



## Full wwPDB EM Validation Report ⓘ

Jun 3, 2026 – 05:21 PM EDT

PDB ID : 9OJM / pdb\_00009ojm  
EMDB ID : EMD-70544  
Title : Human mitochondrial 28S PIC with tRNA and mtIF2  
Authors : Kober, D.L.; Wang, J.  
Deposited on : 2025-05-08  
Resolution : 2.50 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](mailto: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>.

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

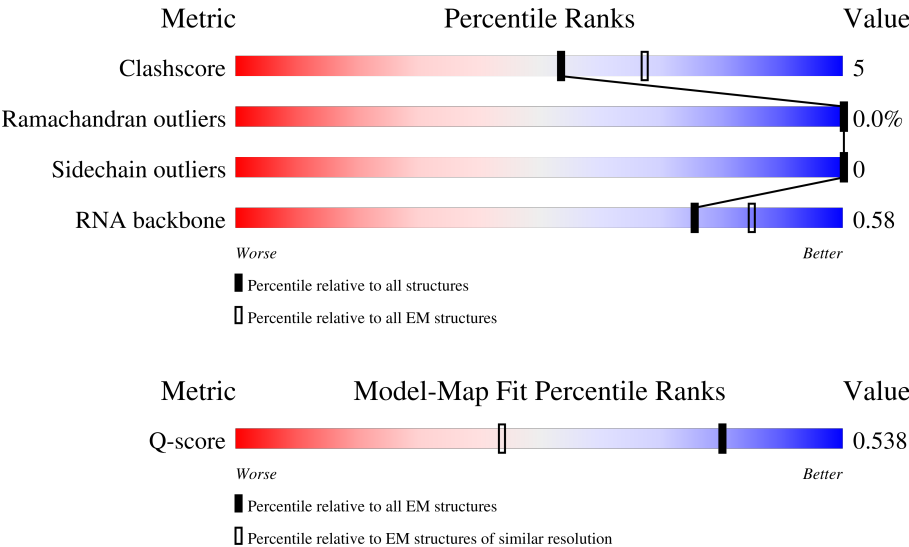
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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.








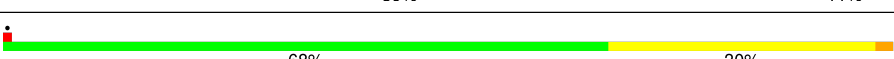
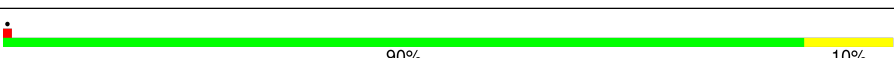


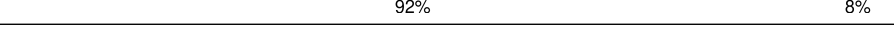
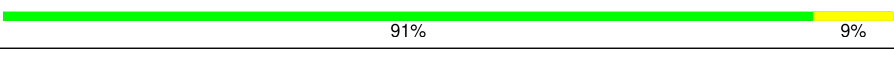
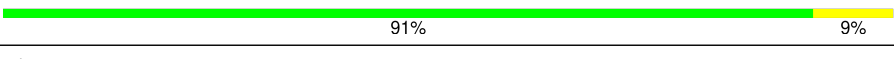




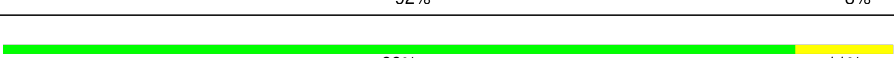



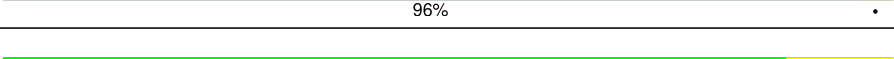


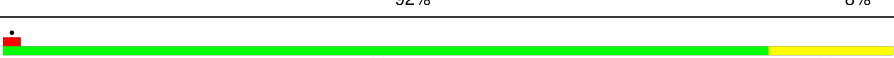

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 ( 2.00 - 3.00 )

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  $\geq 3$ , 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	0	215	
2	1	278	
3	2	118	

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Mol	Chain	Length	Quality of chain
4	3	71	
5	4	616	
6	5	71	
7	6	4	
8	7	571	
9	A	955	
10	B	225	
11	C	132	
12	D	343	
13	E	122	
14	F	208	
15	G	344	
16	H	140	
17	I	137	
18	J	108	
19	K	101	
20	L	174	
21	M	119	
22	N	110	
23	O	193	
24	P	97	
25	Q	87	
26	R	295	
27	S	135	
28	T	168	

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Mol	Chain	Length	Quality of chain
29	U	176	<div><div></div><div>89%11%</div></div>
30	V	379	<div><div>9%</div><div>63%32%</div><div></div></div>
31	W	100	<div><div></div><div>87%12%</div><div></div></div>
32	X	352	<div><div></div><div>88%13%</div></div>
33	Y	149	<div><div>14%</div><div>91%9%</div><div></div></div>
34	Z	100	<div><div></div><div>88%12%</div><div></div></div>

## 2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 74356 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 protein called Small ribosomal subunit protein mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	215	Total	C	N	O	S	0	0
			1787	1130	339	313	5		

- Molecule 2 is a protein called Small ribosomal subunit protein mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	278	Total	C	N	O	S	0	0
			2256	1430	386	429	11		

- Molecule 3 is a protein called Coiled-coil-helix-coiled-coil-helix domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	118	Total	C	N	O	S	0	0
			935	579	182	166	8		

- Molecule 4 is a protein called Small ribosomal subunit protein mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	71	Total	C	N	O	S	0	0
			629	403	135	90	1		

- Molecule 5 is a protein called Small ribosomal subunit protein mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	592	Total	C	N	O	S	0	0
			4795	3070	812	885	28		

- Molecule 6 is a RNA chain called RNA (71-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	71	Total	C	N	O	P	0	0
			1498	673	264	491	70		

- Molecule 7 is a RNA chain called mRNA (5'-R(P\*AP\*UP\*GP\*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	4	Total	C	N	O	P	0	0
			86	38	14	30	4		

- Molecule 8 is a protein called Translation initiation factor IF-2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	571	Total	C	N	O	S	0	0
			4147	2592	741	802	12		

- Molecule 9 is a RNA chain called 12S mitochondrial RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	955	Total	C	N	O	P	0	0
			20282	9098	3652	6577	955		

- Molecule 10 is a protein called Small ribosomal subunit protein uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	225	Total	C	N	O	S	0	0
			1828	1164	331	323	10		

- Molecule 11 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	132	Total	C	N	O	S	0	0
			1083	699	195	185	4		

- Molecule 12 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	343	Total	C	N	O	S	0	0
			2731	1713	518	487	13		

- Molecule 13 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	122	Total	C	N	O	S	0	0
			972	614	177	177	4		

- Molecule 14 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	208	Total	C	N	O	S	0	0
			1725	1104	312	298	11		

- Molecule 15 is a protein called Small ribosomal subunit protein uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	327	Total	C	N	O	S	0	0
			2688	1710	477	487	14		

- Molecule 16 is a protein called Small ribosomal subunit protein uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	140	Total	C	N	O	S	0	0
			1152	745	194	210	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	137	Total	C	N	O	S	0	0
			1019	641	193	181	4		

- Molecule 18 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	108	Total	C	N	O	S	0	0
			839	521	169	143	6		

- Molecule 19 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	101	Total	C	N	O	S	0	0
			862	537	179	141	5		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	174	Total	C	N	O	S	0	0
			1453	925	270	251	7		

- Molecule 21 is a protein called Small ribosomal subunit protein bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	119	Total	C	N	O	S	0	0
			942	594	185	157	6		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	110	Total	C	N	O	S	0	0
			868	562	156	147	3		

- Molecule 23 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	193	Total	C	N	O	S	0	0
			1592	1014	294	277	7		

- Molecule 24 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	97	Total	C	N	O	S	0	0
			781	501	134	138	8		

- Molecule 25 is a protein called 28S ribosomal protein S21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	87	Total	C	N	O	S	0	0
			744	460	150	126	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	50	ARG	CYS	variant	UNP P82921

- Molecule 26 is a protein called Small ribosomal subunit protein mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	295	Total	C	N	O	S	0	0
			2409	1533	413	455	8		

- Molecule 27 is a protein called 28S ribosomal protein S23, mitochondrial.



Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	135	Total	C	N	O	S	0	0
			1111	716	198	196	1		

- Molecule 28 is a protein called Small ribosomal subunit protein mS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	168	Total	C	N	O	S	0	0
			1371	877	239	244	11		

- Molecule 29 is a protein called Small ribosomal subunit protein mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	176	Total	C	N	O	S	0	0
			1488	916	301	267	4		

- Molecule 30 is a protein called Small ribosomal subunit protein mS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	362	Total	C	N	O	S	0	0
			2969	1904	495	558	12		

- Molecule 31 is a protein called Small ribosomal subunit protein bS1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	100	Total	C	N	O	S	0	0
			789	498	141	146	4		

- Molecule 32 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	X	352	Total	C	N	O	S	0	0
			2849	1822	499	517	11		

- Molecule 33 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Y	149	Total	C	N	O	S	0	0
			1246	801	207	234	4		

- Molecule 34 is a protein called Small ribosomal subunit protein mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	100	Total	C	N	O	S	0	0
			839	534	153	148	4		

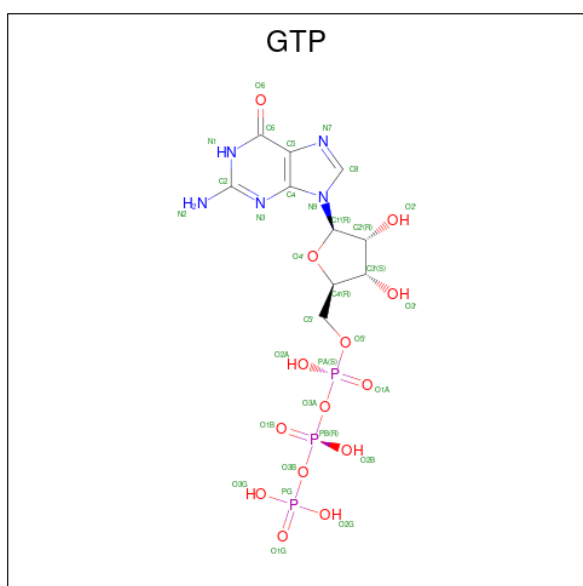
- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	3	1	Total	Mg	0
			1	1	
35	7	1	Total	Mg	0
			1	1	
35	A	68	Total	Mg	0
			68	68	
35	B	1	Total	Mg	0
			1	1	
35	X	1	Total	Mg	0
			1	1	

- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
36	7	1	Total	K	0
			1	1	
36	A	19	Total	K	0
			19	19	

- Molecule 37 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).

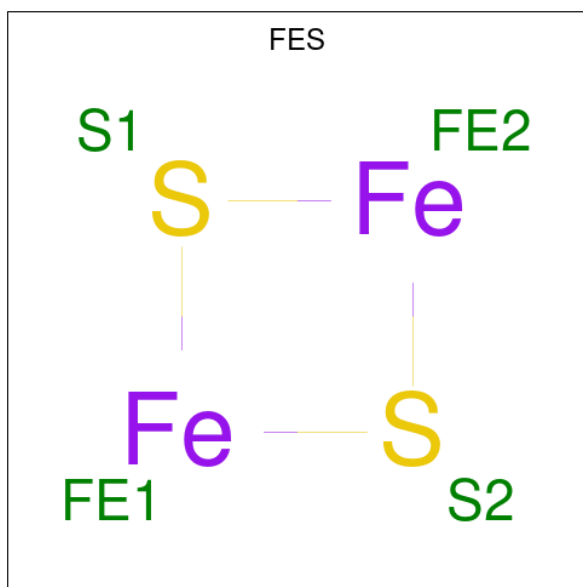


Mol	Chain	Residues	Atoms					AltConf
37	7	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

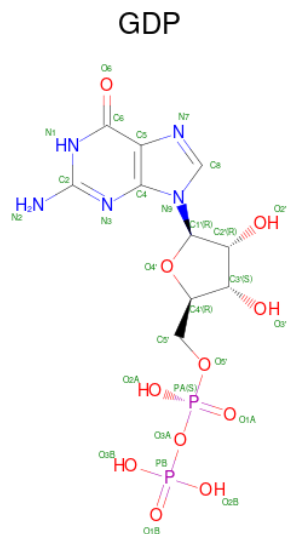
Mol	Chain	Residues	Atoms		AltConf
38	O	1	Total	Zn	0
			1	1	

- Molecule 39 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



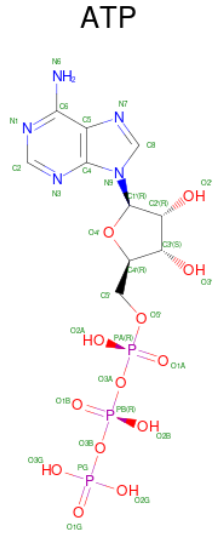
Mol	Chain	Residues	Atoms			AltConf
39	P	1	Total	Fe	S	0
			4	2	2	
39	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 40 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



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

- Molecule 41 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	0	2	Total 2	O 2	0
42	1	21	Total 21	O 21	0
42	2	14	Total 14	O 14	0
42	3	10	Total 10	O 10	0
42	4	14	Total 14	O 14	0
42	5	29	Total 29	O 29	0
42	6	6	Total 6	O 6	0
42	7	14	Total 14	O 14	0
42	A	791	Total 791	O 791	0
42	B	48	Total 48	O 48	0
42	C	14	Total 14	O 14	0
42	D	47	Total 47	O 47	0
42	E	13	Total 13	O 13	0
42	F	22	Total 22	O 22	0
42	G	53	Total 53	O 53	0
42	H	23	Total 23	O 23	0
42	I	22	Total 22	O 22	0
42	J	12	Total 12	O 12	0
42	K	17	Total 17	O 17	0
42	L	30	Total 30	O 30	0
42	M	7	Total 7	O 7	0
42	N	11	Total 11	O 11	0

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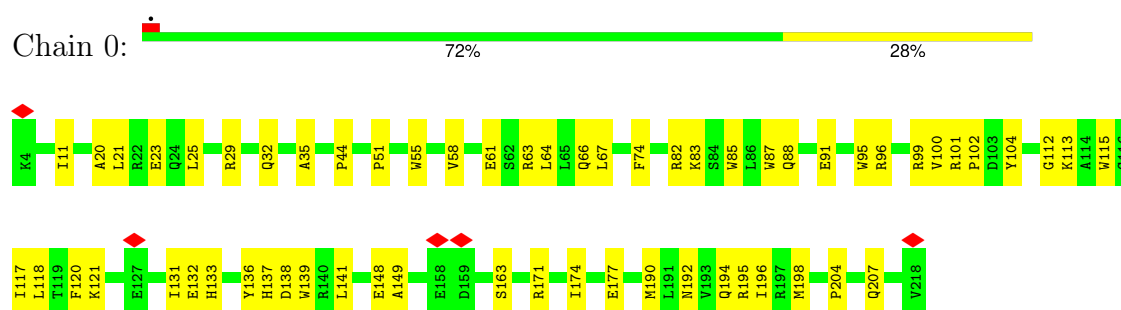
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Mol	Chain	Residues	Atoms		AltConf
42	O	37	Total 37	O 37	0
42	P	13	Total 13	O 13	0
42	Q	20	Total 20	O 20	0
42	R	12	Total 12	O 12	0
42	S	16	Total 16	O 16	0
42	T	13	Total 13	O 13	0
42	U	15	Total 15	O 15	0
42	W	15	Total 15	O 15	0
42	X	12	Total 12	O 12	0
42	Y	13	Total 13	O 13	0
42	Z	13	Total 13	O 13	0

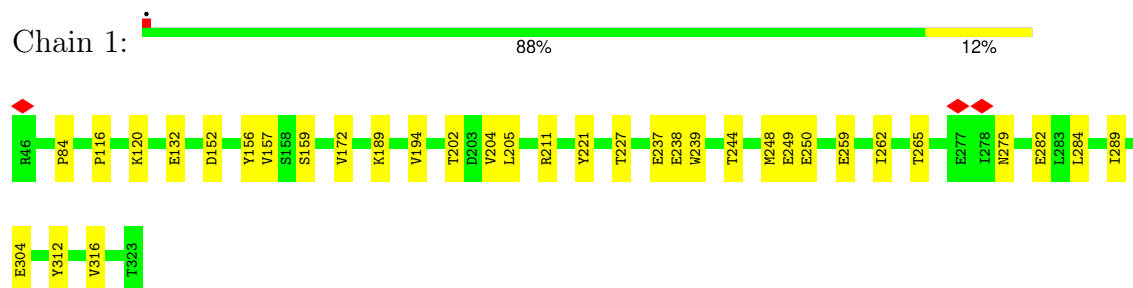
### 3 Residue-property plots

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

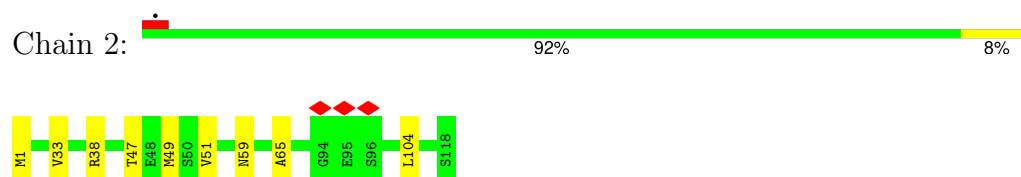
- Molecule 1: Small ribosomal subunit protein mS34



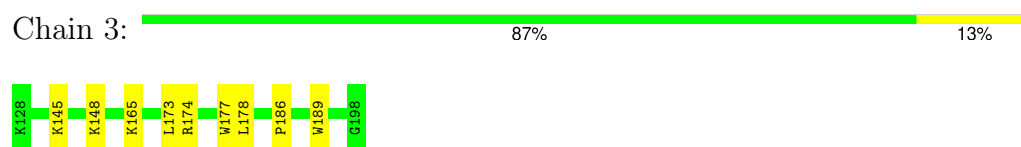
- Molecule 2: Small ribosomal subunit protein mS35



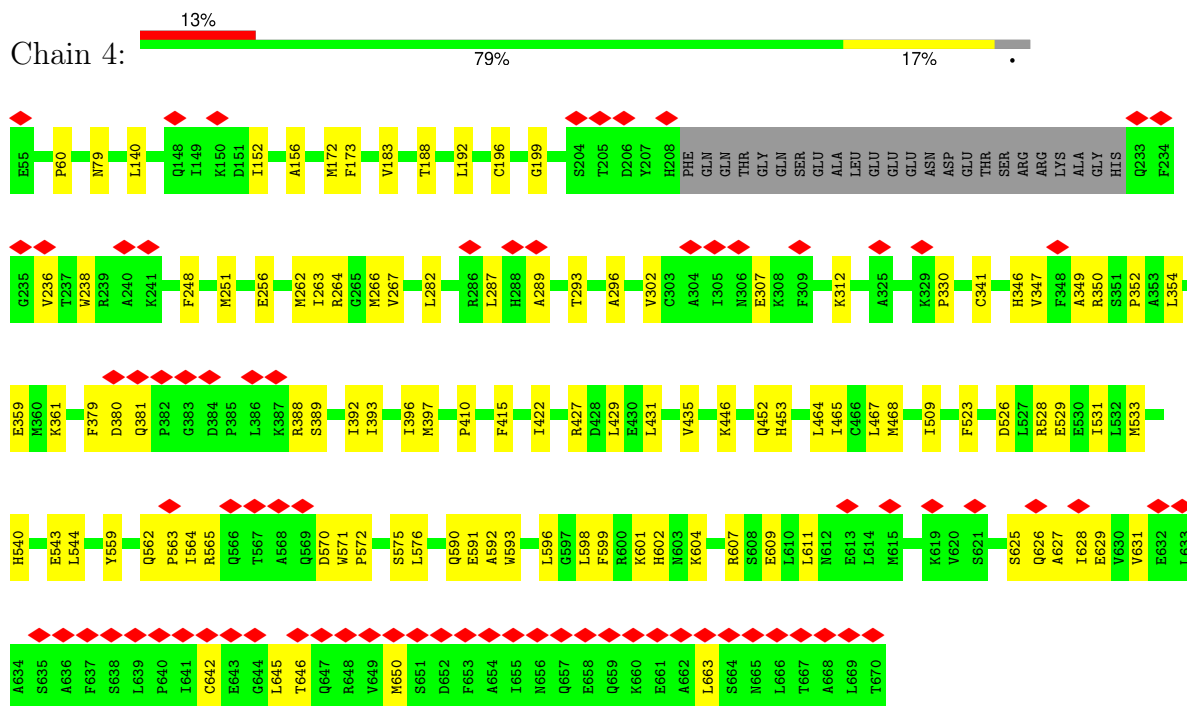
- Molecule 3: Coiled-coil-helix-coiled-coil-helix domain-containing protein 1



