



## Full wwPDB EM Validation Report ⓘ

Oct 1, 2025 – 02:18 PM JST

PDB ID : 9V1J / pdb\_00009v1j  
EMDB ID : EMD-64695  
Title : Cryo- EM structure of small subunit (body) of 75S ribosome with P- tRNA from *Entamoeba histolytica*  
Authors : Sharma, S.; Mishra, S.; Gourinath, S.; Kaushal, P.S.  
Deposited on : 2025-05-19  
Resolution : 3.10 Å (reported)  
Based on initial models : 4UG0, 5XXB

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:

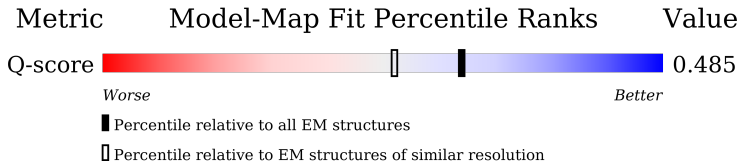
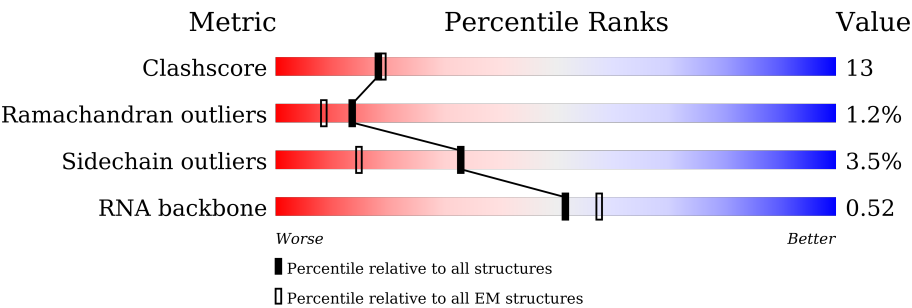
EMDB validation analysis : 0.0.1.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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	14724 ( 2.60 - 3.60 )

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	sB	144	<div><div></div><div>57%</div><div>10%</div><div>•</div><div>32%</div></div>
2	sC	84	<div><div>11%</div><div>65%</div><div>26%</div><div>5%</div><div>••</div></div>
3	sH	76	<div><div>46%</div><div>42%</div><div>11%</div><div>•</div></div>

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Mol	Chain	Length	Quality of chain
4	sK	6	100%
5	sa	1947	27% 19% 50%
6	sb	254	53% 13% 34%
7	sc	255	64% 20% 16%
8	se	256	64% 18% 17%
9	sf	326	54% 23% 21%
10	sh	266	12% 30% 21% 7% 6% 36%
11	si	201	9% 22% 10% 61%
12	sj	237	53% 18% 30%
13	sk	185	70% 15% 15%
14	sm	156	83% 15%
15	so	151	77% 21%
16	sp	146	67% 23% 9%
17	sr	130	78% 21%
18	sx	86	7% 71% 12% 17%
19	sy	141	60% 16% 10% 7% 8%
20	sz	140	8% 21% 19% 60%

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 41917 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 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	sB	98	Total	C	N	O	S	0	0
			787	478	169	134	6		

- Molecule 2 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	sC	83	Total	C	N	O	S	0	0
			641	407	117	111	6		

- Molecule 3 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	sH	75	Total	C	N	O	P	0	0
			1593	712	278	528	75		

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	sK	6	Total	C	N	O	P	0	0
			126	57	21	42	6		

- Molecule 5 is a RNA chain called 17S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	sa	981	Total	C	N	O	P	0	0
			20995	9399	3828	6787	981		

- Molecule 6 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	sb	168	Total	C	N	O	S	0	0
			1327	840	236	240	11		

- Molecule 7 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	sc	215	Total	C	N	O	S	0	0
			1642	1052	291	291	8		

- Molecule 8 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	se	212	Total	C	N	O	S	0	0
			1717	1097	305	306	9		

- Molecule 9 is a protein called 40S ribosomal protein S4, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	sf	256	Total	C	N	O	S	0	0
			2031	1297	378	345	11		

- Molecule 10 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	sh	169	Total	C	N	O	S	0	0
			1345	846	269	224	6		

- Molecule 11 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	si	79	Total	C	N	O	S	0	0
			615	394	114	106	1		

- Molecule 12 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	sj	167	Total	C	N	O	S	0	0
			1329	837	252	236	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	sk	158	Total	C	N	O	S	0	0
			1293	828	246	213	6		

- Molecule 14 is a protein called 40S ribosomal protein S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	sm	154	Total	C	N	O	S	0	0
			1263	796	243	217	7		

- Molecule 15 is a protein called 40S ribosomal protein S13, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	so	150	Total	C	N	O	S	0	0
			1184	756	218	204	6		

- Molecule 16 is a protein called Ribosomal protein S14, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	sp	133	Total	C	N	O	S	0	0
			999	615	192	186	6		

- Molecule 17 is a protein called 40S ribosomal protein S15a, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	sr	129	Total	C	N	O	S	0	0
			1022	650	186	181	5		

- Molecule 18 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	sx	71	Total	C	N	O	S	0	0
			560	356	101	100	3		

- Molecule 19 is a protein called 40S ribosomal protein S23, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	sy	130	Total	C	N	O	S	0	0
			1010	637	200	169	4		

- Molecule 20 is a protein called 40S ribosomal protein S24, putative.

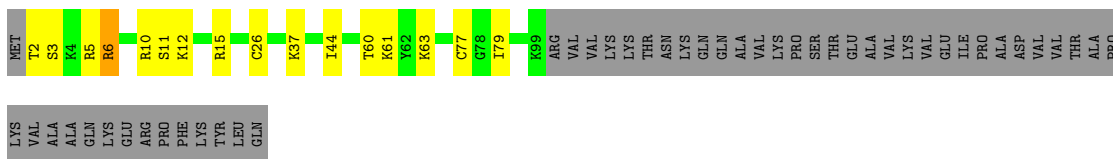
Mol	Chain	Residues	Atoms					AltConf	Trace
20	sz	56	Total	C	N	O	S	0	0
			438	288	74	75	1		

### 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.

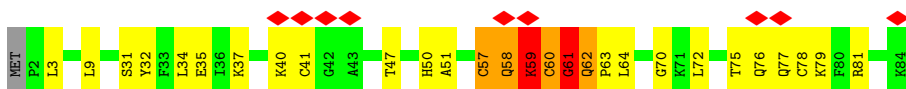
- Molecule 1: 40S ribosomal protein S26

Chain sB: 



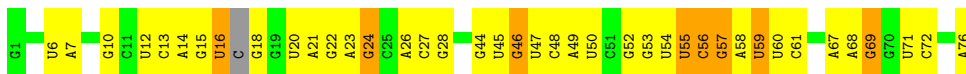
- Molecule 2: Small ribosomal subunit protein eS27

Chain sC: 



- Molecule 3: P-tRNA

Chain sH: 



- Molecule 4: mRNA

Chain sK: 

There are no outlier residues recorded for this chain.

- Molecule 5: 17S rRNA

Chain sa: 

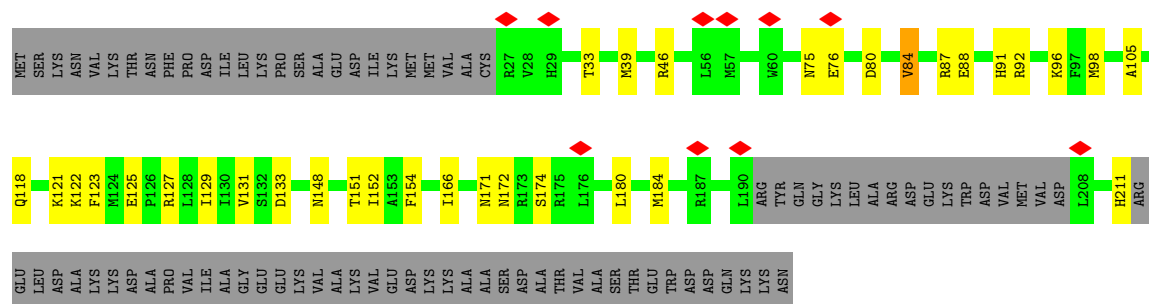




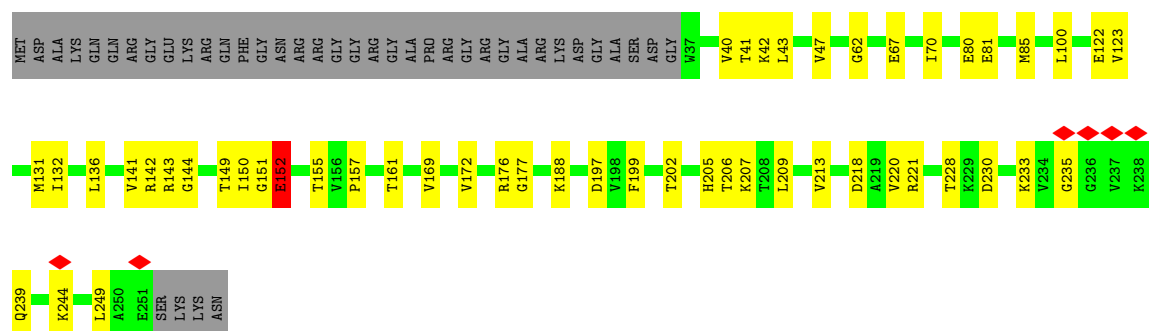


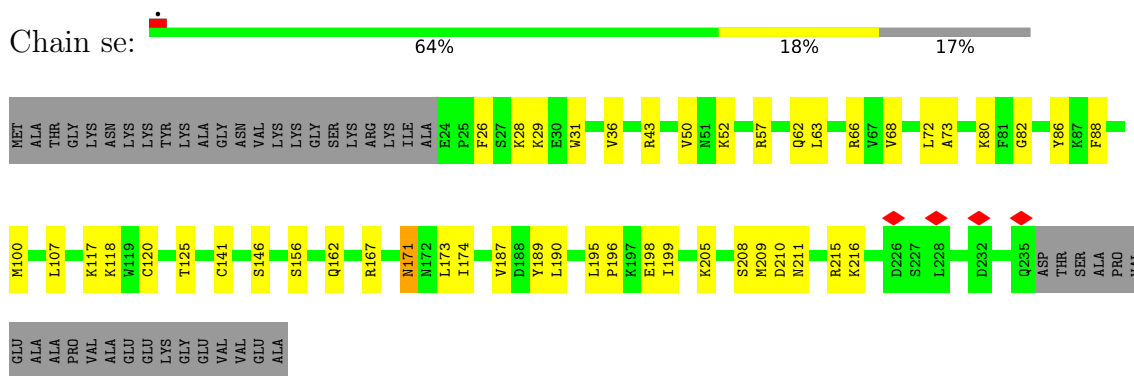


Chain sb: 

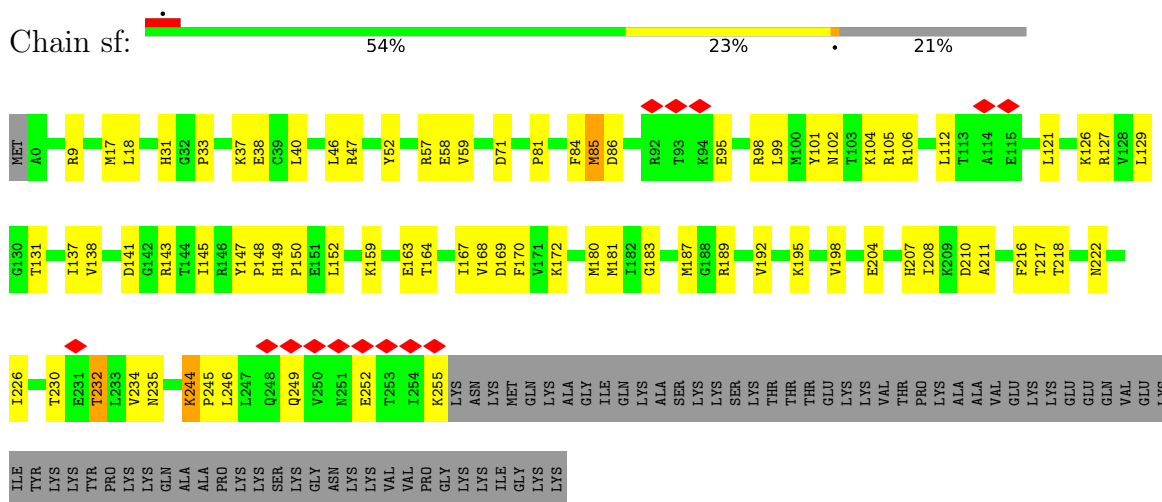


Chain sc: 

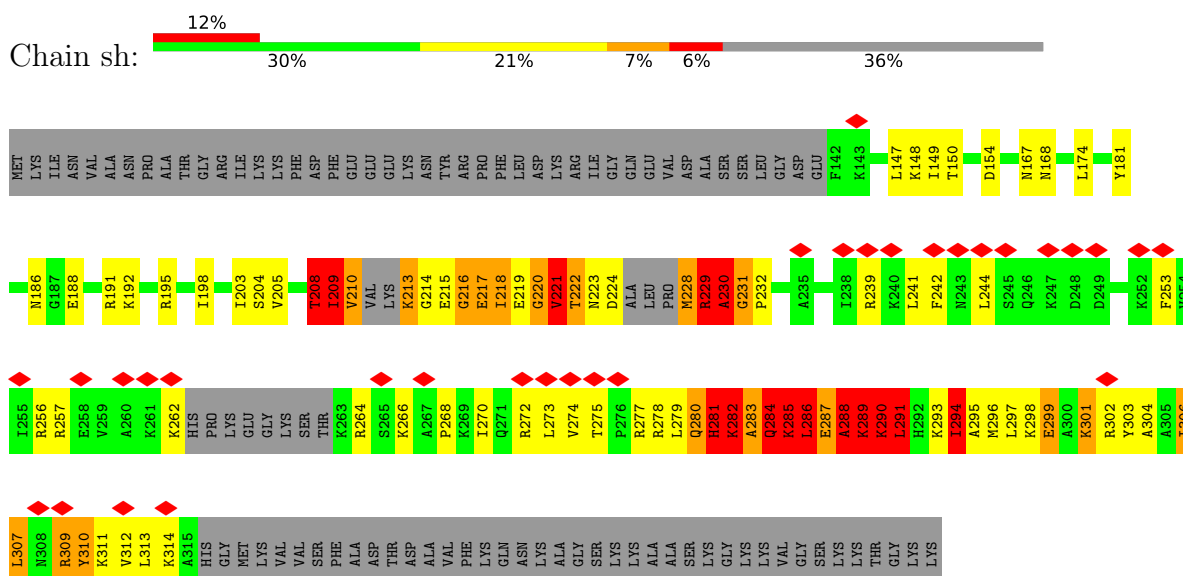




- Molecule 9: 40S ribosomal protein S4, putative



- Molecule 10: 40S ribosomal protein S6



- Molecule 11: 40S ribosomal protein S7



- Molecule 12: 40S ribosomal protein S8

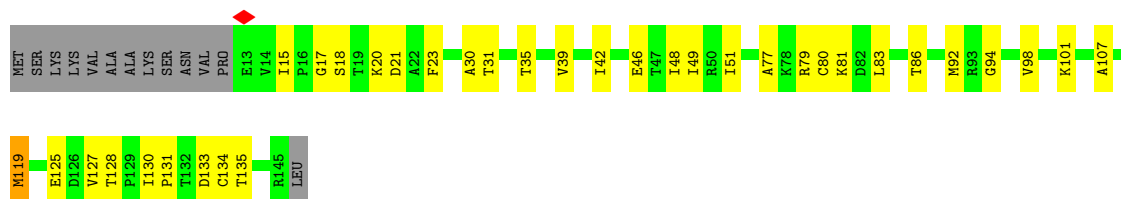
- Molecule 13: Small ribosomal subunit protein uS4

- Molecule 14: 40S ribosomal protein S11, putative


- Molecule 15: 40S ribosomal protein S13, putative

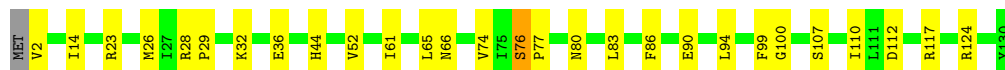
- Molecule 16: Ribosomal protein S14, putative

Chain sp:  67% 23% 9%



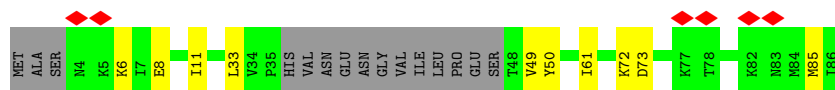
- Molecule 17: 40S ribosomal protein S15a, putative

Chain sr:  78% 21% 1%



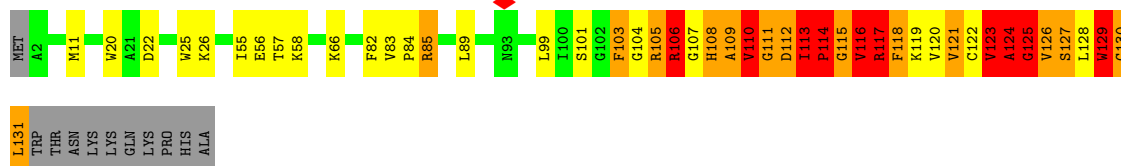
- Molecule 18: 40S ribosomal protein S21

Chain sx:  7% 71% 12% 17%



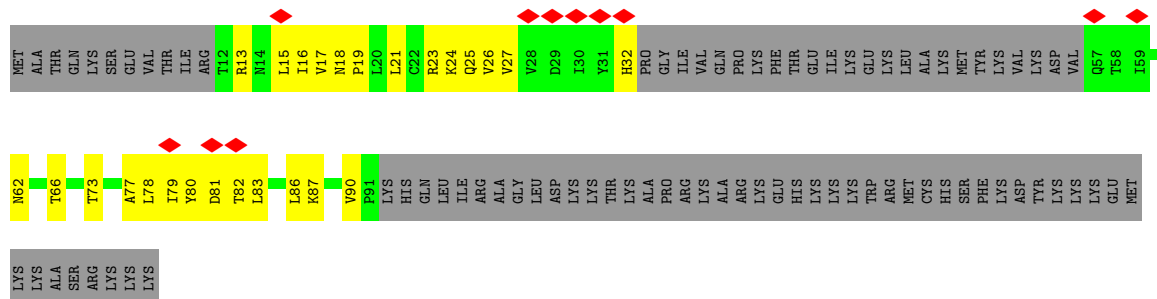
- Molecule 19: 40S ribosomal protein S23, putative

Chain sy:  60% 16% 10% 7% 8%



- Molecule 20: 40S ribosomal protein S24, putative

Chain sz:  8% 21% 19% 60%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53764	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 ( $e^-/\text{\AA}^2$ )	1.106	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	15.439	Depositor
Minimum map value	-4.365	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	288.90002, 288.90002, 288.90002	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	sB	0.15	0/797	0.28	0/1062
2	sC	1.06	11/654 (1.7%)	0.84	10/879 (1.1%)
3	sH	0.12	0/1778	0.29	0/2765
4	sK	0.11	0/140	0.22	0/215
5	sa	0.21	2/23516 (0.0%)	0.32	5/36630 (0.0%)
6	sb	0.15	0/1353	0.32	0/1829
7	sc	0.60	9/1673 (0.5%)	0.48	3/2257 (0.1%)
8	se	0.12	0/1741	0.25	0/2328
9	sf	0.15	0/2072	0.32	0/2792
10	sh	1.56	36/1357 (2.7%)	1.82	30/1799 (1.7%)
11	si	1.67	16/626 (2.6%)	1.47	18/842 (2.1%)
12	sj	0.13	0/1350	0.27	0/1804
13	sk	0.12	0/1313	0.23	0/1756
14	sm	0.14	0/1291	0.28	0/1725
15	so	0.13	0/1204	0.29	0/1613
16	sp	0.14	0/1013	0.30	0/1361
17	sr	0.15	0/1040	0.31	0/1404
18	sx	0.14	0/569	0.26	0/767
19	sy	1.58	34/1027 (3.3%)	1.54	32/1376 (2.3%)
20	sz	0.17	0/445	0.51	0/601
All	All	0.48	108/44959 (0.2%)	0.52	98/65805 (0.1%)

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
10	sh	0	2
17	sr	0	1
19	sy	0	1
All	All	0	4

