1:2:576:G:H21	1.60	0.50
1:2:9:U:N3	1:2:12:U:OP2	2.41	0.49
1:2:1360:A:HO2'	28:K:2:PRO:N	2.10	0.49
1:2:166:C:O2'	6:T:133:LEU:O	2.29	0.49
1:2:567:A:H62	1:2:576:G:N2	2.10	0.49
1:2:1285:U:OP2	1:2:1285:U:H6	1.95	0.49
20:E:63:ALA:HB1	20:E:74:ALA:H	1.76	0.49
1:2:1663:G:N2	1:2:1738:U:O2	2.40	0.49
1:2:1594:G:OP2	1:2:1596:C:N4	2.46	0.49
1:2:1637:C:O2	42:3:31:G:C2	2.64	0.49
1:2:1645:G:H22	1:2:1755:A:H2	1.60	0.49
1:2:1712:A:H3'	1:2:1713:G:H8	1.78	0.48
1:2:1638:G:O6	1:2:1767:G:N2	2.46	0.48
1:2:1470:C:H3'	1:2:1573:A:H62	1.79	0.48
1:2:17:C:O2'	1:2:1137:A:N1	2.38	0.48
1:2:69:G:N2	1:2:82:U:O2	2.38	0.48
37:1:20:A:N3	37:1:20:A:H2'	2.29	0.48
1:2:849:C:H2'	1:2:850:A:H8	1.79	0.48
1:2:5:U:H2'	1:2:6:G:H8	1.78	0.48
1:2:1283:U:H2'	1:2:1284:C:C5	2.49	0.48
1:2:1303:U:O2'	1:2:1322:A:OP2	2.32	0.48
1:2:135:A:H4'	1:2:136:C:H5'	1.95	0.47
1:2:480:G:N2	1:2:508:U:O2	2.40	0.47
1:2:699:U:O2	1:2:739:G:N2	2.34	0.47
1:2:704:C:N4	1:2:732:G:O2'	2.48	0.47
1:2:907:A:N3	1:2:997:G:O2'	2.46	0.47
1:2:593:U:H4'	1:2:595:G:H4'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1171:A:H2'	1:2:1172:G:C8	2.49	0.47
1:2:29:U:H2'	1:2:30:G:H8	1.80	0.47
6:T:57:ASP:HA	6:T:106:LEU:HA	1.95	0.47
8:V:46:VAL:N	8:V:54:LYS:O	2.45	0.47
1:2:2:A:O2'	4:R:198:THR:O	2.32	0.47
1:2:867:G:N2	1:2:961:U:O2	2.34	0.47
1:2:1231:U:O2'	1:2:1258:U:O2'	2.27	0.47
1:2:229:U:OP2	1:2:230:C:N4	2.37	0.47
1:2:538:A:O5'	1:2:543:C:N4	2.46	0.47
1:2:641:G:N2	7:U:177:THR:O	2.48	0.47
1:2:751:G:H2'	1:2:752:A:H8	1.80	0.47
1:2:68:A:N6	6:T:132:ARG:O	2.38	0.46
1:2:1588:G:O6	1:2:1608:U:O4	2.33	0.46
1:2:361:C:N4	1:2:379:U:OP1	2.44	0.46
1:2:1542:G:N1	1:2:1568:C:O2'	2.41	0.46
1:2:69:G:O6	1:2:82:U:O4	2.33	0.46
1:2:993:A:H62	1:2:1011:G:H21	1.63	0.46
1:2:1163:A:N3	1:2:1613:U:O2'	2.40	0.46
1:2:1637:C:C5	37:1:34:C:C2	3.01	0.46
1:2:477:A:H2'	1:2:478:A:H8	1.81	0.46
1:2:699:U:O4	1:2:739:G:O6	2.33	0.46
1:2:1272:U:O2	1:2:1438:G:O6	2.34	0.46
1:2:1756:A:N1	43:A:67:LYS:N	2.63	0.46
1:2:953:G:H2'	1:2:954:G:H8	1.81	0.46
1:2:1311:U:H4'	26:I:2:GLY:HA3	1.98	0.46
1:2:23:G:H1	1:2:602:U:H3	1.63	0.46
1:2:1160:A:O2'	1:2:1620:C:O2	2.34	0.46
1:2:1466:G:O2'	1:2:1602:C:OP1	2.28	0.46
1:2:1713:G:H2'	1:2:1714:A:H8	1.81	0.46
37:1:37:T6A:C12	42:3:28:A:H1'	2.46	0.46
1:2:732:G:HO2'	1:2:735:C:H42	1.62	0.46
1:2:800:U:H2'	1:2:801:G:C8	2.51	0.46
1:2:877:G:H22	1:2:951:A:H2	1.63	0.46
1:2:1158:C:C5	1:2:1581:C:H2'	2.50	0.46
12:Z:60:ALA:HB1	12:Z:101:ALA:HB2	1.97	0.46
1:2:1042:G:H2'	1:2:1043:A:H8	1.81	0.45
1:2:1320:U:O2'	1:2:1322:A:OP1	2.33	0.45
1:2:1474:G:H2'	1:2:1475:A:C8	2.52	0.45
1:2:1637:C:H4'	42:3:31:G:C8	2.47	0.45
1:2:273:G:O6	1:2:283:U:O4	2.34	0.45
1:2:445:A:H61	1:2:462:G:H1'	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1210:C:H2'	1:2:1211:A:H8	1.80	0.45
1:2:1637:C:C5	37:1:34:C:C4	3.04	0.45
1:2:103:A:N7	1:2:358:U:O2	2.50	0.45
1:2:560:U:H2'	1:2:561:G:H8	1.81	0.45
1:2:629:U:C2	1:2:970:A:N7	2.84	0.45
1:2:1060:U:H3'	1:2:1061:A:H5''	1.99	0.45
1:2:1089:U:O2'	1:2:1093:A:N1	2.38	0.45
5:S:181:VAL:HA	5:S:227:VAL:HA	1.99	0.45
1:2:505:A:O2'	1:2:507:U:OP1	2.32	0.45
1:2:523:G:H22	1:2:527:A:H3'	1.82	0.45
1:2:1047:G:O6	1:2:1071:U:O4	2.35	0.45
1:2:1638:G:OP1	42:3:31:G:C2'	2.64	0.45
1:2:444:C:C2	1:2:460:A:N6	2.84	0.45
1:2:1488:G:H3'	1:2:1515:A:H61	1.82	0.45
1:2:1194:A:N6	25:H:143:ARG:O	2.50	0.44
1:2:32:U:O2'	1:2:594:A:N1	2.42	0.44
1:2:1662:G:H2'	1:2:1663:G:H8	1.81	0.44
8:V:57:ALA:HB2	8:V:177:GLY:HA2	1.99	0.44
30:M:39:ALA:H	30:M:71:ILE:HA	1.82	0.44
1:2:1490:C:H5'	1:2:1492:A:H1'	1.98	0.44
1:2:217:A:N1	1:2:844:A:O2'	2.47	0.44
1:2:953:G:H2'	1:2:954:G:C8	2.52	0.44
1:2:1458:G:OP1	27:J:138:THR:N	2.47	0.44
1:2:343:C:H2'	1:2:344:A:H8	1.83	0.44
1:2:534:A:H3'	1:2:535:A:H8	1.82	0.44
1:2:1191:U:C2	37:1:34:C:H5'	2.53	0.44
1:2:867:G:O6	1:2:961:U:O4	2.36	0.44
23:D:55:VAL:HA	23:D:68:LEU:HA	1.99	0.44
1:2:1106:U:H2'	1:2:1107:G:H8	1.81	0.44
32:O:106:TYR:O	32:O:117:LEU:N	2.45	0.44
1:2:1353:U:H3	1:2:1372:U:H3	1.65	0.43
1:2:410:A:H61	1:2:423:G:H1	1.65	0.43
1:2:706:A:H61	1:2:731:C:H5''	1.83	0.43
1:2:922:G:H2'	1:2:923:A:C8	2.54	0.43
1:2:1115:U:C2	1:2:1131:A:N7	2.86	0.43
20:E:16:SER:HA	20:E:21:ASP:HA	2.00	0.43
1:2:871:G:H2'	1:2:872:G:C8	2.54	0.43
1:2:1150:G:O6	42:3:29:A:OP2	2.37	0.43
1:2:340:U:H2'	1:2:341:A:C8	2.54	0.43
1:2:863:A:N7	1:2:964:U:C2	2.85	0.43
1:2:863:A:C8	1:2:964:U:N3	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1371:A:O2'	1:2:1373:C:OP1	2.28	0.43
1:2:1637:C:C5	37:1:34:C:N3	2.87	0.43
42:3:26:A:H2'	42:3:27:A:C8	2.54	0.43
1:2:1151:A:H2'	1:2:1152:A:C8	2.54	0.43
1:2:199:G:H2'	1:2:200:A:H8	1.82	0.43
1:2:50:C:H2'	1:2:424:C:H41	1.83	0.43
1:2:1073:G:H4'	11:Y:10:GLY:HA2	2.01	0.43
1:2:1638:G:P	42:3:31:G:H2'	2.58	0.43
1:2:103:A:N7	1:2:358:U:C2	2.87	0.42
1:2:1170:G:N2	1:2:1571:C:O2'	2.51	0.42
1:2:1643:U:O2	1:2:1780:G:N2	2.49	0.42
1:2:1690:G:H2'	1:2:1691:A:C8	2.54	0.42
1:2:61:A:O2'	1:2:62:A:O4'	2.37	0.42
1:2:62:A:O2'	1:2:268:C:O2	2.37	0.42
1:2:104:A:O4'	1:2:308:C:N4	2.52	0.42
1:2:1287:A:N6	1:2:1329:A:H4'	2.34	0.42
1:2:1315:U:OP2	1:2:1328:G:N1	2.50	0.42
1:2:591:A:H2'	1:2:592:A:C8	2.55	0.42
1:2:1357:A:H2'	1:2:1358:G:C8	2.55	0.42
1:2:1150:G:H1	42:3:29:A:P	2.43	0.42
1:2:751:G:H2'	1:2:752:A:C8	2.55	0.42
1:2:923:A:H2'	1:2:924:A:C8	2.54	0.42
1:2:764:U:O2	1:2:772:G:N2	2.47	0.42
1:2:774:A:N6	1:2:786:C:O2	2.53	0.42
1:2:1637:C:C5'	42:3:31:G:O6	2.68	0.42
1:2:1642:G:N3	1:2:1781:A:O2'	2.48	0.42
1:2:209:U:H2'	1:2:210:A:C8	2.54	0.42
1:2:247:A:O2'	10:X:37:ASN:O	2.29	0.42
1:2:1641:C:H2'	1:2:1642:G:C8	2.55	0.42
1:2:250:C:H2'	1:2:251:A:H8	1.85	0.42
1:2:329:G:H2'	1:2:330:G:H8	1.85	0.42
1:2:992:A:O2'	1:2:1785:U:O2	2.26	0.42
1:2:1626:U:H2'	1:2:1627:U:C6	2.55	0.42
1:2:1171:A:O2'	1:2:1570:A:N3	2.43	0.41
1:2:1484:G:H21	1:2:1606:C:H1'	1.86	0.41
1:2:59:C:O2'	1:2:60:U:O4'	2.37	0.41
1:2:1114:G:N2	1:2:1115:U:O4	2.40	0.41
1:2:1628:U:H2'	1:2:1629:G:C8	2.55	0.41
1:2:1207:C:N4	1:2:1456:C:N3	2.51	0.41
1:2:1761:U:H2'	42:3:29:A:H4'	2.03	0.41
1:2:1187:U:O4	1:2:1200:G:N2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1202:A:H1'	1:2:1207:C:H41	1.84	0.41
1:2:1426:C:H3'	1:2:1427:A:H4'	2.01	0.41
1:2:1658:G:O6	1:2:1743:U:C2	2.74	0.41
1:2:1755:A:HO2'	43:A:46:ARG:N	2.17	0.41
1:2:34:G:O2'	1:2:515:A:O2'	2.39	0.41
1:2:480:G:O6	1:2:508:U:O4	2.39	0.41
1:2:1027:A:OP1	1:2:1789:G:O2'	2.29	0.41
1:2:1504:G:OP1	28:K:98:GLY:N	2.54	0.41
6:T:57:ASP:HA	6:T:107:ALA:H	1.86	0.41
1:2:1693:A:H2'	1:2:1694:A:H8	1.84	0.41
5:S:193:GLY:O	5:S:211:LYS:N	2.54	0.41
1:2:563:U:O2'	1:2:566:C:N3	2.43	0.41
1:2:816:G:H22	1:2:855:A:H2	1.68	0.41
1:2:1132:A:H2'	1:2:1133:A:H8	1.86	0.41
1:2:1511:U:H2'	1:2:1512:G:C8	2.56	0.41
1:2:1585:U:OP1	25:H:125:GLU:N	2.43	0.41
1:2:1591:C:H2'	1:2:1592:A:H8	1.84	0.41
1:2:733:A:N1	1:2:737:A:N6	2.69	0.41
1:2:884:A:H2'	1:2:885:G:C8	2.55	0.41
1:2:1169:G:N1	1:2:1575:G:OP2	2.39	0.41
1:2:1456:C:H5''	1:2:1457:C:H5''	2.03	0.41
20:E:17:TYR:N	20:E:20:VAL:O	2.53	0.41
1:2:139:C:O2'	1:2:177:U:O2	2.39	0.41
1:2:199:G:H2'	1:2:200:A:C8	2.56	0.41
1:2:1110:G:N2	1:2:1135:U:O2	2.44	0.41
1:2:1222:C:H2'	1:2:1223:A:C8	2.56	0.41
1:2:514:G:H2'	1:2:515:A:H8	1.85	0.40
1:2:107:C:H2'	1:2:108:A:C8	2.56	0.40
1:2:890:C:H2'	1:2:891:A:C8	2.56	0.40
1:2:1222:C:H2'	1:2:1223:A:H8	1.87	0.40
1:2:1525:A:N3	1:2:1589:C:O2'	2.42	0.40
6:T:74:LYS:HA	6:T:96:SER:HA	2.02	0.40
1:2:1498:G:H5''	28:K:72:GLY:HA3	2.03	0.40
1:2:20:G:O2'	1:2:554:C:N4	2.39	0.40
1:2:1041:G:H2'	1:2:1042:G:C8	2.57	0.40
1:2:1220:C:H2'	1:2:1221:A:C8	2.57	0.40
1:2:1665:U:O2	1:2:1736:G:C2	2.75	0.40
1:2:272:U:HO2'	1:2:273:G:H8	1.70	0.40
9:W:95:TYR:HA	9:W:98:ALA:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	P	204/252 (81%)	188 (92%)	16 (8%)	0	100	100
3	Q	222/255 (87%)	204 (92%)	17 (8%)	1 (0%)	29	69
4	R	214/254 (84%)	201 (94%)	13 (6%)	0	100	100
5	S	256/261 (98%)	237 (93%)	19 (7%)	0	100	100
6	T	226/236 (96%)	214 (95%)	12 (5%)	0	100	100
7	U	182/190 (96%)	170 (93%)	12 (7%)	0	100	100
8	V	183/200 (92%)	174 (95%)	9 (5%)	0	100	100
9	W	182/197 (92%)	172 (94%)	10 (6%)	0	100	100
10	X	140/155 (90%)	131 (94%)	9 (6%)	0	100	100
11	Y	148/151 (98%)	141 (95%)	7 (5%)	0	100	100
12	Z	125/136 (92%)	111 (89%)	14 (11%)	0	100	100
13	a	85/87 (98%)	79 (93%)	6 (7%)	0	100	100
14	b	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
15	c	142/145 (98%)	129 (91%)	12 (8%)	1 (1%)	22	63
16	d	132/135 (98%)	127 (96%)	5 (4%)	0	100	100
17	e	95/119 (80%)	89 (94%)	6 (6%)	0	100	100
18	f	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
19	g	51/63 (81%)	45 (88%)	6 (12%)	0	100	100
20	E	115/141 (82%)	104 (90%)	11 (10%)	0	100	100
21	B	220/240 (92%)	211 (96%)	9 (4%)	0	100	100
22	C	204/225 (91%)	187 (92%)	17 (8%)	0	100	100
23	D	90/105 (86%)	76 (84%)	14 (16%)	0	100	100
24	F	119/143 (83%)	92 (77%)	24 (20%)	3 (2%)	5	32
25	H	139/143 (97%)	130 (94%)	9 (6%)	0	100	100
26	I	117/136 (86%)	113 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	J	143/146 (98%)	135 (94%)	8 (6%)	0	100	100
28	K	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
29	L	98/121 (81%)	90 (92%)	8 (8%)	0	100	100
30	M	80/108 (74%)	72 (90%)	8 (10%)	0	100	100
31	N	51/56 (91%)	51 (100%)	0	0	100	100
32	O	71/152 (47%)	51 (72%)	20 (28%)	0	100	100
33	h	310/319 (97%)	275 (89%)	35 (11%)	0	100	100
34	i	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
35	l	326/347 (94%)	318 (98%)	8 (2%)	0	100	100
36	r	51/135 (38%)	48 (94%)	3 (6%)	0	100	100
38	m	145/405 (36%)	131 (90%)	13 (9%)	1 (1%)	22	63
39	o	519/964 (54%)	488 (94%)	26 (5%)	5 (1%)	15	54
40	p	638/763 (84%)	583 (91%)	43 (7%)	12 (2%)	8	38
41	q	624/812 (77%)	567 (91%)	45 (7%)	12 (2%)	8	38
43	A	97/153 (63%)	85 (88%)	7 (7%)	5 (5%)	2	19
44	k	575/608 (95%)	522 (91%)	47 (8%)	6 (1%)	15	54
All	All	7727/9481 (82%)	7123 (92%)	558 (7%)	46 (1%)	29	66