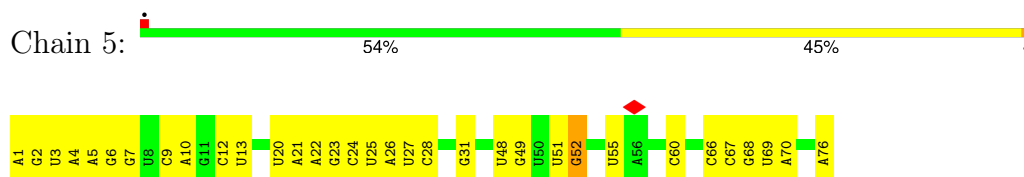
- Molecule 4: Small ribosomal subunit protein mS38



- Molecule 5: Small ribosomal subunit protein mS39



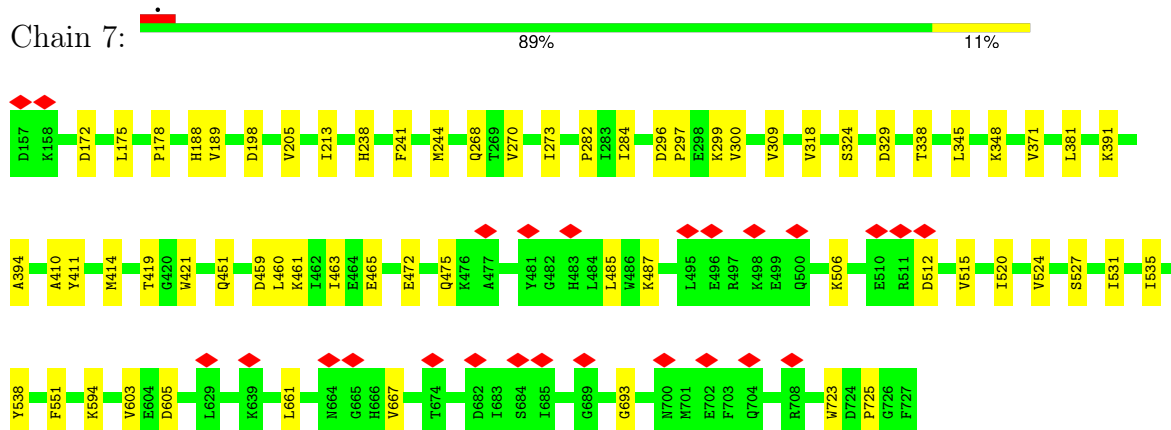
- Molecule 6: RNA (71-MER)



- Molecule 7: mRNA (5'-R(P\*AP\*UP\*GP\*U)-3')

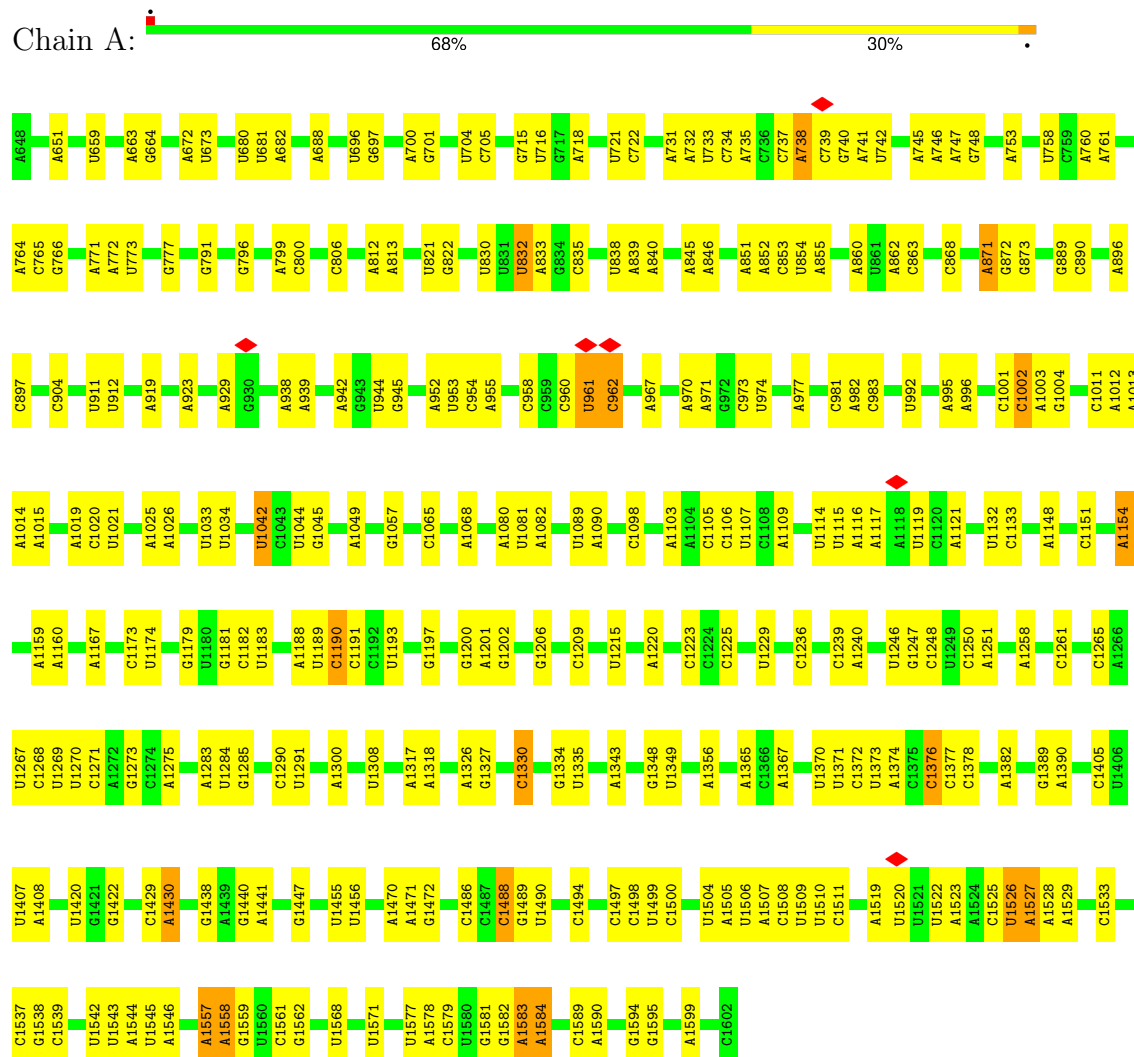


- Molecule 8: Translation initiation factor IF-2, mitochondrial

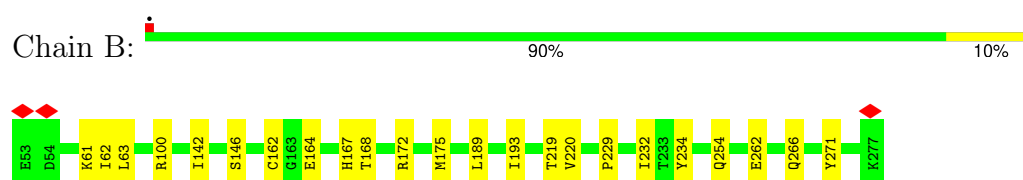




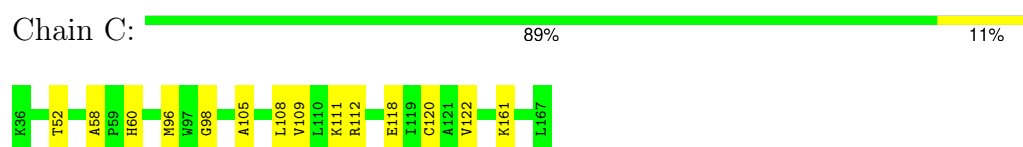
- Molecule 9: 12S mitochondrial RNA



- Molecule 10: Small ribosomal subunit protein uS2m

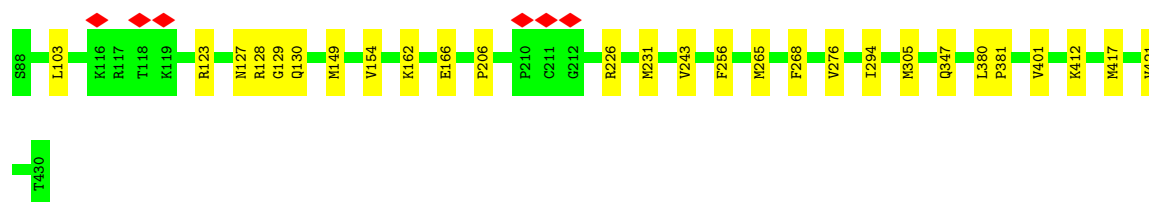


- Molecule 11: 28S ribosomal protein S24, mitochondrial



- Molecule 12: 28S ribosomal protein S5, mitochondrial





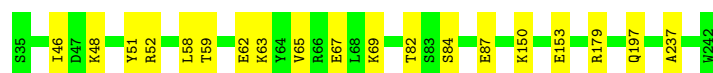
- Molecule 13: 28S ribosomal protein S6, mitochondrial

Chain E: 91% 9%



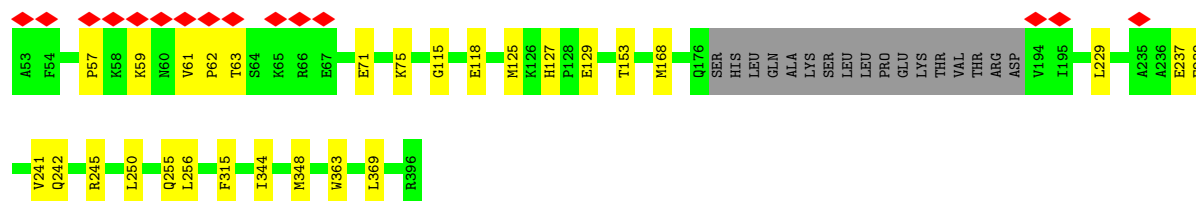
- Molecule 14: 28S ribosomal protein S7, mitochondrial

Chain F: 91% 9%



- Molecule 15: Small ribosomal subunit protein uS9m

Chain G: 87% 8% 5%



- Molecule 16: Small ribosomal subunit protein uS10m

Chain H: 86% 14%



- Molecule 17: Small ribosomal subunit protein uS11m

Chain I: 89% 11%

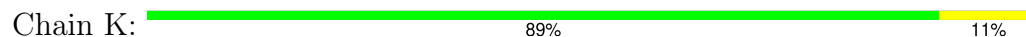


- Molecule 18: 28S ribosomal protein S12, mitochondrial

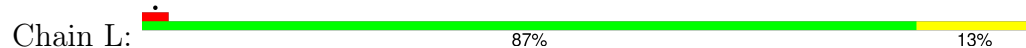
Chain J: 92% 8%



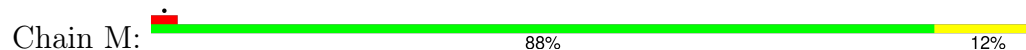
- Molecule 19: 28S ribosomal protein S14, mitochondrial



- Molecule 20: Small ribosomal subunit protein uS15m



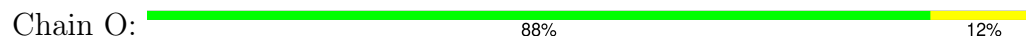
- Molecule 21: Small ribosomal subunit protein bS16m



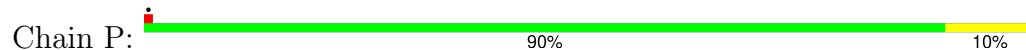
- Molecule 22: Small ribosomal subunit protein uS17m



- Molecule 23: 28S ribosomal protein S18b, mitochondrial



- Molecule 24: 28S ribosomal protein S18c, mitochondrial




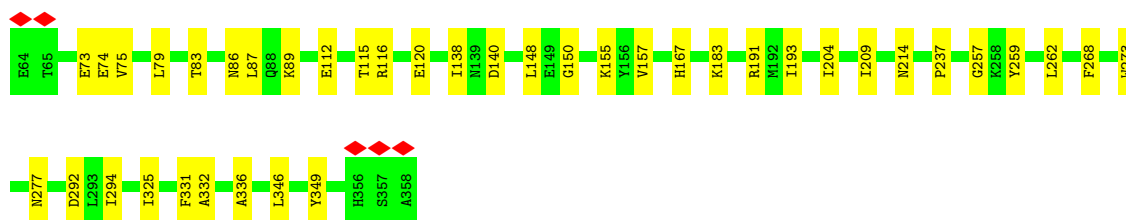
- Molecule 25: 28S ribosomal protein S21, mitochondrial

Chain Q:  92% 8%




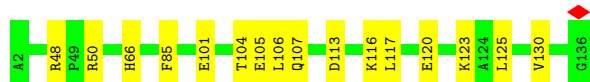
- Molecule 26: Small ribosomal subunit protein mS22

Chain R:  86% 14%




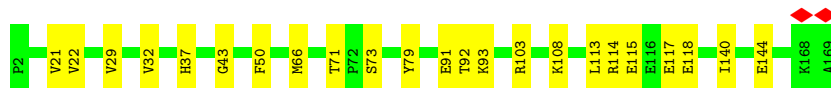
- Molecule 27: 28S ribosomal protein S23, mitochondrial

Chain S:  88% 12%




- Molecule 28: Small ribosomal subunit protein mS25

Chain T:  86% 14%



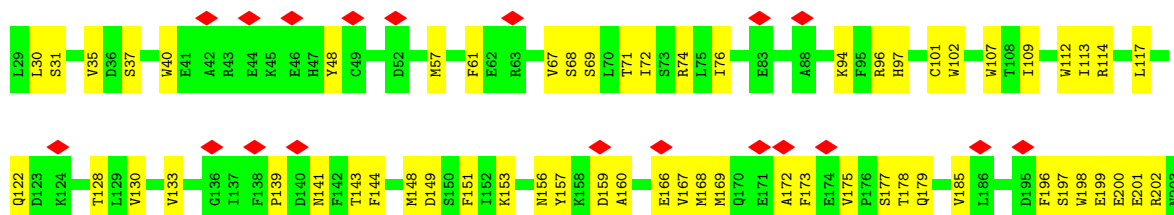
- Molecule 29: Small ribosomal subunit protein mS26

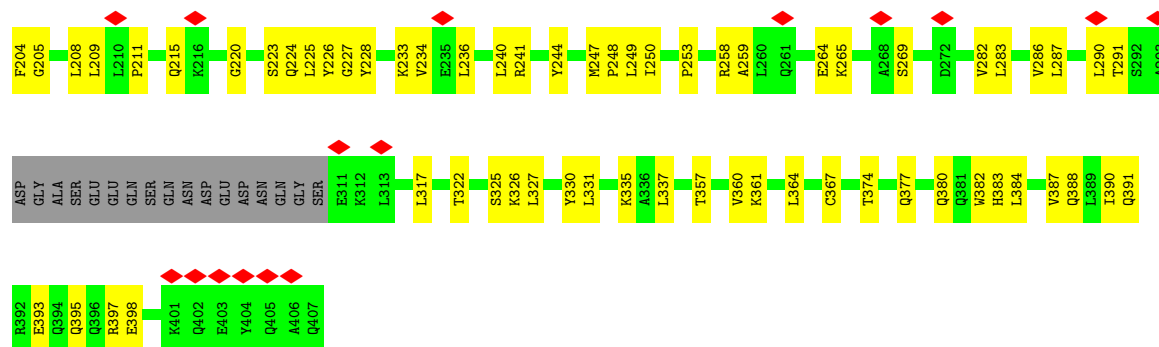
Chain U:  89% 11%



- Molecule 30: Small ribosomal subunit protein mS27

Chain V:  9% 63% 32%





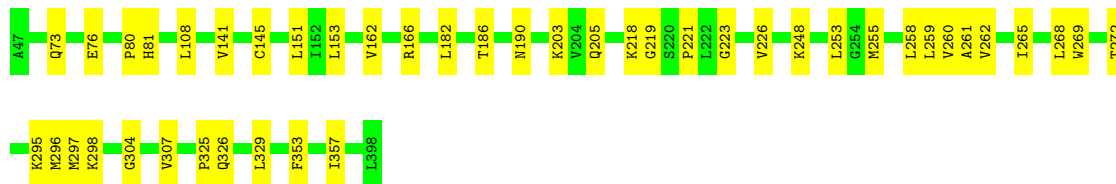
- Molecule 31: Small ribosomal subunit protein bS1m

Chain W: 87% 12%



- Molecule 32: Small ribosomal subunit protein mS29

Chain X: 88% 13%



- Molecule 33: 28S ribosomal protein S27, mitochondrial

Chain Y: 14% 91% 9%



- Molecule 34: Small ribosomal subunit protein mS33

Chain Z: 88% 12%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107666	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.391	Depositor
Minimum map value	-0.122	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.028	Depositor
Map size (Å)	495.59998, 495.59998, 495.59998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.826, 0.826, 0.826	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, ZN, MG, ATP, K, FES, 5MU, GTP, GDP, MA6, B8T

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	0	0.18	0/1834	0.36	0/2484
2	1	0.19	0/2304	0.30	0/3117
3	2	0.36	1/949 (0.1%)	0.37	0/1268
4	3	0.23	0/640	0.40	0/844
5	4	0.16	0/4904	0.33	0/6636
6	5	0.18	0/1673	0.27	0/2602
7	6	0.73	1/95 (1.1%)	0.25	0/144
8	7	0.16	0/4207	0.33	0/5704
9	A	0.29	0/22562	0.28	0/35124
10	B	0.25	0/1871	0.35	0/2531
11	C	0.25	0/1113	0.32	0/1505
12	D	0.24	0/2783	0.31	0/3724
13	E	0.23	0/989	0.33	0/1335
14	F	0.22	0/1767	0.35	0/2373
15	G	0.22	0/2746	0.30	0/3681
16	H	0.25	0/1178	0.35	0/1598
17	I	0.32	0/1039	0.40	0/1400
18	J	0.24	0/855	0.33	0/1148
19	K	0.27	0/880	0.31	0/1182
20	L	0.22	0/1477	0.28	0/1974
21	M	0.24	0/963	0.38	0/1295
22	N	0.24	0/886	0.31	0/1199
23	O	0.21	0/1648	0.32	0/2243
24	P	0.25	0/798	0.32	0/1070
25	Q	0.39	1/756 (0.1%)	0.33	0/1005
26	R	0.18	0/2456	0.29	0/3317
27	S	0.26	0/1138	0.40	0/1533
28	T	0.23	0/1402	0.36	0/1883
29	U	0.18	0/1510	0.32	0/2025
30	V	0.16	0/3030	0.39	0/4093
31	W	0.24	0/801	0.36	0/1079
32	X	0.19	0/2921	0.32	0/3954

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Y	0.20	0/1280	0.32	0/1725
34	Z	0.22	0/857	0.33	0/1141
All	All	0.24	3/76312 (0.0%)	0.32	0/107936

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	1	MET	C-N	8.36	1.45	1.33
25	Q	1	MET	C-N	7.48	1.44	1.33
7	6	1	A	OP3-P	6.50	1.61	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 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	0	1787	0	1796	49	0
2	1	2256	0	2288	24	0
3	2	935	0	970	6	0
4	3	629	0	702	8	0
5	4	4795	0	4796	84	0
6	5	1498	0	766	26	0
7	6	86	0	43	0	0
8	7	4147	0	3941	34	0
9	A	20282	0	10297	152	0
10	B	1828	0	1815	15	0
11	C	1083	0	1088	9	0
12	D	2731	0	2804	20	0
13	E	972	0	1000	10	0
14	F	1725	0	1769	18	0
15	G	2688	0	2687	22	0
16	H	1152	0	1183	14	0
17	I	1019	0	1059	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	J	839	0	887	6	0
19	K	862	0	885	9	0
20	L	1453	0	1540	14	0
21	M	942	0	965	11	0
22	N	868	0	928	3	0
23	O	1592	0	1557	23	0
24	P	781	0	806	10	0
25	Q	744	0	755	5	0
26	R	2409	0	2428	28	0
27	S	1111	0	1115	12	0
28	T	1371	0	1393	15	0
29	U	1488	0	1499	18	0
30	V	2969	0	2961	89	0
31	W	789	0	802	10	0
32	X	2849	0	2843	25	0
33	Y	1246	0	1197	15	0
34	Z	839	0	858	10	0
35	3	1	0	0	0	0
35	7	1	0	0	0	0
35	A	68	0	0	0	0
35	B	1	0	0	0	0
35	X	1	0	0	0	0
36	7	1	0	0	0	0
36	A	19	0	0	0	0
37	7	32	0	12	0	0
38	O	1	0	0	0	0
39	P	4	0	0	0	0
39	T	4	0	0	0	0
40	X	28	0	12	0	0
41	X	31	0	12	0	0
42	0	2	0	0	0	0
42	1	21	0	0	0	0
42	2	14	0	0	0	0
42	3	10	0	0	0	0
42	4	14	0	0	0	0
42	5	29	0	0	0	0
42	6	6	0	0	0	0
42	7	14	0	0	0	0
42	A	791	0	0	0	0
42	B	48	0	0	0	0
42	C	14	0	0	0	0
42	D	47	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	E	13	0	0	0	0
42	F	22	0	0	0	0
42	G	53	0	0	0	0
42	H	23	0	0	0	0
42	I	22	0	0	0	0
42	J	12	0	0	0	0
42	K	17	0	0	0	0
42	L	30	0	0	0	0
42	M	7	0	0	0	0
42	N	11	0	0	0	0
42	O	37	0	0	0	0
42	P	13	0	0	0	0
42	Q	20	0	0	0	0
42	R	12	0	0	0	0
42	S	16	0	0	0	0
42	T	13	0	0	0	0
42	U	15	0	0	0	0
42	W	15	0	0	0	0
42	X	12	0	0	0	0
42	Y	13	0	0	0	0
42	Z	13	0	0	0	0
All	All	74356	0	62459	699	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 5.