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	si	118	LYS	CA-C	-15.53	1.34	1.52
10	sh	283	ALA	CA-C	-14.94	1.34	1.52
10	sh	282	LYS	CA-C	-13.64	1.34	1.52
10	sh	284	GLN	N-CA	-13.17	1.29	1.46
10	sh	218	ILE	CA-C	-12.76	1.36	1.52
11	si	119	PRO	N-CA	-11.42	1.32	1.47
19	sy	123	VAL	CA-CB	-11.36	1.42	1.54
10	sh	216	GLY	CA-C	-10.94	1.36	1.51
11	si	117	TYR	CA-C	-10.72	1.38	1.52
2	sC	59	LYS	CA-C	-10.33	1.39	1.52
19	sy	127	SER	N-CA	-10.16	1.33	1.46
2	sC	61	GLY	CA-C	-10.04	1.37	1.51
19	sy	113	ILE	N-CA	-9.74	1.34	1.46
10	sh	220	GLY	CA-C	-9.53	1.42	1.52
7	sc	151	GLY	CA-C	-9.50	1.39	1.51
2	sC	62	GLN	CA-C	-9.48	1.40	1.52
19	sy	120	VAL	C-O	-9.31	1.15	1.23
10	sh	230	ALA	CA-C	-9.25	1.40	1.52
7	sc	150	ILE	C-O	-9.24	1.13	1.24
10	sh	217	GLU	CA-C	9.01	1.65	1.52
2	sC	62	GLN	C-O	-8.94	1.12	1.24
10	sh	229	ARG	CA-C	-8.87	1.40	1.52
11	si	119	PRO	CA-CB	-8.79	1.41	1.53
11	si	118	LYS	C-O	-8.64	1.13	1.24
7	sc	152	GLU	C-N	-8.63	1.23	1.33
11	si	115	THR	CA-C	-8.59	1.42	1.52
10	sh	230	ALA	CA-CB	-8.45	1.39	1.53
11	si	117	TYR	C-O	-8.38	1.13	1.24
19	sy	126	VAL	CA-C	-8.36	1.42	1.52
10	sh	286	LEU	CA-C	-8.32	1.41	1.52
19	sy	128	LEU	CA-C	-8.23	1.41	1.52
10	sh	281	HIS	N-CA	-8.22	1.35	1.46
11	si	111	GLN	CA-C	-8.05	1.42	1.52
10	sh	288	ALA	CA-CB	-8.02	1.40	1.53
10	sh	290	LYS	CA-CB	-7.94	1.40	1.53
19	sy	130	GLY	CA-C	-7.80	1.40	1.51
10	sh	230	ALA	N-CA	-7.72	1.36	1.46
19	sy	106	ARG	CA-C	-7.70	1.46	1.53
7	sc	152	GLU	C-O	-7.69	1.14	1.23
19	sy	126	VAL	C-N	-7.67	1.24	1.33
19	sy	128	LEU	N-CA	-7.65	1.37	1.46
11	si	139	VAL	CA-C	-7.50	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	sh	231	GLY	CA-C	-7.46	1.41	1.51
19	sy	112	ASP	CA-C	-7.43	1.43	1.52
10	sh	287	GLU	N-CA	-7.25	1.36	1.46
10	sh	283	ALA	C-N	-7.22	1.23	1.33
19	sy	120	VAL	CA-C	-7.22	1.44	1.53
19	sy	106	ARG	C-O	-7.20	1.17	1.24
19	sy	114	PRO	CA-C	-7.18	1.42	1.52
19	sy	125	GLY	CA-C	-7.13	1.41	1.51
19	sy	116	VAL	CA-C	-7.13	1.44	1.52
5	sa	292	A	O3'-P	-7.10	1.50	1.61
19	sy	124	ALA	CA-C	-7.00	1.43	1.52
2	sC	62	GLN	N-CA	-6.95	1.36	1.46
19	sy	119	LYS	C-O	-6.92	1.16	1.24
10	sh	287	GLU	CA-C	-6.92	1.43	1.52
11	si	118	LYS	N-CA	-6.86	1.36	1.46
11	si	137	TYR	CA-C	-6.76	1.44	1.52
10	sh	288	ALA	N-CA	-6.74	1.37	1.46
7	sc	152	GLU	CA-CB	-6.67	1.43	1.53
10	sh	209	ILE	CA-CB	-6.65	1.46	1.54
10	sh	221	VAL	CA-C	-6.61	1.44	1.52
19	sy	114	PRO	CA-CB	-6.53	1.44	1.53
10	sh	284	GLN	C-O	-6.52	1.15	1.24
10	sh	284	GLN	CA-C	-6.45	1.44	1.52
19	sy	117	ARG	C-O	-6.44	1.16	1.24
19	sy	110	VAL	N-CA	-6.41	1.38	1.46
19	sy	122	CYS	CA-C	-6.29	1.44	1.52
19	sy	118	PHE	C-O	-6.22	1.15	1.23
11	si	139	VAL	N-CA	-6.22	1.39	1.46
11	si	110	GLY	CA-C	-6.20	1.44	1.51
7	sc	152	GLU	CA-C	-6.07	1.45	1.52
10	sh	290	LYS	CA-C	-6.07	1.44	1.52
10	sh	283	ALA	C-O	-5.96	1.17	1.24
11	si	118	LYS	CA-CB	-5.91	1.42	1.52
19	sy	118	PHE	CA-CB	-5.86	1.44	1.53
7	sc	149	THR	C-N	-5.85	1.26	1.33
2	sC	60	CYS	CA-CB	-5.84	1.43	1.53
19	sy	128	LEU	CA-CB	-5.81	1.44	1.52
10	sh	285	LYS	CA-C	-5.79	1.45	1.52
7	sc	151	GLY	C-O	-5.76	1.17	1.23
19	sy	120	VAL	CA-CB	-5.69	1.47	1.53
19	sy	110	VAL	CA-CB	-5.68	1.46	1.54
10	sh	282	LYS	CA-CB	-5.67	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	sy	130	GLY	C-O	-5.66	1.16	1.23
19	sy	127	SER	CA-C	-5.66	1.45	1.52
10	sh	286	LEU	N-CA	-5.65	1.39	1.46
10	sh	287	GLU	CA-CB	-5.64	1.44	1.53
2	sC	59	LYS	CA-CB	-5.63	1.44	1.53
5	sa	290	C	O3'-P	-5.62	1.52	1.61
19	sy	119	LYS	CA-C	-5.52	1.46	1.52
10	sh	230	ALA	C-O	-5.47	1.17	1.24
2	sC	61	GLY	N-CA	-5.46	1.37	1.45
7	sc	150	ILE	CA-CB	-5.46	1.46	1.54
2	sC	61	GLY	C-O	-5.43	1.16	1.23
2	sC	62	GLN	C-N	-5.36	1.21	1.33
19	sy	109	ALA	CA-C	-5.36	1.45	1.53
11	si	109	VAL	CA-CB	5.34	1.60	1.55
10	sh	289	LYS	C-O	-5.25	1.17	1.23
10	sh	220	GLY	C-N	-5.22	1.26	1.33
2	sC	58	GLN	N-CA	-5.22	1.39	1.46
19	sy	109	ALA	CA-CB	-5.22	1.44	1.53
19	sy	119	LYS	CA-CB	-5.21	1.45	1.53
11	si	112	SER	CA-C	-5.13	1.45	1.52
10	sh	285	LYS	C-O	-5.10	1.17	1.24
19	sy	112	ASP	CA-CB	-5.08	1.46	1.53
10	sh	281	HIS	CA-C	-5.07	1.45	1.52
10	sh	228	MET	N-CA	5.03	1.55	1.46

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	sh	210	VAL	CB-CA-C	-23.66	66.45	111.40
10	sh	289	LYS	N-CA-C	-22.44	85.24	113.97
10	sh	209	ILE	N-CA-C	22.19	135.28	110.21
10	sh	283	ALA	N-CA-C	-20.04	89.13	110.97
10	sh	231	GLY	CA-C-N	-18.77	99.09	120.11
10	sh	231	GLY	C-N-CA	-18.77	99.09	120.11
19	sy	128	LEU	N-CA-C	-17.94	86.97	111.55
10	sh	281	HIS	N-CA-C	-17.29	92.26	113.01
10	sh	284	GLN	N-CA-C	-12.88	83.37	110.80
10	sh	210	VAL	N-CA-C	12.82	146.91	111.00
11	si	137	TYR	CA-C-N	-12.60	105.06	119.05
11	si	137	TYR	C-N-CA	-12.60	105.06	119.05
19	sy	112	ASP	N-CA-C	-12.12	94.83	111.56
10	sh	210	VAL	N-CA-CB	-12.03	91.05	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	sy	103	PHE	O-C-N	-12.00	106.63	122.59
10	sh	222	THR	N-CA-C	11.54	127.24	108.55
19	sy	106	ARG	CB-CA-C	-11.42	103.41	116.54
10	sh	280	GLN	N-CA-C	-11.24	99.58	113.97
19	sy	125	GLY	CA-C-N	-11.10	111.87	123.08
19	sy	125	GLY	C-N-CA	-11.10	111.87	123.08
5	sa	291	A	C1'-C2'-O2'	-10.98	91.92	108.40
19	sy	124	ALA	N-CA-C	-9.82	89.89	110.80
11	si	118	LYS	CA-CB-CG	-9.74	94.62	114.10
7	sc	150	ILE	CB-CA-C	-9.69	99.20	110.73
19	sy	110	VAL	N-CA-CB	-9.65	95.30	111.23
10	sh	216	GLY	N-CA-C	-9.54	90.58	113.18
5	sa	293	U	C2'-C3'-O3'	-9.23	99.85	113.70
11	si	118	LYS	CA-C-N	-9.05	108.52	119.84
11	si	118	LYS	C-N-CA	-9.05	108.52	119.84
19	sy	129	TRP	N-CA-C	-8.86	91.94	110.80
11	si	110	GLY	N-CA-C	-8.51	101.97	113.37
10	sh	289	LYS	CB-CA-C	-8.42	94.92	109.07
7	sc	151	GLY	N-CA-C	-8.41	100.51	111.52
10	sh	218	ILE	N-CA-C	-8.39	91.89	109.34
10	sh	209	ILE	CB-CA-C	-8.39	102.06	111.45
10	sh	220	GLY	N-CA-C	-8.36	99.58	110.69
19	sy	104	GLY	N-CA-C	-8.25	93.62	113.18
19	sy	110	VAL	N-CA-C	8.22	126.44	109.34
10	sh	288	ALA	N-CA-C	-8.13	93.47	110.80
10	sh	217	GLU	N-CA-C	8.06	122.42	112.59
10	sh	280	GLN	O-C-N	7.66	131.75	122.48
19	sy	113	ILE	N-CA-CB	-7.52	100.68	111.21
11	si	112	SER	N-CA-C	-7.36	95.12	110.80
10	sh	209	ILE	N-CA-CB	-7.36	97.02	111.15
2	sC	62	GLN	N-CA-C	-7.28	93.71	109.81
19	sy	119	LYS	N-CA-C	7.24	120.21	108.34
19	sy	106	ARG	N-CA-C	7.05	119.03	108.31
10	sh	285	LYS	CB-CA-C	6.99	124.32	110.42
19	sy	120	VAL	N-CA-C	6.98	117.48	108.12
11	si	119	PRO	N-CA-C	-6.92	98.21	112.47
19	sy	113	ILE	CB-CA-C	6.92	123.96	111.36
19	sy	123	VAL	CB-CA-C	-6.85	102.97	112.36
11	si	137	TYR	N-CA-C	6.81	124.86	109.81
19	sy	119	LYS	CB-CA-C	-6.79	99.28	110.14
10	sh	282	LYS	CB-CA-C	-6.76	96.97	110.42
2	sC	58	GLN	N-CA-C	-6.73	104.89	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	si	165	VAL	N-CA-C	-6.59	92.56	111.00
19	sy	130	GLY	N-CA-C	-6.57	97.61	113.18
10	sh	224	ASP	N-CA-C	6.54	129.30	111.00
19	sy	127	SER	N-CA-CB	-6.49	100.03	111.39
2	sC	62	GLN	CA-C-N	-6.39	111.85	119.84
2	sC	62	GLN	C-N-CA	-6.39	111.85	119.84
11	si	115	THR	CB-CA-C	-6.32	98.33	109.71
5	sa	1091	C	C1'-C2'-O2'	-6.27	98.99	108.40
10	sh	282	LYS	N-CA-C	-6.17	97.67	110.80
10	sh	284	GLN	CA-C-O	-6.06	111.84	120.51
19	sy	128	LEU	CB-CA-C	-5.99	103.67	111.40
19	sy	112	ASP	N-CA-CB	5.94	120.15	111.54
11	si	119	PRO	CA-C-N	5.93	132.56	122.36
11	si	119	PRO	C-N-CA	5.93	132.56	122.36
5	sa	1091	C	C4'-C3'-O3'	-5.86	104.21	113.00
2	sC	57	CYS	CA-C-N	-5.84	111.38	121.66
2	sC	57	CYS	C-N-CA	-5.84	111.38	121.66
2	sC	59	LYS	CB-CA-C	-5.81	98.86	110.42
19	sy	112	ASP	CB-CA-C	-5.79	102.15	111.18
19	sy	115	GLY	N-CA-C	5.78	126.89	113.18
10	sh	208	THR	O-C-N	5.77	129.37	122.21
2	sC	60	CYS	CA-CB-SG	-5.75	101.17	114.40
10	sh	231	GLY	C-N-CD	5.74	148.52	125.00
19	sy	126	VAL	CB-CA-C	-5.68	106.05	111.44
11	si	118	LYS	CD-CE-NZ	5.67	130.06	111.90
19	sy	126	VAL	CA-C-N	-5.60	110.87	121.63
19	sy	126	VAL	C-N-CA	-5.60	110.87	121.63
19	sy	117	ARG	N-CA-CB	-5.52	103.93	111.65
19	sy	110	VAL	CB-CA-C	-5.38	102.46	111.29
19	sy	116	VAL	N-CA-CB	5.38	121.16	111.21
19	sy	111	GLY	N-CA-C	5.34	125.84	113.18
19	sy	129	TRP	N-CA-CB	5.29	119.43	110.49
10	sh	290	LYS	CB-CA-C	-5.28	99.91	110.42
11	si	109	VAL	N-CA-C	5.25	116.66	111.67
2	sC	60	CYS	CA-C-N	-5.18	111.25	121.41
2	sC	60	CYS	C-N-CA	-5.18	111.25	121.41
5	sa	238	G	C3'-C2'-O2'	-5.14	102.99	110.70
10	sh	281	HIS	CA-CB-CG	5.09	118.89	113.80
11	si	117	TYR	CA-C-N	-5.09	114.54	121.61
11	si	117	TYR	C-N-CA	-5.09	114.54	121.61
11	si	114	LYS	N-CA-CB	-5.08	103.58	111.35
7	sc	149	THR	O-C-N	-5.05	116.22	122.83

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	sh	208	THR	Mainchain
10	sh	284	GLN	Mainchain
17	sr	76	SER	Peptide
19	sy	103	PHE	Mainchain

## 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	sB	787	0	833	15	0
2	sC	641	0	681	33	0
3	sH	1593	0	806	22	0
4	sK	126	0	64	0	0
5	sa	20995	0	10547	337	0
6	sb	1327	0	1327	21	0
7	sc	1642	0	1721	36	0
8	se	1717	0	1824	32	0
9	sf	2031	0	2145	63	0
10	sh	1345	0	1467	189	0
11	si	615	0	648	64	0
12	sj	1329	0	1370	28	0
13	sk	1293	0	1396	22	0
14	sm	1263	0	1279	20	0
15	so	1184	0	1272	26	0
16	sp	999	0	1024	25	0
17	sr	1022	0	1051	21	0
18	sx	560	0	581	6	0
19	sy	1010	0	1067	84	0
20	sz	438	0	465	18	0
All	All	41917	0	31568	940	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 13.