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	F	85	LYS
40	p	337	PRO
40	p	392	PRO
40	p	690	GLN
43	A	31	GLU
43	A	66	ARG
40	p	423	PRO
41	q	160	ASN
41	q	161	TRP
43	A	23	LYS
43	A	116	ASN
43	A	118	THR
44	k	280	ASP
24	F	109	GLU
24	F	126	TRP

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Mol	Chain	Res	Type
39	o	62	LEU
39	o	63	LYS
39	o	251	GLU
40	p	77	GLN
40	p	689	GLU
41	q	460	PRO
41	q	468	THR
41	q	536	ASP
41	q	558	CYS
44	k	364	GLY
3	Q	57	ALA
38	m	12	PRO
40	p	634	GLU
41	q	645	ILE
41	q	650	LYS
39	o	49	GLU
39	o	394	ASN
40	p	207	ASP
40	p	569	PRO
41	q	351	ILE
41	q	514	LYS
41	q	779	GLU
44	k	356	TYR
40	p	198	VAL
40	p	422	VAL
15	c	88	PRO
40	p	478	ILE
41	q	164	PRO
44	k	323	PRO
44	k	404	PRO
44	k	427	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1768/1800 (98%)	474 (26%)	39 (2%)
37	1	72/75 (96%)	28 (38%)	6 (8%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
42	3	7/8 (87%)	1 (14%)	1 (14%)
All	All	1847/1883 (98%)	503 (27%)	46 (2%)

All (503) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	4	C
1	2	17	C
1	2	25	C
1	2	26	A
1	2	34	G
1	2	42	G
1	2	43	A
1	2	45	U
1	2	46	A
1	2	47	A
1	2	56	U
1	2	57	G
1	2	59	C
1	2	61	A
1	2	62	A
1	2	63	G
1	2	65	A
1	2	67	A
1	2	68	A
1	2	69	G
1	2	71	A
1	2	73	U
1	2	74	U
1	2	75	U
1	2	76	A
1	2	78	A
1	2	79	C
1	2	81	G
1	2	104	A
1	2	114	C
1	2	115	G
1	2	116	U
1	2	121	U
1	2	126	A
1	2	127	G

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Mol	Chain	Res	Type
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	138	A
1	2	140	A
1	2	141	U
1	2	142	G
1	2	145	A
1	2	153	G
1	2	155	U
1	2	159	U
1	2	168	A
1	2	171	A
1	2	176	C
1	2	178	U
1	2	179	A
1	2	180	A
1	2	185	U
1	2	186	C
1	2	187	G
1	2	188	A
1	2	191	C
1	2	192	U
1	2	193	U
1	2	194	U
1	2	195	G
1	2	216	U
1	2	217	A
1	2	218	A
1	2	223	U
1	2	224	C
1	2	225	A
1	2	227	U
1	2	228	G
1	2	230	C
1	2	232	U
1	2	233	C
1	2	234	G

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Mol	Chain	Res	Type
1	2	235	G
1	2	236	A
1	2	240	U
1	2	241	U
1	2	243	G
1	2	249	U
1	2	250	C
1	2	255	U
1	2	257	A
1	2	260	U
1	2	265	A
1	2	272	U
1	2	274	G
1	2	276	C
1	2	277	U
1	2	278	U
1	2	279	G
1	2	280	U
1	2	281	G
1	2	287	G
1	2	299	A
1	2	313	U
1	2	314	C
1	2	316	A
1	2	320	U
1	2	322	G
1	2	323	A
1	2	330	G
1	2	333	A
1	2	337	G
1	2	338	C
1	2	352	A
1	2	353	A
1	2	359	A
1	2	361	C
1	2	373	G
1	2	388	G
1	2	390	G
1	2	399	A
1	2	400	A
1	2	401	A
1	2	402	C