All (699) 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)
6:5:5:A:N6	6:5:68:G:H1	1.48	1.10
32:X:108:LEU:HD23	32:X:141:VAL:HG21	1.59	0.83
27:S:106:LEU:HB3	27:S:117:LEU:HD11	1.61	0.82
30:V:240:LEU:HG	30:V:244:TYR:HE1	1.46	0.80
1:0:91:GLU:HG3	1:0:121:LYS:HA	1.60	0.80
5:4:528:ARG:HD2	5:4:559:TYR:HE1	1.46	0.79
9:A:1236:C:H5''	19:K:33:ARG:HE	1.47	0.79
6:5:5:A:N1	6:5:68:G:N2	2.29	0.78
6:5:67:C:H2'	6:5:68:G:H8	1.47	0.77
5:4:602:HIS:CE1	5:4:604:LYS:HZ3	2.05	0.75
5:4:509:ILE:HG23	5:4:531:ILE:HD11	1.68	0.74
9:A:1523:A:H5''	30:V:68:SER:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:393:ILE:HA	5:4:396:ILE:HG12	1.71	0.73
6:5:67:C:H2'	6:5:68:G:C8	2.24	0.72
12:D:130:GLN:HB3	34:Z:72:ARG:HH12	1.52	0.72
28:T:22:VAL:HG21	28:T:113:LEU:HD21	1.71	0.72
12:D:149:MET:HE1	12:D:154:VAL:HG22	1.72	0.71
1:0:100:VAL:HG12	1:0:102:PRO:HD3	1.72	0.71
5:4:392:ILE:HG13	5:4:393:ILE:HD12	1.73	0.71
9:A:1382:A:H5''	32:X:166:ARG:HH21	1.55	0.71
2:1:189:LYS:HG3	34:Z:11:MET:HE1	1.71	0.70
2:1:227:THR:HA	16:H:184:ILE:HD11	1.71	0.70
6:5:76:A:H1'	8:7:693:GLY:HA3	1.74	0.70
23:O:208:PRO:HG2	23:O:213:LEU:HD11	1.74	0.70
15:G:344:ILE:HG22	15:G:348:MET:HE2	1.73	0.70
2:1:84:PRO:HD2	15:G:125:MET:HE3	1.74	0.69
9:A:1201:A:H2'	9:A:1202:G:C8	2.28	0.69
19:K:61:THR:HG21	34:Z:27:ASN:HD21	1.58	0.69
30:V:236:LEU:HD22	30:V:290:LEU:HD22	1.74	0.69
31:W:109:GLU:CD	31:W:110:ASN:H	2.00	0.69
5:4:156:ALA:HB3	5:4:172:MET:HE1	1.74	0.69
25:Q:67:GLU:HG3	31:W:154:LEU:HB2	1.75	0.68
13:E:92:ASN:HB2	24:P:117:MET:HE3	1.76	0.67
1:0:85:TRP:HH2	1:0:95:TRP:HE1	1.43	0.67
32:X:81:HIS:CD2	32:X:190:ASN:HB3	2.30	0.67
30:V:179:GLN:OE1	30:V:215:GLN:NE2	2.27	0.66
24:P:139:ARG:NH1	24:P:141:ARG:HB2	2.10	0.66
30:V:247:MET:HE1	30:V:249:LEU:HD12	1.78	0.66
30:V:291:THR:HG22	30:V:327:LEU:HD21	1.78	0.66
26:R:83:THR:HG22	26:R:268:PHE:HB3	1.78	0.66
30:V:141:ASN:HA	30:V:144:PHE:HD2	1.60	0.65
21:M:63:GLU:HG2	26:R:155:LYS:HE2	1.79	0.65
28:T:21:VAL:HG22	28:T:103:ARG:HB2	1.78	0.65
5:4:598:LEU:HA	5:4:601:LYS:HD2	1.79	0.64
8:7:381:LEU:HB3	8:7:410:ALA:HB3	1.79	0.64
5:4:248:PHE:HA	5:4:251:MET:HE1	1.79	0.64
31:W:139:ARG:HG3	31:W:139:ARG:HH11	1.61	0.64
9:A:1201:A:H2'	9:A:1202:G:H8	1.63	0.64
9:A:845:A:H4'	29:U:60:TYR:CE2	2.34	0.63
30:V:109:ILE:HG21	30:V:139:PRO:HA	1.80	0.63
8:7:371:VAL:HG22	8:7:419:THR:HG22	1.81	0.63
5:4:576:LEU:HB3	5:4:599:PHE:HE1	1.63	0.63
8:7:524:VAL:HG23	8:7:527:SER:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:29:ARG:H	1:0:32:GLN:NE2	1.97	0.63
16:H:104:ILE:HG21	16:H:145:LEU:HD23	1.80	0.63
9:A:961:U:H4'	9:A:962:C:H5''	1.80	0.63
9:A:1025:A:H2'	9:A:1026:A:C8	2.34	0.62
18:J:62:VAL:HA	18:J:83:VAL:HG12	1.81	0.62
21:M:111:ARG:HG3	23:O:236:PRO:HD3	1.81	0.62
9:A:663:A:H2'	9:A:664:G:C8	2.34	0.62
32:X:262:VAL:HG21	32:X:265:ILE:HD13	1.81	0.62
6:5:5:A:H61	6:5:68:G:H1	0.72	0.61
30:V:151:PHE:CE2	30:V:159:ASP:HB2	2.34	0.61
30:V:151:PHE:CE2	30:V:156:ASN:HB3	2.34	0.61
5:4:446:LYS:HG2	33:Y:292:GLN:NE2	2.14	0.61
9:A:1440:G:H2'	9:A:1441:A:C8	2.36	0.61
5:4:570:ASP:HA	5:4:602:HIS:HE1	1.66	0.61
30:V:68:SER:HB3	30:V:71:THR:HG22	1.81	0.61
23:O:235:MET:HG2	26:R:150:GLY:HA3	1.82	0.61
9:A:1068:A:H5''	17:I:190:LYS:HD3	1.82	0.60
9:A:852:A:H3'	9:A:853:C:H6	1.65	0.60
9:A:1119:U:P	27:S:48:ARG:HH22	2.24	0.60
16:H:76:LEU:HG	16:H:148:LEU:HD21	1.84	0.60
6:5:69:U:H2'	6:5:70:A:H8	1.68	0.59
30:V:167:VAL:HG13	30:V:172:ALA:HB3	1.83	0.59
8:7:282:PRO:HG2	8:7:345:LEU:HD11	1.82	0.59
10:B:162:CYS:HB3	10:B:254:GLN:HG3	1.85	0.59
1:0:87:TRP:CD1	23:O:218:ARG:HH12	2.21	0.59
26:R:294:ILE:HG13	26:R:349:TYR:CE2	2.38	0.58
9:A:738:A:H2'	9:A:740:G:C4	2.37	0.58
9:A:740:G:H2'	9:A:741:A:H8	1.68	0.58
8:7:309:VAL:HG13	8:7:318:VAL:HG21	1.85	0.58
30:V:96:ARG:HH21	30:V:133:VAL:HA	1.68	0.58
30:V:233:LYS:HB2	30:V:286:VAL:HG21	1.86	0.58
2:1:211:ARG:HD3	2:1:221:TYR:CE2	2.38	0.58
30:V:199:GLU:HA	30:V:202:ARG:HE	1.69	0.58
8:7:411:TYR:HB2	8:7:414:MET:HE3	1.86	0.58
4:3:174:ARG:HG3	4:3:178:LEU:HD13	1.84	0.57
5:4:397:MET:HE1	5:4:415:PHE:HZ	1.69	0.57
27:S:48:ARG:HH21	27:S:50:ARG:NH2	2.02	0.57
17:I:96:GLN:HE21	17:I:109:PHE:HZ	1.52	0.57
9:A:734:C:P	9:A:735:A:H5''	2.44	0.57
23:O:213:LEU:HB3	23:O:217:ARG:HH12	1.69	0.57
28:T:71:THR:HG22	28:T:73:SER:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1236:C:H5''	19:K:33:ARG:NE	2.18	0.57
5:4:263:ILE:HD11	5:4:293:THR:HG23	1.86	0.57
9:A:777:G:H5''	22:N:21:LYS:HB3	1.86	0.57
9:A:1545:U:H2'	9:A:1546:A:C8	2.39	0.57
32:X:80:PRO:HG2	32:X:81:HIS:HD2	1.69	0.57
24:P:139:ARG:HH12	24:P:141:ARG:HB2	1.70	0.57
30:V:265:LYS:O	30:V:269:SER:HB3	2.05	0.57
30:V:387:VAL:HA	30:V:390:ILE:HD12	1.87	0.57
5:4:410:PRO:HA	33:Y:289:VAL:HG11	1.87	0.56
16:H:76:LEU:HD22	16:H:174:LYS:HG2	1.86	0.56
1:0:95:TRP:CE3	1:0:131:ILE:HG12	2.40	0.56
28:T:29:VAL:HB	28:T:79:TYR:HB2	1.87	0.56
5:4:528:ARG:HD2	5:4:559:TYR:CE1	2.35	0.56
5:4:607:ARG:HD2	5:4:609:GLU:HG2	1.87	0.56
26:R:209:ILE:HD12	26:R:214:ASN:HB3	1.87	0.56
9:A:1269:U:H4'	9:A:1270:U:H3'	1.88	0.55
1:0:174:ILE:O	1:0:177:GLU:HG3	2.06	0.55
16:H:135:GLU:HB3	19:K:126:ALA:HB2	1.87	0.55
5:4:346:HIS:C	5:4:350:ARG:HE	2.14	0.55
1:0:113:LYS:HE3	1:0:115:TRP:HH2	1.70	0.55
9:A:1578:A:H2'	9:A:1579:C:C6	2.41	0.55
27:S:120:GLU:HA	27:S:123:LYS:HZ2	1.72	0.55
5:4:152:ILE:HA	5:4:172:MET:HE3	1.87	0.55
10:B:62:ILE:HG22	10:B:63:LEU:HD22	1.89	0.55
23:O:192:THR:HG23	23:O:197:ASP:HB2	1.89	0.55
24:P:52:ILE:HD13	27:S:66:HIS:CE1	2.42	0.55
30:V:96:ARG:HD2	30:V:101:CYS:SG	2.47	0.55
9:A:1589:C:H2'	9:A:1590:A:C8	2.42	0.55
11:C:52:THR:HG23	11:C:161:LYS:HE3	1.87	0.55
1:0:132:GLU:HA	1:0:207:GLN:HE21	1.72	0.54
4:3:148:LYS:HG3	9:A:1154:A:C2	2.42	0.54
30:V:40:TRP:CZ3	30:V:114:ARG:HB3	2.42	0.54
5:4:199:GLY:HA2	5:4:238:TRP:HZ3	1.70	0.54
9:A:977:A:H1'	17:I:182:PRO:HB3	1.88	0.54
1:0:99:ARG:HD3	9:A:1526:U:H2'	1.90	0.54
10:B:172:ARG:O	10:B:175:MET:HG2	2.07	0.54
16:H:146:GLU:HG2	16:H:147:HIS:CD2	2.42	0.54
6:5:22:A:H2'	6:5:23:G:H8	1.73	0.54
30:V:202:ARG:HG2	30:V:234:VAL:HG11	1.90	0.54
11:C:111:LYS:HB2	11:C:118:GLU:HB2	1.90	0.54
15:G:315:PHE:CD2	15:G:369:LEU:HD21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:361:LYS:NZ	33:Y:251:PHE:HB3	2.23	0.54
6:5:4:A:H2'	6:5:5:A:C8	2.43	0.54
12:D:103:LEU:HD11	12:D:123:ARG:HB2	1.90	0.54
24:P:77:VAL:HG13	24:P:120:MET:HG3	1.90	0.54
10:B:61:LYS:NZ	10:B:271:TYR:HB2	2.23	0.54
10:B:167:HIS:CE1	15:G:153:THR:HA	2.43	0.54
26:R:325:ILE:HG23	26:R:346:LEU:HD21	1.90	0.54
1:0:58:VAL:HG23	1:0:137:HIS:HD1	1.72	0.53
6:5:1:A:H2'	6:5:2:G:H8	1.73	0.53
23:O:177:PHE:CE1	26:R:237:PRO:HG2	2.43	0.53
28:T:114:ARG:HA	28:T:117:GLU:HG2	1.90	0.53
32:X:258:LEU:O	32:X:304:GLY:HA3	2.09	0.53
19:K:54:ILE:HG21	19:K:75:ILE:HB	1.91	0.53
5:4:350:ARG:HH22	5:4:381:GLN:HB2	1.73	0.53
5:4:393:ILE:HG22	5:4:431:LEU:HD11	1.89	0.53
9:A:845:A:H2'	9:A:846:A:C8	2.44	0.53
9:A:732:A:H2'	9:A:733:U:C6	2.44	0.53
11:C:98:GLY:HA3	34:Z:71:TYR:CE1	2.44	0.53
9:A:871:A:H4'	9:A:872:G:H5'	1.89	0.53
19:K:120:LEU:HB3	19:K:123:ILE:HD12	1.91	0.53
3:2:33:VAL:HG21	3:2:104:LEU:HD23	1.91	0.53
9:A:821:U:H2'	9:A:822:G:H8	1.74	0.53
30:V:322:THR:HG23	30:V:325:SER:H	1.73	0.53
8:7:506:LYS:HG2	9:A:1494:C:H5'	1.90	0.52
5:4:262:MET:HE3	5:4:266:MET:HE3	1.91	0.52
30:V:113:ILE:HG21	30:V:143:THR:HG23	1.91	0.52
34:Z:95:LYS:HE3	34:Z:98:GLU:OE1	2.09	0.52
9:A:929:A:H1'	12:D:421:VAL:HG22	1.91	0.52
9:A:1267:U:H2'	9:A:1268:C:C6	2.44	0.52
5:4:256:GLU:HG2	5:4:287:LEU:HB3	1.90	0.52
8:7:297:PRO:HA	8:7:300:VAL:HG22	1.92	0.52
5:4:380:ASP:HB3	5:4:422:ILE:HD11	1.91	0.52
23:O:150:LEU:O	23:O:154:ILE:HG12	2.09	0.52
23:O:208:PRO:HB3	29:U:54:PHE:HD1	1.75	0.52
9:A:1258:A:N7	9:A:1330:C:H5'	2.25	0.52
15:G:61:VAL:HG23	15:G:63:THR:HB	1.92	0.52
1:0:118:LEU:HD21	1:0:120:PHE:HB2	1.92	0.52
25:Q:72:ILE:O	25:Q:76:MET:HG2	2.10	0.52
26:R:140:ASP:HB3	26:R:183:LYS:HD2	1.92	0.52
29:U:129:ARG:O	29:U:132:GLU:HG3	2.10	0.52
10:B:262:GLU:O	10:B:266:GLN:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1014:A:H4'	17:I:184:ASN:HB3	1.91	0.51
23:O:213:LEU:HB3	23:O:217:ARG:NH1	2.25	0.51
29:U:80:ARG:HA	29:U:83:HIS:NE2	2.25	0.51
14:F:82:THR:HG23	15:G:315:PHE:HB2	1.92	0.51
4:3:189:TRP:CE2	20:L:209:LEU:HD12	2.46	0.51
5:4:307:GLU:HG2	5:4:312:LYS:HE3	1.91	0.51
8:7:531:ILE:O	8:7:535:ILE:HG12	2.10	0.51
12:D:294:ILE:HB	12:D:305:MET:HE3	1.93	0.51
3:2:59:ASN:HD22	3:2:65:ALA:HB1	1.75	0.51
9:A:1265:C:H4'	16:H:122:GLN:HG2	1.92	0.51
16:H:118:PHE:HE1	16:H:136:MET:HE2	1.75	0.51
27:S:101:GLU:O	27:S:104:THR:HG22	2.11	0.51
30:V:76:ILE:HD12	30:V:112:TRP:HB2	1.93	0.51
30:V:149:ASP:O	30:V:153:LYS:HG2	2.11	0.51
2:1:159:SER:HB2	11:C:112:ARG:HB3	1.93	0.51
6:5:1:A:H2'	6:5:2:G:C8	2.44	0.50
6:5:22:A:H2'	6:5:23:G:C8	2.45	0.50
5:4:140:LEU:HD21	33:Y:309:LYS:HE3	1.93	0.50
8:7:213:ILE:HD11	8:7:238:HIS:HB2	1.94	0.50
29:U:80:ARG:HA	29:U:83:HIS:CD2	2.47	0.50
30:V:384:LEU:O	30:V:387:VAL:HG22	2.10	0.50
1:0:101:ARG:NH1	9:A:1528:A:H4'	2.26	0.50
12:D:380:LEU:HD12	12:D:381:PRO:HD2	1.93	0.50
13:E:71:PRO:HD3	20:L:97:MET:HE1	1.93	0.50
14:F:65:VAL:O	14:F:69:LYS:HG3	2.10	0.50
26:R:74:GLU:HG2	26:R:75:VAL:N	2.27	0.50
5:4:464:LEU:HD12	5:4:468:MET:HE2	1.94	0.50
20:L:163:ARG:HA	20:L:166:MET:HE2	1.92	0.50
9:A:853:C:H2'	9:A:854:U:C6	2.46	0.50
1:0:132:GLU:HB3	1:0:207:GLN:HB2	1.94	0.50
4:3:177:TRP:CD1	4:3:178:LEU:HD12	2.47	0.50
5:4:593:TRP:CZ2	5:4:626:GLN:HB3	2.47	0.50
5:4:628:ILE:HA	5:4:631:VAL:HG22	1.94	0.50
9:A:672:A:H2'	9:A:673:U:C6	2.46	0.50
9:A:738:A:H5''	9:A:740:G:N7	2.26	0.50
24:P:49:ASP:HA	31:W:85:ARG:HH11	1.77	0.50
30:V:141:ASN:ND2	30:V:175:VAL:HG12	2.27	0.50
30:V:374:THR:HA	30:V:377:GLN:CD	2.37	0.50
5:4:79:ASN:HB3	16:H:50:LEU:HD22	1.93	0.49
5:4:236:VAL:HG12	5:4:238:TRP:H	1.76	0.49
9:A:1470:A:H2'	9:A:1471:A:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:S:113:ASP:HB3	27:S:116:LYS:HE2	1.94	0.49
9:A:1003:A:H2'	9:A:1004:G:C8	2.47	0.49
9:A:1376:C:H4'	9:A:1377:C:H5'	1.94	0.49
30:V:200:GLU:O	30:V:204:PHE:HD2	1.95	0.49
1:O:192:ASN:HD21	1:O:194:GLN:HG3	1.77	0.49
31:W:114:ILE:HG21	31:W:142:LEU:HD11	1.93	0.49
9:A:1132:U:H2'	9:A:1133:C:C6	2.47	0.49
1:O:101:ARG:CZ	9:A:1528:A:H4'	2.42	0.49
12:D:401:VAL:HG21	28:T:50:PHE:CE1	2.48	0.49
4:3:173:LEU:HB3	20:L:209:LEU:HD13	1.93	0.49
19:K:34:MET:HE3	19:K:95:SER:HB2	1.94	0.49
30:V:168:MET:HE1	30:V:169:MET:HE2	1.94	0.49
30:V:377:GLN:HA	30:V:380:GLN:CD	2.37	0.49
1:O:96:ARG:HB3	1:O:117:ILE:HG22	1.95	0.49
9:A:1003:A:H2'	9:A:1004:G:H8	1.78	0.49
11:C:96:MET:HB2	11:C:108:LEU:HD11	1.95	0.49
26:R:332:ALA:HA	26:R:336:ALA:HB3	1.95	0.49
30:V:31:SER:O	30:V:35:VAL:HG23	2.13	0.49
30:V:241:ARG:HA	30:V:244:TYR:CZ	2.48	0.49
12:D:380:LEU:HD13	26:R:87:LEU:HB3	1.94	0.49
2:1:157:VAL:HG13	33:Y:315:ILE:HG13	1.93	0.49
20:L:136:ILE:O	20:L:140:GLU:HG3	2.13	0.49
30:V:197:SER:O	30:V:201:GLU:HG3	2.12	0.49
1:O:51:PRO:HG3	9:A:705:C:H5'	1.95	0.48
30:V:388:GLN:HA	30:V:391:GLN:CD	2.38	0.48
9:A:733:U:H2'	9:A:734:C:C6	2.48	0.48
26:R:191:ARG:HG3	26:R:204:ILE:HG23	1.95	0.48
5:4:611:LEU:HD13	5:4:645:LEU:HD22	1.94	0.48
9:A:911:U:H2'	9:A:912:U:C6	2.49	0.48
30:V:393:GLU:HG3	30:V:397:ARG:HH21	1.77	0.48
9:A:696:U:H2'	9:A:697:G:C8	2.49	0.48
9:A:970:A:H2'	9:A:971:A:C8	2.47	0.48
13:E:26:ILE:HG23	13:E:36:VAL:HG21	1.93	0.48
14:F:84:SER:HB3	14:F:87:GLU:HG2	1.94	0.48
21:M:101:PRO:HB3	29:U:59:ARG:HB3	1.94	0.48
28:T:115:GLU:O	28:T:118:GLU:HG3	2.13	0.48
9:A:1545:U:H2'	9:A:1546:A:H8	1.78	0.48
13:E:23:LYS:O	13:E:27:GLU:HG3	2.14	0.48
23:O:105:CYS:HB2	23:O:142:VAL:HA	1.94	0.48
30:V:264:GLU:HG2	30:V:337:LEU:HD21	1.94	0.48
30:V:198:TRP:O	30:V:202:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1:152:ASP:HB2	2:1:172:VAL:HB	1.96	0.48
5:4:389:SER:HA	5:4:392:ILE:HG12	1.94	0.48
9:A:872:G:H2'	9:A:873:G:C8	2.48	0.48
2:1:237:GLU:CD	2:1:239:TRP:HE1	2.21	0.48
5:4:431:LEU:O	5:4:435:VAL:HG23	2.14	0.48
9:A:1057:G:H4'	9:A:1578:A:H4'	1.96	0.48
14:F:46:ILE:HD12	15:G:315:PHE:HZ	1.78	0.48
27:S:85:PHE:HB2	31:W:100:VAL:HG12	1.96	0.48
28:T:43:GLY:HA3	28:T:93:LYS:O	2.14	0.48
5:4:361:LYS:HZ3	33:Y:251:PHE:HB3	1.77	0.48
5:4:427:ARG:HB3	5:4:468:MET:HE3	1.94	0.48
29:U:125:ARG:O	29:U:128:GLU:HG3	2.14	0.48
30:V:30:LEU:HD12	30:V:149:ASP:HB2	1.96	0.48
1:0:61:GLU:HB2	1:0:137:HIS:O	2.14	0.48
6:5:68:G:H2'	6:5:69:U:H6	1.79	0.48
6:5:69:U:H2'	6:5:70:A:C8	2.48	0.48
9:A:1470:A:H2'	9:A:1471:A:H8	1.79	0.48
8:7:188:HIS:CE1	8:7:268:GLN:HG2	2.49	0.47
8:7:520:ILE:O	8:7:551:PHE:HA	2.14	0.47
30:V:226:TYR:HE1	30:V:282:VAL:HG21	1.79	0.47
9:A:1275:A:H2	9:A:1300:A:H62	1.61	0.47
5:4:238:TRP:CZ2	5:4:266:MET:HE1	2.49	0.47
5:4:238:TRP:CE2	5:4:266:MET:HE1	2.49	0.47
8:7:485:LEU:HG	8:7:487:LYS:H	1.78	0.47
9:A:1308:U:H4'	15:G:118:GLU:HG2	1.96	0.47
9:A:1558:A:H3'	9:A:1559:G:H8	1.80	0.47
18:J:35:GLN:HG2	18:J:38:ARG:HH22	1.80	0.47
23:O:123:LEU:HB3	23:O:154:ILE:HD13	1.96	0.47
27:S:106:LEU:CB	27:S:117:LEU:HD11	2.39	0.47
28:T:91:GLU:HG2	28:T:92:THR:HG23	1.97	0.47
29:U:71:ARG:O	29:U:75:VAL:HG23	2.14	0.47
32:X:153:LEU:HB3	32:X:260:VAL:HG12	1.96	0.47
1:0:198:MET:SD	29:U:65:GLN:HB2	2.54	0.47
5:4:267:VAL:HG21	5:4:296:ALA:HB1	1.96	0.47
14:F:58:LEU:HB2	14:F:63:LYS:NZ	2.30	0.47
23:O:216:LEU:HD11	29:U:53:PHE:HB3	1.96	0.47
30:V:383:HIS:O	30:V:387:VAL:HG13	2.15	0.47
32:X:145:CYS:SG	32:X:259:LEU:HD22	2.54	0.47
9:A:745:A:C4	9:A:746:A:C8	3.03	0.47
5:4:354:LEU:HD11	33:Y:250:ILE:HB	1.95	0.47
5:4:429:LEU:HD11	5:4:465:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:572:PRO:HG2	5:4:575:SER:OG	2.15	0.47
8:7:472:GLU:O	8:7:475:GLN:HG3	2.15	0.47
9:A:715:G:H2'	9:A:716:U:C6	2.49	0.47
9:A:852:A:H3'	9:A:853:C:C6	2.47	0.47
9:A:944:U:H2'	9:A:945:G:C8	2.50	0.47
12:D:162:LYS:O	12:D:166:GLU:HG3	2.15	0.47
14:F:59:THR:O	14:F:63:LYS:HG2	2.14	0.47
1:0:171:ARG:HD3	23:O:199:TRP:HZ2	1.79	0.47
1:0:192:ASN:HB3	1:0:195:ARG:HH12	1.80	0.47
1:0:118:LEU:HD11	1:0:204:PRO:HG2	1.95	0.47
9:A:681:U:H2'	9:A:682:A:H8	1.80	0.47
2:1:132:GLU:O	5:4:60:PRO:HG3	2.15	0.47
3:2:59:ASN:HD22	3:2:65:ALA:CB	2.28	0.47
13:E:92:ASN:CB	24:P:117:MET:HE3	2.45	0.47
32:X:223:GLY:HA2	32:X:226:VAL:HG22	1.96	0.47
6:5:6:G:H2'	6:5:7:G:C8	2.50	0.46
9:A:731:A:H2'	9:A:732:A:H8	1.80	0.46
9:A:1200:G:C2	9:A:1201:A:C8	3.03	0.46
9:A:1440:G:H2'	9:A:1441:A:H8	1.77	0.46
9:A:1577:U:H2'	9:A:1578:A:C8	2.50	0.46
20:L:115:ILE:HG21	20:L:181:ILE:HD13	1.96	0.46
30:V:220:GLY:O	30:V:224:GLN:HG3	2.15	0.46
5:4:592:ALA:O	5:4:596:LEU:HG	2.14	0.46
9:A:1033:U:H2'	9:A:1034:U:C6	2.50	0.46
9:A:1488:5MC:H2'	9:A:1489:G:C8	2.51	0.46
12:D:127:ASN:OD1	34:Z:72:ARG:HD3	2.15	0.46
30:V:208:LEU:HD11	30:V:223:SER:HB2	1.97	0.46
33:Y:386:ILE:HD12	33:Y:386:ILE:H	1.80	0.46
2:1:202:THR:O	2:1:204:VAL:HG23	2.15	0.46
10:B:146:SER:O	10:B:168:THR:HA	2.15	0.46
14:F:58:LEU:HB2	14:F:63:LYS:HZ2	1.80	0.46
30:V:112:TRP:HE1	30:V:128:THR:HG21	1.80	0.46
30:V:395:GLN:HA	30:V:398:GLU:HG2	1.98	0.46
5:4:346:HIS:HB3	5:4:350:ARG:HH21	1.80	0.46
5:4:523:PHE:HB3	5:4:562:GLN:HE22	1.81	0.46
6:5:66:C:H2'	6:5:67:C:C6	2.50	0.46
14:F:63:LYS:O	14:F:67:GLU:OE1	2.33	0.46
30:V:236:LEU:HD13	30:V:290:LEU:HD13	1.97	0.46
1:0:136:TYR:CZ	9:A:705:C:H2'	2.51	0.46
30:V:240:LEU:HG	30:V:244:TYR:CE1	2.38	0.46
30:V:374:THR:HA	30:V:377:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:35:ALA:O	1:0:44:PRO:HD2	2.16	0.46
1:0:74:PHE:HD1	30:V:102:TRP:HD1	1.63	0.46
8:7:270:VAL:O	8:7:273:ILE:HG22	2.15	0.46
9:A:838:U:H2'	9:A:839:A:H8	1.81	0.46
23:O:123:LEU:HB3	23:O:154:ILE:CD1	2.46	0.46
29:U:58:GLU:O	29:U:61:GLN:HG2	2.16	0.46
30:V:48:TYR:HE2	30:V:74:ARG:HD2	1.81	0.46
5:4:289:ALA:HB1	5:4:293:THR:HG21	1.97	0.46
9:A:732:A:H2'	9:A:733:U:H6	1.81	0.46
9:A:659:U:OP1	12:D:226:ARG:HD3	2.15	0.46
9:A:821:U:H2'	9:A:822:G:C8	2.51	0.46
16:H:182:GLU:HA	16:H:185:LYS:NZ	2.31	0.46
26:R:262:LEU:O	26:R:268:PHE:HB2	2.16	0.46
30:V:287:LEU:HD21	30:V:331:LEU:HB2	1.98	0.46
32:X:325:PRO:O	32:X:329:LEU:HB2	2.15	0.46
9:A:1317:A:H3'	9:A:1318:A:H8	1.81	0.46
9:A:1504:U:H2'	9:A:1505:A:C8	2.51	0.46
8:7:198:ASP:OD1	8:7:205:VAL:HG22	2.16	0.45
9:A:1190:C:H2'	9:A:1191:C:H6	1.82	0.45
14:F:48:LYS:O	14:F:52:ARG:HG2	2.15	0.45
15:G:229:LEU:HD21	15:G:241:VAL:HG11	1.98	0.45
9:A:1508:C:H2'	9:A:1509:U:H6	1.81	0.45
5:4:590:GLN:HG2	5:4:591:GLU:N	2.30	0.45
9:A:839:A:H2'	9:A:840:A:H8	1.81	0.45
9:A:1557:A:OP1	18:J:72:LYS:HG2	2.15	0.45
20:L:98:ALA:HB1	20:L:102:GLU:HG3	1.97	0.45
30:V:57:MET:HE3	30:V:67:VAL:HG11	1.98	0.45
30:V:107:TRP:HB3	30:V:382:TRP:CD2	2.52	0.45
31:W:139:ARG:HG3	31:W:139:ARG:NH1	2.29	0.45
1:0:11:ILE:HB	9:A:806:C:C2	2.51	0.45
5:4:350:ARG:HH12	5:4:388:ARG:HH21	1.64	0.45
9:A:981:C:H2'	9:A:982:A:H8	1.81	0.45
9:A:1020:C:C5	9:A:1021:U:C4	3.04	0.45
12:D:256:PHE:HZ	12:D:347:GLN:HG2	1.81	0.45
17:I:60:PHE:CE2	25:Q:15:GLN:HB2	2.52	0.45
1:0:132:GLU:OE1	1:0:133:HIS:ND1	2.47	0.45
8:7:459:ASP:O	8:7:463:ILE:HD12	2.16	0.45
12:D:243:VAL:HG11	12:D:268:PHE:HD1	1.81	0.45
30:V:40:TRP:CE3	30:V:114:ARG:HB3	2.52	0.45
30:V:199:GLU:HA	30:V:202:ARG:NE	2.32	0.45
9:A:733:U:H2'	9:A:734:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:412:LYS:HG3	12:D:417:MET:HB2	1.98	0.45
19:K:50:GLU:O	19:K:54:ILE:HG12	2.17	0.45
27:S:101:GLU:O	27:S:105:GLU:OE1	2.35	0.45
1:O:82:ARG:HB2	1:O:139:TRP:CZ3	2.52	0.45
5:4:446:LYS:HG2	33:Y:292:GLN:HE22	1.78	0.45