All (940) 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)
10:sh:220:GLY:O	10:sh:221:VAL:HG23	1.32	1.22
10:sh:215:GLU:HG2	10:sh:220:GLY:CA	1.73	1.17
10:sh:215:GLU:HG2	10:sh:220:GLY:HA2	1.27	1.14
11:si:104:ALA:HB2	11:si:118:LYS:HE3	1.37	1.03
10:sh:280:GLN:HA	10:sh:283:ALA:HB2	1.41	1.02
10:sh:220:GLY:O	10:sh:221:VAL:CG2	2.09	1.01
10:sh:279:LEU:HB3	10:sh:282:LYS:HB3	1.43	1.01
10:sh:215:GLU:CG	10:sh:220:GLY:HA2	1.91	0.99
5:sa:956:G:H1	5:sa:1003:A:HO2'	0.98	0.97
5:sa:565:G:H4'	19:sy:106:ARG:CZ	1.94	0.96
5:sa:147:U:O4'	10:sh:223:ASN:OD1	1.83	0.96
2:sC:40:LYS:HE2	2:sC:60:CYS:CB	1.96	0.95
10:sh:284:GLN:HA	10:sh:287:GLU:HB3	1.50	0.93
5:sa:65:U:O4	10:sh:230:ALA:HA	1.70	0.92
9:sf:147:TYR:HB3	10:sh:307:LEU:HD13	1.52	0.92
10:sh:215:GLU:HG2	10:sh:220:GLY:HA3	1.55	0.89
10:sh:280:GLN:HA	10:sh:283:ALA:CB	2.03	0.89
2:sC:40:LYS:HE2	2:sC:60:CYS:HB3	1.57	0.86
5:sa:103:U:OP2	5:sa:305:A:N6	2.09	0.86
10:sh:284:GLN:HG3	10:sh:285:LYS:N	1.90	0.86
10:sh:284:GLN:O	10:sh:286:LEU:N	2.09	0.86
19:sy:127:SER:C	19:sy:129:TRP:H	1.82	0.84
10:sh:215:GLU:CB	10:sh:220:GLY:HA2	2.07	0.84
19:sy:106:ARG:HG2	19:sy:110:VAL:HA	1.58	0.82
10:sh:280:GLN:HA	10:sh:283:ALA:CA	2.09	0.82
5:sa:147:U:H1'	10:sh:223:ASN:HD21	1.44	0.82
10:sh:147:LEU:CD2	10:sh:210:VAL:HG11	2.09	0.82
11:si:104:ALA:HB2	11:si:118:LYS:CE	2.09	0.82
11:si:104:ALA:HB3	11:si:118:LYS:CG	2.10	0.81
10:sh:280:GLN:C	10:sh:282:LYS:H	1.87	0.81
10:sh:313:LEU:HD12	10:sh:314:LYS:H	1.44	0.81
5:sa:566:C:OP1	19:sy:106:ARG:HG3	1.82	0.80
10:sh:221:VAL:C	10:sh:222:THR:HG23	2.04	0.80
10:sh:287:GLU:HA	10:sh:289:LYS:HZ1	1.45	0.80
2:sC:62:GLN:O	2:sC:64:LEU:HD23	1.82	0.80
5:sa:389:U:H3	5:sa:396:A:H62	1.31	0.78
2:sC:62:GLN:O	2:sC:63:PRO:C	2.23	0.78
5:sa:262:G:H22	10:sh:285:LYS:HD3	1.48	0.78
19:sy:106:ARG:CD	19:sy:110:VAL:HG12	2.14	0.77
10:sh:215:GLU:C	10:sh:216:GLY:O	2.21	0.77
5:sa:145:U:H4'	10:sh:229:ARG:NH2	1.99	0.77
10:sh:147:LEU:HD22	10:sh:210:VAL:HG21	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:sy:106:ARG:HG2	19:sy:110:VAL:CA	2.14	0.77
5:sa:564:A:N6	19:sy:111:GLY:O	2.17	0.77
10:sh:280:GLN:C	10:sh:282:LYS:N	2.29	0.77
10:sh:209:ILE:HG23	10:sh:213:LYS:HG2	1.66	0.77
15:so:63:VAL:HG11	15:so:71:VAL:HG23	1.66	0.77
12:sj:42:ARG:HE	12:sj:59:ARG:HH21	1.33	0.76
10:sh:284:GLN:O	10:sh:287:GLU:N	2.18	0.76
10:sh:221:VAL:C	10:sh:222:THR:CG2	2.56	0.75
5:sa:401:U:H2'	5:sa:402:A:H8	1.49	0.75
9:sf:210:ASP:OD1	9:sf:211:ALA:N	2.20	0.74
19:sy:57:THR:HG23	19:sy:113:ILE:HG13	1.70	0.74
10:sh:284:GLN:CA	10:sh:287:GLU:HB3	2.17	0.74
11:si:107:LYS:O	11:si:111:GLN:HG2	1.87	0.74
5:sa:972:A:H2	5:sa:992:U:H3	1.35	0.74
9:sf:98:ARG:HB2	9:sf:112:LEU:HD11	1.69	0.74
5:sa:150:G:N2	5:sa:153:U:OP2	2.21	0.74
11:si:118:LYS:HD2	11:si:122:ARG:CB	2.17	0.74
11:si:118:LYS:HD2	11:si:122:ARG:HB3	1.70	0.73
8:se:173:LEU:HD21	8:se:198:GLU:HG2	1.69	0.73
10:sh:167:ASN:O	10:sh:195:ARG:NH1	2.21	0.73
10:sh:282:LYS:HD3	10:sh:286:LEU:HB3	1.68	0.73
3:sH:16:U:N3	3:sH:59:U:O2	2.18	0.73
15:so:99:ARG:NH2	15:so:119:GLU:OE2	2.22	0.73
14:sm:3:GLU:N	14:sm:3:GLU:OE1	2.21	0.73
5:sa:565:G:O2'	19:sy:106:ARG:HD2	1.89	0.73
19:sy:106:ARG:CZ	19:sy:110:VAL:HB	2.18	0.73
10:sh:147:LEU:HA	10:sh:210:VAL:HG11	1.71	0.72
5:sa:563:C:H5''	19:sy:85:ARG:HH11	1.53	0.72
5:sa:114:G:H5'	14:sm:129:ARG:HD2	1.70	0.72
19:sy:110:VAL:HG23	19:sy:111:GLY:H	1.54	0.72
5:sa:67:A:C6	10:sh:229:ARG:HD2	2.25	0.71
10:sh:294:ILE:HG23	10:sh:298:LYS:HB2	1.72	0.71
11:si:114:LYS:HG3	11:si:115:THR:H	1.53	0.71
10:sh:215:GLU:HA	10:sh:220:GLY:HA2	1.73	0.71
10:sh:221:VAL:O	10:sh:222:THR:CG2	2.39	0.71
10:sh:290:LYS:O	10:sh:291:LEU:C	2.28	0.71
10:sh:284:GLN:OE1	10:sh:288:ALA:HB2	1.91	0.71
11:si:137:TYR:HB3	11:si:138:PRO:HD3	1.73	0.70
5:sa:972:A:O2'	5:sa:1932:U:O2	2.09	0.70
5:sa:998:U:OP1	15:so:107:LYS:NZ	2.25	0.70
6:sb:33:THR:O	6:sb:46:ARG:NH1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:sh:147:LEU:HD23	10:sh:210:VAL:HG11	1.72	0.70
10:sh:280:GLN:O	10:sh:285:LYS:HB2	1.91	0.70
10:sh:307:LEU:HD12	10:sh:310:TYR:HE1	1.57	0.70
10:sh:147:LEU:HD22	10:sh:210:VAL:CG2	2.22	0.70
10:sh:280:GLN:CG	10:sh:283:ALA:HB2	2.22	0.70
10:sh:203:ILE:HG22	10:sh:217:GLU:OE2	1.92	0.70
11:si:104:ALA:CB	11:si:118:LYS:CE	2.69	0.70
2:sC:57:CYS:SG	2:sC:59:LYS:HB2	2.32	0.70
9:sf:195:LYS:HB3	9:sf:207:HIS:HB2	1.73	0.69
10:sh:278:ARG:O	10:sh:281:HIS:HB2	1.92	0.69
11:si:104:ALA:CB	11:si:118:LYS:HE3	2.20	0.69
19:sy:106:ARG:N	19:sy:106:ARG:HD3	2.05	0.69
10:sh:147:LEU:CD2	10:sh:210:VAL:HG21	2.22	0.69
6:sb:129:ILE:HB	6:sb:151:THR:HG22	1.75	0.69
11:si:117:TYR:O	11:si:118:LYS:NZ	2.25	0.69
10:sh:209:ILE:C	10:sh:210:VAL:HG13	2.17	0.69
19:sy:127:SER:C	19:sy:129:TRP:N	2.44	0.69
5:sa:797:G:OP2	5:sa:797:G:N2	2.22	0.69
11:si:163:VAL:HG22	11:si:198:PRO:HG3	1.74	0.69
5:sa:563:C:H5''	19:sy:85:ARG:NH1	2.08	0.69
10:sh:209:ILE:HG23	10:sh:213:LYS:N	2.06	0.69
5:sa:604:G:HO2'	5:sa:607:G:HO2'	1.35	0.68
9:sf:58:GLU:OE1	20:sz:23:ARG:NH1	2.26	0.68
2:sC:40:LYS:NZ	2:sC:41:CYS:SG	2.67	0.68
5:sa:783:A:N7	5:sa:784:U:O2'	2.26	0.68
8:se:31:TRP:NE1	16:sp:17:GLY:O	2.27	0.68
10:sh:228:MET:O	10:sh:229:ARG:C	2.35	0.68
5:sa:840:U:C4	5:sa:841:U:O4	2.47	0.68
9:sf:105:ARG:HD3	9:sf:187:MET:HB2	1.75	0.68
5:sa:147:U:H1'	10:sh:223:ASN:ND2	2.07	0.68
10:sh:221:VAL:O	10:sh:222:THR:HG22	1.93	0.68
10:sh:279:LEU:O	10:sh:283:ALA:HA	1.94	0.67
5:sa:295:A:N7	9:sf:37:LYS:NZ	2.40	0.67
5:sa:794:U:H2'	5:sa:795:G:H8	1.59	0.67
16:sp:20:LYS:HE2	16:sp:20:LYS:HA	1.75	0.67
17:sr:80:ASN:OD1	17:sr:124:ARG:NH1	2.28	0.67
5:sa:390:U:O2'	10:sh:186:ASN:ND2	2.27	0.67
9:sf:9:ARG:HH21	9:sf:18:LEU:HD22	1.59	0.67
10:sh:231:GLY:O	10:sh:232:PRO:C	2.31	0.67
3:sH:22:G:N7	3:sH:46:G:O6	2.27	0.67
10:sh:286:LEU:HD22	10:sh:289:LYS:NZ	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:sC:75:THR:OG1	2:sC:78:CYS:SG	2.53	0.66
11:si:117:TYR:O	11:si:117:TYR:CG	2.42	0.66
5:sa:1852:G:O6	5:sa:1863:A:N6	2.28	0.66
5:sa:394:A:OP1	12:sj:49:ARG:NH2	2.28	0.66
5:sa:841:U:OP1	15:so:64:LYS:NZ	2.29	0.66
7:sc:218:ASP:OD1	7:sc:221:ARG:NH1	2.28	0.66
5:sa:125:U:O2'	5:sa:203:C:O2	2.13	0.66
19:sy:131:LEU:O	19:sy:131:LEU:HD13	1.95	0.66
10:sh:290:LYS:O	10:sh:293:LYS:N	2.28	0.66
10:sh:282:LYS:O	10:sh:283:ALA:C	2.35	0.66
10:sh:215:GLU:CA	10:sh:220:GLY:HA2	2.25	0.66
10:sh:282:LYS:HD3	10:sh:287:GLU:H	1.60	0.65
5:sa:774:U:H5''	5:sa:775:G:C5	2.32	0.65
9:sf:71:ASP:OD2	9:sf:143:ARG:NH2	2.29	0.65
10:sh:314:LYS:O	10:sh:314:LYS:HG2	1.96	0.65
2:sC:75:THR:HG1	2:sC:78:CYS:HG	1.44	0.65
5:sa:147:U:C1'	10:sh:223:ASN:OD1	2.45	0.65
5:sa:67:A:N1	10:sh:229:ARG:HD2	2.12	0.65
5:sa:76:U:O2	10:sh:256:ARG:NH1	2.30	0.65
5:sa:781:G:OP1	9:sf:104:LYS:NZ	2.30	0.65
5:sa:67:A:N6	10:sh:229:ARG:HD2	2.12	0.65
5:sa:345:A:H5''	5:sa:346:U:H3'	1.79	0.65
5:sa:565:G:H4'	19:sy:106:ARG:NE	2.11	0.65
9:sf:102:ASN:HD21	9:sf:106:ARG:HB3	1.60	0.65
15:so:4:MET:SD	15:so:124:ARG:NH1	2.70	0.65
8:se:36:VAL:O	8:se:43:ARG:NH1	2.30	0.64
10:sh:220:GLY:C	10:sh:221:VAL:HG23	2.18	0.64
5:sa:1839:A:OP1	10:sh:191:ARG:NH2	2.31	0.64
17:sr:94:LEU:HD12	17:sr:100:GLY:HA3	1.79	0.64
7:sc:169:VAL:HG22	7:sc:202:THR:HG22	1.80	0.64
8:se:174:ILE:HG13	8:se:195:LEU:HD21	1.79	0.64
10:sh:284:GLN:HG3	10:sh:285:LYS:H	1.63	0.64
1:sB:2:THR:OG1	1:sB:3:SER:N	2.19	0.64
15:so:24:SER:O	15:so:27:LYS:NZ	2.31	0.64
5:sa:162:U:H5''	10:sh:232:PRO:HA	1.80	0.64
10:sh:280:GLN:CA	10:sh:283:ALA:HB2	2.22	0.64
12:sj:207:SER:HB3	12:sj:216:GLU:HB2	1.80	0.64
5:sa:324:G:H5''	12:sj:98:LYS:HB3	1.80	0.64
2:sC:31:SER:HB3	2:sC:50:HIS:CD2	2.33	0.63
5:sa:203:C:H5	5:sa:255:G:H21	1.46	0.63
10:sh:147:LEU:HA	10:sh:210:VAL:CG1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:sh:287:GLU:O	10:sh:288:ALA:HB2	1.97	0.63
2:sC:50:HIS:ND1	2:sC:70:GLY:O	2.31	0.63
19:sy:106:ARG:HG2	19:sy:110:VAL:HG12	1.81	0.63
19:sy:106:ARG:CG	19:sy:110:VAL:HG12	2.28	0.63
5:sa:933:A:H2'	5:sa:934:A:C8	2.34	0.63
5:sa:60:A:HO2'	5:sa:262:G:HO2'	1.44	0.63
3:sH:18:G:H1	3:sH:55:U:HO2'	1.45	0.62
5:sa:932:C:H2'	5:sa:933:A:C8	2.34	0.62
10:sh:221:VAL:HG12	10:sh:222:THR:N	2.14	0.62
5:sa:566:C:P	19:sy:106:ARG:HG3	2.39	0.62
5:sa:561:A:H62	5:sa:570:G:H21	1.46	0.62
5:sa:401:U:H2'	5:sa:402:A:C8	2.32	0.62
10:sh:287:GLU:CA	10:sh:289:LYS:HZ1	2.12	0.62
19:sy:106:ARG:CD	19:sy:106:ARG:N	2.61	0.62
19:sy:110:VAL:CG2	19:sy:111:GLY:H	2.07	0.62
8:se:50:VAL:HG11	8:se:63:LEU:HD11	1.81	0.62
10:sh:298:LYS:HA	10:sh:301:LYS:HG3	1.82	0.62
10:sh:309:ARG:O	10:sh:312:VAL:HG12	2.00	0.62
15:so:35:ASP:OD1	15:so:36:GLU:N	2.32	0.62
5:sa:566:C:P	19:sy:106:ARG:HH11	2.23	0.62
5:sa:209:A:N6	5:sa:250:G:O6	2.33	0.61
11:si:105:HIS:HB2	11:si:116:ASP:OD2	1.99	0.61
2:sC:32:TYR:HE1	2:sC:34:LEU:HD23	1.66	0.61
10:sh:181:TYR:OH	10:sh:188:GLU:OE1	2.18	0.61
10:sh:279:LEU:HB3	10:sh:282:LYS:CB	2.26	0.61
3:sH:21:A:H61	3:sH:46:G:H2'	1.65	0.61
5:sa:866:G:N2	16:sp:133:ASP:OD1	2.33	0.61
14:sm:56:LYS:HD3	14:sm:131:LEU:HB3	1.82	0.61
19:sy:110:VAL:HG23	19:sy:111:GLY:N	2.14	0.61
2:sC:61:GLY:O	2:sC:63:PRO:HD3	2.00	0.61
5:sa:138:G:H2'	5:sa:139:G:C8	2.34	0.61
9:sf:17:MET:HE3	9:sf:106:ARG:HG3	1.82	0.61
5:sa:866:G:OP1	8:se:216:LYS:NZ	2.33	0.61
10:sh:242:PHE:HD2	10:sh:253:PHE:HB3	1.66	0.61
19:sy:113:ILE:O	19:sy:114:PRO:C	2.43	0.61
5:sa:1014:C:HO2'	17:sr:2:VAL:N	1.99	0.61
5:sa:366:G:N2	5:sa:606:U:O2	2.34	0.61
5:sa:872:A:H2'	5:sa:873:A:C8	2.36	0.60
10:sh:280:GLN:C	10:sh:283:ALA:H	2.09	0.60
10:sh:280:GLN:HG3	10:sh:283:ALA:HB2	1.82	0.60
3:sH:26:A:H61	3:sH:44:G:H1	1.46	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:sh:229:ARG:O	10:sh:230:ALA:HB3	2.00	0.60
10:sh:239:ARG:HA	10:sh:244:LEU:HB2	1.82	0.60
3:sH:60:U:H5''	3:sH:61:C:H5	1.67	0.60
10:sh:307:LEU:HD11	10:sh:311:LYS:HZ1	1.67	0.59
20:sz:86:LEU:HG	20:sz:90:VAL:HG21	1.84	0.59
10:sh:213:LYS:N	10:sh:213:LYS:HZ2	2.01	0.59
8:se:66:ARG:HH12	16:sp:46:GLU:HG2	1.67	0.59
10:sh:296:MET:O	10:sh:299:GLU:HB3	2.02	0.59
6:sb:87:ARG:NH2	6:sb:172:ASN:O	2.35	0.59
2:sC:62:GLN:OE1	2:sC:63:PRO:HD2	2.03	0.59
5:sa:389:U:O4	5:sa:396:A:N7	2.36	0.59
5:sa:794:U:H2'	5:sa:795:G:C8	2.38	0.59
5:sa:565:G:H5''	19:sy:106:ARG:NH1	2.18	0.59
6:sb:154:PHE:O	6:sb:172:ASN:ND2	2.34	0.59
9:sf:17:MET:HE1	9:sf:106:ARG:HE	1.68	0.59
19:sy:56:GLU:O	19:sy:114:PRO:HG2	2.03	0.59
5:sa:934:A:H2'	5:sa:935:C:H6	1.68	0.58
7:sc:230:ASP:N	7:sc:230:ASP:OD1	2.35	0.58
15:so:16:ILE:HD12	15:so:62:LEU:HD11	1.85	0.58
19:sy:58:LYS:HD2	19:sy:113:ILE:HG23	1.83	0.58
5:sa:387:G:OP1	5:sa:1876:U:O2'	2.21	0.58
11:si:118:LYS:HD3	11:si:119:PRO:CD	2.32	0.58
5:sa:158:A:H4'	10:sh:150:THR:HG23	1.84	0.58
5:sa:328:C:C5	12:sj:49:ARG:HD2	2.38	0.58
5:sa:558:G:N1	5:sa:574:A:OP2	2.35	0.58
10:sh:174:LEU:HD12	10:sh:192:LYS:HB2	1.86	0.58
11:si:162:PHE:CD2	11:si:163:VAL:HG23	2.38	0.58
20:sz:26:VAL:HG23	20:sz:77:ALA:HB3	1.85	0.58
5:sa:1161:U:P	19:sy:117:ARG:HH22	2.26	0.58
10:sh:275:THR:OG1	10:sh:278:ARG:N	2.35	0.58
11:si:128:HIS:ND1	11:si:191:GLU:OE2	2.32	0.58
17:sr:52:VAL:HG22	17:sr:61:ILE:HG12	1.84	0.58
5:sa:395:G:H5''	12:sj:25:LYS:HA	1.85	0.58
5:sa:65:U:C5	10:sh:268:PRO:HG3	2.39	0.58
5:sa:769:C:H2'	5:sa:770:A:C8	2.39	0.58
5:sa:865:A:H2'	5:sa:866:G:C8	2.39	0.57
11:si:118:LYS:C	11:si:119:PRO:O	2.38	0.57
5:sa:746:A:H2'	5:sa:747:A:C8	2.39	0.57
5:sa:295:A:N6	9:sf:38:GLU:OE2	2.37	0.57
8:se:26:PHE:HA	8:se:29:LYS:HG3	1.86	0.57
10:sh:205:VAL:HG22	10:sh:216:GLY:HA2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:se:57:ARG:NH1	8:se:62:GLN:OE1	2.35	0.57
8:se:189:TYR:HE1	8:se:195:LEU:HB2	1.69	0.57
10:sh:307:LEU:HD11	10:sh:311:LYS:NZ	2.19	0.57
15:so:87:ASP:OD1	15:so:87:ASP:N	2.34	0.57
19:sy:99:LEU:HB3	19:sy:121:VAL:HG22	1.86	0.57
19:sy:57:THR:HG22	19:sy:113:ILE:HG21	1.86	0.57
10:sh:298:LYS:O	10:sh:302:ARG:N	2.32	0.57
10:sh:209:ILE:HD13	10:sh:213:LYS:HB2	1.87	0.57
10:sh:282:LYS:NZ	10:sh:287:GLU:HB2	2.18	0.57
5:sa:107:A:H2'	5:sa:108:G:C8	2.40	0.57
10:sh:221:VAL:HG12	10:sh:222:THR:H	1.70	0.57
10:sh:279:LEU:CB	10:sh:282:LYS:HB3	2.26	0.56
5:sa:877:G:H1	5:sa:894:G:HO2'	1.51	0.56
6:sb:152:ILE:HG12	6:sb:166:ILE:HB	1.86	0.56
11:si:118:LYS:CE	11:si:122:ARG:HD2	2.34	0.56
5:sa:380:A:OP1	12:sj:25:LYS:NZ	2.34	0.56
10:sh:313:LEU:HD12	10:sh:314:LYS:N	2.19	0.56
11:si:163:VAL:HA	11:si:198:PRO:HD3	1.87	0.56
1:sB:26:CYS:HB2	1:sB:77:CYS:SG	2.45	0.56
11:si:104:ALA:HB3	11:si:118:LYS:HG3	1.86	0.56
1:sB:10:ARG:NH2	5:sa:1937:A:OP2	2.37	0.56
6:sb:148:ASN:ND2	7:sc:62:GLY:O	2.38	0.56
5:sa:549:A:N3	5:sa:584:C:O2'	2.35	0.56
6:sb:121:LYS:C	6:sb:121:LYS:HD2	2.31	0.56
7:sc:85:MET:HE2	7:sc:123:VAL:HG13	1.88	0.56
10:sh:280:GLN:N	10:sh:282:LYS:H	2.03	0.56
10:sh:287:GLU:O	10:sh:288:ALA:CB	2.54	0.56
19:sy:57:THR:HG22	19:sy:58:LYS:H	1.71	0.56
5:sa:1838:A:H2'	5:sa:1839:A:C8	2.41	0.56
10:sh:282:LYS:HD3	10:sh:286:LEU:CB	2.36	0.56
11:si:137:TYR:HB3	11:si:138:PRO:CD	2.36	0.56
5:sa:64:A:H2	5:sa:83:A:H62	1.54	0.55
10:sh:286:LEU:HD22	10:sh:289:LYS:HZ3	1.70	0.55
5:sa:762:A:OP1	13:sk:9:SER:OG	2.24	0.55
10:sh:209:ILE:HD12	10:sh:213:LYS:N	2.21	0.55
11:si:118:LYS:HZ2	11:si:122:ARG:CD	2.18	0.55
5:sa:622:G:N1	5:sa:950:A:OP2	2.26	0.55
8:se:88:PHE:HB3	8:se:100:MET:HB3	1.89	0.55
10:sh:204:SER:O	10:sh:217:GLU:HG3	2.06	0.55
11:si:117:TYR:O	11:si:118:LYS:CE	2.55	0.55
5:sa:564:A:N1	19:sy:113:ILE:HD11	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:sb:84:VAL:HG22	6:sb:131:VAL:HG12	1.88	0.55
9:sf:198:VAL:HG23	9:sf:204:GLU:HG3	1.89	0.55
12:sj:78:ILE:HA	12:sj:104:ILE:HG22	1.89	0.55
19:sy:112:ASP:O	19:sy:113:ILE:C	2.49	0.55
2:sC:57:CYS:SG	2:sC:58:GLN:N	2.79	0.55
5:sa:919:A:H2'	5:sa:920:A:C8	2.41	0.55
8:se:146:SER:HG	8:se:208:SER:HG	1.53	0.55
19:sy:57:THR:HG23	19:sy:113:ILE:CG1	2.34	0.55
5:sa:17:C:O2'	5:sa:1163:A:N1	2.36	0.55
5:sa:563:C:C4'	19:sy:85:ARG:HH12	2.20	0.55
10:sh:280:GLN:CA	10:sh:283:ALA:N	2.70	0.55
5:sa:145:U:H5'	10:sh:229:ARG:HH12	1.72	0.55
5:sa:563:C:OP1	19:sy:85:ARG:HA	2.06	0.55
5:sa:565:G:C4'	19:sy:106:ARG:CZ	2.79	0.55
6:sb:87:ARG:NH1	6:sb:133:ASP:OD2	2.34	0.55
11:si:161:VAL:HG23	11:si:193:VAL:HG11	1.89	0.55
13:sk:17:VAL:O	13:sk:23:ARG:NH1	2.34	0.55
19:sy:20:TRP:HE3	19:sy:26:LYS:HG3	1.71	0.55
2:sC:3:LEU:HD13	18:sx:61:ILE:HG12	1.89	0.55
9:sf:163:GLU:HG2	9:sf:164:THR:HG23	1.89	0.55
5:sa:243:U:OP1	14:sm:33:TYR:OH	2.21	0.54
8:se:117:LYS:NZ	8:se:210:ASP:OD2	2.39	0.54
20:sz:24:LYS:HB2	20:sz:79:ILE:HB	1.89	0.54
5:sa:1811:G:H22	5:sa:1902:A:H2	1.55	0.54
7:sc:131:MET:HE2	7:sc:131:MET:HA	1.89	0.54
11:si:116:ASP:O	11:si:117:TYR:HB3	2.07	0.54
14:sm:74:VAL:HG22	14:sm:83:ILE:HD12	1.90	0.54
