



# Full wwPDB EM Validation Report ⓘ

Dec 1, 2025 – 12:17 PM JST

PDB ID : 9JSR / pdb\_00009jsr  
EMDB ID : EMD-61781  
Title : 50S precursor - Erm complex (C-I)  
Authors : Sengupta, S.; Mukherjee, R.; Pilsl, M.; Bagale, S.; Adhikary, A.D.; Borkar, A.;  
Pradeepkumar, P.I.; Engel, C.; Chowdhury, A.; Kaushal, P.S.; Anand, R.  
Deposited on : 2024-10-01  
Resolution : 4.00 Å(reported)  
Based on initial model : 6GC7

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:

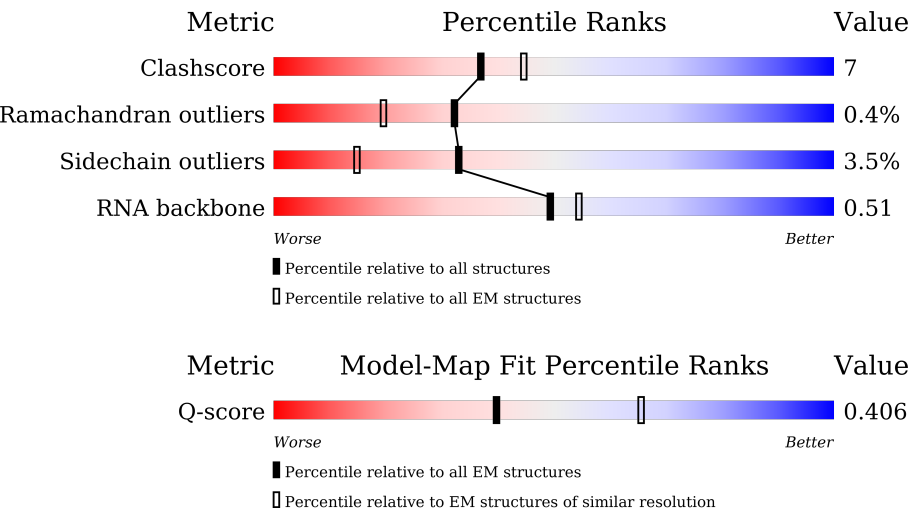
EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the 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) : 2.46

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	7587 ( 3.50 - 4.50 )

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	57	<div><div></div><div>84%</div><div>12%</div><div>.</div></div>
2	2	46	<div>7%</div> <div><div></div><div>76%</div><div>11%</div><div>13%</div></div>
3	A	2904	<div><div></div><div>39%</div><div>14%</div><div>.</div><div>45%</div></div>

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Mol	Chain	Length	Quality of chain
4	C	244	
5	D	209	
6	E	201	
7	J	142	
8	K	123	
9	L	144	
10	N	127	
11	P	115	
12	Q	118	
13	R	103	
14	S	110	
15	T	100	
16	U	104	
17	Y	63	
18	Z	59	

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 49589 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 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	40	Total	C	N	O	S	0	0
			322	193	79	49	1		

- Molecule 3 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	1597	Total	C	N	O	P	0	0
			34307	15307	6352	11051	1597		

- Molecule 4 is a protein called rRNA adenine N-6-methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	235	Total	C	N	O	S	0	0
			1966	1272	339	349	6		

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	178	Total	C	N	O	S	0	0
			1335	841	240	250	4		

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	195	Total	C	N	O	S	0	0
			1508	949	272	282	5		

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	141	Total	C	N	O	S	0	0
			1121	708	211	198	4		

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	120	Total	C	N	O	S	0	0
			923	579	178	160	6		

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	L	103	Total	C	N	O	0	0
			737	458	142	137		

- Molecule 10 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 11 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	113	Total	C	N	O	S	0	0
			912	571	178	162	1		

- Molecule 12 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 13 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 14 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	104	Total	C	N	O	S	0	0
			812	506	153	150	3		

- Molecule 15 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	T	92	Total	C	N	O	S	0	0
			730	461	138	130	1		

- Molecule 16 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	U	102	Total	C	N	O		0	0
			779	492	146	141			

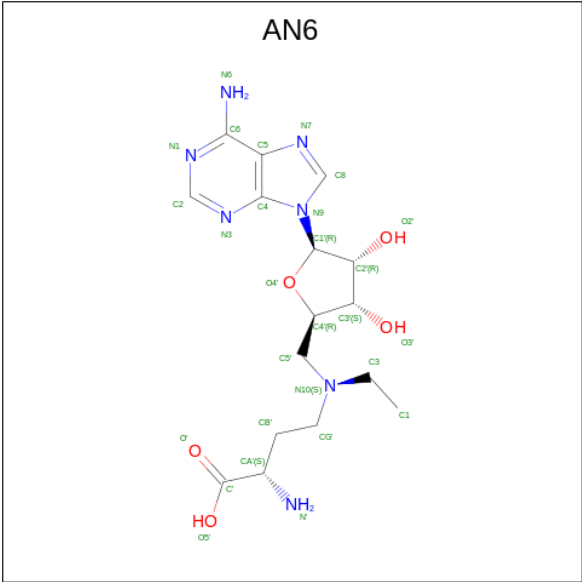
- Molecule 17 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	62	Total	C	N	O	S	0	0
			503	310	98	93	2		

- Molecule 18 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 19 is 5'-{[(3S)-3-amino-3-carboxypropyl](ethyl)amino}-5'-deoxyadenosine (CCD ID: AN6) (formula: C<sub>16</sub>H<sub>25</sub>N<sub>7</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).

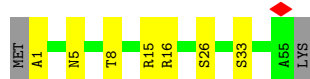
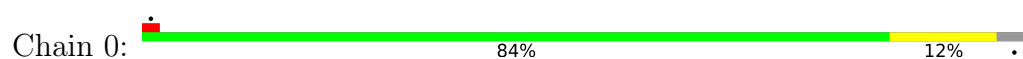


Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	N	O	0
			28	16	7	5	

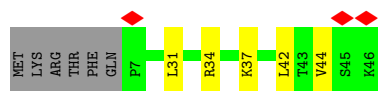
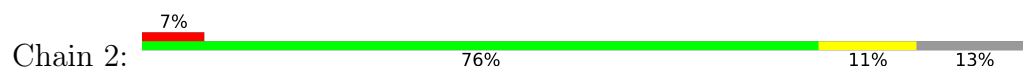
### 3 Residue-property plots

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.

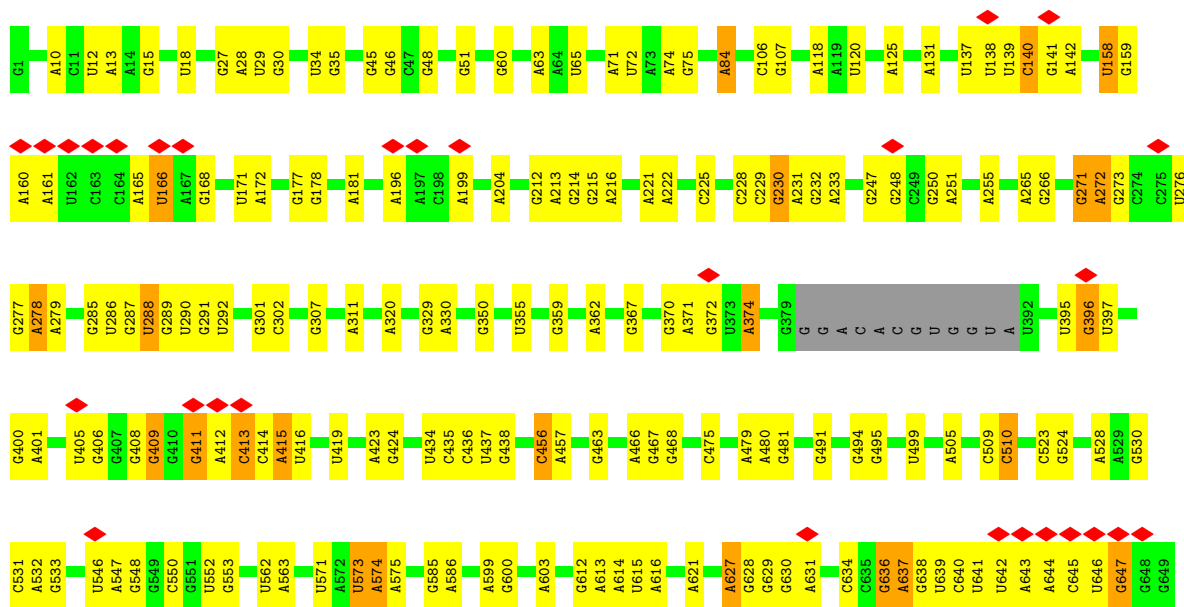
#### • Molecule 1: 50S ribosomal protein L32



#### • Molecule 2: 50S ribosomal protein L34

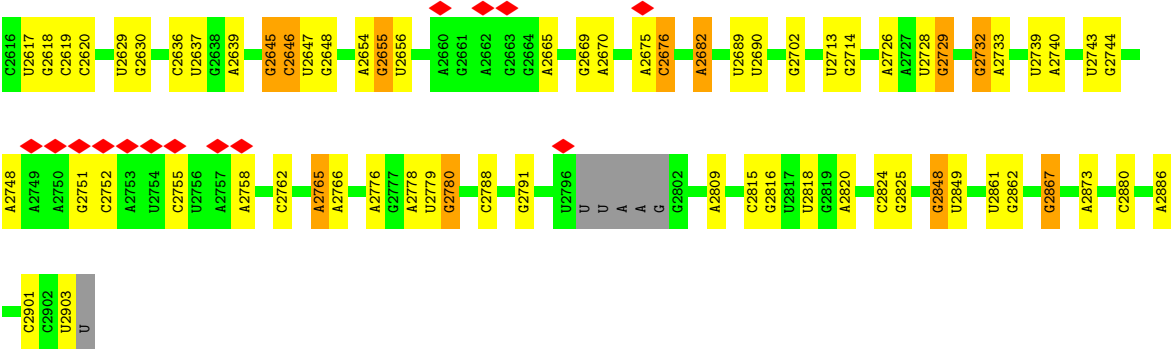
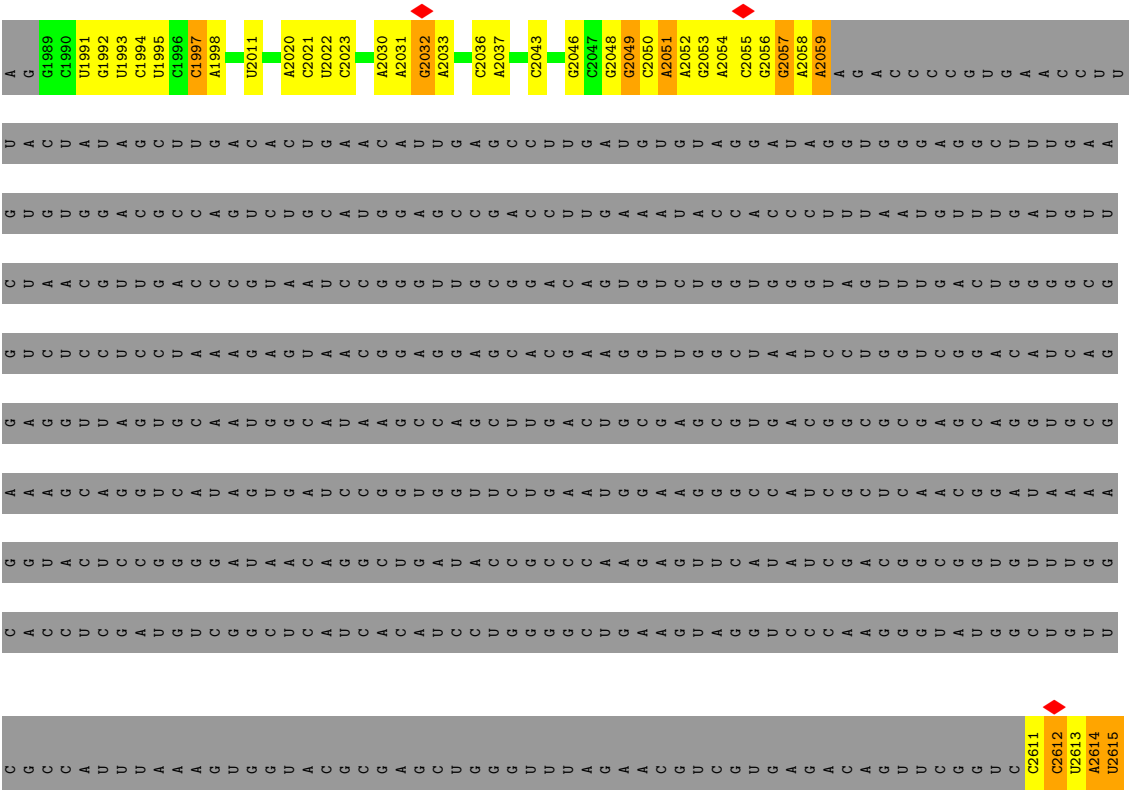


#### • Molecule 3: 23S Ribosomal RNA

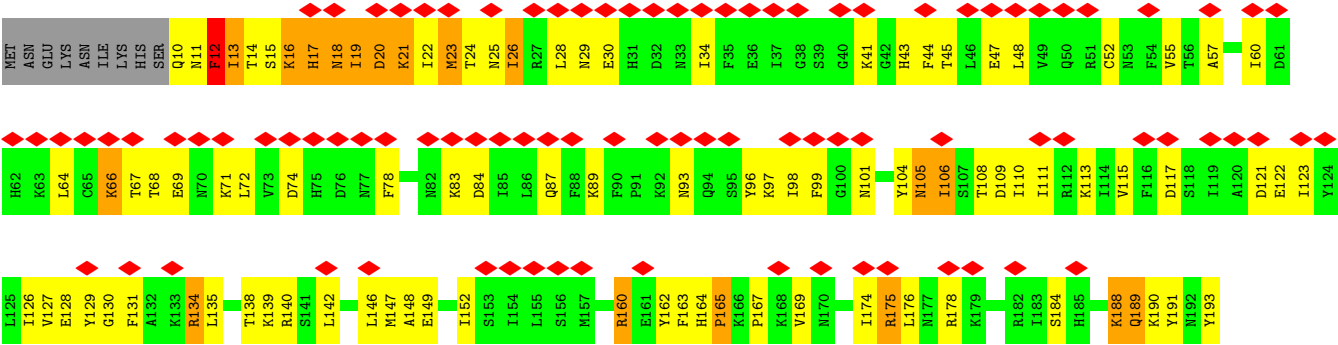




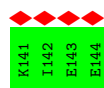




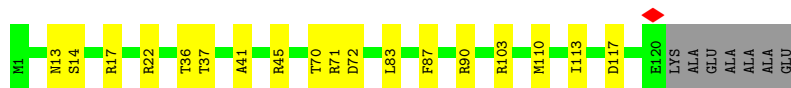
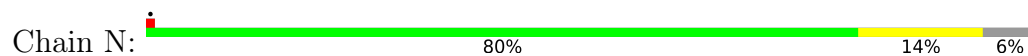
● Molecule 4: rRNA adenine N-6-methyltransferase



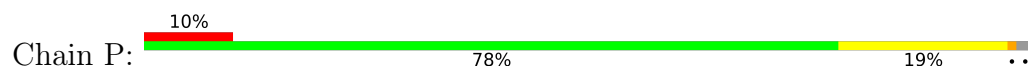




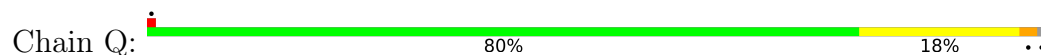
- Molecule 10: 50S ribosomal protein L17



- Molecule 11: 50S ribosomal protein L19



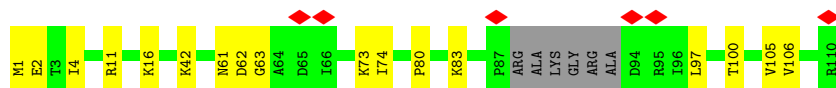
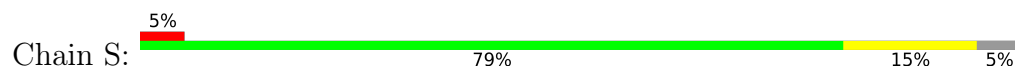
- Molecule 12: 50S ribosomal protein L20



- Molecule 13: 50S ribosomal protein L21




- Molecule 14: 50S ribosomal protein L22

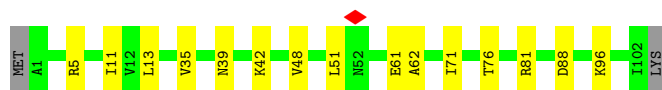


- Molecule 15: 50S ribosomal protein L23




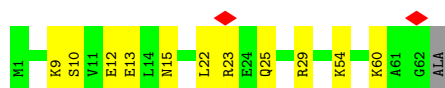
- Molecule 16: 50S ribosomal protein L24

Chain U:  84% 14% .