8:7:603:VAL:HG11	8:7:725:PRO:HG3	1.98	0.45
9:A:740:G:H2'	9:A:741:A:C8	2.51	0.45
30:V:247:MET:HG2	30:V:248:PRO:HD2	1.98	0.45
5:4:627:ALA:O	5:4:631:VAL:HG13	2.17	0.45
8:7:188:HIS:CD2	8:7:189:VAL:H	2.34	0.45
9:A:1561:C:H2'	9:A:1562:G:O4'	2.16	0.45
15:G:238:GLU:O	15:G:242:GLN:HG2	2.17	0.45
23:O:208:PRO:HB3	29:U:54:PHE:CD1	2.52	0.45
32:X:205:GLN:HA	32:X:218:LYS:HG3	1.98	0.45
9:A:764:A:H4'	9:A:765:C:O4'	2.17	0.45
9:A:853:C:H2'	9:A:854:U:H6	1.82	0.45
9:A:1528:A:H2'	9:A:1529:A:C8	2.52	0.45
10:B:193:ILE:O	10:B:219:THR:HA	2.17	0.45
18:J:51:PRO:HG3	18:J:122:LYS:HB3	1.98	0.45
1:O:102:PRO:HA	1:O:112:GLY:HA3	1.98	0.45
2:1:262:ILE:HA	2:1:265:THR:HG22	1.98	0.45
5:4:359:GLU:HG3	33:Y:256:LEU:HD12	1.98	0.45
8:7:172:ASP:HB3	8:7:175:LEU:HG	1.99	0.45
12:D:128:ARG:HG3	12:D:129:GLY:N	2.32	0.45
14:F:153:GLU:HB3	14:F:179:ARG:CG	2.47	0.45
30:V:48:TYR:CE2	30:V:74:ARG:HD2	2.52	0.45
30:V:117:LEU:HD23	30:V:122:GLN:HG2	1.99	0.45
9:A:1116:A:P	10:B:100:ARG:HH22	2.40	0.44
23:O:218:ARG:HD3	30:V:317:LEU:HA	1.99	0.44
26:R:112:GLU:HA	26:R:115:THR:HG22	2.00	0.44
30:V:37:SER:HB2	30:V:40:TRP:HE3	1.82	0.44
30:V:326:LYS:HE3	30:V:330:TYR:OH	2.17	0.44
5:4:563:PRO:HA	5:4:565:ARG:CZ	2.47	0.44
5:4:593:TRP:CH2	5:4:626:GLN:HB3	2.52	0.44
6:5:27:U:H2'	6:5:28:C:H6	1.82	0.44
34:Z:9:PHE:CZ	34:Z:13:ARG:HD2	2.51	0.44
1:O:21:LEU:O	1:O:25:LEU:HG	2.17	0.44
1:O:61:GLU:HB2	1:O:137:HIS:C	2.42	0.44
9:A:740:G:N3	9:A:741:A:C8	2.85	0.44
9:A:1407:U:H2'	9:A:1408:A:C8	2.52	0.44
9:A:1510:U:H2'	9:A:1511:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1527:A:H2'	9:A:1528:A:O4'	2.17	0.44
17:I:129:GLN:HE21	17:I:167:MET:CE	2.30	0.44
26:R:204:ILE:HD12	28:T:144:GLU:HG2	1.98	0.44
5:4:350:ARG:HB3	5:4:379:PHE:HE2	1.83	0.44
9:A:1429:C:H4'	9:A:1430:A:H5'	1.98	0.44
9:A:1499:U:H2'	9:A:1500:C:H6	1.82	0.44
17:I:129:GLN:HE21	17:I:167:MET:HE3	1.82	0.44
20:L:112:MET:O	20:L:116:VAL:HG22	2.17	0.44
30:V:130:VAL:HA	30:V:166:GLU:OE2	2.18	0.44
6:5:27:U:H2'	6:5:28:C:C6	2.53	0.44
15:G:127:HIS:ND1	15:G:129:GLU:HG3	2.33	0.44
23:O:177:PHE:HE1	26:R:237:PRO:HG2	1.81	0.44
30:V:225:LEU:HD11	30:V:283:LEU:HD22	1.98	0.44
5:4:262:MET:O	5:4:266:MET:HG2	2.18	0.44
5:4:625:SER:O	5:4:629:GLU:HG3	2.17	0.44
9:A:862:A:H2'	9:A:863:C:C6	2.53	0.44
9:A:1114:U:H2'	9:A:1115:U:C6	2.53	0.44
12:D:231:MET:HE2	12:D:231:MET:HB2	1.85	0.44
12:D:243:VAL:HG11	12:D:268:PHE:CD1	2.53	0.44
15:G:71:GLU:O	15:G:75:LYS:HG2	2.17	0.44
30:V:148:MET:SD	30:V:185:VAL:HG21	2.58	0.44
33:Y:347:ILE:CD1	33:Y:392:ILE:HG21	2.47	0.44
5:4:529:GLU:O	5:4:533:MET:HG2	2.18	0.44
5:4:570:ASP:HA	5:4:602:HIS:CE1	2.48	0.44
8:7:661:LEU:O	8:7:667:VAL:HA	2.17	0.44
9:A:771:A:H2'	9:A:772:A:C8	2.52	0.44
9:A:1499:U:H2'	9:A:1500:C:C6	2.53	0.44
12:D:206:PRO:HG2	12:D:276:VAL:HG11	1.99	0.44
20:L:175:TYR:HB2	22:N:89:GLY:HA3	2.00	0.44
26:R:257:GLY:HA2	26:R:259:TYR:CE2	2.52	0.44
1:0:63:ARG:HB2	1:0:66:GLN:HB2	1.99	0.44
5:4:302:VAL:HG21	5:4:341:CYS:SG	2.57	0.44
22:N:8:VAL:HB	22:N:68:ALA:HB1	2.00	0.44
30:V:228:TYR:HB3	30:V:259:ALA:HB2	2.00	0.44
30:V:331:LEU:HD11	30:V:335:LYS:HE3	1.98	0.44
5:4:650:MET:HE2	5:4:650:MET:HB2	1.90	0.44
13:E:37:ARG:HG3	29:U:167:PHE:CE1	2.53	0.44
17:I:140:LYS:HD2	17:I:169:GLY:HA3	1.99	0.44
21:M:21:LEU:HD23	21:M:32:TYR:CG	2.53	0.44
26:R:167:HIS:HB3	26:R:193:ILE:HD13	1.99	0.44
30:V:96:ARG:NH2	30:V:133:VAL:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:X:261:ALA:HA	32:X:307:VAL:O	2.17	0.44
1:0:58:VAL:HG23	1:0:137:HIS:ND1	2.32	0.43
3:2:49:MET:HE1	14:F:237:ALA:CB	2.48	0.43
5:4:467:LEU:HG	5:4:468:MET:SD	2.58	0.43
5:4:562:GLN:HG3	5:4:564:ILE:H	1.81	0.43
1:0:67:LEU:HD23	1:0:141:LEU:HB3	2.00	0.43
3:2:38:ARG:HG2	9:A:1183:U:OP1	2.18	0.43
9:A:832:U:H2'	9:A:833:A:C8	2.52	0.43
9:A:1002:C:H2'	9:A:1003:A:H8	1.83	0.43
9:A:1370:U:C2	9:A:1371:U:C5	3.06	0.43
9:A:1507:A:H2'	9:A:1508:C:H6	1.82	0.43
30:V:287:LEU:O	30:V:291:THR:HG23	2.19	0.43
31:W:108:VAL:O	31:W:109:GLU:HG3	2.19	0.43
8:7:594:LYS:HD3	8:7:605:ASP:OD2	2.17	0.43
9:A:995:A:H2'	9:A:996:A:C8	2.54	0.43
9:A:1471:A:H2'	9:A:1472:G:C8	2.53	0.43
27:S:104:THR:O	27:S:107:GLN:HB2	2.18	0.43
27:S:125:LEU:HD12	27:S:130:VAL:HG21	2.00	0.43
30:V:157:TYR:HA	30:V:160:ALA:HB3	2.00	0.43
2:1:244:THR:O	2:1:248:MET:HG2	2.18	0.43
5:4:173:PHE:HE1	5:4:183:VAL:HG21	1.84	0.43
9:A:1239:C:H2'	9:A:1240:A:C8	2.54	0.43
10:B:220:VAL:HG22	10:B:234:TYR:HB2	2.00	0.43
20:L:147:ARG:HG3	20:L:148:LYS:HD3	1.99	0.43
32:X:203:LYS:NZ	32:X:221:PRO:HG3	2.33	0.43
2:1:238:GLU:HG2	2:1:239:TRP:N	2.32	0.43
5:4:429:LEU:HD22	5:4:468:MET:O	2.18	0.43
9:A:845:A:H5'	29:U:64:ARG:HH22	1.84	0.43
20:L:167:LEU:HD11	20:L:187:ILE:HG21	2.00	0.43
1:0:83:LYS:HB3	1:0:138:ASP:OD1	2.19	0.43
5:4:282:LEU:HD21	5:4:289:ALA:HB2	2.00	0.43
6:5:23:G:H2'	6:5:24:C:C6	2.54	0.43
9:A:758:U:O4	9:A:1159:A:HI'	2.19	0.43
9:A:952:A:H2'	9:A:953:U:C6	2.53	0.43
14:F:82:THR:O	14:F:87:GLU:HG3	2.18	0.43
18:J:114:ARG:HA	18:J:122:LYS:HA	2.00	0.43
20:L:73:LEU:HD23	20:L:95:LEU:HD23	2.00	0.43
23:O:55:PRO:HB3	23:O:114:HIS:HB2	2.00	0.43
30:V:173:PHE:CD1	30:V:211:PRO:HB3	2.53	0.43
2:1:259:GLU:HA	2:1:262:ILE:HG22	2.01	0.43
8:7:538:TYR:HA	8:7:723:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1544:A:H2'	9:A:1545:U:C6	2.54	0.43
15:G:241:VAL:O	15:G:245:ARG:HG2	2.18	0.43
1:0:171:ARG:HA	1:0:174:ILE:HG12	2.00	0.43
5:4:330:PRO:HD2	33:Y:262:MET:HE1	2.01	0.43
11:C:96:MET:HE3	11:C:96:MET:HB3	1.90	0.43
30:V:388:GLN:HG3	30:V:391:GLN:HE22	1.84	0.43
32:X:162:VAL:HB	32:X:272:THR:HG22	2.01	0.43
32:X:248:LYS:HB2	32:X:296:MET:SD	2.59	0.43
2:1:156:TYR:CD2	16:H:171:GLU:HG2	2.54	0.43
5:4:452:GLN:HE21	5:4:453:HIS:CE1	2.36	0.43
5:4:642:CYS:HA	5:4:645:LEU:HG	2.00	0.43
9:A:747:A:H2'	9:A:748:G:H8	1.84	0.43
10:B:142:ILE:O	10:B:164:GLU:HB3	2.19	0.43
4:3:145:LYS:NZ	9:A:1583:MA6:H5''	2.34	0.43
8:7:284:ILE:HD12	8:7:338:THR:HG22	2.00	0.43
9:A:1365:A:H4'	9:A:1389:G:H4'	2.01	0.43
17:I:100:VAL:HG12	17:I:106:PRO:HA	2.01	0.43
30:V:322:THR:O	30:V:326:LYS:HG2	2.17	0.43
31:W:120:PHE:HB3	31:W:164:GLU:HA	2.01	0.43
9:A:982:A:H2'	9:A:983:C:H6	1.82	0.42
9:A:1497:C:H2'	9:A:1498:C:H6	1.84	0.42
30:V:205:GLY:O	30:V:209:LEU:HD23	2.19	0.42
31:W:104:ILE:HG21	31:W:107:ILE:HD11	2.01	0.42
32:X:268:LEU:HB2	32:X:269:TRP:CE3	2.54	0.42
32:X:295:LYS:O	32:X:298:LYS:HG2	2.19	0.42
33:Y:285:GLN:O	33:Y:289:VAL:HG13	2.19	0.42
10:B:61:LYS:HZ1	10:B:271:TYR:HB2	1.84	0.42
14:F:153:GLU:HB3	14:F:179:ARG:HG2	2.01	0.42
28:T:114:ARG:O	28:T:117:GLU:HG2	2.19	0.42
1:0:64:LEU:HB2	1:0:139:TRP:CD1	2.55	0.42
9:A:741:A:C6	9:A:742:U:C4	3.07	0.42
9:A:1577:U:H2'	9:A:1578:A:H8	1.84	0.42
13:E:37:ARG:HD2	13:E:69:TYR:HE1	1.83	0.42
14:F:62:GLU:HA	14:F:65:VAL:HG22	2.02	0.42
3:2:47:THR:O	3:2:51:VAL:HG23	2.18	0.42
5:4:350:ARG:HH12	5:4:388:ARG:NH2	2.17	0.42
12:D:265:MET:SD	15:G:57:PRO:HD2	2.58	0.42
28:T:22:VAL:HG23	28:T:108:LYS:HB2	2.02	0.42
30:V:357:THR:HG22	30:V:361:LYS:NZ	2.34	0.42
2:1:279:ASN:CG	2:1:282:GLU:HB2	2.45	0.42
4:3:186:PRO:HB3	20:L:216:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1246:U:C5	34:Z:96:LYS:HD2	2.54	0.42
21:M:19:ILE:HG22	21:M:36:ALA:HB2	2.02	0.42
24:P:124:TYR:HB3	25:Q:9:ALA:HB2	2.00	0.42
26:R:79:LEU:O	26:R:83:THR:HG23	2.20	0.42
26:R:86:ASN:OD1	26:R:89:LYS:HB3	2.20	0.42
26:R:331:PHE:CE2	26:R:336:ALA:HB2	2.53	0.42
32:X:353:PHE:O	32:X:357:ILE:HD12	2.19	0.42
1:O:113:LYS:HE3	1:O:115:TRP:CH2	2.53	0.42
9:A:1181:G:H2'	9:A:1182:C:C6	2.55	0.42
11:C:58:ALA:HB3	11:C:60:HIS:CE1	2.55	0.42
21:M:63:GLU:OE1	26:R:157:VAL:HG21	2.19	0.42
32:X:203:LYS:HD2	32:X:219:GLY:O	2.18	0.42
2:1:249:GLU:HG2	2:1:250:GLU:N	2.33	0.42
2:1:279:ASN:OD1	2:1:282:GLU:HB2	2.19	0.42
9:A:738:A:H2'	9:A:740:G:C5	2.55	0.42
30:V:357:THR:HA	30:V:360:VAL:HG12	2.02	0.42
32:X:182:LEU:O	32:X:186:THR:HG23	2.19	0.42
9:A:715:G:H2'	9:A:716:U:H6	1.84	0.42
9:A:1455:U:H2'	9:A:1456:U:C6	2.55	0.42
30:V:200:GLU:O	30:V:204:PHE:CD2	2.73	0.42
5:4:571:TRP:O	5:4:604:LYS:HE2	2.19	0.42
8:7:178:PRO:HA	8:7:348:LYS:HG2	2.02	0.42
8:7:296:ASP:HB3	8:7:299:LYS:HB3	2.02	0.42
9:A:1542:U:H2'	9:A:1543:U:C6	2.55	0.42
23:O:95:ILE:CD1	23:O:100:VAL:HG22	2.50	0.42
23:O:184:VAL:O	26:R:138:ILE:HD13	2.20	0.42
1:O:88:GLN:HA	23:O:215:ARG:HD3	2.02	0.42
9:A:955:A:OP2	28:T:37:HIS:HE1	2.03	0.42
9:A:1581:G:H2'	9:A:1583:MA6:OP2	2.20	0.42
12:D:128:ARG:HG3	12:D:129:GLY:H	1.85	0.42
34:Z:26:THR:HB	34:Z:31:MET:HE3	2.02	0.42
30:V:175:VAL:HG13	30:V:178:THR:H	1.85	0.41
30:V:250:ILE:HG21	30:V:258:ARG:HH12	1.85	0.41
32:X:73:GLN:HA	32:X:76:GLU:HG2	2.02	0.41
5:4:540:HIS:CG	5:4:544:LEU:HD23	2.55	0.41
6:5:51:U:H2'	6:5:52:G:O4'	2.20	0.41
9:A:1373:U:H2'	9:A:1374:A:H8	1.86	0.41
9:A:1506:U:H2'	9:A:1507:A:C8	2.54	0.41
30:V:240:LEU:HD22	30:V:253:PRO:HG3	2.02	0.41
4:3:165:LYS:HE3	9:A:1148:A:P	2.60	0.41
9:A:1012:A:H2'	9:A:1013:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1044:U:H2'	9:A:1045:G:O4'	2.21	0.41
9:A:1239:C:H2'	9:A:1240:A:H8	1.85	0.41
14:F:51:TYR:HB3	15:G:363:TRP:CD2	2.54	0.41
17:I:129:GLN:NE2	17:I:133:ILE:HD11	2.35	0.41
1:O:163:SER:HB3	1:O:190:MET:HB3	2.00	0.41
9:A:799:A:H2'	9:A:800:C:C6	2.55	0.41
14:F:197:GLN:O	14:F:197:GLN:HG2	2.19	0.41
1:O:192:ASN:HB3	1:O:195:ARG:NH1	2.36	0.41
6:5:23:G:H2'	6:5:24:C:H6	1.84	0.41
9:A:812:A:H2'	9:A:813:A:C8	2.56	0.41
24:P:52:ILE:HD11	24:P:54:MET:HE2	2.01	0.41
30:V:177:SER:HB2	30:V:367:CYS:HB3	2.03	0.41
1:O:20:ALA:O	1:O:23:GLU:HG3	2.20	0.41
2:1:116:PRO:O	2:1:120:LYS:HG3	2.21	0.41
2:1:284:LEU:HA	2:1:289:ILE:HG13	2.01	0.41
6:5:2:G:H2'	6:5:3:U:C6	2.55	0.41
8:7:460:LEU:HB2	18:J:136:GLN:HG3	2.01	0.41
9:A:832:U:H2'	9:A:833:A:H8	1.83	0.41
9:A:1506:U:H2'	9:A:1507:A:H8	1.86	0.41
14:F:82:THR:HG23	15:G:315:PHE:CD1	2.56	0.41
30:V:61:PHE:CZ	30:V:94:LYS:HB3	2.56	0.41
32:X:253:LEU:HB2	32:X:255:MET:HE1	2.01	0.41
5:4:347:VAL:HA	5:4:350:ARG:CG	2.50	0.41
9:A:973:C:O2'	9:A:974:U:H5'	2.21	0.41
9:A:1334:G:H2'	9:A:1335:U:O4'	2.21	0.41
21:M:99:LEU:HD23	26:R:148:LEU:HD21	2.03	0.41
23:O:205:TRP:HZ2	29:U:51:ALA:HB1	1.86	0.41
30:V:69:SER:HA	30:V:72:ILE:HG22	2.02	0.41
32:X:151:LEU:HD12	32:X:151:LEU:HA	1.80	0.41
5:4:349:ALA:C	5:4:352:PRO:HD2	2.46	0.41
8:7:512:ASP:HB3	8:7:515:VAL:HG23	2.02	0.41
9:A:700:A:H4'	9:A:701:G:O5'	2.20	0.41
9:A:746:A:C4	9:A:747:A:C8	3.09	0.41
15:G:250:LEU:HD23	15:G:250:LEU:H	1.85	0.41
15:G:315:PHE:CE2	15:G:369:LEU:HD21	2.56	0.41
30:V:196:PHE:HB3	30:V:201:GLU:HG2	2.03	0.41
30:V:226:TYR:CE1	30:V:282:VAL:HG11	2.55	0.41
33:Y:286:LEU:O	33:Y:289:VAL:HG22	2.21	0.41
2:1:194:VAL:HG11	2:1:205:LEU:HD11	2.03	0.41
5:4:188:THR:O	5:4:192:LEU:HG	2.20	0.41
5:4:256:GLU:HG3	5:4:287:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:646:THR:HG23	5:4:663:LEU:HD22	2.03	0.41
8:7:461:LYS:O	8:7:465:GLU:HG2	2.21	0.41
9:A:854:U:H2'	9:A:855:A:C8	2.56	0.41
9:A:1348:G:H2'	9:A:1349:U:C6	2.56	0.41
9:A:1372:C:H2'	9:A:1373:U:H6	1.86	0.41
13:E:37:ARG:HD2	13:E:69:TYR:CE1	2.55	0.41
13:E:108:ILE:HD11	24:P:100:CYS:HB3	2.02	0.41
14:F:150:LYS:HA	14:F:153:GLU:HG3	2.03	0.41
16:H:185:LYS:HE2	16:H:185:LYS:HB2	1.79	0.41
17:I:181:ILE:HD11	25:Q:39:ILE:HD11	2.03	0.41
20:L:207:LYS:O	20:L:211:ILE:HG12	2.21	0.41
21:M:55:ASP:HB2	28:T:140:ILE:HD13	2.02	0.41
30:V:209:LEU:CD2	30:V:227:GLY:HA3	2.50	0.41
5:4:526:ASP:O	5:4:529:GLU:HG3	2.21	0.41
6:5:12:C:H2'	6:5:13:U:H6	1.86	0.41
6:5:68:G:H2'	6:5:69:U:C6	2.56	0.41
8:7:324:SER:HB3	8:7:329:ASP:HB3	2.03	0.41
9:A:862:A:H2'	9:A:863:C:H6	1.86	0.41
9:A:896:A:H2'	9:A:897:C:C6	2.55	0.41
9:A:1089:U:H2'	9:A:1090:A:H8	1.85	0.41
10:B:193:ILE:HB	10:B:219:THR:HG22	2.02	0.41
11:C:105:ALA:HB3	11:C:122:VAL:HG12	2.03	0.41
30:V:74:ARG:HH22	30:V:390:ILE:HD11	1.85	0.41
30:V:360:VAL:O	30:V:364:LEU:HB2	2.21	0.41
32:X:265:ILE:HG12	32:X:297:MET:HE2	2.03	0.41
1:0:104:TYR:HB2	30:V:97:HIS:O	2.21	0.40
5:4:264:ARG:NH2	33:Y:278:TRP:HB3	2.35	0.40
5:4:543:GLU:HG2	5:4:544:LEU:N	2.35	0.40
6:5:12:C:H2'	6:5:13:U:C6	2.56	0.40
6:5:25:U:C2	6:5:26:A:C8	3.09	0.40
8:7:391:LYS:HE2	8:7:451:GLN:OE1	2.20	0.40
9:A:1173:C:H2'	9:A:1174:U:C6	2.56	0.40
11:C:109:VAL:HB	11:C:120:CYS:HB2	2.02	0.40
15:G:115:GLY:HA3	16:H:84:ASP:OD1	2.22	0.40
19:K:54:ILE:O	19:K:58:ARG:HG3	2.21	0.40
26:R:273:TRP:NE1	26:R:277:ASN:HD21	2.18	0.40
26:R:292:ASP:OD2	26:R:349:TYR:HE1	2.04	0.40
28:T:32:VAL:HB	28:T:66:MET:HG3	2.03	0.40
1:0:55:TRP:HA	1:0:58:VAL:HG12	2.02	0.40
1:0:198:MET:HE1	29:U:61:GLN:HA	2.02	0.40
2:1:304:GLU:OE1	32:X:326:GLN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:4:393:ILE:HD13	5:4:422:ILE:HG21	2.04	0.40
9:A:955:A:O4'	9:A:1042:U:H1'	2.21	0.40
9:A:1489:G:H2'	9:A:1490:U:H6	1.87	0.40
30:V:199:GLU:HB2	30:V:202:ARG:HH21	1.85	0.40
1:0:58:VAL:CG2	1:0:137:HIS:HD1	2.34	0.40
2:1:239:TRP:CG	34:Z:10:ARG:HE	2.39	0.40
5:4:388:ARG:O	5:4:392:ILE:HG12	2.22	0.40
8:7:241:PHE:HB3	8:7:244:MET:HB3	2.02	0.40
10:B:189:LEU:HD23	10:B:189:LEU:HA	1.94	0.40
10:B:229:PRO:HA	10:B:232:ILE:HD12	2.02	0.40
15:G:59:LYS:HE2	15:G:62:PRO:HA	2.04	0.40
16:H:78:VAL:HG22	16:H:172:VAL:HG23	2.04	0.40
21:M:54:TYR:CD1	21:M:66:VAL:HG22	2.56	0.40
21:M:78:GLY:O	29:U:75:VAL:HG22	2.21	0.40
21:M:83:LEU:HD12	21:M:88:GLU:HG3	2.03	0.40
26:R:73:GLU:HG2	26:R:74:GLU:N	2.37	0.40
26:R:116:ARG:O	26:R:120:GLU:HG2	2.21	0.40
1:0:148:GLU:HG2	1:0:149:ALA:N	2.36	0.40
8:7:394:ALA:HB2	8:7:421:TRP:CD2	2.56	0.40
9:A:1190:C:H2'	9:A:1191:C:C6	2.57	0.40
9:A:1372:C:H2'	9:A:1373:U:C6	2.56	0.40
15:G:168:MET:HE2	15:G:237:GLU:HG3	2.02	0.40
17:I:122:LYS:HB2	17:I:122:LYS:HE3	1.87	0.40
30:V:74:ARG:HA	30:V:74:ARG:HD3	1.89	0.40
1:0:196:ILE:HG13	1:0:196:ILE:O	2.21	0.40
2:1:312:TYR:O	2:1:316:VAL:HG23	2.22	0.40
5:4:196:CYS:SG	5:4:262:MET:HA	2.61	0.40
9:A:731:A:H2'	9:A:732:A:C8	2.56	0.40
13:E:118:TYR:HB3	13:E:123:ARG:NH2	2.37	0.40
15:G:255:GLN:HG3	15:G:256:LEU:O	2.21	0.40
29:U:97:LYS:O	29:U:101:GLU:HG2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	213/215 (99%)	209 (98%)	4 (2%)	0	100	100
2	1	276/278 (99%)	270 (98%)	6 (2%)	0	100	100
3	2	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
4	3	69/71 (97%)	68 (99%)	1 (1%)	0	100	100
5	4	588/616 (96%)	573 (97%)	15 (3%)	0	100	100
8	7	569/571 (100%)	554 (97%)	15 (3%)	0	100	100
10	B	223/225 (99%)	220 (99%)	3 (1%)	0	100	100
11	C	130/132 (98%)	127 (98%)	3 (2%)	0	100	100
12	D	341/343 (99%)	331 (97%)	10 (3%)	0	100	100
13	E	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
14	F	206/208 (99%)	201 (98%)	5 (2%)	0	100	100
15	G	323/344 (94%)	316 (98%)	7 (2%)	0	100	100
16	H	138/140 (99%)	134 (97%)	3 (2%)	1 (1%)	18	34
17	I	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
18	J	106/108 (98%)	105 (99%)	1 (1%)	0	100	100
19	K	99/101 (98%)	98 (99%)	1 (1%)	0	100	100
20	L	172/174 (99%)	170 (99%)	2 (1%)	0	100	100
21	M	117/119 (98%)	115 (98%)	2 (2%)	0	100	100
22	N	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
23	O	191/193 (99%)	188 (98%)	3 (2%)	0	100	100
24	P	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
25	Q	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
26	R	293/295 (99%)	285 (97%)	8 (3%)	0	100	100
27	S	133/135 (98%)	133 (100%)	0	0	100	100
28	T	166/168 (99%)	166 (100%)	0	0	100	100
29	U	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
30	V	358/379 (94%)	349 (98%)	9 (2%)	0	100	100
31	W	98/100 (98%)	97 (99%)	0	1 (1%)	12	24
32	X	350/352 (99%)	345 (99%)	5 (1%)	0	100	100
33	Y	147/149 (99%)	140 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Z	98/100 (98%)	98 (100%)	0	0	100	100
All	All	6237/6363 (98%)	6109 (98%)	126 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	H	126	ILE
31	W	109	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	188/188 (100%)	188 (100%)	0	100	100
2	1	256/256 (100%)	256 (100%)	0	100	100
3	2	100/101 (99%)	100 (100%)	0	100	100
4	3	65/65 (100%)	65 (100%)	0	100	100
5	4	529/549 (96%)	529 (100%)	0	100	100
8	7	396/481 (82%)	396 (100%)	0	100	100
10	B	198/198 (100%)	198 (100%)	0	100	100
11	C	115/115 (100%)	115 (100%)	0	100	100
12	D	286/286 (100%)	286 (100%)	0	100	100
13	E	104/104 (100%)	104 (100%)	0	100	100
14	F	185/185 (100%)	185 (100%)	0	100	100
15	G	285/301 (95%)	285 (100%)	0	100	100
16	H	130/130 (100%)	130 (100%)	0	100	100
17	I	105/105 (100%)	105 (100%)	0	100	100
18	J	93/93 (100%)	93 (100%)	0	100	100
19	K	91/91 (100%)	91 (100%)	0	100	100
20	L	158/158 (100%)	158 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	M	97/97 (100%)	97 (100%)	0	100	100
22	N	96/96 (100%)	96 (100%)	0	100	100
23	O	174/174 (100%)	174 (100%)	0	100	100
24	P	88/88 (100%)	88 (100%)	0	100	100
25	Q	78/79 (99%)	78 (100%)	0	100	100
26	R	264/264 (100%)	264 (100%)	0	100	100
27	S	116/116 (100%)	116 (100%)	0	100	100
28	T	153/153 (100%)	153 (100%)	0	100	100
29	U	152/152 (100%)	152 (100%)	0	100	100
30	V	325/339 (96%)	325 (100%)	0	100	100
31	W	87/87 (100%)	87 (100%)	0	100	100
32	X	311/311 (100%)	311 (100%)	0	100	100
33	Y	137/137 (100%)	137 (100%)	0	100	100
34	Z	90/90 (100%)	90 (100%)	0	100	100
All	All	5452/5589 (98%)	5452 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	192	ASN
1	0	207	GLN
5	4	148	GLN
5	4	189	ASN
5	4	269	HIS
5	4	346	HIS
5	4	373	HIS
5	4	452	GLN
5	4	504	ASN
5	4	562	GLN
5	4	602	HIS
8	7	274	GLN
12	D	341	ASN
14	F	122	GLN
17	I	96	GLN
17	I	129	GLN