11:si:137:TYR:O	11:si:138:PRO:C	2.41	0.54
19:sy:123:VAL:C	19:sy:125:GLY:H	2.16	0.54
11:si:118:LYS:HD2	11:si:122:ARG:HB2	1.88	0.54
11:si:114:LYS:HG3	11:si:115:THR:N	2.23	0.54
14:sm:61:SER:OG	14:sm:62:ASP:N	2.40	0.54
17:sr:112:ASP:OD1	17:sr:112:ASP:N	2.39	0.54
5:sa:775:G:C8	5:sa:776:U:C5	2.95	0.54
16:sp:94:GLY:H	16:sp:128:THR:HG1	1.56	0.54
5:sa:1134:G:OP2	5:sa:1134:G:N2	2.34	0.54
9:sf:33:PRO:HD2	9:sf:81:PRO:HG2	1.90	0.54
5:sa:147:U:O3'	10:sh:221:VAL:HG11	2.07	0.54
5:sa:443:U:H2'	5:sa:444:U:C6	2.43	0.54
7:sc:233:LYS:HG3	7:sc:235:GLY:H	1.73	0.54
19:sy:55:ILE:HG21	19:sy:114:PRO:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:sH:27:C:H2'	3:sH:28:G:H8	1.72	0.53
5:sa:70:A:OP1	5:sa:71:C:O2'	2.23	0.53
5:sa:774:U:H5''	5:sa:775:G:C6	2.43	0.53
9:sf:46:LEU:HD12	9:sf:59:VAL:HG13	1.90	0.53
5:sa:262:G:N2	10:sh:285:LYS:HD3	2.20	0.53
5:sa:292:A:C2'	5:sa:293:U:H5'	2.38	0.53
5:sa:934:A:H2'	5:sa:935:C:C6	2.42	0.53
9:sf:104:LYS:NZ	9:sf:249:GLN:OE1	2.42	0.53
15:so:102:LEU:HD21	15:so:112:LYS:HG2	1.91	0.53
2:sC:40:LYS:HE2	2:sC:60:CYS:HB2	1.85	0.53
11:si:104:ALA:CB	11:si:118:LYS:CG	2.85	0.53
19:sy:113:ILE:HB	19:sy:114:PRO:HD3	1.90	0.53
19:sy:129:TRP:O	19:sy:130:GLY:C	2.46	0.53
5:sa:864:C:H2'	5:sa:865:A:C8	2.44	0.53
7:sc:144:GLY:N	7:sc:155:THR:O	2.33	0.53
10:sh:273:LEU:O	10:sh:278:ARG:HD2	2.08	0.53
12:sj:11:ARG:O	14:sm:133:LYS:NZ	2.33	0.53
5:sa:147:U:O3'	10:sh:221:VAL:CG1	2.57	0.53
9:sf:147:TYR:CD2	10:sh:307:LEU:HD22	2.43	0.53
5:sa:208:C:H2'	5:sa:209:A:H8	1.72	0.53
8:se:73:ALA:HB2	8:se:82:GLY:HA2	1.90	0.53
5:sa:785:A:H2'	5:sa:786:U:O4'	2.08	0.53
7:sc:80:GLU:CD	7:sc:131:MET:HE1	2.33	0.53
10:sh:215:GLU:O	10:sh:216:GLY:O	2.26	0.53
6:sb:98:MET:HE3	6:sb:105:ALA:HB3	1.91	0.53
10:sh:195:ARG:NH2	10:sh:198:ILE:O	2.41	0.53
11:si:118:LYS:NZ	11:si:122:ARG:HD2	2.24	0.53
19:sy:106:ARG:HG3	19:sy:106:ARG:HH11	1.73	0.53
19:sy:117:ARG:O	19:sy:118:PHE:CG	2.62	0.53
1:sB:12:LYS:HG3	1:sB:15:ARG:HG2	1.91	0.53
5:sa:366:G:H1	5:sa:607:G:H1	1.57	0.53
5:sa:585:A:H2'	5:sa:586:A:C8	2.44	0.53
11:si:117:TYR:O	11:si:119:PRO:HD3	2.08	0.53
19:sy:112:ASP:HB2	19:sy:116:VAL:HG13	1.91	0.53
5:sa:774:U:H5''	5:sa:775:G:C4	2.44	0.53
10:sh:289:LYS:O	10:sh:293:LYS:N	2.32	0.53
19:sy:22:ASP:HB3	19:sy:25:TRP:HB3	1.91	0.53
1:sB:60:THR:OG1	1:sB:61:LYS:N	2.42	0.52
8:se:187:VAL:HA	8:se:190:LEU:HD12	1.91	0.52
2:sC:35:GLU:OE2	2:sC:81:ARG:HG2	2.09	0.52
5:sa:565:G:O3'	19:sy:106:ARG:HG3	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:sa:773:A:OP1	5:sa:774:U:H3'	2.09	0.52
10:sh:280:GLN:HA	10:sh:283:ALA:N	2.23	0.52
11:si:107:LYS:HA	11:si:111:GLN:NE2	2.24	0.52
9:sf:85:MET:SD	9:sf:121:LEU:HB2	2.50	0.52
14:sm:56:LYS:NZ	14:sm:131:LEU:O	2.40	0.52
5:sa:361:A:OP1	5:sa:749:A:O2'	2.26	0.52
5:sa:781:G:H4'	5:sa:782:A:H4'	1.91	0.52
5:sa:959:A:H4'	5:sa:1933:G:N2	2.24	0.52
10:sh:277:ARG:O	10:sh:280:GLN:N	2.42	0.52
5:sa:933:A:H2'	5:sa:934:A:H8	1.71	0.52
10:sh:299:GLU:O	10:sh:303:TYR:N	2.40	0.52
20:sz:23:ARG:NH2	20:sz:25:GLN:OE1	2.42	0.52
5:sa:880:A:H3'	5:sa:881:G:H21	1.73	0.52
19:sy:127:SER:HB2	19:sy:130:GLY:O	2.10	0.52
5:sa:887:A:H2'	5:sa:888:A:H8	1.75	0.52
17:sr:32:LYS:O	17:sr:36:GLU:HG2	2.09	0.52
19:sy:112:ASP:HB2	19:sy:116:VAL:CG1	2.40	0.52
2:sC:37:LYS:HD2	2:sC:37:LYS:O	2.10	0.52
5:sa:442:U:H2'	5:sa:443:U:O4'	2.09	0.52
5:sa:773:A:C8	20:sz:15:LEU:HD22	2.44	0.52
9:sf:137:ILE:HG23	9:sf:148:PRO:HG3	1.92	0.52
10:sh:147:LEU:HD22	10:sh:210:VAL:HG11	1.89	0.52
2:sC:57:CYS:SG	2:sC:59:LYS:N	2.67	0.52
10:sh:208:THR:N	10:sh:209:ILE:HG12	2.25	0.52
11:si:104:ALA:HB3	11:si:118:LYS:HG2	1.91	0.52
14:sm:1:MET:SD	14:sm:1:MET:N	2.77	0.52
5:sa:264:A:H2'	5:sa:265:G:C8	2.45	0.52
5:sa:619:C:H2'	5:sa:620:U:C6	2.44	0.52
5:sa:948:U:OP1	5:sa:1013:U:O2'	2.28	0.52
5:sa:1161:U:OP2	19:sy:117:ARG:NH2	2.43	0.52
5:sa:1816:U:H2'	5:sa:1817:A:C8	2.44	0.52
5:sa:1907:G:H1'	5:sa:1928:A:H2	1.75	0.52
9:sf:169:ASP:OD1	9:sf:170:PHE:N	2.43	0.52
12:sj:43:VAL:HG12	12:sj:57:ALA:HA	1.91	0.52
13:sk:59:MET:HE2	13:sk:72:GLU:HB2	1.92	0.52
5:sa:137:A:OP2	10:sh:272:ARG:HD3	2.10	0.51
9:sf:145:ILE:HD13	9:sf:167:ILE:HD11	1.92	0.51
12:sj:193:LEU:O	12:sj:197:GLN:HG3	2.09	0.51
14:sm:3:GLU:H	14:sm:3:GLU:CD	2.16	0.51
5:sa:442:U:OP1	9:sf:47:ARG:NH1	2.42	0.51
5:sa:443:U:H2'	5:sa:444:U:H6	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:sa:746:A:H2'	5:sa:747:A:H8	1.75	0.51
2:sC:62:GLN:NE2	2:sC:62:GLN:HA	2.24	0.51
3:sH:53:G:H2'	3:sH:54:U:C6	2.45	0.51
11:si:136:LEU:O	11:si:139:VAL:N	2.41	0.51
16:sp:23:PHE:HB3	16:sp:42:ILE:HD11	1.92	0.51
11:si:107:LYS:O	11:si:108:LYS:HB2	2.09	0.51
5:sa:69:G:H21	5:sa:80:A:H62	1.57	0.51
10:sh:280:GLN:O	10:sh:285:LYS:HG3	2.11	0.51
11:si:136:LEU:O	11:si:139:VAL:HG23	2.10	0.51
20:sz:66:THR:HA	20:sz:73:THR:HA	1.91	0.51
5:sa:90:G:OP1	5:sa:392:A:N6	2.44	0.51
5:sa:594:U:H2'	5:sa:595:A:H8	1.75	0.51
10:sh:273:LEU:H	10:sh:278:ARG:NE	2.09	0.51
16:sp:79:ARG:HD2	16:sp:83:LEU:HD13	1.92	0.51
5:sa:61:A:H1'	5:sa:262:G:H1'	1.93	0.51
5:sa:72:C:H2'	5:sa:73:A:C8	2.46	0.51
9:sf:192:VAL:HG21	9:sf:230:THR:HG22	1.93	0.51
10:sh:147:LEU:CB	10:sh:210:VAL:HG11	2.41	0.51
15:so:91:LEU:HD21	15:so:121:LYS:HB3	1.93	0.51
5:sa:147:U:O2'	10:sh:221:VAL:HG12	2.11	0.51
5:sa:383:G:OP2	5:sa:418:G:O2'	2.29	0.51
5:sa:623:U:OP2	5:sa:949:C:N4	2.37	0.51
10:sh:147:LEU:CA	10:sh:210:VAL:HG11	2.40	0.51
11:si:104:ALA:CB	11:si:118:LYS:CD	2.89	0.51
15:so:136:GLU:OE1	15:so:136:GLU:N	2.23	0.51
10:sh:221:VAL:CG1	10:sh:222:THR:N	2.74	0.50
11:si:140:GLU:OE2	15:so:21:SER:OG	2.27	0.50
12:sj:57:ALA:HB2	12:sj:213:GLY:HA2	1.92	0.50
2:sC:31:SER:OG	5:sa:939:G:OP1	2.28	0.50
5:sa:72:C:H2'	5:sa:73:A:H8	1.76	0.50
5:sa:563:C:C4'	19:sy:85:ARG:NH1	2.75	0.50
20:sz:18:ASN:ND2	20:sz:21:LEU:HB2	2.26	0.50
5:sa:205:A:OP1	9:sf:131:THR:HG21	2.11	0.50
5:sa:213:A:H2	5:sa:245:A:N1	2.08	0.50
5:sa:959:A:N3	5:sa:1922:U:O2'	2.43	0.50
5:sa:1850:C:H2'	5:sa:1851:U:C6	2.47	0.50
10:sh:286:LEU:O	10:sh:287:GLU:C	2.51	0.50
19:sy:106:ARG:HD3	19:sy:110:VAL:HG12	1.91	0.50
5:sa:243:U:H4'	5:sa:244:U:OP2	2.10	0.50
7:sc:239:GLN:HG2	7:sc:244:LYS:HB3	1.93	0.50
10:sh:147:LEU:HD22	10:sh:210:VAL:CG1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:sj:208:ARG:HH11	12:sj:211:GLN:HG3	1.77	0.50
18:sx:6:LYS:HE3	18:sx:8:GLU:O	2.10	0.50
5:sa:402:A:O2'	5:sa:1837:A:N3	2.35	0.50
6:sb:121:LYS:HD2	6:sb:122:LYS:N	2.26	0.50
11:si:107:LYS:HA	11:si:111:GLN:HE21	1.76	0.50
16:sp:101:LYS:HD3	16:sp:130:ILE:HD12	1.93	0.50
15:so:37:MET:HE1	15:so:63:VAL:HG21	1.92	0.50
5:sa:563:C:C5'	19:sy:85:ARG:NH1	2.73	0.50
9:sf:38:GLU:OE1	9:sf:38:GLU:N	2.45	0.50
5:sa:867:A:H2	16:sp:135:THR:HG23	1.77	0.49
10:sh:209:ILE:CG2	10:sh:213:LYS:N	2.74	0.49
10:sh:215:GLU:HA	10:sh:220:GLY:CA	2.41	0.49
10:sh:273:LEU:H	10:sh:278:ARG:CZ	2.25	0.49
10:sh:299:GLU:HA	10:sh:302:ARG:HB2	1.94	0.49
20:sz:23:ARG:HD2	20:sz:78:LEU:CD1	2.42	0.49
5:sa:563:C:O3'	19:sy:85:ARG:NH1	2.38	0.49
5:sa:751:A:H61	5:sa:784:U:H3	1.59	0.49
14:sm:20:ASN:HD21	14:sm:22:LYS:HE3	1.77	0.49
1:sB:11:SER:O	1:sB:11:SER:OG	2.26	0.49
6:sb:80:ASP:HB3	6:sb:127:ARG:HG3	1.94	0.49
10:sh:257:ARG:O	10:sh:266:LYS:N	2.39	0.49
10:sh:279:LEU:C	10:sh:282:LYS:H	2.21	0.49
2:sC:3:LEU:HB3	18:sx:61:ILE:HD11	1.94	0.49
3:sH:6:U:H2'	3:sH:7:A:C8	2.46	0.49
5:sa:467:C:O2'	5:sa:760:A:N3	2.38	0.49
5:sa:563:C:C3'	19:sy:85:ARG:HH12	2.25	0.49
5:sa:936:U:OP1	5:sa:1097:C:O2'	2.28	0.49
13:sk:89:ASP:OD1	13:sk:89:ASP:N	2.44	0.49
5:sa:540:U:H2'	5:sa:541:U:C6	2.47	0.49
19:sy:113:ILE:HB	19:sy:114:PRO:CD	2.42	0.49
8:se:50:VAL:HB	8:se:63:LEU:HD21	1.94	0.49
10:sh:282:LYS:HZ2	10:sh:287:GLU:N	2.09	0.49
10:sh:289:LYS:O	10:sh:290:LYS:C	2.55	0.49
5:sa:777:U:C4	5:sa:779:A:H1'	2.47	0.49
3:sH:14:A:H2'	3:sH:15:G:O4'	2.13	0.49
8:se:173:LEU:HD23	8:se:199:ILE:HG12	1.94	0.49
9:sf:127:ARG:HH22	9:sf:150:PRO:HA	1.77	0.49
10:sh:284:GLN:C	10:sh:286:LEU:N	2.69	0.49
19:sy:101:SER:O	19:sy:101:SER:OG	2.26	0.49
5:sa:294:G:H4'	5:sa:295:A:H5''	1.94	0.49
5:sa:751:A:H2'	5:sa:752:A:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:sa:415:A:O2'	5:sa:416:A:H5'	2.12	0.49
5:sa:1126:G:H1'	17:sr:76:SER:HB2	1.95	0.49
5:sa:245:A:C8	9:sf:129:LEU:HB2	2.48	0.48
5:sa:558:G:N2	5:sa:571:G:OP1	2.44	0.48
11:si:118:LYS:HZ2	11:si:122:ARG:HD3	1.78	0.48
5:sa:412:A:H4'	5:sa:413:G:O5'	2.13	0.48
5:sa:887:A:H2'	5:sa:888:A:C8	2.48	0.48
11:si:111:GLN:O	11:si:112:SER:CB	2.61	0.48
5:sa:911:C:H5'	8:se:118:LYS:HA	1.95	0.48
6:sb:125:GLU:HG2	7:sc:42:LYS:HD2	1.95	0.48
18:sx:50:TYR:OH	18:sx:73:ASP:OD2	2.23	0.48
5:sa:789:A:H5''	14:sm:92:TYR:HD2	1.78	0.48
19:sy:131:LEU:O	19:sy:131:LEU:CD1	2.60	0.48
5:sa:58:G:H4'	5:sa:448:A:H5'	1.94	0.48
5:sa:327:U:H5''	12:sj:31:ARG:NH1	2.29	0.48
7:sc:122:GLU:N	7:sc:122:GLU:OE1	2.47	0.48
5:sa:148:G:H2'	5:sa:149:U:H6	1.78	0.48
5:sa:1828:A:H2'	5:sa:1829:A:C8	2.49	0.48
7:sc:42:LYS:HB3	7:sc:249:LEU:HD13	1.96	0.48
20:sz:62:ASN:OD1	20:sz:62:ASN:N	2.46	0.48
6:sb:92:ARG:O	6:sb:96:LYS:HG2	2.13	0.48
9:sf:101:TYR:HB2	9:sf:180:MET:HE2	1.96	0.48
10:sh:279:LEU:O	10:sh:283:ALA:CA	2.61	0.48
10:sh:290:LYS:HA	10:sh:293:LYS:HB3	1.96	0.48
11:si:140:GLU:O	11:si:165:VAL:C	2.56	0.48
5:sa:1887:A:H2'	5:sa:1888:U:C6	2.48	0.48
10:sh:208:THR:H	10:sh:209:ILE:CD1	2.27	0.48
5:sa:145:U:H4'	10:sh:229:ARG:HH22	1.72	0.48
5:sa:242:G:O2'	5:sa:243:U:OP1	2.25	0.48
5:sa:329:G:H2'	5:sa:330:A:H8	1.78	0.48
5:sa:332:G:O2'	12:sj:10:LYS:NZ	2.47	0.48
5:sa:563:C:H4'	19:sy:85:ARG:NH1	2.28	0.48
5:sa:783:A:H3'	5:sa:784:U:H4'	1.95	0.48
5:sa:870:A:H2'	5:sa:871:U:H6	1.78	0.48
5:sa:1808:G:H2'	5:sa:1809:U:H6	1.78	0.48
9:sf:85:MET:HB2	9:sf:98:ARG:HE	1.79	0.48
5:sa:106:C:H2'	5:sa:107:A:H8	1.78	0.47
5:sa:866:G:H2'	5:sa:867:A:C8	2.49	0.47
6:sb:123:PHE:HE2	7:sc:41:THR:HG22	1.79	0.47
8:se:125:THR:HG22	8:se:141:CYS:HB3	1.96	0.47
8:se:210:ASP:OD1	8:se:211:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:sf:244:LYS:H	9:sf:244:LYS:HD2	1.79	0.47
10:sh:275:THR:O	10:sh:278:ARG:HB3	2.14	0.47
20:sz:24:LYS:NZ	20:sz:81:ASP:OD2	2.47	0.47
5:sa:841:U:O2'	5:sa:842:A:O4'	2.32	0.47
10:sh:209:ILE:CD1	10:sh:213:LYS:HB2	2.44	0.47
20:sz:81:ASP:OD1	20:sz:82:THR:N	2.47	0.47
1:sB:61:LYS:HD2	1:sB:61:LYS:C	2.40	0.47
3:sH:26:A:N6	3:sH:44:G:H1	2.12	0.47
3:sH:60:U:H5''	3:sH:61:C:C5	2.49	0.47
16:sp:77:ALA:O	16:sp:81:LYS:HG3	2.14	0.47
19:sy:123:VAL:O	19:sy:124:ALA:CB	2.62	0.47
5:sa:26:U:H2'	5:sa:27:A:H8	1.79	0.47
5:sa:554:U:O2'	5:sa:555:G:H8	1.97	0.47
5:sa:870:A:H2'	5:sa:871:U:C6	2.49	0.47
5:sa:1107:A:H2'	5:sa:1108:G:H8	1.79	0.47
7:sc:132:ILE:O	7:sc:136:LEU:HD12	2.13	0.47
5:sa:4:C:OP1	7:sc:202:THR:OG1	2.30	0.47
5:sa:7:G:O6	7:sc:207:LYS:NZ	2.43	0.47
8:se:209:MET:HE2	8:se:209:MET:HB3	1.81	0.47
10:sh:221:VAL:CG1	10:sh:222:THR:H	2.27	0.47
15:so:101:HIS:CD2	15:so:105:ASN:HD22	2.33	0.47
16:sp:30:ALA:HB3	16:sp:107:ALA:HB2	1.97	0.47
19:sy:106:ARG:HG2	19:sy:110:VAL:CG1	2.45	0.47
19:sy:107:GLY:O	19:sy:108:HIS:HB2	2.15	0.47
5:sa:864:C:H2'	5:sa:865:A:H8	1.79	0.47
5:sa:875:G:H2'	5:sa:876:G:C8	2.50	0.47
5:sa:1802:C:O2	5:sa:1912:A:N6	2.48	0.47
9:sf:159:LYS:N	9:sf:169:ASP:O	2.44	0.47
10:sh:168:ASN:OD1	10:sh:168:ASN:N	2.48	0.47
10:sh:299:GLU:HG2	10:sh:303:TYR:CD1	2.49	0.47
12:sj:188:PHE:HB3	12:sj:192:LEU:HD23	1.95	0.47
14:sm:56:LYS:HB3	14:sm:131:LEU:HD13	1.97	0.47
16:sp:21:ASP:OD1	16:sp:86:THR:OG1	2.33	0.47
3:sH:68:A:H2'	3:sH:69:G:C8	2.50	0.47
5:sa:293:U:O2	9:sf:31:HIS:HB3	2.14	0.47
5:sa:401:U:C2	5:sa:402:A:C8	3.03	0.47
5:sa:1879:A:H2'	5:sa:1880:U:C6	2.49	0.47
5:sa:1932:U:H2'	5:sa:1933:G:H8	1.80	0.47
8:se:156:SER:O	8:se:156:SER:OG	2.33	0.47
5:sa:1831:G:H2'	5:sa:1832:A:H8	1.79	0.47
11:si:118:LYS:HD3	11:si:119:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:sa:584:C:H2'	5:sa:585:A:H8	1.78	0.46
5:sa:906:A:H2'	5:sa:907:U:O4'	2.14	0.46
6:sb:118:GLN:HA	6:sb:123:PHE:CG	2.50	0.46
13:sk:63:ASP:HB3	13:sk:66:ASP:OD1	2.16	0.46
5:sa:444:U:H2'	5:sa:445:C:H6	1.80	0.46
5:sa:601:G:N1	5:sa:607:G:H5'	2.30	0.46
9:sf:84:PHE:O	9:sf:86:ASP:N	2.47	0.46
10:sh:280:GLN:CA	10:sh:282:LYS:H	2.27	0.46
10:sh:298:LYS:HB3	10:sh:302:ARG:NH2	2.30	0.46
11:si:117:TYR:O	11:si:117:TYR:CD2	2.68	0.46
5:sa:748:A:C5	5:sa:749:A:C8	3.03	0.46
5:sa:1124:A:OP1	7:sc:161:THR:OG1	2.22	0.46
19:sy:106:ARG:HB2	19:sy:109:ALA:O	2.16	0.46
1:sB:2:THR:HG23	5:sa:1168:A:H5''	1.97	0.46
5:sa:966:G:H2'	5:sa:967:G:O4'	2.15	0.46
7:sc:81:GLU:OE1	7:sc:188:LYS:HB3	2.15	0.46
13:sk:55:ILE:O	13:sk:59:MET:HG2	2.16	0.46
1:sB:2:THR:HG21	5:sa:612:U:H1'	1.97	0.46
5:sa:401:U:C2	5:sa:402:A:N7	2.84	0.46
5:sa:767:A:H2'	5:sa:769:C:N4	2.31	0.46
12:sj:110:ARG:NH2	12:sj:120:ASP:OD2	2.48	0.46
5:sa:5:U:O2'	5:sa:547:G:H4'	2.15	0.46
5:sa:51:U:H2'	5:sa:52:G:H8	1.80	0.46
9:sf:52:TYR:OH	9:sf:95:GLU:OE2	2.25	0.46
16:sp:39:VAL:HG23	16:sp:48:ILE:HB	1.96	0.46
5:sa:111:A:O2'	14:sm:66:ARG:NH1	2.49	0.46
5:sa:287:A:H2'	5:sa:288:A:C8	2.50	0.46
5:sa:594:U:H2'	5:sa:595:A:C8	2.50	0.46
7:sc:177:GLY:HA3	13:sk:53:ARG:NE	2.31	0.46
7:sc:228:THR:OG1	7:sc:230:ASP:OD1	2.25	0.46
10:sh:278:ARG:C	10:sh:280:GLN:H	2.24	0.46
10:sh:286:LEU:HD22	10:sh:289:LYS:HZ2	1.79	0.46
5:sa:40:A:O2'	5:sa:432:A:O2'	2.17	0.46
5:sa:867:A:H1'	16:sp:131:PRO:HB3	1.98	0.46
5:sa:871:U:H2'	5:sa:872:A:H8	1.80	0.46
7:sc:41:THR:OG1	7:sc:67:GLU:OE2	2.25	0.46
10:sh:209:ILE:HG12	10:sh:209:ILE:H	0.97	0.46
11:si:153:LYS:HD3	11:si:153:LYS:N	2.31	0.46
11:si:192:LYS:H	11:si:192:LYS:HG2	1.58	0.46
5:sa:564:A:N6	19:sy:111:GLY:C	2.73	0.46
5:sa:565:G:HO2'	19:sy:106:ARG:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:sc:142:ARG:HG2	7:sc:157:PRO:HG3	1.97	0.46
10:sh:280:GLN:O	10:sh:285:LYS:CB	2.63	0.46
3:sH:6:U:H2'	3:sH:7:A:H8	1.81	0.46
5:sa:444:U:H2'	5:sa:445:C:C6	2.51	0.46
5:sa:869:A:H2'	5:sa:870:A:H8	1.81	0.46
5:sa:1831:G:H2'	5:sa:1832:A:C8	2.51	0.46
9:sf:255:LYS:HB2	9:sf:255:LYS:HE3	1.70	0.46
5:sa:69:G:H4'	5:sa:70:A:OP2	2.16	0.45
5:sa:908:G:O2'	5:sa:925:U:H5'	2.16	0.45
5:sa:26:U:H2'	5:sa:27:A:C8	2.51	0.45
5:sa:208:C:H2'	5:sa:209:A:C8	2.51	0.45
5:sa:561:A:H62	5:sa:570:G:N2	2.14	0.45
5:sa:1158:A:H2'	5:sa:1159:A:H8	1.82	0.45
8:se:68:VAL:HG13	16:sp:42:ILE:HG22	1.97	0.45
9:sf:127:ARG:NH2	9:sf:150:PRO:O	2.49	0.45
11:si:118:LYS:NZ	11:si:122:ARG:CD	2.79	0.45
5:sa:561:A:H8	5:sa:561:A:OP2	2.00	0.45
5:sa:932:C:H2'	5:sa:933:A:H8	1.77	0.45
12:sj:107:ALA:HB3	12:sj:108:PRO:HD3	1.98	0.45
19:sy:58:LYS:H	19:sy:113:ILE:HG21	1.81	0.45
20:sz:78:LEU:HD12	20:sz:80:TYR:CE2	2.52	0.45
5:sa:5:U:OP2	7:sc:206:THR:OG1	2.35	0.45
5:sa:336:A:H2'	5:sa:337:C:C6	2.52	0.45