- Molecule 17: 50S ribosomal protein L29

Chain Y:  81% 17% .



- Molecule 18: 50S ribosomal protein L30

Chain Z:  86% 10% . .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	6081	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 ( $e^-/\text{\AA}^2$ )	41.25	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.122	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0158	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AN6

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	0.20	0/440	0.65	0/588
2	2	0.20	0/324	0.50	0/424
3	A	0.18	0/38423	0.33	1/59917 (0.0%)
4	C	0.48	0/2008	1.02	14/2697 (0.5%)
5	D	0.23	0/1350	0.41	0/1814
6	E	0.17	0/1526	0.41	0/2053
7	J	0.19	0/1143	0.50	0/1537
8	K	0.34	1/931 (0.1%)	0.67	0/1245
9	L	0.18	0/737	0.52	0/980
10	N	0.21	0/973	0.55	0/1301
11	P	0.24	0/923	0.60	1/1232 (0.1%)
12	Q	0.18	0/960	0.48	2/1278 (0.2%)
13	R	0.18	0/829	0.49	0/1107
14	S	0.20	0/818	0.50	0/1095
15	T	0.33	0/736	0.68	1/984 (0.1%)
16	U	0.17	0/787	0.47	1/1051 (0.1%)
17	Y	0.29	0/504	0.72	1/670 (0.1%)
18	Z	0.21	0/453	0.59	1/605 (0.2%)
All	All	0.21	1/53865 (0.0%)	0.42	22/80578 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	C	0	1
6	E	0	1
8	K	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	93	GLN	C-N	5.35	1.40	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	17	HIS	CA-CB-CG	-15.89	97.91	113.80
4	C	105	ASN	CB-CA-C	10.60	127.39	111.17
4	C	26	ILE	N-CA-C	-9.87	94.89	108.12
4	C	21	LYS	N-CA-C	9.53	123.95	111.75
4	C	18	ASN	N-CA-C	-9.10	102.10	113.02
4	C	26	ILE	CB-CA-C	8.78	120.92	111.35
4	C	17	HIS	CB-CA-C	7.46	122.54	110.09
12	Q	91	ARG	N-CA-C	6.61	120.61	112.54
18	Z	5	LYS	CB-CG-CD	6.24	125.65	111.30
4	C	165	PRO	N-CA-C	-6.11	99.89	112.47
4	C	129	TYR	CA-CB-CG	5.86	124.45	113.90
17	Y	9	LYS	CA-CB-CG	5.71	125.52	114.10
16	U	51	LEU	CA-CB-CG	5.43	135.30	116.30
4	C	21	LYS	CB-CA-C	-5.43	99.93	110.46
4	C	105	ASN	N-CA-CB	-5.36	103.04	110.65
4	C	189	GLN	CA-CB-CG	5.23	124.55	114.10
4	C	20	ASP	CB-CA-C	5.22	120.81	110.42
11	P	28	LYS	CB-CG-CD	5.21	123.29	111.30
15	T	52	GLU	CA-CB-CG	5.20	124.49	114.10
12	Q	90	ASP	CB-CA-C	-5.18	100.71	110.51
4	C	12	PHE	N-CA-CB	5.03	118.99	110.49
3	A	271	G	P-O3'-C3'	5.02	127.73	120.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	C	160	ARG	Sidechain
6	E	61	ARG	Sidechain
8	K	49	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

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	434	0	448	8	0
2	2	322	0	357	3	0
3	A	34307	0	17269	186	0
4	C	1966	0	2001	248	0
5	D	1335	0	1390	14	0
6	E	1508	0	1571	12	0
7	J	1121	0	1150	8	0
8	K	923	0	1000	24	0
9	L	737	0	796	13	0
10	N	960	0	1000	20	0
11	P	912	0	959	37	0
12	Q	947	0	1022	28	0
13	R	816	0	839	4	0
14	S	812	0	869	12	0
15	T	730	0	795	35	0
16	U	779	0	834	6	0
17	Y	503	0	538	25	0
18	Z	449	0	491	4	0
19	A	28	0	23	2	0
All	All	49589	0	33352	600	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 7.

