



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 07:48 PM UTC

PDB ID : 5LMR / pdb_00005lmr
EMDB ID : EMD-4077
Title : Structure of bacterial 30S-IF1-IF3-mRNA-tRNA translation pre-initiation complex(state-2B)
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on : 2016-08-01
Resolution : 4.45 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

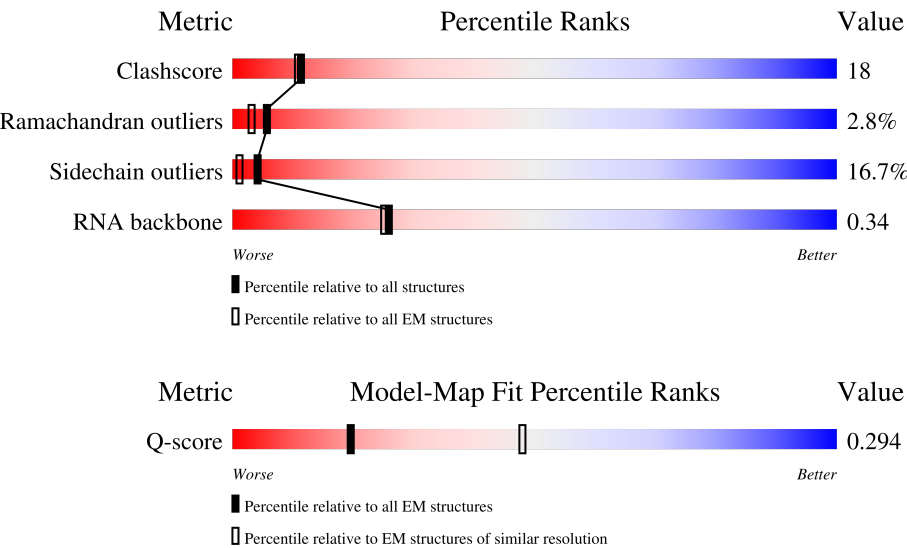
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.45 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3027 (3.95 - 4.95)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	27%54%16% 62% 54%32%5%9%
2	B	256	5% 46%33%7%14%
3	C	239	

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Mol	Chain	Length	Quality of chain
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	W	72	
23	X	171	
24	Y	42	
25	Z	77	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	ZN	D	300	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 55662 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1515	Total	C	N	O	P	0	0
			32542	14490	6022	10519	1511		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	208	Total	C	N	O	S	0	0
			1703	1066	339	291	7		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	101	Total	C	N	O	S	0	0
			843	531	155	154	3		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	138	Total	C	N	O	S	0	0
			1116	705	215	193	3		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	127	Total	C	N	O	0	0
			1010	639	197	174		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			792	498	156	137	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	119	Total	C	N	O	S	0	0
			885	549	168	165	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	121	Total	C	N	O	S	0	0
			964	597	199	166	2		

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	88	Total	C	N	O	S	0	0
			734	459	147	126	2		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0
			823	528	151	142	2		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	73	Total	C	N	O	0	0
			598	381	118	99		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			655	419	120	114	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	99	Total	C	N	O	S	0	0
			763	470	162	129	2		

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	71	Total	C	N	O	S	0	0
			570	362	103	103	2		

- Molecule 23 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	168	Total	C	N	O	S	0	0
			1356	853	249	245	9		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	17	Total	C	N	O	P	0	0
			373	166	74	116	17		

- Molecule 25 is a RNA chain called tRNAi.

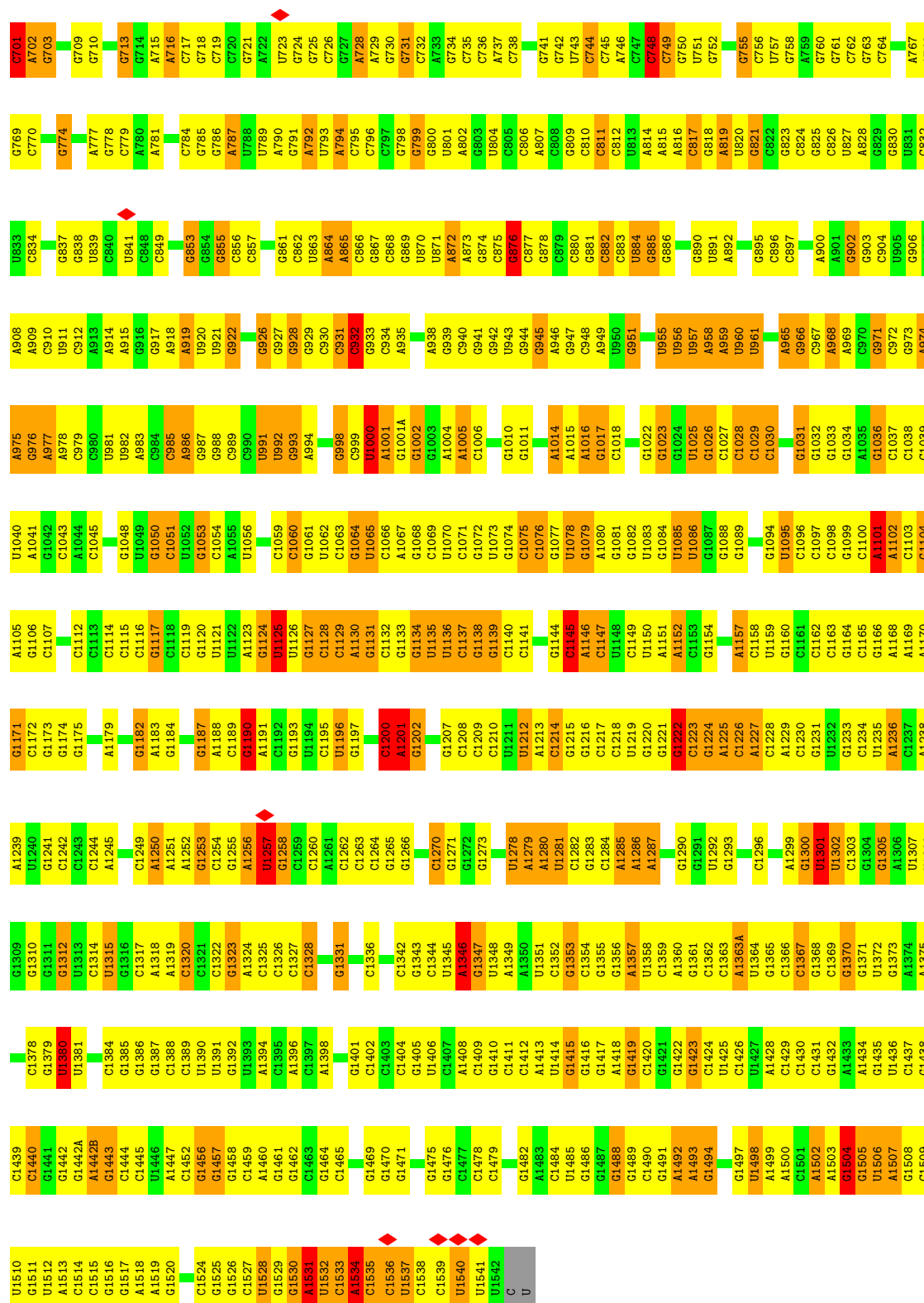
Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	77	Total	C	N	O	P	S	0	0
			1646	735	297	536	77	1		

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	D	1	Total	Zn	0
			1	1	
26	N	1	Total	Zn	0
			1	1	

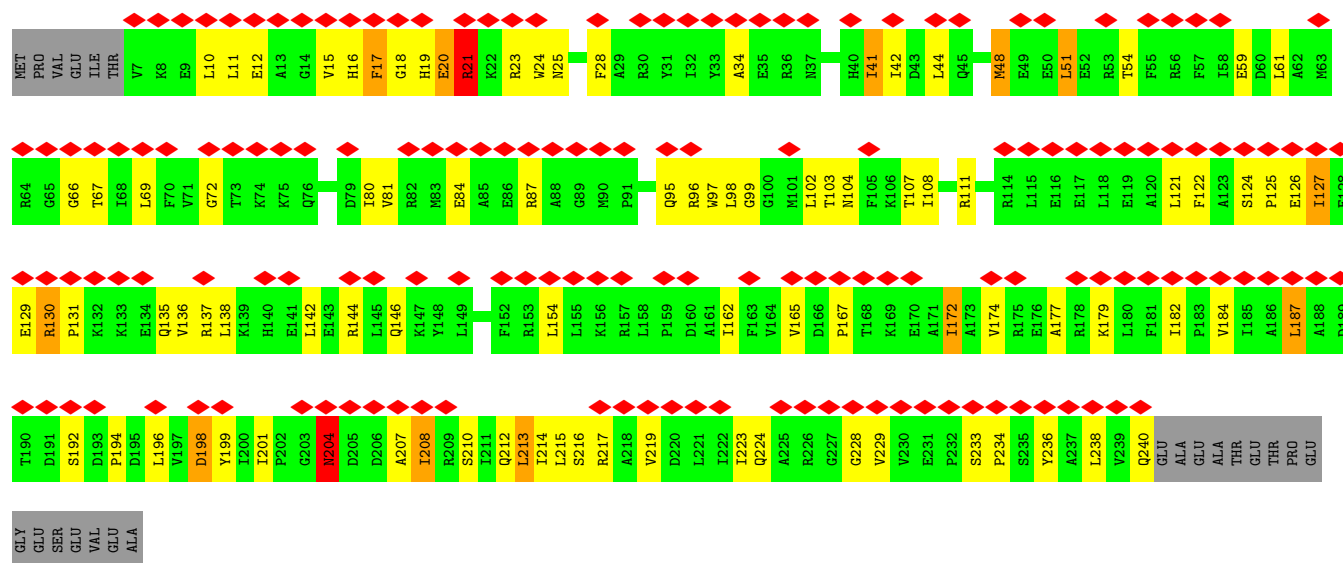
- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
27	W	1	Total	Mg	0
			1	1	
27	Z	1	Total	Mg	0
			1	1	

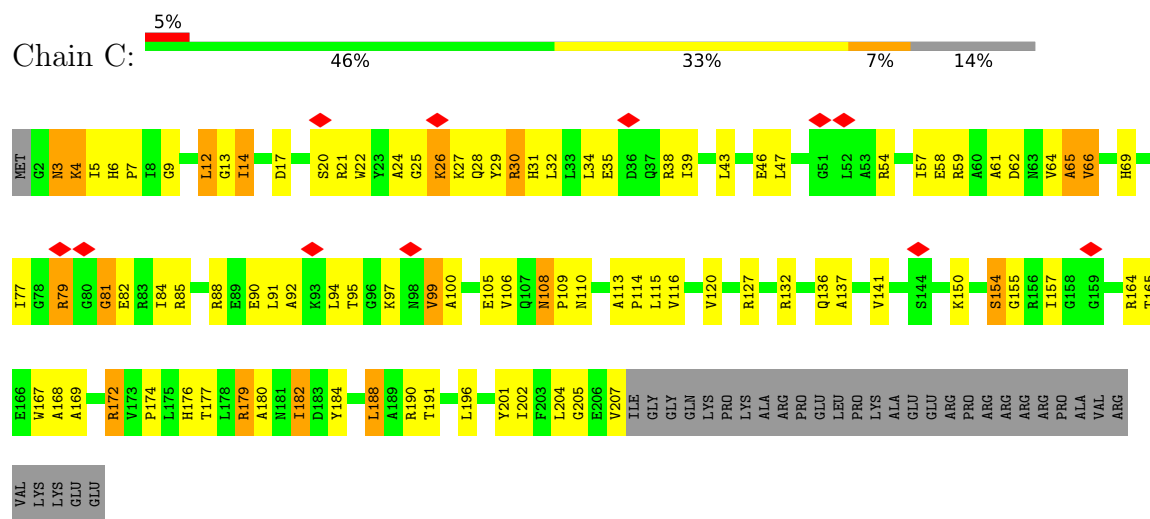


• Molecule 2: 30S ribosomal protein S2

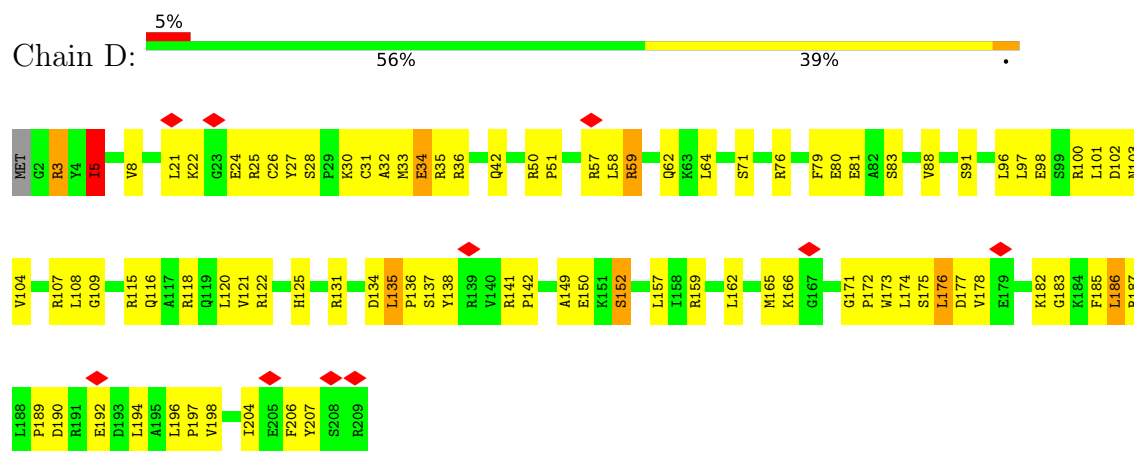




• Molecule 3: 30S ribosomal protein S3

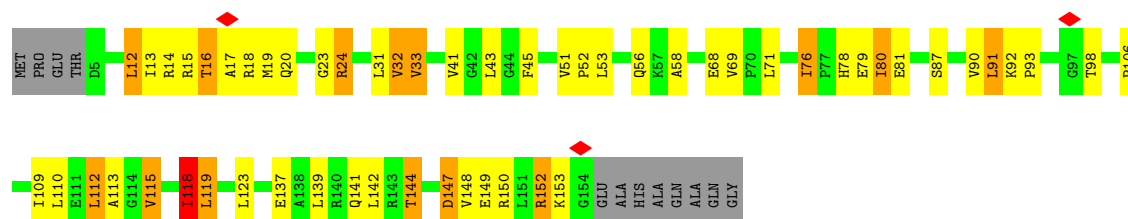


• Molecule 4: 30S ribosomal protein S4



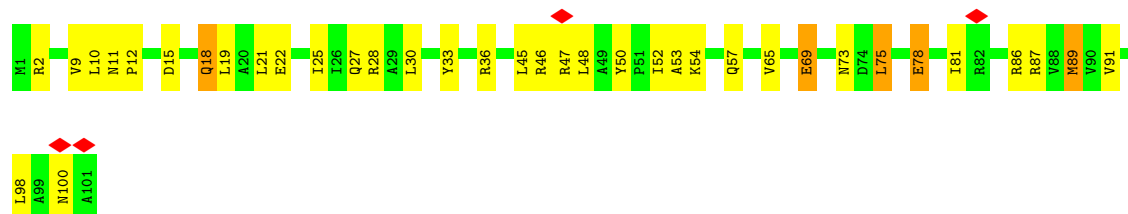
• Molecule 5: 30S ribosomal protein S5

Chain E: 



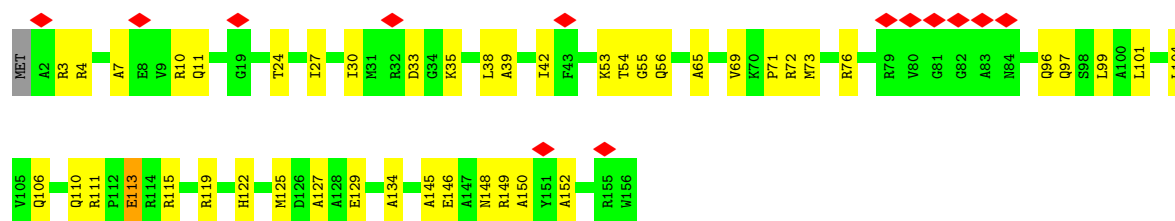
- Molecule 6: 30S ribosomal protein S6

Chain F: 



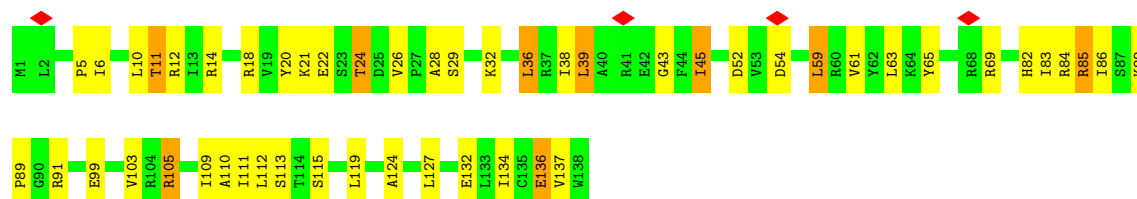
- Molecule 7: 30S ribosomal protein S7

Chain G: 



- Molecule 8: 30S ribosomal protein S8

Chain H: 



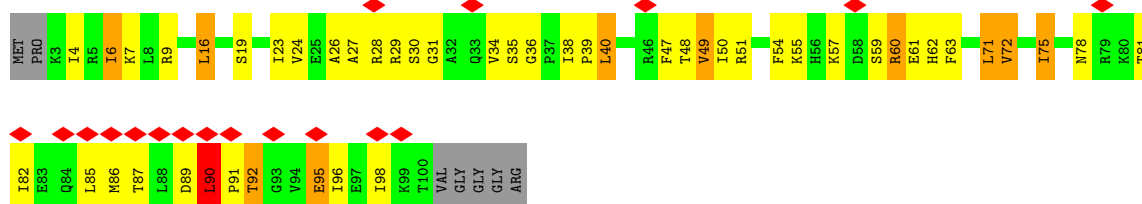
- Molecule 9: 30S ribosomal protein S9

Chain I: 

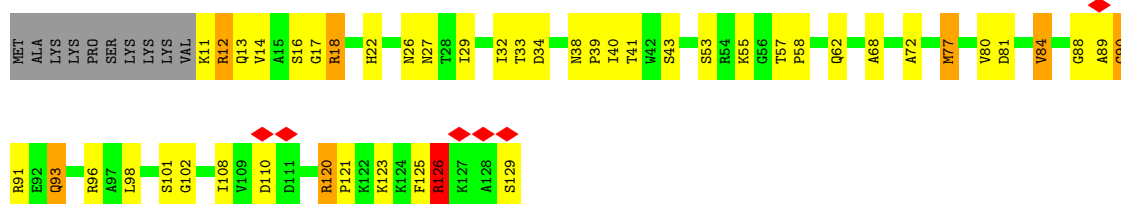




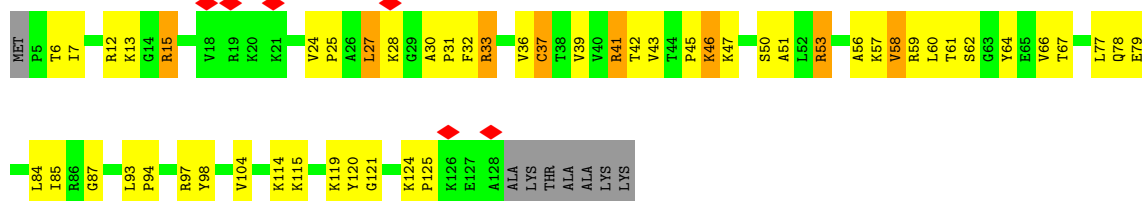
- Molecule 10: 30S ribosomal protein S10



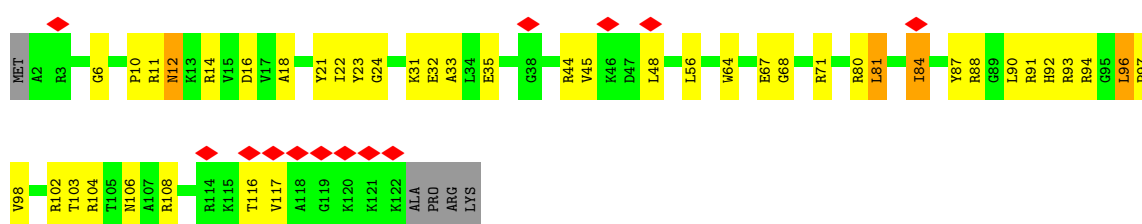
- Molecule 11: 30S ribosomal protein S11



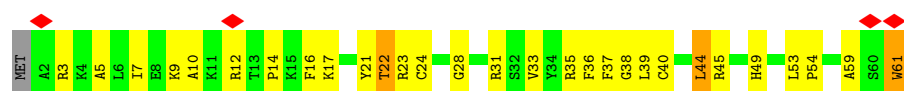
- Molecule 12: 30S ribosomal protein S12



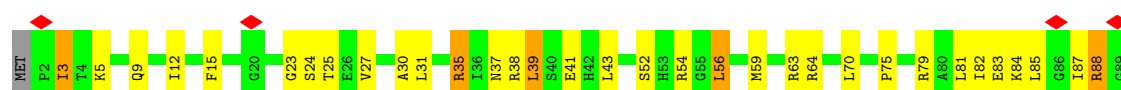
- Molecule 13: 30S ribosomal protein S13



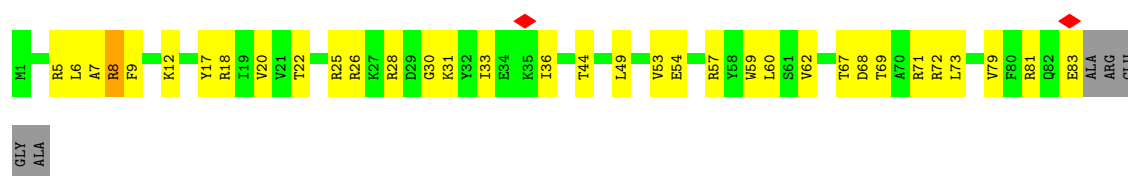
- Molecule 14: 30S ribosomal protein S14 type Z



- Molecule 15: 30S ribosomal protein S15



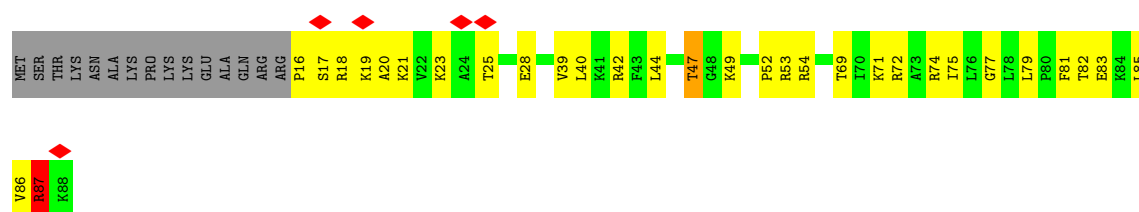
- Molecule 16: 30S ribosomal protein S16



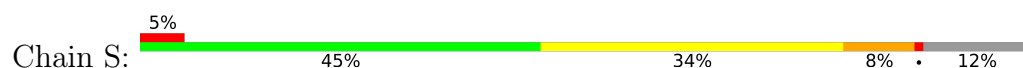
- Molecule 17: 30S ribosomal protein S17

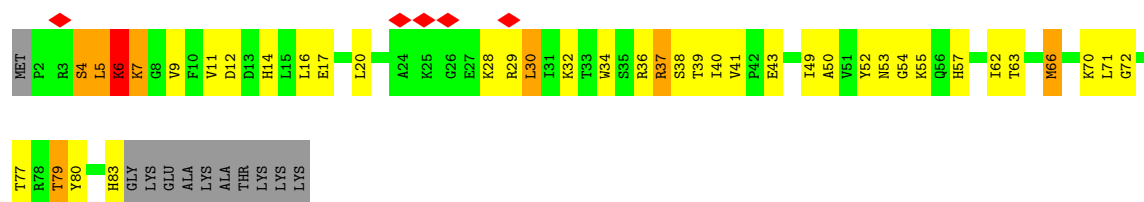


- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19

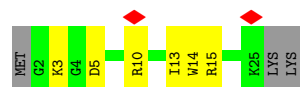




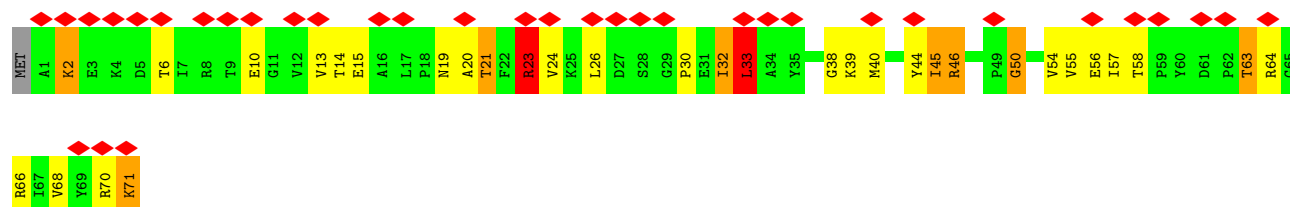
- Molecule 20: 30S ribosomal protein S20



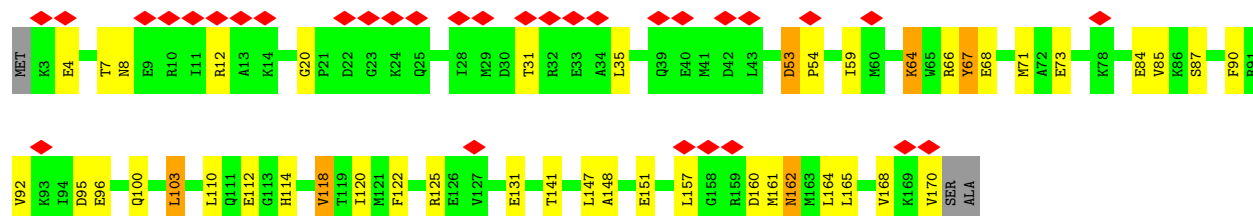
- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: Translation initiation factor IF-1



- Molecule 23: Translation initiation factor IF-3



- Molecule 24: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17176	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.438	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	348.4, 348.4, 348.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, MG, 4SU, ZN, OMC, PSU, G7M

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	A	0.43	0/36416	0.82	71/56813 (0.1%)
2	B	0.69	0/1935	1.18	1/2609 (0.0%)
3	C	0.55	0/1636	1.16	6/2205 (0.3%)
4	D	0.52	0/1733	1.16	2/2318 (0.1%)
5	E	0.55	0/1162	1.20	6/1564 (0.4%)
6	F	0.50	0/856	0.99	0/1154
7	G	0.56	0/1276	1.12	0/1709
8	H	0.51	0/1136	1.04	0/1527
9	I	0.52	0/1029	0.98	0/1379
10	J	0.71	0/805	1.06	6/1082 (0.6%)
11	K	0.61	0/900	1.19	4/1213 (0.3%)
12	L	0.51	0/986	1.03	3/1320 (0.2%)
13	M	0.61	0/974	1.15	2/1303 (0.2%)
14	N	0.51	0/501	1.02	1/664 (0.2%)
15	O	0.56	0/745	1.21	0/992
16	P	0.50	0/716	1.02	1/963 (0.1%)
17	Q	0.49	0/836	1.02	1/1117 (0.1%)
18	R	0.60	0/604	1.12	0/801
19	S	0.64	0/670	1.14	2/903 (0.2%)
20	T	0.60	0/765	1.29	2/1007 (0.2%)
21	V	0.55	0/212	0.97	0/277
22	W	0.75	0/580	1.30	3/782 (0.4%)
23	X	0.66	0/1375	1.17	4/1844 (0.2%)
24	Y	0.53	0/418	0.83	0/649
25	Z	0.55	2/1719 (0.1%)	0.95	4/2674 (0.1%)
All	All	0.50	2/59985 (0.0%)	0.93	119/88869 (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
2	B	0	1
23	X	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	8	4SU	O3'-P	6.04	1.62	1.56
25	Z	46	G7M	O3'-P	5.56	1.61	1.56