5:sa:765:A:OP2	5:sa:781:G:N1	2.50	0.45
7:sc:100:LEU:HG	7:sc:123:VAL:HG22	1.99	0.45
9:sf:17:MET:CE	9:sf:106:ARG:HG3	2.46	0.45
12:sj:110:ARG:HD2	12:sj:122:ALA:HB2	1.99	0.45
3:sH:23:A:H5'	3:sH:24:G:OP2	2.17	0.45
5:sa:155:A:H2'	5:sa:156:U:O4'	2.16	0.45
5:sa:250:G:H2'	5:sa:251:C:C6	2.51	0.45
10:sh:293:LYS:O	10:sh:295:ALA:N	2.46	0.45
10:sh:298:LYS:HB3	10:sh:302:ARG:HH21	1.82	0.45
5:sa:889:U:H2'	5:sa:890:C:H6	1.82	0.45
10:sh:203:ILE:CG2	10:sh:217:GLU:OE2	2.63	0.45
13:sk:59:MET:HA	13:sk:62:LYS:HG3	1.99	0.45
16:sp:98:VAL:HG12	16:sp:134:CYS:HB2	1.98	0.45
5:sa:147:U:H1'	10:sh:223:ASN:CG	2.42	0.45
5:sa:148:G:H2'	5:sa:149:U:C6	2.50	0.45
5:sa:840:U:O4	5:sa:841:U:O4	2.35	0.45
5:sa:960:G:H4'	5:sa:1923:A:H4'	1.97	0.45
5:sa:1864:G:H2'	5:sa:1865:A:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:so:73:ARG:HG2	15:so:73:ARG:HH11	1.82	0.45
5:sa:389:U:H2'	5:sa:390:U:C6	2.52	0.45
5:sa:563:C:H4'	19:sy:85:ARG:HH12	1.81	0.45
5:sa:584:C:H2'	5:sa:585:A:C8	2.51	0.45
9:sf:183:GLY:HA3	9:sf:222:ASN:CG	2.42	0.45
12:sj:37:ARG:NH2	12:sj:59:ARG:HD3	2.32	0.45
1:sB:6:ARG:NH2	5:sa:1116:U:OP2	2.49	0.45
5:sa:545:G:H2'	5:sa:546:G:H8	1.81	0.45
5:sa:619:C:H2'	5:sa:620:U:H6	1.82	0.45
5:sa:762:A:H5'	13:sk:7:ASN:HB2	1.98	0.45
10:sh:284:GLN:CG	10:sh:285:LYS:N	2.70	0.45
17:sr:90:GLU:HA	17:sr:94:LEU:HD23	1.99	0.45
3:sH:56:C:H2'	3:sH:57:G:C8	2.51	0.44
5:sa:775:G:C8	5:sa:776:U:C4	3.06	0.44
9:sf:249:GLN:HA	9:sf:252:GLU:HG2	1.99	0.44
13:sk:107:ARG:HH21	13:sk:148:VAL:HG23	1.82	0.44
15:so:39:LYS:HB2	15:so:39:LYS:HE2	1.79	0.44
16:sp:49:ILE:HD11	16:sp:51:ILE:HD11	1.98	0.44
17:sr:99:PHE:CD1	17:sr:99:PHE:C	2.95	0.44
5:sa:752:A:OP1	13:sk:51:HIS:NE2	2.41	0.44
10:sh:209:ILE:HD12	10:sh:213:LYS:CA	2.47	0.44
11:si:117:TYR:CZ	11:si:119:PRO:HG3	2.52	0.44
5:sa:147:U:O2'	10:sh:221:VAL:CG1	2.65	0.44
5:sa:153:U:H2'	5:sa:155:A:H5'	1.99	0.44
5:sa:566:C:P	19:sy:106:ARG:NH1	2.89	0.44
5:sa:773:A:H5'	5:sa:774:U:C5	2.52	0.44
5:sa:15:U:O2'	5:sa:614:A:N6	2.50	0.44
10:sh:280:GLN:O	10:sh:285:LYS:HE2	2.18	0.44
12:sj:111:LEU:HD11	12:sj:115:LYS:NZ	2.33	0.44
16:sp:92:MET:SD	16:sp:107:ALA:HB1	2.57	0.44
5:sa:65:U:C4	10:sh:268:PRO:HG3	2.52	0.44
5:sa:381:G:H2'	5:sa:382:A:C8	2.52	0.44
5:sa:580:G:H2'	5:sa:581:C:C6	2.52	0.44
5:sa:926:U:O2'	5:sa:927:U:O5'	2.35	0.44
5:sa:1863:A:H2'	5:sa:1864:G:H8	1.82	0.44
7:sc:47:VAL:HG21	7:sc:70:ILE:HG12	1.99	0.44
11:si:104:ALA:HB3	11:si:118:LYS:CD	2.48	0.44
13:sk:25:ASP:OD1	13:sk:26:ALA:N	2.50	0.44
3:sH:15:G:N2	3:sH:21:A:H1'	2.33	0.44
5:sa:796:G:O2'	17:sr:107:SER:HB3	2.18	0.44
5:sa:1089:A:O2'	5:sa:1090:C:P	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:sh:279:LEU:CB	10:sh:282:LYS:CB	2.94	0.44
17:sr:36:GLU:HB2	17:sr:110:ILE:HD12	1.99	0.44
5:sa:561:A:H5''	5:sa:562:G:OP2	2.18	0.44
5:sa:776:U:C4	5:sa:777:U:C4	3.06	0.44
15:so:91:LEU:HD12	15:so:91:LEU:HA	1.82	0.44
17:sr:86:PHE:O	17:sr:90:GLU:HG3	2.17	0.44
5:sa:1089:A:C2'	5:sa:1090:C:O5'	2.65	0.44
7:sc:43:LEU:HD22	7:sc:70:ILE:HD13	1.98	0.44
7:sc:172:VAL:HB	7:sc:199:PHE:HB2	1.98	0.44
10:sh:209:ILE:HD11	10:sh:214:GLY:H	1.82	0.44
17:sr:76:SER:HB3	17:sr:77:PRO:CD	2.47	0.44
3:sH:58:A:H1'	3:sH:60:U:OP2	2.17	0.44
9:sf:159:LYS:HD2	9:sf:168:VAL:HB	2.00	0.44
10:sh:209:ILE:HG22	10:sh:210:VAL:H	1.83	0.44
1:sB:79:ILE:HD11	5:sa:1942:U:H5'	1.99	0.43
5:sa:1863:A:H2'	5:sa:1864:G:C8	2.53	0.43
10:sh:148:LYS:HD2	10:sh:148:LYS:HA	1.70	0.43
13:sk:63:ASP:OD1	13:sk:64:ALA:N	2.50	0.43
14:sm:15:HIS:HB2	14:sm:30:VAL:HG11	1.99	0.43
17:sr:90:GLU:OE2	17:sr:117:ARG:NH1	2.49	0.43
5:sa:851:A:H2'	5:sa:852:A:C8	2.53	0.43
5:sa:1115:C:N4	5:sa:1116:U:O4	2.51	0.43
5:sa:1133:A:O2'	5:sa:1134:G:H5'	2.17	0.43
6:sb:88:GLU:HA	6:sb:91:HIS:CE1	2.53	0.43
6:sb:125:GLU:CD	7:sc:42:LYS:HD2	2.43	0.43
7:sc:141:VAL:HG13	7:sc:220:VAL:HG13	1.99	0.43
11:si:107:LYS:HB2	11:si:107:LYS:HE3	1.51	0.43
14:sm:58:PRO:HA	14:sm:63:VAL:HG23	1.99	0.43
5:sa:440:A:O5'	9:sf:57:ARG:NH2	2.51	0.43
5:sa:455:A:H3'	5:sa:456:G:H8	1.82	0.43
5:sa:623:U:H2'	5:sa:624:A:H8	1.82	0.43
5:sa:788:C:N4	5:sa:789:A:H62	2.16	0.43
10:sh:203:ILE:CB	10:sh:217:GLU:OE2	2.65	0.43
15:so:3:ARG:NH1	15:so:10:GLY:H	2.16	0.43
16:sp:15:ILE:O	16:sp:18:SER:OG	2.31	0.43
18:sx:72:LYS:HG3	18:sx:85:MET:HE1	2.01	0.43
19:sy:66:LYS:HG2	19:sy:89:LEU:HD13	2.00	0.43
19:sy:82:PHE:CD1	19:sy:112:ASP:CG	2.97	0.43
2:sC:37:LYS:HD2	2:sC:37:LYS:C	2.44	0.43
2:sC:51:ALA:HB3	2:sC:72:LEU:HG	2.01	0.43
2:sC:60:CYS:HB3	2:sC:61:GLY:H	1.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:se:28:LYS:O	8:se:52:LYS:N	2.42	0.43
13:sk:57:LYS:HB2	13:sk:57:LYS:HE3	1.69	0.43
5:sa:441:C:H41	5:sa:456:G:H21	1.67	0.43
5:sa:563:C:C5'	19:sy:85:ARG:HH11	2.26	0.43
6:sb:180:LEU:HD11	6:sb:184:MET:HE3	1.99	0.43
7:sc:155:THR:OG1	7:sc:197:ASP:O	2.26	0.43
19:sy:20:TRP:CE3	19:sy:26:LYS:HG3	2.52	0.43
5:sa:301:U:O2	14:sm:68:ARG:NH2	2.42	0.43
5:sa:1011:U:H4'	5:sa:1012:G:OP2	2.17	0.43
11:si:116:ASP:N	11:si:116:ASP:OD1	2.51	0.43
15:so:73:ARG:HD2	15:so:73:ARG:HA	1.78	0.43
16:sp:125:GLU:HG2	16:sp:127:VAL:HG13	1.99	0.43
1:sB:37:LYS:HE2	1:sB:37:LYS:HB2	1.76	0.43
9:sf:181:MET:HE1	9:sf:208:ILE:HD12	1.99	0.43
10:sh:209:ILE:CG2	10:sh:213:LYS:NZ	2.82	0.43
5:sa:151:A:H2'	5:sa:152:A:O4'	2.19	0.43
7:sc:80:GLU:OE1	7:sc:80:GLU:HA	2.18	0.43
9:sf:232:THR:OG1	9:sf:234:VAL:O	2.35	0.43
10:sh:282:LYS:HZ2	10:sh:287:GLU:CA	2.32	0.43
11:si:161:VAL:H	11:si:193:VAL:HG12	1.83	0.43
19:sy:105:ARG:C	19:sy:106:ARG:HD3	2.44	0.43
2:sC:79:LYS:HD3	2:sC:79:LYS:HA	1.83	0.43
5:sa:860:G:H2'	5:sa:861:A:C8	2.53	0.43
5:sa:906:A:OP1	5:sa:996:C:O2'	2.31	0.43
5:sa:1879:A:H2'	5:sa:1880:U:H6	1.84	0.43
9:sf:126:LYS:HE2	9:sf:138:VAL:HG21	2.01	0.43
12:sj:5:ARG:NH1	12:sj:29:MET:O	2.52	0.43
13:sk:87:PRO:HB2	13:sk:89:ASP:OD1	2.18	0.43
14:sm:151:LYS:HE2	14:sm:151:LYS:HB2	1.73	0.43
19:sy:127:SER:HB2	19:sy:130:GLY:N	2.34	0.43
5:sa:305:A:OP2	14:sm:102:ARG:NH1	2.42	0.43
5:sa:773:A:N3	5:sa:773:A:H2'	2.34	0.43
5:sa:942:C:H2'	5:sa:943:A:O4'	2.19	0.43
5:sa:1850:C:H2'	5:sa:1851:U:H6	1.84	0.43
5:sa:1880:U:H2'	5:sa:1881:C:C6	2.54	0.43
8:se:107:LEU:HG	8:se:215:ARG:HA	2.00	0.43
10:sh:149:ILE:H	10:sh:149:ILE:HD12	1.83	0.43
10:sh:282:LYS:HA	10:sh:286:LEU:HB2	2.00	0.43
11:si:104:ALA:CB	11:si:118:LYS:HG2	2.48	0.43
5:sa:124:U:H2'	5:sa:125:U:C6	2.53	0.42
5:sa:399:G:H2'	5:sa:400:C:H6	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:sa:866:G:H2'	5:sa:867:A:H8	1.83	0.42
7:sc:152:GLU:O	7:sc:176:ARG:NH2	2.49	0.42
8:se:195:LEU:HB3	8:se:196:PRO:HD3	2.01	0.42
13:sk:48:MET:O	13:sk:52:MET:HG3	2.19	0.42
5:sa:1111:A:H2'	5:sa:1112:A:C8	2.54	0.42
5:sa:1865:A:H2'	5:sa:1866:A:C8	2.54	0.42
8:se:117:LYS:HG3	8:se:120:CYS:HB2	2.01	0.42
17:sr:28:ARG:HB3	17:sr:29:PRO:HD3	2.01	0.42
19:sy:129:TRP:HB3	19:sy:130:GLY:H	1.70	0.42
2:sC:76:GLN:HG2	2:sC:77:GLN:HG2	2.01	0.42
19:sy:109:ALA:C	19:sy:110:VAL:HG13	2.44	0.42
5:sa:1816:U:H2'	5:sa:1817:A:H8	1.84	0.42
8:se:29:LYS:NZ	16:sp:46:GLU:OE1	2.51	0.42
9:sf:152:LEU:HD23	9:sf:152:LEU:HA	1.86	0.42
11:si:125:LYS:HE2	11:si:125:LYS:HB3	1.87	0.42
11:si:160:THR:O	11:si:160:THR:OG1	2.36	0.42
19:sy:106:ARG:CG	19:sy:106:ARG:HH11	2.32	0.42
20:sz:13:ARG:HG3	20:sz:13:ARG:HH11	1.83	0.42
5:sa:5:U:H2'	5:sa:6:G:H8	1.85	0.42
5:sa:209:A:C6	5:sa:250:G:C6	3.07	0.42
5:sa:252:C:H3'	5:sa:253:A:H8	1.84	0.42
9:sf:189:ARG:HD3	9:sf:216:PHE:CZ	2.54	0.42
12:sj:34:ALA:HB3	12:sj:56:ARG:HD2	2.02	0.42
17:sr:44:HIS:NE2	17:sr:112:ASP:OD2	2.43	0.42
5:sa:1090:C:OP1	8:se:162:GLN:NE2	2.52	0.42
5:sa:1849:U:HO2'	5:sa:1850:C:H6	1.68	0.42
17:sr:66:ASN:N	17:sr:66:ASN:OD1	2.52	0.42
2:sC:59:LYS:HD2	2:sC:59:LYS:HA	1.32	0.42
5:sa:77:A:O2'	5:sa:78:G:O4'	2.38	0.42
5:sa:872:A:H2'	5:sa:873:A:H8	1.80	0.42
6:sb:171:ASN:OD1	6:sb:174:SER:OG	2.25	0.42
10:sh:286:LEU:O	10:sh:288:ALA:N	2.52	0.42
11:si:137:TYR:CD2	11:si:137:TYR:C	2.96	0.42
15:so:36:GLU:OE2	15:so:36:GLU:HA	2.19	0.42
16:sp:92:MET:HE3	16:sp:92:MET:HB3	1.78	0.42
2:sC:37:LYS:HE3	2:sC:79:LYS:H	1.84	0.42
5:sa:768:A:H3'	5:sa:769:C:C5	2.55	0.42
6:sb:75:ASN:OD1	6:sb:76:GLU:N	2.52	0.42
9:sf:99:LEU:HD12	9:sf:99:LEU:HA	1.84	0.42
10:sh:241:LEU:HD12	10:sh:242:PHE:N	2.34	0.42
5:sa:426:C:C2	5:sa:427:G:C8	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:sa:593:A:H2'	5:sa:594:U:C6	2.54	0.42
5:sa:784:U:OP1	9:sf:105:ARG:NH1	2.52	0.42
10:sh:210:VAL:HG22	10:sh:213:LYS:HZ3	1.84	0.42
10:sh:229:ARG:HA	10:sh:229:ARG:HD3	1.45	0.42
10:sh:279:LEU:HA	10:sh:282:LYS:HB2	2.02	0.42
13:sk:45:VAL:HG12	13:sk:101:GLU:HG2	2.02	0.42
14:sm:74:VAL:HG12	14:sm:119:GLU:HA	2.01	0.42
19:sy:113:ILE:CB	19:sy:114:PRO:HD3	2.49	0.42
5:sa:1030:G:C6	5:sa:1094:G:C6	3.08	0.42
3:sH:71:U:H2'	3:sH:72:C:C6	2.55	0.41
5:sa:150:G:N2	5:sa:152:A:H3'	2.35	0.41
9:sf:172:LYS:HA	9:sf:172:LYS:HD3	1.83	0.41
15:so:5:TYR:HE2	15:so:121:LYS:HG3	1.85	0.41
5:sa:768:A:H2'	5:sa:768:A:N3	2.35	0.41
5:sa:882:G:H2'	5:sa:883:U:C6	2.55	0.41
9:sf:40:LEU:HD12	9:sf:40:LEU:HA	1.94	0.41
10:sh:282:LYS:HA	10:sh:286:LEU:H	1.85	0.41
11:si:162:PHE:CZ	11:si:198:PRO:HA	2.55	0.41
13:sk:88:ARG:HE	13:sk:88:ARG:HB3	1.66	0.41
20:sz:17:VAL:HG12	20:sz:19:PRO:HD3	2.02	0.41
2:sC:47:THR:OG1	15:so:56:ASP:O	2.35	0.41
3:sH:71:U:H2'	3:sH:72:C:H6	1.85	0.41
5:sa:447:A:OP2	5:sa:448:A:N6	2.53	0.41
5:sa:801:A:H2'	5:sa:802:U:C6	2.55	0.41
7:sc:80:GLU:CD	7:sc:81:GLU:H	2.29	0.41
9:sf:58:GLU:HB3	20:sz:21:LEU:HD11	2.02	0.41
9:sf:149:HIS:ND1	9:sf:150:PRO:HD2	2.34	0.41
10:sh:209:ILE:C	10:sh:210:VAL:CG1	2.89	0.41
10:sh:304:ALA:O	10:sh:307:LEU:HB3	2.19	0.41
13:sk:17:VAL:HB	13:sk:20:GLU:OE2	2.19	0.41
15:so:35:ASP:OD1	15:so:35:ASP:C	2.63	0.41
2:sC:61:GLY:O	2:sC:63:PRO:CD	2.68	0.41
12:sj:101:ILE:HD12	12:sj:220:LEU:HD11	2.02	0.41
12:sj:220:LEU:HD22	12:sj:224:GLU:HG2	2.02	0.41
16:sp:80:CYS:HB2	16:sp:119:MET:HE1	2.02	0.41
19:sy:112:ASP:O	19:sy:114:PRO:HD2	2.20	0.41
3:sH:21:A:N6	3:sH:46:G:H2'	2.33	0.41
5:sa:1818:C:H2'	5:sa:1819:C:H6	1.86	0.41
5:sa:1864:G:H2'	5:sa:1865:A:C8	2.55	0.41
10:sh:154:ASP:HB2	10:sh:195:ARG:HG3	2.02	0.41
1:sB:5:ARG:HH21	5:sa:1942:U:H3'	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:sB:61:LYS:HD2	1:sB:61:LYS:O	2.21	0.41
5:sa:77:A:H2'	5:sa:78:G:C4	2.55	0.41
5:sa:443:U:P	9:sf:47:ARG:HH22	2.43	0.41
5:sa:583:C:HO2'	5:sa:584:C:H6	1.67	0.41
5:sa:611:U:H5'	5:sa:1011:U:O4'	2.20	0.41
10:sh:309:ARG:HE	10:sh:309:ARG:HB3	1.30	0.41
11:si:114:LYS:HE3	11:si:114:LYS:HB2	1.61	0.41
15:so:54:MET:HE3	15:so:54:MET:HB3	1.86	0.41
17:sr:23:ARG:HD3	17:sr:23:ARG:HA	1.70	0.41
8:se:205:LYS:HD2	8:se:205:LYS:HA	1.73	0.41
9:sf:141:ASP:OD1	9:sf:141:ASP:C	2.64	0.41
2:sC:72:LEU:HD23	2:sC:72:LEU:HA	1.94	0.41
5:sa:446:G:H3'	5:sa:448:A:H62	1.86	0.41
5:sa:878:A:C2	5:sa:895:A:C5	3.09	0.41
5:sa:905:G:N2	5:sa:968:A:H1'	2.36	0.41
10:sh:262:LYS:HD2	10:sh:262:LYS:C	2.46	0.41
10:sh:286:LEU:C	10:sh:289:LYS:NZ	2.79	0.41
12:sj:106:PRO:HB2	12:sj:196:PHE:CE1	2.55	0.41
13:sk:59:MET:HE3	13:sk:59:MET:HB3	1.95	0.41
18:sx:33:LEU:HD22	18:sx:49:VAL:HG22	2.03	0.41
19:sy:11:MET:HE2	19:sy:11:MET:HB3	1.66	0.41
20:sz:16:ILE:N	20:sz:16:ILE:HD12	2.35	0.41
5:sa:77:A:O2'	5:sa:78:G:OP1	2.26	0.41
5:sa:783:A:H2'	5:sa:785:A:OP1	2.21	0.41
5:sa:840:U:C4	5:sa:841:U:C4	3.09	0.41
5:sa:840:U:O4'	11:si:120:ARG:HG2	2.20	0.41
9:sf:163:GLU:OE1	9:sf:163:GLU:N	2.39	0.41
11:si:118:LYS:CD	11:si:122:ARG:HD2	2.50	0.41
12:sj:197:GLN:HG3	12:sj:197:GLN:H	1.68	0.41
15:so:55:ARG:HH21	15:so:56:ASP:CG	2.29	0.41
20:sz:32:HIS:NE2	20:sz:73:THR:OG1	2.45	0.41
5:sa:15:U:H2'	5:sa:16:G:O4'	2.20	0.41
5:sa:468:A:H2'	5:sa:469:C:O4'	2.21	0.41
5:sa:782:A:H3'	5:sa:784:U:O4'	2.20	0.41
5:sa:868:A:H2	5:sa:905:G:H22	1.69	0.41
5:sa:1804:G:H2'	5:sa:1805:C:O4'	2.21	0.41
7:sc:205:HIS:CE1	7:sc:207:LYS:HB2	2.56	0.41
9:sf:169:ASP:OD1	9:sf:169:ASP:C	2.64	0.41
10:sh:213:LYS:O	10:sh:221:VAL:O	2.39	0.41
17:sr:26:MET:HE2	17:sr:26:MET:HB3	1.88	0.41
1:sB:63:LYS:HE3	1:sB:63:LYS:HB3	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:se:167:ARG:O	8:se:171:ASN:HB2	2.20	0.40
12:sj:113:PHE:CZ	12:sj:121:ILE:HD11	2.56	0.40
13:sk:130:ARG:HA	13:sk:130:ARG:HD2	1.94	0.40
2:sC:40:LYS:CE	2:sC:60:CYS:HB3	2.38	0.40
5:sa:238:G:N3	5:sa:238:G:O4'	2.54	0.40
5:sa:287:A:H2'	5:sa:288:A:H8	1.86	0.40
5:sa:416:A:O2'	5:sa:417:G:H8	2.04	0.40
5:sa:611:U:H2'	5:sa:612:U:C6	2.56	0.40
5:sa:926:U:O2'	5:sa:927:U:H6	2.04	0.40
9:sf:181:MET:HE3	9:sf:218:THR:HG21	2.03	0.40
9:sf:244:LYS:HB3	9:sf:244:LYS:HE3	1.82	0.40
10:sh:242:PHE:CD2	10:sh:253:PHE:HB3	2.51	0.40
10:sh:280:GLN:O	10:sh:285:LYS:CG	2.70	0.40
13:sk:5:LEU:HD23	13:sk:5:LEU:HA	1.89	0.40
17:sr:14:ILE:HG23	17:sr:65:LEU:HD21	2.02	0.40
19:sy:106:ARG:NE	19:sy:110:VAL:HG12	2.35	0.40
5:sa:898:G:H2'	5:sa:899:C:C6	2.57	0.40
8:se:72:LEU:HD13	8:se:86:TYR:CE1	2.57	0.40
9:sf:112:LEU:HD23	9:sf:235:ASN:HD21	1.87	0.40
9:sf:244:LYS:HA	9:sf:245:PRO:HD3	1.95	0.40
10:sh:302:ARG:O	10:sh:306:ILE:HG23	2.21	0.40
17:sr:124:ARG:H	17:sr:124:ARG:HG2	1.56	0.40
19:sy:106:ARG:HB3	19:sy:107:GLY:H	1.62	0.40
5:sa:149:U:H5'	10:sh:205:VAL:HG21	2.02	0.40
5:sa:341:G:C2	5:sa:342:A:C8	3.10	0.40
5:sa:1887:A:H2'	5:sa:1888:U:H6	1.84	0.40
7:sc:244:LYS:NZ	7:sc:244:LYS:HB2	2.36	0.40
16:sp:30:ALA:HA	16:sp:35:THR:HA	2.03	0.40
19:sy:82:PHE:CD1	19:sy:112:ASP:OD2	2.73	0.40
3:sH:27:C:H2'	3:sH:28:G:C8	2.54	0.40
5:sa:1015:A:C2	5:sa:1016:A:N7	2.90	0.40
5:sa:1089:A:H2'	5:sa:1090:C:H6	1.86	0.40
5:sa:1930:C:H2'	5:sa:1931:C:C6	2.57	0.40
11:si:107:LYS:CA	11:si:111:GLN:HE21	2.34	0.40
11:si:113:GLY:O	11:si:114:LYS:HB2	2.21	0.40
11:si:163:VAL:HG13	11:si:165:VAL:HG13	2.02	0.40
16:sp:39:VAL:HG21	16:sp:80:CYS:SG	2.62	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	sB	96/144 (67%)	93 (97%)	3 (3%)	0	100	100
2	sC	81/84 (96%)	73 (90%)	7 (9%)	1 (1%)	11	38
6	sb	164/254 (65%)	157 (96%)	7 (4%)	0	100	100
7	sc	213/255 (84%)	201 (94%)	12 (6%)	0	100	100
8	se	210/256 (82%)	204 (97%)	6 (3%)	0	100	100
9	sf	254/326 (78%)	237 (93%)	15 (6%)	2 (1%)	16	48
10	sh	161/266 (60%)	133 (83%)	17 (11%)	11 (7%)	1	6
11	si	75/201 (37%)	64 (85%)	7 (9%)	4 (5%)	1	10
12	sj	163/237 (69%)	159 (98%)	4 (2%)	0	100	100
13	sk	156/185 (84%)	154 (99%)	2 (1%)	0	100	100
14	sm	152/156 (97%)	145 (95%)	7 (5%)	0	100	100
15	so	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
16	sp	131/146 (90%)	125 (95%)	6 (5%)	0	100	100
17	sr	127/130 (98%)	117 (92%)	10 (8%)	0	100	100
18	sx	67/86 (78%)	67 (100%)	0	0	100	100
19	sy	128/141 (91%)	109 (85%)	10 (8%)	9 (7%)	1	5
20	sz	52/140 (37%)	45 (86%)	6 (12%)	1 (2%)	6	27
All	All	2378/3158 (75%)	2228 (94%)	122 (5%)	28 (1%)	14	38