All (600) 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)
4:C:164:HIS:CD2	4:C:165:PRO:HD3	1.39	1.55
9:L:107:PHE:CE1	9:L:126:ARG:NH2	1.78	1.44
4:C:13:ILE:HD11	4:C:164:HIS:CG	1.50	1.43
3:A:2645:G:C6	4:C:209:LYS:HE3	1.57	1.39
3:A:1252:G:O6	12:Q:35:PHE:CE2	1.77	1.37
4:C:138:THR:HG22	4:C:229:PHE:CE1	1.59	1.37
4:C:97:LYS:CD	4:C:122:GLU:HB3	1.57	1.35
4:C:57:ALA:CB	4:C:78:PHE:HZ	1.39	1.35
3:A:1252:G:O6	12:Q:35:PHE:CD2	1.79	1.34
4:C:55:VAL:HB	4:C:78:PHE:CD1	1.61	1.34
4:C:164:HIS:CG	4:C:165:PRO:HD3	1.66	1.30
4:C:13:ILE:HG12	4:C:164:HIS:ND1	1.46	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:97:LYS:HD2	4:C:122:GLU:CB	1.62	1.29
4:C:13:ILE:CG1	4:C:164:HIS:ND1	1.96	1.26
4:C:26:ILE:HD13	4:C:99:PHE:CE2	1.71	1.25
4:C:41:LYS:NZ	4:C:64:LEU:HD21	1.50	1.25
4:C:138:THR:CG2	4:C:229:PHE:CE1	2.20	1.25
9:L:107:PHE:HE1	9:L:126:ARG:NH2	1.21	1.21
15:T:12:ARG:CZ	17:Y:29:ARG:NH2	2.03	1.21
4:C:57:ALA:CB	4:C:78:PHE:CZ	2.25	1.20
11:P:61:ARG:NH1	11:P:100:ARG:HA	1.55	1.18
3:A:2645:G:O6	4:C:209:LYS:HE3	1.43	1.18
4:C:131:PHE:CZ	4:C:135:LEU:HD11	1.79	1.18
4:C:41:LYS:HD2	4:C:67:THR:HG21	1.20	1.17
4:C:122:GLU:OE2	4:C:175:ARG:CZ	1.93	1.17
4:C:26:ILE:CD1	4:C:99:PHE:HE2	1.57	1.16
4:C:138:THR:CG2	4:C:229:PHE:HE1	1.55	1.16
4:C:13:ILE:CD1	4:C:164:HIS:ND1	2.08	1.16
11:P:61:ARG:HH12	11:P:100:ARG:CA	1.58	1.16
3:A:2645:G:N1	4:C:209:LYS:HE3	1.63	1.13
4:C:101:ASN:HD22	4:C:126:ILE:CG2	1.60	1.13
4:C:55:VAL:CB	4:C:78:PHE:HD1	1.61	1.13
15:T:12:ARG:NH1	17:Y:29:ARG:HH12	1.46	1.12
4:C:164:HIS:CD2	4:C:165:PRO:CD	2.33	1.12
15:T:12:ARG:CZ	17:Y:29:ARG:HH22	1.59	1.11
4:C:131:PHE:CE2	4:C:135:LEU:HD11	1.85	1.11
4:C:18:ASN:HB2	4:C:162:TYR:CE1	1.86	1.10
4:C:57:ALA:HB2	4:C:78:PHE:CZ	1.84	1.10
4:C:14:THR:HG23	4:C:15:SER:H	1.13	1.09
4:C:41:LYS:NZ	4:C:64:LEU:CD2	2.14	1.09
15:T:12:ARG:NH1	17:Y:29:ARG:NH1	1.98	1.09
4:C:57:ALA:HB3	4:C:78:PHE:HZ	1.10	1.09
4:C:106:ILE:O	4:C:106:ILE:HD12	1.50	1.09
15:T:12:ARG:NH1	17:Y:29:ARG:HH22	1.49	1.08
15:T:12:ARG:NH1	17:Y:29:ARG:NH2	2.00	1.08
4:C:13:ILE:CD1	4:C:164:HIS:CG	2.37	1.07
4:C:23:MET:HE1	4:C:44:PHE:CD2	1.89	1.06
4:C:106:ILE:CD1	4:C:110:ILE:HD11	1.85	1.06
8:K:105:ARG:NH2	11:P:31:VAL:CG2	2.18	1.05
4:C:106:ILE:HD12	4:C:110:ILE:HD11	1.35	1.05
4:C:26:ILE:CD1	4:C:99:PHE:CE2	2.37	1.03
4:C:13:ILE:HD11	4:C:164:HIS:CB	1.88	1.03
4:C:13:ILE:HD11	4:C:164:HIS:ND1	1.71	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:55:VAL:HB	4:C:78:PHE:HD1	0.86	1.01
15:T:12:ARG:NH1	17:Y:29:ARG:CZ	2.25	0.99
4:C:57:ALA:HB3	4:C:78:PHE:CZ	1.92	0.99
15:T:12:ARG:HH12	17:Y:29:ARG:NH1	1.62	0.96
4:C:122:GLU:CD	4:C:175:ARG:CZ	2.38	0.96
3:A:1252:G:C6	12:Q:35:PHE:CD2	2.52	0.96
4:C:97:LYS:NZ	4:C:122:GLU:HB2	1.81	0.96
4:C:26:ILE:HD13	4:C:99:PHE:HE2	0.79	0.95
4:C:14:THR:CG2	4:C:15:SER:H	1.79	0.95
8:K:35:VAL:HG21	8:K:69:VAL:HG21	1.48	0.95
12:Q:57:ARG:HH21	12:Q:91:ARG:NH1	1.62	0.95
4:C:48:LEU:O	4:C:52:CYS:SG	2.24	0.95
4:C:14:THR:HG23	4:C:15:SER:N	1.75	0.94
4:C:17:HIS:NE2	4:C:20:ASP:OD2	1.98	0.94
4:C:23:MET:CE	4:C:44:PHE:CD2	2.50	0.94
4:C:101:ASN:ND2	4:C:126:ILE:CG2	2.30	0.94
4:C:138:THR:HG22	4:C:229:PHE:HE1	0.77	0.93
4:C:147:MET:HG2	4:C:229:PHE:CE2	2.03	0.93
4:C:41:LYS:HZ1	4:C:64:LEU:HD21	1.15	0.93
3:A:290:U:H3	3:A:350:G:H1	1.05	0.93
6:E:76:PRO:HG3	6:E:84:THR:HG22	1.50	0.92
3:A:2645:G:O6	4:C:209:LYS:CE	2.17	0.92
4:C:41:LYS:HZ2	4:C:64:LEU:CD2	1.81	0.92
4:C:18:ASN:HB3	4:C:162:TYR:CD1	2.03	0.92
4:C:121:ASP:HA	4:C:178:ARG:HG2	1.50	0.92
8:K:105:ARG:NH2	11:P:31:VAL:HG22	1.85	0.92
4:C:18:ASN:CB	4:C:162:TYR:CE1	2.53	0.92
4:C:164:HIS:CG	4:C:165:PRO:CD	2.51	0.91
4:C:41:LYS:HZ2	4:C:64:LEU:HD21	1.30	0.91
4:C:55:VAL:CB	4:C:78:PHE:CD1	2.43	0.91
3:A:1631:G:H21	3:A:1635:A:H62	1.17	0.91
1:O:1:ALA:CB	3:A:2613:U:O2'	2.19	0.91
4:C:18:ASN:CB	4:C:162:TYR:CD1	2.54	0.91
8:K:105:ARG:NH2	11:P:31:VAL:HG21	1.82	0.90
4:C:131:PHE:CE2	4:C:135:LEU:CD1	2.54	0.90
3:A:2645:G:C6	4:C:209:LYS:CE	2.53	0.89
4:C:18:ASN:HB2	4:C:162:TYR:HE1	1.31	0.89
4:C:160:ARG:HB2	4:C:167:PRO:HG2	1.56	0.88
3:A:1252:G:O6	12:Q:35:PHE:HE2	1.51	0.88
4:C:101:ASN:HD22	4:C:126:ILE:HG21	1.38	0.88
3:A:1252:G:O6	12:Q:35:PHE:HD2	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:41:LYS:HZ1	4:C:64:LEU:CD2	1.80	0.87
8:K:35:VAL:HG21	8:K:69:VAL:CG2	2.05	0.87
4:C:106:ILE:HD12	4:C:110:ILE:CD1	2.04	0.86
4:C:41:LYS:CD	4:C:67:THR:HG21	2.03	0.86
4:C:13:ILE:CD1	4:C:164:HIS:HB3	2.06	0.86
4:C:101:ASN:ND2	4:C:126:ILE:HG21	1.91	0.85
4:C:23:MET:HE1	4:C:44:PHE:HD2	1.39	0.85
4:C:121:ASP:HA	4:C:178:ARG:CG	2.06	0.85
4:C:97:LYS:HD2	4:C:122:GLU:HB3	0.85	0.84
11:P:87:ARG:HG2	11:P:88:ARG:H	1.42	0.84
9:L:107:PHE:CD1	9:L:126:ARG:NH2	2.44	0.83
11:P:61:ARG:HH12	11:P:100:ARG:HA	0.71	0.83
4:C:57:ALA:HB2	4:C:78:PHE:HZ	1.19	0.83
1:O:1:ALA:HB1	3:A:2613:U:O2'	1.79	0.83
3:A:2051:A:N7	3:A:2614:A:N6	2.27	0.82
4:C:34:ILE:HG21	4:C:48:LEU:HD11	1.61	0.82
3:A:2645:G:N1	4:C:209:LYS:CE	2.43	0.82
4:C:122:GLU:OE2	4:C:175:ARG:NH2	2.12	0.82
4:C:193:TYR:CE2	4:C:239:TYR:OH	2.32	0.82
4:C:97:LYS:CD	4:C:122:GLU:CB	2.39	0.82
4:C:97:LYS:HZ2	4:C:122:GLU:HB2	1.42	0.81
4:C:109:ASP:O	4:C:113:LYS:HG2	1.80	0.81
4:C:101:ASN:HD22	4:C:126:ILE:HG22	1.44	0.81
4:C:106:ILE:O	4:C:106:ILE:CD1	2.29	0.81
8:K:21:CYS:SG	8:K:39:ILE:HD12	2.20	0.81
15:T:12:ARG:NE	17:Y:29:ARG:HH22	1.78	0.81
11:P:25:VAL:HG12	11:P:46:VAL:HG23	1.64	0.80
4:C:101:ASN:ND2	4:C:126:ILE:HG22	1.98	0.79
3:A:2645:G:H1	4:C:209:LYS:HE3	1.44	0.78
4:C:13:ILE:HG13	4:C:164:HIS:H	1.49	0.78
11:P:87:ARG:NH2	11:P:109:ILE:HD11	1.99	0.78
3:A:1631:G:N2	3:A:1635:A:H62	1.80	0.78
4:C:23:MET:HE1	4:C:44:PHE:CE2	2.19	0.78
4:C:122:GLU:CD	4:C:175:ARG:NH1	2.42	0.77
4:C:122:GLU:CD	4:C:175:ARG:NH2	2.42	0.77
3:A:2645:G:H1	4:C:209:LYS:CD	1.98	0.77
15:T:12:ARG:NE	17:Y:29:ARG:NH2	2.33	0.77
4:C:122:GLU:HG3	4:C:175:ARG:HH22	1.49	0.77
4:C:72:LEU:HD12	4:C:72:LEU:O	1.86	0.76
4:C:68:THR:O	4:C:72:LEU:HG	1.85	0.75
3:A:1631:G:H21	3:A:1635:A:N6	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:61:ARG:HD2	11:P:70:GLU:OE2	1.87	0.75
12:Q:61:ILE:HD11	12:Q:91:ARG:HD3	1.69	0.75
4:C:12:PHE:HB3	4:C:43:HIS:HE1	1.52	0.74
10:N:87:PHE:CD1	10:N:90:ARG:NH1	2.55	0.74
15:T:12:ARG:CD	17:Y:29:ARG:HH22	1.99	0.74
11:P:25:VAL:CG1	11:P:46:VAL:HG23	2.18	0.73
4:C:122:GLU:HG3	4:C:175:ARG:NH2	2.03	0.73
15:T:12:ARG:HH12	17:Y:29:ARG:HH12	1.14	0.73
4:C:193:TYR:HE2	4:C:239:TYR:OH	1.70	0.73
4:C:97:LYS:HD2	4:C:122:GLU:CG	2.18	0.73
15:T:20:ALA:O	15:T:24:MET:HG2	1.89	0.73
11:P:87:ARG:HG2	11:P:88:ARG:N	2.04	0.72
4:C:55:VAL:HG12	4:C:78:PHE:CE1	2.24	0.72
4:C:12:PHE:HB3	4:C:43:HIS:CE1	2.24	0.72
4:C:23:MET:CE	4:C:44:PHE:CE2	2.73	0.72
5:D:12:THR:HG23	11:P:8:GLU:OE1	1.89	0.72
10:N:14:SER:HB2	10:N:17:ARG:HH21	1.54	0.72
11:P:105:LYS:HA	11:P:108:ARG:HH12	1.54	0.72
15:T:12:ARG:HD2	17:Y:29:ARG:HH22	1.56	0.71
3:A:2055:C:H42	3:A:2612:C:H42	1.35	0.71
4:C:184:SER:O	4:C:188:LYS:HG3	1.89	0.71
4:C:147:MET:CG	4:C:229:PHE:CE2	2.72	0.71
12:Q:57:ARG:NH2	12:Q:91:ARG:NH1	2.39	0.71
4:C:21:LYS:O	4:C:21:LYS:HG3	1.90	0.70
8:K:105:ARG:HH21	11:P:31:VAL:HG21	1.54	0.70
11:P:61:ARG:CD	11:P:70:GLU:OE2	2.39	0.70
11:P:105:LYS:HA	11:P:108:ARG:NH1	2.06	0.70
3:A:2645:G:H1	4:C:209:LYS:CE	2.00	0.70
4:C:13:ILE:HD11	4:C:164:HIS:HB3	1.63	0.70
1:O:1:ALA:HB2	3:A:2613:U:O2'	1.89	0.70
4:C:57:ALA:HB2	4:C:78:PHE:CE1	2.26	0.70
11:P:87:ARG:HH21	11:P:109:ILE:HD11	1.55	0.70
4:C:19:ILE:HG12	4:C:162:TYR:OH	1.92	0.70
3:A:630:G:H1'	3:A:640:C:H4'	1.74	0.69
4:C:138:THR:HG23	4:C:229:PHE:CE1	2.23	0.69
10:N:14:SER:HA	10:N:17:ARG:HE	1.57	0.69
4:C:83:LYS:HZ3	4:C:87:GLN:CB	2.06	0.69
15:T:64:LYS:HA	15:T:79:ASP:OD1	1.93	0.69
4:C:13:ILE:HG12	4:C:164:HIS:CE1	2.26	0.69
4:C:17:HIS:CD2	4:C:20:ASP:OD2	2.45	0.69
4:C:26:ILE:HD11	4:C:99:PHE:CE2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:105:ARG:HH21	11:P:31:VAL:CG2	2.07	0.68
4:C:26:ILE:HG22	4:C:28:LEU:HG	1.74	0.68
3:A:1252:G:C6	12:Q:35:PHE:HD2	2.05	0.67
4:C:55:VAL:HG12	4:C:78:PHE:HE1	1.58	0.67
14:S:62:ASP:CG	14:S:63:GLY:H	2.02	0.67
3:A:2056:G:H22	3:A:2611:C:H2'	1.60	0.67
4:C:60:ILE:HG22	4:C:83:LYS:O	1.93	0.67
3:A:2645:G:H1	4:C:209:LYS:HG3	1.59	0.67
4:C:109:ASP:O	4:C:113:LYS:CG	2.42	0.67
15:T:12:ARG:HH11	17:Y:29:ARG:HH22	1.42	0.66
3:A:1282:U:H3	3:A:1286:A:H62	1.41	0.66
4:C:13:ILE:O	4:C:43:HIS:CD2	2.49	0.66
4:C:55:VAL:C	4:C:78:PHE:CD1	2.74	0.65
3:A:374:A:H61	3:A:400:G:H2'	1.61	0.65
4:C:19:ILE:O	4:C:22:ILE:N	2.28	0.65
4:C:18:ASN:HB2	4:C:162:TYR:CD1	2.25	0.65
4:C:68:THR:HG22	4:C:72:LEU:CD2	2.27	0.65
4:C:55:VAL:O	4:C:78:PHE:CD1	2.50	0.64
4:C:83:LYS:HZ1	4:C:87:GLN:C	2.04	0.64
11:P:25:VAL:HG11	11:P:46:VAL:CG2	2.27	0.64
3:A:2645:G:H1	4:C:209:LYS:CG	2.10	0.64
15:T:65:GLY:N	15:T:79:ASP:OD1	2.30	0.64
4:C:13:ILE:O	4:C:43:HIS:CG	2.51	0.64
4:C:15:SER:O	4:C:17:HIS:N	2.29	0.64
4:C:164:HIS:NE2	4:C:165:PRO:HD3	2.05	0.64
3:A:2682:A:C2	5:D:23:PRO:HB3	2.33	0.64
3:A:955:U:H3	3:A:962:G:H1	1.46	0.63
10:N:14:SER:CA	10:N:17:ARG:HH21	2.11	0.63
15:T:44:LYS:HG3	15:T:55:VAL:HG11	1.81	0.63
3:A:2051:A:H2	3:A:2618:G:H1	1.45	0.63
4:C:23:MET:HE2	4:C:44:PHE:CD2	2.33	0.63
4:C:97:LYS:HD3	4:C:122:GLU:HB3	1.72	0.63
3:A:645:C:H2'	3:A:647:G:C8	2.34	0.62
4:C:97:LYS:NZ	4:C:122:GLU:CB	2.59	0.62
3:A:996:A:OP1	13:R:10:LYS:HD3	2.00	0.62
10:N:14:SER:CB	10:N:17:ARG:HH21	2.12	0.62
4:C:10:GLN:HA	4:C:165:PRO:HG2	1.81	0.62
4:C:122:GLU:CG	4:C:175:ARG:NH2	2.62	0.61
4:C:24:THR:HG23	4:C:25:ASN:N	2.15	0.61
10:N:87:PHE:CE1	10:N:90:ARG:NH1	2.68	0.61
4:C:13:ILE:CD1	4:C:164:HIS:CB	2.61	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:106:ILE:HD11	4:C:110:ILE:HD11	1.77	0.61
10:N:14:SER:HA	10:N:17:ARG:HH21	1.64	0.61
3:A:1031:G:H21	3:A:1125:G:H5''	1.65	0.61
4:C:83:LYS:HZ3	4:C:87:GLN:HB2	1.64	0.61
4:C:122:GLU:OE2	4:C:175:ARG:NE	2.32	0.61
4:C:83:LYS:NZ	4:C:87:GLN:C	2.59	0.61
4:C:127:VAL:HG11	4:C:131:PHE:CD2	2.36	0.61
4:C:127:VAL:HG21	4:C:131:PHE:HD2	1.66	0.61
11:P:87:ARG:HH21	11:P:109:ILE:CD1	2.14	0.61
11:P:87:ARG:NH2	11:P:109:ILE:CD1	2.64	0.60
4:C:131:PHE:CZ	4:C:135:LEU:CD1	2.72	0.60
8:K:35:VAL:CG2	8:K:69:VAL:CG2	2.78	0.60
9:L:107:PHE:HE1	9:L:126:ARG:CZ	2.06	0.60
3:A:2656:U:O2	3:A:2665:A:N7	2.34	0.60
12:Q:57:ARG:HH21	12:Q:91:ARG:CZ	2.12	0.60
4:C:11:ASN:HA	4:C:163:PHE:HB3	1.82	0.60
8:K:19:VAL:HG21	8:K:41:ILE:HD12	1.83	0.60
12:Q:36:GLN:HG3	12:Q:40:LYS:HE3	1.84	0.60
12:Q:57:ARG:NH2	12:Q:91:ARG:CZ	2.64	0.60
5:D:32:ASN:ND2	5:D:52:THR:OG1	2.34	0.60
4:C:55:VAL:CG1	4:C:78:PHE:CD1	2.84	0.59
11:P:25:VAL:CG1	11:P:46:VAL:CG2	2.80	0.59
4:C:147:MET:HG2	4:C:229:PHE:HE2	1.62	0.59
4:C:117:ASP:OD1	4:C:117:ASP:O	2.20	0.59
3:A:628:G:H4'	3:A:651:G:H4'	1.85	0.59
3:A:861:A:C8	3:A:916:G:N2	2.69	0.59
13:R:48:LYS:NZ	13:R:49:ILE:O	2.36	0.58
3:A:861:A:N6	3:A:916:G:O2'	2.36	0.58
8:K:105:ARG:HH22	11:P:31:VAL:CG2	2.14	0.58
4:C:55:VAL:CG1	4:C:78:PHE:CE1	2.86	0.58
4:C:127:VAL:HG11	4:C:131:PHE:CE2	2.37	0.58
19:A:3001:AN6:H2	4:C:104:TYR:OH	2.03	0.58
4:C:17:HIS:CE1	4:C:20:ASP:OD2	2.57	0.58
4:C:26:ILE:CG2	4:C:28:LEU:HG	2.33	0.58
4:C:135:LEU:HD22	4:C:146:LEU:HD22	1.85	0.58
3:A:1138:G:H21	7:J:108:MET:HE2	1.67	0.58
3:A:2743:U:OP2	3:A:2755:C:N4	2.36	0.58
4:C:152:ILE:HD12	4:C:176:LEU:HD22	1.85	0.57
3:A:1140:C:OP2	7:J:68:LYS:NZ	2.37	0.57
4:C:83:LYS:NZ	4:C:87:GLN:CB	2.68	0.57
4:C:105:ASN:O	4:C:106:ILE:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:12:ARG:HD2	17:Y:29:ARG:NH2	2.19	0.57
3:A:954:G:N2	3:A:963:U:O2	2.37	0.57
3:A:463:G:N2	3:A:466:A:OP2	2.38	0.57
3:A:957:C:H2'	3:A:959:A:C8	2.39	0.57
3:A:1031:G:N2	3:A:1125:G:OP2	2.38	0.57
4:C:13:ILE:CG1	4:C:164:HIS:CG	2.81	0.57
11:P:87:ARG:CG	11:P:88:ARG:H	2.13	0.57
3:A:954:G:H1	3:A:963:U:H3	1.53	0.57
4:C:14:THR:O	4:C:19:ILE:HD11	2.05	0.57
5:D:18:ASP:OD1	5:D:18:ASP:N	2.38	0.57
3:A:1324:G:N2	3:A:1647:U:O4	2.38	0.56
4:C:69:GLU:OE1	4:C:72:LEU:HD11	2.05	0.56
10:N:36:THR:HG23	10:N:37:THR:O	2.05	0.56
4:C:106:ILE:O	4:C:110:ILE:HD12	2.05	0.56
3:A:1390:U:H3	3:A:1395:A:H62	1.54	0.56
15:T:64:LYS:HA	15:T:79:ASP:CG	2.31	0.56
4:C:68:THR:HG22	4:C:72:LEU:HD23	1.88	0.56
3:A:2614:A:O2'	3:A:2615:U:H5'	2.06	0.56
3:A:411:G:N2	3:A:413:C:O2'	2.36	0.56
4:C:55:VAL:C	4:C:78:PHE:HD1	2.13	0.56
4:C:121:ASP:HA	4:C:178:ARG:HG3	1.86	0.55
10:N:13:ASN:O	10:N:17:ARG:HG3	2.06	0.55
3:A:495:G:H21	14:S:61:ASN:HD21	1.55	0.55
3:A:1154:G:OP2	12:Q:57:ARG:NH1	2.39	0.55
4:C:34:ILE:HG21	4:C:48:LEU:CD1	2.35	0.55
4:C:19:ILE:O	4:C:20:ASP:C	2.49	0.55
10:N:103:ARG:HG3	10:N:110:MET:HE2	1.89	0.55
14:S:62:ASP:CG	14:S:63:GLY:N	2.64	0.55
3:A:627:A:N6	9:L:112:LEU:O	2.39	0.55
15:T:34:VAL:HG21	15:T:43:ILE:HD11	1.88	0.55
18:Z:26:LEU:O	18:Z:37:ARG:NH1	2.39	0.55
3:A:2780:G:O6	7:J:99:ARG:NH1	2.39	0.54
3:A:2054:A:H2'	3:A:2055:C:C6	2.42	0.54
4:C:13:ILE:HG13	4:C:164:HIS:N	2.21	0.54
4:C:222:ASP:O	4:C:222:ASP:OD1	2.25	0.54
7:J:31:GLU:HG2	7:J:142:ILE:HG12	1.88	0.54
3:A:2740:A:O2'	4:C:244:LYS:NZ	2.41	0.54
4:C:15:SER:HB3	4:C:162:TYR:HE1	1.72	0.54
4:C:60:ILE:CG2	4:C:83:LYS:O	2.55	0.54
8:K:93:GLN:HB2	8:K:114:LYS:HZ1	1.73	0.53
4:C:83:LYS:NZ	4:C:87:GLN:HB2	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:T:12:ARG:CZ	17:Y:29:ARG:CZ	2.74	0.53
3:A:1255:U:H3'	6:E:68:ALA:HB2	1.90	0.53
3:A:2636:C:H4'	5:D:81:GLU:OE1	2.08	0.53
4:C:97:LYS:CE	4:C:122:GLU:CB	2.86	0.53
4:C:14:THR:C	4:C:16:LYS:H	2.17	0.53
3:A:65:U:O2'	3:A:456:C:N3	2.40	0.53
3:A:320:A:OP1	6:E:130:LYS:NZ	2.42	0.53
4:C:97:LYS:HZ3	4:C:122:GLU:HB2	1.67	0.53
6:E:105:LEU:HD23	6:E:200:LEU:HD11	1.91	0.53
3:A:960:A:H1'	4:C:89:LYS:HG3	1.89	0.52
3:A:2057:G:H1'	3:A:2611:C:H42	1.74	0.52
4:C:24:THR:CG2	4:C:25:ASN:N	2.72	0.52
4:C:41:LYS:NZ	4:C:64:LEU:HD23	2.20	0.52
4:C:72:LEU:O	4:C:72:LEU:CD1	2.55	0.52
4:C:175:ARG:NH1	4:C:176:LEU:O	2.43	0.52
3:A:2011:U:OP2	14:S:16:LYS:NZ	2.38	0.52
4:C:68:THR:HG22	4:C:72:LEU:HD21	1.90	0.52
3:A:1352:U:O2	3:A:1378:A:N7	2.43	0.52
6:E:149:ILE:HB	6:E:188:MET:HG2	1.92	0.52
3:A:1666:G:H4'	8:K:6:THR:HG23	1.92	0.52
12:Q:80:ASN:OD1	12:Q:84:LYS:HE2	2.10	0.52
1:O:15:ARG:NH1	3:A:1266:G:OP1	2.42	0.52
3:A:212:G:H2'	3:A:213:A:C8	2.45	0.52
3:A:643:A:H3'	3:A:644:A:H8	1.74	0.52
3:A:1415:U:H2'	3:A:1587:G:N3	2.25	0.52
9:L:76:GLU:HG3	9:L:111:ILE:HD12	1.91	0.52
15:T:24:MET:SD	15:T:30:ILE:HG22	2.50	0.52
3:A:955:U:O2	3:A:962:G:N2	2.41	0.51
3:A:2824:C:OP2	3:A:2825:G:N2	2.44	0.51
4:C:20:ASP:HA	4:C:23:MET:HB2	1.91	0.51
4:C:55:VAL:O	4:C:78:PHE:HA	2.11	0.51
4:C:122:GLU:CG	4:C:175:ARG:HH22	2.20	0.51
3:A:48:G:N2	3:A:177:G:OP2	2.37	0.51
3:A:374:A:N6	3:A:400:G:C2	2.79	0.51
3:A:571:U:O2'	3:A:573:U:OP2	2.29	0.51
3:A:957:C:H2'	3:A:959:A:H8	1.76	0.51
4:C:148:ALA:HB2	4:C:191:TYR:CE2	2.45	0.51
4:C:138:THR:CG2	4:C:229:PHE:CD1	2.89	0.51
3:A:396:G:H4'	3:A:397:U:C5	2.45	0.51
3:A:159:G:N1	3:A:166:U:OP2	2.44	0.50
3:A:1252:G:N2	12:Q:32:ARG:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:10:GLN:C	4:C:12:PHE:H	2.19	0.50
4:C:230:GLU:HA	4:C:233:LEU:HG	1.92	0.50
3:A:414:C:H2'	3:A:415:A:C8	2.46	0.50
3:A:1029:A:C5	3:A:1125:G:C2	2.99	0.50
4:C:83:LYS:HZ3	4:C:87:GLN:HB3	1.75	0.50
3:A:627:A:H61	3:A:637:A:H5''	1.75	0.50
3:A:2619:C:H2'	3:A:2620:C:H6	1.76	0.50
4:C:106:ILE:O	4:C:106:ILE:CG1	2.56	0.50
5:D:12:THR:CG2	11:P:8:GLU:OE1	2.60	0.50
4:C:34:ILE:HG13	4:C:48:LEU:HD11	1.94	0.50
9:L:77:ILE:HD11	9:L:82:LEU:HB2	1.94	0.50
15:T:2:ILE:O	15:T:3:ARG:C	2.55	0.50
11:P:13:LYS:HE3	11:P:76:HIS:HA	1.94	0.50
3:A:285:G:N2	3:A:355:U:O2	2.45	0.50
4:C:13:ILE:CG1	4:C:164:HIS:H	2.23	0.50
8:K:34:GLY:N	8:K:37:ASP:OD2	2.45	0.50
12:Q:23:TYR:HB2	12:Q:28:SER:HB3	1.93	0.50
15:T:2:ILE:O	15:T:2:ILE:HG22	2.11	0.50
2:2:37:LYS:NZ	3:A:468:G:OP2	2.45	0.49
3:A:848:C:H2'	3:A:849:A:H8	1.76	0.49
3:A:1336:A:OP2	15:T:68:LYS:NZ	2.43	0.49
5:D:24:VAL:HG21	5:D:188:LEU:HD23	1.93	0.49
3:A:1327:A:N6	3:A:1647:U:O2	2.44	0.49
4:C:57:ALA:N	4:C:78:PHE:CE1	2.81	0.49
3:A:677:A:H61	3:A:800:A:H61	1.60	0.49
4:C:10:GLN:C	4:C:12:PHE:N	2.67	0.49
4:C:34:ILE:CG2	4:C:48:LEU:HD11	2.37	0.49
3:A:552:U:H2'	3:A:553:G:H8	1.76	0.49
3:A:2647:U:H2'	3:A:2648:G:H8	1.77	0.49
3:A:784:G:H21	3:A:793:A:H62	1.59	0.49
5:D:125:TRP:CG	5:D:160:LYS:HB3	2.47	0.49
3:A:301:G:OP2	16:U:81:ARG:NH2	2.46	0.49
1:0:8:THR:CG2	3:A:2020:A:H5'	2.43	0.49
3:A:814:C:H1'	3:A:1225:G:H21	1.78	0.49
4:C:18:ASN:CB	4:C:162:TYR:HD1	2.20	0.49
17:Y:10:SER:HA	17:Y:13:GLU:HB2	1.95	0.49
3:A:84:A:OP1	16:U:5:ARG:NH1	2.46	0.49
3:A:639:U:H2'	3:A:640:C:C6	2.48	0.49
3:A:161:A:OP2	3:A:165:A:N6	2.45	0.48
3:A:2645:G:N1	4:C:209:LYS:CD	2.73	0.48
11:P:61:ARG:NH1	11:P:100:ARG:CA	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:80:PRO:O	14:S:100:THR:OG1	2.30	0.48
4:C:13:ILE:C	4:C:43:HIS:CD2	2.91	0.48
4:C:55:VAL:CA	4:C:78:PHE:HD1	2.23	0.48
10:N:14:SER:HB2	10:N:17:ARG:NH2	2.24	0.48
3:A:72:U:OP2	17:Y:54:LYS:NZ	2.46	0.48
3:A:667:U:O4	3:A:668:A:N6	2.47	0.48
3:A:993:G:OP2	12:Q:50:ARG:NH2	2.46	0.48
9:L:80:SER:HB2	9:L:115:GLU:HG3	1.95	0.48
3:A:1019:U:H3	3:A:1142:A:H62	1.62	0.48
4:C:184:SER:O	4:C:188:LYS:N	2.46	0.48
3:A:230:G:H2'	3:A:231:A:H8	1.77	0.48
3:A:2011:U:OP1	14:S:42:LYS:NZ	2.47	0.48
4:C:115:VAL:HA	4:C:178:ARG:HH22	1.78	0.48
3:A:1668:A:H1'	3:A:1670:C:H41	1.78	0.48
3:A:2788:C:O2'	3:A:2809:A:N3	2.42	0.48
4:C:131:PHE:CE2	4:C:135:LEU:HD12	2.45	0.48
4:C:135:LEU:HD22	4:C:146:LEU:CD2	2.43	0.48
9:L:2:ARG:O	9:L:5:THR:OG1	2.32	0.48
4:C:14:THR:OG1	4:C:16:LYS:HE3	2.13	0.48
3:A:1668:A:N3	3:A:1670:C:N4	2.62	0.47
4:C:15:SER:HB3	4:C:162:TYR:CE1	2.48	0.47
8:K:25:LEU:HD11	8:K:40:LYS:HG3	1.96	0.47
4:C:74:ASP:OD1	4:C:74:ASP:N	2.43	0.47
4:C:96:TYR:HE1	4:C:98:ILE:HD11	1.79	0.47
4:C:110:ILE:O	4:C:113:LYS:HB2	2.14	0.47
4:C:122:GLU:OE1	4:C:175:ARG:NH1	2.47	0.47
6:E:76:PRO:CG	6:E:84:THR:HG22	2.32	0.47
12:Q:108:LEU:HD13	13:R:48:LYS:HE3	1.96	0.47
16:U:39:ASN:HB3	16:U:62:ALA:HB3	1.97	0.47
17:Y:22:LEU:HD23	17:Y:23:ARG:HG2	1.96	0.47
4:C:29:ASN:CG	4:C:30:GLU:H	2.23	0.47
8:K:2:ILE:HB	8:K:33:ALA:HB3	1.96	0.47
3:A:2052:A:C2	3:A:2053:G:C8	3.02	0.47
3:A:2054:A:H2'	3:A:2055:C:H6	1.79	0.47
15:T:64:LYS:CA	15:T:79:ASP:OD1	2.61	0.47
3:A:276:U:O2'	3:A:278:A:N6	2.48	0.47
3:A:475:C:H4'	3:A:510:C:H5''	1.96	0.47
4:C:26:ILE:CD1	4:C:99:PHE:CZ	2.95	0.47
11:P:29:VAL:HG13	11:P:40:GLN:HB3	1.97	0.47
11:P:105:LYS:HB3	11:P:105:LYS:HE3	1.69	0.47
4:C:26:ILE:HD11	4:C:99:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:396:G:H4'	3:A:397:U:H5	1.81	0.46
3:A:2848:G:O2'	3:A:2867:G:N2	2.48	0.46
4:C:60:ILE:HG21	4:C:84:ASP:HA	1.98	0.46
4:C:149:GLU:N	4:C:149:GLU:OE1	2.48	0.46
5:D:3:GLY:O	5:D:4:LEU:HD23	2.15	0.46
18:Z:8:GLN:HB2	18:Z:28:LEU:HD13	1.96	0.46
1:O:16:ARG:NE	3:A:1266:G:OP2	2.46	0.46
4:C:188:LYS:C	4:C:190:LYS:H	2.23	0.46
3:A:247:G:N2	3:A:251:A:OP2	2.41	0.46
3:A:574:A:H61	3:A:2032:G:H2'	1.81	0.46
4:C:47:GLU:OE1	4:C:47:GLU:N	2.48	0.46
3:A:18:U:OP1	12:Q:29:ARG:NH2	2.49	0.46
4:C:18:ASN:HD22	4:C:162:TYR:HD1	1.61	0.46
10:N:87:PHE:HD1	10:N:90:ARG:NH1	2.11	0.46
15:T:5:GLU:OE2	15:T:5:GLU:N	2.44	0.46
17:Y:12:GLU:HA	17:Y:15:ASN:HB3	1.98	0.46
1:O:26:SER:O	1:O:26:SER:OG	2.26	0.46
3:A:171:U:H2'	3:A:172:A:H8	1.81	0.46
3:A:643:A:H3'	3:A:644:A:C8	2.51	0.46
3:A:1383:A:O2'	3:A:1405:U:O2'	2.33	0.46
19:A:3001:AN6:HN6	4:C:130:GLY:HA3	1.80	0.46
7:J:141:ASP:OD1	7:J:141:ASP:N	2.38	0.46
15:T:12:ARG:CD	17:Y:29:ARG:NH2	2.68	0.46
4:C:106:ILE:O	4:C:110:ILE:CD1	2.65	0.45
6:E:2:GLU:N	6:E:2:GLU:OE2	2.49	0.45
12:Q:80:ASN:ND2	12:Q:84:LYS:HE2	2.31	0.45
4:C:23:MET:SD	4:C:44:PHE:CE2	3.09	0.45
4:C:108:THR:HA	4:C:111:ILE:HG22	1.97	0.45
3:A:177:G:H3'	3:A:178:G:H8	1.82	0.45
3:A:629:G:H21	3:A:640:C:H5'	1.82	0.45
3:A:1997:C:H2'	3:A:1998:A:H8	1.81	0.45
3:A:2765:A:O2'	4:C:214:ASN:OD1	2.34	0.45
4:C:163:PHE:HB2	4:C:167:PRO:HD3	1.98	0.45
3:A:2057:G:N2	3:A:2059:A:OP2	2.50	0.45
12:Q:61:ILE:CD1	12:Q:91:ARG:HD3	2.45	0.45
3:A:1415:U:H2'	3:A:1587:G:C2	2.52	0.45
6:E:4:VAL:HG22	6:E:6:LYS:H	1.82	0.45
8:K:42:THR:HG22	8:K:57:VAL:HG22	1.99	0.45
17:Y:25:GLN:O	17:Y:29:ARG:HG3	2.16	0.45
3:A:641:U:H2'	3:A:642:U:O4'	2.16	0.44
4:C:21:LYS:O	4:C:21:LYS:CG	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:1:MET:HG3	14:S:2:GLU:N	2.32	0.44
3:A:599:A:H2'	3:A:600:G:H8	1.81	0.44
3:A:628:G:N2	3:A:639:U:H4'	2.32	0.44
8:K:53:LYS:HE2	8:K:53:LYS:HB2	1.81	0.44
3:A:171:U:H2'	3:A:172:A:C8	2.52	0.44
4:C:131:PHE:HA	4:C:134:ARG:HG2	1.99	0.44
5:D:13:ARG:HD3	11:P:55:HIS:ND1	2.31	0.44
12:Q:93:ILE:HA	12:Q:96:ASP:HB2	1.99	0.44
3:A:434:U:O2	3:A:436:C:N4	2.50	0.44
3:A:585:G:H21	3:A:1254:A:N6	2.16	0.44
3:A:629:G:N2	3:A:640:C:H5'	2.33	0.44
3:A:2728:U:HO2'	3:A:2729:G:H8	1.66	0.44
3:A:2646:C:OP2	3:A:2732:G:O2'	2.36	0.44
18:Z:38:GLU:OE2	18:Z:38:GLU:N	2.47	0.44
3:A:288:U:H2'	3:A:289:G:C8	2.53	0.44
3:A:1009:A:N3	3:A:1153:C:O2'	2.49	0.44
3:A:1278:C:H2'	3:A:1279:G:H8	1.82	0.44
10:N:22:ARG:HG3	10:N:70:THR:HA	2.00	0.44
3:A:2619:C:O2	5:D:161:MET:HE1	2.17	0.44
10:N:36:THR:CG2	10:N:41:ALA:HB2	2.48	0.44
12:Q:61:ILE:HD11	12:Q:91:ARG:CD	2.45	0.44
15:T:12:ARG:HA	17:Y:29:ARG:NH2	2.33	0.44
18:Z:5:LYS:HB2	18:Z:57:GLU:HB2	1.99	0.44
3:A:1407:G:H2'	3:A:1408:G:H8	1.82	0.44
4:C:66:LYS:HA	4:C:66:LYS:HD3	1.71	0.44
4:C:184:SER:C	4:C:188:LYS:HG3	2.43	0.44
3:A:137:U:H2'	3:A:140:C:H41	1.83	0.43
3:A:2655:G:N2	3:A:2665:A:OP2	2.51	0.43
4:C:164:HIS:NE2	4:C:165:PRO:CD	2.75	0.43
10:N:71:ARG:HA	10:N:71:ARG:HD2	1.83	0.43
4:C:14:THR:C	4:C:16:LYS:N	2.76	0.43
4:C:24:THR:CG2	4:C:25:ASN:H	2.31	0.43
4:C:128:GLU:HG3	4:C:131:PHE:H	1.83	0.43
7:J:3:THR:HG21	12:Q:60:TRP:HE1	1.82	0.43
10:N:45:ARG:HE	10:N:45:ARG:HB3	1.56	0.43
12:Q:80:ASN:HD21	12:Q:84:LYS:HE2	1.84	0.43
3:A:973:A:O2'	3:A:974:G:N2	2.48	0.43
4:C:19:ILE:CG1	4:C:162:TYR:OH	2.64	0.43
10:N:14:SER:HA	10:N:17:ARG:NE	2.28	0.43
14:S:74:ILE:HG13	14:S:105:VAL:HG22	2.00	0.43
12:Q:82:LEU:HD12	12:Q:82:LEU:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:S:4:ILE:HG23	14:S:106:VAL:HG22	2.00	0.43
3:A:1412:U:H3	3:A:1591:A:H61	1.67	0.43
8:K:105:ARG:NH1	11:P:32:VAL:O	2.51	0.43
16:U:81:ARG:HG3	16:U:96:LYS:HG3	2.01	0.43
3:A:1136:G:H2'	3:A:1137:G:H8	1.84	0.43
9:L:9:ALA:O	9:L:12:SER:OG	2.37	0.43
11:P:61:ARG:CG	11:P:70:GLU:OE2	2.67	0.43
3:A:2049:G:N2	3:A:2050:C:O2	2.52	0.43
3:A:2637:U:H3	3:A:2776:A:H62	1.66	0.43
8:K:103:VAL:HG21	8:K:116:ILE:HG22	2.01	0.43
12:Q:80:ASN:CG	12:Q:84:LYS:HE2	2.44	0.43
1:O:8:THR:HG21	3:A:2020:A:H5'	2.01	0.42
3:A:651:G:H2'	3:A:652:U:O4'	2.19	0.42
5:D:175:LEU:HD23	5:D:175:LEU:HA	1.86	0.42
10:N:117:ASP:OD1	10:N:117:ASP:N	2.52	0.42
3:A:13:A:O2'	3:A:15:G:N7	2.49	0.42
3:A:409:G:C2	3:A:419:U:O2	2.72	0.42
3:A:411:G:C4'	3:A:413:C:H5	2.14	0.42
4:C:139:LYS:HG2	4:C:140:ARG:HH11	1.84	0.42
14:S:83:LYS:HE3	14:S:97:LEU:HD21	2.02	0.42
3:A:2669:G:H2'	3:A:2670:A:H8	1.84	0.42
3:A:2676:C:O2	3:A:2732:G:N2	2.46	0.42
3:A:2861:U:H2'	3:A:2862:G:C8	2.55	0.42
6:E:123:LYS:HB3	6:E:123:LYS:HE3	1.88	0.42
15:T:58:VAL:HG22	15:T:85:VAL:HG23	2.01	0.42
3:A:612:G:H21	3:A:616:A:H62	1.67	0.42
2:2:31:LEU:HD22	2:2:42:LEU:HD13	2.00	0.42
7:J:4:PHE:O	12:Q:63:ARG:NH2	2.47	0.42
9:L:14:LYS:HE3	9:L:14:LYS:HB3	1.88	0.42
10:N:71:ARG:O	10:N:72:ASP:OD1	2.38	0.42
16:U:13:LEU:HD23	16:U:13:LEU:HA	1.92	0.42
3:A:2056:G:C6	3:A:2612:C:C4	3.07	0.42
4:C:69:GLU:HA	4:C:72:LEU:HG	2.02	0.42
15:T:12:ARG:HH11	17:Y:29:ARG:HH12	1.50	0.42
3:A:213:A:H2'	3:A:214:G:C8	2.55	0.42
3:A:2619:C:H2'	3:A:2620:C:C6	2.54	0.42
4:C:14:THR:CG2	4:C:15:SER:N	2.43	0.42
4:C:57:ALA:CB	4:C:78:PHE:CE1	2.92	0.42
6:E:35:TYR:OH	6:E:176:ASP:OD2	2.33	0.42
8:K:105:ARG:HH22	11:P:31:VAL:HG22	1.79	0.42
3:A:437:U:H2'	3:A:438:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:959:A:H3'	3:A:960:A:H8	1.85	0.42
3:A:960:A:C2	3:A:962:G:H1'	2.55	0.42
5:D:84:LEU:HD23	5:D:84:LEU:HA	1.71	0.42
6:E:76:PRO:HG3	6:E:84:THR:CG2	2.35	0.42
3:A:1414:C:O2	3:A:1588:G:N2	2.53	0.41
4:C:45:THR:HA	4:C:48:LEU:HB3	2.02	0.41
3:A:1024:G:OP2	3:A:1025:G:O2'	2.36	0.41
10:N:103:ARG:HE	10:N:110:MET:HE2	1.85	0.41
3:A:499:U:H5''	16:U:42:LYS:HD2	2.02	0.41
3:A:1029:A:C5	3:A:1125:G:N2	2.89	0.41
4:C:123:ILE:H	4:C:175:ARG:HH12	1.68	0.41
17:Y:60:LYS:HE2	17:Y:60:LYS:HB2	1.72	0.41
3:A:158:U:H3	3:A:168:G:H1	1.67	0.41
4:C:20:ASP:O	4:C:23:MET:N	2.53	0.41
6:E:1:MET:HE2	6:E:1:MET:HB3	1.98	0.41
7:J:36:LEU:HD11	7:J:122:LEU:HB2	2.03	0.41
9:L:107:PHE:HE1	9:L:126:ARG:HH22	0.64	0.41
11:P:67:GLU:N	11:P:67:GLU:OE1	2.53	0.41
4:C:174:ILE:HB	4:C:176:LEU:HD21	2.02	0.41
2:2:34:ARG:NE	2:2:42:LEU:O	2.54	0.41
3:A:926:G:H2'	3:A:927:A:C8	2.56	0.41
4:C:147:MET:HE2	4:C:229:PHE:CG	2.54	0.41
8:K:48:PRO:HD2	8:K:49:ARG:CZ	2.50	0.41
3:A:272:A:H2'	3:A:273:G:H8	1.85	0.41
3:A:636:G:OP1	9:L:129:LYS:NZ	2.50	0.41
4:C:121:ASP:CA	4:C:178:ARG:HG2	2.36	0.41
13:R:58:VAL:H	13:R:102:SER:HB3	1.86	0.41
14:S:11:ARG:HE	14:S:11:ARG:HB3	1.75	0.41
3:A:1029:A:C6	3:A:1125:G:C2	3.09	0.41
3:A:1386:C:H2'	3:A:1387:A:C8	2.56	0.41
3:A:1386:C:H2'	3:A:1387:A:H8	1.85	0.41
15:T:26:LYS:HD3	15:T:26:LYS:HA	1.86	0.41
15:T:69:ARG:HB2	15:T:74:ILE:HG22	2.03	0.41
3:A:106:C:H2'	3:A:107:G:H8	1.85	0.41
4:C:71:LYS:HD2	4:C:71:LYS:HA	1.91	0.41
4:C:83:LYS:HD2	4:C:84:ASP:H	1.85	0.41
4:C:149:GLU:HG2	4:C:178:ARG:NH1	2.35	0.41
11:P:93:LYS:HE3	11:P:93:LYS:HB3	1.93	0.41
3:A:1161:C:H2'	3:A:1162:G:H8	1.85	0.40
5:D:127:PHE:HD1	5:D:127:PHE:HA	1.75	0.40
15:T:53:VAL:HG11	15:T:87:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:523:C:H2'	3:A:524:G:H8	1.87	0.40
3:A:1190:G:H2'	3:A:1191:G:H8	1.86	0.40
3:A:2036:C:H2'	3:A:2037:A:C8	2.57	0.40
4:C:138:THR:HG22	4:C:229:PHE:CD1	2.36	0.40
8:K:105:ARG:HH22	11:P:31:VAL:HG21	1.75	0.40
14:S:73:LYS:HB2	14:S:106:VAL:HB	2.03	0.40
3:A:2815:C:H2'	3:A:2816:G:H8	1.86	0.40
4:C:105:ASN:O	4:C:106:ILE:CG2	2.68	0.40
8:K:51:LYS:HB3	8:K:51:LYS:HE2	1.67	0.40
3:A:861:A:H62	3:A:916:G:H1'	1.87	0.40
3:A:1608:A:O2'	3:A:1610:A:OP2	2.39	0.40
3:A:2055:C:C4	3:A:2056:G:N7	2.90	0.40
3:A:29:U:H2'	3:A:30:G:H8	1.86	0.40
3:A:1316:U:H2'	3:A:1317:G:H8	1.86	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	53/57 (93%)	53 (100%)	0	0	100	100
2	2	38/46 (83%)	36 (95%)	2 (5%)	0	100	100
4	C	233/244 (96%)	206 (88%)	21 (9%)	6 (3%)	4	30
5	D	174/209 (83%)	163 (94%)	11 (6%)	0	100	100
6	E	191/201 (95%)	189 (99%)	2 (1%)	0	100	100
7	J	137/142 (96%)	132 (96%)	5 (4%)	0	100	100
8	K	116/123 (94%)	109 (94%)	6 (5%)	1 (1%)	14	49
9	L	95/144 (66%)	86 (90%)	9 (10%)	0	100	100
10	N	118/127 (93%)	106 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	P	109/115 (95%)	103 (94%)	6 (6%)	0	100	100
12	Q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
13	R	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
14	S	100/110 (91%)	95 (95%)	5 (5%)	0	100	100
15	T	90/100 (90%)	86 (96%)	4 (4%)	0	100	100
16	U	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
17	Y	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
18	Z	56/59 (95%)	56 (100%)	0	0	100	100
All	All	1886/2065 (91%)	1778 (94%)	101 (5%)	7 (0%)	32	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	13	ILE
4	C	16	LYS
4	C	106	ILE
4	C	189	GLN
4	C	188	LYS
4	C	12	PHE
8	K	95	ILE