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	23	ARG	N-CA-C	-19.63	79.19	110.20
5	E	15	ARG	CB-CA-C	-13.92	85.65	109.72
5	E	15	ARG	N-CA-C	-13.48	87.37	109.07
3	C	65	ALA	CB-CA-C	-12.66	87.83	109.72
1	A	1145	C	C2'-C3'-O3'	11.49	126.74	109.50
3	C	65	ALA	N-CA-C	-11.37	90.77	109.07
1	A	266	G	C2'-C3'-O3'	11.34	126.51	109.50
3	C	13	GLY	N-CA-C	10.67	125.54	112.73
3	C	66	VAL	N-CA-C	-10.52	87.46	109.34
1	A	1498	U	C2'-C3'-O3'	10.38	125.08	109.50
25	Z	47	U	C2'-C3'-O3'	9.68	124.01	109.50
1	A	1301	U	C2'-C3'-O3'	9.66	123.99	109.50
1	A	687	A	C2'-C3'-O3'	9.38	123.57	109.50
1	A	1346	A	C2'-C3'-O3'	9.09	123.14	109.50
10	J	61	GLU	N-CA-CB	-9.04	95.61	111.08
1	A	792	A	C2'-C3'-O3'	9.01	123.01	109.50
1	A	328	C	C2'-C3'-O3'	8.80	122.70	109.50
1	A	965	A	C2'-C3'-O3'	8.60	122.41	109.50
1	A	51	A	C4'-C3'-O3'	8.56	122.24	109.40
1	A	1101	A	C4'-C3'-O3'	8.37	121.95	109.40
1	A	115	G	C4'-C3'-O3'	8.23	121.75	109.40
1	A	197	A	C2'-C3'-O3'	8.09	121.64	109.50
1	A	1065	U	C2'-C3'-O3'	8.07	121.61	109.50
1	A	428	G	C2'-C3'-O3'	8.03	121.55	109.50
1	A	115	G	C2'-C3'-O3'	8.03	121.54	109.50
1	A	559	A	C2'-C3'-O3'	7.92	121.38	109.50
4	D	34	GLU	N-CA-C	7.85	119.84	111.28
1	A	748	C	C2'-C3'-O3'	7.62	120.93	109.50
1	A	181	G	C2'-C3'-O3'	7.60	120.89	109.50
1	A	1190	G	C2'-C3'-O3'	7.53	125.00	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1065	U	C4'-C3'-O3'	7.36	120.45	109.40
1	A	1300	G	C2'-C3'-O3'	7.33	120.50	109.50
1	A	1201	A	C4'-C3'-O3'	7.22	120.22	109.40
22	W	33	LEU	N-CA-C	-7.06	99.37	109.96
1	A	1380	U	C4'-C3'-O3'	7.03	119.95	109.40
10	J	61	GLU	N-CA-C	-6.97	98.56	109.72
1	A	344	A	C2'-C3'-O3'	6.73	119.59	109.50
1	A	484	G	C4'-C3'-O3'	6.67	119.40	109.40
1	A	992	U	C2'-C3'-O3'	6.66	119.48	109.50
1	A	181	G	C4'-C3'-O3'	6.63	119.35	109.40
1	A	572	A	C4'-C3'-O3'	-6.62	103.08	113.00
5	E	16	THR	N-CA-C	-6.57	100.23	109.69
1	A	932	C	C4'-C3'-O3'	-6.54	103.19	113.00
1	A	1285	A	C2'-C3'-O3'	6.52	119.28	109.50
5	E	118	ILE	N-CA-C	6.48	116.91	108.35
25	Z	58	A	C2'-C3'-O3'	6.48	119.22	109.50
1	A	78	G	C2'-C3'-O3'	-6.47	104.00	113.70
1	A	60	A	C2'-C3'-O3'	6.41	119.11	109.50
1	A	1257	U	C2'-C3'-O3'	6.38	119.07	109.50
23	X	53	ASP	CA-C-N	6.35	126.92	120.38
23	X	53	ASP	C-N-CA	6.35	126.92	120.38
23	X	96	GLU	N-CA-C	6.33	117.87	110.97
14	N	22	THR	N-CA-C	6.32	118.17	111.28
12	L	46	LYS	N-CA-C	6.28	113.93	108.78
1	A	1000	U	C2'-C3'-O3'	6.22	123.02	113.70
11	K	102	GLY	N-CA-C	-6.20	106.48	114.85
1	A	701	C	C2'-C3'-O3'	6.19	118.79	109.50
1	A	1380	U	C2'-C3'-O3'	6.16	118.74	109.50
25	Z	36	U	C2'-C3'-O3'	6.07	122.80	113.70
25	Z	17	C	C2'-C3'-O3'	6.05	118.57	109.50
1	A	1101	A	C2'-C3'-O3'	6.04	118.56	109.50
4	D	207	TYR	N-CA-C	5.99	118.77	111.82
1	A	281	G	C2'-C3'-O3'	5.97	122.66	113.70
1	A	1534	A	C2'-C3'-O3'	5.87	118.30	109.50
1	A	1182	G	C3'-C2'-O2'	5.86	119.48	110.70
1	A	577	G	C4'-C3'-O3'	-5.84	104.24	113.00
1	A	1200	C	C4'-C3'-O3'	-5.74	104.39	113.00
16	P	30	GLY	N-CA-C	5.71	119.91	112.25
1	A	1285	A	C4'-C3'-O3'	5.64	117.86	109.40
11	K	17	GLY	N-CA-C	5.63	117.77	110.45
5	E	78	HIS	N-CA-C	5.61	117.60	109.07
1	A	1531	A	C2'-C3'-O3'	5.53	122.00	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	49	VAL	N-CA-C	5.53	116.08	108.12
23	X	84	GLU	CB-CA-C	-5.52	109.22	115.79
10	J	90	LEU	N-CA-C	5.50	121.97	109.81
1	A	1214	C	C4'-C3'-O3'	5.50	117.65	109.40
1	A	64	G	C2'-C3'-O3'	5.46	117.69	109.50
11	K	89	ALA	N-CA-C	-5.46	99.02	108.52
11	K	77	MET	N-CA-C	5.45	119.12	109.96
10	J	6	ILE	N-CA-C	5.44	114.20	106.53
2	B	66	GLY	N-CA-C	5.43	118.30	112.33
1	A	993	G	C4'-C3'-O3'	5.43	117.54	109.40
5	E	16	THR	N-CA-CB	-5.43	102.67	110.87
1	A	496	A	C4'-C3'-O3'	5.42	117.54	109.40
13	M	108	ARG	N-CA-C	5.42	116.99	111.14
1	A	1222	G	C3'-C2'-O2'	5.40	118.80	110.70
1	A	509	A	C4'-C3'-O3'	5.38	121.07	113.00
1	A	372	C	C4'-C3'-O3'	5.36	117.43	109.40
1	A	1504	G	C2'-C3'-O3'	5.35	117.53	109.50
12	L	30	ALA	CA-C-N	5.29	125.10	119.28
12	L	30	ALA	C-N-CA	5.29	125.10	119.28
1	A	428	G	C4'-C3'-O3'	5.28	117.32	109.40
1	A	243	A	C2'-C3'-O3'	5.25	117.38	109.50
22	W	24	VAL	N-CA-CB	-5.25	105.52	112.34
1	A	1196	U	C4'-C3'-O3'	5.24	117.26	109.40
1	A	279	A	C4'-C3'-O3'	5.21	117.21	109.40
1	A	559	A	C4'-C3'-O3'	5.20	117.20	109.40
1	A	1182	G	C2'-C3'-O3'	5.18	121.47	113.70
19	S	4	SER	N-CA-C	5.17	117.02	108.49
1	A	243	A	C4'-C3'-O3'	5.17	117.15	109.40
1	A	60	A	C4'-C3'-O3'	5.14	117.11	109.40
1	A	1145	C	C4'-C3'-O3'	-5.13	101.70	109.40
19	S	54	GLY	N-CA-C	-5.12	108.38	114.48
1	A	372	C	C2'-C3'-O3'	5.12	117.18	109.50
17	Q	62	SER	N-CA-C	5.12	116.76	109.14
1	A	306	G	C4'-C3'-O3'	-5.10	105.35	113.00
1	A	484	G	C2'-C3'-O3'	5.10	117.15	109.50
20	T	13	LEU	CA-C-N	5.08	127.35	120.38
20	T	13	LEU	C-N-CA	5.08	127.35	120.38
1	A	1504	G	C4'-C3'-O3'	5.08	117.02	109.40
1	A	1147	C	C3'-C2'-O2'	5.07	118.30	110.70
13	M	81	LEU	CA-CB-CG	5.06	134.00	116.30
1	A	78	G	C3'-C2'-O2'	5.05	118.28	110.70
1	A	876	G	C4'-C3'-O3'	-5.04	105.43	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	12	LEU	CA-C-N	5.03	125.57	119.98
3	C	12	LEU	C-N-CA	5.03	125.57	119.98
10	J	16	LEU	N-CA-C	-5.03	108.89	114.62
1	A	1125	U	C4'-C3'-O3'	-5.00	105.49	113.00
1	A	315	A	C2'-C3'-O3'	5.00	117.00	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	HIS	Peptide
23	X	53	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32542	0	16447	1120	0
2	B	1900	0	1951	41	0
3	C	1612	0	1674	77	0
4	D	1703	0	1766	44	0
5	E	1146	0	1207	47	0
6	F	843	0	857	16	0
7	G	1257	0	1296	28	0
8	H	1116	0	1177	40	0
9	I	1010	0	1037	33	0
10	J	792	0	835	48	0
11	K	885	0	904	20	0
12	L	970	0	1057	32	0
13	M	964	0	1034	24	0
14	N	492	0	529	28	0
15	O	734	0	771	13	0
16	P	700	0	720	19	0
17	Q	823	0	891	20	0
18	R	598	0	670	17	0
19	S	655	0	672	34	0
20	T	763	0	861	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	V	208	0	221	3	0
22	W	570	0	599	25	0
23	X	1356	0	1401	15	0
24	Y	373	0	186	17	0
25	Z	1646	0	845	108	0
26	D	1	0	0	4	0
26	N	1	0	0	0	0
27	W	1	0	0	0	0
27	Z	1	0	0	0	0
All	All	55662	0	39608	1700	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 18.

