



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:32 am GMT

PDB ID : 5LMO
EMDB ID : EMD-4074
Title : Structure of bacterial 30S-IF1-IF3-mRNA translation pre-initiation complex (state-1B)
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on : 2016-08-01
Resolution : 4.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

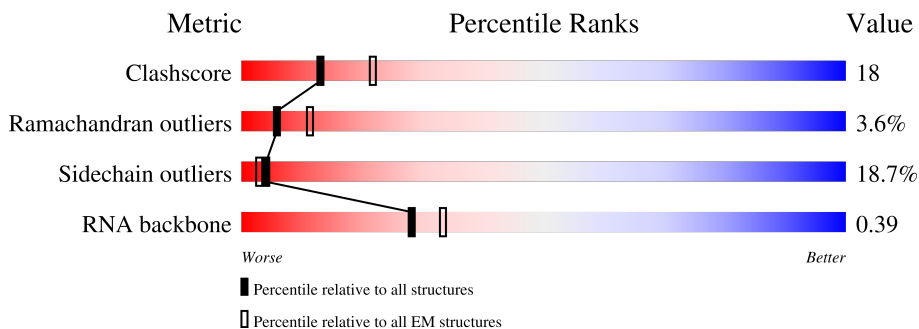
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	

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Mol	Chain	Length	Quality of chain
8	H	138	60% 33% 7%
9	I	128	65% 30% 5% .
10	J	105	52% 34% 7% 7% 10%
11	K	129	53% 33% 6% 8%
12	L	132	60% 27% 8% 6%
13	M	126	67% 24% . 7%
14	N	61	54% 36% 8% .
15	O	89	48% 44% 7% .
16	P	88	55% 35% 5% 6%
17	Q	105	69% 21% 5% 6%
18	R	88	39% 41% . 17%
19	S	93	54% 29% . 14%
20	T	106	56% 33% 5% 7%
21	V	27	74% 15% 11%
22	W	72	68% 25% 6% . 49%
23	X	171	70% 26% . . 23%
24	Y	39	15% 15% . 67%

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
28	ZN	D	300	-	-	X	-

2 Entry composition i

There are 29 unique types of molecules in this entry. The entry contains 54110 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
			Total	C	N	O	P		
1	A	1514	32525	14481	6019	10514	1511	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	117	933	577	192	162	2	0	0

- 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	80	Total	C	N	O	S	0	0
			647	414	119	112	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		

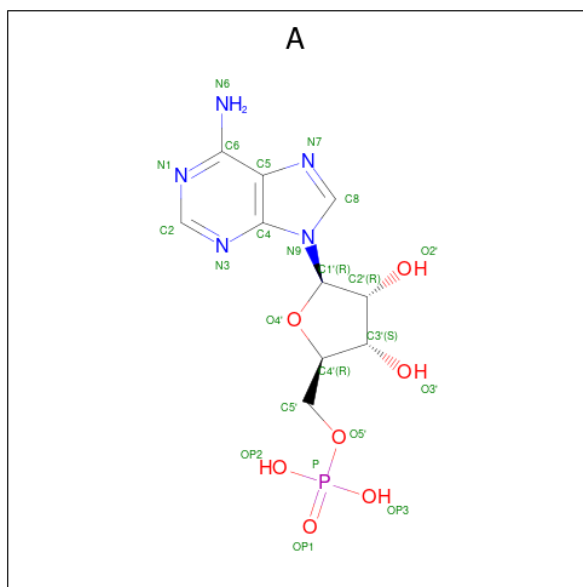
- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	13	Total	C	N	O	P	0	0
			288	128	60	87	13		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