### 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	46/48 (96%)	44 (96%)	2 (4%)	25	48
2	2	32/38 (84%)	31 (97%)	1 (3%)	35	56
4	C	223/232 (96%)	213 (96%)	10 (4%)	23	46
5	D	139/164 (85%)	132 (95%)	7 (5%)	20	44
6	E	161/165 (98%)	158 (98%)	3 (2%)	52	70
7	J	115/116 (99%)	111 (96%)	4 (4%)	31	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	101/104 (97%)	97 (96%)	4 (4%)	27	49
9	L	72/103 (70%)	69 (96%)	3 (4%)	25	48
10	N	100/103 (97%)	98 (98%)	2 (2%)	50	68
11	P	99/100 (99%)	96 (97%)	3 (3%)	36	57
12	Q	89/90 (99%)	85 (96%)	4 (4%)	23	46
13	R	84/84 (100%)	80 (95%)	4 (5%)	21	45
14	S	90/93 (97%)	90 (100%)	0	100	100
15	T	79/84 (94%)	76 (96%)	3 (4%)	28	51
16	U	83/85 (98%)	76 (92%)	7 (8%)	9	31
17	Y	55/55 (100%)	55 (100%)	0	100	100
18	Z	48/49 (98%)	48 (100%)	0	100	100
All	All	1616/1713 (94%)	1559 (96%)	57 (4%)	33	53