All (1700) 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)
22:W:21:THR:CG2	22:W:33:LEU:HD11	1.53	1.36
10:J:7:LYS:HG3	10:J:71:LEU:CD2	1.55	1.33
1:A:1358:U:H3	1:A:1363(A):A:N6	1.36	1.24
1:A:1345:U:N3	1:A:1375:A:N6	1.87	1.21
5:E:93:PRO:HG3	8:H:105:ARG:NH2	1.53	1.20
9:I:5:TYR:CE2	9:I:7:THR:OG1	1.95	1.19
1:A:1358:U:O4	1:A:1363(A):A:N1	1.75	1.19
5:E:93:PRO:CG	8:H:105:ARG:NH2	2.05	1.18
22:W:21:THR:HG22	22:W:33:LEU:CD1	1.79	1.12
22:W:21:THR:HG21	22:W:33:LEU:HD11	1.24	1.11
1:A:92:C:H2'	1:A:93:G:C8	1.85	1.11
10:J:7:LYS:HG3	10:J:71:LEU:HD21	1.18	1.11
1:A:918:A:H2	1:A:1079:G:N2	1.46	1.11
1:A:1256:A:H3'	3:C:27:LYS:NZ	1.66	1.11
3:C:29:TYR:OH	14:N:54:PRO:HG2	1.50	1.09
1:A:92:C:H2'	1:A:93:G:H8	0.99	1.09
10:J:7:LYS:CG	10:J:71:LEU:HD21	1.84	1.07
22:W:21:THR:CG2	22:W:33:LEU:CD1	2.31	1.07
25:Z:1:C:H2'	25:Z:2:G:H8	1.14	1.06
5:E:93:PRO:CG	8:H:105:ARG:HH22	1.63	1.04
1:A:827:U:O4	1:A:872:A:N1	1.91	1.04
1:A:1532:U:H5''	1:A:1533:C:OP2	1.58	1.04
10:J:7:LYS:HG3	10:J:71:LEU:HD23	1.37	1.02
1:A:1256:A:H5''	3:C:27:LYS:CE	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:G:H3'	1:A:81:U:H5''	1.39	1.01
1:A:827:U:H3	1:A:872:A:N6	1.57	1.01
10:J:7:LYS:CG	10:J:71:LEU:CD2	2.39	1.00
1:A:1219:U:H2'	1:A:1220:G:C8	1.97	0.97
4:D:31:CYS:SG	26:D:300:ZN:ZN	1.54	0.97
10:J:40:LEU:HD11	10:J:71:LEU:HG	1.44	0.97
1:A:1074:G:H1'	2:B:104:ASN:HD21	1.27	0.95
16:P:59:TRP:O	16:P:62:VAL:CG2	2.14	0.94
1:A:864:A:H2'	1:A:865:A:C8	2.03	0.93
1:A:918:A:C2	1:A:1079:G:N2	2.33	0.93
1:A:827:U:N3	1:A:872:A:N6	2.13	0.93
3:C:28:GLN:HA	3:C:31:HIS:CD2	2.04	0.93
9:I:5:TYR:HE2	9:I:7:THR:OG1	1.40	0.93
1:A:918:A:H2	1:A:1079:G:H22	1.05	0.92
10:J:50:ILE:HG13	10:J:60:ARG:HD2	1.51	0.92
1:A:1492:A:H8	22:W:19:ASN:HB3	1.34	0.92
1:A:1227:A:C2	19:S:83:HIS:HB3	2.04	0.92
1:A:958:A:N1	19:S:55:LYS:HB2	1.85	0.92
3:C:92:ALA:O	3:C:95:THR:O	1.87	0.91
16:P:59:TRP:O	16:P:62:VAL:HG22	1.71	0.90
5:E:93:PRO:HG2	8:H:105:ARG:CZ	2.01	0.90
1:A:1358:U:N3	1:A:1363(A):A:N6	2.05	0.90
1:A:13:U:H5'	1:A:14:U:H5	1.38	0.89
1:A:1061:G:H5'	10:J:59:SER:OG	1.71	0.89
1:A:664:G:H22	1:A:741:G:H1	1.19	0.88
1:A:745:C:H2'	1:A:746:A:C8	2.08	0.88
1:A:1256:A:H5''	3:C:27:LYS:HE2	1.54	0.88
1:A:1071:C:H2'	1:A:1072:G:H8	1.38	0.88
1:A:1345:U:C2	1:A:1375:A:N6	2.41	0.88
13:M:84:ILE:HG22	19:S:66:MET:HE3	1.55	0.88
1:A:1535:C:N3	1:A:1536:C:C5	2.42	0.88
25:Z:50:U:H2'	25:Z:51:C:C6	2.09	0.88
1:A:67:C:H2'	1:A:68:G:C8	2.09	0.87
1:A:1000:U:H2'	1:A:1001:A:H1'	1.56	0.87
10:J:62:HIS:HB3	14:N:59:ALA:HB3	1.56	0.87
3:C:30:ARG:NH1	14:N:35:ARG:O	2.06	0.87
9:I:82:ALA:HB1	9:I:96:LEU:HD21	1.57	0.87
1:A:966:G:C2	25:Z:34:C:H5'	2.10	0.86
1:A:1073:U:H3	1:A:1102:A:H61	1.24	0.86
1:A:1227:A:N1	19:S:83:HIS:HB3	1.89	0.86
25:Z:1:C:H2'	25:Z:2:G:C8	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1530:G:H2'	1:A:1531:A:O4'	1.76	0.86
5:E:93:PRO:CB	8:H:105:ARG:HH22	1.89	0.85
22:W:32:ILE:HB	22:W:63:THR:C	2.01	0.85
1:A:1256:A:C3'	3:C:27:LYS:NZ	2.38	0.85
1:A:1227:A:C2	19:S:83:HIS:CB	2.59	0.85
1:A:1061:G:C5'	10:J:59:SER:OG	2.25	0.85
1:A:1345:U:H3	1:A:1375:A:N6	1.72	0.85
1:A:1077:G:N2	1:A:1079:G:H3'	1.92	0.85
5:E:93:PRO:CG	8:H:105:ARG:CZ	2.56	0.84
1:A:1101:A:H4'	1:A:1102:A:O5'	1.76	0.84
10:J:7:LYS:HA	10:J:71:LEU:HD22	1.60	0.84
1:A:501:C:H2'	1:A:502:G:C8	2.14	0.83
1:A:920:U:H2'	1:A:921:U:C6	2.13	0.83
9:I:112:LYS:HG2	9:I:119:ALA:H	1.41	0.83
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.59	0.83
1:A:1070:U:H2'	1:A:1071:C:C6	2.14	0.83
1:A:67:C:H2'	1:A:68:G:H8	1.43	0.82
1:A:1535:C:C4	1:A:1536:C:C5	2.68	0.82
1:A:1531:A:H2'	1:A:1532:U:O4'	1.79	0.82
1:A:1000:U:H2'	1:A:1001:A:C1'	2.09	0.82
1:A:17:U:H2'	1:A:18:C:C6	2.15	0.81
1:A:19:C:H2'	1:A:20:U:C6	2.15	0.81
1:A:1071:C:H2'	1:A:1072:G:C8	2.14	0.81
1:A:501:C:H2'	1:A:502:G:H8	1.43	0.80
1:A:674:G:H2'	1:A:675:A:H8	1.44	0.80
5:E:93:PRO:HG3	8:H:105:ARG:HH22	1.23	0.80
1:A:123:C:H2'	1:A:124:G:H8	1.46	0.80
1:A:958:A:C2	19:S:55:LYS:HB2	2.17	0.80
1:A:13:U:H5'	1:A:14:U:C5	2.16	0.80
25:Z:55:PSU:H3'	25:Z:56:C:H5''	1.63	0.80
1:A:1014:A:H4'	19:S:14:HIS:HB3	1.62	0.79
5:E:93:PRO:HB2	8:H:105:ARG:HH12	1.47	0.79
1:A:78:G:H2'	1:A:79:G:O4'	1.82	0.79
4:D:26:CYS:HG	26:D:300:ZN:ZN	0.94	0.79
25:Z:34:C:H2'	25:Z:35:A:C8	2.18	0.79
3:C:29:TYR:HD1	14:N:36:PHE:CE2	2.02	0.78
1:A:1492:A:C8	22:W:19:ASN:HB3	2.19	0.78
25:Z:3:C:H2'	25:Z:4:G:C8	2.18	0.78
2:B:72:GLY:HA3	2:B:81:VAL:HG21	1.66	0.78
25:Z:66:C:H2'	25:Z:67:C:O4'	1.82	0.78
1:A:24:U:H2'	1:A:25:C:C6	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:G:H2'	1:A:918:A:C8	2.18	0.77
3:C:9:GLY:HA2	3:C:12:LEU:HG	1.66	0.77
1:A:662:G:H2'	1:A:663:A:C8	2.19	0.77
25:Z:56:C:H2'	25:Z:57:A:C8	2.20	0.77
3:C:29:TYR:OH	14:N:54:PRO:CG	2.33	0.77
25:Z:39:C:H2'	25:Z:40:C:C6	2.20	0.77
1:A:745:C:H2'	1:A:746:A:H8	1.49	0.76
1:A:1535:C:C2	1:A:1536:C:C6	2.73	0.76
1:A:299:G:H2'	1:A:300:A:C8	2.21	0.76
4:D:26:CYS:SG	26:D:300:ZN:ZN	1.75	0.76
19:S:34:TRP:HA	19:S:52:TYR:HB2	1.68	0.76
5:E:93:PRO:HG2	8:H:105:ARG:NH1	2.01	0.76
10:J:40:LEU:HD11	10:J:71:LEU:CG	2.16	0.76
1:A:80:G:H3'	1:A:81:U:C5'	2.16	0.76
1:A:21:G:H2'	1:A:22:G:C8	2.21	0.75
1:A:1123:A:H4'	10:J:36:GLY:HA3	1.67	0.75
19:S:11:VAL:HA	19:S:38:SER:HB2	1.68	0.75
1:A:1296:C:H5'	13:M:14:ARG:HD2	1.69	0.75
1:A:316:G:H1	1:A:337:C:H42	1.33	0.74
1:A:1536:C:H1'	24:Y:30:G:H22	1.50	0.74
3:C:30:ARG:HH21	3:C:30:ARG:HB2	1.51	0.74
9:I:44:VAL:HG12	9:I:51:ARG:HH12	1.52	0.74
16:P:59:TRP:O	16:P:62:VAL:HG23	1.85	0.74
1:A:170:U:H2'	1:A:171:A:H8	1.52	0.74
1:A:543:C:H2'	1:A:544:G:H8	1.52	0.74
10:J:16:LEU:HA	10:J:19:SER:HB3	1.69	0.74
1:A:90:U:H2'	1:A:91:C:C6	2.23	0.73
1:A:977:A:N7	1:A:1223:C:H2'	2.03	0.73
1:A:966:G:N3	25:Z:34:C:H5'	2.03	0.73
1:A:1080:A:H5''	5:E:16:THR:HB	1.70	0.73
1:A:524:G:C6	1:A:525:C:N4	2.57	0.73
1:A:1218:C:H2'	1:A:1219:U:C6	2.22	0.73
1:A:1386:G:H2'	1:A:1387:G:H8	1.54	0.72
1:A:45:U:H2'	1:A:46:G:H8	1.53	0.72
1:A:1219:U:H2'	1:A:1220:G:H8	1.54	0.72
3:C:28:GLN:HA	3:C:31:HIS:NE2	2.04	0.72
11:K:58:PRO:HB2	11:K:93:GLN:HG3	1.71	0.72
1:A:1270:C:H2'	1:A:1271:G:H8	1.53	0.72
1:A:729:A:H2'	1:A:730:G:H8	1.55	0.72
10:J:6:ILE:HG22	10:J:98:ILE:HG12	1.71	0.72
4:D:25:ARG:HA	4:D:28:SER:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:86:VAL:O	18:R:87:ARG:HB2	1.88	0.72
1:A:69:G:H1	1:A:100:C:H42	1.38	0.71
1:A:1103:C:H2'	1:A:1104:G:O4'	1.89	0.71
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.72	0.71
22:W:21:THR:HG22	22:W:33:LEU:HD12	1.71	0.71
1:A:584:G:H2'	1:A:585:G:H8	1.56	0.71
3:C:29:TYR:CZ	14:N:54:PRO:HG2	2.24	0.71
1:A:45:U:H2'	1:A:46:G:C8	2.25	0.71
1:A:19:C:H2'	1:A:20:U:H6	1.53	0.71
1:A:78:G:O2'	1:A:79:G:O4'	2.07	0.71
3:C:77:ILE:HA	3:C:84:ILE:HB	1.73	0.71
23:X:90:PHE:HB2	23:X:120:ILE:HG12	1.72	0.71
1:A:584:G:H2'	1:A:585:G:C8	2.24	0.71
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.73	0.71
1:A:1000:U:H3'	1:A:1000:U:H6	1.55	0.71
1:A:1098:C:H1'	1:A:1168:A:H2	1.55	0.71
1:A:1359:C:H3'	14:N:35:ARG:NH2	2.05	0.70
1:A:1475:G:H2'	1:A:1476:G:H8	1.55	0.70
1:A:123:C:H2'	1:A:124:G:C8	2.26	0.70
1:A:743:U:H2'	1:A:744:C:C6	2.26	0.70
1:A:1360:A:H8	1:A:1360:A:OP1	1.74	0.70
2:B:130:ARG:HB3	2:B:131:PRO:HD2	1.73	0.70
1:A:1036:G:H2'	1:A:1037:C:O4'	1.92	0.70
1:A:1342:C:H2'	1:A:1343:G:C8	2.26	0.70
17:Q:81:ARG:HE	17:Q:84:LEU:HD12	1.55	0.70
24:Y:24:A:H2'	24:Y:25:A:H8	1.57	0.69
25:Z:48:C:H2'	25:Z:59:A:H4'	1.74	0.69
1:A:78:G:C2'	1:A:79:G:O4'	2.40	0.69
1:A:398:C:H2'	1:A:399:G:H8	1.56	0.69
1:A:1099:G:H5''	2:B:96:ARG:HE	1.58	0.69
4:D:101:LEU:HB2	4:D:138:TYR:HB3	1.74	0.69
1:A:1064:G:N2	1:A:1190:G:H2'	2.08	0.69
1:A:181:G:H4'	1:A:182:U:H5'	1.74	0.69
1:A:1081:G:C8	1:A:1081:G:H5''	2.27	0.69
1:A:1280:A:H3'	1:A:1281:U:H5''	1.74	0.69
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.75	0.69
10:J:7:LYS:HA	10:J:71:LEU:CD2	2.23	0.69
1:A:536:C:H2'	1:A:537:G:C8	2.28	0.69
1:A:1264:C:H2'	1:A:1265:G:H8	1.58	0.68
25:Z:36:U:H2'	25:Z:37:A:H8	1.58	0.68
1:A:671:G:C2	1:A:736:C:N3	2.62	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:7:LYS:CB	10:J:71:LEU:HD21	2.22	0.68
1:A:10:A:H2'	1:A:11:G:C8	2.29	0.68
1:A:718:G:H21	18:R:49:LYS:HE3	1.59	0.68
1:A:1234:C:H2'	1:A:1235:U:C6	2.28	0.68
25:Z:50:U:N3	25:Z:51:C:N4	2.42	0.68
1:A:736:C:H2'	1:A:737:A:C8	2.27	0.68
1:A:1346:A:H2'	7:G:10:ARG:HH22	1.59	0.68
3:C:62:ASP:HA	3:C:97:LYS:HD3	1.76	0.68
1:A:662:G:H2'	1:A:663:A:H8	1.56	0.68
3:C:28:GLN:O	3:C:32:LEU:HG	1.94	0.68
3:C:29:TYR:CD1	14:N:36:PHE:CE2	2.82	0.68
1:A:398:C:H2'	1:A:399:G:C8	2.29	0.68
2:B:69:LEU:HB3	2:B:162:ILE:HG12	1.76	0.68
25:Z:35:A:H2'	25:Z:36:U:C6	2.28	0.68
1:A:16:A:C2	1:A:1080:A:H1'	2.29	0.67
1:A:1073:U:H3	1:A:1102:A:N6	1.91	0.67
1:A:579:G:H5'	1:A:728:A:H1'	1.76	0.67
1:A:1103:C:H5''	2:B:98:LEU:HD23	1.76	0.67
1:A:1218:C:H2'	1:A:1219:U:H6	1.59	0.67
1:A:701:C:H1'	1:A:703:G:C5	2.30	0.67
5:E:12:LEU:HG	5:E:31:LEU:HD12	1.77	0.67
1:A:1342:C:H2'	1:A:1343:G:H8	1.59	0.67
1:A:1264:C:H2'	1:A:1265:G:C8	2.30	0.67
3:C:30:ARG:NH2	14:N:35:ARG:O	2.26	0.67
1:A:302:G:H2'	1:A:303:A:C8	2.30	0.67
1:A:524:G:C2	1:A:525:C:N3	2.62	0.67
1:A:1356:G:H2'	1:A:1357:A:C8	2.30	0.67
1:A:1536:C:H1'	24:Y:30:G:N2	2.10	0.67
1:A:1384:C:H2'	1:A:1385:G:C8	2.29	0.67
15:O:75:PRO:O	15:O:79:ARG:HG3	1.95	0.67
1:A:457:C:H2'	1:A:458:C:C6	2.29	0.67
10:J:47:PHE:HB2	10:J:63:PHE:HB2	1.76	0.67
1:A:674:G:H2'	1:A:675:A:C8	2.30	0.66
1:A:1227:A:C2	19:S:83:HIS:HB2	2.30	0.66
22:W:15:GLU:HB3	22:W:23:ARG:HB2	1.76	0.66
1:A:956:U:O2'	19:S:80:TYR:HB3	1.95	0.66
1:A:1280:A:OP1	1:A:1281:U:H5	1.78	0.66
1:A:6:G:H2'	5:E:119:LEU:HD21	1.76	0.66
7:G:39:ALA:HA	7:G:42:ILE:HD12	1.78	0.66
1:A:562:C:H41	1:A:884:U:H2'	1.61	0.66
1:A:1016:A:H2'	1:A:1017:G:O4'	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:SER:HB3	3:C:22:TRP:HE1	1.61	0.65
24:Y:28:A:H3'	24:Y:29:G:C8	2.32	0.65
1:A:101:A:H2'	1:A:102:G:H8	1.61	0.65
3:C:21:ARG:HG3	3:C:58:GLU:HG2	1.78	0.65
12:L:25:PRO:C	12:L:27:LEU:H	2.01	0.65
1:A:1438:G:N2	1:A:1439:C:C2	2.64	0.65
5:E:149:GLU:O	5:E:153:LYS:HB2	1.97	0.65
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.78	0.65
1:A:1345:U:N3	1:A:1375:A:C6	2.63	0.65
8:H:105:ARG:NH2	8:H:105:ARG:HG2	2.10	0.65
12:L:27:LEU:HG	12:L:28:LYS:HG3	1.79	0.65
16:P:59:TRP:C	16:P:62:VAL:HG22	2.21	0.65
1:A:543:C:H2'	1:A:544:G:C8	2.31	0.65
1:A:671:G:N2	1:A:736:C:C2	2.64	0.65
1:A:279:A:H5''	1:A:280:C:H3'	1.77	0.65
1:A:1442(A):G:H5''	1:A:1442(B):A:H5'	1.79	0.65
1:A:701:C:H4'	1:A:702:A:O5'	1.97	0.65
17:Q:67:LYS:O	17:Q:68:ARG:HB3	1.97	0.65
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.32	0.65
1:A:814:A:H2'	1:A:816:A:H5''	1.78	0.65
1:A:943:U:H2'	1:A:944:G:H8	1.62	0.65
1:A:998:G:N2	1:A:999:C:C2	2.65	0.65
1:A:1151:A:HO2'	1:A:1152:A:H8	1.43	0.65
1:A:1354:C:H2'	1:A:1355:G:H8	1.62	0.65
22:W:32:ILE:HD11	22:W:55:VAL:HG11	1.79	0.65
1:A:1004:A:H5''	1:A:1025:U:C5	2.32	0.64
2:B:34:ALA:HB3	2:B:41:ILE:HD12	1.79	0.64
5:E:93:PRO:CB	8:H:105:ARG:HH12	2.09	0.64
6:F:52:ILE:HD11	18:R:77:GLY:HA3	1.78	0.64
1:A:1125:U:H5'	1:A:1126:U:H5	1.62	0.64
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.78	0.64
10:J:50:ILE:CG1	10:J:60:ARG:HD2	2.26	0.64
1:A:1099:G:C6	1:A:1100:C:N3	2.65	0.64
1:A:79:G:H2'	1:A:80:G:H8	1.62	0.64
1:A:1443:G:C6	1:A:1444:C:N4	2.66	0.64
10:J:7:LYS:CB	10:J:71:LEU:CD2	2.76	0.64
25:Z:36:U:H2'	25:Z:37:A:C8	2.32	0.64
1:A:266:G:C8	1:A:266:G:H5''	2.33	0.64
1:A:1105:A:H2'	1:A:1106:G:H8	1.62	0.64
1:A:61:G:H2'	1:A:62:U:O4'	1.98	0.64
1:A:525:C:H2'	1:A:526:C:C6	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:C:O2'	12:L:50:SER:HB3	1.97	0.64
1:A:1081:G:H2'	1:A:1082:G:C8	2.33	0.64
1:A:1392:G:N2	1:A:1502:A:H8	1.95	0.64
4:D:176:LEU:HA	4:D:183:GLY:HA2	1.79	0.64
1:A:1074:G:C1'	2:B:104:ASN:HD21	2.06	0.64
19:S:6:LYS:HB2	19:S:7:LYS:HE3	1.80	0.64
1:A:988:G:N1	1:A:989:C:C2	2.67	0.63
1:A:1070:U:H2'	1:A:1071:C:H6	1.64	0.63
24:Y:28:A:H3'	24:Y:29:G:H8	1.62	0.63
1:A:880:C:H2'	1:A:881:G:H8	1.63	0.63
1:A:1358:U:C4	1:A:1363(A):A:N1	2.62	0.63
2:B:184:VAL:H	2:B:198:ASP:HB2	1.63	0.63
1:A:335:C:H2'	1:A:336:C:C6	2.33	0.63
1:A:1081:G:H2'	1:A:1082:G:H8	1.64	0.63
1:A:1475:G:H2'	1:A:1476:G:C8	2.33	0.63
1:A:926:G:H3'	1:A:1505:G:H21	1.63	0.63
1:A:1128:C:H2'	1:A:1139:G:N7	2.13	0.63
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.80	0.63
1:A:919:A:C2	1:A:1080:A:H2	2.16	0.63
25:Z:51:C:H2'	25:Z:52:G:O4'	1.99	0.63
1:A:1391:U:H2'	1:A:1392:G:C8	2.33	0.63
1:A:1445:C:C2	1:A:1458:G:C2	2.87	0.63
1:A:1048:G:H5''	14:N:3:ARG:HG2	1.79	0.63
25:Z:52:G:C2	25:Z:63:G:C2	2.86	0.63
1:A:316:G:H1	1:A:337:C:N4	1.97	0.62
3:C:154:SER:HA	3:C:165:THR:HG23	1.79	0.62
1:A:920:U:H2'	1:A:921:U:H6	1.63	0.62
1:A:1061:G:H5''	10:J:59:SER:OG	1.99	0.62
1:A:1125:U:H5'	1:A:1126:U:C5	2.34	0.62
25:Z:49:G:C6	25:Z:50:U:C2	2.87	0.62
1:A:1535:C:N3	1:A:1536:C:C6	2.67	0.62
2:B:204:ASN:HB3	2:B:210:SER:OG	2.00	0.62
1:A:1354:C:H2'	1:A:1355:G:C8	2.34	0.62
1:A:877:C:H2'	1:A:878:G:H8	1.64	0.62
1:A:973:G:H3'	1:A:974:A:H5''	1.80	0.62
23:X:4:GLU:HA	23:X:66:ARG:HH12	1.64	0.62
1:A:69:G:H1	1:A:100:C:N4	1.97	0.62
1:A:1014:A:C2	19:S:34:TRP:CG	2.88	0.62
25:Z:33:U:O2	25:Z:36:U:H5	1.82	0.62
1:A:234:C:H2'	1:A:235:C:C6	2.34	0.62
1:A:1256:A:N6	1:A:1278:U:C2	2.68	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:7:LYS:CA	10:J:71:LEU:HD22	2.30	0.62
23:X:64:LYS:O	23:X:68:GLU:HG2	2.00	0.62
1:A:17:U:O2	1:A:1079:G:N3	2.32	0.62
1:A:313:A:H2'	1:A:314:C:C6	2.34	0.62
1:A:1014:A:C2	19:S:34:TRP:CD2	2.87	0.62
1:A:1102:A:H2'	1:A:1103:C:C6	2.35	0.62
3:C:108:ASN:HD21	3:C:110:ASN:HB2	1.65	0.62
23:X:157:LEU:HB2	23:X:160:ASP:HB2	1.82	0.62
25:Z:55:PSU:H6	25:Z:55:PSU:H5'	1.65	0.62
1:A:868:C:H2'	1:A:869:G:O4'	2.00	0.62
1:A:1127:G:H21	1:A:1147:C:H41	1.47	0.62
8:H:105:ARG:HG2	8:H:105:ARG:HH21	1.65	0.62
9:I:5:TYR:CZ	9:I:7:THR:OG1	2.26	0.62
1:A:24:U:H2'	1:A:25:C:H6	1.64	0.61
1:A:694:A:H5'	11:K:53:SER:HB2	1.81	0.61
1:A:695:A:H2'	1:A:696:A:C8	2.35	0.61
10:J:57:LYS:O	10:J:60:ARG:HD3	2.00	0.61
1:A:939:G:H1'	1:A:1375:A:C2	2.35	0.61
8:H:11:THR:HA	8:H:14:ARG:NH1	2.15	0.61
9:I:5:TYR:OH	9:I:7:THR:OG1	2.05	0.61
1:A:582:U:H2'	1:A:583:A:C8	2.35	0.61
1:A:1164:G:N2	1:A:1165:C:C2	2.69	0.61
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.81	0.61
1:A:1386:G:H2'	1:A:1387:G:C8	2.35	0.61
10:J:38:ILE:HD12	10:J:71:LEU:O	1.99	0.61
1:A:588:G:N2	1:A:589:C:C2	2.68	0.61
1:A:302:G:H2'	1:A:303:A:H8	1.64	0.61
23:X:90:PHE:HE2	23:X:118:VAL:HG12	1.66	0.61
24:Y:24:A:H2'	24:Y:25:A:C8	2.35	0.61
1:A:509:A:H4'	1:A:510:A:OP1	2.00	0.61
1:A:960:U:H4'	1:A:961:U:H5''	1.82	0.61
1:A:1256:A:H5''	3:C:27:LYS:NZ	2.14	0.61
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.33	0.61
1:A:312:C:H2'	1:A:313:A:C8	2.36	0.61
1:A:1349:A:H5''	9:I:121:ARG:HB2	1.83	0.61
9:I:17:VAL:HG22	9:I:63:ILE:HG12	1.82	0.61
9:I:118:LYS:O	9:I:120:ARG:N	2.33	0.61
13:M:87:TYR:HA	13:M:90:LEU:HD12	1.83	0.61
1:A:376:G:H2'	1:A:377:G:H8	1.65	0.60
1:A:568:G:N2	1:A:883:C:C2	2.69	0.60
25:Z:47:U:H4'	25:Z:48:C:H5'	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:GLN:CA	3:C:31:HIS:CD2	2.82	0.60
1:A:623:C:H2'	1:A:624:C:O4'	2.01	0.60
14:N:24:CYS:HB3	14:N:28:GLY:H	1.67	0.60
1:A:1132:C:H2'	1:A:1133:G:C8	2.35	0.60
1:A:1384:C:H2'	1:A:1385:G:H8	1.65	0.60
1:A:370:C:C2	1:A:392:G:N2	2.69	0.60
1:A:1000:U:H3'	1:A:1000:U:C6	2.35	0.60
1:A:96:U:H2'	1:A:97:G:H8	1.66	0.60
1:A:677:U:H2'	1:A:678:U:C6	2.37	0.60
1:A:960:U:H4'	1:A:961:U:C5'	2.31	0.60
1:A:1464:G:N2	1:A:1465:C:C2	2.70	0.60
18:R:52:PRO:HG2	18:R:54:ARG:CZ	2.31	0.60
1:A:399:G:H2'	1:A:400:C:C6	2.37	0.60
1:A:932:C:H5'	7:G:3:ARG:HB3	1.84	0.60
1:A:999:C:O2	1:A:1043:C:O2	2.18	0.60
3:C:7:PRO:HG2	3:C:184:TYR:HB2	1.83	0.60
3:C:30:ARG:CZ	14:N:35:ARG:O	2.49	0.60
4:D:5:ILE:H	4:D:115:ARG:HH22	1.48	0.60
20:T:44:ALA:HB1	20:T:91:LEU:HB2	1.84	0.60
1:A:884:U:H4'	1:A:885:G:H5''	1.84	0.60
1:A:1532:U:H2'	1:A:1533:C:H1'	1.83	0.60
23:X:157:LEU:HD11	23:X:162:ASN:HB3	1.84	0.60
1:A:390:C:H2'	1:A:391:G:H8	1.67	0.59
1:A:1411:C:H5'	22:W:64:ARG:HH22	1.66	0.59
1:A:1513:A:H2'	1:A:1514:C:C6	2.37	0.59
10:J:9:ARG:HG3	10:J:95:GLU:HB3	1.82	0.59
14:N:12:ARG:O	14:N:14:PRO:HD3	2.02	0.59
19:S:40:ILE:HG21	19:S:62:ILE:HD11	1.84	0.59
1:A:170:U:H2'	1:A:171:A:C8	2.35	0.59
1:A:921:U:H5'	1:A:1081:G:O2'	2.02	0.59
25:Z:37:A:H2'	25:Z:38:A:C8	2.37	0.59
25:Z:40:C:H2'	25:Z:41:C:C6	2.37	0.59
1:A:189(L):G:H2'	1:A:190:U:C6	2.38	0.59
1:A:735:C:H5'	18:R:71:LYS:HD3	1.84	0.59
1:A:1005:A:O4'	1:A:1036:G:N2	2.35	0.59
1:A:1430:C:C2	1:A:1471:G:N2	2.71	0.59
1:A:556:C:H2'	1:A:557:G:O4'	2.02	0.59
25:Z:64:G:H2'	25:Z:65:C:O4'	2.03	0.59
1:A:59:A:H5''	1:A:387:U:H5''	1.83	0.59
1:A:521:G:N2	1:A:522:C:C2	2.71	0.59
5:E:33:VAL:HG21	5:E:109:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:G:H3'	11:K:26:ASN:HD21	1.66	0.59
1:A:1074:G:O2'	1:A:1101:A:N1	2.35	0.59
1:A:1081:G:H5''	1:A:1081:G:H8	1.66	0.59
25:Z:53:G:C2	25:Z:62:C:C2	2.90	0.59
1:A:1435:G:H2'	1:A:1436:U:C6	2.38	0.59
5:E:18:ARG:HD3	5:E:20:GLN:HE21	1.67	0.59
1:A:17:U:H2'	1:A:18:C:C5	2.38	0.58
1:A:1310:G:N2	1:A:1328:C:C2	2.71	0.58
1:A:1493:A:C2	22:W:46:ARG:HA	2.38	0.58
2:B:17:PHE:HD1	2:B:18:GLY:H	1.51	0.58
8:H:105:ARG:HH21	8:H:105:ARG:CG	2.14	0.58
1:A:258:G:N2	1:A:269:C:C2	2.71	0.58
3:C:26:LYS:HE3	3:C:26:LYS:H	1.68	0.58
1:A:216:G:C6	1:A:217:C:N4	2.71	0.58
1:A:757:U:H2'	1:A:758:G:O4'	2.03	0.58
1:A:1022:G:H2'	1:A:1023:G:C8	2.39	0.58
1:A:1025:U:H2'	1:A:1026:G:C8	2.39	0.58
3:C:20:SER:HB3	3:C:22:TRP:NE1	2.18	0.58
13:M:87:TYR:O	13:M:91:ARG:HG2	2.03	0.58
1:A:820:U:H3'	1:A:821:G:C5'	2.34	0.58
1:A:1162:C:C2	1:A:1175:G:C2	2.92	0.58
2:B:135:GLN:HA	2:B:138:LEU:HD12	1.84	0.58
4:D:196:LEU:HB3	4:D:198:VAL:HG12	1.84	0.58
25:Z:50:U:H3	25:Z:51:C:N4	2.01	0.58
10:J:57:LYS:HB2	10:J:60:ARG:NH1	2.19	0.58
1:A:576:G:H3'	1:A:577:G:H5''	1.85	0.58
1:A:824:C:H2'	1:A:825:G:C8	2.39	0.58
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.86	0.58
1:A:109:A:H2'	1:A:326:G:N2	2.18	0.58
25:Z:3:C:H2'	25:Z:4:G:H8	1.69	0.58
1:A:1456:G:C2	1:A:1457:G:C8	2.92	0.58
2:B:122:PHE:HA	2:B:127:ILE:HG12	1.85	0.58
1:A:725:G:N2	1:A:726:C:C2	2.72	0.58
1:A:1241:G:N2	1:A:1242:C:C2	2.71	0.58
25:Z:17:C:OP1	25:Z:18:G:H5'	2.04	0.58
1:A:243:A:H4'	1:A:244:U:O5'	2.04	0.57
1:A:928:G:H1	1:A:1389:C:H42	1.51	0.57
5:E:93:PRO:CG	8:H:105:ARG:NH1	2.66	0.57
1:A:911:U:H2'	1:A:912:C:C6	2.40	0.57
1:A:1515:C:H2'	1:A:1516:G:C8	2.39	0.57
9:I:10:ARG:HE	9:I:11:LYS:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:50:ILE:HA	10:J:59:SER:O	2.04	0.57
1:A:1106:G:N2	1:A:1107:C:C2	2.73	0.57
25:Z:64:G:C5	25:Z:65:C:C4	2.92	0.57
1:A:354:G:N2	1:A:355:C:C2	2.72	0.57
4:D:166:LYS:HG3	4:D:178:VAL:HG11	1.87	0.57
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.86	0.57
9:I:96:LEU:HG	9:I:101:PHE:HB2	1.86	0.57
15:O:24:SER:HB3	15:O:27:VAL:HG23	1.87	0.57
1:A:769:G:N2	1:A:770:C:C2	2.73	0.57
1:A:1347:G:N2	1:A:1373:G:H2'	2.20	0.57
8:H:12:ARG:HB3	8:H:24:THR:HG21	1.87	0.57
10:J:6:ILE:HG13	10:J:72:VAL:O	2.05	0.57
1:A:524:G:C2	1:A:525:C:C4	2.93	0.57
1:A:551:U:H2'	1:A:552:U:C6	2.39	0.57
1:A:1391:U:H2'	1:A:1392:G:H8	1.68	0.57
1:A:558:G:H3'	1:A:559:A:H5''	1.86	0.57
1:A:958:A:H8	1:A:958:A:O5'	1.88	0.57
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.87	0.57
1:A:18:C:H4'	1:A:1078:U:H1'	1.87	0.57
1:A:384:G:H2'	1:A:385:C:C6	2.40	0.57
1:A:1095:U:H2'	1:A:1096:C:C6	2.40	0.57
1:A:1530:G:C2'	1:A:1531:A:O4'	2.50	0.57
5:E:14:ARG:HE	5:E:45:PHE:HZ	1.53	0.57
25:Z:50:U:C2	25:Z:51:C:C5	2.93	0.57
1:A:1106:G:C6	1:A:1107:C:N4	2.73	0.57
3:C:106:VAL:HG21	3:C:115:LEU:HD11	1.86	0.57
25:Z:1:C:H42	25:Z:72:A:H61	1.50	0.57
25:Z:39:C:H2'	25:Z:40:C:H6	1.66	0.57
1:A:874:G:N2	1:A:875:C:C2	2.73	0.57
1:A:943:U:H2'	1:A:944:G:C8	2.40	0.57
1:A:1464:G:N1	1:A:1465:C:C4	2.73	0.57
2:B:130:ARG:HH22	3:C:207:VAL:HG22	1.70	0.57
1:A:128:G:N2	1:A:234:C:C2	2.73	0.56
1:A:590:C:C2	1:A:650:G:C2	2.93	0.56
1:A:1076:C:H2'	1:A:1077:G:C8	2.40	0.56
1:A:1270:C:H2'	1:A:1271:G:C8	2.37	0.56
5:E:33:VAL:HG12	5:E:112:LEU:HD12	1.86	0.56
10:J:23:ILE:HG23	10:J:85:LEU:HD22	1.87	0.56
23:X:122:PHE:HE2	23:X:161:MET:HB2	1.69	0.56
25:Z:37:A:H3'	25:Z:38:A:H8	1.70	0.56
25:Z:55:PSU:C3'	25:Z:56:C:H5''	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:G:H2'	1:A:764:C:C6	2.40	0.56
1:A:90:U:O2'	1:A:91:C:H5'	2.05	0.56
1:A:253:U:H2'	1:A:254:G:H8	1.70	0.56
1:A:589:C:O2	1:A:651:C:O2	2.24	0.56
1:A:598:U:H2'	1:A:599:C:C6	2.40	0.56
1:A:810:C:H2'	1:A:811:C:O4'	2.05	0.56
1:A:974:A:H8	1:A:974:A:OP1	1.88	0.56
1:A:975:A:H4'	1:A:976:G:O5'	2.05	0.56
1:A:1222:G:C6	1:A:1223:C:N4	2.73	0.56
1:A:1314:C:H2'	1:A:1315:U:C6	2.40	0.56
1:A:1404:C:H42	1:A:1497:G:H1	1.51	0.56
1:A:1438:G:N1	1:A:1439:C:C4	2.73	0.56
5:E:106:PRO:HA	5:E:109:ILE:HD12	1.87	0.56
16:P:54:GLU:HA	16:P:57:ARG:HD2	1.87	0.56
17:Q:51:TYR:HE1	17:Q:76:LEU:HB2	1.70	0.56
1:A:755:G:N2	1:A:756:C:C2	2.73	0.56
1:A:1164:G:N1	1:A:1165:C:C4	2.74	0.56
1:A:1323:G:H2'	1:A:1324:A:C8	2.41	0.56
1:A:1500:A:H5''	1:A:1508:G:H5''	1.88	0.56
20:T:43:LEU:HD22	20:T:51:GLU:HG3	1.88	0.56
22:W:32:ILE:HB	22:W:63:THR:O	2.05	0.56
25:Z:41:C:H2'	25:Z:42:G:C8	2.40	0.56
1:A:417:C:N4	1:A:418:C:N4	2.54	0.56
6:F:22:GLU:HA	6:F:25:ILE:HD12	1.88	0.56
1:A:96:U:H2'	1:A:97:G:C8	2.39	0.56
1:A:930:C:H2'	1:A:931:C:O4'	2.05	0.56
7:G:115:ARG:O	7:G:119:ARG:HG3	2.05	0.56
1:A:255:G:H2'	1:A:256:U:C6	2.41	0.56
1:A:678:U:H2'	1:A:679:C:C6	2.41	0.56
1:A:914:A:H2'	1:A:915:A:H8	1.69	0.56
1:A:998:G:N1	1:A:999:C:C4	2.74	0.56
1:A:1537:U:H3	24:Y:28:A:H61	1.52	0.56
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.87	0.56
1:A:78:G:HO2'	1:A:79:G:C4'	2.19	0.56
1:A:538:G:H2'	1:A:539:A:H8	1.71	0.56
1:A:790:A:H2'	1:A:791:G:C8	2.40	0.56
1:A:939:G:H1'	1:A:1375:A:H2	1.71	0.56
1:A:999:C:C2'	1:A:1000:U:H5'	2.36	0.56
1:A:1233:G:C6	1:A:1234:C:N4	2.73	0.56
1:A:377:G:H1	1:A:386:C:H42	1.53	0.56
1:A:891:U:H2'	1:A:892:A:H8	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:4:G:H2'	25:Z:5:G:C8	2.41	0.56
1:A:1005:A:OP1	1:A:1006:C:C5	2.58	0.55
1:A:1353:G:N2	1:A:1354:C:C2	2.74	0.55
4:D:30:LYS:C	4:D:32:ALA:H	2.14	0.55
13:M:10:PRO:CB	13:M:18:ALA:HB1	2.35	0.55
1:A:60:A:H4'	1:A:61:G:O5'	2.06	0.55
1:A:1098:C:H1'	1:A:1168:A:C2	2.39	0.55
1:A:1515:C:H2'	1:A:1516:G:H8	1.70	0.55
8:H:113:SER:HB3	8:H:132:GLU:HB3	1.87	0.55
18:R:47:THR:HA	18:R:83:GLU:HB2	1.87	0.55
25:Z:63:G:N1	25:Z:64:G:C5	2.75	0.55
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.70	0.55
1:A:128:G:C2	1:A:234:C:C2	2.95	0.55
1:A:910:C:H4'	1:A:1413:A:H4'	1.88	0.55
1:A:1227:A:N1	19:S:83:HIS:CB	2.67	0.55
1:A:189(K):U:H2'	1:A:189(L):G:H8	1.72	0.55
1:A:279:A:H4'	1:A:280:C:OP2	2.06	0.55
1:A:1540:U:H3	24:Y:25:A:H61	1.53	0.55
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.87	0.55
1:A:233:C:H2'	1:A:234:C:H6	1.72	0.55
1:A:390:C:H2'	1:A:391:G:C8	2.42	0.55
1:A:457:C:H2'	1:A:458:C:H6	1.71	0.55
1:A:1127:G:H21	1:A:1147:C:N4	2.05	0.55
1:A:1485:U:H2'	1:A:1486:G:H8	1.72	0.55
2:B:54:THR:HG21	2:B:201:ILE:HD11	1.89	0.55
5:E:93:PRO:HB2	8:H:105:ARG:NH1	2.21	0.55
8:H:85:ARG:HH21	8:H:134:ILE:HG23	1.72	0.55
1:A:530:G:O2'	22:W:39:LYS:HG2	2.07	0.55
1:A:774:G:N2	1:A:806:C:C2	2.74	0.55
1:A:1223:C:H5''	1:A:1224:G:H5''	1.89	0.55
1:A:939:G:C6	1:A:940:C:N4	2.74	0.55
1:A:1166:G:N2	1:A:1170:A:OP2	2.30	0.55
7:G:24:THR:HA	7:G:27:ILE:HD12	1.89	0.55
13:M:88:ARG:HG3	13:M:98:VAL:CG1	2.37	0.55
1:A:397:A:H3'	1:A:397:A:N3	2.21	0.54
1:A:695:A:H2'	1:A:696:A:H8	1.71	0.54
1:A:1000:U:H2'	1:A:1001:A:O4'	2.06	0.54
3:C:30:ARG:HH21	3:C:30:ARG:CB	2.20	0.54
10:J:7:LYS:CA	10:J:71:LEU:CD2	2.86	0.54
25:Z:56:C:H2'	25:Z:57:A:H8	1.66	0.54
1:A:683:G:H2'	1:A:684:A:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:A:OP1	1:A:1006:C:H5	1.91	0.54
1:A:1010:G:H2'	1:A:1011:G:C8	2.42	0.54
1:A:1134:G:N2	1:A:1141:C:C2	2.75	0.54
1:A:1491:G:H5''	12:L:47:LYS:HE2	1.89	0.54
8:H:88:LYS:HB2	8:H:91:ARG:HB3	1.89	0.54
22:W:10:GLU:HG2	22:W:54:VAL:HG22	1.88	0.54
24:Y:36:A:C2	24:Y:37:U:C2	2.95	0.54
1:A:691:G:H8	11:K:26:ASN:HD22	1.53	0.54
1:A:1368:G:N2	1:A:1369:C:C2	2.76	0.54
25:Z:48:C:H2'	25:Z:59:A:C4'	2.38	0.54
1:A:729:A:H2'	1:A:730:G:C8	2.38	0.54
1:A:878:G:H5'	8:H:89:PRO:HG2	1.89	0.54
1:A:946:A:H2'	1:A:947:G:C8	2.42	0.54
1:A:1079:G:H5''	5:E:14:ARG:NH2	2.22	0.54
1:A:1359:C:H3'	14:N:35:ARG:HH22	1.71	0.54
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.90	0.54
25:Z:17:C:O2	25:Z:17:C:C2'	2.55	0.54
1:A:33:A:H2'	1:A:34:C:C6	2.43	0.54
1:A:35:G:H2'	1:A:36:C:C6	2.42	0.54
1:A:999:C:N3	1:A:1043:C:N3	2.55	0.54
1:A:1169:A:H2'	1:A:1170:A:O4'	2.07	0.54
1:A:1370:G:H4'	9:I:12:GLU:OE2	2.07	0.54
8:H:28:ALA:HA	8:H:59:LEU:HD12	1.90	0.54
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.89	0.54
1:A:34:C:H2'	1:A:35:G:C8	2.43	0.54
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.90	0.54
1:A:761:G:C2	1:A:762:C:C2	2.96	0.54
1:A:1098:C:C1'	1:A:1168:A:H2	2.20	0.54
1:A:1112:C:H1'	3:C:179:ARG:HH21	1.72	0.54
1:A:1244:C:H2'	1:A:1245:A:C8	2.43	0.54
1:A:1378:C:N3	7:G:76:ARG:NH2	2.56	0.54
3:C:113:ALA:HA	3:C:202:ILE:HD12	1.89	0.54
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.88	0.54
17:Q:68:ARG:HG3	17:Q:68:ARG:O	2.08	0.54
1:A:1230:C:C5'	25:Z:30:G:H5''	2.38	0.54
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.89	0.54
1:A:530:G:H8	22:W:38:GLY:HA3	1.73	0.54
1:A:434:U:H2'	1:A:435:C:C6	2.43	0.54
1:A:582:U:H2'	1:A:583:A:H8	1.72	0.54
1:A:1262:C:H2'	1:A:1263:C:C6	2.43	0.54
1:A:1325:C:H2'	1:A:1326:C:C6	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:ALA:N	3:C:114:PRO:CD	2.71	0.54
8:H:91:ARG:HD3	12:L:7:ILE:HG21	1.90	0.54
12:L:37:CYS:SG	12:L:58:VAL:HG22	2.48	0.54
1:A:504:C:N3	1:A:542:G:C2	2.76	0.53
1:A:555:C:H2'	1:A:556:C:C6	2.43	0.53
1:A:827:U:C4	1:A:872:A:N1	2.72	0.53
1:A:1312:G:C2	1:A:1326:C:C2	2.95	0.53
1:A:500:G:C6	1:A:501:C:N4	2.76	0.53
1:A:522:C:H5''	12:L:120:TYR:OH	2.08	0.53
9:I:104:ARG:HH11	9:I:106:ALA:HA	1.73	0.53
23:X:110:LEU:HD13	23:X:148:ALA:HB2	1.89	0.53
25:Z:70:G:H2'	25:Z:71:C:O4'	2.08	0.53
1:A:948:C:H2'	1:A:949:A:H8	1.74	0.53
1:A:1133:G:H1	1:A:1141:C:H42	1.55	0.53
1:A:79:G:H2'	1:A:80:G:C8	2.42	0.53
1:A:532:A:N6	3:C:127:ARG:HB3	2.23	0.53
12:L:58:VAL:HG21	12:L:85:ILE:HD11	1.91	0.53
25:Z:37:A:H2'	25:Z:38:A:O4'	2.09	0.53
1:A:521:G:N1	1:A:522:C:C4	2.77	0.53
1:A:910:C:H5''	12:L:97:ARG:NH2	2.24	0.53
1:A:975:A:H5''	1:A:975:A:C8	2.44	0.53
1:A:1027:C:H2'	1:A:1028:C:H5'	1.89	0.53
1:A:1314:C:H42	19:S:4:SER:HB2	1.74	0.53
8:H:36:LEU:HD21	8:H:61:VAL:HG22	1.91	0.53
1:A:975:A:H4'	1:A:976:G:C5'	2.39	0.53
4:D:109:GLY:HA3	4:D:165:MET:HG3	1.91	0.53
7:G:33:ASP:HB2	7:G:35:LYS:HG3	1.90	0.53
1:A:138:G:H1	1:A:225:C:H42	1.57	0.53
1:A:216:G:C2	1:A:217:C:N3	2.77	0.53
1:A:1414:U:H2'	1:A:1415:G:C8	2.43	0.53
1:A:1418:A:N6	1:A:1482:G:O2'	2.40	0.53
1:A:1437:C:H2'	1:A:1438:G:H8	1.74	0.53
25:Z:48:C:H5''	25:Z:50:U:OP2	2.09	0.53
1:A:974:A:H4'	1:A:975:A:H3'	1.90	0.53
1:A:1510:U:H2'	1:A:1511:G:C8	2.44	0.53
2:B:10:LEU:HG	2:B:48:MET:HG3	1.89	0.53
1:A:376:G:H5''	16:P:5:ARG:HD2	1.90	0.53
1:A:598:U:H2'	1:A:599:C:H6	1.74	0.53
1:A:662:G:C2	1:A:744:C:O2	2.62	0.53
1:A:928:G:H1	1:A:1389:C:N4	2.07	0.53
5:E:20:GLN:HB2	5:E:23:GLY:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:112:GLU:HB3	23:X:114:HIS:CD2	2.43	0.53
1:A:46:G:H2'	1:A:366:C:C5	2.43	0.52
1:A:1105:A:H2'	1:A:1106:G:C8	2.44	0.52
10:J:90:LEU:H	10:J:91:PRO:HD2	1.74	0.52
1:A:266:G:O2'	1:A:267:C:OP2	2.22	0.52
1:A:317:G:P	1:A:353:A:H61	2.33	0.52
1:A:369:C:H2'	1:A:370:C:C6	2.44	0.52
1:A:529:G:H5'	1:A:530:G:OP2	2.09	0.52
1:A:1050:G:C6	1:A:1051:C:N4	2.77	0.52
1:A:1106:G:C2	1:A:1107:C:C4	2.98	0.52
1:A:1456:G:N2	1:A:1457:G:N7	2.57	0.52
2:B:80:ILE:O	2:B:84:GLU:HG2	2.09	0.52
1:A:122:G:C2	1:A:123:C:C2	2.96	0.52
1:A:148:G:C2	1:A:175:C:C2	2.98	0.52
1:A:312:C:H2'	1:A:313:A:H8	1.75	0.52
1:A:392:G:H2'	1:A:393:A:C8	2.44	0.52
1:A:1114:C:H2'	1:A:1115:C:C6	2.45	0.52
1:A:1125:U:C5'	1:A:1126:U:H5	2.20	0.52
1:A:1525:G:H2'	1:A:1526:G:H8	1.75	0.52
1:A:568:G:C2	1:A:883:C:C2	2.98	0.52
1:A:890:G:O2'	1:A:906:G:O6	2.24	0.52
1:A:1251:A:H2'	1:A:1252:A:O4'	2.09	0.52
1:A:1534:A:C4	1:A:1535:C:C5	2.98	0.52
13:M:94:ARG:HB3	13:M:96:LEU:HD12	1.92	0.52
15:O:82:ILE:HA	15:O:87:ILE:HD12	1.90	0.52
1:A:437:U:H2'	1:A:438:G:O4'	2.09	0.52
1:A:1124:G:H1	1:A:1149:C:H42	1.57	0.52
1:A:1162:C:C2	1:A:1175:G:N2	2.77	0.52
4:D:108:LEU:HD21	4:D:174:LEU:HD22	1.91	0.52
25:Z:52:G:C4	25:Z:53:G:C8	2.97	0.52
25:Z:64:G:C2	25:Z:65:C:C2	2.98	0.52
1:A:145:G:N2	1:A:178:C:C2	2.78	0.52
1:A:876:G:C6	1:A:877:C:N4	2.77	0.52
1:A:1096:C:H2'	1:A:1097:C:C6	2.44	0.52
8:H:6:ILE:O	8:H:10:LEU:HG	2.09	0.52
1:A:333:G:N2	1:A:334:C:C2	2.77	0.52
1:A:505:G:H2'	1:A:506:G:H8	1.74	0.52
1:A:674:G:O5'	1:A:674:G:H8	1.93	0.52
1:A:1229:A:H2'	1:A:1230:C:H6	1.75	0.52
3:C:26:LYS:N	3:C:26:LYS:CE	2.73	0.52
1:A:99:U:H2'	1:A:100:C:C6	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001(A):G:N1	1:A:1002:G:C6	2.78	0.52
1:A:1365:G:C2	1:A:1366:C:C2	2.98	0.52
1:A:1365:G:C6	1:A:1366:C:C4	2.98	0.52
1:A:1424:C:H42	1:A:1476:G:H1	1.56	0.52
25:Z:17(A):U:C3'	25:Z:18:G:H5''	2.40	0.52
1:A:130:A:H8	1:A:130:A:OP1	1.93	0.52
1:A:200:G:C2	1:A:218:C:C2	2.98	0.52
1:A:269:C:H2'	1:A:270:A:C8	2.44	0.52
1:A:413:G:N2	1:A:429:U:OP2	2.38	0.52
1:A:1129:C:O5'	1:A:1130:A:H5'	2.10	0.52
5:E:139:LEU:HA	5:E:142:LEU:HD12	1.91	0.52
9:I:10:ARG:CD	9:I:105:ASP:HB3	2.40	0.52
1:A:100:C:H2'	1:A:101:A:C8	2.45	0.52
1:A:124:G:H2'	1:A:125:U:O4'	2.10	0.52
1:A:1010:G:H2'	1:A:1011:G:H8	1.74	0.52
1:A:1434:A:H2'	1:A:1435:G:O4'	2.10	0.52
8:H:11:THR:HA	8:H:14:ARG:HH12	1.75	0.52
13:M:33:ALA:HB2	13:M:64:TRP:HH2	1.74	0.52
19:S:6:LYS:HD2	19:S:7:LYS:H	1.75	0.52
1:A:70:G:C2	1:A:100:C:C2	2.98	0.51
10:J:57:LYS:HB2	10:J:60:ARG:HH12	1.74	0.51
19:S:17:GLU:HA	19:S:20:LEU:HG	1.91	0.51
1:A:560:U:H2'	5:E:123:LEU:HD22	1.91	0.51
1:A:1029:C:H2'	1:A:1030:C:C6	2.45	0.51
1:A:1137:C:H4'	1:A:1138:G:C2	2.45	0.51
1:A:1392:G:H21	1:A:1502:A:H8	1.59	0.51
5:E:92:LYS:HG2	5:E:93:PRO:HD2	1.91	0.51
15:O:30:ALA:HA	15:O:85:LEU:HD11	1.92	0.51
17:Q:34:LYS:HG3	17:Q:36:ILE:HG23	1.91	0.51
25:Z:68:C:H2'	25:Z:69:C:C6	2.45	0.51
1:A:967:C:H2'	1:A:968:A:C8	2.45	0.51
1:A:1280:A:OP1	1:A:1281:U:C5	2.62	0.51
23:X:67:TYR:O	23:X:71:MET:HG2	2.11	0.51
1:A:277:C:H5'	17:Q:68:ARG:NH1	2.25	0.51
1:A:476:G:H2'	1:A:477:A:C8	2.45	0.51
1:A:681:C:H42	1:A:709:G:H1	1.58	0.51
1:A:1068:G:N2	1:A:1069:C:C2	2.78	0.51
1:A:1369:C:H2'	1:A:1370:G:O4'	2.10	0.51
1:A:1389:C:H2'	1:A:1390:U:O4'	2.11	0.51
3:C:30:ARG:NH2	3:C:30:ARG:CB	2.73	0.51
7:G:111:ARG:CZ	7:G:122:HIS:HB3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:G:H2'	1:A:185:A:H8	1.75	0.51
1:A:522:C:H41	12:L:53:ARG:HH21	1.59	0.51
1:A:737:A:H2'	1:A:738:C:C6	2.46	0.51
1:A:838:G:C2	1:A:849:C:C2	2.99	0.51
1:A:1126:U:O2	1:A:1126:U:H2'	2.09	0.51
1:A:1431:C:C2	1:A:1470:G:N2	2.79	0.51
1:A:1443:G:N2	1:A:1444:C:C2	2.79	0.51
1:A:1493:A:H2'	22:W:20:ALA:H	1.75	0.51
5:E:19:MET:SD	5:E:24:ARG:HB3	2.51	0.51
1:A:1244:C:H2'	1:A:1245:A:H8	1.75	0.51
1:A:1367:C:H4'	10:J:48:THR:HG21	1.91	0.51
1:A:1464:G:C2	1:A:1465:C:C4	2.98	0.51
3:C:26:LYS:N	3:C:26:LYS:CD	2.73	0.51
6:F:78:GLU:HA	6:F:81:ILE:HD12	1.92	0.51
13:M:90:LEU:HA	13:M:93:ARG:HD2	1.91	0.51
22:W:13:VAL:HB	22:W:50:GLY:H	1.75	0.51
1:A:880:C:H2'	1:A:881:G:C8	2.46	0.51
1:A:1405:G:H2'	1:A:1406:U:H6	1.75	0.51
20:T:45:GLN:HG2	20:T:91:LEU:HD22	1.93	0.51
1:A:70:G:C2	1:A:100:C:O2	2.64	0.51
1:A:264:U:H2'	1:A:265:G:O4'	2.11	0.51
1:A:1048:G:H1	1:A:1209:C:H42	1.59	0.51
1:A:1230:C:H5''	25:Z:30:G:H5''	1.92	0.51
1:A:1283:G:N2	1:A:1284:C:C2	2.79	0.51
1:A:173:U:H5'	1:A:197:A:O4'	2.11	0.51
1:A:824:C:H2'	1:A:825:G:H8	1.74	0.51
1:A:864:A:C2	1:A:865:A:C2	2.99	0.51
1:A:1027:C:C2'	1:A:1028:C:H5'	2.40	0.51
1:A:1064:G:H21	1:A:1190:G:H2'	1.75	0.51
1:A:1079:G:H2'	1:A:1080:A:C8	2.46	0.51
1:A:1325:C:H2'	1:A:1326:C:H6	1.75	0.51
1:A:1363(A):A:H1'	1:A:1365:G:C5	2.45	0.51
25:Z:70:G:C6	25:Z:71:C:C4	2.99	0.51
1:A:504:C:C2	1:A:542:G:N2	2.79	0.51
1:A:1201:A:H4'	1:A:1202:G:O5'	2.11	0.51
1:A:1534:A:C4	1:A:1535:C:C6	2.99	0.51
25:Z:31:G:H2'	25:Z:32:OMC:H6	1.76	0.51
1:A:1360:A:OP2	14:N:35:ARG:NH2	2.44	0.50
17:Q:93:GLN:O	17:Q:96:GLU:HB2	2.12	0.50
25:Z:29:G:H2'	25:Z:30:G:O4'	2.11	0.50
1:A:17:U:O2	1:A:1079:G:C2	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:G:H2'	1:A:877:C:C6	2.45	0.50
1:A:1130:A:H2'	1:A:1131:G:C8	2.46	0.50
1:A:1229:A:H2'	1:A:1230:C:C6	2.46	0.50
1:A:10:A:H2'	1:A:11:G:H8	1.72	0.50
1:A:967:C:H4'	9:I:128:ARG:NE	2.26	0.50
1:A:1507:A:H2'	1:A:1508:G:C8	2.45	0.50
5:E:152:ARG:HB3	8:H:43:GLY:HA3	1.94	0.50
7:G:65:ALA:O	7:G:69:VAL:HG23	2.12	0.50
25:Z:69:C:H2'	25:Z:70:G:O4'	2.11	0.50
1:A:132:C:C2	1:A:231:G:N2	2.80	0.50
1:A:309:G:H2'	1:A:310:G:H8	1.76	0.50
1:A:558:G:H3'	1:A:559:A:C5'	2.42	0.50
1:A:914:A:H2'	1:A:915:A:C8	2.46	0.50
4:D:149:ALA:HB3	4:D:152:SER:HB2	1.93	0.50
7:G:97:GLN:O	7:G:101:LEU:HG	2.11	0.50
24:Y:36:A:H2'	24:Y:37:U:O4'	2.12	0.50
1:A:56:U:H2'	1:A:57:G:C8	2.45	0.50
1:A:236:G:C2	1:A:237:C:C2	3.00	0.50
1:A:381:C:H2'	1:A:382:A:O4'	2.12	0.50
1:A:1106:G:H5''	3:C:172:ARG:HD2	1.92	0.50
1:A:1128:C:H1'	1:A:1146:A:H61	1.77	0.50
3:C:188:LEU:HD12	3:C:190:ARG:HG3	1.92	0.50
4:D:79:PHE:CZ	4:D:204:ILE:HA	2.47	0.50
1:A:777:A:H2'	1:A:778:G:C8	2.46	0.50
1:A:966:G:C4	25:Z:34:C:H5'	2.46	0.50
1:A:1255:G:H2'	1:A:1279:A:N6	2.26	0.50
1:A:1361:G:C6	1:A:1362:C:N3	2.80	0.50
2:B:51:LEU:HG	2:B:201:ILE:HG23	1.93	0.50
4:D:121:VAL:O	4:D:134:ASP:HA	2.12	0.50
10:J:51:ARG:N	10:J:59:SER:O	2.37	0.50
1:A:16:A:N3	1:A:1080:A:H1'	2.27	0.50
1:A:229:U:H2'	1:A:230:G:C8	2.47	0.50
1:A:648:A:H2'	1:A:649:G:H8	1.77	0.50
1:A:1081:G:O5'	5:E:18:ARG:HB2	2.12	0.50
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.93	0.50
25:Z:53:G:N2	25:Z:62:C:C2	2.80	0.50
1:A:22:G:C6	1:A:23:C:C4	2.99	0.50
1:A:142:G:H2'	1:A:143:A:C8	2.47	0.50
1:A:474:G:H2'	1:A:475:G:C8	2.47	0.50
1:A:1028:C:H2'	1:A:1029:C:O4'	2.12	0.50
1:A:1132:C:H2'	1:A:1133:G:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1532:U:H5''	1:A:1533:C:P	2.51	0.50
6:F:27:GLN:HA	6:F:30:LEU:HD12	1.93	0.50
1:A:399:G:C6	1:A:400:C:N4	2.80	0.50
1:A:784:C:C2	1:A:799:G:N2	2.80	0.50
1:A:939:G:H2'	1:A:940:C:C6	2.47	0.50
1:A:1000:U:C6	1:A:1000:U:C3'	2.95	0.50
1:A:1017:G:C2	1:A:1018:C:C2	2.99	0.50
1:A:1280:A:C3'	1:A:1281:U:H5''	2.41	0.50
1:A:1518:A:H2'	1:A:1519:A:C8	2.47	0.50
7:G:145:ALA:O	7:G:146:GLU:HB2	2.11	0.50
1:A:1135:U:H4'	1:A:1136:U:C5	2.47	0.49
10:J:62:HIS:CB	14:N:59:ALA:HB3	2.37	0.49
14:N:7:ILE:HG22	14:N:10:ALA:HB2	1.93	0.49
16:P:22:THR:HA	16:P:33:ILE:HD12	1.93	0.49
25:Z:22:G:N2	25:Z:23:C:C2	2.79	0.49
1:A:416:G:C6	1:A:417:C:C4	3.00	0.49
1:A:538:G:H2'	1:A:539:A:C8	2.46	0.49
1:A:1059:C:O3'	14:N:45:ARG:NH2	2.45	0.49
1:A:1172:C:H2'	1:A:1173:G:H8	1.77	0.49
1:A:1220:G:H2'	1:A:1221:G:C8	2.47	0.49
1:A:1385:G:H2'	1:A:1386:G:H8	1.77	0.49
1:A:1525:G:H2'	1:A:1526:G:C8	2.47	0.49
2:B:174:VAL:HG13	2:B:184:VAL:HG11	1.94	0.49
8:H:12:ARG:HD3	8:H:26:VAL:HG12	1.94	0.49
10:J:57:LYS:HA	10:J:60:ARG:HH11	1.77	0.49
1:A:105:G:H2'	1:A:106:C:C6	2.46	0.49
1:A:115:G:O2'	1:A:289:G:H5''	2.13	0.49
1:A:384:G:C6	1:A:385:C:N4	2.80	0.49
1:A:1405:G:H2'	1:A:1406:U:C6	2.46	0.49
25:Z:52:G:H2'	25:Z:53:G:O4'	2.13	0.49
1:A:41:G:H2'	1:A:42:G:H8	1.78	0.49
1:A:293:G:C6	1:A:294:U:C4	3.00	0.49
1:A:919:A:C2	1:A:1080:A:C2	2.99	0.49
1:A:1114:C:C2	1:A:1187:G:C2	3.00	0.49
1:A:1222:G:OP1	19:S:77:THR:HG23	2.12	0.49
1:A:1256:A:H1'	1:A:1258:G:C4	2.48	0.49
1:A:1493:A:H4'	1:A:1494:G:OP1	2.13	0.49
3:C:25:GLY:O	3:C:29:TYR:HB2	2.12	0.49
15:O:39:LEU:HD22	15:O:56:LEU:HB2	1.94	0.49
25:Z:37:A:H3'	25:Z:38:A:C8	2.47	0.49
1:A:270:A:H2'	1:A:271:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:G:C2	1:A:417:C:C2	3.01	0.49
1:A:544:G:OP1	4:D:62:GLN:HG3	2.12	0.49
1:A:1262:C:H42	1:A:1273:G:H1	1.60	0.49
1:A:1345:U:H4'	1:A:1346:A:O5'	2.12	0.49
1:A:1416:G:H2'	1:A:1417:G:O4'	2.12	0.49
1:A:1428:A:H2'	1:A:1429:C:C6	2.48	0.49
5:E:139:LEU:O	5:E:142:LEU:HB2	2.12	0.49
12:L:37:CYS:SG	12:L:56:ALA:HB1	2.52	0.49
20:T:22:ARG:HG2	20:T:25:ARG:HH22	1.76	0.49
1:A:22:G:C2	1:A:23:C:C2	3.01	0.49
1:A:122:G:C6	1:A:123:C:C4	3.00	0.49
1:A:132:C:N3	1:A:231:G:C2	2.81	0.49