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Mol	Chain	Res	Type
1	2	404	G
1	2	416	A
1	2	417	A
1	2	422	G
1	2	423	G
1	2	424	C
1	2	425	A
1	2	426	G
1	2	434	G
1	2	436	A
1	2	439	U
1	2	444	C
1	2	446	A
1	2	448	C
1	2	452	A
1	2	454	U
1	2	460	A
1	2	468	A
1	2	471	A
1	2	477	A
1	2	482	U
1	2	483	A
1	2	485	A
1	2	486	G
1	2	487	G
1	2	489	C
1	2	491	C
1	2	492	A
1	2	493	U
1	2	494	U
1	2	496	G
1	2	498	G
1	2	499	U
1	2	500	C
1	2	502	U
1	2	505	A
1	2	506	A
1	2	507	U
1	2	510	G
1	2	511	A
1	2	527	A
1	2	534	A

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Mol	Chain	Res	Type
1	2	538	A
1	2	540	G
1	2	541	A
1	2	542	A
1	2	544	A
1	2	556	A
1	2	557	G
1	2	558	U
1	2	559	C
1	2	565	C
1	2	568	G
1	2	572	C
1	2	579	A
1	2	580	A
1	2	594	A
1	2	595	G
1	2	606	A
1	2	610	G
1	2	611	U
1	2	617	U
1	2	619	A
1	2	620	A
1	2	621	A
1	2	622	A
1	2	623	A
1	2	624	G
1	2	635	A
1	2	638	U
1	2	639	U
1	2	640	U
1	2	641	G
1	2	643	G
1	2	648	G
1	2	653	C
1	2	654	C
1	2	655	G
1	2	677	G
1	2	678	A
1	2	680	U
1	2	681	U
1	2	682	C
1	2	683	C

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Mol	Chain	Res	Type
1	2	687	G
1	2	693	U
1	2	694	U
1	2	696	C
1	2	698	U
1	2	700	C
1	2	702	G
1	2	703	G
1	2	704	C
1	2	705	U
1	2	706	A
1	2	707	A
1	2	708	C
1	2	709	C
1	2	710	U
1	2	711	U
1	2	712	G
1	2	713	A
1	2	714	G
1	2	728	U
1	2	729	G
1	2	730	G
1	2	731	C
1	2	732	G
1	2	733	A
1	2	734	A
1	2	736	C
1	2	737	A
1	2	738	G
1	2	739	G
1	2	741	C
1	2	742	U
1	2	743	U
1	2	756	A
1	2	765	G
1	2	766	U
1	2	767	U
1	2	774	A
1	2	775	G
1	2	778	G
1	2	779	U
1	2	780	A

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Mol	Chain	Res	Type
1	2	781	U
1	2	782	U
1	2	783	G
1	2	789	A
1	2	812	A
1	2	813	U
1	2	814	A
1	2	815	G
1	2	818	C
1	2	819	G
1	2	820	U
1	2	821	U
1	2	823	G
1	2	833	U
1	2	835	U
1	2	840	U
1	2	841	U
1	2	846	G
1	2	851	U
1	2	852	C
1	2	855	A
1	2	856	A
1	2	857	U
1	2	863	A
1	2	899	G
1	2	901	G
1	2	902	G
1	2	903	U
1	2	912	U
1	2	913	G
1	2	929	A
1	2	933	A
1	2	934	C
1	2	935	U
1	2	942	G
1	2	960	U
1	2	964	U
1	2	966	A
1	2	970	A
1	2	971	A
1	2	988	A
1	2	992	A

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Mol	Chain	Res	Type
1	2	993	A
1	2	998	A
1	2	1004	U
1	2	1005	A
1	2	1020	A
1	2	1021	C
1	2	1024	U
1	2	1026	A
1	2	1028	C
1	2	1039	A
1	2	1052	U
1	2	1053	G
1	2	1058	U
1	2	1059	U
1	2	1060	U
1	2	1061	A
1	2	1063	U
1	2	1076	A
1	2	1080	U
1	2	1081	A
1	2	1082	C
1	2	1092	A
1	2	1093	A
1	2	1096	C
1	2	1100	G
1	2	1138	A
1	2	1150	G
1	2	1153	G
1	2	1156	C
1	2	1158	C
1	2	1160	A
1	2	1164	G
1	2	1166	A
1	2	1167	G
1	2	1170	G
1	2	1185	U
1	2	1194	A
1	2	1196	A
1	2	1199	G
1	2	1200	G
1	2	1202	A
1	2	1208	A

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Mol	Chain	Res	Type
1	2	1216	C
1	2	1217	A
1	2	1218	G
1	2	1227	A
1	2	1229	G
1	2	1241	G
1	2	1243	G
1	2	1244	A
1	2	1245	G
1	2	1246	C
1	2	1251	U
1	2	1252	C
1	2	1256	A
1	2	1257	U
1	2	1274	C
1	2	1275	A
1	2	1285	U
1	2	1287	A
1	2	1291	G
1	2	1301	U
1	2	1314	U
1	2	1315	U
1	2	1316	G
1	2	1318	G
1	2	1321	A
1	2	1322	A
1	2	1325	A
1	2	1337	A
1	2	1344	A
1	2	1345	A
1	2	1346	A
1	2	1348	A
1	2	1349	G
1	2	1354	G
1	2	1355	C
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

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Mol	Chain	Res	Type
1	2	1382	A
1	2	1383	G
1	2	1389	C
1	2	1390	U
1	2	1398	U
1	2	1399	C
1	2	1400	A
1	2	1402	G
1	2	1414	U
1	2	1425	A
1	2	1427	A
1	2	1431	C
1	2	1432	U
1	2	1433	G
1	2	1445	G
1	2	1446	A
1	2	1459	C
1	2	1460	A
1	2	1466	G
1	2	1469	A
1	2	1470	C
1	2	1471	A
1	2	1472	C
1	2	1479	A
1	2	1486	G
1	2	1491	U
1	2	1492	A
1	2	1493	A
1	2	1496	U
1	2	1503	A
1	2	1506	G
1	2	1514	U
1	2	1516	A
1	2	1517	U
1	2	1518	C
1	2	1521	G
1	2	1523	G
1	2	1524	A
1	2	1528	U
1	2	1531	G
1	2	1535	U
1	2	1537	C

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Mol	Chain	Res	Type
1	2	1540	G
1	2	1542	G
1	2	1543	A
1	2	1554	U
1	2	1557	U
1	2	1558	U
1	2	1559	A
1	2	1570	A
1	2	1572	G
1	2	1573	A
1	2	1574	G
1	2	1575	G
1	2	1576	A
1	2	1577	A
1	2	1583	A
1	2	1584	G
1	2	1590	G
1	2	1601	G
1	2	1607	G
1	2	1611	A
1	2	1614	A
1	2	1616	G
1	2	1622	G
1	2	1631	A
1	2	1634	C
1	2	1635	A
1	2	1636	C
1	2	1637	C
1	2	1657	U
1	2	1658	G
1	2	1678	A
1	2	1688	U
1	2	1693	A
1	2	1700	C
1	2	1701	A
1	2	1703	C
1	2	1708	U
1	2	1709	C
1	2	1715	G
1	2	1716	C
1	2	1717	G
1	2	1743	U

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Mol	Chain	Res	Type
1	2	1753	A
1	2	1756	A
1	2	1757	G
1	2	1760	G
1	2	1762	A
1	2	1766	A
1	2	1767	G
1	2	1769	U
1	2	1771	U
1	2	1780	G
1	2	1782	A
1	2	1783	C
1	2	1792	G
1	2	1793	G
1	2	1794	A
1	2	1796	C
1	2	1798	U
1	2	1799	U
37	1	8	U
37	1	9	1MG
37	1	10	2MG
37	1	15	G
37	1	16	H2U
37	1	19	G
37	1	20	A
37	1	21	A
37	1	22	G
37	1	23	C
37	1	26	M2G
37	1	40	C
37	1	44	A
37	1	46	G7M
37	1	47	H2U
37	1	48	5MC
37	1	49	5MC
37	1	52	G
37	1	58	1MA
37	1	59	A
37	1	60	A
37	1	61	C
37	1	64	RIA
37	1	68	G

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Mol	Chain	Res	Type
37	1	71	C
37	1	74	C
37	1	75	C
37	1	76	A
42	3	27	A

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	68	A
1	2	77	U
1	2	139	C
1	2	141	U
1	2	224	C
1	2	278	U
1	2	280	U
1	2	313	U
1	2	322	G
1	2	352	A
1	2	387	A
1	2	400	A
1	2	539	G
1	2	541	A
1	2	555	A
1	2	609	U
1	2	639	U
1	2	640	U
1	2	705	U
1	2	711	U
1	2	755	A
1	2	765	G
1	2	819	G
1	2	912	U
1	2	928	U
1	2	1023	A
1	2	1226	A
1	2	1256	A
1	2	1273	G
1	2	1274	C
1	2	1344	A
1	2	1382	A
1	2	1430	U

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Mol	Chain	Res	Type
1	2	1471	A
1	2	1573	A
1	2	1633	A
1	2	1636	C
1	2	1742	U
1	2	1791	A
37	1	7	G
37	1	43	G
37	1	47	H2U
37	1	48	5MC
37	1	58	1MA
37	1	74	C
42	3	28	A

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

11 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	$\# Z > 2$
37	T6A	1	37	37	27,34,35	1.04	2 (7%)	29,49,52	2.65	9 (31%)
37	H2U	1	16	37	18,21,22	0.80	1 (5%)	21,30,33	1.47	4 (19%)
37	1MG	1	9	37	18,26,27	0.99	0	19,39,42	1.48	4 (21%)
37	M2G	1	26	37	20,27,28	1.75	3 (15%)	22,40,43	1.18	4 (18%)
37	1MA	1	58	37	16,25,26	1.81	3 (18%)	18,37,40	1.42	3 (16%)
37	2MG	1	10	37	18,26,27	1.02	1 (5%)	16,38,41	1.19	2 (12%)
37	H2U	1	47	37	18,21,22	0.79	0	21,30,33	1.37	4 (19%)
37	G7M	1	46	37	20,26,27	2.75	3 (15%)	17,39,42	1.01	1 (5%)
37	5MC	1	48	37	18,22,23	0.99	1 (5%)	26,32,35	1.31	4 (15%)
37	RIA	1	64	37	31,38,39	0.53	0	39,57,60	0.65	0
37	5MC	1	49	37	18,22,23	1.08	1 (5%)	26,32,35	1.33	5 (19%)