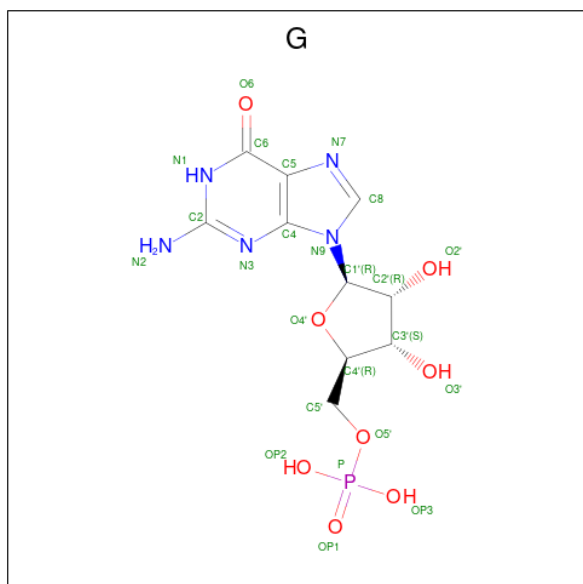
Mol	Chain	Residues	Atoms		AltConf
25	A	107	Total	Mg	0
			107	107	
25	W	1	Total	Mg	0
			1	1	

- Molecule 26 is ADENOSINE-5'-MONOPHOSPHATE (three-letter code: A) (formula: C₁₀H₁₄N₅O₇P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
26	A	1	Total	C	N	O	P	0
			44	20	10	12	2	
26	A	1	Total	C	N	O	P	0
			44	20	10	12	2	
26	X	1	Total	C	N	O	P	0
			22	10	5	6	1	

- Molecule 27 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: G) (formula: $C_{10}H_{14}N_5O_8P$).

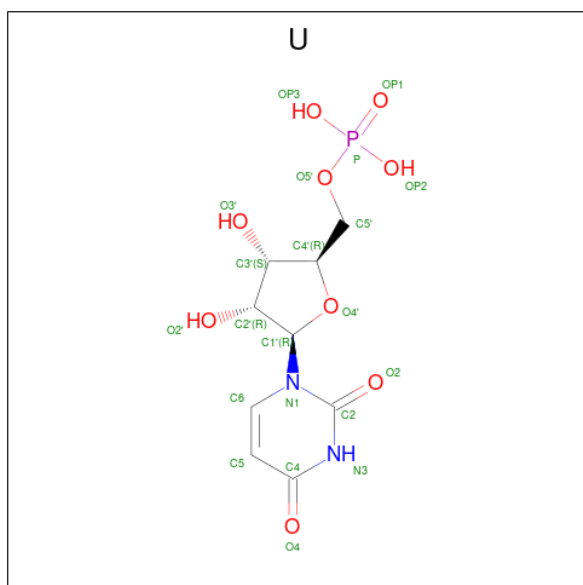


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
27	A	1	23	10	5	7	1	0

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 29 is URIDINE-5'-MONOPHOSPHATE (three-letter code: U) (formula: C₉H₁₃N₂O₉P).