1:A:744:C:H2'	1:A:745:C:C6	2.48	0.49
1:A:1409:C:H2'	1:A:1410:G:H8	1.77	0.49
1:A:1443:G:C2	1:A:1444:C:C4	3.00	0.49
11:K:33:THR:HA	11:K:39:PRO:HA	1.94	0.49
20:T:43:LEU:HB3	20:T:52:ALA:HB2	1.94	0.49
22:W:56:GLU:HB3	22:W:66:ARG:HH11	1.76	0.49
23:X:141:THR:HG22	23:X:165:LEU:HD11	1.93	0.49
1:A:940:C:H2'	1:A:941:G:C8	2.48	0.49
1:A:20:U:H2'	1:A:21:G:O4'	2.13	0.49
1:A:125:U:H2'	1:A:126:G:C8	2.47	0.49
1:A:552:U:H2'	1:A:553:A:C8	2.48	0.49
1:A:864:A:O2'	1:A:865:A:O4'	2.31	0.49
1:A:1456:G:N2	1:A:1457:G:C8	2.81	0.49
1:A:15:G:H2'	1:A:16:A:H8	1.78	0.49
1:A:28:G:O2'	1:A:296:U:OP1	2.31	0.49
1:A:148:G:H2'	1:A:149:A:C8	2.47	0.49
1:A:940:C:H2'	1:A:941:G:H8	1.78	0.49
5:E:51:VAL:HG13	5:E:52:PRO:HD3	1.95	0.49
13:M:94:ARG:HH22	19:S:80:TYR:HA	1.77	0.49
25:Z:64:G:C6	25:Z:65:C:C4	3.00	0.49
1:A:189:G:C2	1:A:189(A):C:C2	3.00	0.49
1:A:224:C:H2'	1:A:225:C:C6	2.48	0.49
1:A:1217:C:N4	1:A:1218:C:N4	2.61	0.49
1:A:1484:C:H2'	1:A:1485:U:O4'	2.13	0.49
1:A:977:A:H2'	1:A:978:A:H5''	1.95	0.48
1:A:1030:C:C2	1:A:1032:G:N2	2.81	0.48
1:A:1357:A:N6	1:A:1363(A):A:C2	2.80	0.48
18:R:69:THR:HA	18:R:72:ARG:HD2	1.94	0.48
25:Z:36:U:H2'	25:Z:37:A:O4'	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:64:G:H2'	25:Z:65:C:C6	2.48	0.48
1:A:427:U:OP2	4:D:36:ARG:NH2	2.46	0.48
1:A:568:G:C6	1:A:569:C:N4	2.81	0.48
1:A:648:A:H2'	1:A:649:G:C8	2.48	0.48
1:A:1266:G:N2	1:A:1270:C:C2	2.81	0.48
4:D:31:CYS:C	4:D:33:MET:H	2.21	0.48
10:J:7:LYS:CG	10:J:71:LEU:HD23	2.24	0.48
12:L:32:PHE:HB3	12:L:84:LEU:HD11	1.95	0.48
25:Z:70:G:C2	25:Z:71:C:C2	3.01	0.48
1:A:130:A:H5'	17:Q:63:ARG:HE	1.79	0.48
1:A:198:G:H2'	1:A:199:G:C8	2.48	0.48
1:A:229:U:H2'	1:A:230:G:H8	1.78	0.48
1:A:261:U:N3	1:A:264:U:OP2	2.39	0.48
1:A:442:C:H2'	1:A:443:C:C6	2.49	0.48
1:A:778:G:C6	1:A:779:C:C4	3.01	0.48
1:A:778:G:C2	1:A:779:C:C2	3.02	0.48
1:A:823:G:N2	1:A:824:C:C2	2.81	0.48
1:A:1226:C:H2'	13:M:103:THR:HB	1.94	0.48
3:C:29:TYR:CE2	14:N:54:PRO:HG2	2.48	0.48
5:E:71:LEU:HD21	5:E:115:VAL:HG22	1.96	0.48
12:L:57:LYS:HG2	12:L:67:THR:HG22	1.96	0.48
1:A:588:G:N1	1:A:589:C:C4	2.81	0.48
1:A:719:C:H1'	18:R:49:LYS:HG2	1.94	0.48
1:A:877:C:H2'	1:A:878:G:C8	2.46	0.48
1:A:947:G:H2'	1:A:948:C:O4'	2.13	0.48
1:A:951:G:C6	1:A:1231:G:C6	3.02	0.48
2:B:21:ARG:HD3	2:B:21:ARG:H	1.79	0.48
1:A:35:G:O2'	12:L:121:GLY:HA2	2.12	0.48
1:A:253:U:H2'	1:A:254:G:C8	2.48	0.48
1:A:361:G:H2'	1:A:362:G:O4'	2.13	0.48
1:A:1345:U:O4	1:A:1375:A:N1	2.47	0.48
10:J:26:ALA:HA	10:J:29:ARG:HH21	1.78	0.48
19:S:32:LYS:HA	19:S:50:ALA:HB3	1.95	0.48
25:Z:1:C:N4	25:Z:72:A:H61	2.12	0.48
1:A:1385:G:H2'	1:A:1386:G:C8	2.49	0.48
1:A:1443:G:C2	1:A:1444:C:N3	2.81	0.48
25:Z:50:U:H2'	25:Z:51:C:H6	1.71	0.48
1:A:434:U:H2'	1:A:435:C:H6	1.79	0.48
1:A:518:C:O2'	1:A:519:C:OP2	2.25	0.48
1:A:600:C:C2	1:A:639:G:C2	3.01	0.48
1:A:602:A:H2'	1:A:603:U:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:G:N3	15:O:23:GLY:HA3	2.28	0.48
1:A:988:G:C6	1:A:989:C:N3	2.82	0.48
1:A:1216:G:N2	1:A:1217:C:C2	2.81	0.48
3:C:54:ARG:H	3:C:69:HIS:HB2	1.79	0.48
3:C:132:ARG:HG2	3:C:136:GLN:HE21	1.79	0.48
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.94	0.48
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.94	0.48
7:G:53:LYS:HD2	7:G:125:MET:HE1	1.95	0.48
10:J:24:VAL:HG22	10:J:72:VAL:HG21	1.95	0.48
15:O:9:GLN:HA	15:O:12:ILE:HD12	1.95	0.48
1:A:169:C:H2'	1:A:170:U:C6	2.49	0.48
1:A:568:G:C2	1:A:883:C:N3	2.82	0.48
1:A:603:U:H2'	1:A:604:G:H8	1.78	0.48
1:A:1077:G:H22	1:A:1079:G:H3'	1.78	0.48
25:Z:62:C:H2'	25:Z:63:G:C8	2.48	0.48
1:A:110:C:H4'	16:P:25:ARG:HB3	1.96	0.48
1:A:296:U:H2'	1:A:297:G:C8	2.49	0.48
1:A:715:A:H2'	1:A:716:A:O4'	2.14	0.48
1:A:1038:C:H2'	1:A:1039:C:H6	1.79	0.48
3:C:57:ILE:HA	3:C:65:ALA:O	2.13	0.48
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.54	0.48
21:V:14:TRP:HZ3	21:V:15:ARG:HE	1.62	0.48
25:Z:63:G:C2	25:Z:64:G:C5	3.01	0.48
1:A:761:G:C6	1:A:762:C:C4	3.01	0.47
1:A:1508:G:C2	1:A:1509:C:C2	3.02	0.47
7:G:125:MET:O	7:G:129:GLU:HG2	2.14	0.47
1:A:403:C:H5''	4:D:136:PRO:HD2	1.96	0.47
1:A:577:G:C2	1:A:578:C:C2	3.01	0.47
1:A:784:C:H42	1:A:798:G:H1	1.60	0.47
1:A:1301:U:H1'	1:A:1302:U:OP1	2.13	0.47
12:L:114:LYS:HE2	12:L:125:PRO:HB3	1.96	0.47
25:Z:16:C:O4'	25:Z:59:A:C2	2.67	0.47
1:A:263:A:OP1	20:T:79:ARG:HD3	2.14	0.47
1:A:538:G:OP2	12:L:115:LYS:HB2	2.14	0.47
1:A:636:U:H2'	1:A:637:G:C8	2.49	0.47
1:A:975:A:H4'	1:A:976:G:H5'	1.95	0.47
3:C:116:VAL:O	3:C:120:VAL:HG23	2.13	0.47
3:C:155:GLY:O	3:C:196:LEU:HG	2.13	0.47
5:E:32:VAL:HB	5:E:58:ALA:HB1	1.95	0.47
1:A:669:U:H2'	1:A:670:G:H8	1.79	0.47
1:A:988:G:H2'	1:A:989:C:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.96	0.47
4:D:31:CYS:HG	26:D:300:ZN:ZN	1.24	0.47
8:H:86:ILE:HD11	8:H:136:GLU:HB3	1.96	0.47
1:A:377:G:H1	1:A:386:C:N4	2.12	0.47
1:A:669:U:H2'	1:A:670:G:C8	2.49	0.47
1:A:681:C:C2	1:A:710:G:N2	2.82	0.47
1:A:875:C:O2'	8:H:14:ARG:HD2	2.14	0.47
1:A:881:G:C2	1:A:882:C:C2	3.02	0.47
1:A:1444:C:O5'	1:A:1444:C:H6	1.97	0.47
3:C:64:VAL:O	3:C:99:VAL:HG23	2.14	0.47
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.49	0.47
25:Z:12:G:N1	25:Z:13:C:C2	2.83	0.47
1:A:172:A:H2'	1:A:174:C:H5	1.78	0.47
1:A:189:G:C6	1:A:189(A):C:C4	3.03	0.47
1:A:883:C:H2'	1:A:884:U:C6	2.50	0.47
1:A:945:G:H2'	1:A:945:G:N3	2.30	0.47
1:A:949:A:OP2	13:M:106:ASN:HB2	2.13	0.47
1:A:1084:G:H1'	1:A:1103:C:H41	1.78	0.47
1:A:1188:A:H2'	1:A:1189:C:O4'	2.15	0.47
1:A:1283:G:C6	1:A:1284:C:N4	2.82	0.47
1:A:1346:A:H2'	7:G:10:ARG:NH2	2.26	0.47
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.95	0.47
25:Z:31:G:C2	25:Z:40:C:C2	3.02	0.47
25:Z:52:G:C5	25:Z:53:G:N7	2.82	0.47
1:A:333:G:C6	1:A:334:C:N4	2.82	0.47
1:A:590:C:N3	1:A:650:G:C2	2.83	0.47
1:A:960:U:H4'	1:A:961:U:O5'	2.13	0.47
1:A:1119:C:H2'	1:A:1120:G:H8	1.78	0.47
1:A:1228:C:H4'	13:M:116:THR:HA	1.96	0.47
2:B:187:LEU:HA	2:B:201:ILE:HB	1.97	0.47
3:C:54:ARG:HB3	3:C:69:HIS:CD2	2.50	0.47
8:H:103:VAL:HG21	8:H:110:ALA:HB2	1.95	0.47
12:L:25:PRO:C	12:L:27:LEU:N	2.69	0.47
24:Y:28:A:H5'	24:Y:29:G:OP2	2.15	0.47
25:Z:4:G:H2'	25:Z:5:G:H8	1.80	0.47
1:A:362:G:H5''	12:L:61:THR:HB	1.97	0.47
1:A:1050:G:N2	1:A:1051:C:C2	2.83	0.47
3:C:99:VAL:CG2	3:C:100:ALA:N	2.78	0.47
4:D:120:LEU:HA	4:D:125:HIS:HD2	1.79	0.47
15:O:15:PHE:HE2	15:O:84:LYS:HB3	1.79	0.47
16:P:49:LEU:HD13	16:P:73:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:G:C6	1:A:237:C:C4	3.03	0.47
1:A:628:G:H2'	1:A:629:G:C8	2.50	0.47
1:A:643:C:H2'	1:A:644:G:H8	1.80	0.47
1:A:823:G:H2'	1:A:824:C:C6	2.50	0.47
1:A:928:G:H2'	1:A:929:G:C8	2.49	0.47
1:A:957:U:H4'	19:S:79:THR:HG23	1.96	0.47
1:A:1030:C:H42	1:A:1031:G:H1	1.62	0.47
1:A:1038:C:H2'	1:A:1039:C:C6	2.49	0.47
2:B:177:ALA:HA	2:B:182:ILE:HD12	1.96	0.47
3:C:34:LEU:O	3:C:38:ARG:HG2	2.15	0.47
1:A:988:G:C6	1:A:989:C:C2	3.03	0.47
1:A:1533:C:H2'	1:A:1534:A:N1	2.30	0.47
6:F:53:ALA:HB3	6:F:86:ARG:HH11	1.79	0.47
19:S:36:ARG:HD3	19:S:72:GLY:HA3	1.97	0.47
22:W:32:ILE:HG22	22:W:63:THR:HA	1.97	0.47
1:A:14:U:H1'	1:A:17:U:H5	1.80	0.46
1:A:199:G:N2	1:A:219:C:C2	2.83	0.46
2:B:80:ILE:HG21	2:B:212:GLN:HA	1.96	0.46
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.97	0.46
1:A:199:G:C2	1:A:219:C:N3	2.83	0.46
1:A:201:C:H42	1:A:216:G:H1	1.63	0.46
1:A:269:C:H2'	1:A:270:A:H8	1.79	0.46
1:A:1119:C:OP2	9:I:9:ARG:NH2	2.44	0.46
1:A:1171:G:N2	1:A:1172:C:C2	2.82	0.46
1:A:1320:C:OP1	19:S:70:LYS:HE3	2.15	0.46
17:Q:61:GLU:HA	17:Q:71:PHE:CE1	2.50	0.46
25:Z:33:U:O2'	25:Z:35:A:N7	2.46	0.46
1:A:290:C:H2'	1:A:291:C:O4'	2.16	0.46
1:A:585:G:C2	1:A:586:C:C2	3.04	0.46
1:A:908:A:H2'	1:A:909:A:H8	1.80	0.46
1:A:1084:G:H2'	1:A:1085:U:C5	2.51	0.46
1:A:1127:G:N2	1:A:1145:C:C2	2.83	0.46
3:C:137:ALA:O	3:C:141:VAL:HG23	2.15	0.46
5:E:110:LEU:HD13	5:E:118:ILE:HD12	1.97	0.46
9:I:7:THR:O	9:I:83:ARG:CD	2.64	0.46
1:A:23:C:C4	1:A:24:U:C4	3.03	0.46
1:A:35:G:C6	1:A:36:C:N4	2.84	0.46
1:A:277:C:H5'	17:Q:68:ARG:HH12	1.79	0.46
1:A:725:G:N1	1:A:726:C:C4	2.83	0.46
1:A:806:C:H2'	1:A:807:A:C8	2.51	0.46
1:A:834:C:C2	1:A:853:G:C2	3.02	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1535:C:C4	1:A:1536:C:H5	2.29	0.46
6:F:100:ASN:HB3	18:R:28:GLU:HA	1.96	0.46
10:J:31:GLY:HA2	10:J:78:ASN:HD22	1.81	0.46
13:M:88:ARG:HG3	13:M:98:VAL:HG11	1.97	0.46
16:P:7:ALA:O	16:P:17:TYR:HA	2.15	0.46
25:Z:49:G:C8	25:Z:49:G:O5'	2.68	0.46
1:A:194:C:H4'	20:T:64:ASP:HB3	1.96	0.46
1:A:376:G:H5''	16:P:5:ARG:HB2	1.96	0.46
1:A:895:G:H1	1:A:904:C:H42	1.63	0.46
1:A:1431:C:H3'	1:A:1432:G:H8	1.81	0.46
2:B:213:LEU:O	2:B:217:ARG:HG2	2.15	0.46
11:K:22:HIS:HB3	11:K:29:ILE:HG23	1.98	0.46
20:T:56:MET:HE2	20:T:85:MET:HA	1.98	0.46
1:A:259:G:C2	1:A:268:C:C2	3.04	0.46
1:A:663:A:H2'	1:A:664:G:O4'	2.16	0.46
1:A:838:G:N2	1:A:849:C:C2	2.83	0.46
1:A:977:A:O2'	1:A:979:C:OP2	2.21	0.46
1:A:1077:G:N2	1:A:1080:A:OP2	2.41	0.46
14:N:44:LEU:HD22	14:N:53:LEU:HD11	1.98	0.46
1:A:289:G:N2	1:A:290:C:C2	2.84	0.46
1:A:931:C:H3'	1:A:932:C:H5''	1.98	0.46
1:A:1050:G:C2	1:A:1209:C:C2	3.04	0.46
17:Q:92:ARG:HB3	17:Q:92:ARG:HH11	1.81	0.46
1:A:127:G:N2	1:A:235:C:C2	2.84	0.46
1:A:389:A:H3'	1:A:390:C:C6	2.51	0.46
1:A:392:G:H5'	16:P:12:LYS:HG3	1.98	0.46
1:A:1078:U:H5	1:A:1079:G:N1	2.14	0.46
1:A:1419:G:C2	1:A:1420:C:C2	3.04	0.46
1:A:1533:C:H4'	24:Y:32:A:H61	1.80	0.46
5:E:93:PRO:CB	8:H:105:ARG:NH1	2.78	0.46
22:W:26:LEU:HD12	22:W:30:PRO:HD2	1.98	0.46
25:Z:58:A:O2'	25:Z:60:U:OP2	2.34	0.46
1:A:919:A:N3	1:A:1080:A:H2	2.13	0.46
1:A:971:G:OP1	1:A:972:C:H5''	2.16	0.46
1:A:986:A:H2'	1:A:987:G:C8	2.50	0.46
1:A:1119:C:H42	1:A:1154:G:H1	1.63	0.46
1:A:1440:C:H42	1:A:1461:G:H1	1.63	0.46
1:A:1508:G:C6	1:A:1509:C:C4	3.04	0.46
3:C:26:LYS:H	3:C:26:LYS:CE	2.28	0.46
11:K:88:GLY:O	11:K:90:GLY:N	2.47	0.46
1:A:200:G:N2	1:A:218:C:C2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:917:G:H2'	1:A:918:A:H8	1.79	0.46
1:A:928:G:H2'	1:A:929:G:H8	1.80	0.46
1:A:1074:G:C6	1:A:1075:C:C4	3.03	0.46
1:A:1430:C:C2	1:A:1471:G:C2	3.03	0.46
4:D:59:ARG:HH12	4:D:62:GLN:HG3	1.81	0.46
12:L:41:ARG:HD2	12:L:43:VAL:HG22	1.98	0.46
1:A:18:C:H2'	1:A:19:C:C6	2.51	0.45
1:A:21:G:H21	1:A:914:A:H62	1.62	0.45
1:A:113:G:H1'	1:A:354:G:H5'	1.98	0.45
1:A:763:G:C2	1:A:764:C:C2	3.04	0.45
1:A:908:A:H2'	1:A:909:A:C8	2.50	0.45
1:A:932:C:O5'	7:G:4:ARG:HG2	2.15	0.45
1:A:988:G:C6	1:A:989:C:C4	3.04	0.45
3:C:157:ILE:HD12	3:C:164:ARG:HB2	1.97	0.45
4:D:116:GLN:O	4:D:120:LEU:HG	2.16	0.45
7:G:101:LEU:HA	7:G:104:LEU:HD12	1.98	0.45
1:A:579:G:H2'	1:A:580:U:C6	2.51	0.45
1:A:781:A:N6	1:A:802:A:H1'	2.31	0.45
1:A:1256:A:C5'	3:C:27:LYS:CE	2.81	0.45
5:E:144:THR:HB	5:E:147:ASP:H	1.81	0.45
7:G:54:THR:C	7:G:56:GLN:H	2.24	0.45
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.97	0.45
17:Q:48:GLU:HB2	17:Q:50:LYS:HB2	1.97	0.45
25:Z:70:G:N1	25:Z:71:C:C2	2.85	0.45
1:A:291:C:H2'	1:A:292:G:H8	1.81	0.45
1:A:548:G:C2	1:A:549:C:C2	3.04	0.45
1:A:1033:G:H2'	1:A:1034:G:C8	2.52	0.45
2:B:87:ARG:HE	2:B:219:VAL:CG1	2.29	0.45
11:K:32:ILE:HG22	11:K:40:ILE:HD12	1.98	0.45
16:P:6:LEU:HD11	16:P:73:LEU:HD12	1.98	0.45
1:A:184:G:H2'	1:A:185:A:C8	2.51	0.45
1:A:233:C:H2'	1:A:234:C:C6	2.52	0.45
1:A:399:G:C2	1:A:400:C:C2	3.04	0.45
1:A:662:G:N1	1:A:744:C:C2	2.84	0.45
1:A:671:G:C2	1:A:736:C:C2	3.04	0.45
1:A:774:G:C2	1:A:806:C:N3	2.84	0.45
11:K:84:VAL:HG23	11:K:110:ASP:HA	1.98	0.45
1:A:122:G:N1	1:A:123:C:C2	2.85	0.45
1:A:439:A:C6	1:A:441:A:H1'	2.51	0.45
1:A:865:A:H2'	1:A:866:C:C6	2.51	0.45
1:A:872:A:C4	1:A:874:G:N7	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:G:H8	1:A:1081:G:OP2	2.00	0.45
1:A:1401:G:H2'	1:A:1402:C:O4'	2.16	0.45
1:A:1459:C:H2'	1:A:1460:A:H8	1.82	0.45
1:A:1536:C:C2	24:Y:30:G:N1	2.85	0.45
13:M:68:GLY:HA2	13:M:71:ARG:HD2	1.98	0.45
1:A:19:C:O2	1:A:917:G:C2	2.69	0.45
1:A:226:G:H2'	1:A:227:G:O4'	2.17	0.45
1:A:500:G:C2	1:A:501:C:N3	2.84	0.45
1:A:968:A:H8	1:A:968:A:OP1	1.99	0.45
1:A:991:U:C4	1:A:1212:U:H1'	2.51	0.45
1:A:1106:G:N1	1:A:1107:C:C4	2.85	0.45
3:C:30:ARG:NH2	14:N:38:GLY:N	2.65	0.45
11:K:43:SER:HB3	11:K:68:ALA:HB2	1.98	0.45
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.99	0.45
25:Z:10:G:N2	25:Z:26:G:H1'	2.32	0.45
25:Z:17:C:OP1	25:Z:60:U:O2'	2.26	0.45
1:A:63:C:H42	1:A:104:G:H1	1.65	0.45
1:A:571:U:H3'	1:A:572:A:H5''	1.98	0.45
1:A:767:A:H2'	1:A:768:A:O4'	2.17	0.45
1:A:880:C:H5''	12:L:12:ARG:HH21	1.81	0.45
1:A:977:A:H3'	1:A:977:A:N3	2.32	0.45
1:A:1017:G:C6	1:A:1018:C:C4	3.04	0.45
1:A:1305:G:OP2	21:V:5:ASP:HB2	2.17	0.45
1:A:1478:C:H2'	1:A:1479:C:C6	2.52	0.45
1:A:1508:G:H2'	1:A:1509:C:O4'	2.16	0.45
4:D:171:GLY:C	4:D:173:TRP:H	2.25	0.45
20:T:63:ILE:HG23	20:T:77:ALA:HB1	1.97	0.45
1:A:187:C:N3	1:A:191:G:C2	2.84	0.45
1:A:571:U:C3'	1:A:572:A:H5''	2.47	0.45
1:A:929:G:C2	1:A:930:C:C2	3.04	0.45
1:A:939:G:C2	1:A:940:C:N3	2.85	0.45
1:A:1390:U:H2'	1:A:1391:U:C6	2.52	0.45
3:C:174:PRO:HD2	3:C:182:ILE:HD11	1.99	0.45
1:A:15:G:N2	5:E:17:ALA:O	2.47	0.45
1:A:15:G:C5	1:A:16:A:N7	2.85	0.45
1:A:370:C:N3	1:A:392:G:C2	2.85	0.45
1:A:886:G:C2	1:A:912:C:O2	2.70	0.45
1:A:1120:G:H2'	1:A:1121:U:C6	2.51	0.45
1:A:1488:G:H2'	1:A:1489:G:H8	1.81	0.45
6:F:48:LEU:HD13	6:F:52:ILE:HB	1.99	0.45
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:70:G:C6	25:Z:71:C:N3	2.85	0.45
1:A:145:G:C2	1:A:178:C:N3	2.86	0.45
1:A:743:U:H2'	1:A:744:C:H6	1.81	0.45
1:A:1171:G:C2	1:A:1172:C:C2	3.05	0.45
1:A:1343:G:C6	1:A:1344:C:N3	2.85	0.45
4:D:88:VAL:HG12	4:D:91:SER:H	1.82	0.45
17:Q:29:HIS:CE1	17:Q:31:LEU:HB3	2.52	0.45
1:A:105:G:C2	1:A:106:C:C2	3.05	0.44
1:A:127:G:C2	1:A:235:C:N3	2.85	0.44
1:A:252:U:H2'	1:A:253:U:C6	2.52	0.44
1:A:443:C:C2	1:A:492:G:N2	2.85	0.44
1:A:864:A:C2'	1:A:865:A:C8	2.88	0.44
1:A:1086:U:O5'	1:A:1086:U:H6	2.00	0.44
1:A:1327:C:H2'	1:A:1328:C:C6	2.52	0.44
1:A:1526:G:H2'	1:A:1527:C:C6	2.51	0.44
3:C:57:ILE:HG12	3:C:66:VAL:HG22	1.99	0.44
5:E:93:PRO:CB	8:H:105:ARG:NH2	2.64	0.44
1:A:101:A:C4	1:A:102:G:C8	3.05	0.44
1:A:823:G:C2	1:A:824:C:C2	3.05	0.44
1:A:1222:G:C2	1:A:1223:C:N3	2.85	0.44
1:A:1225:A:H2'	1:A:1225:A:N3	2.31	0.44
1:A:1252:A:H2'	1:A:1253:G:O4'	2.17	0.44
1:A:1371:G:H2'	1:A:1372:U:C6	2.52	0.44
1:A:1478:C:H2'	1:A:1479:C:H6	1.81	0.44
9:I:89:ASN:HB3	9:I:92:TYR:CE2	2.52	0.44
13:M:88:ARG:O	13:M:92:HIS:HD2	2.00	0.44
1:A:514:C:H42	1:A:537:G:H1	1.65	0.44
1:A:518:C:H2'	1:A:530:G:C8	2.52	0.44
1:A:914:A:C4	1:A:915:A:N7	2.86	0.44
1:A:1134:G:C2	1:A:1141:C:N3	2.85	0.44
4:D:57:ARG:HH11	4:D:57:ARG:HG3	1.82	0.44
17:Q:21:VAL:HG11	17:Q:59:ILE:HG13	1.99	0.44
25:Z:37:A:C5	25:Z:38:A:C5	3.06	0.44
1:A:255:G:C2	1:A:272:C:C2	3.06	0.44
1:A:262:A:H5''	20:T:76:ALA:HB2	2.00	0.44
1:A:748:C:H1'	1:A:749:C:H5	1.82	0.44
1:A:982:U:H4'	1:A:983:A:O4'	2.18	0.44
1:A:1014:A:N1	19:S:34:TRP:CE2	2.86	0.44
1:A:1129:C:O2'	1:A:1131:G:OP2	2.34	0.44
1:A:1133:G:H1	1:A:1141:C:N4	2.15	0.44
1:A:1537:U:H3	24:Y:28:A:N6	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:GLU:HA	2:B:129:GLU:HG3	1.99	0.44
3:C:24:ALA:HB3	3:C:29:TYR:CD2	2.53	0.44
5:E:18:ARG:HD3	5:E:20:GLN:NE2	2.32	0.44
23:X:4:GLU:HA	23:X:66:ARG:NH1	2.32	0.44
1:A:109:A:C6	1:A:326:G:C6	3.06	0.44
1:A:138:G:H1	1:A:225:C:N4	2.15	0.44
1:A:256:U:H2'	1:A:257:G:C8	2.52	0.44
1:A:354:G:N1	1:A:355:C:C4	2.86	0.44
1:A:577:G:C6	1:A:578:C:C4	3.05	0.44
1:A:590:C:C2	1:A:650:G:N2	2.85	0.44
1:A:932:C:C2	1:A:1386:G:N2	2.85	0.44
1:A:1220:G:H2'	1:A:1221:G:O4'	2.17	0.44
1:A:1464:G:C2	1:A:1465:C:N3	2.86	0.44
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.98	0.44
9:I:3:GLN:HA	9:I:19:LEU:O	2.18	0.44
15:O:85:LEU:HD12	15:O:87:ILE:HD11	1.98	0.44
1:A:1129:C:O5'	1:A:1130:A:H8	2.00	0.44
1:A:1380:U:C5	7:G:3:ARG:HG3	2.53	0.44
5:E:76:ILE:HD12	5:E:118:ILE:HG21	2.00	0.44
1:A:230:G:H2'	1:A:231:G:O4'	2.18	0.44
1:A:372:C:H4'	1:A:373:A:O5'	2.17	0.44
1:A:701:C:H3'	23:X:67:TYR:OH	2.17	0.44
1:A:806:C:H2'	1:A:807:A:H8	1.83	0.44
1:A:929:G:C6	1:A:930:C:C4	3.06	0.44
1:A:975:A:C5'	1:A:975:A:H8	2.31	0.44
1:A:1004:A:H5''	1:A:1025:U:C4	2.52	0.44
1:A:1353:G:N1	1:A:1354:C:C4	2.86	0.44
1:A:1419:G:C6	1:A:1420:C:C4	3.05	0.44
3:C:79:ARG:HG3	3:C:82:GLU:HG2	1.99	0.44
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.99	0.44
4:D:107:ARG:HD3	4:D:173:TRP:HZ2	1.82	0.44
25:Z:49:G:O5'	25:Z:49:G:H8	2.00	0.44
1:A:90:U:H2'	1:A:91:C:C5	2.52	0.44
1:A:585:G:C6	1:A:586:C:C4	3.05	0.44
1:A:769:G:H4'	1:A:1513:A:H4'	2.00	0.44
1:A:823:G:C6	1:A:824:C:N4	2.85	0.44
1:A:947:G:C2	1:A:948:C:C2	3.06	0.44
1:A:956:U:O2	1:A:956:U:C2'	2.66	0.44
19:S:34:TRP:HA	19:S:52:TYR:CB	2.43	0.44
25:Z:16:C:H2'	25:Z:17:C:C5	2.53	0.44
25:Z:18:G:H21	25:Z:57:A:H2'	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:G:C5	1:A:106:C:C4	3.05	0.44
1:A:223:U:H5'	20:T:68:LYS:NZ	2.33	0.44
1:A:524:G:N2	1:A:525:C:N3	2.66	0.44
1:A:874:G:N1	1:A:875:C:C4	2.85	0.44
1:A:1408:A:H2'	1:A:1409:C:C6	2.53	0.44
1:A:1422:G:H1	1:A:1478:C:H42	1.66	0.44
1:A:1437:C:H2'	1:A:1438:G:C8	2.53	0.44
1:A:1464:G:C6	1:A:1465:C:N4	2.86	0.44
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.52	0.44
25:Z:37:A:C3'	25:Z:38:A:H8	2.31	0.44
25:Z:40:C:H2'	25:Z:41:C:H6	1.80	0.44
25:Z:60:U:H2'	25:Z:61:C:C5	2.53	0.44
25:Z:65:C:H2'	25:Z:66:C:O4'	2.18	0.44
1:A:819:A:H5'	1:A:820:U:H5	1.82	0.43
1:A:1257:U:H4'	1:A:1258:G:O5'	2.18	0.43
1:A:1422:G:H1	1:A:1478:C:N4	2.16	0.43
1:A:1504:G:H4'	1:A:1505:G:O5'	2.17	0.43
1:A:1507:A:C2	1:A:1508:G:C4	3.06	0.43
1:A:1534:A:N1	24:Y:31:U:O4	2.51	0.43
4:D:100:ARG:CZ	4:D:137:SER:HA	2.48	0.43
6:F:33:TYR:HB2	6:F:75:LEU:HD23	1.99	0.43
25:Z:19:G:H5''	25:Z:60:U:O4	2.18	0.43
1:A:51:A:H4'	1:A:52:G:C5'	2.48	0.43
1:A:130:A:OP1	1:A:130:A:C8	2.71	0.43
1:A:825:G:C2	1:A:826:C:C2	3.06	0.43
1:A:1119:C:H2'	1:A:1120:G:C8	2.53	0.43
1:A:1233:G:C2	1:A:1234:C:N3	2.87	0.43
1:A:1526:G:C2	1:A:1527:C:C2	3.06	0.43
7:G:69:VAL:HG11	7:G:134:ALA:HB1	2.00	0.43
12:L:64:TYR:HB3	12:L:66:VAL:HG13	2.00	0.43
16:P:59:TRP:HA	16:P:62:VAL:HG22	2.00	0.43
22:W:15:GLU:HB3	22:W:23:ARG:CB	2.45	0.43
22:W:70:ARG:HB2	22:W:71:LYS:HD2	2.00	0.43
25:Z:52:G:N2	25:Z:63:G:N3	2.65	0.43
1:A:320:C:H2'	1:A:321:A:C8	2.52	0.43
1:A:389:A:H3'	1:A:390:C:H6	1.82	0.43
1:A:774:G:C2	1:A:806:C:C2	3.05	0.43
1:A:861:G:C2	1:A:862:C:C2	3.06	0.43
1:A:1014:A:C2	19:S:34:TRP:CD1	3.06	0.43
1:A:1096:C:H2'	1:A:1097:C:H6	1.81	0.43
1:A:1425:U:H2'	1:A:1426:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:ILE:H	2:B:172:ILE:HG13	1.43	0.43
1:A:25:C:H2'	1:A:26:A:C8	2.53	0.43
1:A:198:G:H1	1:A:219:C:N4	2.16	0.43
1:A:352:C:H4'	1:A:354:G:OP1	2.17	0.43
1:A:769:G:N1	1:A:770:C:C4	2.86	0.43
1:A:1050:G:C2	1:A:1209:C:O2	2.71	0.43
1:A:1356:G:C2	1:A:1367:C:C2	3.07	0.43
6:F:11:ASN:HB2	6:F:86:ARG:HH21	1.83	0.43
9:I:104:ARG:NH1	9:I:106:ALA:HA	2.33	0.43
25:Z:67:C:H2'	25:Z:68:C:C6	2.54	0.43
1:A:394:G:C2	1:A:395:C:C2	3.06	0.43
1:A:926:G:N2	24:Y:37:U:OP2	2.52	0.43
1:A:1063:C:H42	1:A:1193:G:H1	1.65	0.43
1:A:1241:G:N1	1:A:1242:C:C4	2.86	0.43
10:J:71:LEU:HD22	10:J:71:LEU:HA	1.71	0.43
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.53	0.43
20:T:43:LEU:HD13	20:T:52:ALA:HA	1.99	0.43
25:Z:50:U:C2	25:Z:51:C:C4	3.07	0.43
1:A:34:C:H2'	1:A:35:G:H8	1.83	0.43
1:A:456:C:C4	1:A:457:C:N4	2.87	0.43
1:A:1022:G:H2'	1:A:1023:G:H8	1.79	0.43
1:A:1053:G:N7	1:A:1200:C:H5''	2.34	0.43
1:A:1249:C:H4'	9:I:73:GLN:HE22	1.83	0.43
1:A:1286:A:H2'	1:A:1287:A:H4'	2.01	0.43
1:A:1365:G:C5	1:A:1366:C:C4	3.07	0.43
4:D:177:ASP:HB3	4:D:182:LYS:HB2	2.01	0.43
1:A:384:G:C2	1:A:385:C:C2	3.07	0.43
1:A:1149:C:H2'	1:A:1150:U:O4'	2.19	0.43
1:A:1431:C:H2'	1:A:1432:G:O4'	2.18	0.43
1:A:1505:G:H4'	1:A:1506:U:H5''	2.01	0.43
2:B:142:LEU:O	2:B:146:GLN:HB2	2.18	0.43
15:O:3:ILE:HA	15:O:38:ARG:HH22	1.84	0.43
25:Z:37:A:C2'	25:Z:38:A:C8	3.02	0.43
1:A:70:G:C6	1:A:100:C:N3	2.87	0.43
1:A:504:C:C2	1:A:542:G:C2	3.07	0.43
1:A:881:G:C6	1:A:882:C:C4	3.06	0.43
1:A:955:U:H1'	1:A:1227:A:H61	1.84	0.43
1:A:1074:G:C2	1:A:1075:C:C2	3.07	0.43
1:A:1207:G:C6	1:A:1208:C:C4	3.07	0.43
3:C:32:LEU:HG	3:C:32:LEU:H	1.70	0.43
9:I:89:ASN:HA	9:I:90:PRO:HD2	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:87:ILE:HG22	15:O:88:ARG:H	1.82	0.43
19:S:11:VAL:HB	19:S:16:LEU:HD22	2.00	0.43
23:X:20:GLY:HA2	23:X:59:ILE:HD12	2.00	0.43
1:A:235:C:OP1	17:Q:70:ARG:NH1	2.51	0.43
1:A:524:G:N2	1:A:525:C:C2	2.87	0.43
1:A:1250:A:H4'	9:I:67:GLY:HA2	2.00	0.43
2:B:124:SER:O	2:B:127:ILE:HG13	2.19	0.43
13:M:18:ALA:O	13:M:21:TYR:HB2	2.19	0.43
25:Z:52:G:C6	25:Z:53:G:C5	3.07	0.43
1:A:17:U:O2'	1:A:1079:G:H1'	2.18	0.43
1:A:101:A:H2'	1:A:102:G:C8	2.48	0.43
1:A:385:C:H2'	1:A:386:C:O4'	2.19	0.43
1:A:500:G:H1	1:A:545:C:H42	1.67	0.43
1:A:876:G:C2	1:A:877:C:N3	2.87	0.43
1:A:966:G:C2	1:A:967:C:C2	3.07	0.43
1:A:1077:G:C2	1:A:1079:G:H3'	2.50	0.43
1:A:1135:U:H4'	1:A:1136:U:H5	1.84	0.43
4:D:25:ARG:C	4:D:27:TYR:H	2.25	0.43
8:H:39:LEU:HB3	8:H:45:ILE:HG12	2.00	0.43
13:M:23:TYR:HB3	13:M:67:GLU:HA	2.00	0.43
14:N:9:LYS:HG3	14:N:21:TYR:O	2.19	0.43
25:Z:17:C:O2	25:Z:17:C:H2'	2.18	0.43
1:A:79:G:C2'	1:A:80:G:H8	2.32	0.42
1:A:102:G:C2	1:A:103:C:C2	3.07	0.42
1:A:216:G:H2'	1:A:217:C:C6	2.53	0.42
1:A:685:G:H5'	11:K:12:ARG:HH12	1.84	0.42
1:A:1163:C:C2	1:A:1174:G:N2	2.87	0.42
1:A:1524:C:H5''	11:K:120:ARG:NH2	2.34	0.42
2:B:18:GLY:HA3	2:B:41:ILE:HA	2.00	0.42
17:Q:26:GLN:HE21	17:Q:26:GLN:HB2	1.74	0.42
1:A:91:C:C6	1:A:91:C:H3'	2.54	0.42
1:A:164:U:H2'	1:A:165:C:C6	2.53	0.42
1:A:374:A:C6	1:A:375:U:C4	3.08	0.42
1:A:402:G:C2	1:A:403:C:C2	3.07	0.42
1:A:550:G:H2'	1:A:551:U:C6	2.54	0.42
1:A:855:G:C6	1:A:856:C:C4	3.07	0.42
1:A:867:G:N2	1:A:868:C:C2	2.87	0.42
1:A:903:G:C2	1:A:904:C:C2	3.07	0.42
1:A:1179:A:OP2	9:I:93:ARG:NH2	2.51	0.42
1:A:1207:G:C2	1:A:1208:C:C2	3.07	0.42
1:A:1489:G:C2	1:A:1490:C:C2	3.06	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:GLU:HB3	3:C:59:ARG:HH22	1.83	0.42
10:J:50:ILE:N	10:J:60:ARG:HG3	2.34	0.42
19:S:5:LEU:HD13	19:S:9:VAL:HA	2.01	0.42
25:Z:18:G:H8	25:Z:18:G:O5'	2.01	0.42
25:Z:55:PSU:H2'	25:Z:56:C:H3'	2.00	0.42
1:A:110:C:H2'	1:A:111:G:O4'	2.20	0.42
1:A:728:A:H2'	1:A:729:A:C8	2.54	0.42
1:A:926:G:C6	1:A:1505:G:C6	3.08	0.42
1:A:1231:G:H4'	9:I:126:SER:HB3	2.01	0.42
2:B:124:SER:C	2:B:126:GLU:H	2.28	0.42
3:C:150:LYS:HB3	3:C:201:TYR:HB2	2.01	0.42
1:A:64:G:H4'	1:A:65:U:H5''	2.01	0.42
1:A:342:C:C2	1:A:348:G:N2	2.87	0.42
1:A:500:G:N2	1:A:501:C:C2	2.88	0.42
1:A:562:C:H1'	12:L:15:ARG:HG3	2.01	0.42
1:A:682:G:H2'	1:A:683:G:O4'	2.19	0.42
1:A:872:A:H2'	1:A:872:A:N3	2.35	0.42
1:A:918:A:H2	1:A:1079:G:H21	1.50	0.42
1:A:1050:G:C2	1:A:1051:C:C2	3.07	0.42
1:A:1078:U:O2'	1:A:1079:G:O4'	2.36	0.42
1:A:1097:C:H2'	1:A:1098:C:C6	2.55	0.42
1:A:1165:C:H42	1:A:1171:G:H1	1.68	0.42
1:A:1363(A):A:H1'	1:A:1365:G:N7	2.34	0.42
12:L:93:LEU:HA	12:L:94:PRO:HD3	1.91	0.42
1:A:245:C:C2	1:A:284:G:C2	3.07	0.42
1:A:309:G:H2'	1:A:310:G:C8	2.53	0.42
1:A:318:G:N2	1:A:336:C:C2	2.88	0.42
1:A:500:G:C2	1:A:501:C:C2	3.08	0.42
1:A:734:G:C2	1:A:735:C:C2	3.07	0.42
1:A:917:G:C6	1:A:918:A:C6	3.08	0.42
1:A:1088:G:H2'	1:A:1089:G:O4'	2.20	0.42
1:A:1220:G:H2'	1:A:1221:G:H8	1.84	0.42
1:A:1230:C:H5'	25:Z:30:G:H5''	2.01	0.42
1:A:1353:G:C6	1:A:1354:C:N4	2.88	0.42
1:A:1540:U:H3	24:Y:25:A:N6	2.17	0.42
3:C:177:THR:HG23	3:C:180:ALA:HB2	2.01	0.42
22:W:40:MET:HA	22:W:45:ILE:HD12	2.01	0.42
25:Z:41:C:H2'	25:Z:42:G:H8	1.82	0.42
1:A:1253:G:C2	1:A:1254:C:C2	3.08	0.42
1:A:1310:G:C2	1:A:1328:C:N3	2.88	0.42
10:J:24:VAL:HG12	10:J:28:ARG:HE	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:G:OP2	1:A:198:G:C8	2.72	0.42
1:A:444:C:H42	1:A:490:G:H1	1.67	0.42
1:A:742:G:H2'	1:A:743:U:O4'	2.20	0.42
1:A:786:G:H2'	1:A:787:A:O4'	2.20	0.42
1:A:975:A:C8	1:A:975:A:C5'	3.02	0.42
1:A:1116:C:H2'	1:A:1117:G:O4'	2.20	0.42
1:A:1305:G:N2	1:A:1331:G:H1'	2.34	0.42
1:A:1445:C:O2	1:A:1458:G:C2	2.72	0.42
1:A:1526:G:C6	1:A:1527:C:N4	2.88	0.42
2:B:233:SER:HA	2:B:234:PRO:HD3	1.77	0.42
2:B:234:PRO:C	2:B:236:TYR:H	2.28	0.42
9:I:13:ALA:HB2	9:I:68:GLY:HA3	2.00	0.42
13:M:102:ARG:NH1	13:M:104:ARG:HB3	2.34	0.42
18:R:47:THR:HG22	18:R:83:GLU:H	1.84	0.42
1:A:42:G:C6	1:A:43:C:C4	3.07	0.42
1:A:147:G:C2	1:A:176:C:C2	3.07	0.42
1:A:321:A:H2'	1:A:322:C:H6	1.85	0.42
1:A:416:G:C6	1:A:417:C:N3	2.88	0.42
1:A:553:A:H1'	12:L:31:PRO:HG3	2.02	0.42
1:A:736:C:H2'	1:A:737:A:H8	1.83	0.42
1:A:800:G:H2'	1:A:801:U:C6	2.54	0.42
1:A:855:G:C2	1:A:856:C:C2	3.08	0.42
1:A:1074:G:N1	1:A:1075:C:C2	2.88	0.42
1:A:1084:G:H2'	1:A:1085:U:C6	2.54	0.42
1:A:1144:G:N2	1:A:1146:A:H62	2.17	0.42
12:L:124:LYS:HA	12:L:125:PRO:HD2	1.82	0.42
1:A:79:G:N1	1:A:91:C:C2	2.87	0.42
1:A:370:C:O2	1:A:482:A:O2'	2.38	0.42
1:A:409:G:OP1	4:D:24:GLU:HB3	2.20	0.42
1:A:445:G:H2'	1:A:446:G:O4'	2.19	0.42
1:A:689:C:H42	1:A:698:G:H1	1.67	0.42
1:A:784:C:N3	1:A:799:G:C2	2.88	0.42
1:A:817:C:C2	1:A:819:A:O4'	2.73	0.42
1:A:895:G:C2	1:A:896:C:C2	3.07	0.42
1:A:918:A:H2'	1:A:919:A:O4'	2.20	0.42
1:A:1080:A:H5''	5:E:16:THR:CB	2.46	0.42
1:A:1371:G:OP1	9:I:68:GLY:HA2	2.20	0.42
1:A:1538:C:C5	18:R:16:PRO:HA	2.55	0.42
2:B:28:PHE:HA	2:B:194:PRO:HG3	2.02	0.42
3:C:46:GLU:HB2	3:C:47:LEU:HD12	2.02	0.42
4:D:185:PHE:HZ	4:D:189:PRO:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:24:VAL:HG13	12:L:98:TYR:HE1	1.85	0.42
20:T:73:HIS:HB3	20:T:74:LYS:HG3	2.01	0.42
1:A:354:G:C6	1:A:355:C:N4	2.88	0.42
1:A:356:A:H2'	1:A:357:G:O4'	2.20	0.42
1:A:376:G:H2'	1:A:377:G:C8	2.50	0.42
1:A:505:G:H2'	1:A:506:G:C8	2.53	0.42
1:A:1064:G:N2	1:A:1190:G:C2'	2.79	0.42
1:A:1106:G:C2	1:A:1107:C:N3	2.88	0.42
10:J:75:ILE:H	10:J:75:ILE:HG13	1.55	0.42
15:O:35:ARG:HB3	15:O:59:MET:SD	2.60	0.42
17:Q:29:HIS:HE1	17:Q:31:LEU:HB3	1.85	0.42
25:Z:60:U:H2'	25:Z:61:C:H5	1.85	0.42
1:A:43:C:H2'	1:A:44:G:C8	2.55	0.41
1:A:81:U:H1'	1:A:88:A:H62	1.86	0.41
1:A:104:G:C2	1:A:105:G:C5	3.08	0.41
1:A:319:G:C2	1:A:320:C:C2	3.07	0.41
1:A:338:A:H2'	1:A:339:C:O4'	2.20	0.41
1:A:402:G:C6	1:A:403:C:C4	3.07	0.41
1:A:407:G:C2	1:A:436:C:C2	3.08	0.41
1:A:524:G:N1	1:A:525:C:N4	2.68	0.41
1:A:903:G:C6	1:A:904:C:C4	3.08	0.41
1:A:949:A:O2'	1:A:971:G:O6	2.25	0.41
1:A:959:A:H1'	1:A:985:C:H1'	2.01	0.41
1:A:1116:C:H3'	1:A:1117:G:H5''	2.02	0.41
1:A:1241:G:C6	1:A:1242:C:N4	2.88	0.41
1:A:1314:C:OP2	19:S:6:LYS:HB3	2.19	0.41
1:A:1387:G:C2	1:A:1388:C:C2	3.08	0.41
1:A:1423:G:C2	1:A:1424:C:C2	3.08	0.41
1:A:1488:G:H2'	1:A:1489:G:C8	2.54	0.41
6:F:15:ASP:OD1	6:F:18:GLN:HB2	2.20	0.41
11:K:27:ASN:HB2	11:K:55:LYS:HB3	2.01	0.41
19:S:12:ASP:OD1	19:S:37:ARG:HB2	2.20	0.41
25:Z:18:G:O5'	25:Z:18:G:C8	2.73	0.41
1:A:28:G:H2'	1:A:29:G:O4'	2.20	0.41
1:A:258:G:C2	1:A:269:C:C2	3.09	0.41
1:A:295:C:C4	1:A:296:U:C4	3.08	0.41
1:A:333:G:C2	1:A:334:C:C2	3.08	0.41
1:A:344:A:H5''	1:A:345:C:H5	1.85	0.41
1:A:662:G:C6	1:A:744:C:N3	2.88	0.41
1:A:681:C:N4	1:A:709:G:H1	2.18	0.41
1:A:825:G:C6	1:A:826:C:C4	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:U:H2'	1:A:1041:A:C8	2.55	0.41
2:B:19:HIS:CD2	2:B:20:GLU:HG2	2.55	0.41
3:C:30:ARG:HB2	3:C:30:ARG:NH2	2.23	0.41
18:R:19:LYS:HB3	18:R:20:ALA:H	1.69	0.41
25:Z:22:G:C2	25:Z:23:C:C2	3.08	0.41
1:A:310:G:H5'	16:P:31:LYS:HB2	2.01	0.41
1:A:321:A:H2'	1:A:322:C:C6	2.54	0.41
1:A:414:A:H2'	1:A:415:A:O4'	2.19	0.41
1:A:453:A:H2'	1:A:454:C:C6	2.55	0.41
1:A:576:G:H3'	1:A:577:G:C5'	2.49	0.41
1:A:646:U:H2'	1:A:647:C:C6	2.55	0.41
1:A:794:A:H2'	1:A:795:C:C6	2.55	0.41
1:A:981:U:O4	1:A:1223:C:N4	2.53	0.41
1:A:1074:G:H1	1:A:1083:U:H3	1.69	0.41
1:A:1078:U:H5	1:A:1079:G:C6	2.39	0.41
1:A:1166:G:N2	1:A:1169:A:H3'	2.35	0.41
1:A:1190:G:H5'	3:C:176:HIS:HE1	1.84	0.41
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.21	0.41
1:A:1375:A:N3	1:A:1375:A:H2'	2.34	0.41
3:C:3:ASN:HB2	3:C:4:LYS:H	1.72	0.41
4:D:3:ARG:HH21	4:D:71:SER:HB2	1.85	0.41
6:F:12:PRO:HG3	6:F:57:GLN:O	2.20	0.41
7:G:73:MET:HE3	7:G:145:ALA:HB1	2.01	0.41
8:H:82:HIS:CE1	8:H:84:ARG:HB2	2.55	0.41
25:Z:36:U:C2	25:Z:37:A:C8	3.09	0.41
1:A:77:G:H3'	1:A:77:G:C8	2.56	0.41
1:A:157:G:C6	1:A:165:C:N3	2.89	0.41
1:A:446:G:N2	1:A:489:C:C2	2.88	0.41
1:A:519:C:H2'	1:A:520:A:C8	2.54	0.41
1:A:660:G:H2'	1:A:661:G:O4'	2.20	0.41
1:A:876:G:C2	1:A:877:C:C2	3.08	0.41
1:A:1424:C:N4	1:A:1476:G:H1	2.18	0.41
2:B:54:THR:HG23	2:B:199:TYR:HB3	2.02	0.41
4:D:8:VAL:HG11	4:D:21:LEU:HB2	2.03	0.41
11:K:110:ASP:HB3	18:R:85:LEU:HB3	2.02	0.41
20:T:36:LEU:HD23	20:T:36:LEU:HA	1.90	0.41
25:Z:22:G:N1	25:Z:23:C:C4	2.89	0.41
1:A:15:G:O4'	1:A:1396:A:O2'	2.39	0.41
1:A:317:G:H2'	1:A:318:G:O4'	2.20	0.41
1:A:518:C:H4'	1:A:519:C:O5'	2.21	0.41
1:A:830:G:N2	1:A:857:C:C2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:G:C6	1:A:948:C:C4	3.08	0.41
1:A:1157:A:H4'	1:A:1158:C:O5'	2.19	0.41
4:D:175:SER:HB3	4:D:186:LEU:HD11	2.02	0.41
8:H:119:LEU:HD13	8:H:124:ALA:HB2	2.03	0.41
1:A:41:G:H2'	1:A:42:G:C8	2.56	0.41
1:A:42:G:C2	1:A:43:C:C2	3.08	0.41
1:A:289:G:C2	1:A:290:C:C2	3.08	0.41
1:A:363:A:C6	12:L:31:PRO:HD2	2.56	0.41
1:A:551:U:H2'	1:A:552:U:H6	1.82	0.41
1:A:832:C:O2	1:A:855:G:C2	2.74	0.41
1:A:910:C:H5''	12:L:97:ARG:HH21	1.86	0.41
1:A:1171:G:N1	1:A:1172:C:C4	2.89	0.41
2:B:184:VAL:N	2:B:198:ASP:HB2	2.30	0.41
3:C:108:ASN:HA	3:C:109:PRO:HD2	1.77	0.41
8:H:29:SER:HB3	8:H:32:LYS:HB2	2.02	0.41
17:Q:62:SER:OG	17:Q:72:ARG:HG3	2.20	0.41
21:V:10:ARG:HA	21:V:13:ILE:HD12	2.03	0.41
23:X:100:GLN:HA	23:X:103:LEU:HD23	2.02	0.41
1:A:299:G:C6	1:A:300:A:C6	3.09	0.41
1:A:336:C:H2'	1:A:337:C:C6	2.56	0.41
1:A:456:C:C2	1:A:476:G:C2	3.09	0.41
1:A:671:G:C6	1:A:736:C:N4	2.88	0.41
1:A:763:G:C6	1:A:764:C:C4	3.09	0.41
1:A:872:A:C8	1:A:874:G:C8	3.09	0.41
1:A:1292:U:H2'	1:A:1293:G:C8	2.56	0.41
1:A:1368:G:N1	1:A:1369:C:C4	2.88	0.41
3:C:6:HIS:CG	14:N:49:HIS:HB3	2.56	0.41
7:G:148:ASN:C	7:G:150:ALA:N	2.79	0.41
8:H:83:ILE:HG13	8:H:137:VAL:HG22	2.03	0.41
9:I:74:ILE:HA	9:I:77:ILE:HD12	2.02	0.41
1:A:146:G:C2	1:A:177:C:C2	3.09	0.41
1:A:217:C:H2'	1:A:218:C:H6	1.85	0.41
1:A:319:G:C6	1:A:320:C:C4	3.09	0.41
1:A:741:G:H2'	1:A:742:G:O4'	2.21	0.41
1:A:863:U:H2'	1:A:865:A:OP2	2.21	0.41
1:A:1068:G:C2	1:A:1069:C:C2	3.09	0.41
1:A:1235:U:H2'	1:A:1236:A:O4'	2.20	0.41
1:A:1253:G:C6	1:A:1254:C:C4	3.08	0.41
2:B:167:PRO:HG2	2:B:192:SER:OG	2.20	0.41
4:D:50:ARG:HA	4:D:51:PRO:HD3	1.87	0.41
4:D:135:LEU:HA	4:D:136:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.89	0.41
5:E:69:VAL:HG21	5:E:113:ALA:HB1	2.02	0.41
5:E:79:GLU:C	5:E:80:ILE:HG13	2.46	0.41
10:J:50:ILE:HG13	10:J:60:ARG:CD	2.35	0.41
11:K:18:ARG:HA	11:K:81:ASP:H	1.84	0.41
15:O:39:LEU:HD13	15:O:56:LEU:HA	2.03	0.41
25:Z:60:U:H3'	25:Z:61:C:C5	2.55	0.41
1:A:77:G:C8	1:A:77:G:C3'	3.04	0.41
1:A:119:A:H2'	1:A:240:C:H41	1.85	0.41
1:A:392:G:P	16:P:8:ARG:HH22	2.44	0.41
1:A:433:C:H2'	1:A:434:U:C6	2.56	0.41
1:A:542:G:C6	1:A:543:C:N4	2.89	0.41
1:A:544:G:C2	1:A:545:C:C2	3.09	0.41
1:A:579:G:H1	1:A:762:C:H42	1.68	0.41
1:A:643:C:H2'	1:A:644:G:C8	2.55	0.41
1:A:691:G:H3'	11:K:26:ASN:ND2	2.35	0.41
1:A:725:G:C2	1:A:726:C:C2	3.09	0.41
1:A:832:C:C2	1:A:855:G:C2	3.09	0.41
1:A:837:G:H2'	1:A:838:G:O4'	2.21	0.41
1:A:862:C:H2'	1:A:863:U:O4'	2.20	0.41
1:A:895:G:C6	1:A:896:C:C4	3.09	0.41
1:A:918:A:C6	1:A:919:A:C6	3.09	0.41
1:A:999:C:H2'	1:A:1000:U:H5'	2.03	0.41
1:A:1000:U:C5	1:A:1001:A:C8	3.08	0.41
1:A:1028:C:H2'	1:A:1029:C:C4'	2.51	0.41
1:A:1075:C:H5'	1:A:1101:A:N6	2.36	0.41
1:A:1076:C:H2'	1:A:1077:G:H8	1.83	0.41
1:A:1080:A:P	5:E:14:ARG:HH22	2.43	0.41
1:A:1151:A:O2'	1:A:1152:A:H8	2.02	0.41
1:A:1255:G:O2'	1:A:1258:G:H1'	2.21	0.41
1:A:1292:U:H2'	1:A:1293:G:H8	1.86	0.41
1:A:1307:U:H2'	1:A:1308:U:C6	2.55	0.41
1:A:1369:C:OP1	14:N:61:TRP:NE1	2.51	0.41
2:B:12:GLU:HG3	2:B:15:VAL:HB	2.02	0.41
4:D:98:GLU:HG3	4:D:103:ASN:ND2	2.36	0.41
6:F:69:GLU:H	6:F:69:GLU:HG3	1.57	0.41
6:F:89:MET:HE2	6:F:91:VAL:HB	2.02	0.41
7:G:69:VAL:O	7:G:71:PRO:HD3	2.21	0.41
7:G:149:ARG:HG2	7:G:152:ALA:HB2	2.03	0.41
11:K:121:PRO:HB2	11:K:125:PHE:HB2	2.02	0.41
17:Q:61:GLU:HA	17:Q:71:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:44:LEU:HD12	18:R:79:LEU:HD22	2.03	0.41
20:T:53:LEU:HD22	20:T:102:GLY:HA3	2.01	0.41
20:T:89:ARG:HD2	20:T:104:LEU:HD22	2.03	0.41
1:A:13:U:H3'	1:A:14:U:H6	1.86	0.41
1:A:324:G:N2	1:A:326:G:H3'	2.36	0.41
1:A:625:G:H2'	1:A:626:U:C6	2.56	0.41
1:A:896:C:H2'	1:A:897:C:O4'	2.21	0.41
1:A:919:A:N3	1:A:1080:A:C2	2.89	0.41
1:A:975:A:H5''	1:A:975:A:H8	1.85	0.41
1:A:1348:U:H2'	1:A:1349:A:H8	1.86	0.41
1:A:1492:A:H2'	22:W:19:ASN:HA	2.02	0.41
7:G:113:GLU:HG2	7:G:119:ARG:HG2	2.03	0.41
16:P:59:TRP:CA	16:P:62:VAL:HG22	2.50	0.41
25:Z:51:C:H42	25:Z:63:G:H1	1.68	0.41
1:A:44:G:OP2	16:P:12:LYS:HE3	2.20	0.40
1:A:527:G:N2	1:A:528:C:C2	2.89	0.40
1:A:942:G:C6	1:A:1342:C:N3	2.89	0.40
1:A:956:U:H2'	1:A:957:U:O4'	2.22	0.40
1:A:1050:G:N1	1:A:1051:C:C4	2.89	0.40
1:A:1314:C:N4	19:S:4:SER:HB2	2.35	0.40
1:A:1345:U:C4	1:A:1375:A:N6	2.60	0.40
1:A:1411:C:H4'	12:L:43:VAL:HG11	2.03	0.40
1:A:1423:G:C6	1:A:1424:C:C4	3.10	0.40
13:M:96:LEU:HD23	13:M:97:PRO:HD2	2.03	0.40
1:A:289:G:C6	1:A:290:C:C4	3.09	0.40
1:A:373:A:H2'	1:A:374:A:H8	1.86	0.40
1:A:552:U:H2'	1:A:553:A:H8	1.86	0.40
1:A:751:U:H2'	1:A:752:G:O4'	2.21	0.40
1:A:861:G:C6	1:A:862:C:C4	3.09	0.40
1:A:921:U:H2'	1:A:922:G:O4'	2.20	0.40
1:A:986:A:H2'	1:A:987:G:O4'	2.20	0.40
1:A:988:G:C2	1:A:989:C:C2	3.08	0.40
1:A:1060:C:P	14:N:45:ARG:HH22	2.44	0.40
1:A:1077:G:N1	1:A:1080:A:OP2	2.51	0.40
1:A:1312:G:N2	1:A:1326:C:C2	2.89	0.40
1:A:1371:G:H2'	1:A:1372:U:H6	1.85	0.40
1:A:1528:U:H1'	1:A:1530:G:H5'	2.03	0.40
7:G:106:GLN:O	7:G:110:GLN:HG2	2.21	0.40
9:I:89:ASN:C	9:I:91:ASP:H	2.29	0.40
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.20	0.40
12:L:60:LEU:HD21	12:L:66:VAL:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:C:H2'	1:A:175:C:C6	2.56	0.40
1:A:394:G:C6	1:A:395:C:C4	3.09	0.40
1:A:677:U:H3	1:A:713:G:H1	1.68	0.40
1:A:678:U:H2'	1:A:679:C:H6	1.82	0.40
1:A:731:G:C6	1:A:732:C:C4	3.10	0.40
1:A:1129:C:H1'	1:A:1132:C:H5	1.86	0.40
1:A:1409:C:H2'	1:A:1410:G:C8	2.55	0.40
1:A:1431:C:H42	1:A:1469:G:H1	1.69	0.40
1:A:1512:U:H2'	1:A:1513:A:C8	2.57	0.40
6:F:50:TYR:HE1	18:R:77:GLY:HA2	1.86	0.40
25:Z:2:G:C2	25:Z:3:C:C2	3.10	0.40
25:Z:31:G:H2'	25:Z:32:OMC:C6	2.55	0.40
1:A:105:G:C6	1:A:106:C:C4	3.09	0.40
1:A:671:G:H2'	1:A:672:U:O4'	2.21	0.40
1:A:1351:U:H2'	1:A:1352:C:H6	1.85	0.40
1:A:1361:G:C2	1:A:1362:C:O2	2.74	0.40
1:A:1440:C:N4	1:A:1461:G:H1	2.19	0.40
1:A:1461:G:H2'	1:A:1462:G:C8	2.56	0.40
3:C:39:ILE:O	3:C:43:LEU:HG	2.21	0.40
3:C:82:GLU:O	3:C:85:ARG:HB3	2.20	0.40
5:E:80:ILE:HD12	5:E:91:LEU:HB2	2.03	0.40
13:M:22:ILE:HG22	13:M:24:GLY:H	1.86	0.40
25:Z:18:G:C4	25:Z:57:A:C6	3.09	0.40
1:A:16:A:C2	1:A:17:U:C6	3.09	0.40
1:A:123:C:H5''	1:A:311:C:O2'	2.21	0.40
1:A:137:C:C2	1:A:227:G:C2	3.09	0.40
1:A:200:G:C6	1:A:201:C:N3	2.90	0.40
1:A:328:C:H4'	1:A:329:A:H5'	2.03	0.40
1:A:542:G:C2	1:A:543:C:C2	3.10	0.40
1:A:629:G:H2'	1:A:630:G:O4'	2.21	0.40
1:A:902:G:H2'	1:A:903:G:H8	1.86	0.40
1:A:968:A:C8	1:A:1062:U:H4'	2.56	0.40
4:D:25:ARG:C	4:D:27:TYR:N	2.80	0.40
7:G:96:GLN:HA	7:G:99:LEU:HD12	2.03	0.40
11:K:123:LYS:HA	11:K:126:ARG:HG3	2.03	0.40
13:M:45:VAL:HA	13:M:48:LEU:HD12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	195 (84%)	24 (10%)	13 (6%)	1	15
3	C	204/239 (85%)	177 (87%)	18 (9%)	9 (4%)	2	17
4	D	206/209 (99%)	191 (93%)	12 (6%)	3 (2%)	8	38
5	E	148/162 (91%)	140 (95%)	8 (5%)	0	100	100
6	F	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	G	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	9	41
8	H	136/138 (99%)	129 (95%)	6 (4%)	1 (1%)	18	55
9	I	125/128 (98%)	107 (86%)	15 (12%)	3 (2%)	4	27
10	J	96/105 (91%)	72 (75%)	16 (17%)	8 (8%)	0	9
11	K	117/129 (91%)	99 (85%)	13 (11%)	5 (4%)	2	17
12	L	122/132 (92%)	101 (83%)	17 (14%)	4 (3%)	3	21
13	M	119/126 (94%)	102 (86%)	16 (13%)	1 (1%)	16	53
14	N	58/61 (95%)	51 (88%)	5 (9%)	2 (3%)	3	21
15	O	86/89 (97%)	84 (98%)	1 (1%)	1 (1%)	10	43
16	P	81/88 (92%)	73 (90%)	7 (9%)	1 (1%)	10	43
17	Q	97/105 (92%)	88 (91%)	6 (6%)	3 (3%)	3	22
18	R	71/88 (81%)	66 (93%)	4 (6%)	1 (1%)	9	39
19	S	80/93 (86%)	66 (82%)	11 (14%)	3 (4%)	2	19
20	T	97/106 (92%)	80 (82%)	12 (12%)	5 (5%)	1	15
21	V	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
22	W	69/72 (96%)	58 (84%)	7 (10%)	4 (6%)	1	14
23	X	166/171 (97%)	150 (90%)	13 (8%)	3 (2%)	6	33
All	All	2584/2781 (93%)	2288 (88%)	224 (9%)	72 (3%)	6	24