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
37	T6A	1	37	37	-	8/19/41/42	0/3/3/3
37	H2U	1	16	37	-	1/7/38/39	0/2/2/2
37	1MG	1	9	37	-	2/3/25/26	0/3/3/3
37	M2G	1	26	37	-	6/7/29/30	0/3/3/3
37	1MA	1	58	37	-	0/3/25/26	0/3/3/3
37	2MG	1	10	37	-	2/5/27/28	0/3/3/3
37	H2U	1	47	37	-	5/7/38/39	0/2/2/2
37	G7M	1	46	37	-	1/3/25/26	0/3/3/3
37	5MC	1	48	37	-	3/7/25/26	0/2/2/2
37	RIA	1	64	37	-	3/13/51/52	0/4/4/4
37	5MC	1	49	37	-	2/7/25/26	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1	46	G7M	C8-N9	7.81	1.47	1.33
37	1	46	G7M	C8-N7	7.29	1.46	1.33
37	1	26	M2G	C2-N3	5.69	1.37	1.30
37	1	58	1MA	C2-N3	5.57	1.35	1.29
37	1	46	G7M	C5-C4	4.76	1.48	1.39
37	1	26	M2G	C2-N2	3.61	1.42	1.35
37	1	58	1MA	C6-N6	3.47	1.36	1.27
37	1	49	5MC	C6-C5	3.37	1.40	1.34
37	1	48	5MC	C6-C5	2.88	1.39	1.34
37	1	37	T6A	C5-C4	2.49	1.47	1.40
37	1	10	2MG	O4'-C1'	2.23	1.44	1.41
37	1	37	T6A	O4'-C1'	2.20	1.44	1.41
37	1	26	M2G	O4'-C1'	2.13	1.44	1.41
37	1	58	1MA	C5-C4	2.05	1.48	1.43
37	1	16	H2U	C2-N3	-2.04	1.34	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	1	37	T6A	C12-N11-C10	8.55	136.18	121.94
37	1	37	T6A	C2-N1-C6	7.15	122.72	116.59
37	1	16	H2U	O4'-C1'-N1	3.92	114.64	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	1	37	T6A	C14-C12-C13	3.63	116.37	110.19
37	1	37	T6A	N3-C2-N1	-3.58	123.08	128.68
37	1	58	1MA	C3'-C2'-C1'	3.48	106.21	100.98
37	1	37	T6A	N6-C6-N1	3.08	122.84	118.72
37	1	9	1MG	C5-C6-N1	3.07	118.52	113.90
37	1	49	5MC	C5-C4-N3	-2.95	118.50	121.67
37	1	37	T6A	O10-C10-N6	-2.93	118.67	123.62
37	1	49	5MC	O2-C2-N3	-2.86	117.67	122.33
37	1	47	H2U	C4-N3-C2	-2.81	123.46	125.79
37	1	46	G7M	CN7-N7-C8	-2.77	112.07	125.43
37	1	48	5MC	O2-C2-N3	-2.77	117.83	122.33
37	1	9	1MG	C3'-C2'-C1'	2.71	105.06	100.98
37	1	37	T6A	C14-C12-N11	2.71	118.65	111.72
37	1	16	H2U	C5-C4-N3	2.70	119.68	116.65
37	1	37	T6A	C4-C5-N7	-2.67	106.61	109.40
37	1	9	1MG	O6-C6-C5	-2.66	119.49	124.19
37	1	16	H2U	C4-N3-C2	-2.61	123.62	125.79
37	1	48	5MC	C5-C6-N1	-2.60	120.67	123.34
37	1	47	H2U	C3'-C2'-C1'	2.54	106.26	101.43
37	1	47	H2U	C5-C4-N3	2.54	119.50	116.65
37	1	48	5MC	C5-C4-N3	-2.46	119.02	121.67
37	1	26	M2G	C5-C6-N1	2.45	118.27	113.95
37	1	9	1MG	C8-N7-C5	2.38	107.53	102.99
37	1	10	2MG	C5-C6-N1	2.35	118.11	113.95
37	1	58	1MA	C8-N7-C5	2.33	107.44	102.99
37	1	10	2MG	C8-N7-C5	2.33	107.42	102.99
37	1	26	M2G	C8-N7-C5	2.30	107.37	102.99
37	1	49	5MC	C3'-C2'-C1'	2.30	105.79	101.43
37	1	58	1MA	C5-C6-N1	2.24	117.23	113.90
37	1	49	5MC	O4'-C1'-N1	2.20	113.38	108.36
37	1	47	H2U	C5-C6-N1	-2.17	104.47	111.61
37	1	26	M2G	O6-C6-C5	-2.15	120.17	124.37
37	1	16	H2U	C3'-C2'-C1'	2.15	105.52	101.43
37	1	48	5MC	CM5-C5-C6	-2.15	119.98	122.85
37	1	49	5MC	CM5-C5-C6	-2.11	120.03	122.85
37	1	26	M2G	N1-C2-N2	2.09	119.82	118.04
37	1	37	T6A	N6-C10-N11	2.08	116.67	113.76

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	1	9	1MG	O4'-C4'-C5'-O5'
37	1	9	1MG	C3'-C4'-C5'-O5'
37	1	16	H2U	C4'-C5'-O5'-P
37	1	26	M2G	C3'-C4'-C5'-O5'
37	1	26	M2G	N1-C2-N2-CM1
37	1	26	M2G	N3-C2-N2-CM1
37	1	26	M2G	N3-C2-N2-CM2
37	1	37	T6A	C14-C12-N11-C10
37	1	47	H2U	C4'-C5'-O5'-P
37	1	47	H2U	C3'-C4'-C5'-O5'
37	1	47	H2U	O4'-C1'-N1-C6
37	1	48	5MC	C4'-C5'-O5'-P
37	1	64	RIA	C3'-C4'-C5'-O5'
37	1	10	2MG	O4'-C4'-C5'-O5'
37	1	10	2MG	C3'-C4'-C5'-O5'
37	1	48	5MC	O4'-C4'-C5'-O5'
37	1	48	5MC	C3'-C4'-C5'-O5'
37	1	26	M2G	O4'-C4'-C5'-O5'
37	1	64	RIA	O1'-C4'-C5'-O5'
37	1	37	T6A	C14-C12-C13-ODB
37	1	47	H2U	O4'-C4'-C5'-O5'
37	1	37	T6A	C13-C12-C14-C15
37	1	37	T6A	C14-C12-C13-ODA
37	1	26	M2G	N1-C2-N2-CM2
37	1	46	G7M	C4'-C5'-O5'-P
37	1	47	H2U	O4'-C1'-N1-C2
37	1	64	RIA	C4A-C5A-O5A-P
37	1	37	T6A	O4'-C4'-C5'-O5'
37	1	37	T6A	N11-C12-C13-ODA
37	1	37	T6A	N11-C12-C13-ODB
37	1	49	5MC	O4'-C4'-C5'-O5'
37	1	37	T6A	C13-C12-N11-C10
37	1	49	5MC	C3'-C4'-C5'-O5'

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	1	37	T6A	8	0
37	1	9	1MG	1	0
37	1	48	5MC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
48	ATP	k	703	45	26,33,33	0.93	1 (3%)	31,52,52	1.60	5 (16%)
49	SF4	k	705	-	0,12,12	-	-	-		
49	SF4	k	706	-	0,12,12	-	-	-		
47	ADP	k	701	45	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	ATP	k	703	45	-	2/18/38/38	0/3/3/3
49	SF4	k	705	-	-	-	0/6/5/5
49	SF4	k	706	-	-	-	0/6/5/5
47	ADP	k	701	45	-	5/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	k	703	ATP	C5-C4	2.50	1.47	1.40
47	k	701	ADP	C5-C4	2.47	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	k	701	ADP	PA-O3A-PB	-3.70	120.12	132.83
48	k	703	ATP	PB-O3B-PG	-3.64	120.35	132.83
48	k	703	ATP	PA-O3A-PB	-3.49	120.84	132.83
48	k	703	ATP	C3'-C2'-C1'	3.43	106.14	100.98
48	k	703	ATP	N3-C2-N1	-3.19	123.69	128.68
47	k	701	ADP	N3-C2-N1	-3.14	123.77	128.68
47	k	701	ADP	C3'-C2'-C1'	2.95	105.42	100.98
48	k	703	ATP	C4-C5-N7	-2.71	106.57	109.40
47	k	701	ADP	C4-C5-N7	-2.68	106.60	109.40

There are no chirality outliers.

All (7) torsion outliers are listed below:

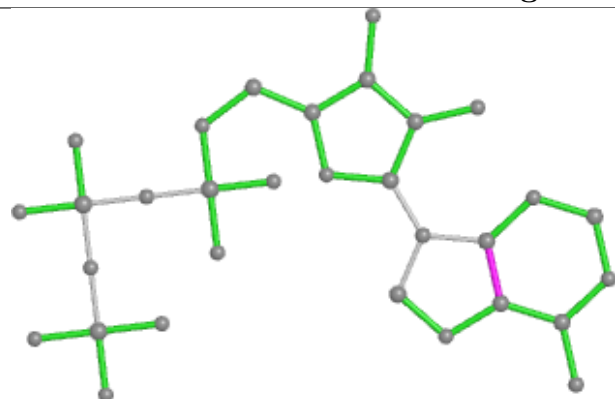
Mol	Chain	Res	Type	Atoms
47	k	701	ADP	C5'-O5'-PA-O1A
47	k	701	ADP	C5'-O5'-PA-O2A
48	k	703	ATP	O4'-C4'-C5'-O5'
47	k	701	ADP	PA-O3A-PB-O2B
47	k	701	ADP	C5'-O5'-PA-O3A
48	k	703	ATP	C3'-C4'-C5'-O5'
47	k	701	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

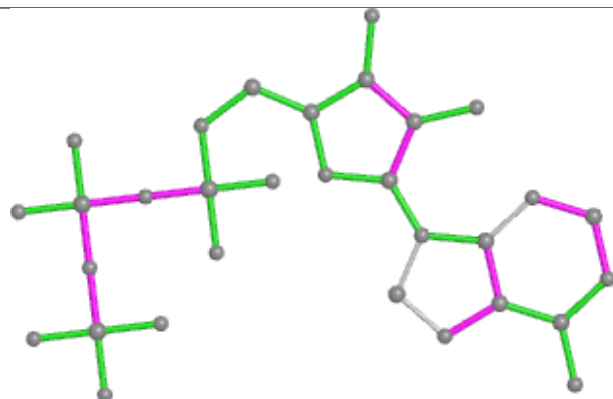
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