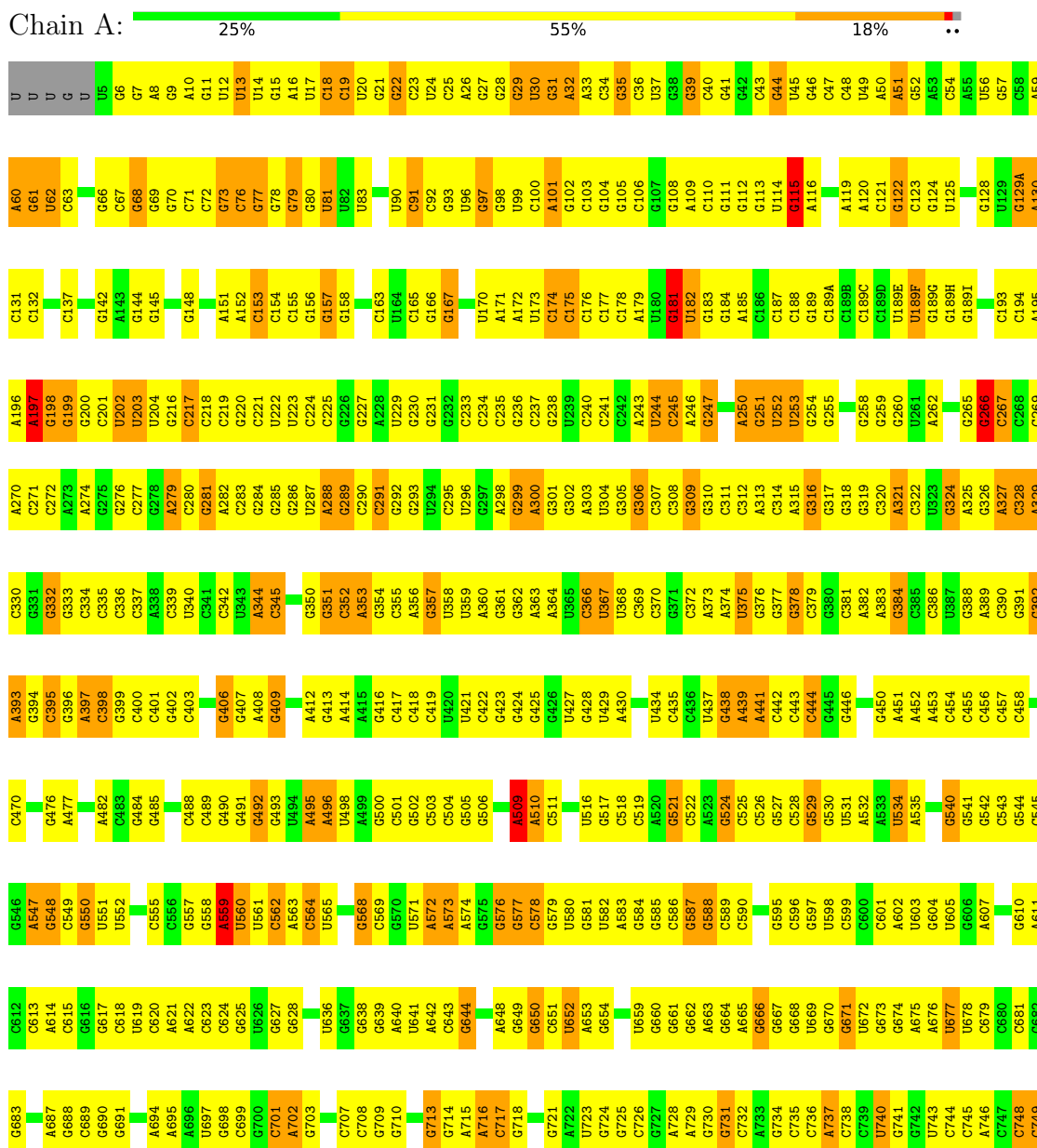


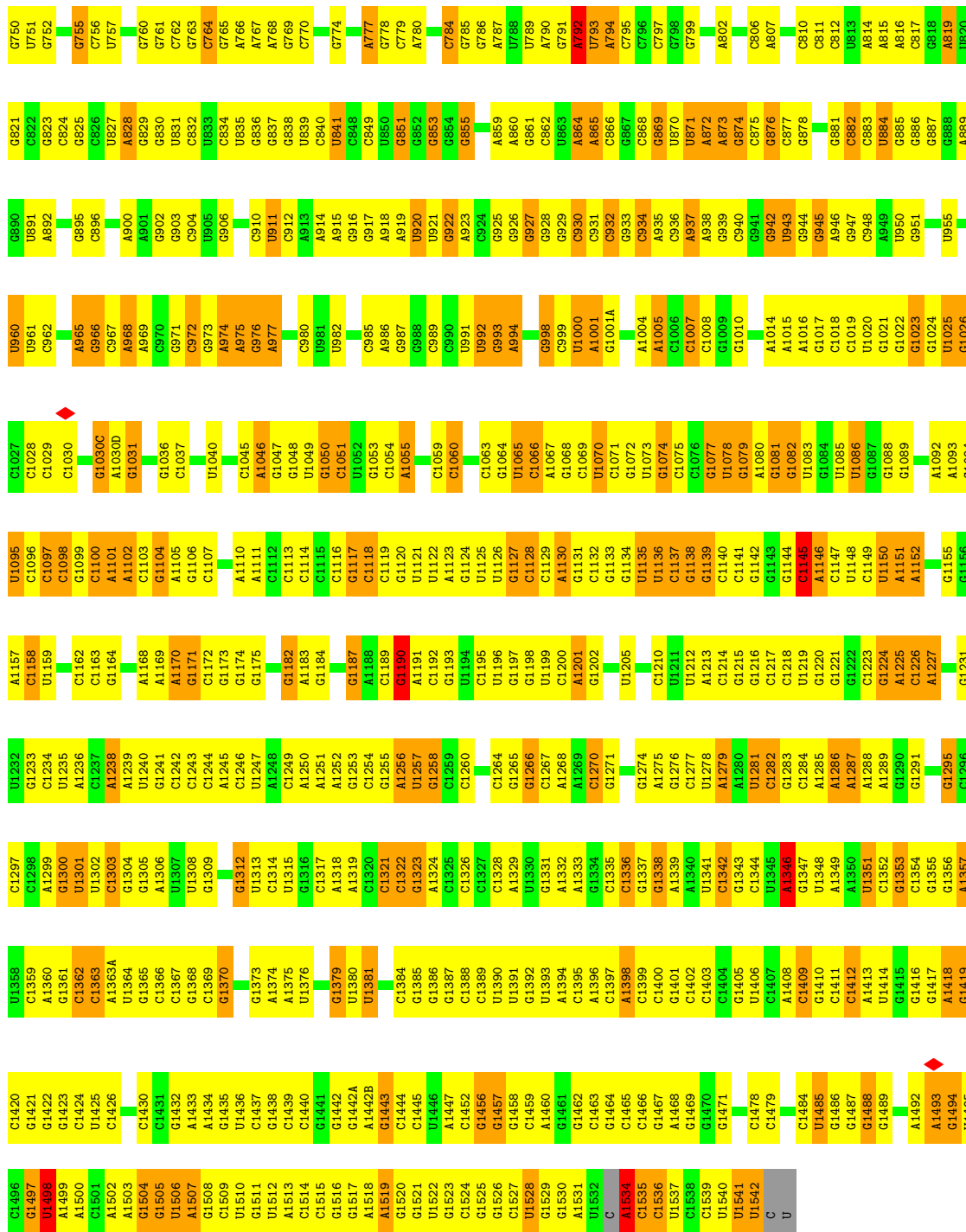
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
29	W	1	20	9	2	8	1	0
29	X	1	20	9	2	8	1	0