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
2	B	24	TRP
9	I	119	ALA
11	K	101	SER
12	L	79	GLU
18	R	87	ARG
20	T	94	ALA
23	X	8	ASN
23	X	54	PRO
2	B	17	PHE
2	B	207	ALA
3	C	61	ALA
3	C	154	SER
3	C	179	ARG
7	G	7	ALA
9	I	56	LEU
10	J	55	LYS
16	P	81	ARG
19	S	30	LEU
20	T	13	LEU
20	T	49	ALA
2	B	20	GLU
2	B	99	GLY
2	B	204	ASN
2	B	228	GLY
3	C	14	ILE
10	J	30	SER
10	J	34	VAL
10	J	35	SER
10	J	90	LEU
11	K	126	ARG
12	L	27	LEU
14	N	31	ARG
15	O	88	ARG
17	Q	68	ARG
19	S	6	LYS
22	W	2	LYS
2	B	95	GLN
3	C	4	LYS
3	C	81	GLY
3	C	108	ASN
3	C	168	ALA
4	D	5	ILE

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Mol	Chain	Res	Type
4	D	172	PRO
9	I	58	HIS
14	N	23	ARG
17	Q	99	SER
19	S	71	LEU
20	T	97	ALA
22	W	44	TYR
2	B	229	VAL
10	J	39	PRO
10	J	54	PHE
11	K	12	ARG
11	K	13	GLN
12	L	45	PRO
17	Q	80	GLY
20	T	9	ASN
23	X	73	GLU
2	B	130	ARG
7	G	55	GLY
10	J	40	LEU
12	L	51	ALA
13	M	6	GLY
22	W	45	ILE
3	C	205	GLY
4	D	142	PRO
8	H	5	PRO
11	K	90	GLY
2	B	125	PRO
2	B	208	ILE
22	W	50	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
2	B	202/220 (92%)	164 (81%)	38 (19%)	1 9
3	C	160/188 (85%)	141 (88%)	19 (12%)	5 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	180/181 (99%)	149 (83%)	31 (17%)	2	11
5	E	115/123 (94%)	89 (77%)	26 (23%)	1	6
6	F	90/90 (100%)	72 (80%)	18 (20%)	1	8
7	G	126/127 (99%)	122 (97%)	4 (3%)	34	55
8	H	119/119 (100%)	97 (82%)	22 (18%)	1	10
9	I	98/99 (99%)	84 (86%)	14 (14%)	3	15
10	J	87/92 (95%)	73 (84%)	14 (16%)	2	12
11	K	90/99 (91%)	73 (81%)	17 (19%)	1	9
12	L	104/109 (95%)	87 (84%)	17 (16%)	2	12
13	M	97/101 (96%)	85 (88%)	12 (12%)	4	18
14	N	49/50 (98%)	43 (88%)	6 (12%)	5	18
15	O	79/80 (99%)	62 (78%)	17 (22%)	1	6
16	P	72/74 (97%)	57 (79%)	15 (21%)	1	7
17	Q	94/97 (97%)	78 (83%)	16 (17%)	2	11
18	R	64/77 (83%)	50 (78%)	14 (22%)	1	6
19	S	71/80 (89%)	56 (79%)	15 (21%)	1	6
20	T	76/82 (93%)	57 (75%)	19 (25%)	0	4
21	V	19/22 (86%)	18 (95%)	1 (5%)	20	42
22	W	62/63 (98%)	49 (79%)	13 (21%)	1	6
23	X	145/150 (97%)	125 (86%)	20 (14%)	3	15
All	All	2199/2323 (95%)	1831 (83%)	368 (17%)	4	12