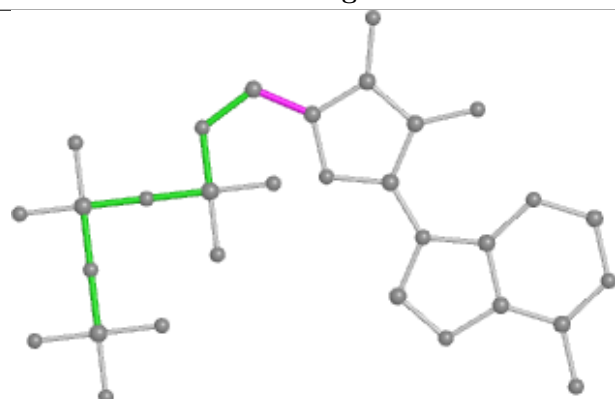
Ligand ATP k 703



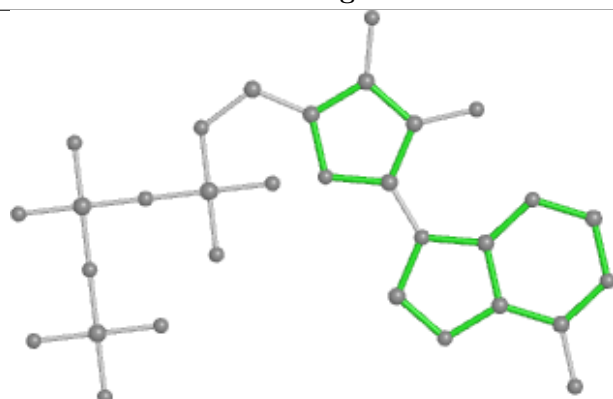
Bond lengths



Bond angles

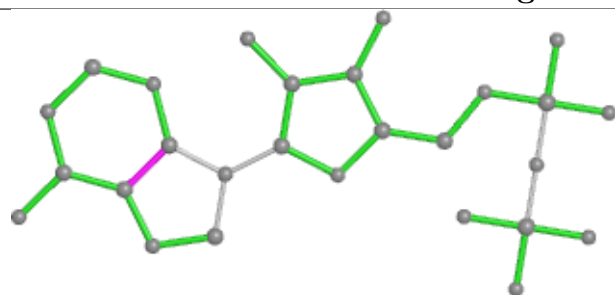


Torsions

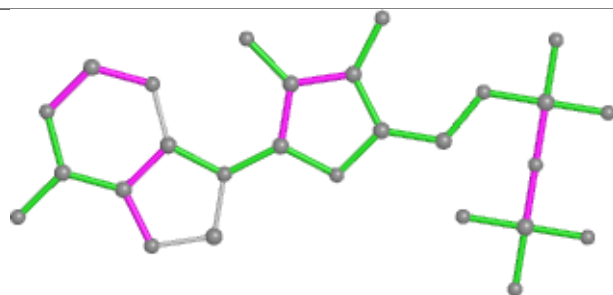


Rings

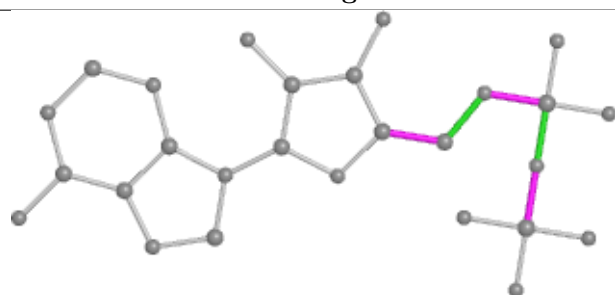
Ligand ADP k 701



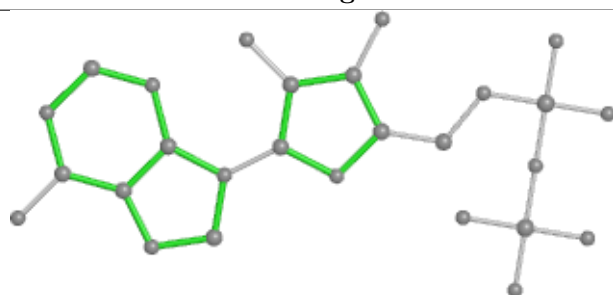
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	q	2
37	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	16:H2U	O3'	18:G	P	5.01
1	q	582:GLN	C	583:GLN	N	3.87
1	q	605:CYS	C	606:LEU	N	3.34

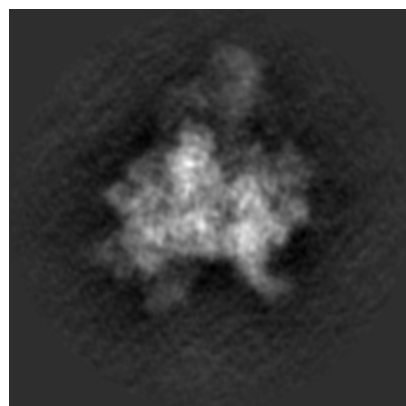
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11439. These allow visual inspection of the internal detail of the map and identification of artifacts.

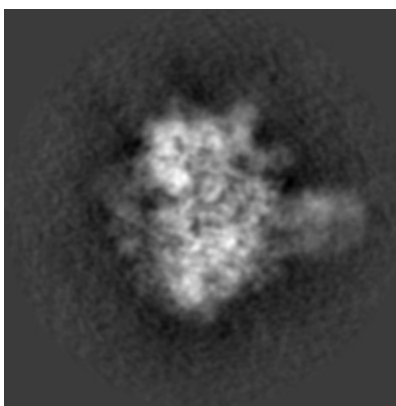
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

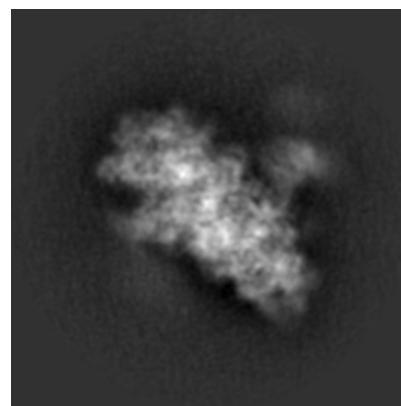
6.1.1 Primary map



X

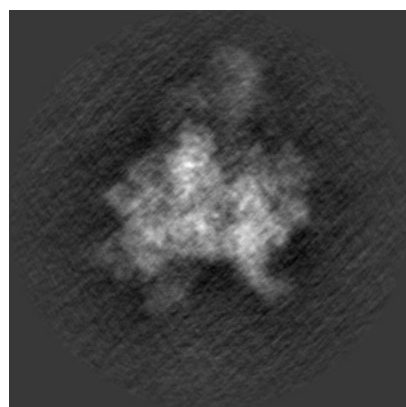


Y

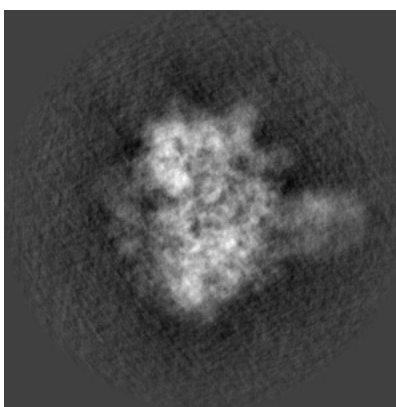


Z

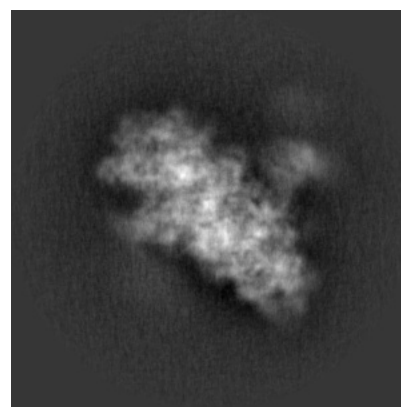
6.1.2 Raw map



X



Y

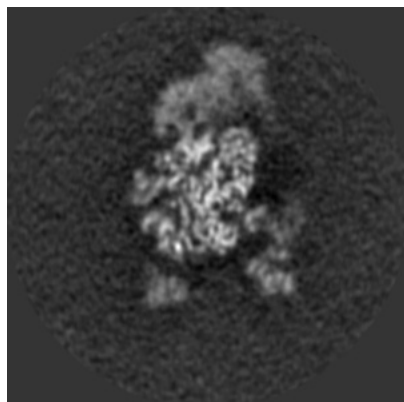


Z

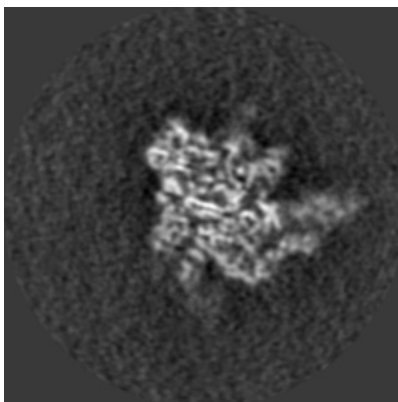
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

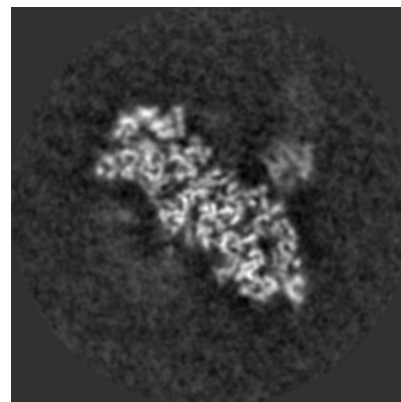
6.2.1 Primary map



X Index: 180

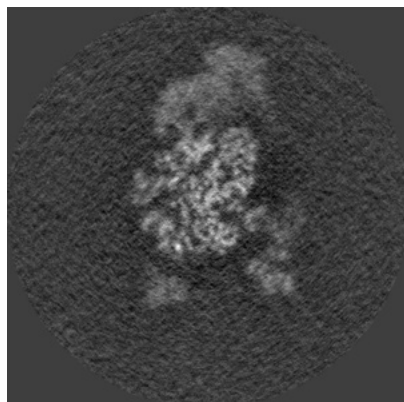


Y Index: 180

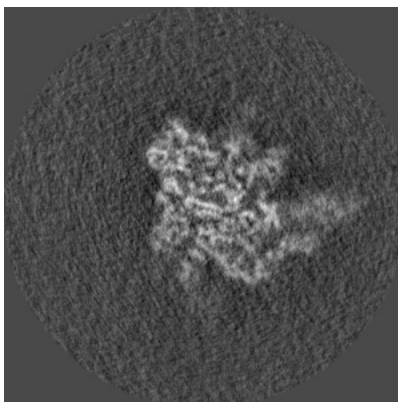


Z Index: 180

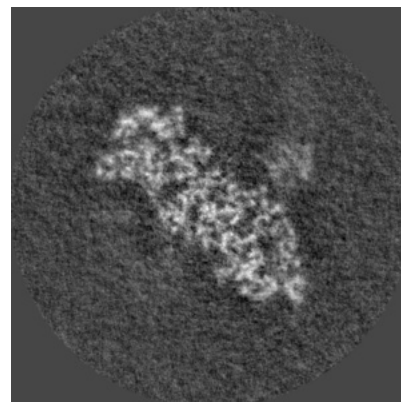
6.2.2 Raw map



X Index: 180



Y Index: 180

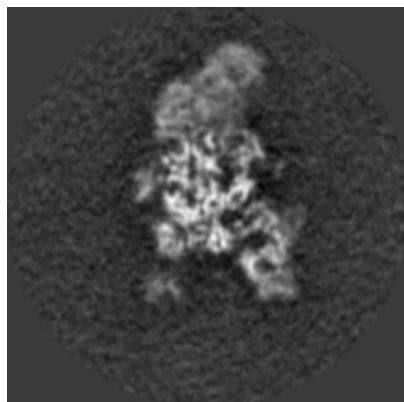


Z Index: 180

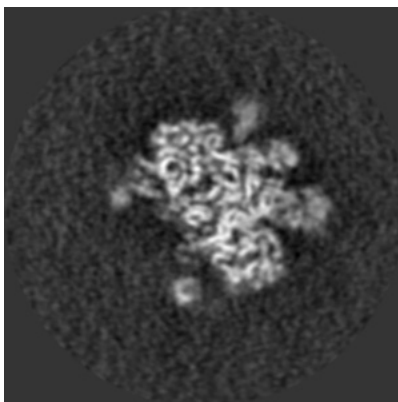
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