3 Residue-property plots

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

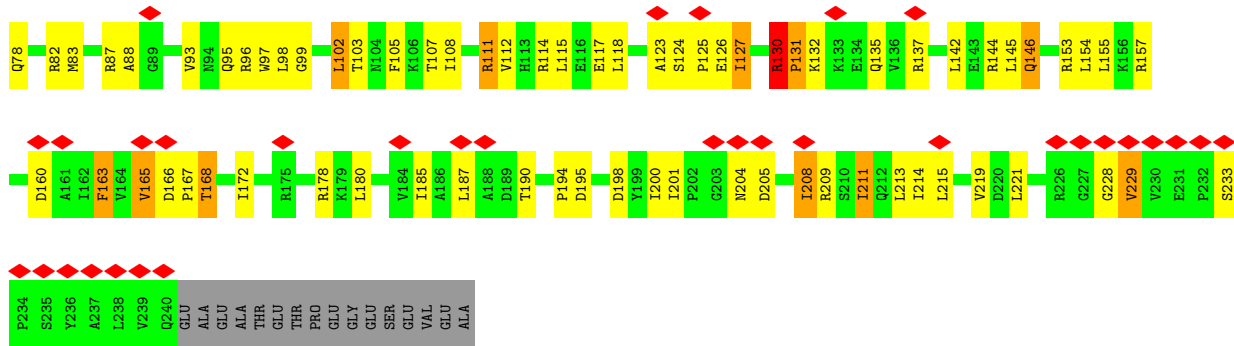
• Molecule 1: 16S rRNA



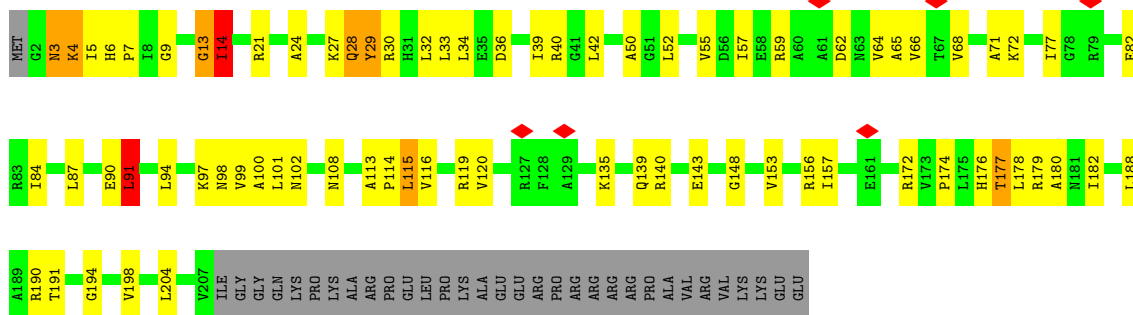


• Molecule 2: 30S ribosomal protein S2

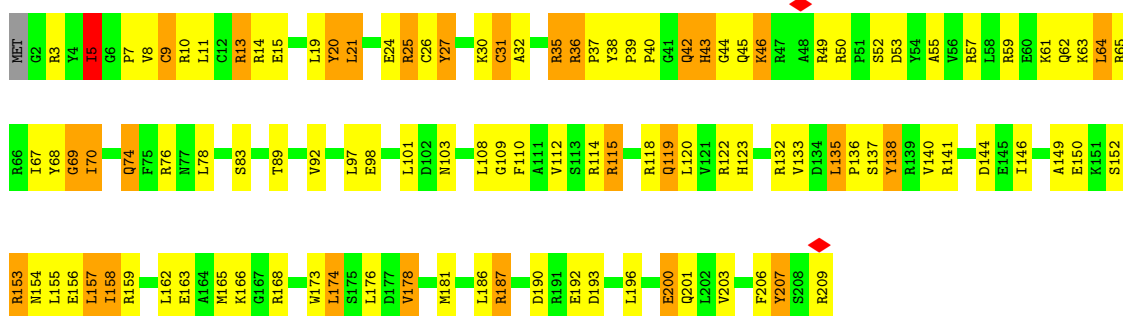




• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

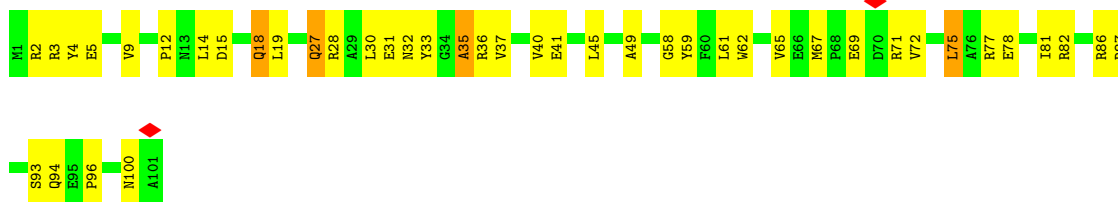


• Molecule 5: 30S ribosomal protein S5




GLN
GLY

- Molecule 6: 30S ribosomal protein S6

Chain F:  57% 39%

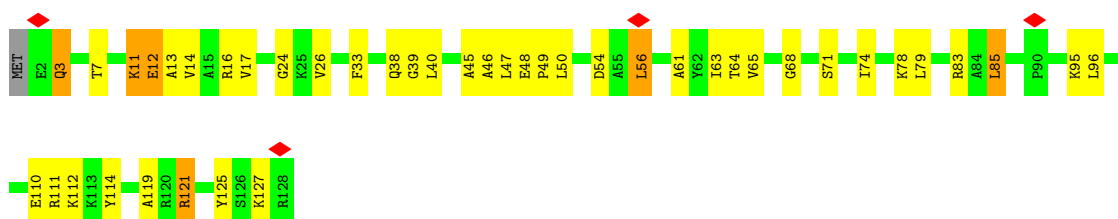