All (368) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	11	LEU
2	B	21	ARG
2	B	23	ARG
2	B	25	ASN
2	B	41	ILE
2	B	42	ILE
2	B	44	LEU
2	B	48	MET
2	B	51	LEU
2	B	59	GLU

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Mol	Chain	Res	Type
2	B	61	LEU
2	B	67	THR
2	B	103	THR
2	B	107	THR
2	B	108	ILE
2	B	111	ARG
2	B	121	LEU
2	B	127	ILE
2	B	136	VAL
2	B	137	ARG
2	B	144	ARG
2	B	154	LEU
2	B	165	VAL
2	B	172	ILE
2	B	179	LYS
2	B	187	LEU
2	B	196	LEU
2	B	198	ASP
2	B	204	ASN
2	B	208	ILE
2	B	213	LEU
2	B	214	ILE
2	B	215	LEU
2	B	216	SER
2	B	223	ILE
2	B	224	GLN
2	B	238	LEU
2	B	240	GLN
3	C	3	ASN
3	C	5	ILE
3	C	14	ILE
3	C	17	ASP
3	C	26	LYS
3	C	30	ARG
3	C	79	ARG
3	C	88	ARG
3	C	90	GLU
3	C	91	LEU
3	C	94	LEU
3	C	99	VAL
3	C	105	GLU
3	C	167	TRP

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Mol	Chain	Res	Type
3	C	172	ARG
3	C	182	ILE
3	C	188	LEU
3	C	191	THR
3	C	204	LEU
4	D	3	ARG
4	D	5	ILE
4	D	34	GLU
4	D	35	ARG
4	D	42	GLN
4	D	58	LEU
4	D	59	ARG
4	D	64	LEU
4	D	76	ARG
4	D	80	GLU
4	D	81	GLU
4	D	83	SER
4	D	96	LEU
4	D	97	LEU
4	D	104	VAL
4	D	118	ARG
4	D	122	ARG
4	D	131	ARG
4	D	135	LEU
4	D	141	ARG
4	D	150	GLU
4	D	152	SER
4	D	157	LEU
4	D	159	ARG
4	D	162	LEU
4	D	176	LEU
4	D	186	LEU
4	D	187	ARG
4	D	190	ASP
4	D	192	GLU
4	D	194	LEU
5	E	12	LEU
5	E	13	ILE
5	E	24	ARG
5	E	32	VAL
5	E	33	VAL
5	E	41	VAL

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Mol	Chain	Res	Type
5	E	43	LEU
5	E	53	LEU
5	E	56	GLN
5	E	68	GLU
5	E	76	ILE
5	E	80	ILE
5	E	87	SER
5	E	91	LEU
5	E	98	THR
5	E	112	LEU
5	E	115	VAL
5	E	118	ILE
5	E	119	LEU
5	E	137	GLU
5	E	141	GLN
5	E	144	THR
5	E	147	ASP
5	E	148	VAL
5	E	150	ARG
5	E	152	ARG
6	F	2	ARG
6	F	10	LEU
6	F	18	GLN
6	F	19	LEU
6	F	21	LEU
6	F	28	ARG
6	F	36	ARG
6	F	45	LEU
6	F	46	ARG
6	F	47	ARG
6	F	54	LYS
6	F	65	VAL
6	F	69	GLU
6	F	73	ASN
6	F	75	LEU
6	F	78	GLU
6	F	89	MET
6	F	98	LEU
7	G	11	GLN
7	G	38	LEU
7	G	72	ARG
7	G	113	GLU

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Mol	Chain	Res	Type
8	H	11	THR
8	H	18	ARG
8	H	21	LYS
8	H	22	GLU
8	H	24	THR
8	H	36	LEU
8	H	38	ILE
8	H	39	LEU
8	H	45	ILE
8	H	52	ASP
8	H	54	ASP
8	H	59	LEU
8	H	63	LEU
8	H	69	ARG
8	H	85	ARG
8	H	99	GLU
8	H	105	ARG
8	H	109	ILE
8	H	112	LEU
8	H	115	SER
8	H	127	LEU
8	H	136	GLU
9	I	2	GLU
9	I	3	GLN
9	I	12	GLU
9	I	14	VAL
9	I	34	ASN
9	I	35	GLU
9	I	38	GLN
9	I	65	VAL
9	I	71	SER
9	I	79	LEU
9	I	102	LEU
9	I	111	ARG
9	I	112	LYS
9	I	118	LYS
10	J	4	ILE
10	J	49	VAL
10	J	60	ARG
10	J	71	LEU
10	J	72	VAL
10	J	75	ILE