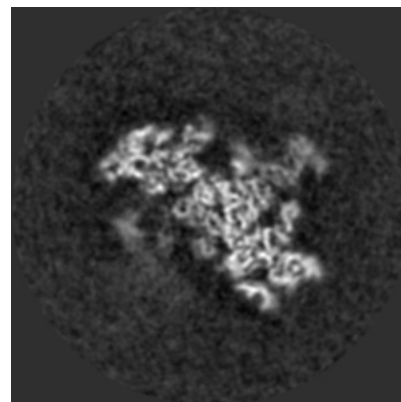
6.3.1 Primary map



X Index: 174

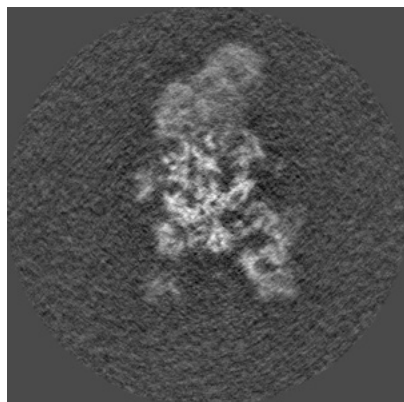


Y Index: 160

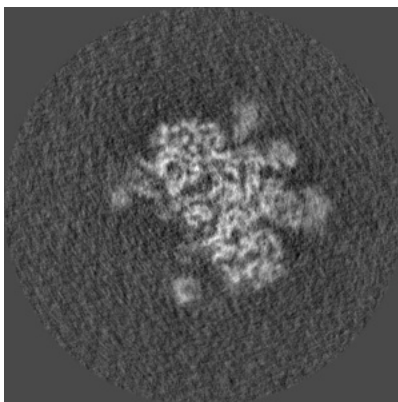


Z Index: 154

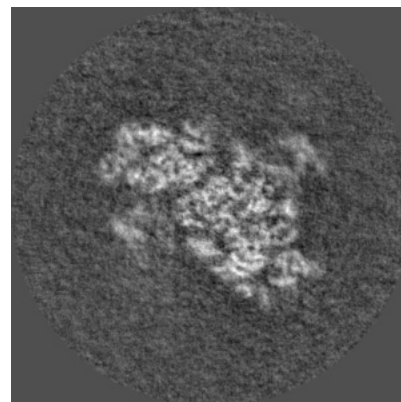
6.3.2 Raw map



X Index: 174



Y Index: 159

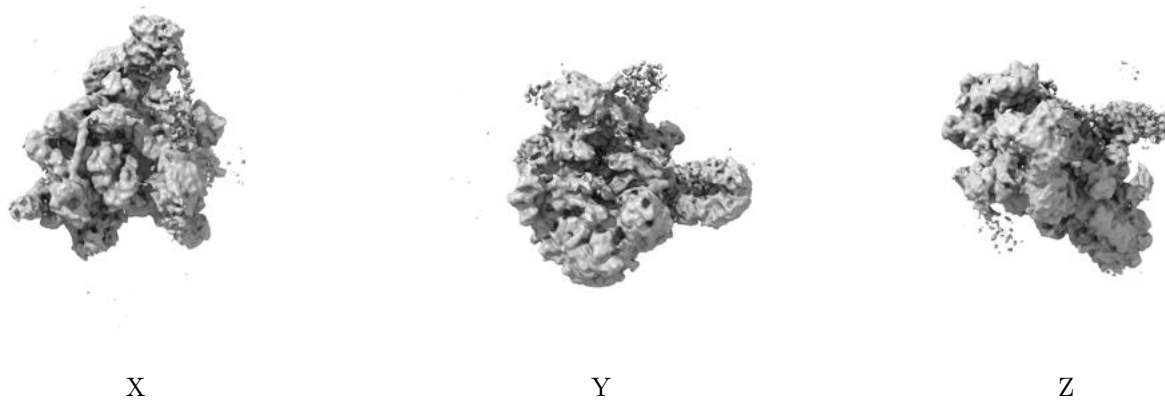


Z Index: 159

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

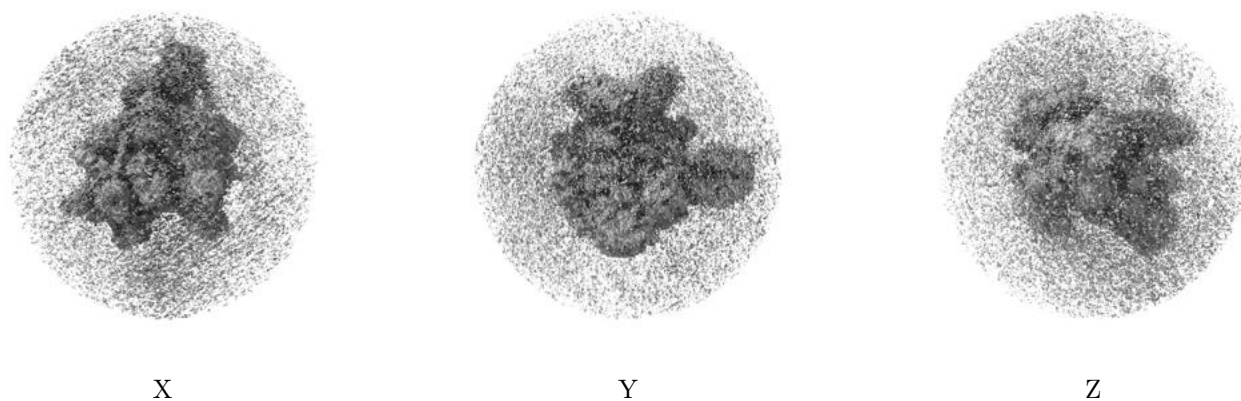
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.009. 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.

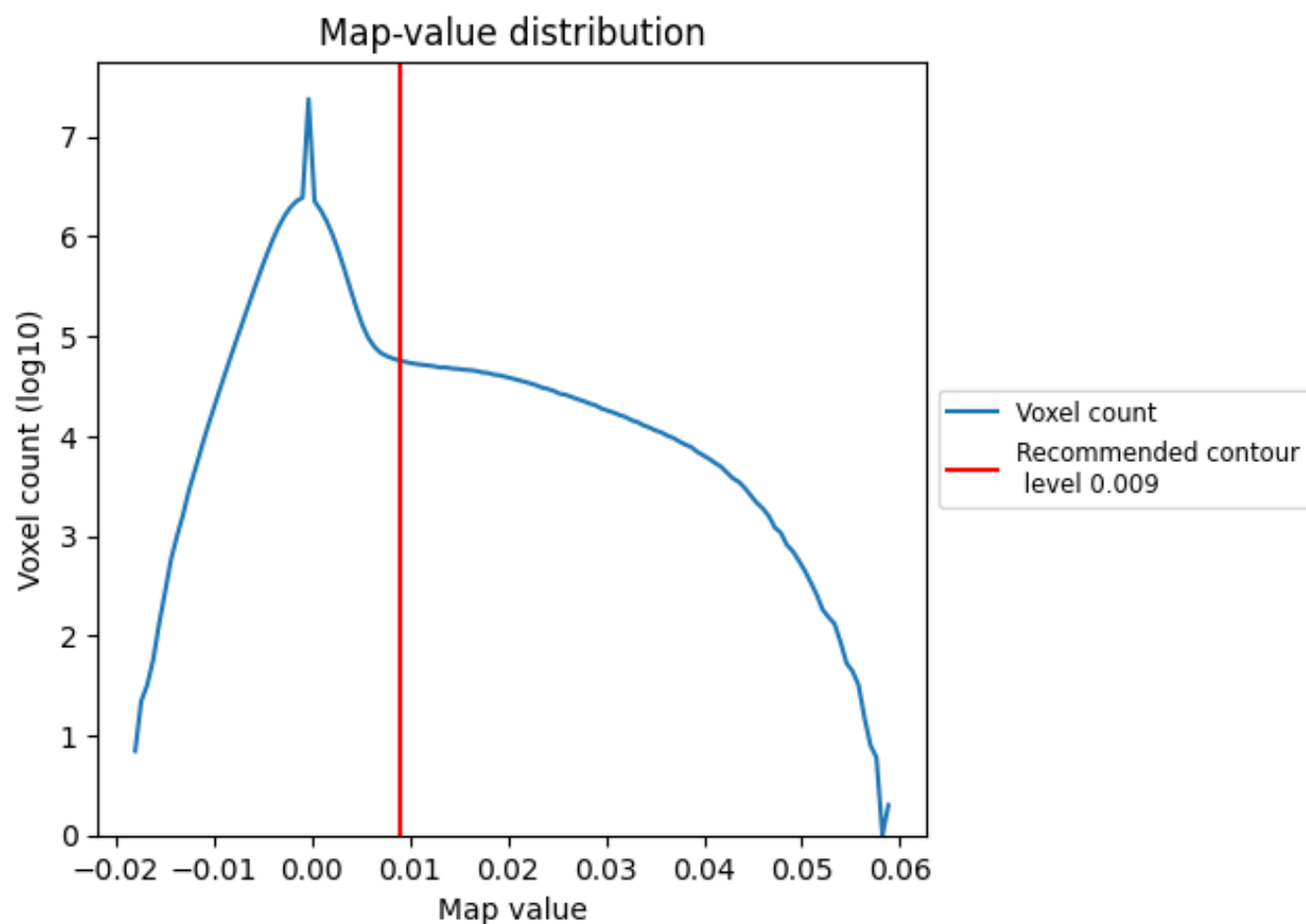
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