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	5	ASN
1	0	33	SER
2	2	44	VAL
4	C	19	ILE
4	C	23	MET
4	C	66	LYS
4	C	93	ASN
4	C	134	ARG
4	C	142	LEU
4	C	169	VAL
4	C	175	ARG
4	C	214	ASN
4	C	227	ILE
5	D	12	THR
5	D	37	VAL
5	D	40	LEU
5	D	58	ASN
5	D	176	ASP
5	D	180	VAL
5	D	197	THR
6	E	49	ARG
6	E	61	ARG

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Mol	Chain	Res	Type
6	E	73	ILE
7	J	24	THR
7	J	28	LEU
7	J	57	LEU
7	J	73	VAL
8	K	22	ILE
8	K	49	ARG
8	K	51	LYS
8	K	52	VAL
9	L	6	LEU
9	L	19	LEU
9	L	100	ILE
10	N	83	LEU
10	N	113	ILE
11	P	27	VAL
11	P	31	VAL
11	P	79	VAL
12	Q	79	ILE
12	Q	93	ILE
12	Q	94	LEU
12	Q	103	VAL
13	R	19	THR
13	R	38	VAL
13	R	75	VAL
13	R	98	ILE
15	T	3	ARG
15	T	62	VAL
15	T	78	SER
16	U	11	ILE
16	U	35	VAL
16	U	48	VAL
16	U	61	GLU
16	U	71	ILE
16	U	76	THR
16	U	88	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	18	ASN
4	C	43	HIS
4	C	50	GLN

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Mol	Chain	Res	Type
4	C	62	HIS
4	C	101	ASN
4	C	189	GLN
4	C	218	HIS
4	C	226	ASN
6	E	29	HIS
6	E	156	ASN
11	P	11	GLN
11	P	40	GLN
14	S	9	HIS
15	T	91	GLN
16	U	45	GLN
17	Y	31	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	A	1585/2904 (54%)	300 (18%)	8 (0%)

All (300) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	A	10	A
3	A	12	U
3	A	27	G
3	A	28	A
3	A	34	U
3	A	35	G
3	A	45	G
3	A	46	G
3	A	51	G
3	A	60	G
3	A	63	A
3	A	71	A
3	A	74	A
3	A	75	G
3	A	84	A
3	A	118	A
3	A	120	U
3	A	125	A
3	A	131	A

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Mol	Chain	Res	Type
3	A	138	U
3	A	139	U
3	A	140	C
3	A	141	G
3	A	142	A
3	A	158	U
3	A	160	A
3	A	166	U
3	A	181	A
3	A	196	A
3	A	199	A
3	A	204	A
3	A	215	G
3	A	216	A
3	A	221	A
3	A	222	A
3	A	225	C
3	A	228	C
3	A	229	C
3	A	230	G
3	A	232	G
3	A	233	A
3	A	248	G
3	A	250	G
3	A	255	A
3	A	265	A
3	A	266	G
3	A	271	G
3	A	272	A
3	A	277	G
3	A	278	A
3	A	279	A
3	A	286	U
3	A	287	G
3	A	288	U
3	A	291	G
3	A	292	U
3	A	302	C
3	A	307	G
3	A	311	A
3	A	329	G
3	A	330	A

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Mol	Chain	Res	Type
3	A	359	G
3	A	362	A
3	A	367	G
3	A	370	G
3	A	371	A
3	A	372	G
3	A	374	A
3	A	395	U
3	A	396	G
3	A	401	A
3	A	405	U
3	A	406	G
3	A	408	G
3	A	409	G
3	A	411	G
3	A	412	A
3	A	413	C
3	A	415	A
3	A	416	U
3	A	423	A
3	A	424	G
3	A	435	C
3	A	456	C
3	A	457	A
3	A	467	G
3	A	480	A
3	A	481	G
3	A	491	G
3	A	494	G
3	A	505	A
3	A	509	C
3	A	510	C
3	A	528	A
3	A	530	G
3	A	531	C
3	A	532	A
3	A	533	G
3	A	546	U
3	A	547	A
3	A	548	G
3	A	550	C
3	A	562	U

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Mol	Chain	Res	Type
3	A	563	A
3	A	573	U
3	A	574	A
3	A	575	A
3	A	586	A
3	A	603	A
3	A	613	A
3	A	614	A
3	A	615	U
3	A	621	A
3	A	627	A
3	A	631	A
3	A	634	C
3	A	636	G
3	A	637	A
3	A	638	G
3	A	646	U
3	A	647	G
3	A	650	C
3	A	651	G
3	A	653	U
3	A	654	A
3	A	669	G
3	A	780	G
3	A	782	A
3	A	784	G
3	A	785	G
3	A	792	A
3	A	793	A
3	A	801	G
3	A	812	C
3	A	819	A
3	A	827	U
3	A	828	U
3	A	829	A
3	A	830	G
3	A	831	G
3	A	845	A
3	A	846	U
3	A	847	U
3	A	855	G
3	A	858	G

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Mol	Chain	Res	Type
3	A	859	G
3	A	861	A
3	A	862	G
3	A	914	G
3	A	915	C
3	A	917	A
3	A	920	A
3	A	931	U
3	A	934	U
3	A	945	A
3	A	957	C
3	A	958	U
3	A	959	A
3	A	960	A
3	A	961	C
3	A	962	G
3	A	963	U
3	A	964	C
3	A	965	C
3	A	966	G
3	A	974	G
3	A	980	A
3	A	982	C
3	A	983	A
3	A	985	C
3	A	995	C
3	A	996	A
3	A	1005	C
3	A	1012	U
3	A	1013	C
3	A	1022	G
3	A	1026	G
3	A	1030	C
3	A	1124	G
3	A	1125	G
3	A	1126	A
3	A	1128	G
3	A	1135	C
3	A	1136	G
3	A	1142	A
3	A	1173	U
3	A	1174	U

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Mol	Chain	Res	Type
3	A	1175	A
3	A	1176	U
3	A	1182	G
3	A	1186	G
3	A	1212	G
3	A	1238	G
3	A	1247	A
3	A	1253	A
3	A	1256	G
3	A	1266	G
3	A	1271	G
3	A	1272	A
3	A	1300	G
3	A	1301	A
3	A	1302	A
3	A	1345	C
3	A	1376	C
3	A	1378	A
3	A	1379	U
3	A	1380	G
3	A	1384	A
3	A	1386	C
3	A	1395	A
3	A	1403	A
3	A	1408	G
3	A	1410	G
3	A	1411	U
3	A	1412	U
3	A	1414	C
3	A	1415	U
3	A	1416	G
3	A	1588	G
3	A	1591	A
3	A	1593	A
3	A	1595	C
3	A	1598	A
3	A	1633	G
3	A	1634	A
3	A	1646	C
3	A	1647	U
3	A	1648	U
3	A	1654	A