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Mol	Chain	Res	Type
10	J	81	THR
10	J	82	ILE
10	J	86	MET
10	J	87	THR
10	J	89	ASP
10	J	92	THR
10	J	95	GLU
10	J	96	ILE
11	K	11	LYS
11	K	14	VAL
11	K	16	SER
11	K	18	ARG
11	K	41	THR
11	K	57	THR
11	K	62	GLN
11	K	80	VAL
11	K	84	VAL
11	K	91	ARG
11	K	93	GLN
11	K	96	ARG
11	K	98	LEU
11	K	108	ILE
11	K	120	ARG
11	K	126	ARG
11	K	129	SER
12	L	6	THR
12	L	13	LYS
12	L	15	ARG
12	L	33	ARG
12	L	36	VAL
12	L	37	CYS
12	L	39	VAL
12	L	41	ARG
12	L	42	THR
12	L	46	LYS
12	L	53	ARG
12	L	58	VAL
12	L	59	ARG
12	L	77	LEU
12	L	78	GLN
12	L	104	VAL
12	L	119	LYS

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Mol	Chain	Res	Type
13	M	12	ASN
13	M	16	ASP
13	M	31	LYS
13	M	32	GLU
13	M	35	GLU
13	M	44	ARG
13	M	56	LEU
13	M	80	ARG
13	M	81	LEU
13	M	84	ILE
13	M	96	LEU
13	M	117	VAL
14	N	16	PHE
14	N	17	LYS
14	N	22	THR
14	N	33	VAL
14	N	44	LEU
14	N	61	TRP
15	O	3	ILE
15	O	5	LYS
15	O	25	THR
15	O	31	LEU
15	O	35	ARG
15	O	37	ASN
15	O	39	LEU
15	O	41	GLU
15	O	43	LEU
15	O	52	SER
15	O	54	ARG
15	O	56	LEU
15	O	63	ARG
15	O	64	ARG
15	O	70	LEU
15	O	81	LEU
15	O	83	GLU
16	P	8	ARG
16	P	20	VAL
16	P	26	ARG
16	P	28	ARG
16	P	36	ILE
16	P	44	THR
16	P	53	VAL

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Mol	Chain	Res	Type
16	P	60	LEU
16	P	67	THR
16	P	68	ASP
16	P	69	THR
16	P	71	ARG
16	P	72	ARG
16	P	79	VAL
16	P	83	GLU
17	Q	5	VAL
17	Q	9	VAL
17	Q	23	VAL
17	Q	24	GLU
17	Q	26	GLN
17	Q	34	LYS
17	Q	38	ARG
17	Q	53	LEU
17	Q	57	VAL
17	Q	58	GLU
17	Q	70	ARG
17	Q	72	ARG
17	Q	91	ARG
17	Q	92	ARG
17	Q	98	LEU
17	Q	100	LYS
18	R	17	SER
18	R	18	ARG
18	R	21	LYS
18	R	23	LYS
18	R	25	THR
18	R	39	VAL
18	R	42	ARG
18	R	47	THR
18	R	53	ARG
18	R	74	ARG
18	R	75	ILE
18	R	81	PHE
18	R	82	THR
18	R	87	ARG
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	28	LYS

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Mol	Chain	Res	Type
19	S	29	ARG
19	S	30	LEU
19	S	37	ARG
19	S	39	THR
19	S	41	VAL
19	S	43	GLU
19	S	49	ILE
19	S	53	ASN
19	S	63	THR
19	S	66	MET
19	S	79	THR
20	T	8	ARG
20	T	10	LEU
20	T	13	LEU
20	T	17	ARG
20	T	19	SER
20	T	20	LEU
20	T	25	ARG
20	T	38	LYS
20	T	39	LYS
20	T	42	GLN
20	T	45	GLN
20	T	53	LEU
20	T	55	ILE
20	T	56	MET
20	T	64	ASP
20	T	68	LYS
20	T	73	HIS
20	T	74	LYS
20	T	84	LEU
21	V	3	LYS
22	W	2	LYS
22	W	6	THR
22	W	14	THR
22	W	21	THR
22	W	23	ARG
22	W	32	ILE
22	W	33	LEU
22	W	46	ARG
22	W	57	ILE
22	W	58	THR
22	W	63	THR

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Mol	Chain	Res	Type
22	W	68	VAL
22	W	71	LYS
23	X	7	THR
23	X	12	ARG
23	X	31	THR
23	X	35	LEU
23	X	64	LYS
23	X	67	TYR
23	X	85	VAL
23	X	87	SER
23	X	92	VAL
23	X	95	ASP
23	X	103	LEU
23	X	118	VAL
23	X	125	ARG
23	X	131	GLU
23	X	147	LEU
23	X	151	GLU
23	X	162	ASN
23	X	164	LEU
23	X	168	VAL
23	X	170	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	94	ASN
2	B	104	ASN
2	B	135	GLN
2	B	212	GLN
3	C	6	HIS
3	C	31	HIS
3	C	37	GLN
3	C	69	HIS
3	C	102	ASN
3	C	108	ASN
3	C	110	ASN
3	C	136	GLN
4	D	45	GLN
4	D	62	GLN
4	D	161	ASN

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Mol	Chain	Res	Type
5	E	20	GLN
6	F	27	GLN
6	F	100	ASN
7	G	28	ASN
7	G	37	ASN
7	G	51	GLN
7	G	109	ASN
9	I	23	ASN
9	I	38	GLN
9	I	87	GLN
10	J	76	ASN
10	J	78	ASN
10	J	84	GLN
11	K	26	ASN
11	K	27	ASN
11	K	38	ASN
11	K	62	GLN
11	K	104	GLN
11	K	117	ASN
12	L	76	ASN
12	L	78	GLN
13	M	92	HIS
15	O	37	ASN
16	P	76	GLN
17	Q	26	GLN
19	S	56	GLN
19	S	83	HIS
23	X	100	GLN
23	X	129	HIS
23	X	162	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	423 (28%)	103 (6%)
24	Y	15/42 (35%)	7 (46%)	0
25	Z	75/77 (97%)	35 (46%)	9 (12%)
All	All	1597/1641 (97%)	465 (29%)	112 (7%)

All (465) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	13	U
1	A	19	C
1	A	22	G
1	A	29	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	43	C
1	A	44	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	54	C
1	A	58	C
1	A	60	A
1	A	61	G
1	A	66	G
1	A	68	G
1	A	72	C
1	A	76	C
1	A	77	G
1	A	78	G
1	A	79	G
1	A	81	U
1	A	91	C
1	A	97	G
1	A	100	C
1	A	108	G
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	122	G
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	144	G
1	A	151	A

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Mol	Chain	Res	Type
1	A	157	G
1	A	163	C
1	A	181	G
1	A	182	U
1	A	189(E)	U
1	A	189(F)	U
1	A	189(G)	G
1	A	189(H)	G
1	A	195	A
1	A	197	A
1	A	198	G
1	A	199	G
1	A	201	C
1	A	203	U
1	A	217	C
1	A	220	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	253	U
1	A	266	G
1	A	267	C
1	A	280	C
1	A	281	G
1	A	282	A
1	A	283	C
1	A	288	A
1	A	289	G
1	A	291	C
1	A	298	A
1	A	301	G
1	A	306	G
1	A	313	A
1	A	315	A
1	A	316	G
1	A	325	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	342	C
1	A	344	A

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Mol	Chain	Res	Type
1	A	345	C
1	A	347	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	366	C
1	A	367	U
1	A	372	C
1	A	373	A
1	A	375	U
1	A	378	G
1	A	384	G
1	A	388	G
1	A	389	A
1	A	390	C
1	A	392	G
1	A	393	A
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	419	C
1	A	421	U
1	A	422	C
1	A	423	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	441	A
1	A	450	G
1	A	452	A
1	A	453	A
1	A	454	C
1	A	455	C
1	A	470	C
1	A	481	G

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Mol	Chain	Res	Type
1	A	484	G
1	A	485	G
1	A	495	A
1	A	496	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	521	G
1	A	524	G
1	A	527	G
1	A	528	C
1	A	529	G
1	A	531	U
1	A	532	A
1	A	534	U
1	A	535	A
1	A	540	G
1	A	543	C
1	A	545	C
1	A	547	A
1	A	550	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	574	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	596	C
1	A	607	A
1	A	619	U
1	A	641	U
1	A	642	A
1	A	653	A

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Mol	Chain	Res	Type
1	A	665	A
1	A	666	G
1	A	671	G
1	A	687	A
1	A	688	G
1	A	693	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	713	G
1	A	716	A
1	A	717	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	728	A
1	A	731	G
1	A	744	C
1	A	748	C
1	A	749	C
1	A	755	G
1	A	760	G
1	A	774	G
1	A	785	G
1	A	787	A
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	796	C
1	A	799	G
1	A	804	U
1	A	809	G
1	A	811	C
1	A	812	C
1	A	815	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	821	G
1	A	828	A
1	A	839	U

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Mol	Chain	Res	Type
1	A	841	U
1	A	853	G
1	A	855	G
1	A	864	A
1	A	865	A
1	A	870	U
1	A	871	U
1	A	873	A
1	A	876	G
1	A	882	C
1	A	885	G
1	A	900	A
1	A	902	G
1	A	919	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	928	G
1	A	931	C
1	A	932	C
1	A	933	G
1	A	934	C
1	A	935	A
1	A	938	A
1	A	945	G
1	A	951	G
1	A	955	U
1	A	956	U
1	A	957	U
1	A	958	A
1	A	959	A
1	A	961	U
1	A	965	A
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	985	C
1	A	986	A

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Mol	Chain	Res	Type
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	998	G
1	A	1000	U
1	A	1001	A
1	A	1002	G
1	A	1005	A
1	A	1014	A
1	A	1015	A
1	A	1016	A
1	A	1017	G
1	A	1023	G
1	A	1025	U
1	A	1026	G
1	A	1028	C
1	A	1029	C
1	A	1030	C
1	A	1031	G
1	A	1036	G
1	A	1045	C
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1054	C
1	A	1056	U
1	A	1060	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1067	A
1	A	1075	C
1	A	1076	C
1	A	1078	U
1	A	1079	G
1	A	1085	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A

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Mol	Chain	Res	Type
1	A	1104	G
1	A	1117	G
1	A	1124	G
1	A	1125	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1134	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1171	G
1	A	1183	A
1	A	1184	G
1	A	1187	G
1	A	1190	G
1	A	1191	A
1	A	1195	C
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1210	C
1	A	1212	U
1	A	1213	A
1	A	1215	G
1	A	1222	G
1	A	1223	C
1	A	1224	G
1	A	1225	A

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Mol	Chain	Res	Type
1	A	1226	C
1	A	1227	A
1	A	1236	A
1	A	1238	A
1	A	1250	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1290	G
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1312	G
1	A	1315	U
1	A	1317	C
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1328	C
1	A	1336	C
1	A	1346	A
1	A	1347	G
1	A	1353	G
1	A	1357	A
1	A	1363	C
1	A	1363(A)	A

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Mol	Chain	Res	Type
1	A	1364	U
1	A	1367	C
1	A	1370	G
1	A	1379	G
1	A	1380	U
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1412	C
1	A	1419	G
1	A	1423	G
1	A	1440	C
1	A	1442	G
1	A	1443	G
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1457	G
1	A	1488	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1520	G
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U
1	A	1533	C
1	A	1534	A
1	A	1535	C
1	A	1536	C
1	A	1537	U
1	A	1539	C

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Mol	Chain	Res	Type
1	A	1540	U
1	A	1541	U
24	Y	28	A
24	Y	30	G
24	Y	31	U
24	Y	32	A
24	Y	37	U
24	Y	38	G
24	Y	39	U
25	Z	3	C
25	Z	6	G
25	Z	7	G
25	Z	8	4SU
25	Z	9	G
25	Z	13	C
25	Z	16	C
25	Z	17	C
25	Z	17(A)	U
25	Z	18	G
25	Z	19	G
25	Z	20	U
25	Z	26	G
25	Z	34	C
25	Z	36	U
25	Z	37	A
25	Z	40	C
25	Z	42	G
25	Z	43	A
25	Z	47	U
25	Z	48	C
25	Z	50	U
25	Z	51	C
25	Z	53	G
25	Z	55	PSU
25	Z	56	C
25	Z	59	A
25	Z	66	C
25	Z	67	C
25	Z	68	C
25	Z	69	C
25	Z	70	G
25	Z	71	C

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Mol	Chain	Res	Type
25	Z	72	A
25	Z	76	A

All (112) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	31	G
1	A	48	C
1	A	49	U
1	A	51	A
1	A	60	A
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	189(F)	U
1	A	197	A
1	A	202	U
1	A	243	A
1	A	250	A
1	A	266	G
1	A	279	A
1	A	281	G
1	A	305	G
1	A	315	A
1	A	328	C
1	A	329	A
1	A	344	A
1	A	351	G
1	A	372	C
1	A	389	A
1	A	428	G
1	A	429	U
1	A	484	G
1	A	495	A
1	A	496	A
1	A	508	C
1	A	509	A
1	A	518	C
1	A	531	U

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Mol	Chain	Res	Type
1	A	535	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	575	G
1	A	576	G
1	A	595	G
1	A	641	U
1	A	687	A
1	A	701	C
1	A	703	G
1	A	717	C
1	A	748	C
1	A	792	A
1	A	864	A
1	A	872	A
1	A	884	U
1	A	931	C
1	A	933	G
1	A	934	C
1	A	956	U
1	A	958	A
1	A	960	U
1	A	965	A
1	A	968	A
1	A	975	A
1	A	992	U
1	A	993	G
1	A	1000	U
1	A	1065	U
1	A	1078	U
1	A	1101	A
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1212	U
1	A	1214	C
1	A	1222	G
1	A	1224	G

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Mol	Chain	Res	Type
1	A	1225	A
1	A	1226	C
1	A	1239	A
1	A	1257	U
1	A	1278	U
1	A	1279	A
1	A	1285	A
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1318	A
1	A	1331	G
1	A	1346	A
1	A	1363(A)	A
1	A	1380	U
1	A	1415	G
1	A	1442(B)	A
1	A	1447	A
1	A	1493	A
1	A	1498	U
1	A	1504	G
1	A	1531	A
1	A	1533	C
1	A	1534	A
1	A	1536	C
25	Z	17	C
25	Z	36	U
25	Z	47	U
25	Z	50	U
25	Z	51	C
25	Z	55	PSU
25	Z	58	A
25	Z	60	U
25	Z	71	C

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	G7M	Z	46	25	23,26,27	2.47	4 (17%)	34,39,42	2.99	12 (35%)
25	4SU	Z	8	25	18,21,22	1.85	5 (27%)	25,30,33	2.01	6 (24%)
25	5MU	Z	54	25	19,22,23	1.58	3 (15%)	27,32,35	2.01	7 (25%)
25	OMC	Z	32	25	19,22,23	0.94	1 (5%)	25,31,34	1.32	3 (12%)
25	PSU	Z	55	25	18,21,22	1.54	1 (5%)	21,30,33	2.07	5 (23%)

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
25	G7M	Z	46	25	-	0/7/25/26	0/3/3/3
25	4SU	Z	8	25	-	0/7/25/26	0/2/2/2
25	5MU	Z	54	25	-	0/7/25/26	0/2/2/2
25	OMC	Z	32	25	-	0/9/27/28	0/2/2/2
25	PSU	Z	55	25	-	2/7/25/26	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	46	G7M	C8-N7	7.91	1.46	1.33
25	Z	55	PSU	C6-C5	5.17	1.41	1.35
25	Z	8	4SU	C4-S4	-4.89	1.60	1.68
25	Z	46	G7M	C8-N9	4.59	1.48	1.35
25	Z	46	G7M	C5-N7	-4.36	1.34	1.39
25	Z	54	5MU	C6-C5	4.33	1.41	1.34
25	Z	46	G7M	C5-C4	4.23	1.48	1.38
25	Z	8	4SU	C4-N3	-3.34	1.34	1.37
25	Z	54	5MU	C4-C5	3.12	1.49	1.44
25	Z	8	4SU	C2-N1	2.91	1.43	1.38
25	Z	54	5MU	C4-N3	-2.49	1.34	1.38
25	Z	8	4SU	C6-C5	2.27	1.40	1.35
25	Z	32	OMC	C6-C5	2.15	1.40	1.35
25	Z	8	4SU	C5-C4	-2.07	1.40	1.42

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	46	G7M	CN7-N7-C8	-7.82	112.94	124.79
25	Z	46	G7M	N9-C8-N7	-6.26	97.28	112.48
25	Z	46	G7M	N9-C4-N3	6.09	138.13	125.95
25	Z	54	5MU	N3-C2-N1	5.98	122.67	114.89
25	Z	55	PSU	N1-C2-N3	5.89	121.38	115.17
25	Z	46	G7M	C8-N7-C5	5.89	115.14	107.78
25	Z	46	G7M	C5-C4-N3	-5.41	117.94	128.15
25	Z	8	4SU	C4-N3-C2	-5.11	122.42	127.31
25	Z	8	4SU	C5-C4-N3	4.85	119.27	114.75
25	Z	46	G7M	C2-N3-C4	4.79	120.55	112.30
25	Z	8	4SU	N3-C2-N1	4.15	120.30	114.89
25	Z	46	G7M	CN7-N7-C5	4.11	131.92	126.80
25	Z	55	PSU	O2-C2-N1	-3.99	118.68	122.79
25	Z	46	G7M	C8-N9-C4	3.76	116.39	107.09
25	Z	54	5MU	O2-C2-N1	-3.74	117.93	122.80
25	Z	54	5MU	C4-N3-C2	-3.62	122.60	127.34
25	Z	32	OMC	O2-C2-N3	-3.27	117.17	122.33
25	Z	54	5MU	C6-N1-C2	-3.24	118.08	121.30
25	Z	55	PSU	C6-C5-C4	-3.23	115.99	118.17
25	Z	46	G7M	O6-C6-C5	-3.21	120.83	128.01
25	Z	55	PSU	C4-N3-C2	-3.20	121.96	126.37
25	Z	46	G7M	C1'-N9-C8	-2.75	117.47	126.74
25	Z	8	4SU	C6-N1-C2	-2.70	117.70	121.00
25	Z	54	5MU	C1'-N1-C6	2.61	125.45	121.15
25	Z	8	4SU	C5-C4-S4	-2.46	121.49	124.31
25	Z	32	OMC	O4'-C1'-N1	2.41	113.83	108.36
25	Z	46	G7M	C5-C6-N1	2.26	116.52	111.84
25	Z	54	5MU	C5-C4-N3	2.26	117.29	115.32
25	Z	8	4SU	O2-C2-N3	-2.12	117.58	121.49
25	Z	46	G7M	C2'-C1'-N9	2.10	119.10	113.25
25	Z	55	PSU	O2'-C2'-C1'	-2.09	106.26	111.21
25	Z	32	OMC	O3'-C3'-C2'	2.06	116.96	111.19
25	Z	54	5MU	O4-C4-C5	-2.02	122.61	124.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	Z	55	PSU	C4'-C5'-O5'-P
25	Z	55	PSU	O4'-C1'-C5-C4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	32	OMC	2	0
25	Z	55	PSU	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	7
25	Z	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	841:U	O3'	848:C	P	5.77
1	A	84:U	O3'	88:A	P	5.45
1	A	93:G	O3'	96:U	P	5.02
1	A	204:U	O3'	216:G	P	3.93
1	A	1442(A):G	O3'	1442(B):A	P	3.82
1	Z	21:A	O3'	22:G	P	3.81

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1389:C	O3'	1390:U	P	3.33
1	Z	14:A	O3'	15:G	P	3.31
1	A	927:G	O3'	928:G	P	3.06

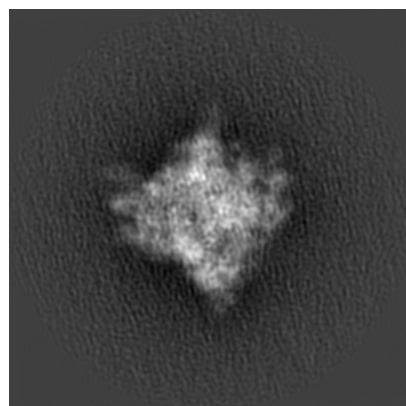
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4077. These allow visual inspection of the internal detail of the map and identification of artifacts.

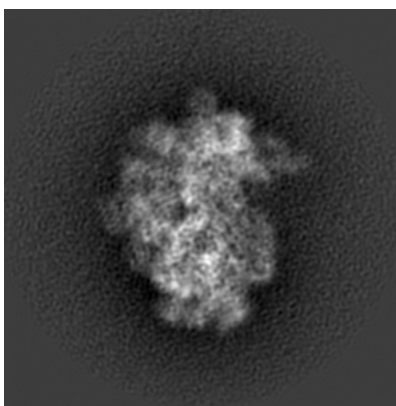
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

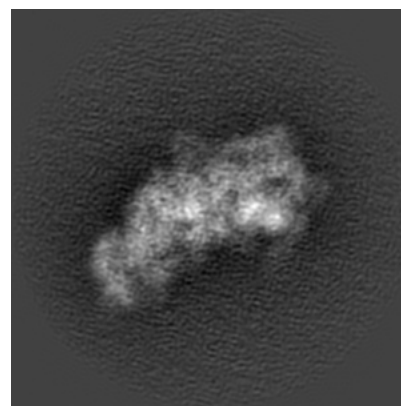
6.1.1 Primary map



X

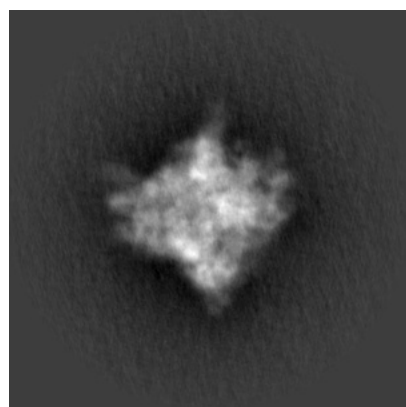


Y

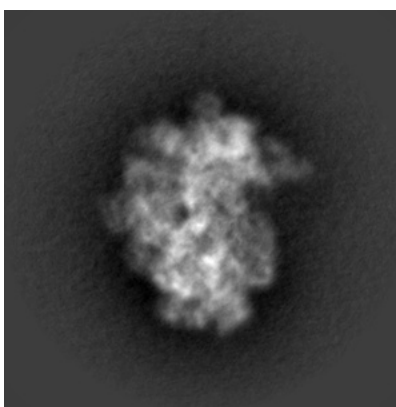


Z

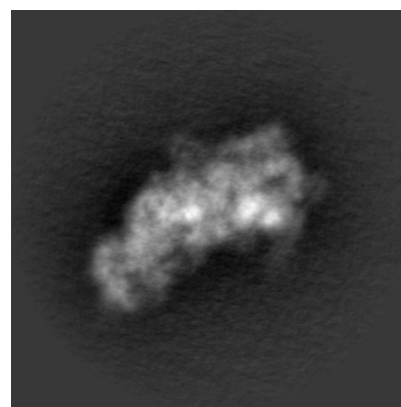
6.1.2 Raw map



X



Y

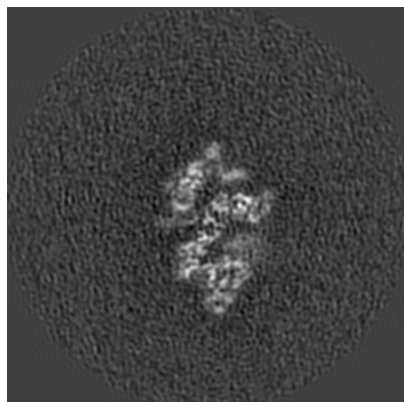


Z

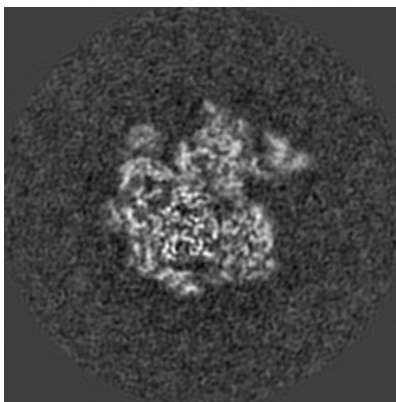
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

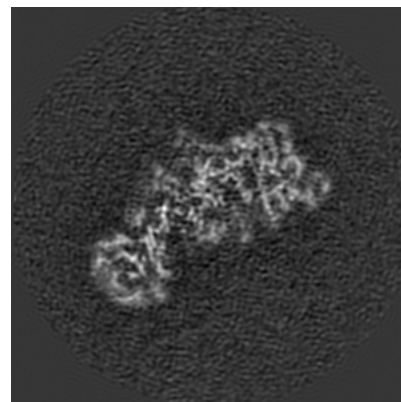
6.2.1 Primary map



X Index: 130

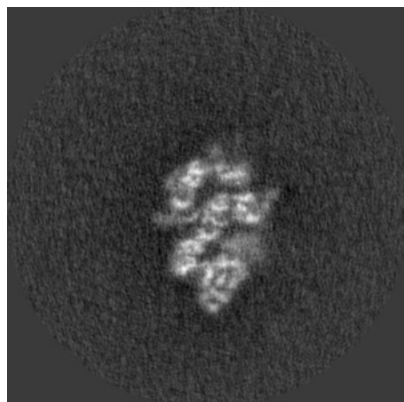


Y Index: 130

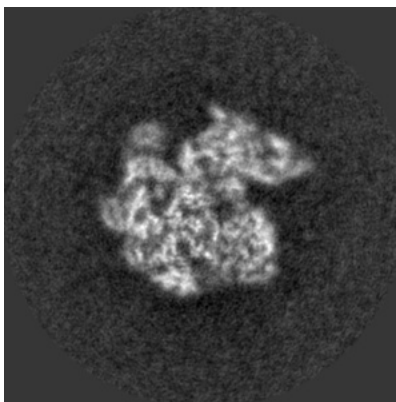


Z Index: 130

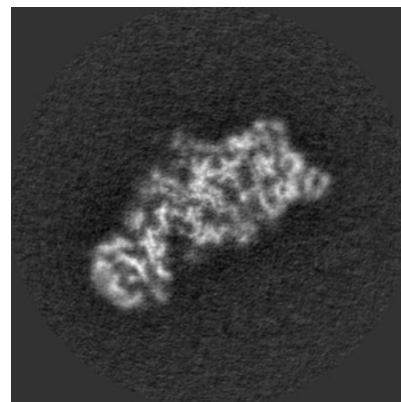
6.2.2 Raw map



X Index: 130



Y Index: 130

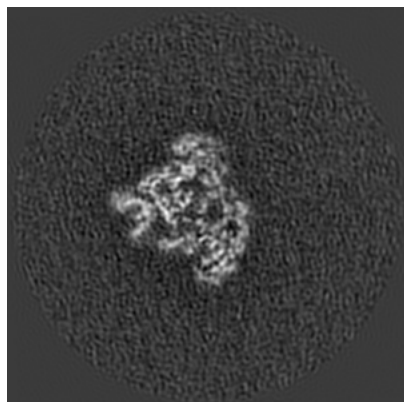


Z Index: 130

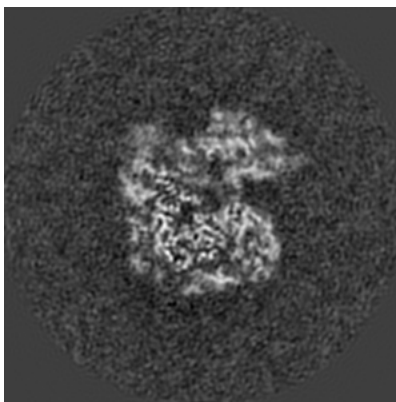
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

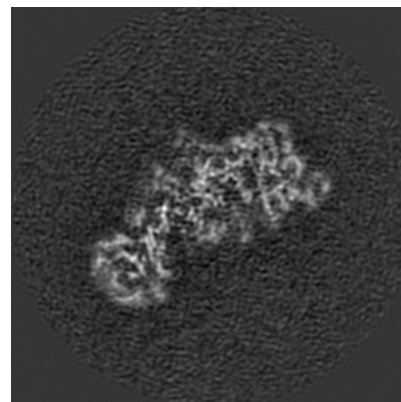
6.3.1 Primary map



X Index: 95

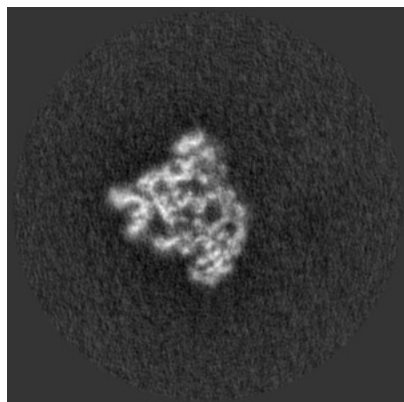


Y Index: 125

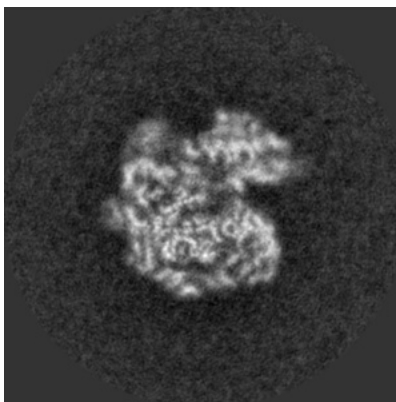


Z Index: 130

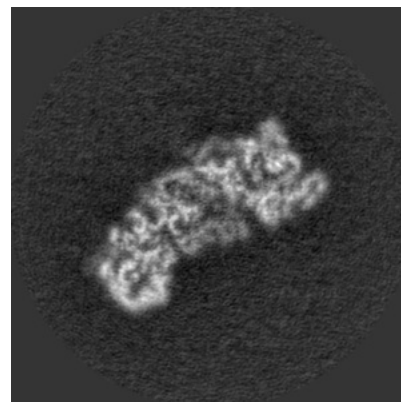
6.3.2 Raw map



X Index: 95



Y Index: 127

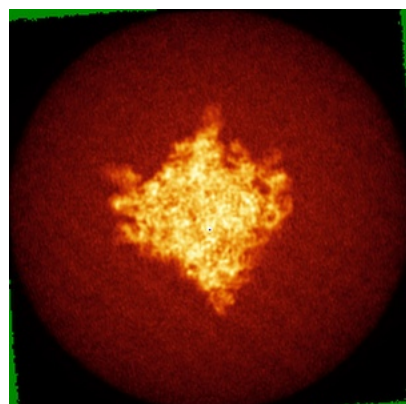


Z Index: 136

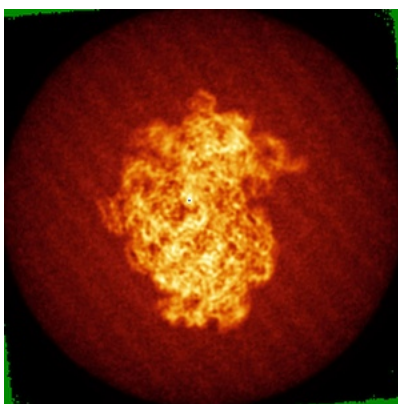
The images above show the largest variance slices of the map in three orthogonal directions.