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	sh	219	GLU
10	sh	285	LYS
10	sh	288	ALA
11	si	112	SER
11	si	137	TYR

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Mol	Chain	Res	Type
19	sy	84	PRO
19	sy	85	ARG
19	sy	108	HIS
19	sy	113	ILE
20	sz	87	LYS
10	sh	221	VAL
10	sh	229	ARG
10	sh	230	ALA
10	sh	294	ILE
19	sy	115	GLY
19	sy	124	ALA
10	sh	218	ILE
10	sh	290	LYS
11	si	119	PRO
9	sf	246	LEU
10	sh	264	ARG
10	sh	291	LEU
11	si	163	VAL
9	sf	85	MET
19	sy	114	PRO
19	sy	110	VAL
2	sC	61	GLY
19	sy	125	GLY

### 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	sB	87/127 (68%)	85 (98%)	2 (2%)	45	70
2	sC	72/73 (99%)	70 (97%)	2 (3%)	38	66
6	sb	145/218 (66%)	142 (98%)	3 (2%)	48	72
7	sc	172/199 (86%)	167 (97%)	5 (3%)	37	65
8	se	193/225 (86%)	191 (99%)	2 (1%)	73	86
9	sf	223/283 (79%)	219 (98%)	4 (2%)	54	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	sh	141/220 (64%)	122 (86%)	19 (14%)	3	13
11	si	66/167 (40%)	55 (83%)	11 (17%)	2	7
12	sj	140/205 (68%)	138 (99%)	2 (1%)	62	81
13	sk	140/164 (85%)	140 (100%)	0	100	100
14	sm	136/138 (99%)	135 (99%)	1 (1%)	81	90
15	so	128/129 (99%)	126 (98%)	2 (2%)	58	79
16	sp	103/114 (90%)	101 (98%)	2 (2%)	52	75
17	sr	112/113 (99%)	110 (98%)	2 (2%)	54	76
18	sx	64/77 (83%)	63 (98%)	1 (2%)	58	79
19	sy	104/114 (91%)	92 (88%)	12 (12%)	4	19
20	sz	49/125 (39%)	47 (96%)	2 (4%)	26	57
All	All	2075/2691 (77%)	2003 (96%)	72 (4%)	33	61

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

Mol	Chain	Res	Type
1	sB	6	ARG
1	sB	44	ILE
2	sC	9	LEU
2	sC	59	LYS
6	sb	39	MET
6	sb	84	VAL
6	sb	211	HIS
7	sc	40	VAL
7	sc	143	ARG
7	sc	152	GLU
7	sc	209	LEU
7	sc	213	VAL
8	se	80	LYS
8	se	171	ASN
9	sf	217	THR
9	sf	226	ILE
9	sf	232	THR
9	sf	244	LYS
10	sh	209	ILE
10	sh	213	LYS
10	sh	229	ARG
10	sh	270	ILE

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Mol	Chain	Res	Type
10	sh	274	VAL
10	sh	281	HIS
10	sh	282	LYS
10	sh	286	LEU
10	sh	289	LYS
10	sh	290	LYS
10	sh	291	LEU
10	sh	294	ILE
10	sh	297	LEU
10	sh	299	GLU
10	sh	301	LYS
10	sh	306	ILE
10	sh	307	LEU
10	sh	309	ARG
10	sh	310	TYR
11	si	107	LYS
11	si	108	LYS
11	si	111	GLN
11	si	114	LYS
11	si	115	THR
11	si	116	ASP
11	si	118	LYS
11	si	139	VAL
11	si	149	THR
11	si	160	THR
11	si	165	VAL
12	sj	27	ASN
12	sj	189	ASP
14	sm	108	VAL
15	so	87	ASP
15	so	150	VAL
16	sp	31	THR
16	sp	119	MET
17	sr	74	VAL
17	sr	83	LEU
18	sx	11	ILE
19	sy	83	VAL
19	sy	105	ARG
19	sy	106	ARG
19	sy	113	ILE
19	sy	114	PRO
19	sy	116	VAL

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Mol	Chain	Res	Type
19	sy	117	ARG
19	sy	121	VAL
19	sy	123	VAL
19	sy	126	VAL
19	sy	129	TRP
19	sy	131	LEU
20	sz	27	VAL
20	sz	83	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	sC	54	GLN
6	sb	48	ASN
6	sb	211	HIS
7	sc	57	GLN
7	sc	91	GLN
7	sc	205	HIS
9	sf	34	HIS
10	sh	186	ASN
10	sh	281	HIS
12	sj	44	HIS
12	sj	80	ASN
14	sm	10	GLN
15	so	105	ASN
19	sy	6	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	sH	73/76 (96%)	20 (27%)	0
4	sK	5/6 (83%)	0	0
5	sa	970/1947 (49%)	197 (20%)	0
All	All	1048/2029 (51%)	217 (20%)	0

All (217) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	sH	10	G
3	sH	12	U

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Mol	Chain	Res	Type
3	sH	13	C
3	sH	16	U
3	sH	20	U
3	sH	24	G
3	sH	45	U
3	sH	46	G
3	sH	47	U
3	sH	48	C
3	sH	49	A
3	sH	50	U
3	sH	52	G
3	sH	55	U
3	sH	56	C
3	sH	57	G
3	sH	59	U
3	sH	67	A
3	sH	69	G
3	sH	76	A
5	sa	4	C
5	sa	17	C
5	sa	25	A
5	sa	26	U
5	sa	33	A
5	sa	41	G
5	sa	42	A
5	sa	44	U
5	sa	46	A
5	sa	49	C
5	sa	56	G
5	sa	61	A
5	sa	62	G
5	sa	64	A
5	sa	65	U
5	sa	67	A
5	sa	68	A
5	sa	69	G
5	sa	70	A
5	sa	72	C
5	sa	74	A
5	sa	75	G
5	sa	76	U
5	sa	77	A

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Mol	Chain	Res	Type
5	sa	78	G
5	sa	79	G
5	sa	103	U
5	sa	104	A
5	sa	113	A
5	sa	114	G
5	sa	115	U
5	sa	123	G
5	sa	135	C
5	sa	136	A
5	sa	139	G
5	sa	141	U
5	sa	148	G
5	sa	154	G
5	sa	171	A
5	sa	173	A
5	sa	213	A
5	sa	214	A
5	sa	243	U
5	sa	244	U
5	sa	246	G
5	sa	251	C
5	sa	252	C
5	sa	253	A
5	sa	262	G
5	sa	263	U
5	sa	264	A
5	sa	283	A
5	sa	287	A
5	sa	288	A
5	sa	292	A
5	sa	294	G
5	sa	295	A
5	sa	296	G
5	sa	299	U
5	sa	310	U
5	sa	311	C
5	sa	313	A
5	sa	317	G
5	sa	332	G
5	sa	333	A
5	sa	345	A

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Mol	Chain	Res	Type
5	sa	347	A
5	sa	350	G
5	sa	354	A
5	sa	355	A
5	sa	356	C
5	sa	385	G
5	sa	394	A
5	sa	395	G
5	sa	396	A
5	sa	397	U
5	sa	399	G
5	sa	411	A
5	sa	412	A
5	sa	413	G
5	sa	417	G
5	sa	419	C
5	sa	420	A
5	sa	421	G
5	sa	430	U
5	sa	434	U
5	sa	439	C
5	sa	448	A
5	sa	449	U
5	sa	455	A
5	sa	463	A
5	sa	470	A
5	sa	549	A
5	sa	551	G
5	sa	553	C
5	sa	555	G
5	sa	559	C
5	sa	561	A
5	sa	562	G
5	sa	568	G
5	sa	571	G
5	sa	572	U
5	sa	576	U
5	sa	579	A
5	sa	584	C
5	sa	588	A
5	sa	589	G
5	sa	600	A

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Mol	Chain	Res	Type
5	sa	602	U
5	sa	605	C
5	sa	613	A
5	sa	614	A
5	sa	616	A
5	sa	617	C
5	sa	618	G
5	sa	628	G
5	sa	742	G
5	sa	746	A
5	sa	756	G
5	sa	757	U
5	sa	765	A
5	sa	767	A
5	sa	768	A
5	sa	769	C
5	sa	771	U
5	sa	772	U
5	sa	773	A
5	sa	774	U
5	sa	775	G
5	sa	776	U
5	sa	777	U
5	sa	782	A
5	sa	783	A
5	sa	784	U
5	sa	785	A
5	sa	803	G
5	sa	840	U
5	sa	843	A
5	sa	845	A
5	sa	852	A
5	sa	853	U
5	sa	856	G
5	sa	877	G
5	sa	894	G
5	sa	902	U
5	sa	911	C
5	sa	913	A
5	sa	915	A
5	sa	922	G
5	sa	924	A

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Mol	Chain	Res	Type
5	sa	927	U
5	sa	930	C
5	sa	932	C
5	sa	939	G
5	sa	940	U
5	sa	946	A
5	sa	972	A
5	sa	973	A
5	sa	984	U
5	sa	985	A
5	sa	1006	A
5	sa	1008	C
5	sa	1012	G
5	sa	1020	A
5	sa	1033	A
5	sa	1090	C
5	sa	1101	A
5	sa	1106	A
5	sa	1117	U
5	sa	1118	G
5	sa	1122	U
5	sa	1123	U
5	sa	1135	G
5	sa	1140	G
5	sa	1164	A
5	sa	1797	A
5	sa	1800	C
5	sa	1801	A
5	sa	1824	G
5	sa	1846	G
5	sa	1849	U
5	sa	1850	C
5	sa	1897	A
5	sa	1903	A
5	sa	1907	G
5	sa	1909	A
5	sa	1913	A
5	sa	1916	U
5	sa	1927	G
5	sa	1929	A
5	sa	1930	C
5	sa	1939	G

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Mol	Chain	Res	Type
5	sa	1940	G
5	sa	1941	A
5	sa	1942	U
5	sa	1943	C
5	sa	1945	U

There are no RNA pucker outliers to report.