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Mol	Chain	Res	Type
3	A	1663	G
3	A	1669	A
3	A	1674	G
3	A	1675	C
3	A	1991	U
3	A	1992	G
3	A	1993	U
3	A	1994	C
3	A	1995	U
3	A	1997	C
3	A	2021	C
3	A	2022	U
3	A	2023	C
3	A	2030	A
3	A	2031	A
3	A	2032	G
3	A	2033	A
3	A	2043	C
3	A	2046	G
3	A	2048	G
3	A	2049	G
3	A	2051	A
3	A	2057	G
3	A	2058	A
3	A	2059	A
3	A	2612	C
3	A	2614	A
3	A	2615	U
3	A	2617	U
3	A	2629	U
3	A	2630	G
3	A	2639	A
3	A	2645	G
3	A	2646	C
3	A	2654	A
3	A	2655	G
3	A	2675	A
3	A	2676	C
3	A	2682	A
3	A	2689	U
3	A	2690	U
3	A	2702	G

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Mol	Chain	Res	Type
3	A	2713	U
3	A	2714	G
3	A	2726	A
3	A	2729	G
3	A	2732	G
3	A	2733	A
3	A	2739	U
3	A	2744	G
3	A	2748	A
3	A	2751	G
3	A	2752	C
3	A	2758	A
3	A	2762	C
3	A	2765	A
3	A	2766	A
3	A	2778	A
3	A	2779	U
3	A	2780	G
3	A	2791	G
3	A	2818	U
3	A	2820	A
3	A	2848	G
3	A	2849	U
3	A	2867	G
3	A	2873	A
3	A	2880	C
3	A	2886	A
3	A	2901	C
3	A	2903	U

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	271	G
3	A	287	G
3	A	396	G
3	A	411	G
3	A	412	A
3	A	479	A
3	A	958	U
3	A	1414	C

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
19	AN6	A	3001	3	26,30,30	0.65	0	27,43,43	0.64	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
19	AN6	A	3001	3	-	10/15/35/35	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	3001	AN6	O'-C'-CA'-N'
19	A	3001	AN6	CA'-CB'-CG'-N10
19	A	3001	AN6	CB'-CG'-N10-C3
19	A	3001	AN6	O5'-C'-CA'-N'

*Continued on next page...*

*Continued from previous page...*

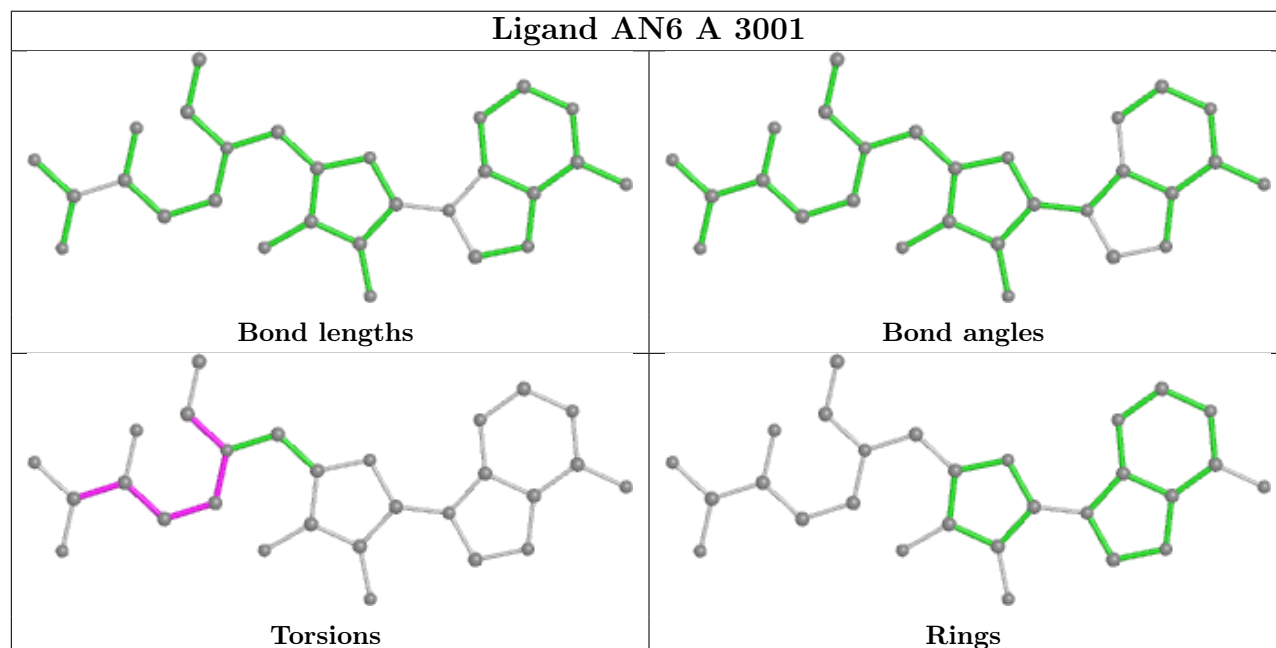
Mol	Chain	Res	Type	Atoms
19	A	3001	AN6	N'-CA'-CB'-CG'
19	A	3001	AN6	CB'-CG'-N10-C5'
19	A	3001	AN6	O'-C'-CA'-CB'
19	A	3001	AN6	O5'-C'-CA'-CB'
19	A	3001	AN6	C1-C3-N10-CG'
19	A	3001	AN6	C1-C3-N10-C5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	3001	AN6	2	0

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

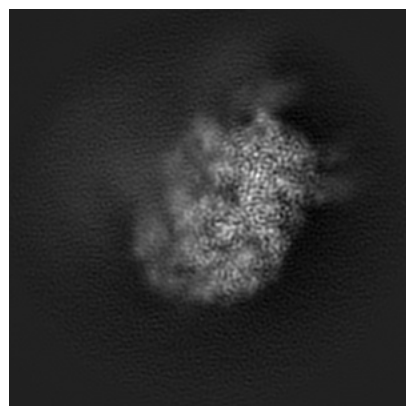
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61781. These allow visual inspection of the internal detail of the map and identification of artifacts.

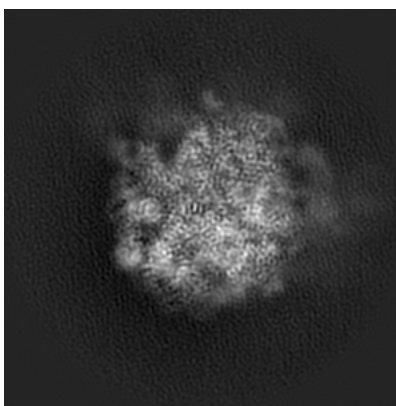
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

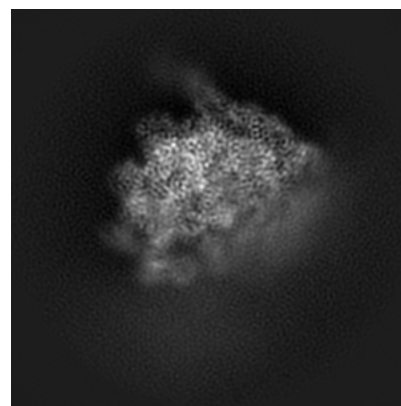
#### 6.1.1 Primary map



X

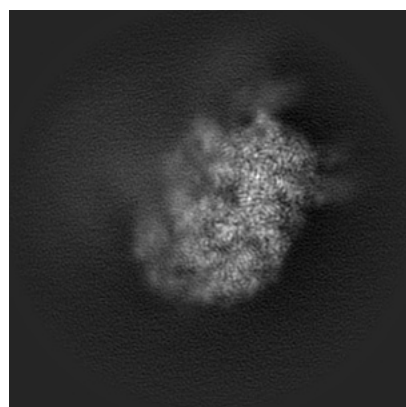


Y

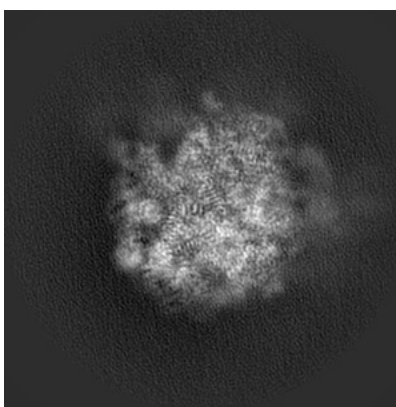


Z

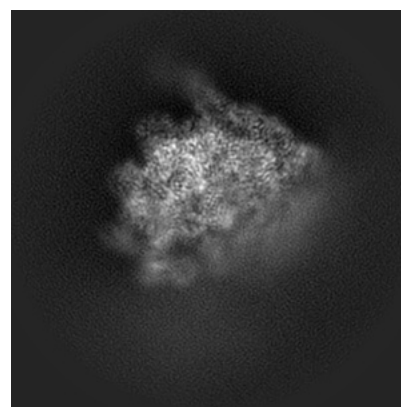
#### 6.1.2 Raw map



X



Y

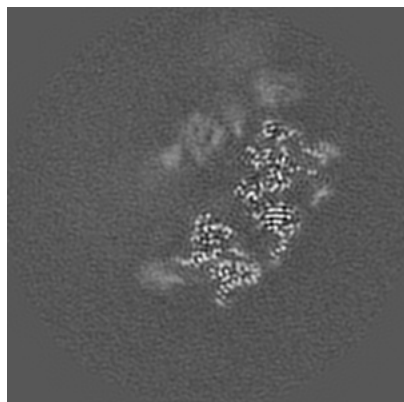


Z

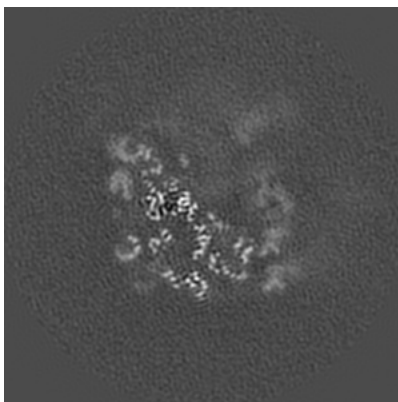
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

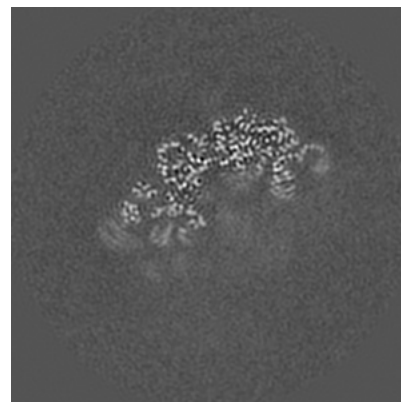
### 6.2.1 Primary map



X Index: 120

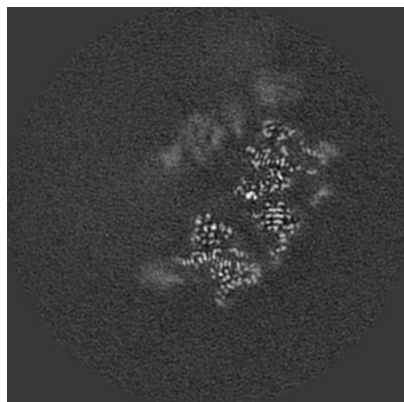


Y Index: 120

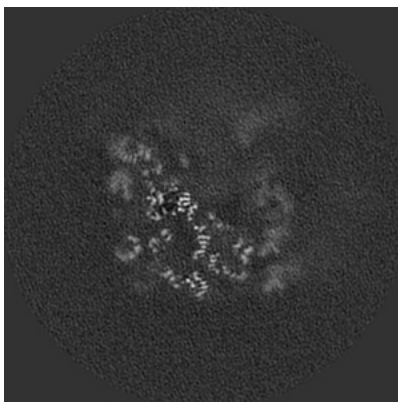


Z Index: 120

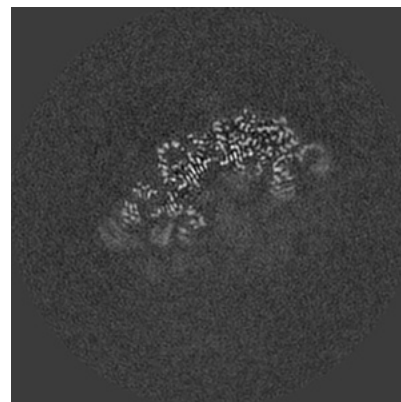
### 6.2.2 Raw map



X Index: 120



Y Index: 120



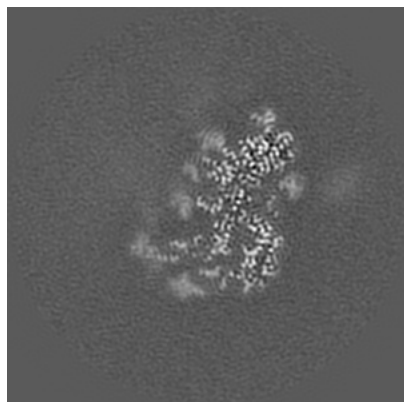
Z Index: 120

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

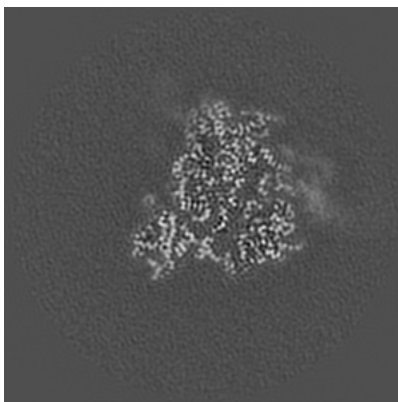


## 6.3 Largest variance slices [i](#)

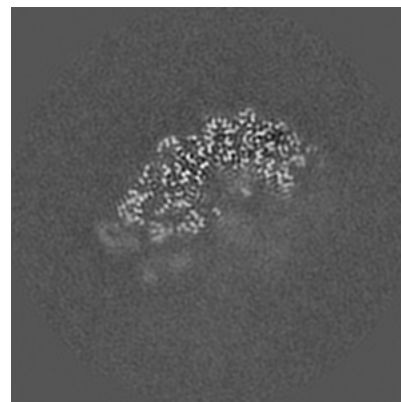
### 6.3.1 Primary map



X Index: 95

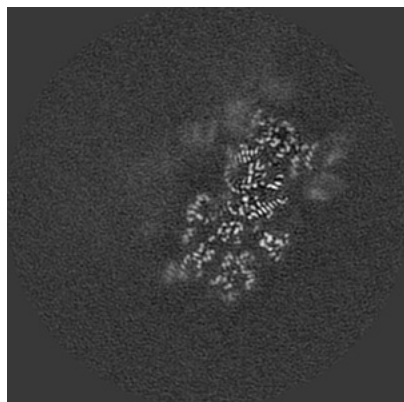


Y Index: 157

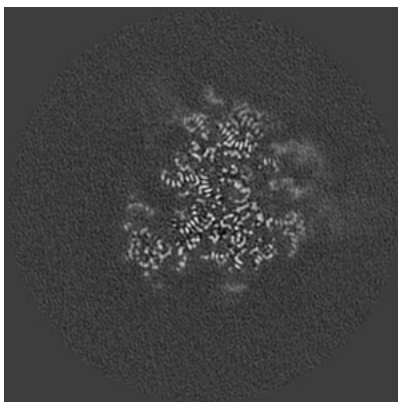


Z Index: 117

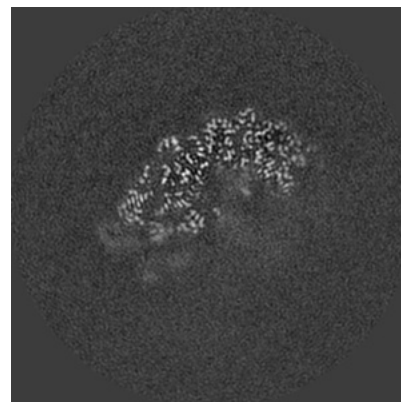
### 6.3.2 Raw map



X Index: 113



Y Index: 149

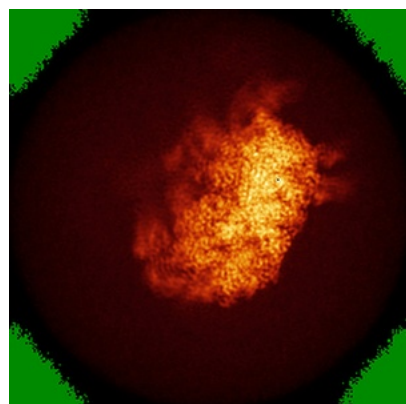


Z Index: 117

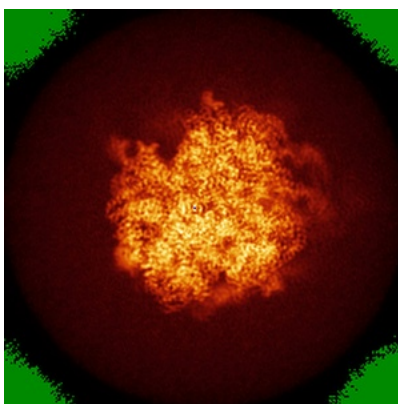
The images above show the largest variance slices of the map in three orthogonal directions.