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Mol	Chain	Res	Type
19	K	28	HIS
20	L	169	ASN
22	N	44	ASN
26	R	108	GLN
26	R	278	ASN
26	R	305	HIS
27	S	66	HIS
27	S	91	ASN
28	T	54	GLN
30	V	38	HIS
30	V	383	HIS
31	W	121	HIS
32	X	81	HIS
32	X	291	HIS
32	X	302	HIS
32	X	394	HIS
33	Y	285	GLN
33	Y	292	GLN
33	Y	337	HIS
34	Z	27	ASN
34	Z	56	HIS
34	Z	63	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	5	70/71 (98%)	10 (14%)	0
7	6	3/4 (75%)	1 (33%)	0
9	A	954/955 (99%)	121 (12%)	0
All	All	1027/1030 (99%)	132 (12%)	0

All (132) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	5	9	C
6	5	10	A
6	5	20	U
6	5	21	A
6	5	31	G
6	5	48	U
6	5	49	G

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Mol	Chain	Res	Type
6	5	52	G
6	5	55	U
6	5	60	C
7	6	4	U
9	A	651	A
9	A	680	U
9	A	688	A
9	A	704	U
9	A	718	A
9	A	721	U
9	A	722	C
9	A	737	C
9	A	738	A
9	A	739	C
9	A	753	A
9	A	760	A
9	A	761	A
9	A	766	G
9	A	773	U
9	A	791	G
9	A	796	G
9	A	830	U
9	A	832	U
9	A	835	C
9	A	851	A
9	A	860	A
9	A	868	C
9	A	871	A
9	A	889	G
9	A	890	C
9	A	904	C
9	A	919	A
9	A	923	A
9	A	938	A
9	A	939	A
9	A	942	A
9	A	954	C
9	A	958	C
9	A	960	C
9	A	961	U
9	A	962	C
9	A	967	A

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Mol	Chain	Res	Type
9	A	992	U
9	A	1001	C
9	A	1002	C
9	A	1011	C
9	A	1015	A
9	A	1019	A
9	A	1042	U
9	A	1049	A
9	A	1065	C
9	A	1080	A
9	A	1081	U
9	A	1082	A
9	A	1098	C
9	A	1103	A
9	A	1105	C
9	A	1106	C
9	A	1107	U
9	A	1109	A
9	A	1117	A
9	A	1121	A
9	A	1151	C
9	A	1154	A
9	A	1160	A
9	A	1167	A
9	A	1179	G
9	A	1188	A
9	A	1189	U
9	A	1190	C
9	A	1193	U
9	A	1197	G
9	A	1206	G
9	A	1209	C
9	A	1215	U
9	A	1220	A
9	A	1223	C
9	A	1225	C
9	A	1229	U
9	A	1247	G
9	A	1248	C
9	A	1250	C
9	A	1251	A
9	A	1261	C

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Mol	Chain	Res	Type
9	A	1271	C
9	A	1273	G
9	A	1283	A
9	A	1284	U
9	A	1285	G
9	A	1290	C
9	A	1291	U
9	A	1326	A
9	A	1327	G
9	A	1330	C
9	A	1343	A
9	A	1356	A
9	A	1367	A
9	A	1376	C
9	A	1378	C
9	A	1390	A
9	A	1405	C
9	A	1420	U
9	A	1422	G
9	A	1430	A
9	A	1438	G
9	A	1447	G
9	A	1519	A
9	A	1520	U
9	A	1522	U
9	A	1525	C
9	A	1526	U
9	A	1527	A
9	A	1533	C
9	A	1537	C
9	A	1538	G
9	A	1539	C
9	A	1557	A
9	A	1558	A
9	A	1568	U
9	A	1571	U
9	A	1582	G
9	A	1584	MA6
9	A	1594	G
9	A	1595	G
9	A	1599	A

There are no RNA pucker outliers to report.