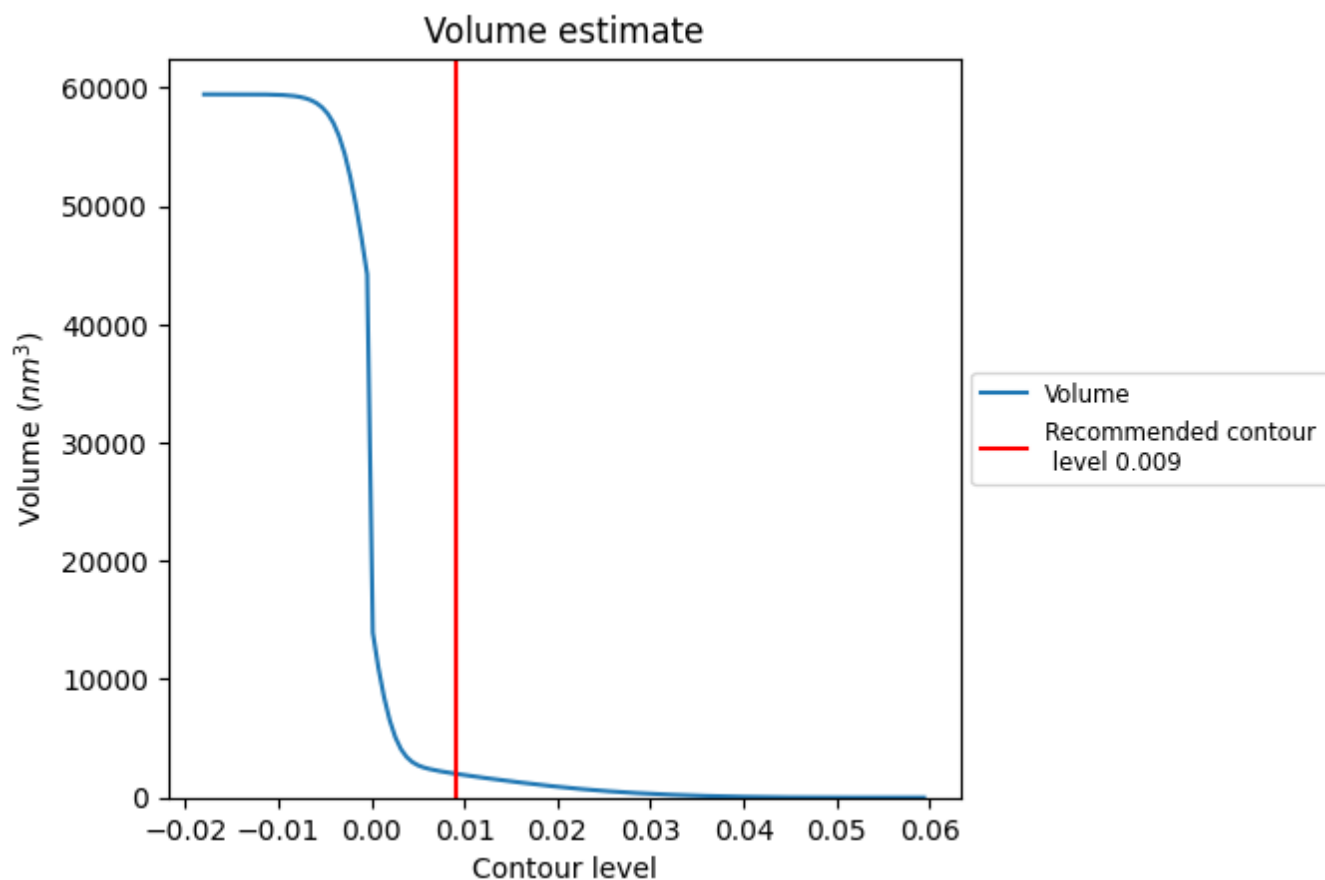
This section contains the results of statistical analysis of the map.

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.

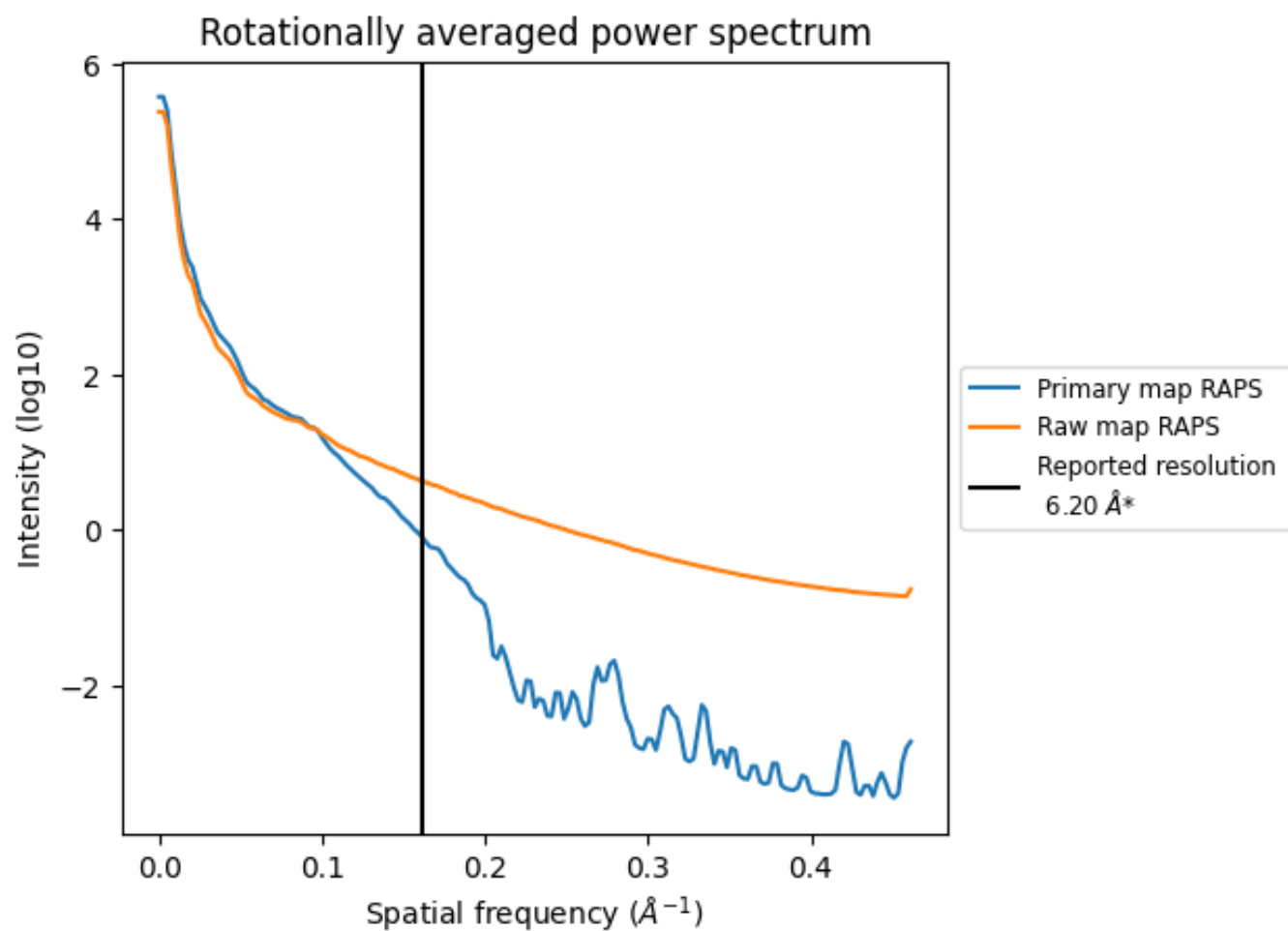
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2020 nm³; this corresponds to an approximate mass of 1824 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](#)

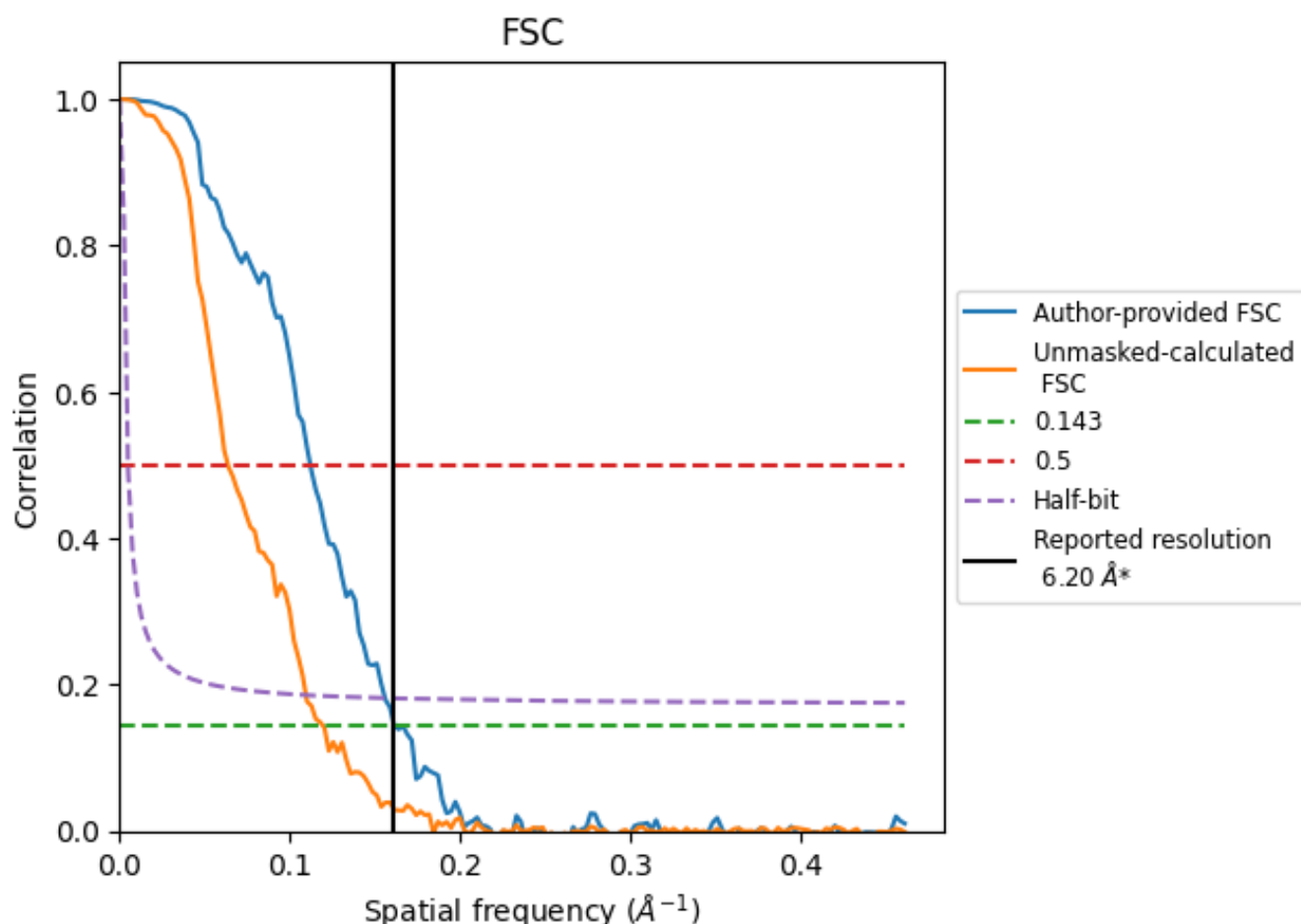


*Reported resolution corresponds to spatial frequency of 0.161 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.161 Å⁻¹

8.2 Resolution estimates [i](#)

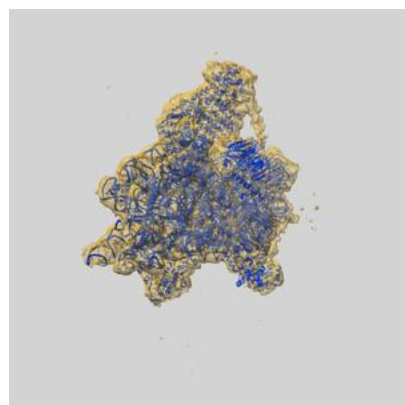
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.19	8.92	6.41
Unmasked-calculated*	8.35	15.70	9.13

*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 8.35 differs from the reported value 6.2 by more than 10 %

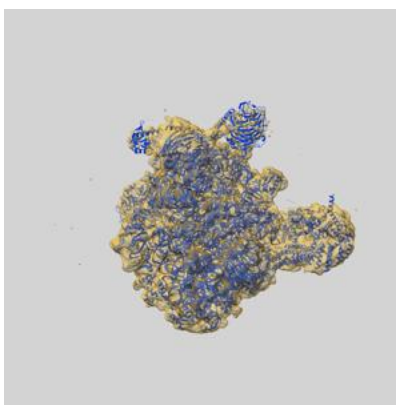
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11439 and PDB model 6ZU9. Per-residue inclusion information can be found in section [3](#) on page [14](#).