- Molecule 7: 30S ribosomal protein S7

Chain G:  77% 21%

- Molecule 8: 30S ribosomal protein S8

Chain H:  60% 33% 7%

- Molecule 9: 30S ribosomal protein S9

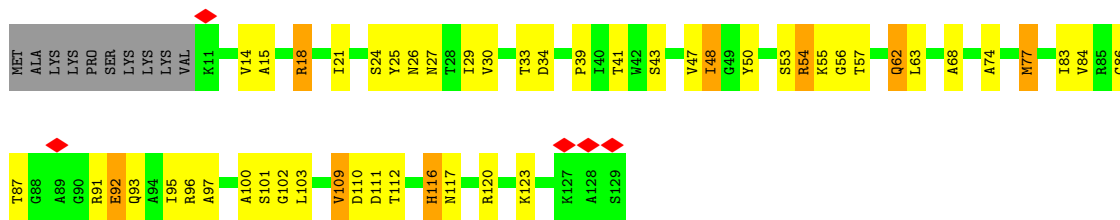
Chain I:  65% 30% 5%

- Molecule 10: 30S ribosomal protein S10

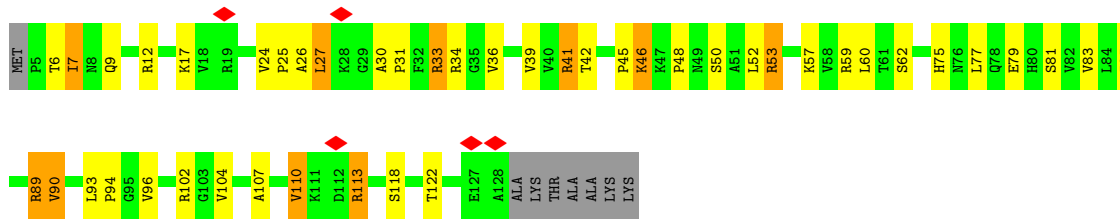
Chain J:  10% 52% 34% 7% 7%



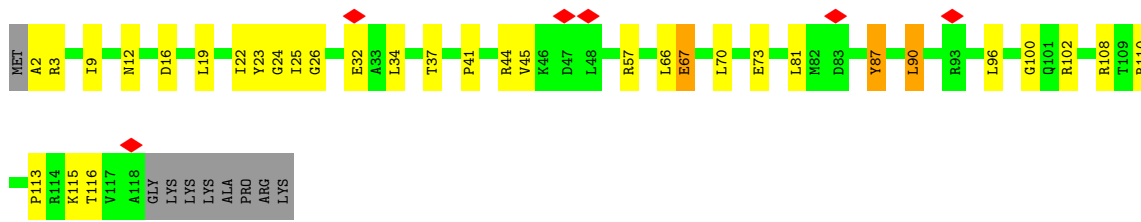
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12



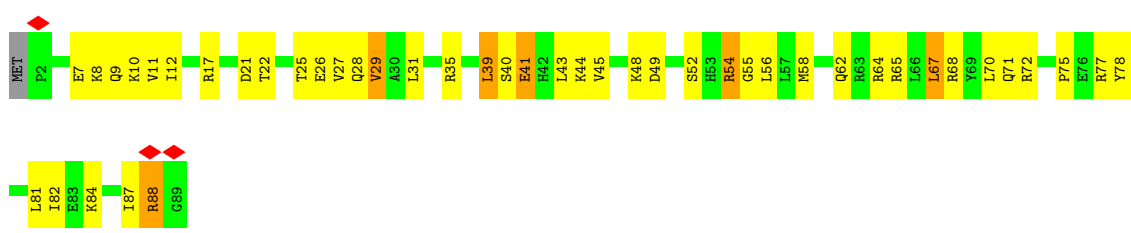
• Molecule 13: 30S ribosomal protein S13