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

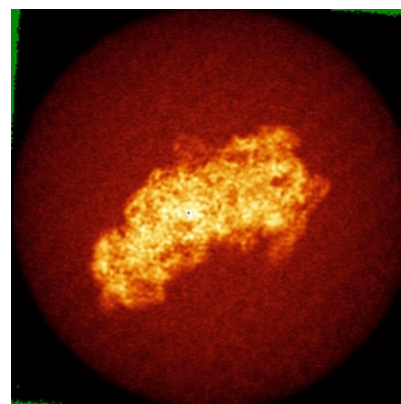
6.4.1 Primary map



X

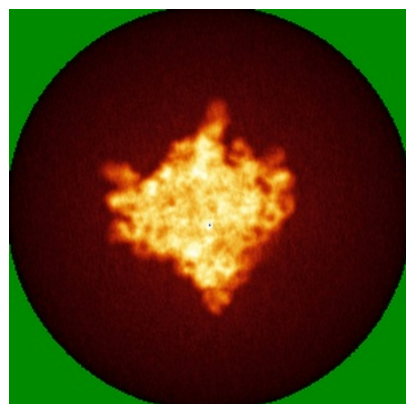


Y

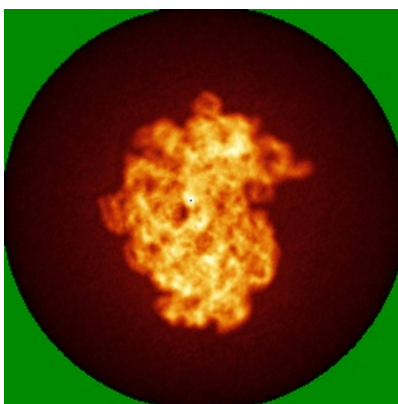


Z

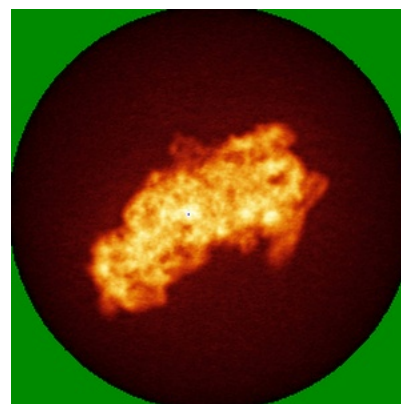
6.4.2 Raw map



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.

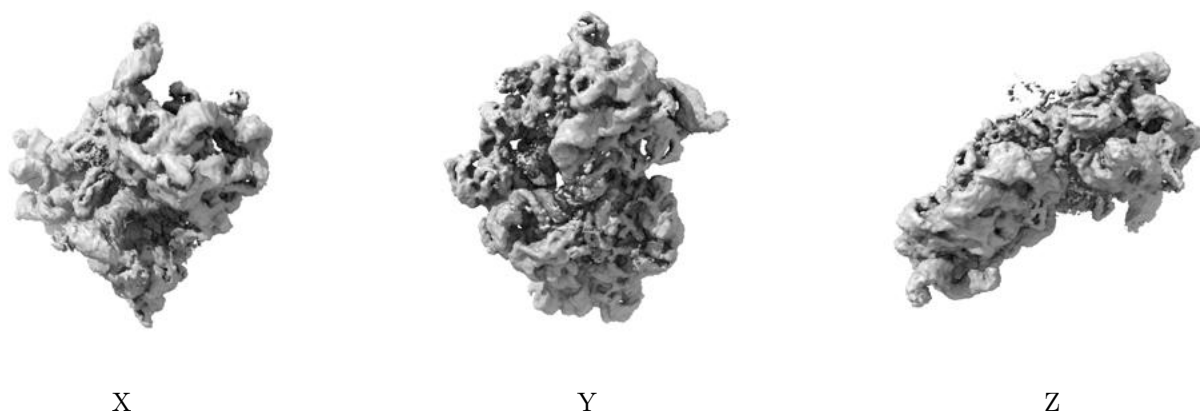
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. 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.

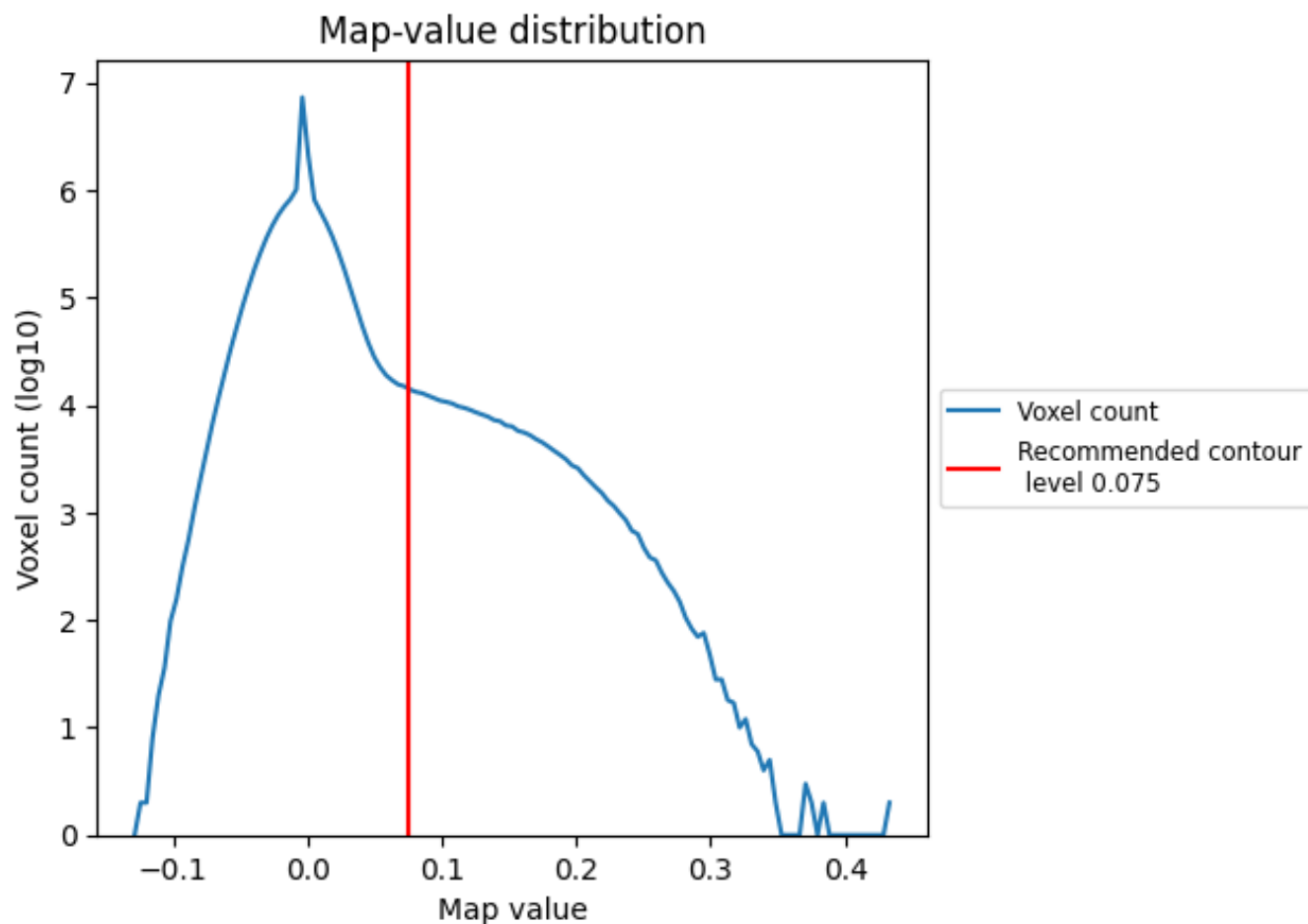
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

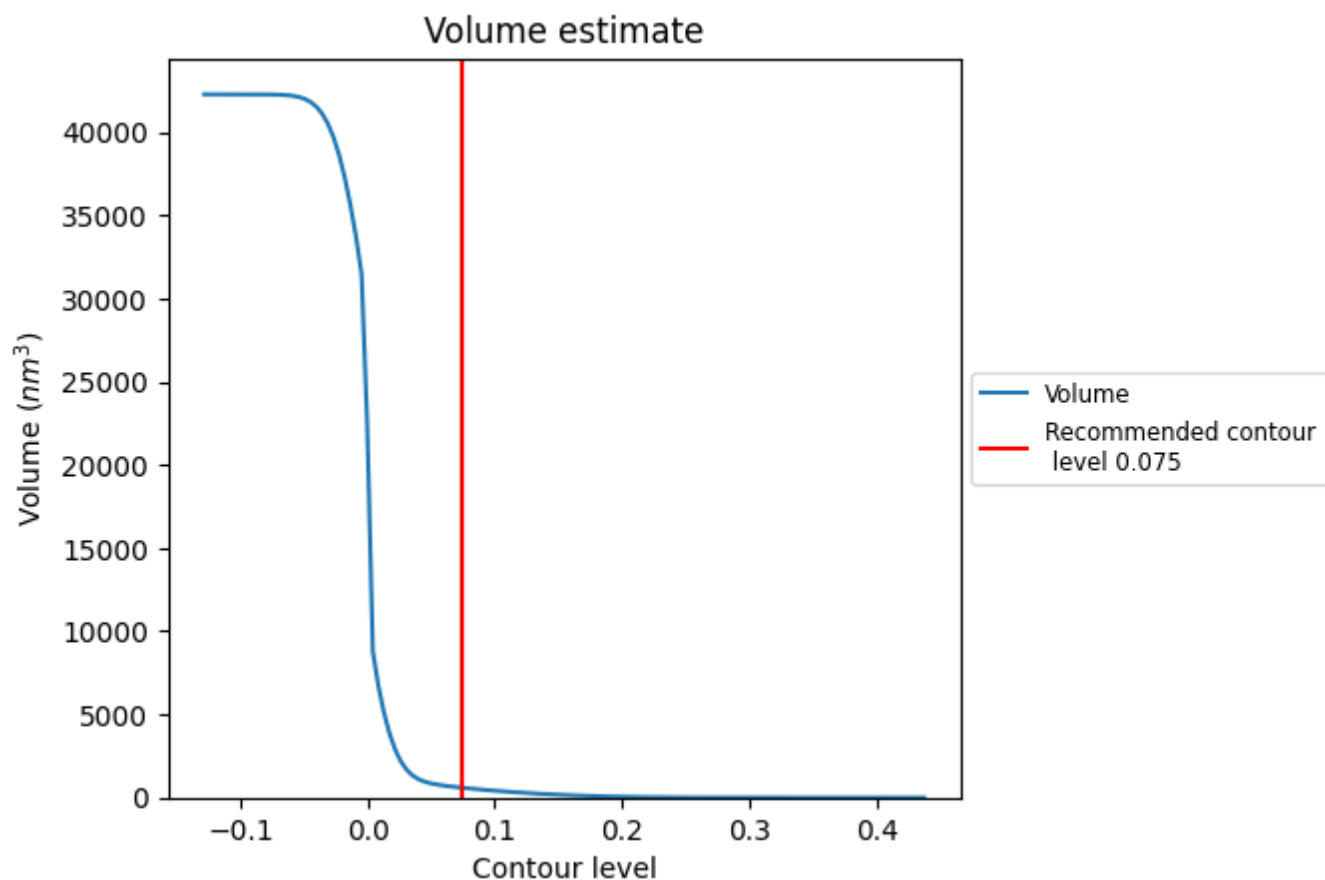
This section contains the results of statistical analysis of the map.

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.

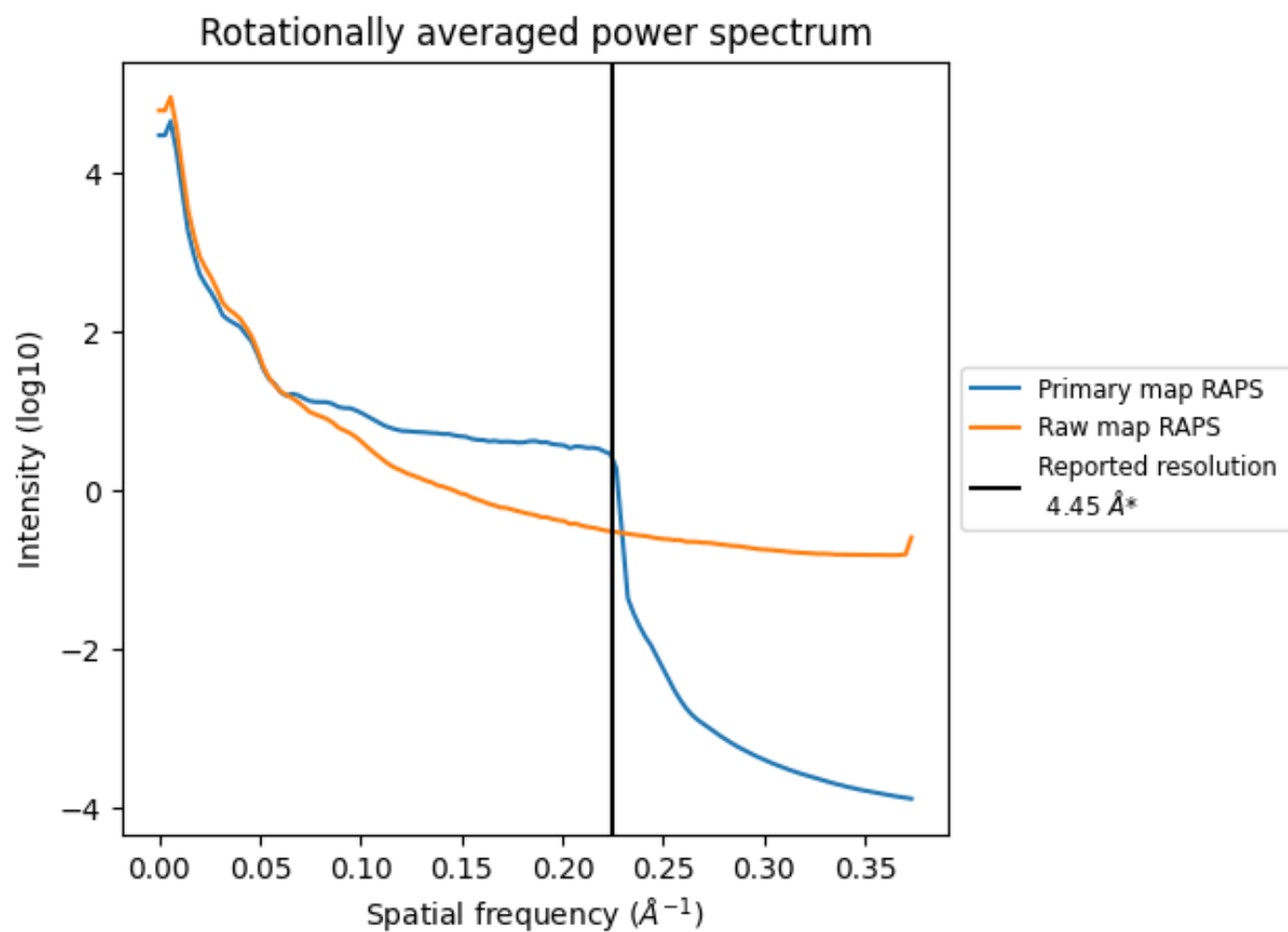
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 583 nm³; this corresponds to an approximate mass of 527 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 ⓘ

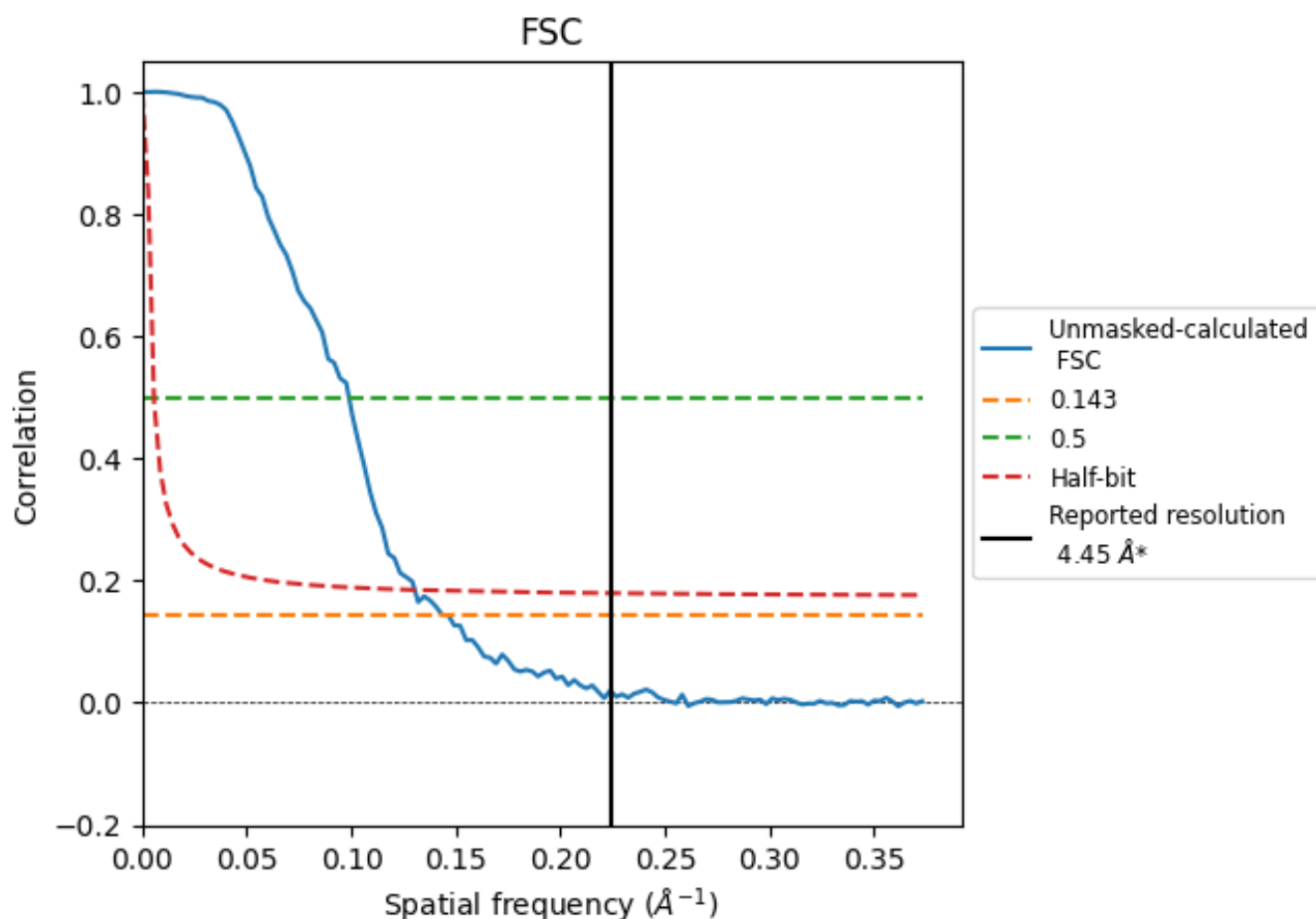


*Reported resolution corresponds to spatial frequency of 0.225 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.225 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

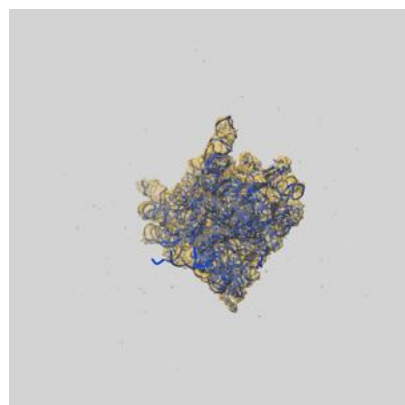
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.45	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.84	10.11	7.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.84 differs from the reported value 4.45 by more than 10 %

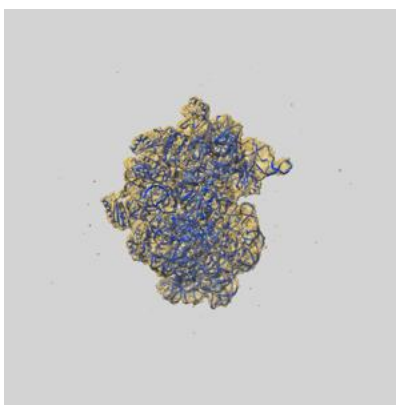
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4077 and PDB model 5LMR. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

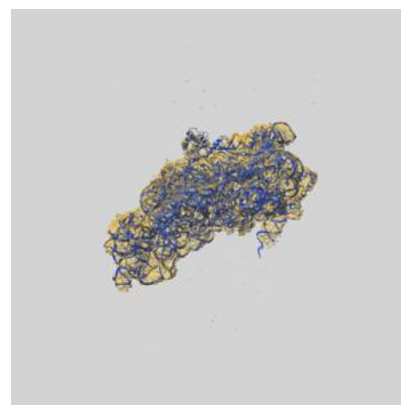
9.1 Map-model overlay [i](#)



X



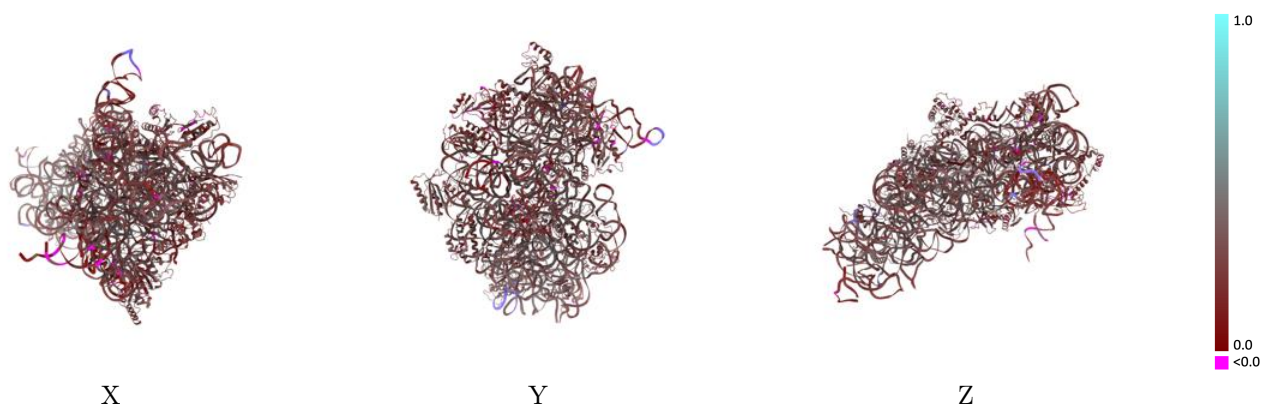
Y



Z

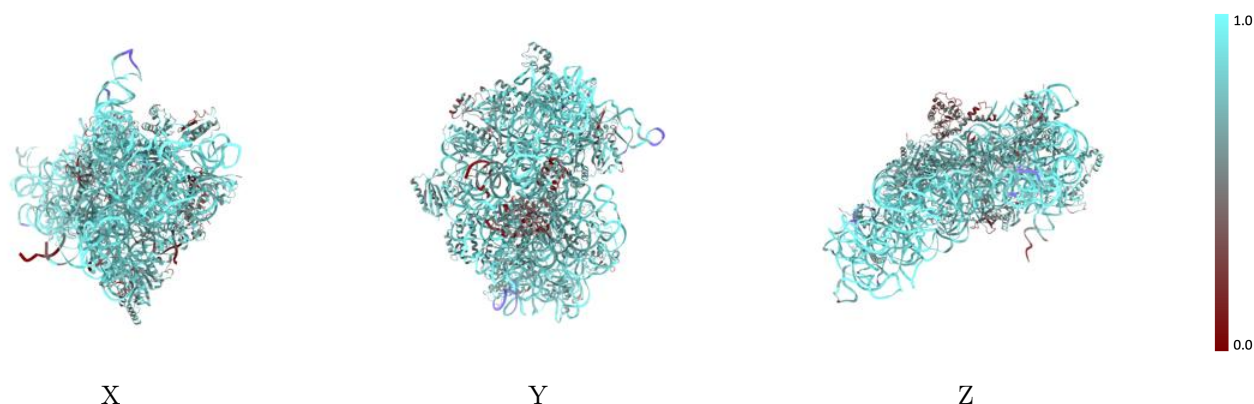
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



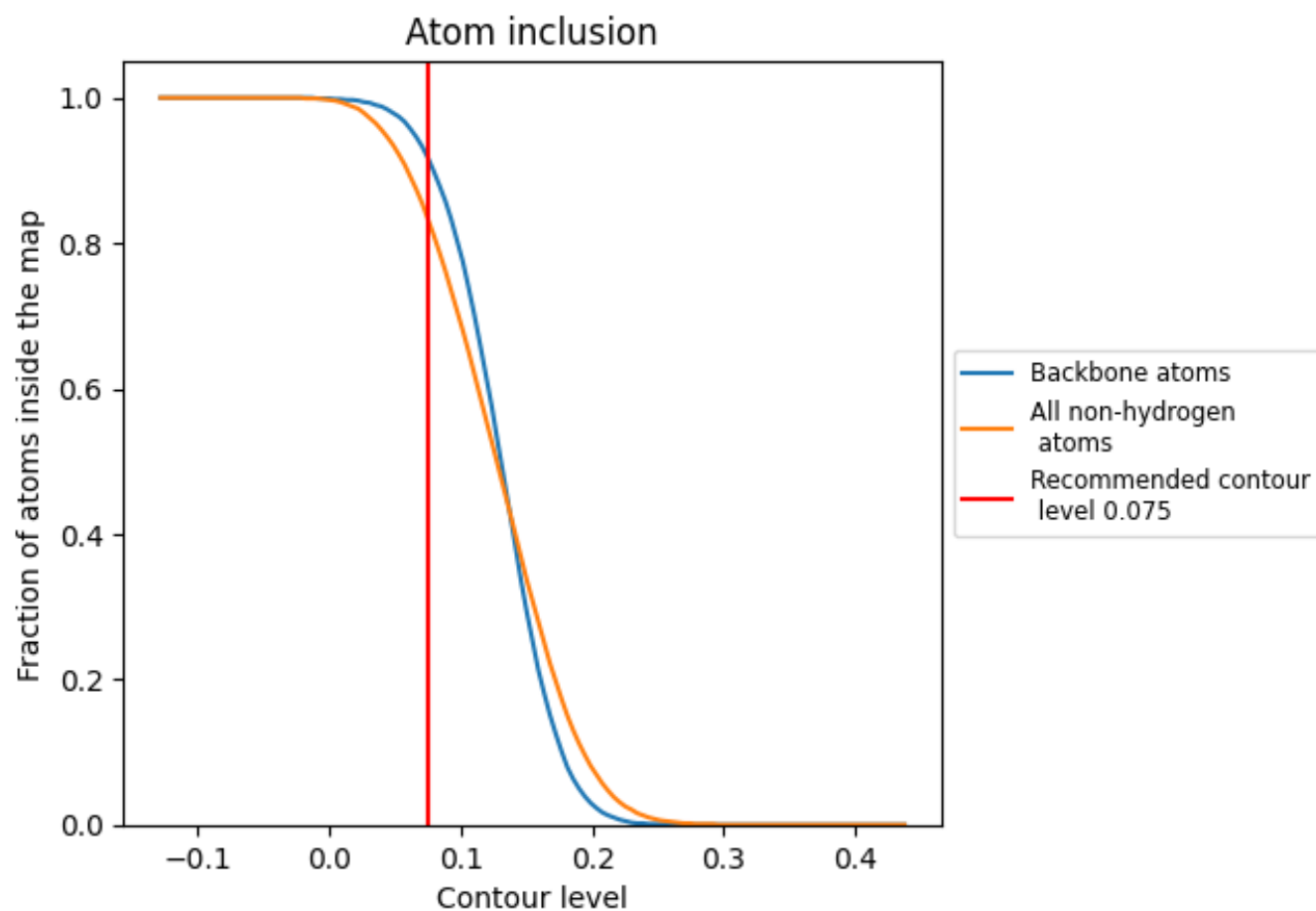
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 83% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8330	 0.2940
A	 0.9430	 0.3120
B	 0.3130	 0.2260
C	 0.7170	 0.2930
D	 0.7150	 0.2800
E	 0.7230	 0.3300
F	 0.7210	 0.2950
G	 0.6980	 0.2660
H	 0.7320	 0.3230
I	 0.7440	 0.2770
J	 0.6070	 0.2560
K	 0.7540	 0.2800
L	 0.7290	 0.3350
M	 0.7100	 0.2440
N	 0.7240	 0.3030
O	 0.7350	 0.2900
P	 0.7650	 0.3080
Q	 0.7330	 0.3140
R	 0.7130	 0.2900
S	 0.7180	 0.1960
T	 0.7130	 0.2700
V	 0.7440	 0.2620
W	 0.4100	 0.2570
X	 0.6090	 0.2370
Y	 0.5150	 0.1950
Z	 0.7830	 0.1610