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

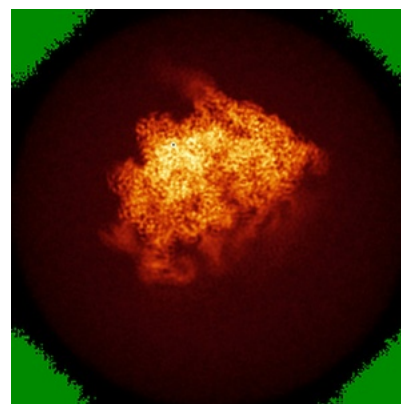
### 6.4.1 Primary map



X

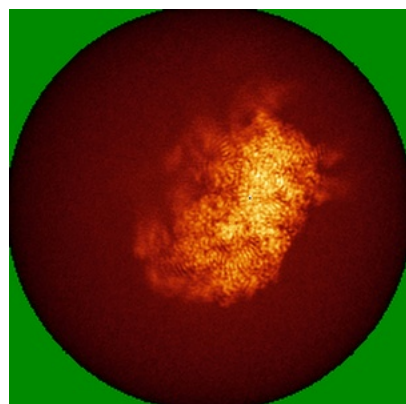


Y

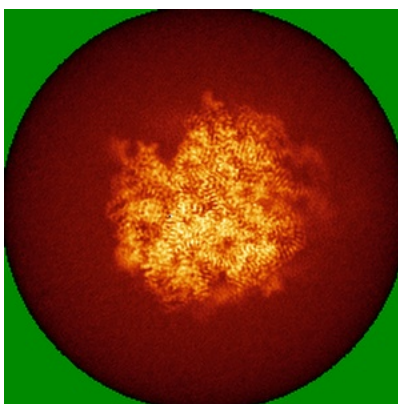


Z

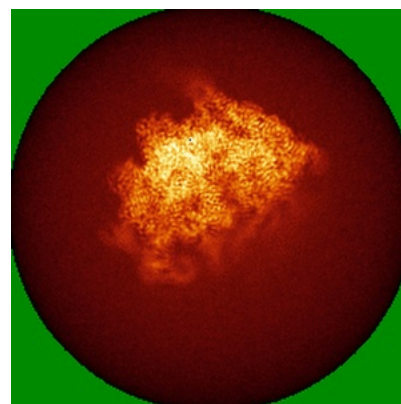
### 6.4.2 Raw map



X



Y

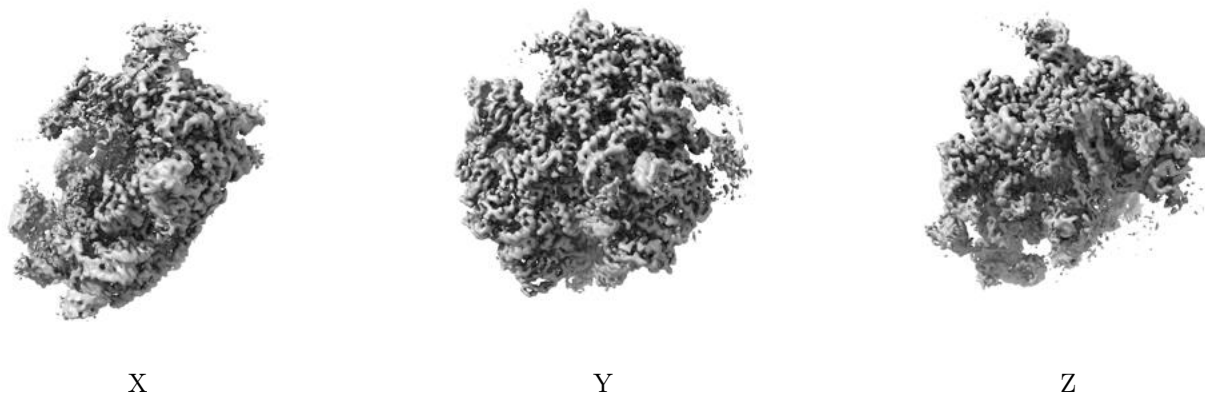


Z

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.

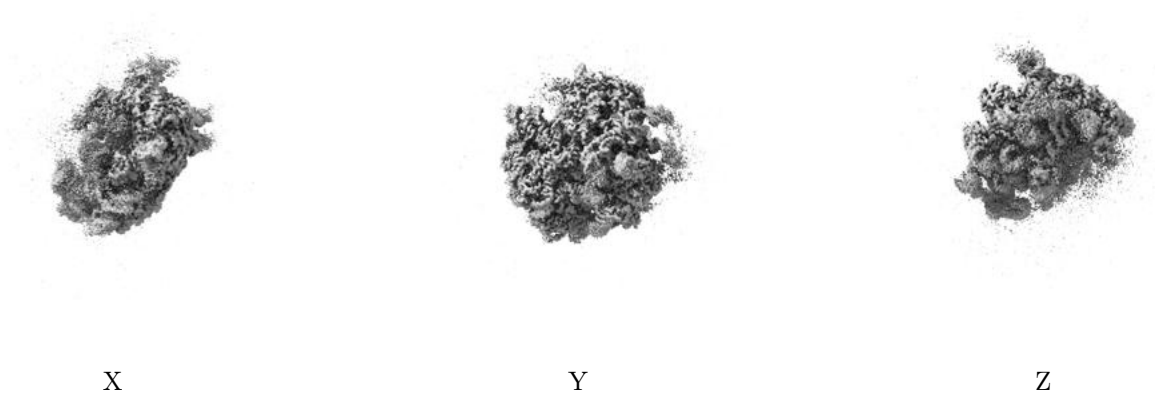
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0158. 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



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.

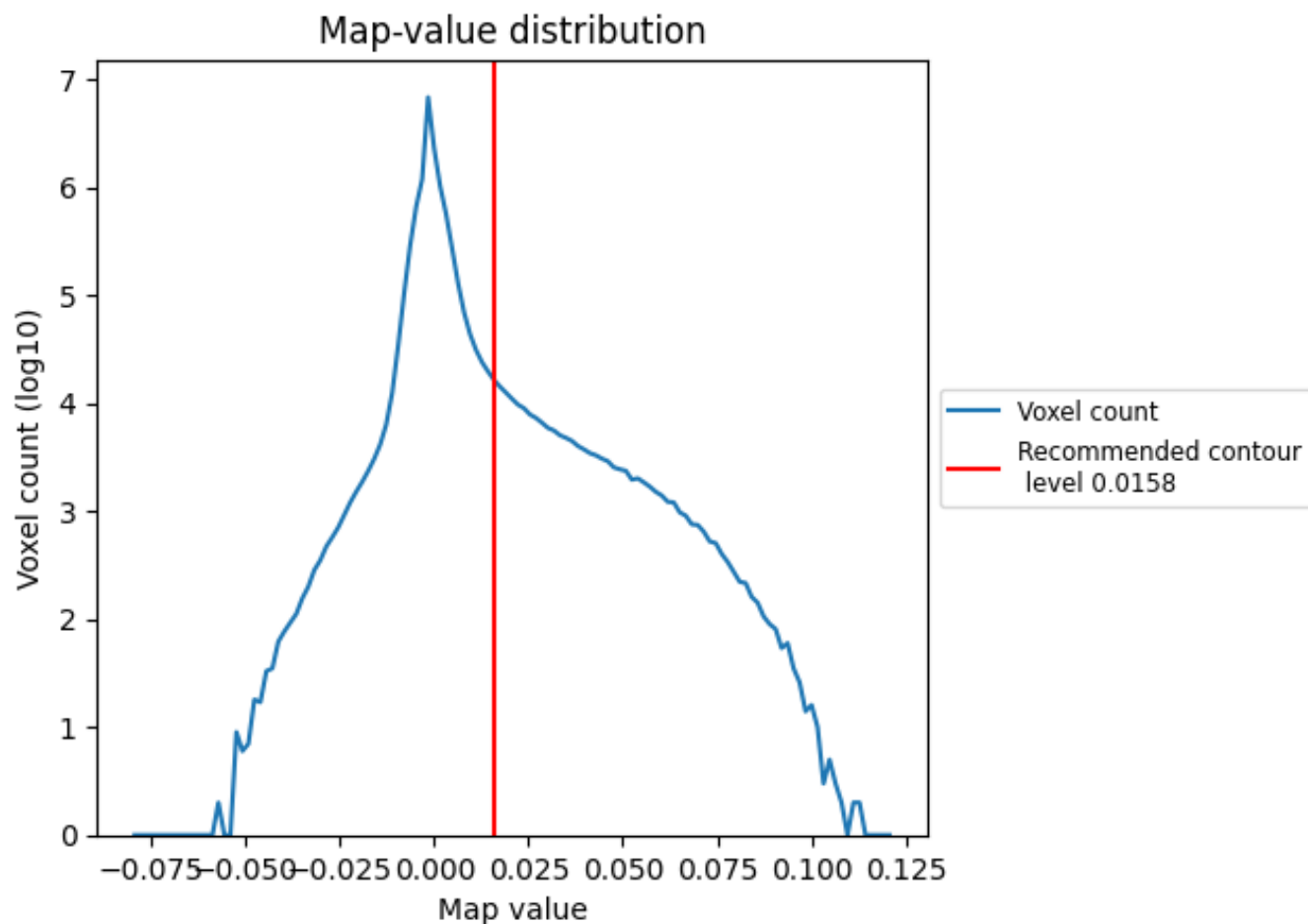
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

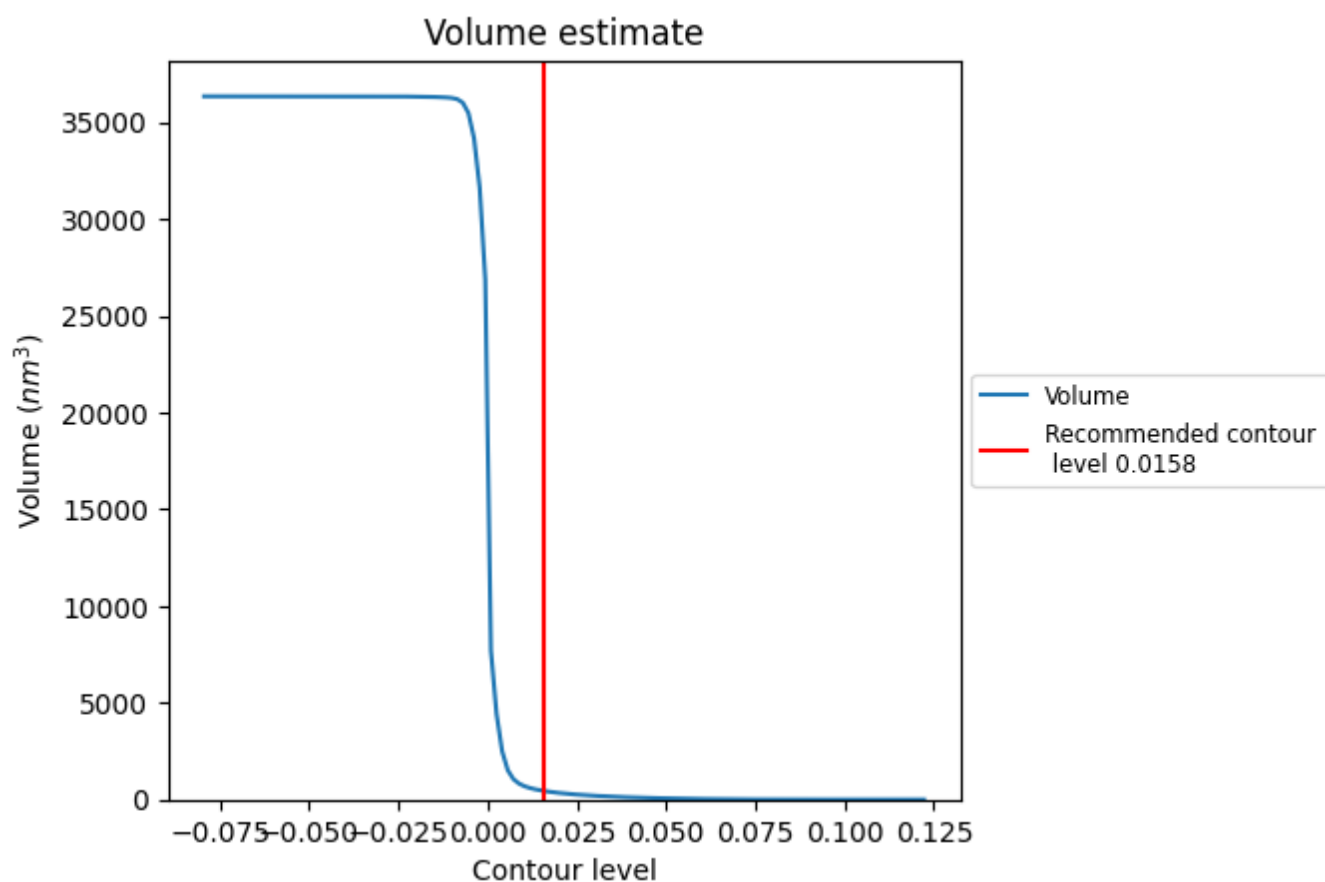
This section contains the results of statistical analysis of the map.