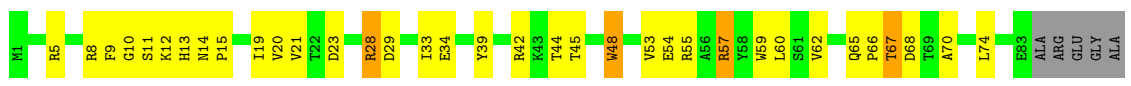
• Molecule 14: 30S ribosomal protein S14 type Z



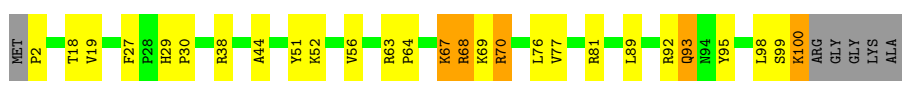
• Molecule 15: 30S ribosomal protein S15



• Molecule 16: 30S ribosomal protein S16



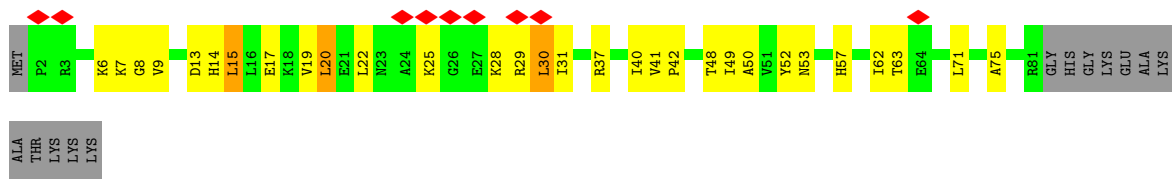
• Molecule 17: 30S ribosomal protein S17



• Molecule 18: 30S ribosomal protein S18

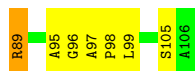


• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20

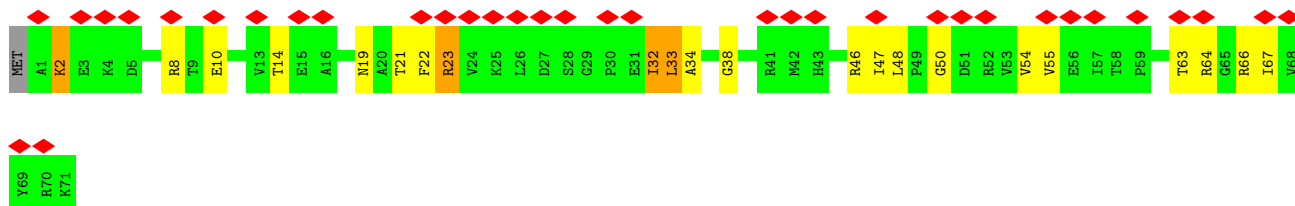




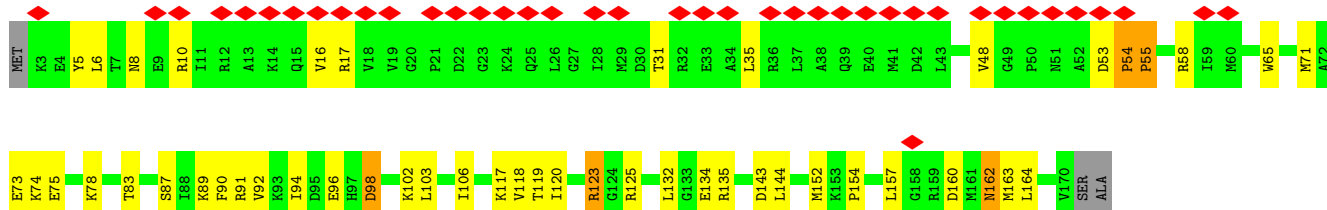
- Molecule 21: 30S ribosomal protein Thx



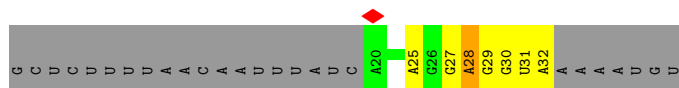
- Molecule 22: Translation initiation factor IF-1