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

5 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
9	MA6	A	1583	9	23,26,27	1.43	5 (21%)	33,38,41	2.78	14 (42%)
9	B8T	A	1486	9,35	19,22,23	3.08	8 (42%)	25,31,34	0.86	1 (4%)
9	5MC	A	1488	9	19,22,23	4.24	8 (42%)	26,32,35	0.95	1 (3%)
9	MA6	A	1584	9	23,26,27	1.44	6 (26%)	33,38,41	2.80	14 (42%)
9	5MU	A	1076	9	19,22,23	0.55	0	27,32,35	0.59	0

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
9	MA6	A	1583	9	-	0/11/29/30	0/3/3/3
9	B8T	A	1486	9,35	-	1/7/27/28	0/2/2/2
9	5MC	A	1488	9	-	0/7/25/26	0/2/2/2
9	MA6	A	1584	9	-	1/11/29/30	0/3/3/3
9	5MU	A	1076	9	-	0/7/25/26	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1488	5MC	C6-C5	9.62	1.50	1.34
9	A	1488	5MC	C5-C4	7.99	1.50	1.44
9	A	1488	5MC	C4-N3	7.38	1.45	1.34
9	A	1486	B8T	C4-N3	6.81	1.44	1.32
9	A	1488	5MC	C2-N3	6.69	1.49	1.36
9	A	1486	B8T	C2-N3	6.08	1.48	1.36
9	A	1486	B8T	C6-C5	5.89	1.48	1.35
9	A	1488	5MC	C4-N4	5.53	1.48	1.34
9	A	1488	5MC	C6-N1	5.39	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1486	B8T	C4-N4	4.15	1.44	1.36
9	A	1488	5MC	C2-N1	4.06	1.48	1.40
9	A	1486	B8T	C2-N1	3.87	1.48	1.40
9	A	1584	MA6	C5-C4	-3.59	1.32	1.39
9	A	1583	MA6	C5-C4	-3.52	1.32	1.39
9	A	1486	B8T	C5-C4	3.37	1.48	1.41
9	A	1486	B8T	O2-C2	-3.06	1.18	1.23
9	A	1486	B8T	C6-N1	2.88	1.44	1.38
9	A	1584	MA6	C6-N6	2.87	1.44	1.36
9	A	1583	MA6	C6-N6	2.83	1.44	1.36
9	A	1488	5MC	O2-C2	-2.72	1.18	1.23
9	A	1584	MA6	C5-N7	-2.64	1.34	1.39
9	A	1583	MA6	C5-N7	-2.53	1.34	1.39
9	A	1583	MA6	C8-N9	-2.51	1.33	1.37
9	A	1584	MA6	C8-N9	-2.47	1.33	1.37
9	A	1583	MA6	C4-N9	-2.33	1.32	1.37
9	A	1584	MA6	C4-N9	-2.22	1.33	1.37
9	A	1584	MA6	C5-C6	-2.01	1.36	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1583	MA6	N1-C6-N6	-8.00	107.11	116.86
9	A	1584	MA6	N1-C6-N6	-8.00	107.11	116.86
9	A	1583	MA6	N1-C2-N3	-5.89	119.67	128.58
9	A	1584	MA6	N1-C2-N3	-5.72	119.92	128.58
9	A	1583	MA6	C5-C6-N6	4.93	133.14	125.33
9	A	1584	MA6	C5-C6-N6	4.91	133.11	125.33
9	A	1583	MA6	N9-C8-N7	-4.60	107.41	113.94
9	A	1584	MA6	C1'-N9-C8	-4.42	117.28	127.09
9	A	1584	MA6	N9-C8-N7	-4.40	107.69	113.94
9	A	1584	MA6	C5-C4-N3	-4.28	120.83	126.72
9	A	1583	MA6	C1'-N9-C8	-4.27	117.62	127.09
9	A	1583	MA6	C5-C4-N3	-4.02	121.18	126.72
9	A	1583	MA6	C2-N1-C6	3.68	120.83	111.83
9	A	1584	MA6	C2-N1-C6	3.53	120.45	111.83
9	A	1584	MA6	C4-C5-C6	3.35	119.37	115.91
9	A	1584	MA6	C4-N9-C1'	3.24	134.20	126.63
9	A	1584	MA6	C2-N3-C4	3.20	119.66	111.83
9	A	1583	MA6	C2-N3-C4	3.16	119.55	111.83
9	A	1583	MA6	C4-N9-C8	3.08	108.97	105.74
9	A	1583	MA6	C4-C5-C6	3.02	119.03	115.91

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1583	MA6	C4-N9-C1'	2.90	133.41	126.63
9	A	1488	5MC	C5-C6-N1	-2.89	120.18	123.31
9	A	1583	MA6	C5-N7-C8	2.87	107.96	103.45
9	A	1584	MA6	C5-N7-C8	2.84	107.92	103.45
9	A	1584	MA6	C4-N9-C8	2.62	108.48	105.74
9	A	1584	MA6	N3-C4-N9	2.41	131.27	127.17
9	A	1583	MA6	N3-C4-N9	2.37	131.19	127.17
9	A	1486	B8T	C6-C5-C4	2.33	119.81	117.00
9	A	1584	MA6	C4-C5-N7	-2.26	108.00	110.58
9	A	1583	MA6	C4-C5-N7	-2.22	108.04	110.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1584	MA6	C4'-C5'-O5'-P
9	A	1486	B8T	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1583	MA6	2	0
9	A	1488	5MC	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 98 ligands modelled in this entry, 93 are monoatomic - leaving 5 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
39	FES	P	201	24,13	0,4,4	-	-	-		
39	FES	T	201	21,28	0,4,4	-	-	-		
37	GTP	7	803	35	33,34,34	0.95	1 (3%)	50,54,54	1.60	9 (18%)
40	GDP	X	401	-	29,30,30	3.83	16 (55%)	45,47,47	1.74	10 (22%)
41	ATP	X	403	35	32,33,33	0.56	1 (3%)	48,52,52	0.33	0

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
39	FES	P	201	24,13	-	-	0/1/1/1
39	FES	T	201	21,28	-	-	0/1/1/1
37	GTP	7	803	35	-	5/22/38/38	0/3/3/3
40	GDP	X	401	-	-	1/16/32/32	0/3/3/3
41	ATP	X	403	35	-	4/22/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	X	401	GDP	C2'-C3'	-10.92	1.23	1.53
40	X	401	GDP	C4-N3	6.61	1.49	1.34
40	X	401	GDP	O4'-C4'	-6.43	1.30	1.45
40	X	401	GDP	C2-N3	5.49	1.46	1.33
40	X	401	GDP	C1'-N9	-5.44	1.32	1.47
40	X	401	GDP	C3'-C4'	5.39	1.66	1.53
40	X	401	GDP	PA-O3A	5.35	1.65	1.59
40	X	401	GDP	C2-N2	4.82	1.45	1.34
40	X	401	GDP	O4'-C1'	3.95	1.51	1.42
40	X	401	GDP	O2'-C2'	3.05	1.50	1.43
40	X	401	GDP	C5-N7	-2.98	1.33	1.39
40	X	401	GDP	C2-N1	2.69	1.44	1.37
40	X	401	GDP	O6-C6	-2.62	1.18	1.23
40	X	401	GDP	C5-C6	2.46	1.53	1.44
40	X	401	GDP	C6-N1	2.34	1.43	1.38
40	X	401	GDP	C2'-C1'	2.29	1.60	1.53
37	7	803	GTP	C2-N3	2.12	1.38	1.33
41	X	403	ATP	PB-O3B	-2.10	1.57	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	X	401	GDP	C5-C4-N3	-5.30	119.95	128.39
37	7	803	GTP	C5-C4-N3	-5.09	120.30	128.39
40	X	401	GDP	C2-N3-C4	4.58	120.19	112.30
37	7	803	GTP	C2-N3-C4	4.51	120.07	112.30
37	7	803	GTP	N9-C4-N3	3.33	132.62	125.95
40	X	401	GDP	C2-N1-C6	-3.18	119.34	125.11
40	X	401	GDP	N9-C4-N3	3.15	132.25	125.95
37	7	803	GTP	C2-N1-C6	-2.92	119.82	125.11
40	X	401	GDP	N9-C8-N7	-2.90	108.01	113.40
40	X	401	GDP	C5-C6-N1	2.73	120.21	113.25
37	7	803	GTP	N9-C8-N7	-2.56	108.65	113.40
40	X	401	GDP	O6-C6-C5	-2.53	119.85	126.53
37	7	803	GTP	C8-N7-C5	2.49	108.70	104.26
37	7	803	GTP	C5-C6-N1	2.43	119.44	113.25
37	7	803	GTP	O6-C6-C5	-2.42	120.15	126.53
40	X	401	GDP	C8-N7-C5	2.15	108.08	104.26
37	7	803	GTP	C3'-C2'-C1'	2.11	105.46	101.46
40	X	401	GDP	C1'-N9-C4	-2.10	120.30	126.49
40	X	401	GDP	C3'-C2'-C1'	2.04	105.32	101.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

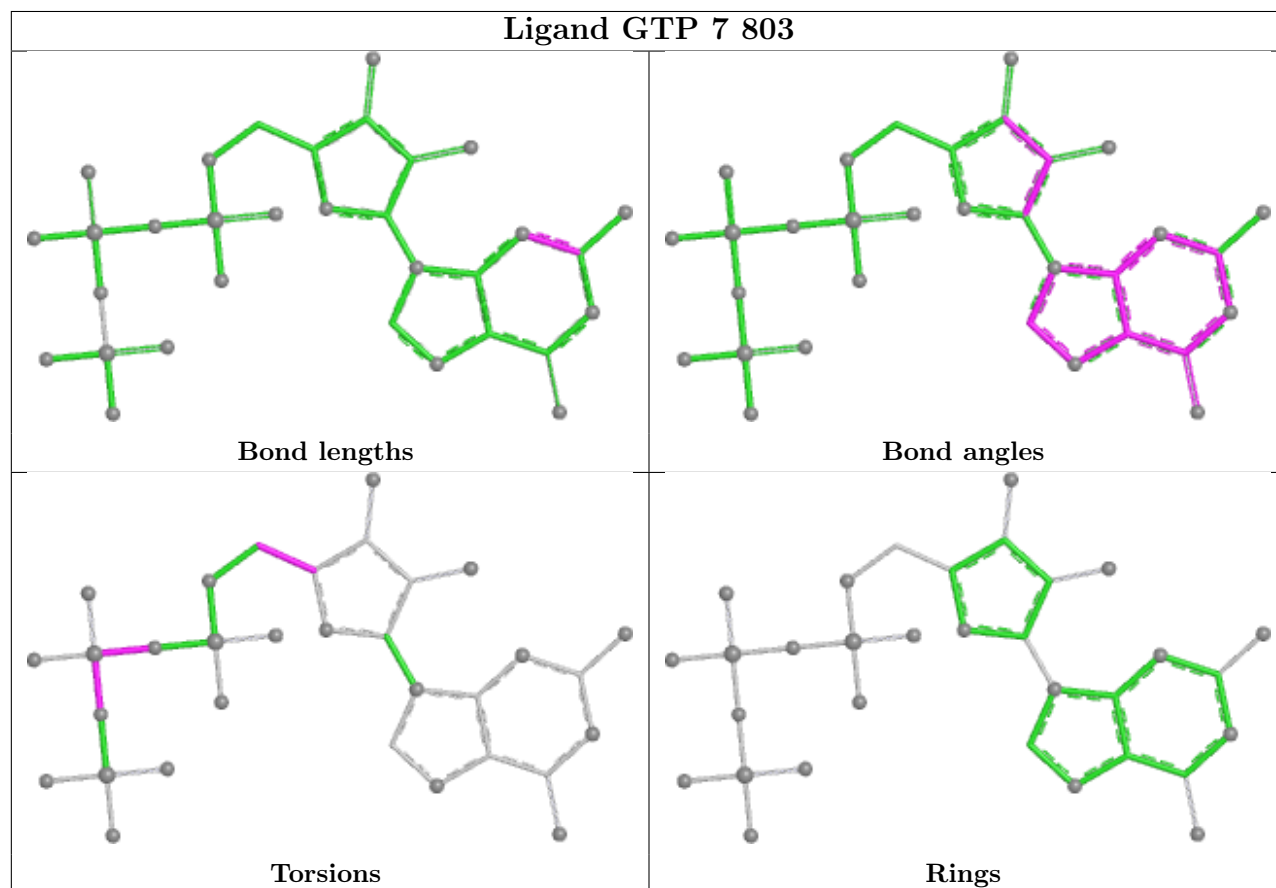
Mol	Chain	Res	Type	Atoms
37	7	803	GTP	PA-O3A-PB-O3B
41	X	403	ATP	PB-O3B-PG-O3G
37	7	803	GTP	PG-O3B-PB-O2B
41	X	403	ATP	PA-O3A-PB-O1B
40	X	401	GDP	C5'-O5'-PA-O1A
37	7	803	GTP	O4'-C4'-C5'-O5'
37	7	803	GTP	PA-O3A-PB-O2B
37	7	803	GTP	C3'-C4'-C5'-O5'
41	X	403	ATP	PG-O3B-PB-O2B
41	X	403	ATP	PA-O3A-PB-O2B

There are no ring outliers.

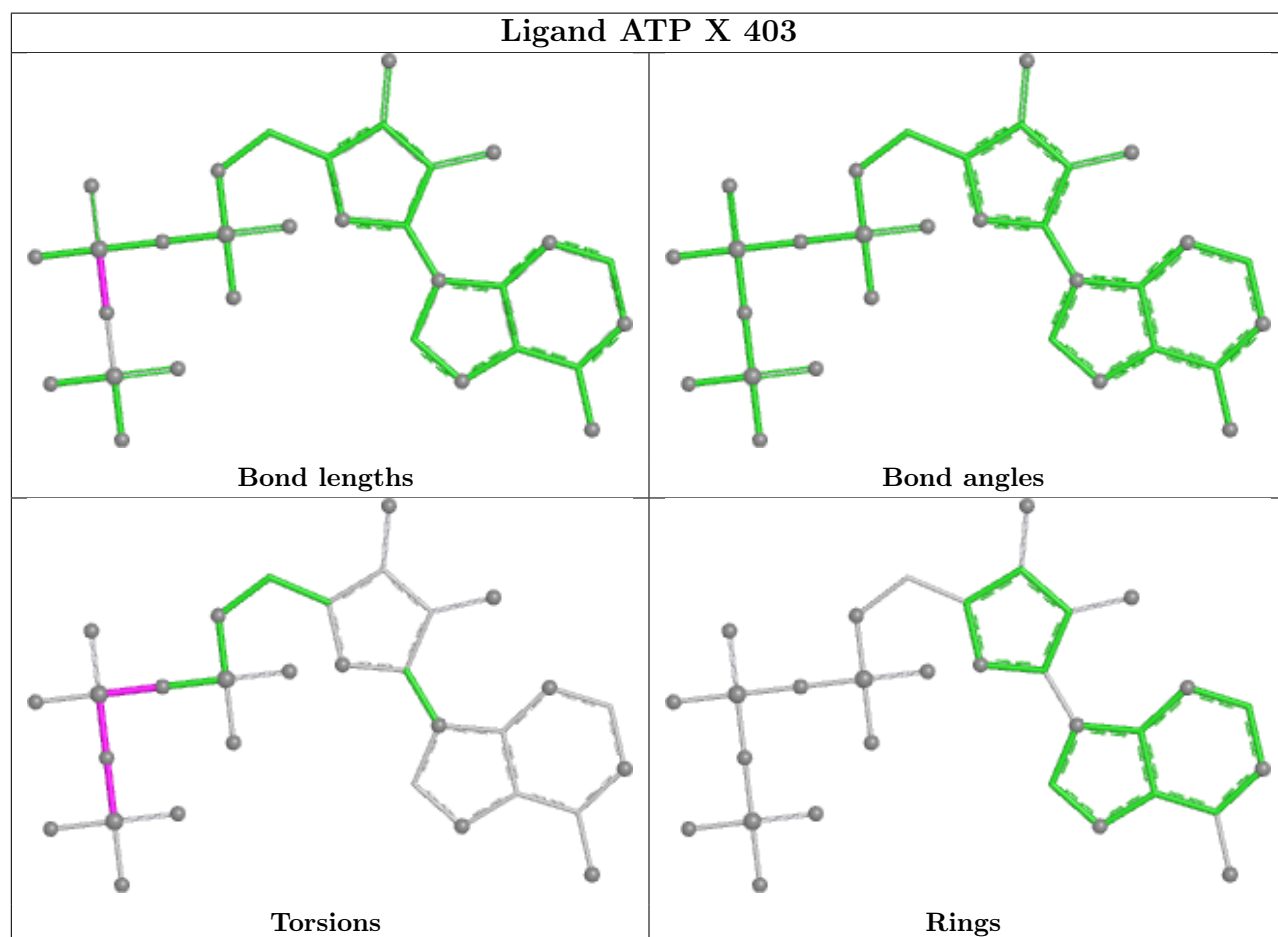
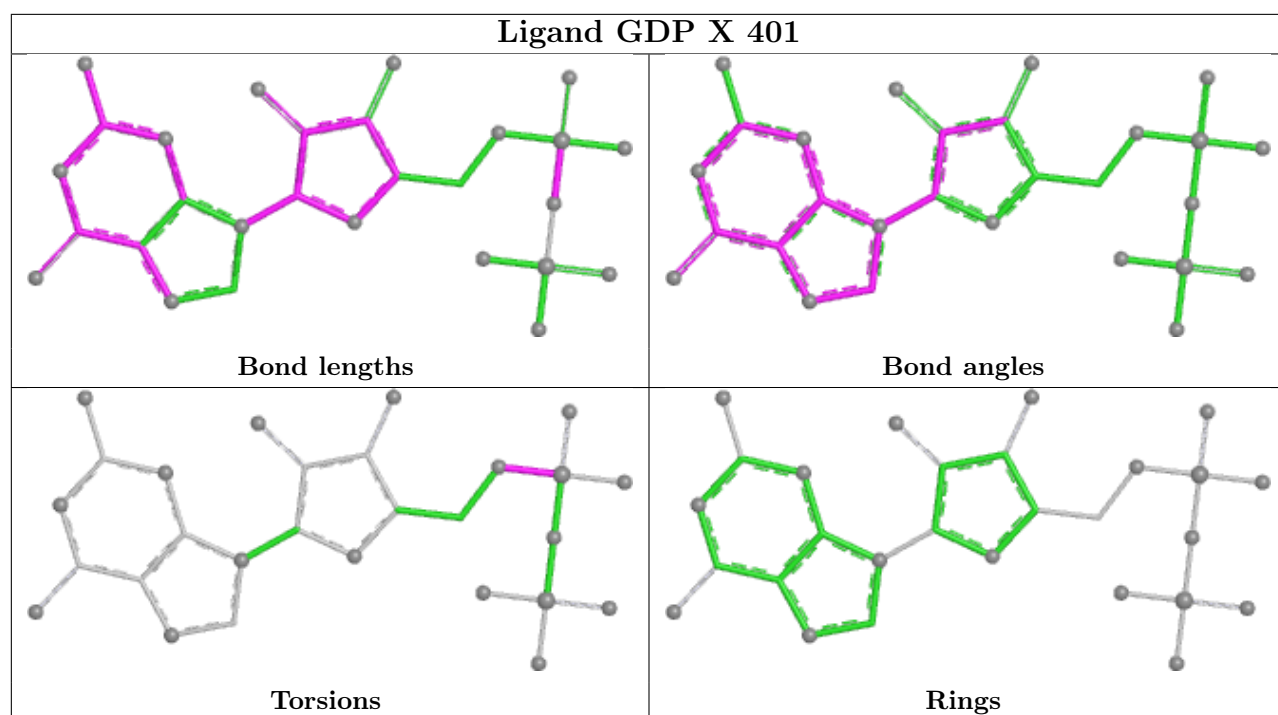
No monomer is involved in short contacts.