### 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.

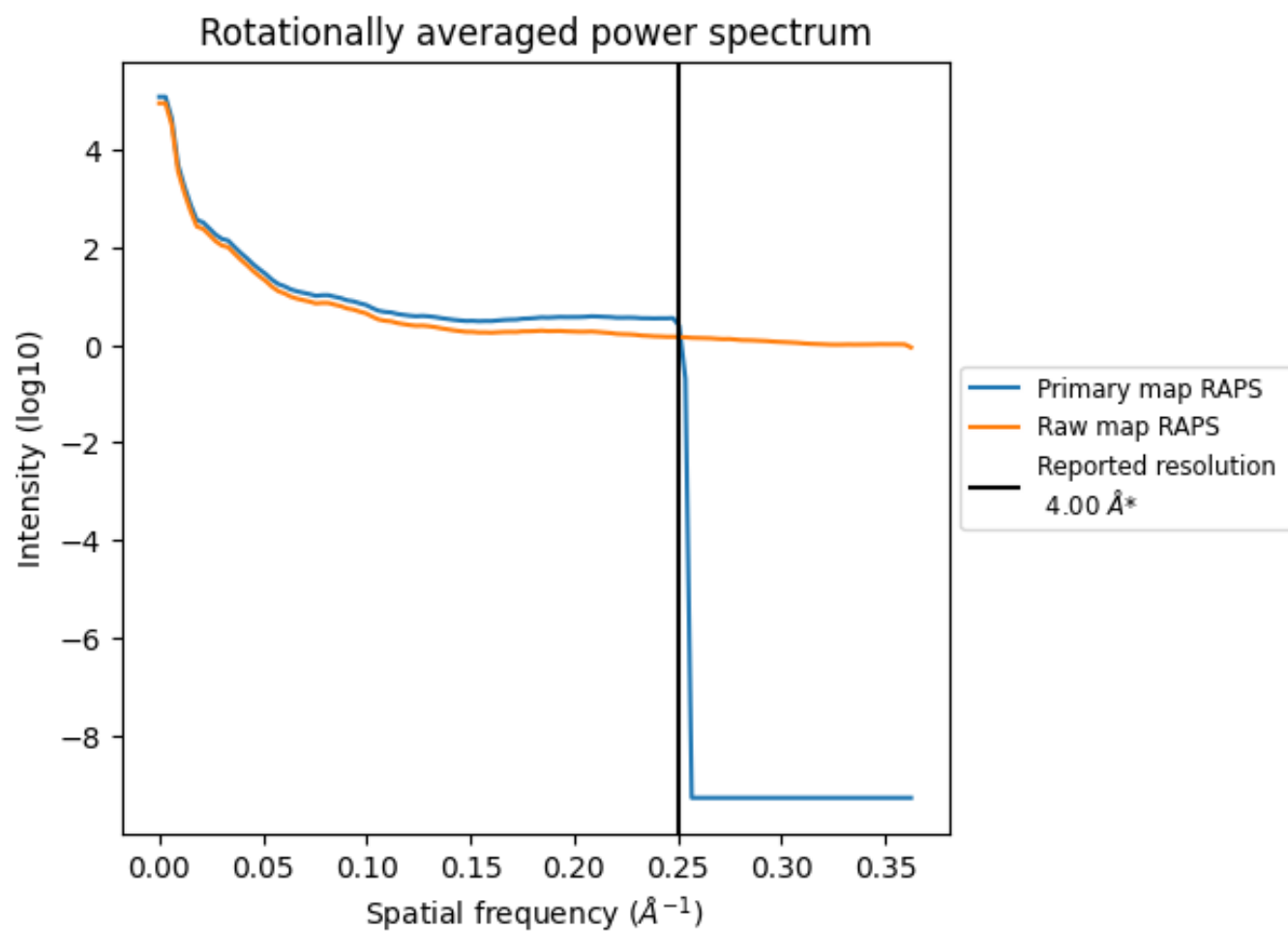
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 447 nm<sup>3</sup>; this corresponds to an approximate mass of 404 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 ⓘ

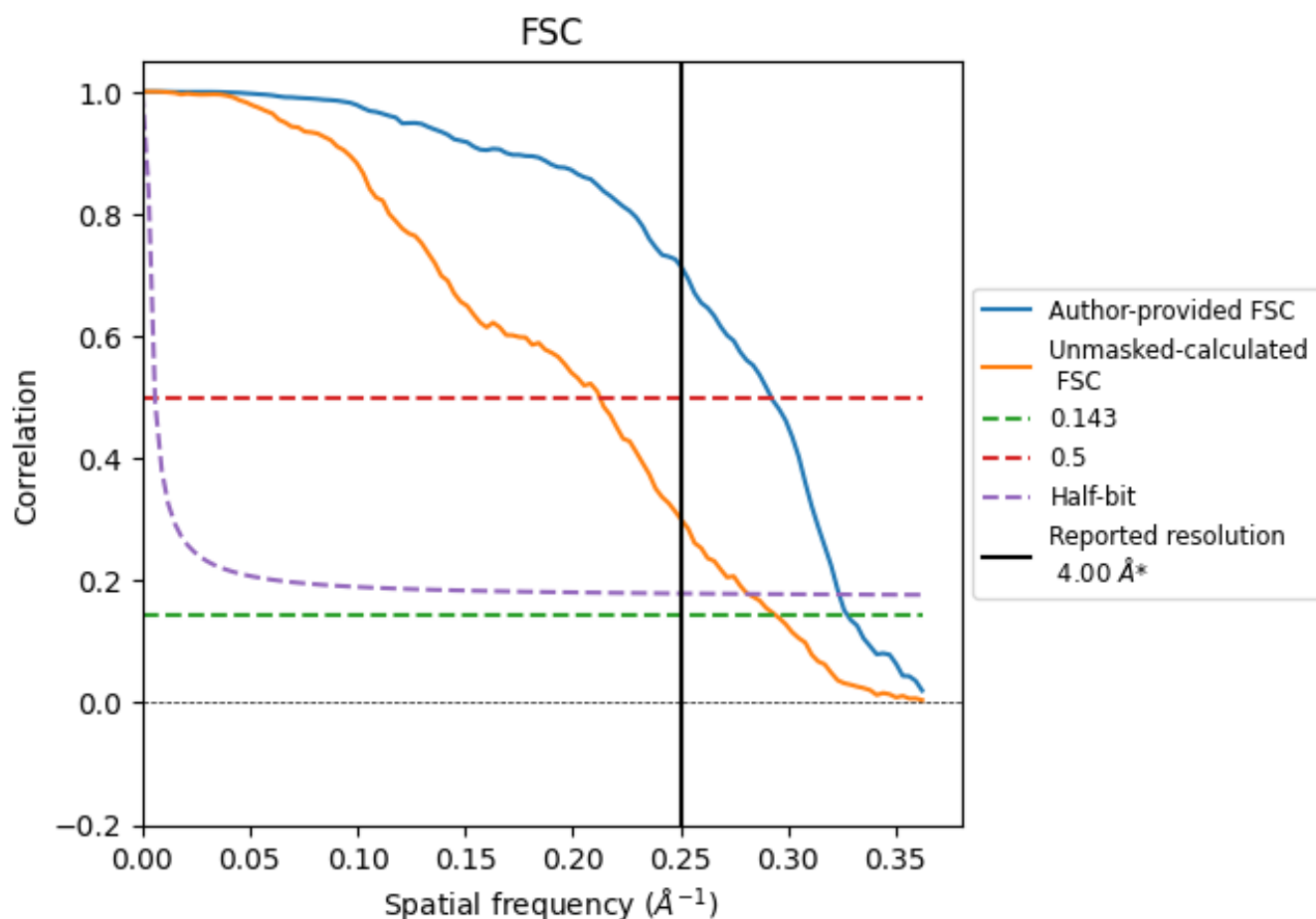


\*Reported resolution corresponds to spatial frequency of 0.250 Å<sup>-1</sup>

## 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  $0.250 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.05	3.42	3.09
Unmasked-calculated*	3.40	4.71	3.55

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.05 differs from the reported value 4.0 by more than 10 %

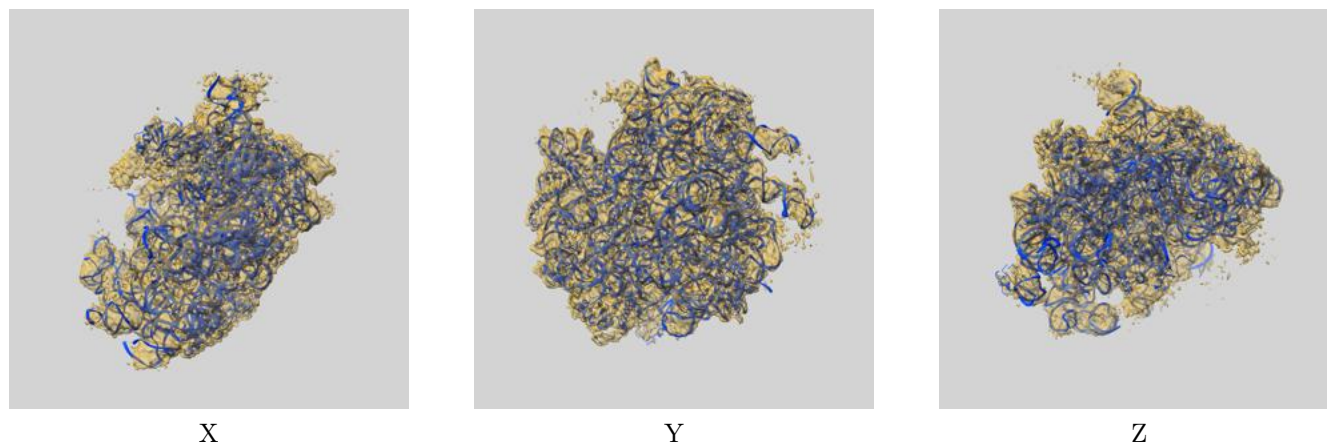
The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.40 differs from the reported value 4.0 by more than 10 %



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

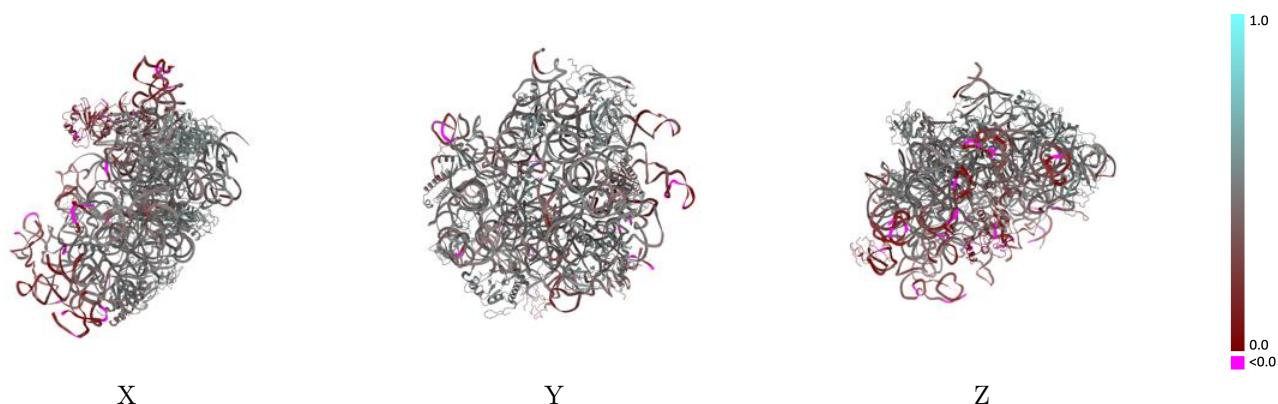
This section contains information regarding the fit between EMDB map EMD-61781 and PDB model 9JSR. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



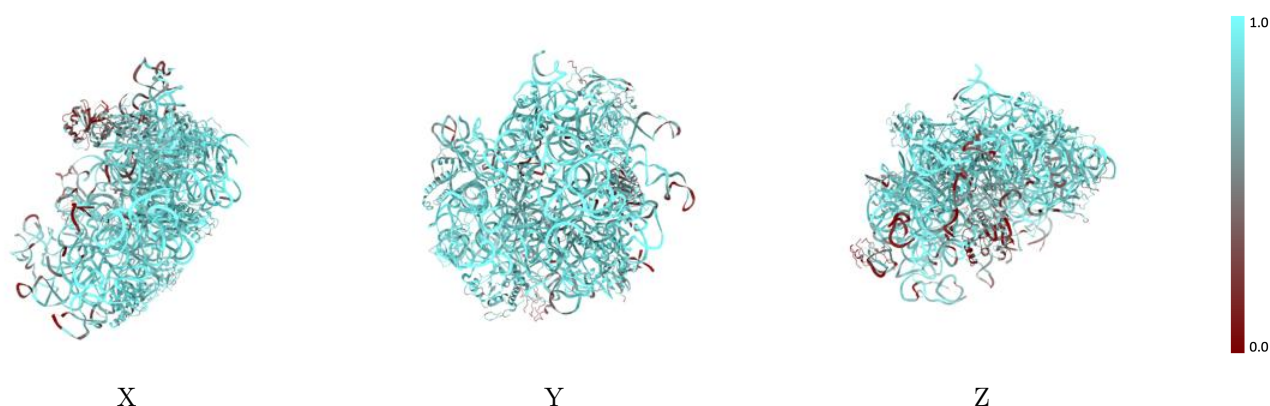
The images above show the 3D surface view of the map at the recommended contour level 0.0158 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



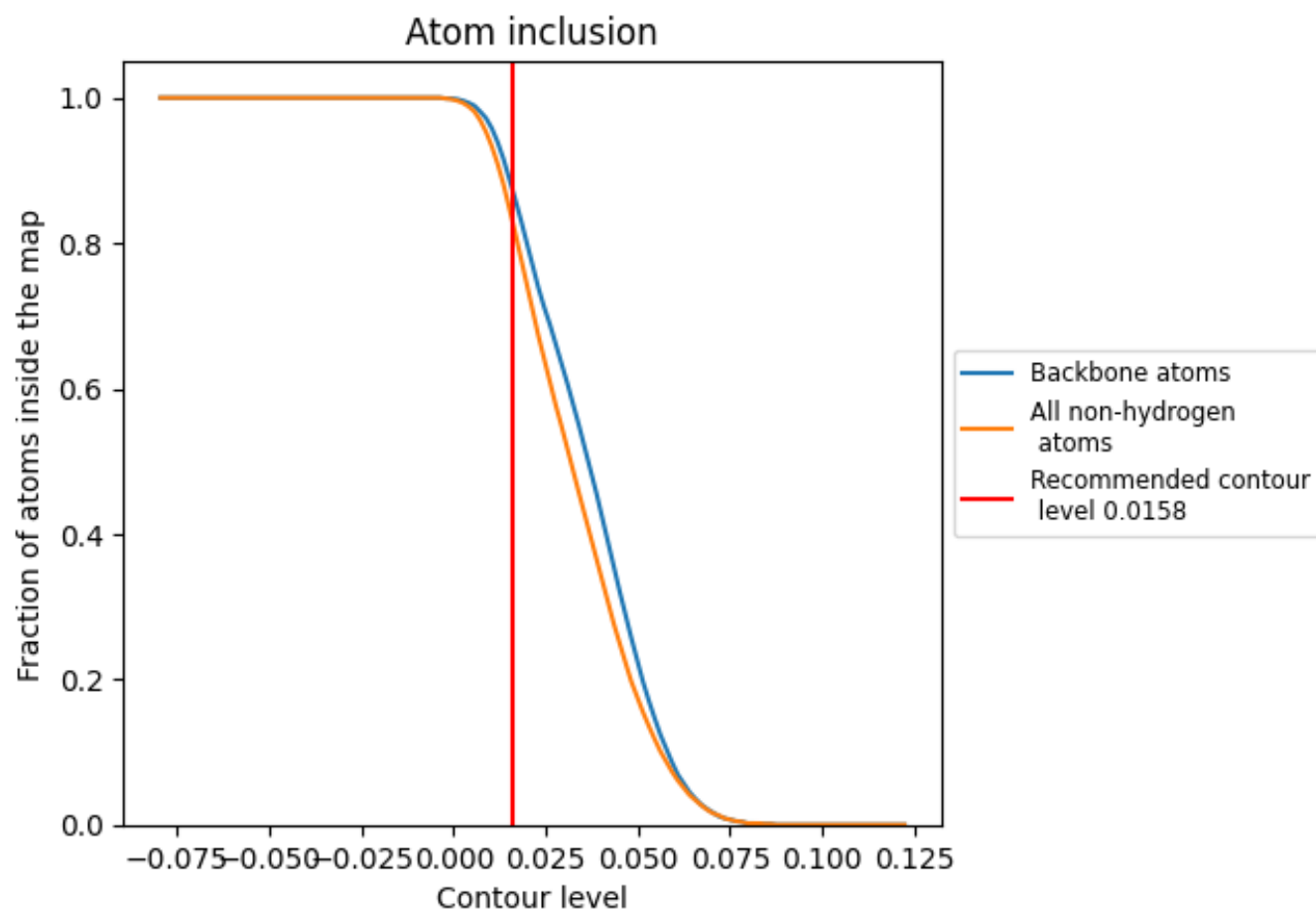
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0158).







































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.0158) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8350	 0.4060
0	 0.8730	 0.4990
2	 0.8310	 0.4830
A	 0.8650	 0.3870
C	 0.4810	 0.2510
D	 0.8630	 0.5150
E	 0.7930	 0.4840
J	 0.8490	 0.5000
K	 0.7390	 0.4470
L	 0.3860	 0.2860
N	 0.9010	 0.5050
P	 0.7620	 0.4730
Q	 0.8910	 0.5020
R	 0.8570	 0.5010
S	 0.8240	 0.5010
T	 0.8090	 0.4690
U	 0.8850	 0.4960
Y	 0.8330	 0.4300
Z	 0.7830	 0.4620