#### 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](#)

There are no ligands in this entry.

#### 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

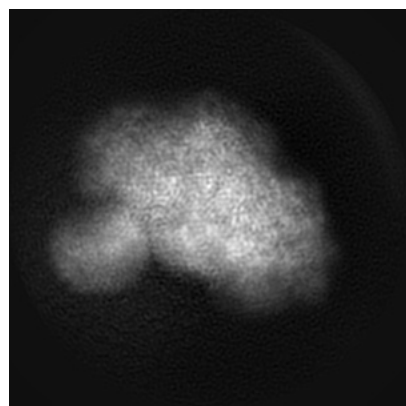
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64695. These allow visual inspection of the internal detail of the map and identification of artifacts.

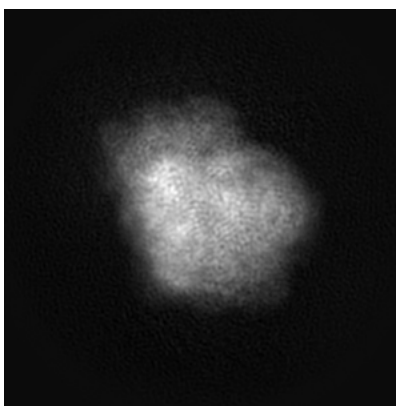
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

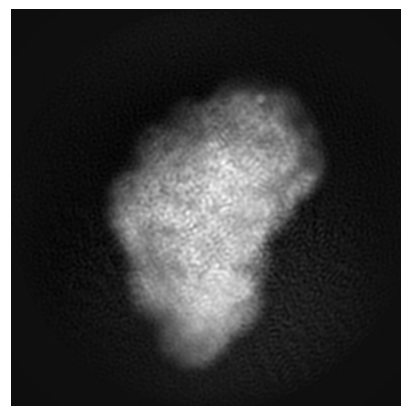
#### 6.1.1 Primary map



X

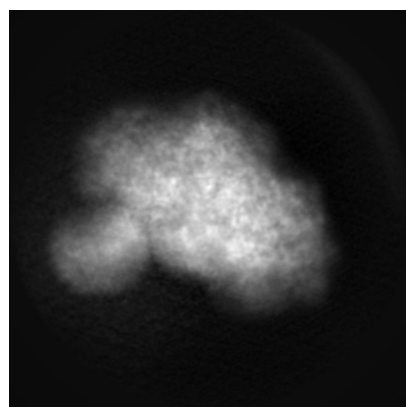


Y

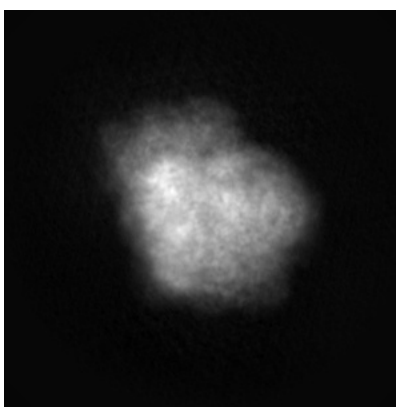


Z

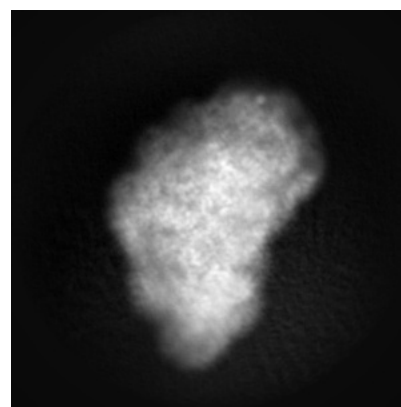
#### 6.1.2 Raw map



X



Y

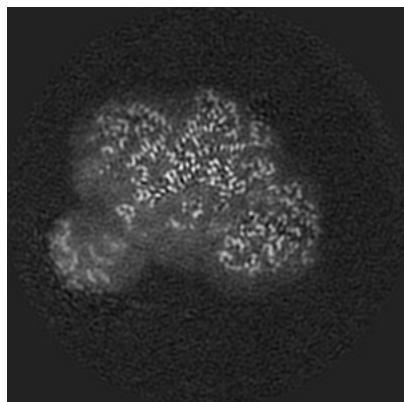


Z

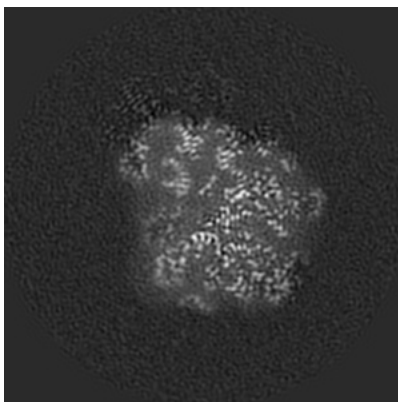
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

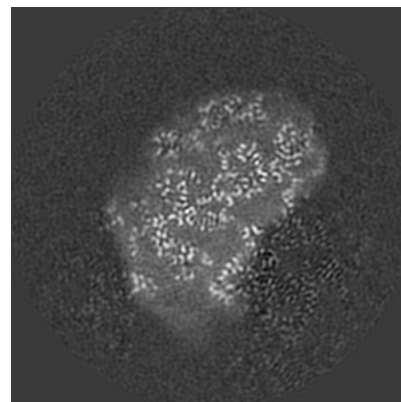
### 6.2.1 Primary map



X Index: 135

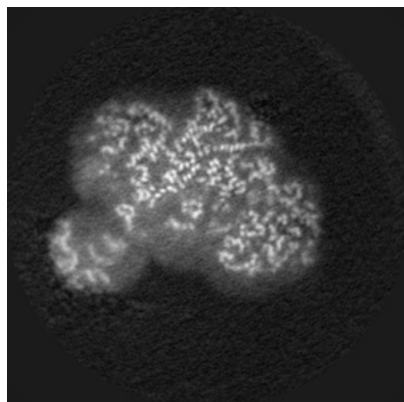


Y Index: 135

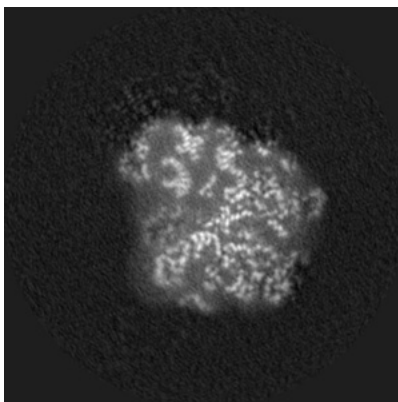


Z Index: 135

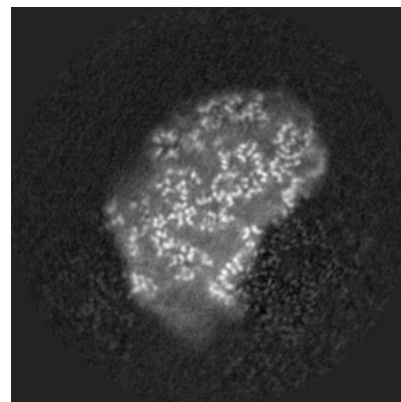
### 6.2.2 Raw map



X Index: 135



Y Index: 135



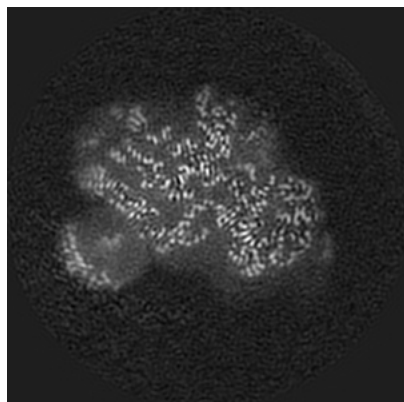
Z Index: 135

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

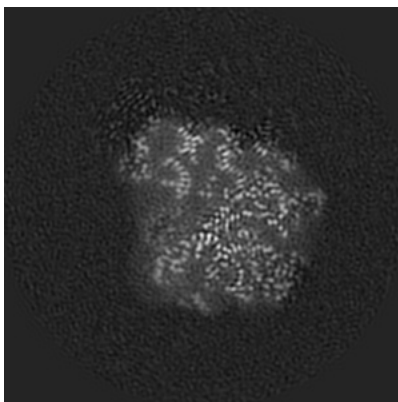


## 6.3 Largest variance slices [i](#)

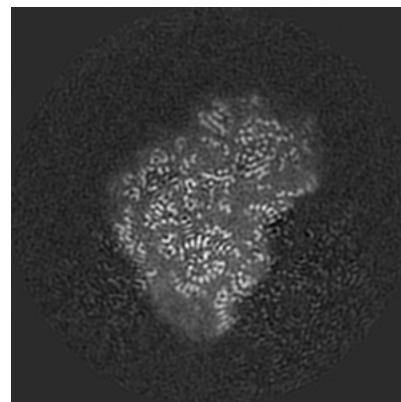
### 6.3.1 Primary map



X Index: 142

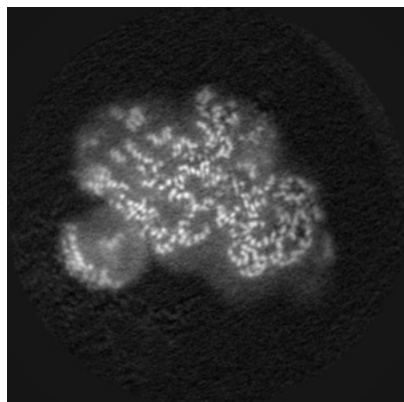


Y Index: 134

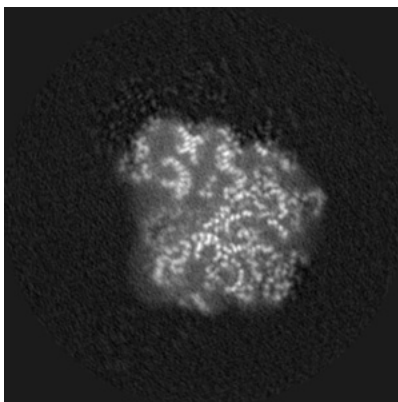


Z Index: 149

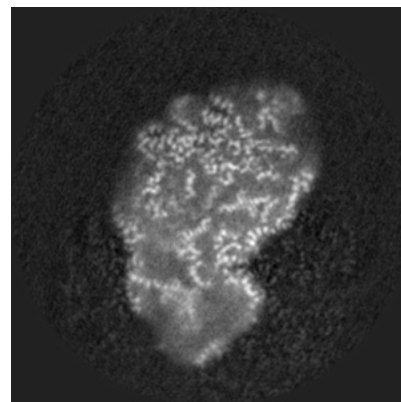
### 6.3.2 Raw map



X Index: 143



Y Index: 134

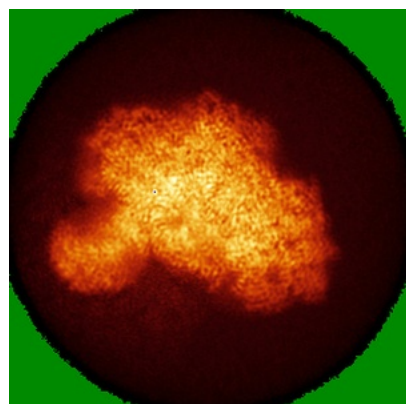


Z Index: 118

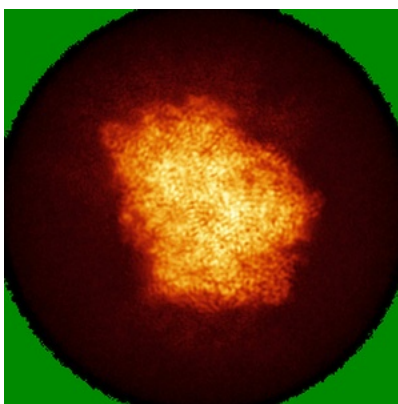
The images above show the largest variance slices of the map in three orthogonal directions.

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

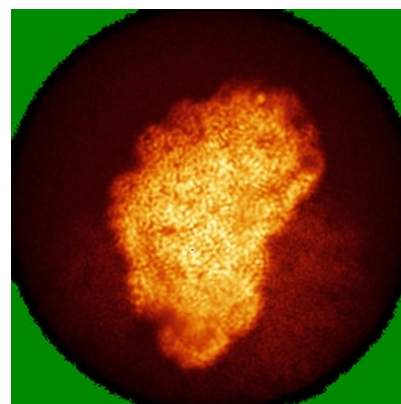
### 6.4.1 Primary map



X

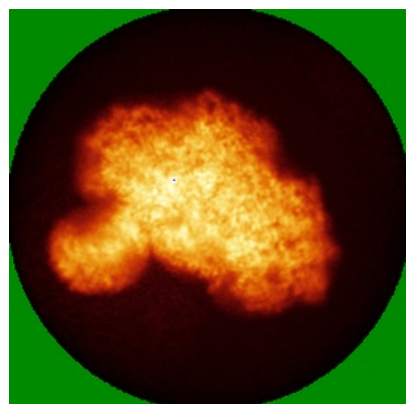


Y

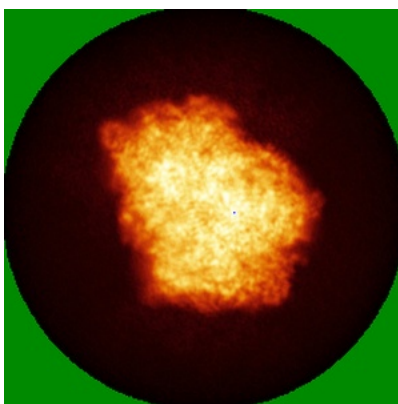


Z

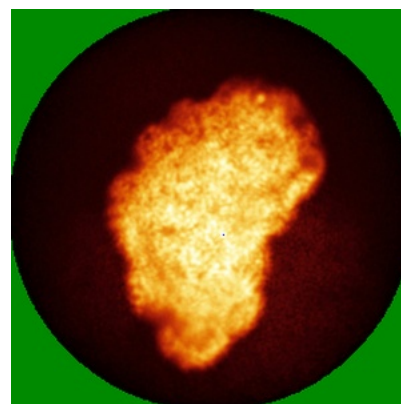
### 6.4.2 Raw map



X



Y

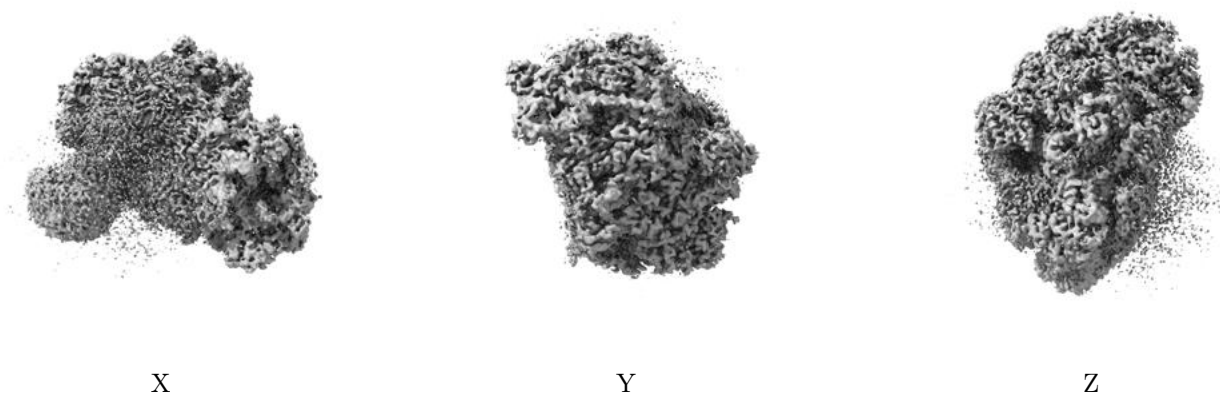


Z

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.

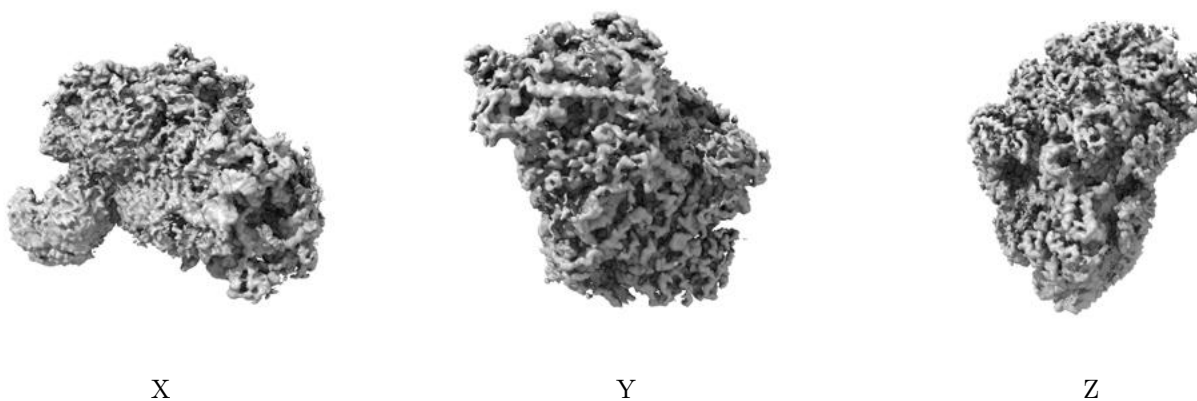
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.5. 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.

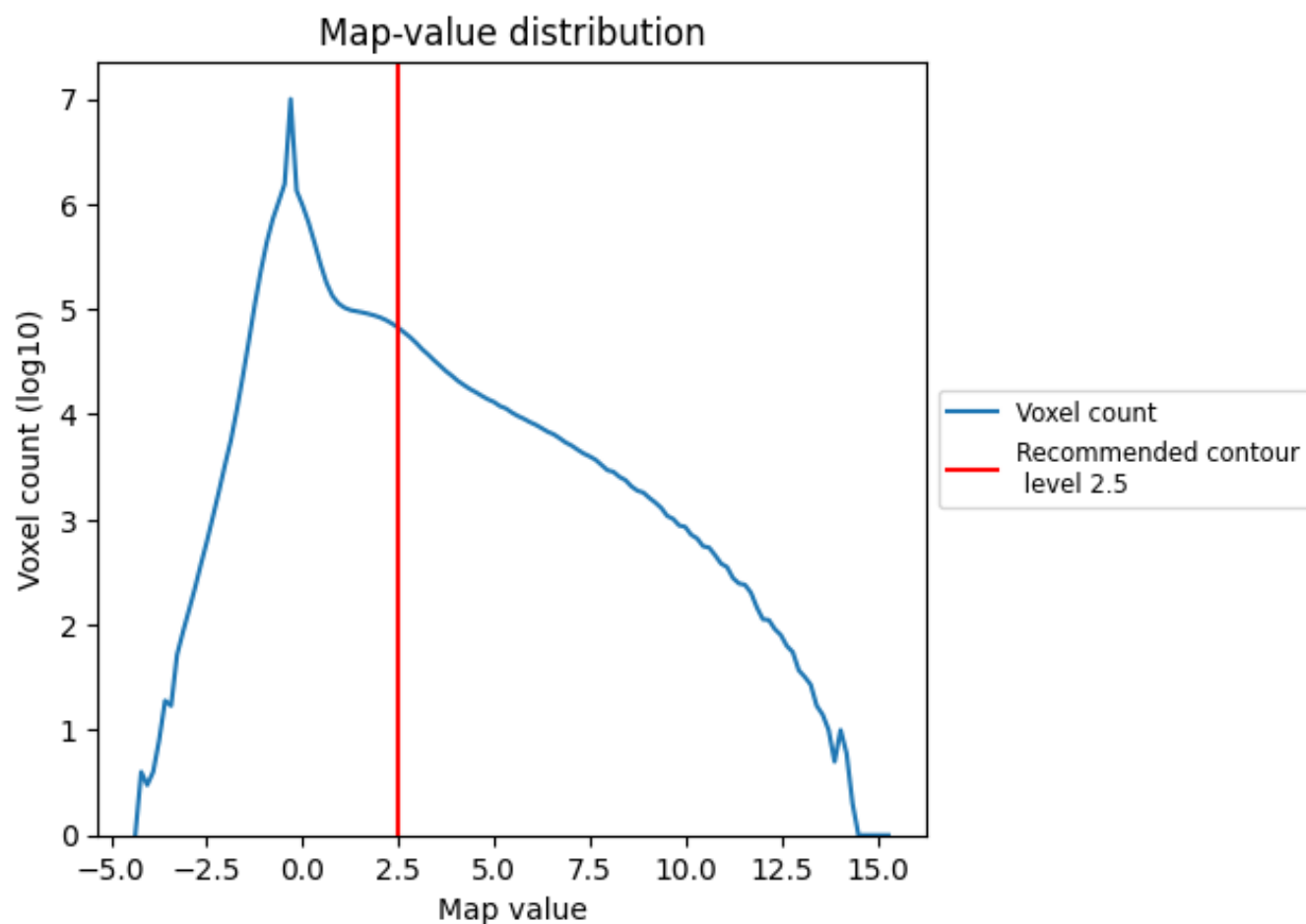
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