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.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

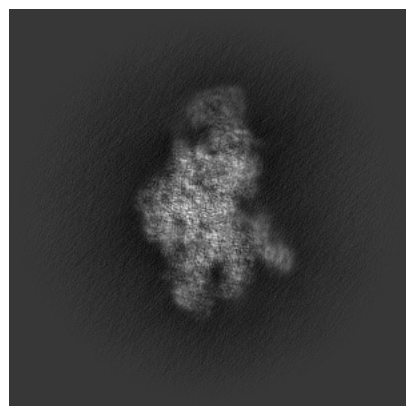
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70544. These allow visual inspection of the internal detail of the map and identification of artifacts.

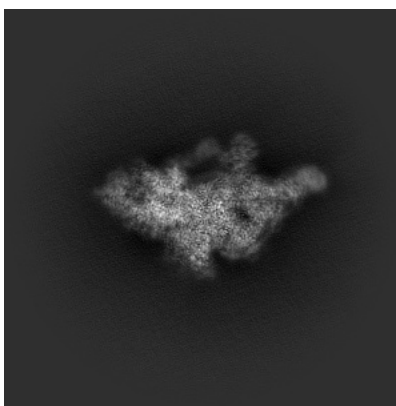
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

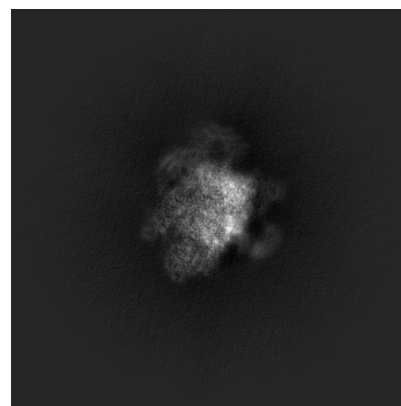
#### 6.1.1 Primary map



X

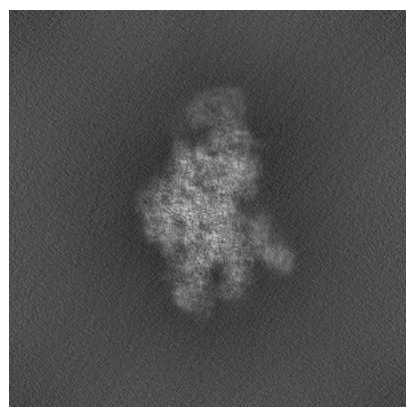


Y

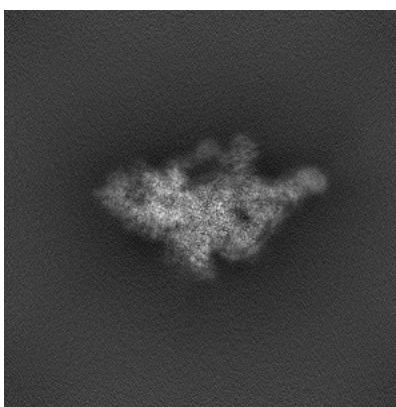


Z

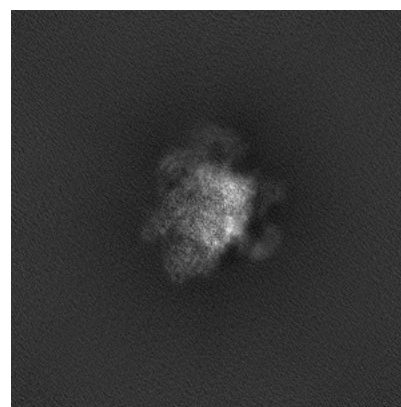
#### 6.1.2 Raw map



X



Y

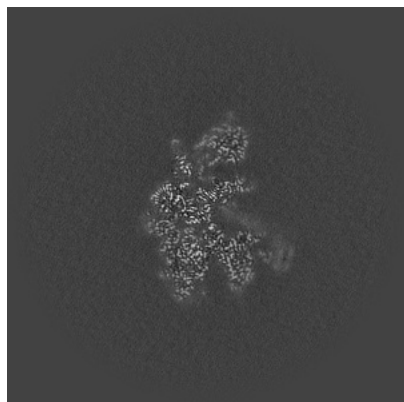


Z

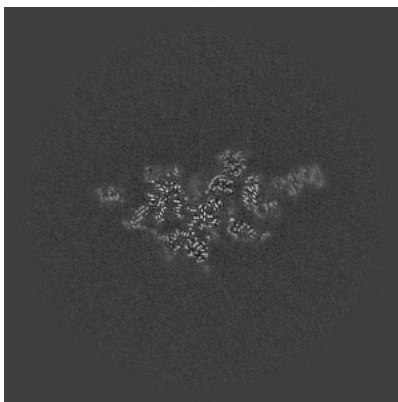
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

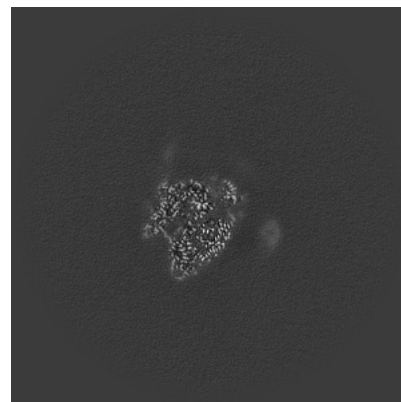
### 6.2.1 Primary map



X Index: 300

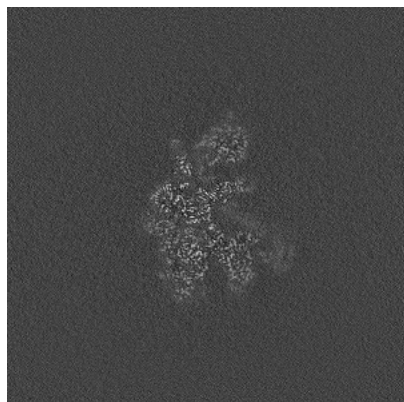


Y Index: 300

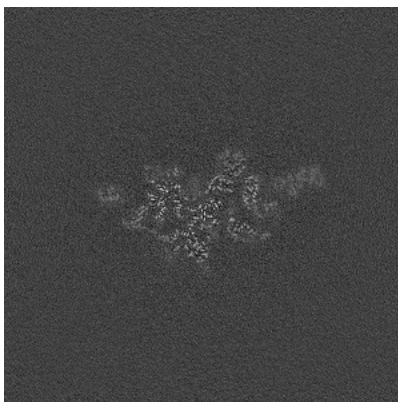


Z Index: 300

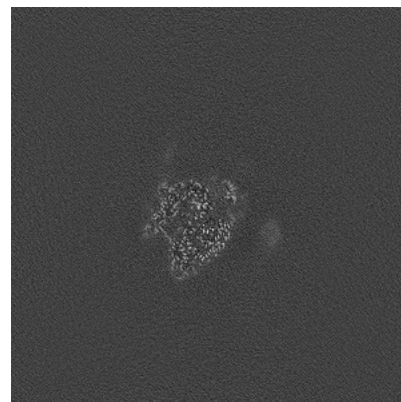
### 6.2.2 Raw map



X Index: 300



Y Index: 300

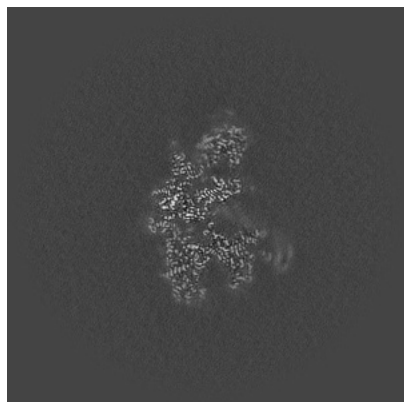


Z Index: 300

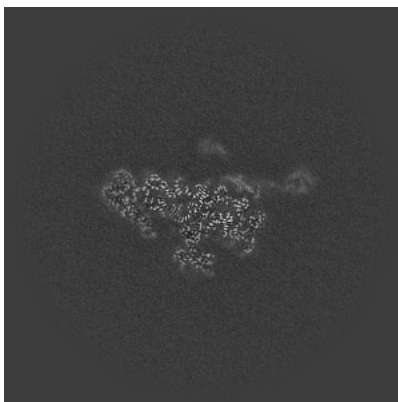
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

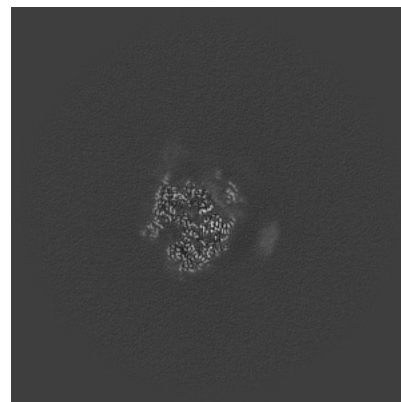
### 6.3.1 Primary map



X Index: 303

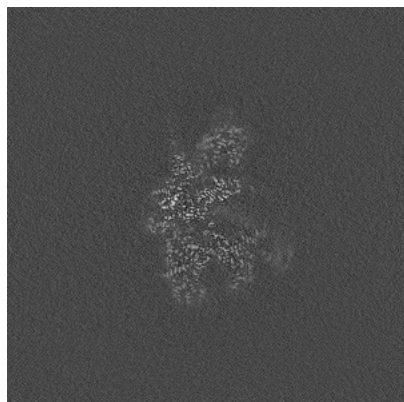


Y Index: 273

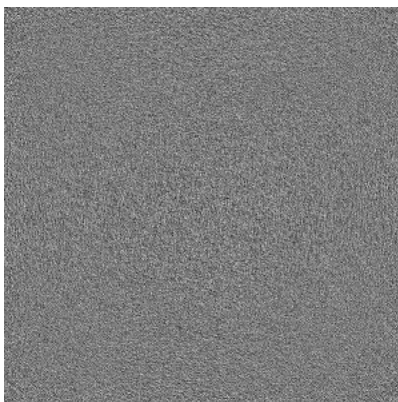


Z Index: 294

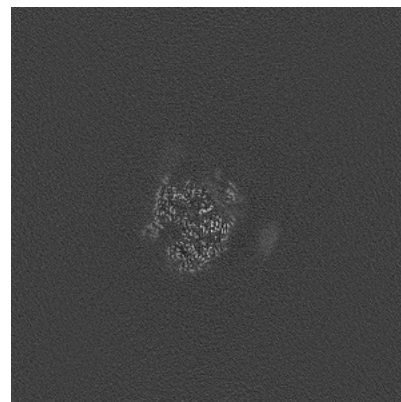
### 6.3.2 Raw map



X Index: 303



Y Index: 0



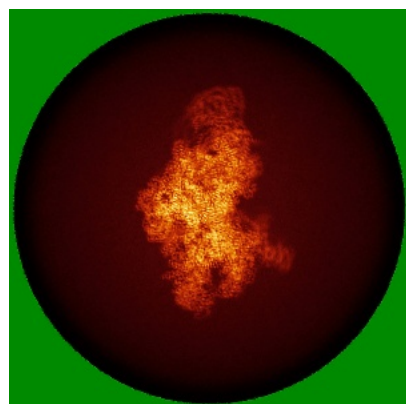
Z Index: 294

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

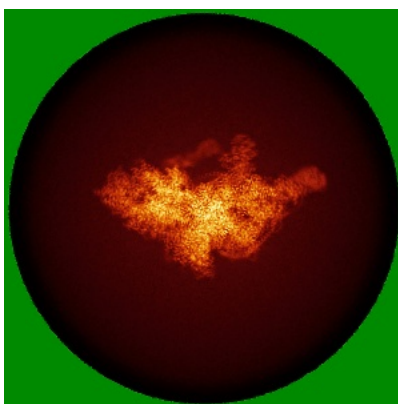


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

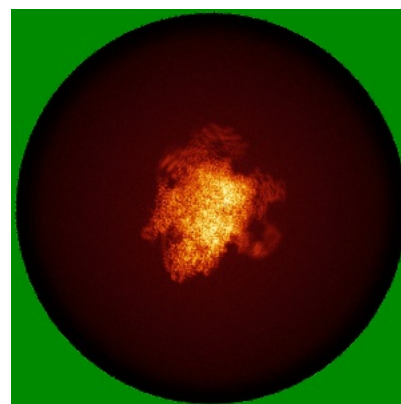
### 6.4.1 Primary map



X

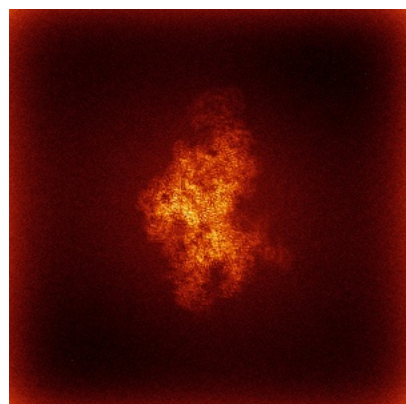


Y

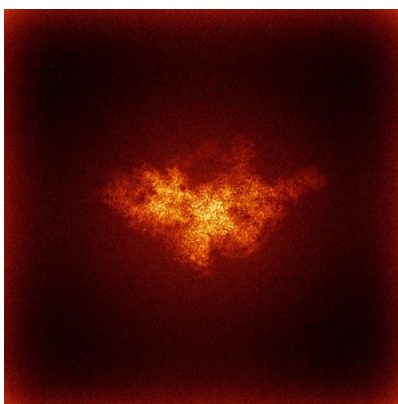


Z

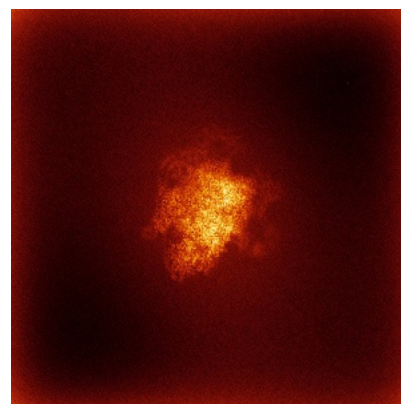
### 6.4.2 Raw map



X



Y



Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



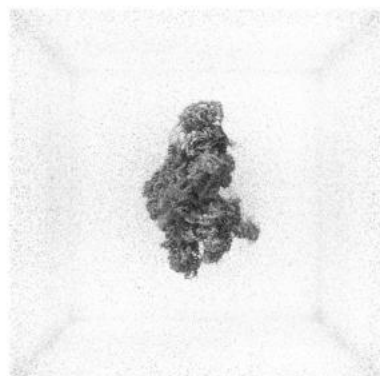
Y



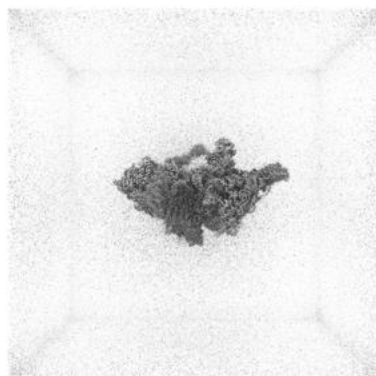
Z

The images above show the 3D surface view of the map at the recommended contour level 0.028. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

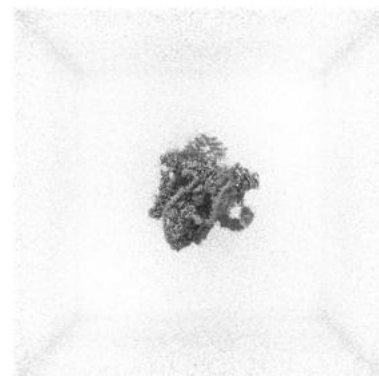
### 6.5.2 Raw map



X



Y



Z

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

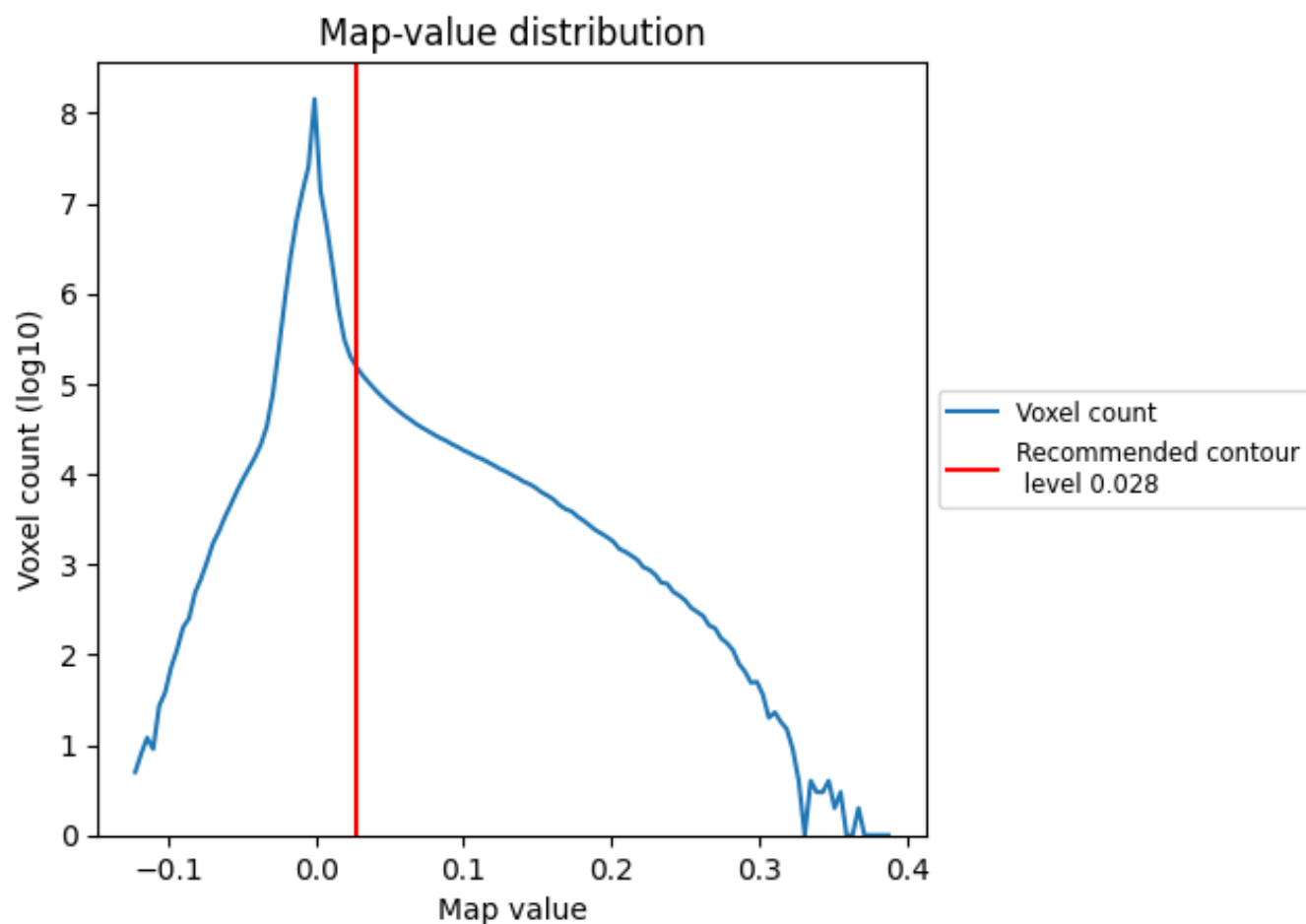
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

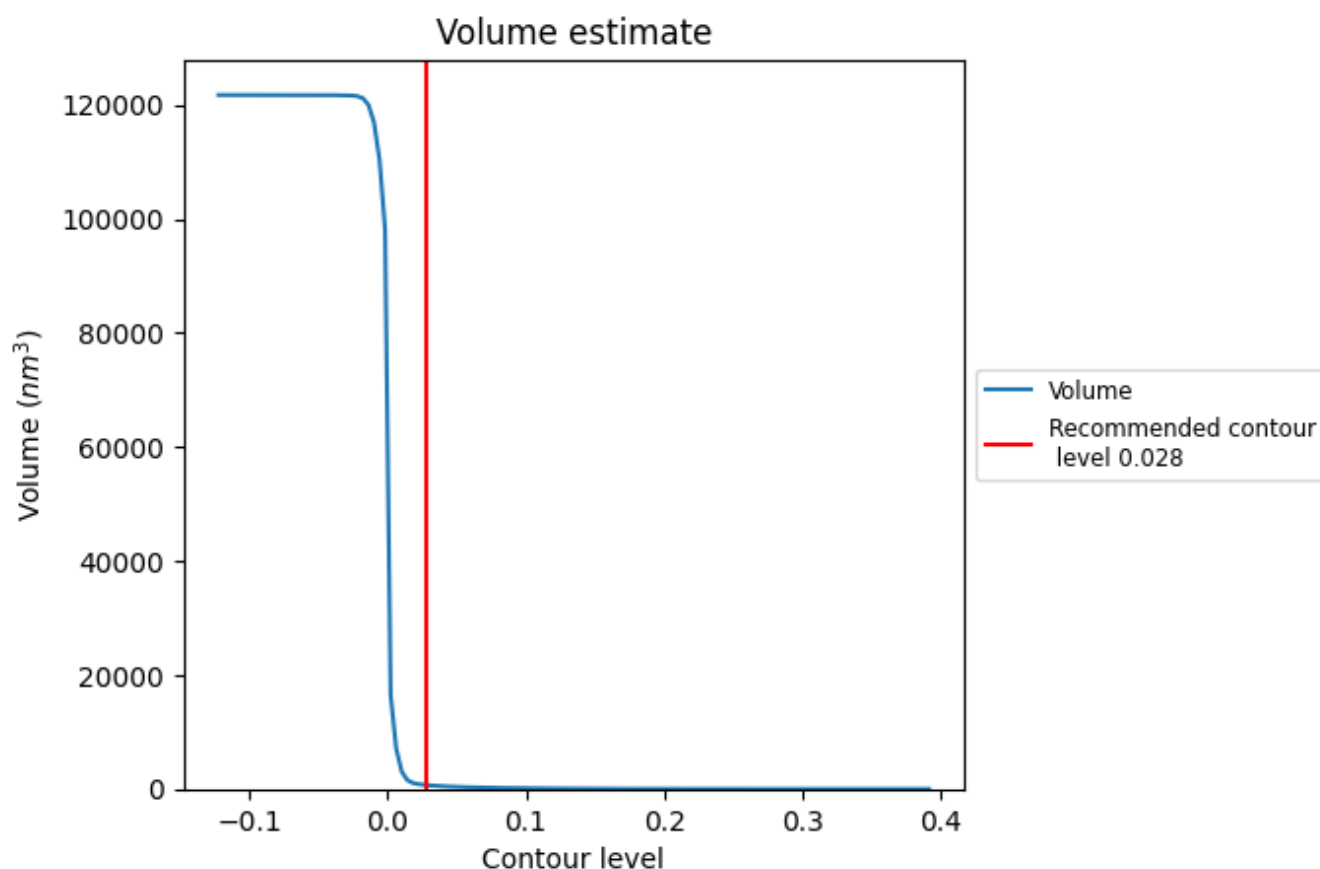
### 7.1 Map-value distribution [i](#)



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.