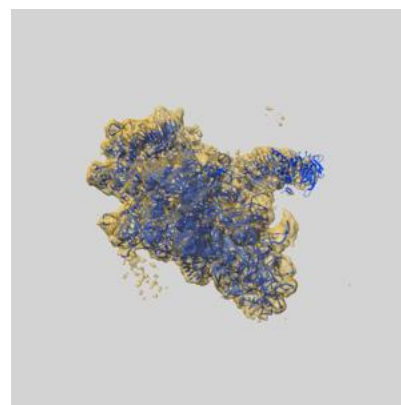
9.1 Map-model overlay [i](#)



X



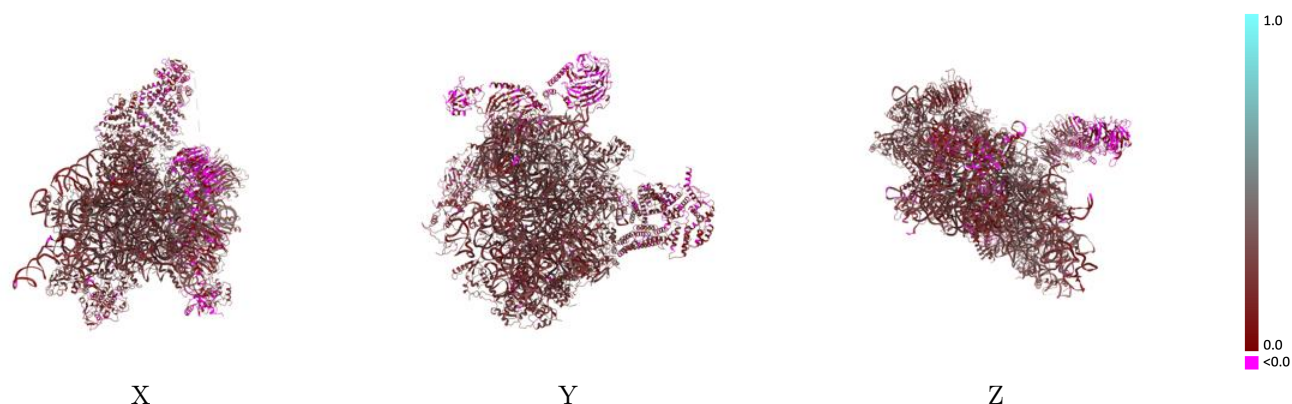
Y



Z

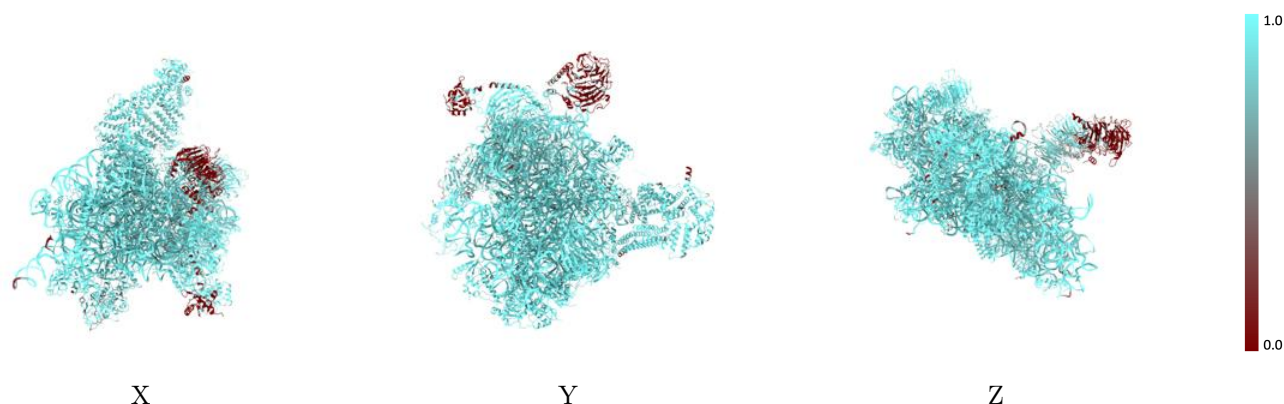
The images above show the 3D surface view of the map at the recommended contour level 0.009 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



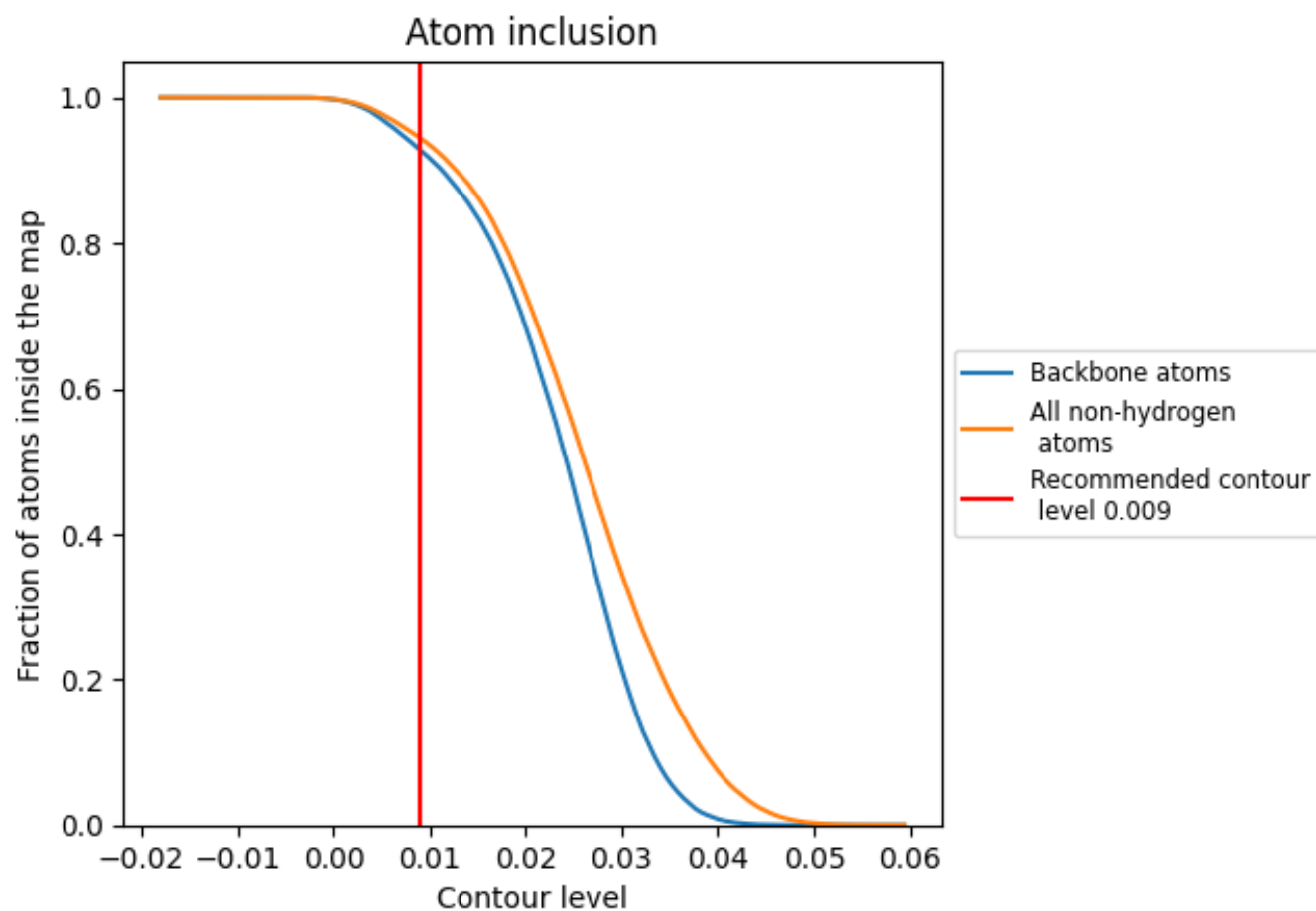
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 93% of all backbone atoms, 94% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9448	 0.2200
1	 0.9128	 0.1270
2	 0.9917	 0.2340
3	 0.8772	 0.1710
A	 0.9497	 0.2640
B	 0.9918	 0.2580
C	 0.9971	 0.2500
D	 1.0000	 0.2660
E	 0.9826	 0.2310
F	 0.9429	 0.2140
H	 1.0000	 0.2470
I	 0.9967	 0.2680
J	 0.9902	 0.2410
K	 0.9914	 0.2350
L	 0.9980	 0.2760
M	 0.8919	 0.2410
N	 1.0000	 0.2370
O	 0.9586	 0.2270
P	 0.9961	 0.2790
Q	 0.9946	 0.2440
R	 0.9962	 0.2870
S	 0.9984	 0.2800
T	 0.9982	 0.2560
U	 0.9945	 0.2700
V	 0.9924	 0.2680
W	 0.9912	 0.2580
X	 0.9858	 0.2870
Y	 0.9906	 0.2590
Z	 0.9952	 0.2350
a	 0.9977	 0.2680
b	 0.9968	 0.2640
c	 0.9901	 0.2800
d	 0.9803	 0.2520
e	 0.9855	 0.2600
f	 0.7850	 0.0690



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Chain	Atom inclusion	Q-score
g	 0.9080	 0.2430
h	 0.9948	 0.2360
i	 0.9774	 0.2290
k	 0.8907	 0.1740
l	 0.1349	 0.0260
m	 0.6327	 0.1700
o	 0.9157	 0.1460
p	 0.7295	 0.1280
q	 0.9530	 0.1670
r	 0.0460	 0.0810