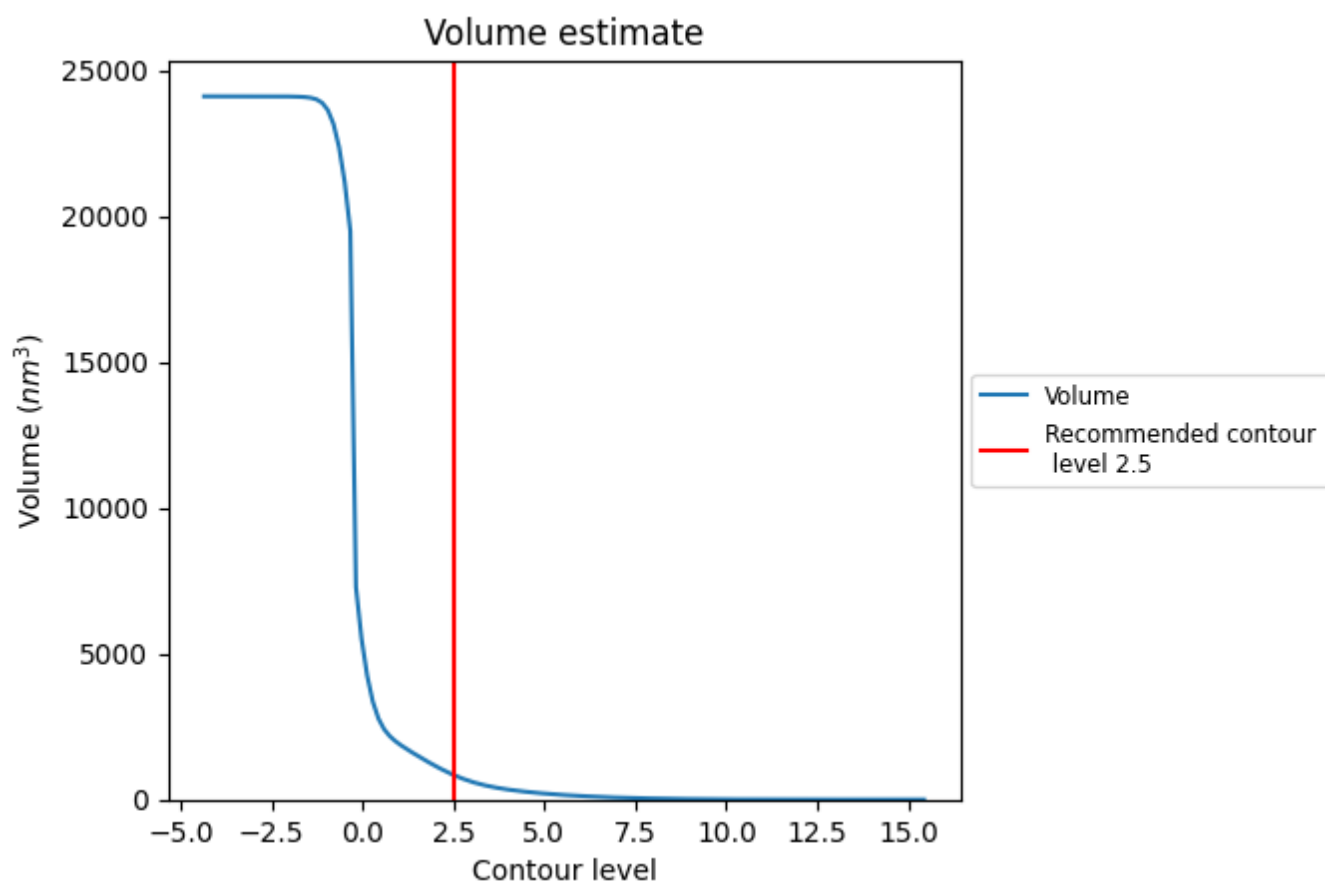
This section contains the results of statistical analysis of the map.

### 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.

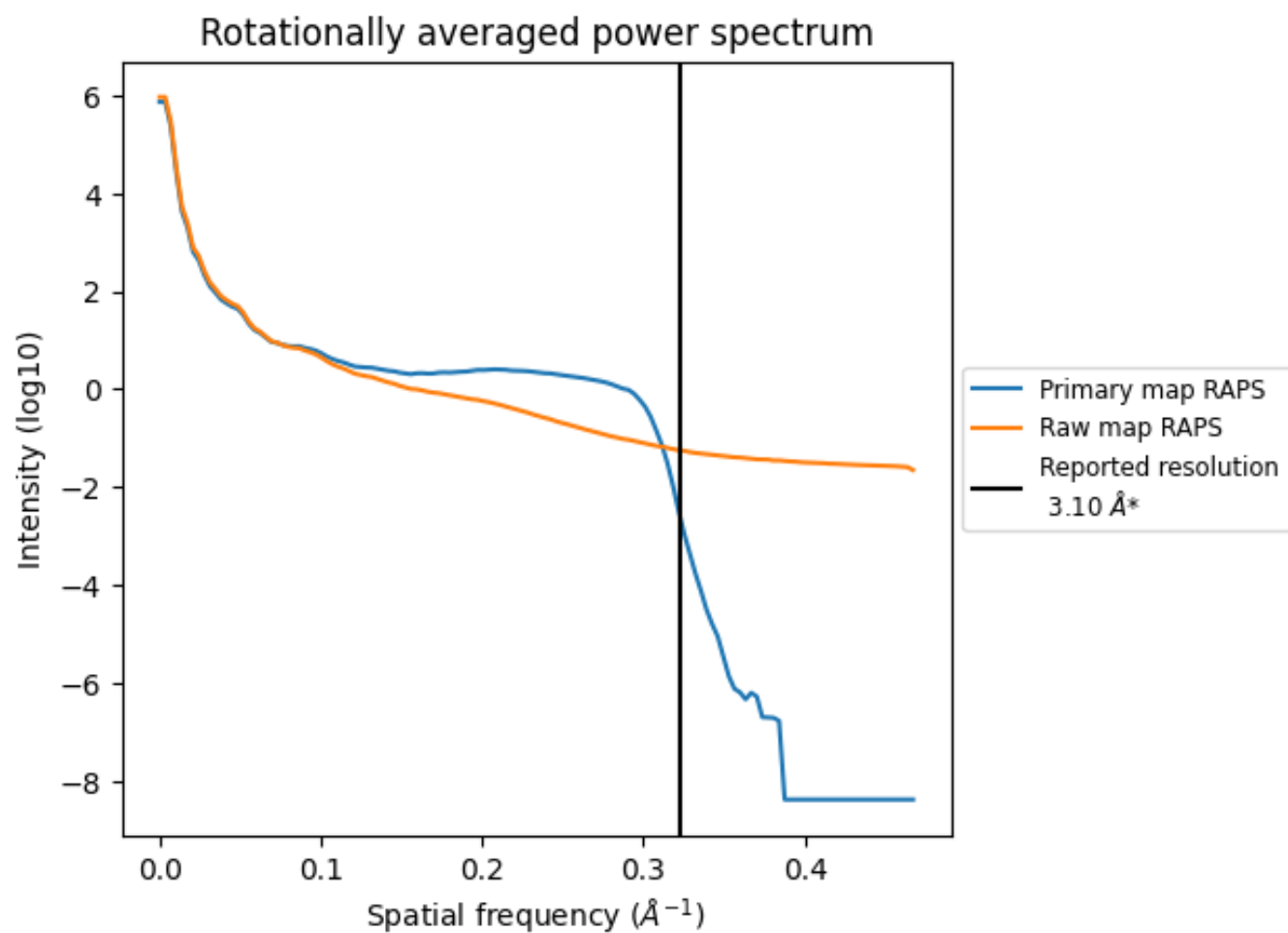
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 843  $\text{nm}^3$ ; this corresponds to an approximate mass of 761 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 ⓘ

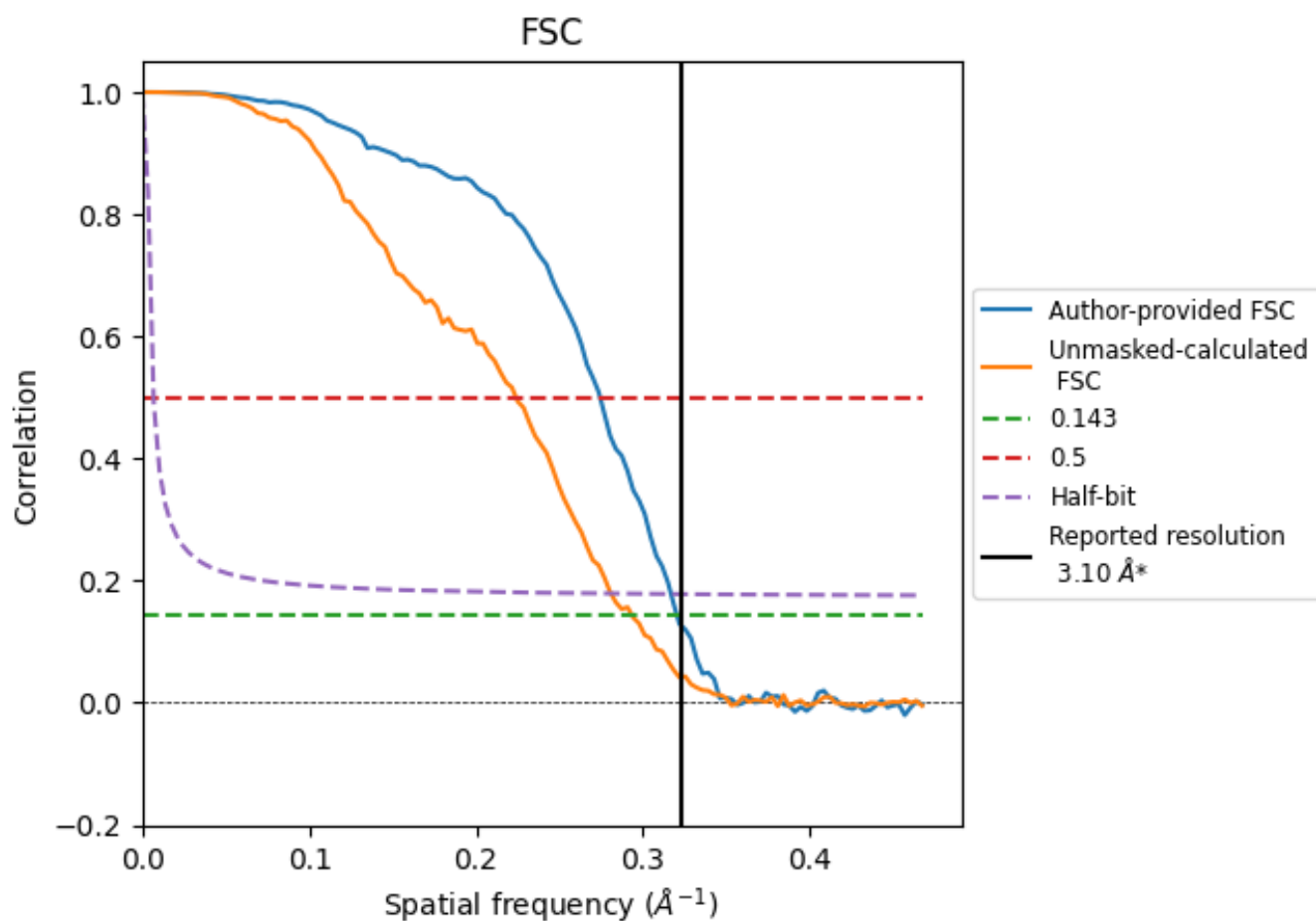


\*Reported resolution corresponds to spatial frequency of  $0.323 \text{ \AA}^{-1}$

## 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 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.12	3.65	3.16
Unmasked-calculated*	3.41	4.46	3.56

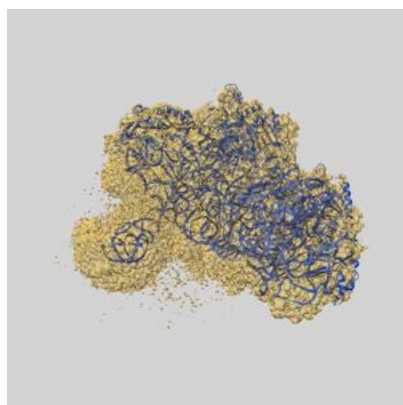
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.41 differs from the reported value 3.1 by more than 10 %



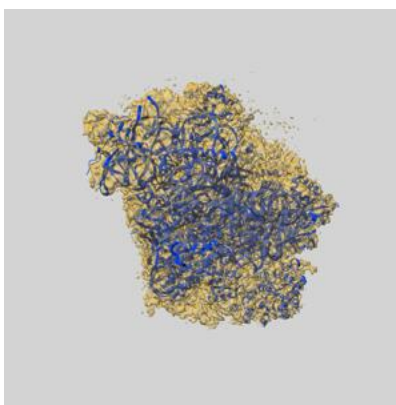
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-64695 and PDB model 9V1J. Per-residue inclusion information can be found in section [3](#) on page [7](#).

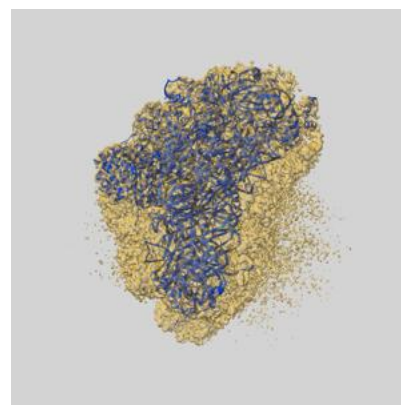
### 9.1 Map-model overlay [i](#)



X



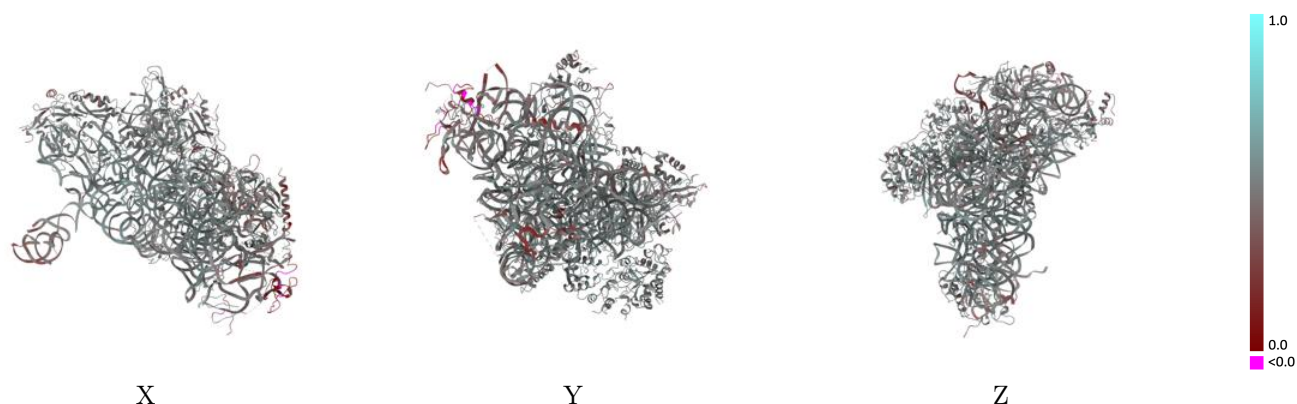
Y



Z

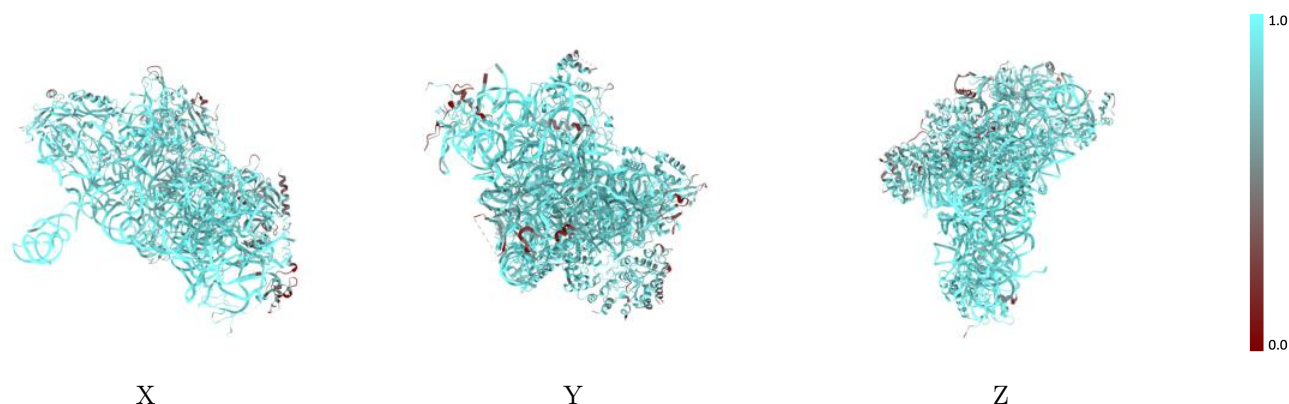
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



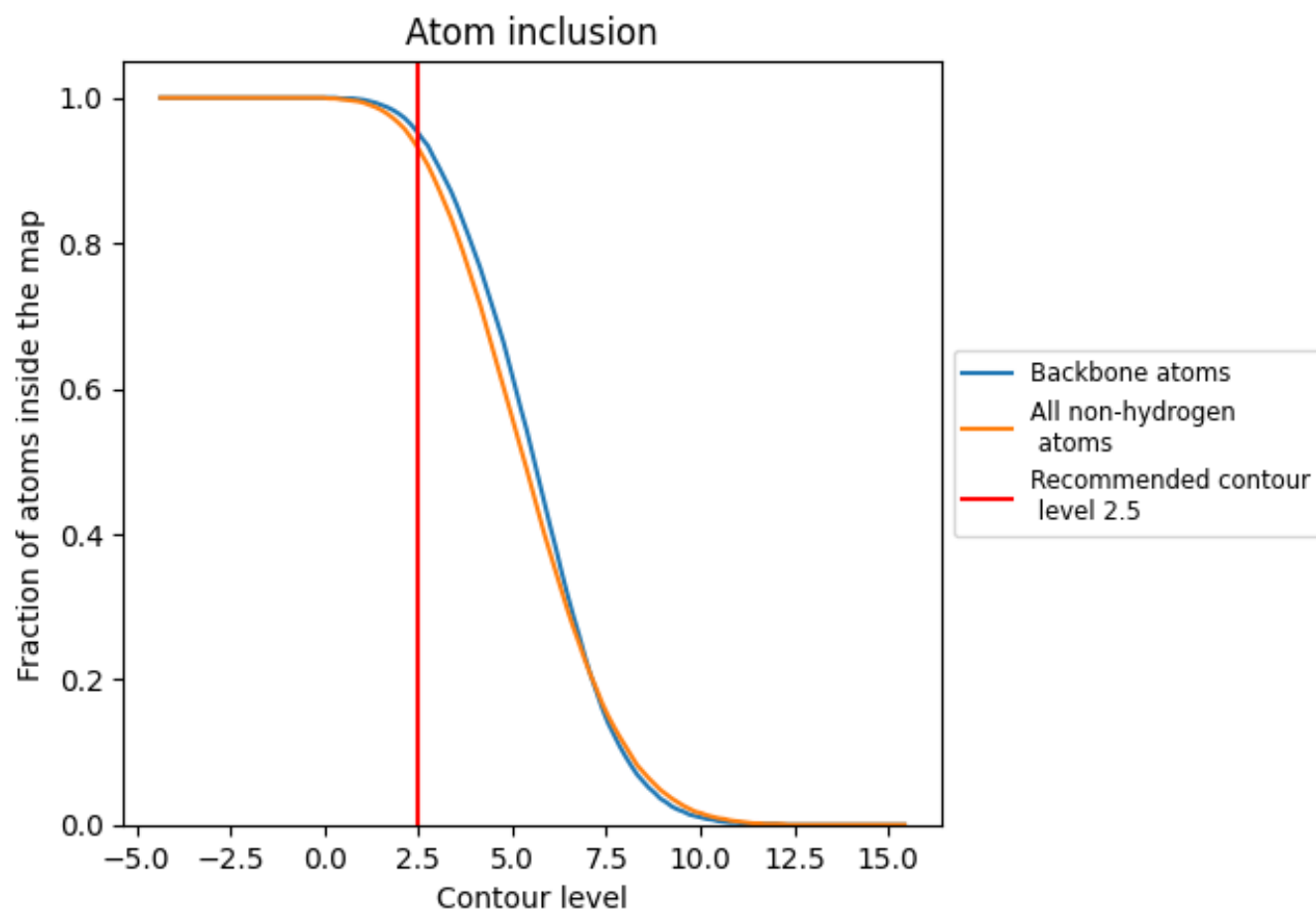
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).











































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 93% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9300	 0.4850
sB	 0.9640	 0.5220
sC	 0.8080	 0.4780
sH	 0.9900	 0.4240
sK	 1.0000	 0.5280
sa	 0.9830	 0.4930
sb	 0.8290	 0.4940
sc	 0.8970	 0.5150
se	 0.8990	 0.4820
sf	 0.8380	 0.4850
sh	 0.7020	 0.3390
si	 0.6390	 0.4510
sj	 0.9080	 0.4850
sk	 0.8720	 0.4950
sm	 0.9360	 0.4960
so	 0.9280	 0.4790
sp	 0.9580	 0.4980
sr	 0.9490	 0.5120
sx	 0.8150	 0.5000
sy	 0.9140	 0.4930
sz	 0.5850	 0.4450