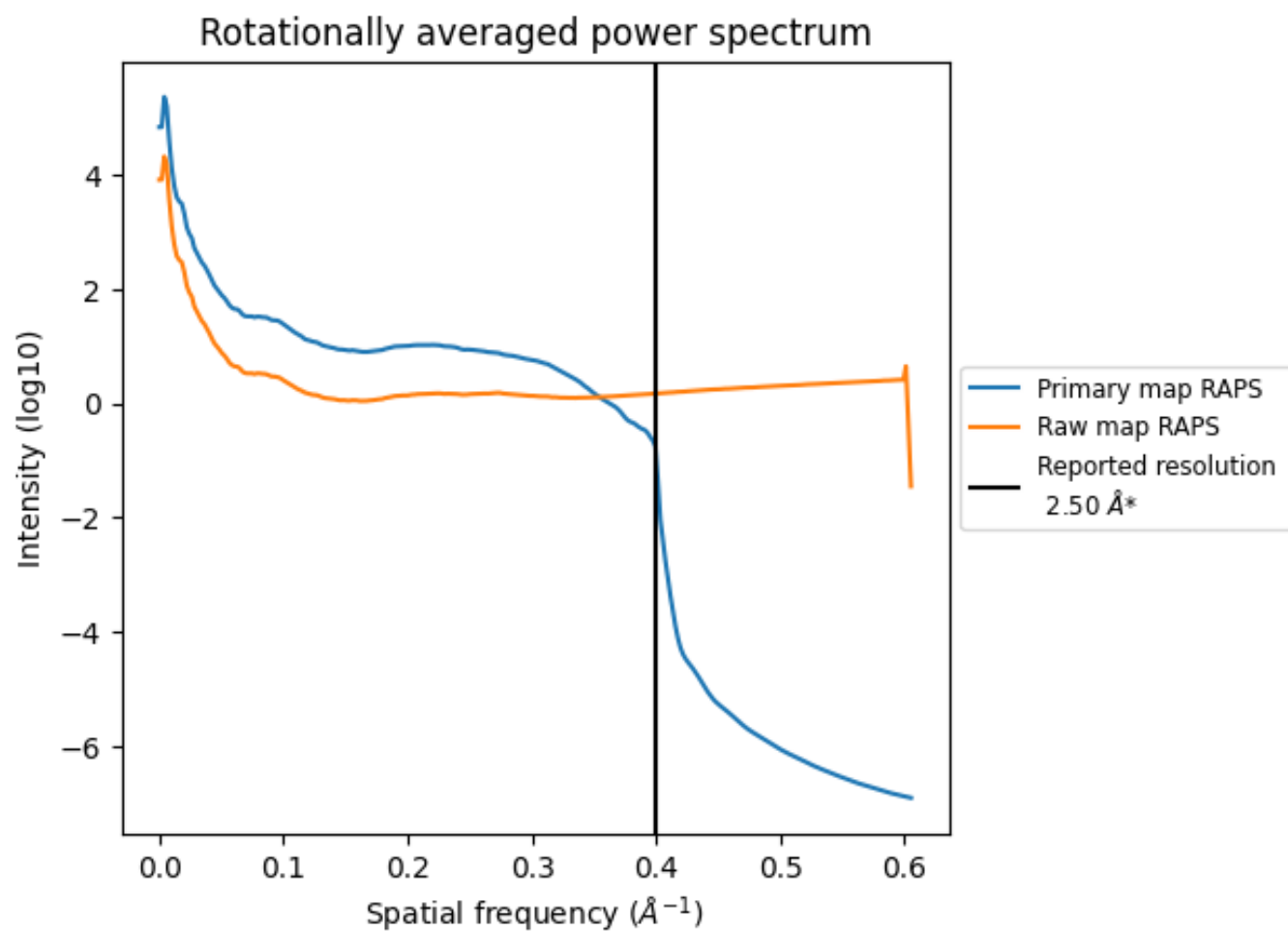
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 687  $\text{nm}^3$ ; this corresponds to an approximate mass of 621 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 ⓘ

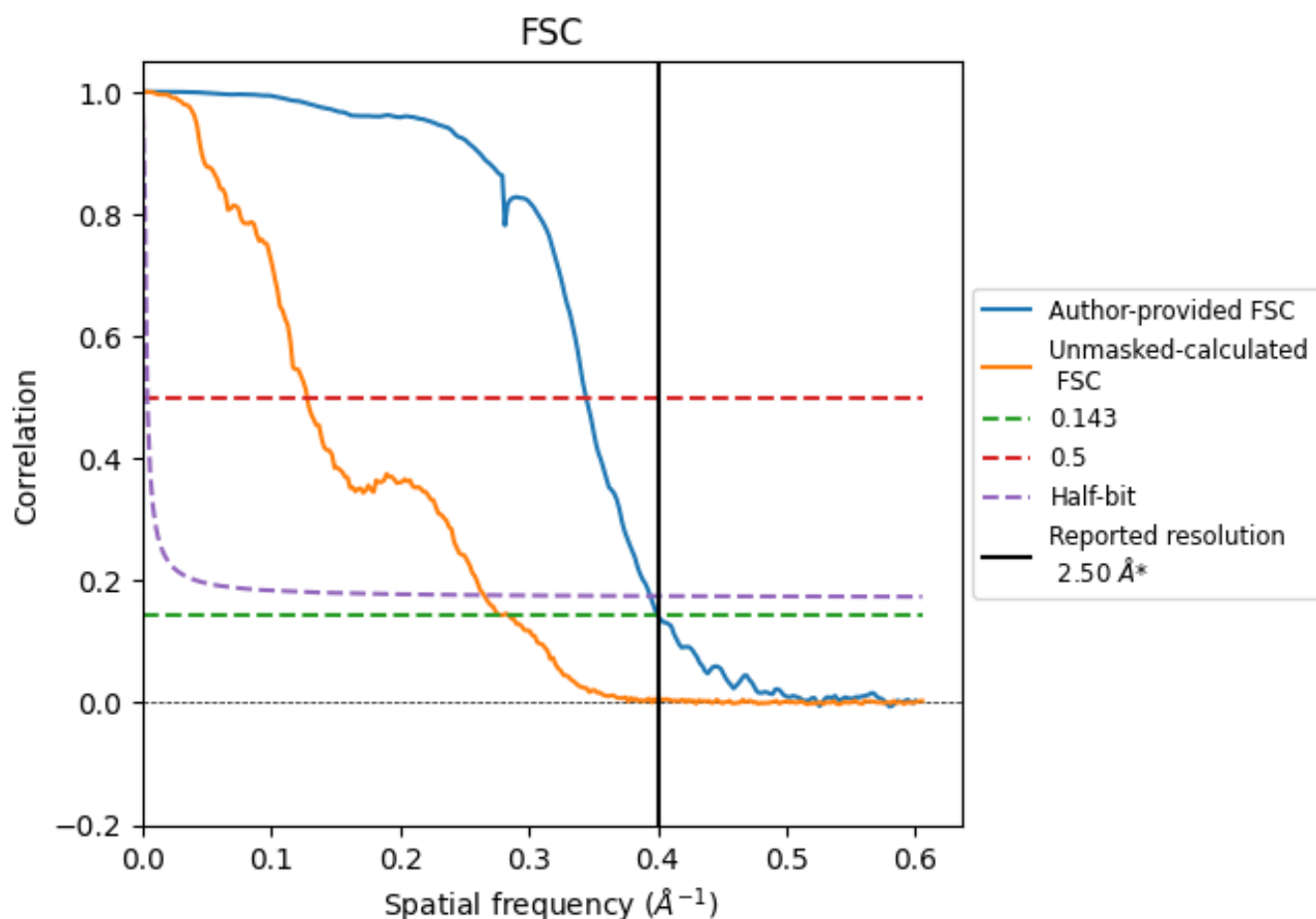


\*Reported resolution corresponds to spatial frequency of 0.400  $\text{\AA}^{-1}$

## 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 0.400  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

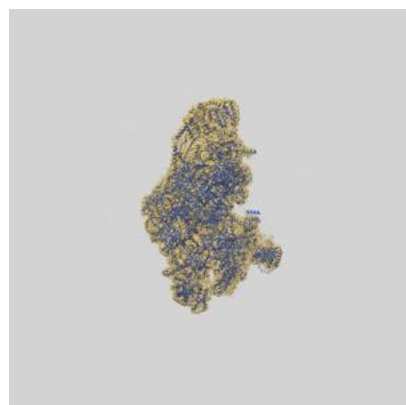
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.50	2.90	2.54
Unmasked-calculated*	3.59	7.81	3.77

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.59 differs from the reported value 2.5 by more than 10 %

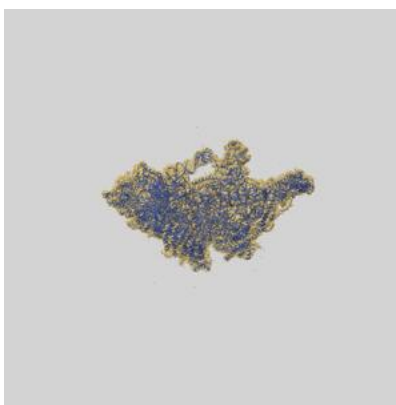
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70544 and PDB model 9OJM. Per-residue inclusion information can be found in section [3](#) on page [15](#).

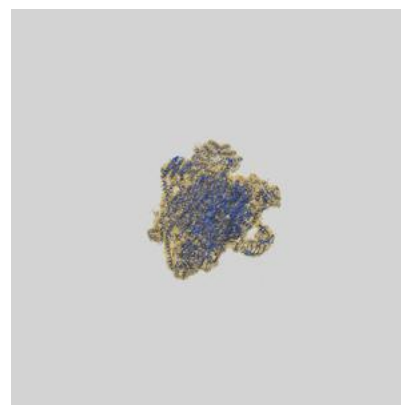
### 9.1 Map-model overlay [i](#)



X



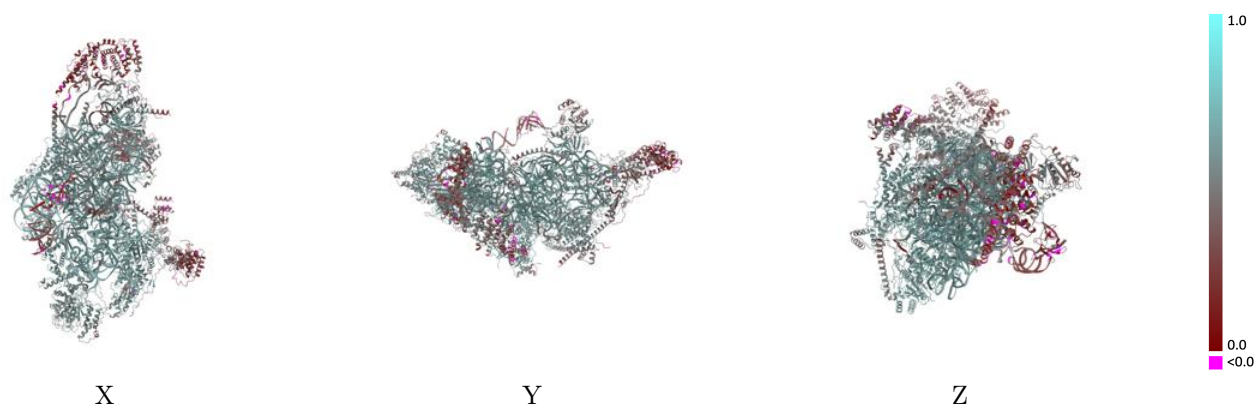
Y



Z

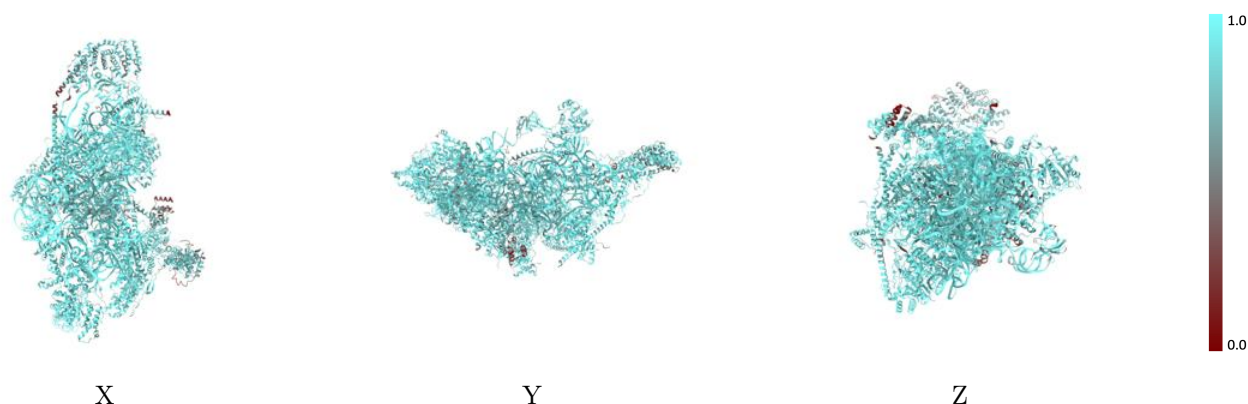
The images above show the 3D surface view of the map at the recommended contour level 0.028 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



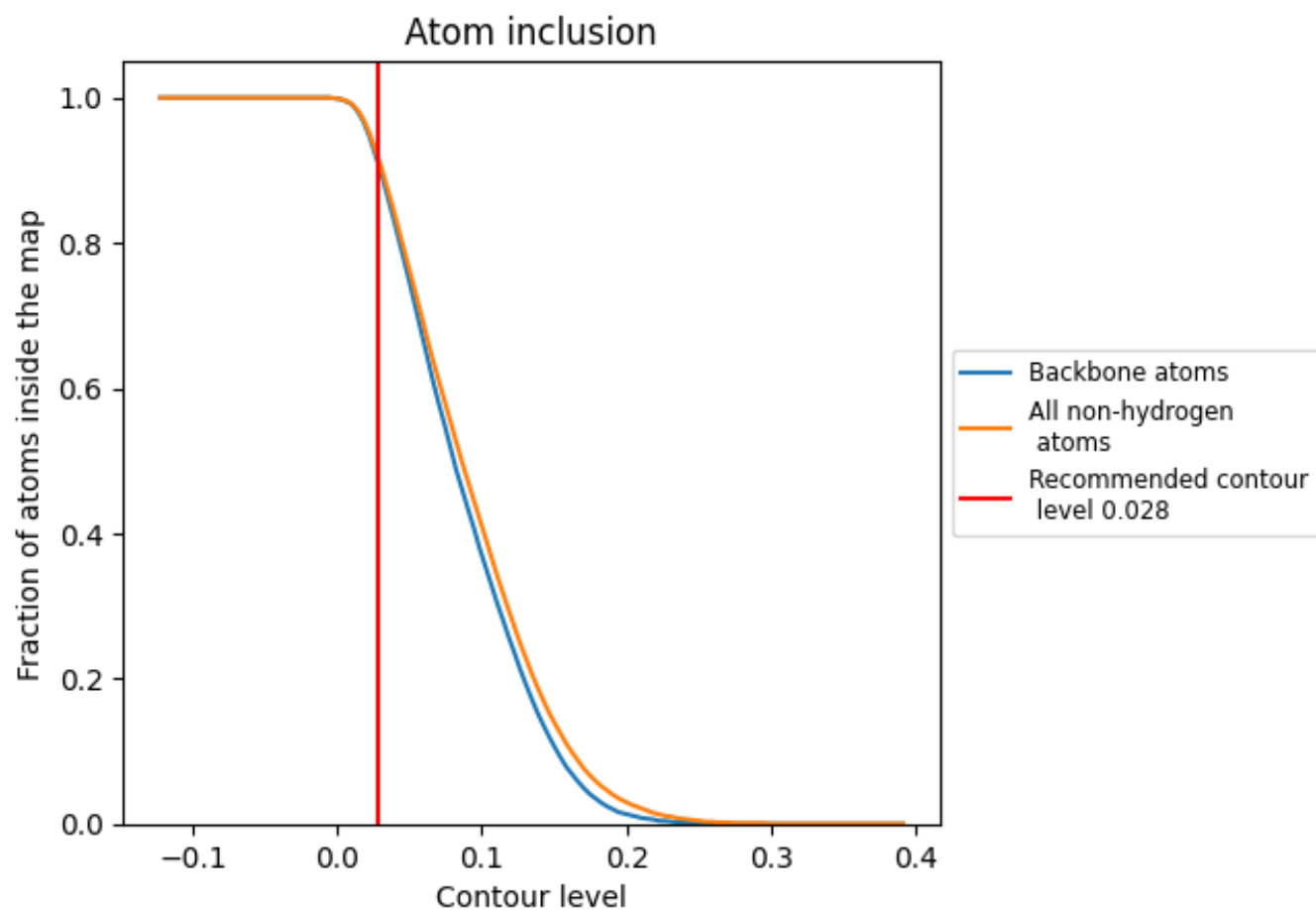
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.028).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 92% 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 (0.028) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9200	 0.5380
0	 0.8790	 0.4410
1	 0.9260	 0.5530
2	 0.9120	 0.5690
3	 0.9630	 0.6070
4	 0.7340	 0.3450
5	 0.9410	 0.3780
6	 0.9880	 0.5970
7	 0.8500	 0.4420
A	 0.9850	 0.6080
B	 0.9640	 0.6110
C	 0.9820	 0.6310
D	 0.9270	 0.5820
E	 0.9580	 0.6020
F	 0.9550	 0.5830
G	 0.9080	 0.5630
H	 0.9390	 0.5900
I	 0.9650	 0.6050
J	 0.9560	 0.6040
K	 0.9770	 0.6320
L	 0.9310	 0.5680
M	 0.9280	 0.5520
N	 0.9640	 0.6200
O	 0.9520	 0.5590
P	 0.9530	 0.6120
Q	 0.9760	 0.6310
R	 0.9240	 0.5240
S	 0.9390	 0.5600
T	 0.9420	 0.5870
U	 0.8970	 0.4960
V	 0.7370	 0.2380
W	 0.9530	 0.5990
X	 0.9420	 0.5500
Y	 0.7790	 0.4670
Z	 0.9320	 0.5740