- 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	57382	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	0.377	Depositor
Minimum map value	-0.084	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.05	Depositor
Map size (\AA)	348.4, 348.4, 348.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.34, 1.34, 1.34	Depositor

5 Model quality i

5.1 Standard geometry i

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

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	0.37	0/36397	0.77	20/56783 (0.0%)
2	B	0.57	0/1935	0.84	2/2609 (0.1%)
3	C	0.54	0/1636	0.86	5/2205 (0.2%)
4	D	0.47	0/1733	0.86	2/2318 (0.1%)
5	E	0.48	0/1162	0.92	1/1564 (0.1%)
6	F	0.46	0/856	0.86	1/1154 (0.1%)
7	G	0.56	0/1276	0.83	0/1709
8	H	0.43	0/1136	0.83	0/1527
9	I	0.54	0/1029	1.01	5/1379 (0.4%)
10	J	0.55	0/805	0.76	0/1082
11	K	0.52	0/900	0.78	0/1213
12	L	0.38	0/986	0.76	0/1320
13	M	0.59	0/943	0.84	2/1265 (0.2%)
14	N	0.49	0/501	0.82	1/664 (0.2%)
15	O	0.49	0/745	0.88	0/992
16	P	0.42	0/716	0.78	0/963
17	Q	0.42	0/836	0.80	0/1117
18	R	0.51	0/604	0.89	0/801
19	S	0.64	0/661	0.85	2/890 (0.2%)
20	T	0.48	0/765	0.90	0/1007
21	V	0.50	0/212	0.77	0/277
22	W	0.58	0/580	0.88	1/782 (0.1%)
23	X	0.55	0/1373	0.84	1/1838 (0.1%)
24	Y	0.58	0/324	0.77	0/505
All	All	0.43	0/58111	0.80	43/85964 (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
5	E	1	0
12	L	0	1
16	P	0	1
23	X	0	1
All	All	1	3

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	11	LYS	CB-CA-C	21.20	152.79	110.40
5	E	21	ALA	CB-CA-C	17.11	135.76	110.10
22	W	23	ARG	N-CA-C	-11.55	79.83	111.00
1	A	266	G	C2'-C3'-O3'	9.66	130.75	109.50
1	A	792	A	C2'-C3'-O3'	8.32	127.80	109.50
1	A	1534	A	C2'-C3'-O3'	7.77	126.60	109.50
3	C	91	LEU	CA-CB-CG	7.62	132.83	115.30
1	A	1190	G	C2'-C3'-O3'	7.60	126.22	109.50
6	F	75	LEU	CA-CB-CG	7.60	132.77	115.30
23	X	103	LEU	CA-CB-CG	7.42	132.37	115.30
1	A	1346	A	C2'-C3'-O3'	7.13	125.19	109.50
9	I	11	LYS	N-CA-C	-7.07	91.91	111.00
1	A	281	G	C2'-C3'-O3'	6.98	124.86	113.70
1	A	1498	U	C2'-C3'-O3'	6.87	124.69	113.70
1	A	1301	U	C2'-C3'-O3'	6.71	124.43	113.70
3	C	42	LEU	CA-CB-CG	6.61	130.51	115.30
1	A	1145	C	C2'-C3'-O3'	6.44	124.01	113.70
1	A	197	A	C2'-C3'-O3'	6.34	123.84	113.70
1	A	181	G	C2'-C3'-O3'	6.15	123.54	113.70
4	D	36	ARG	C-N-CD	-6.12	107.13	120.60
1	A	1182	G	C2'-C3'-O3'	6.07	123.42	113.70
13	M	90	LEU	CA-CB-CG	5.93	128.93	115.30
1	A	559	A	C2'-C3'-O3'	5.85	123.06	113.70
9	I	12	GLU	N-CA-C	-5.76	95.46	111.00
1	A	328	C	C2'-C3'-O3'	5.69	122.80	113.70
4	D	157	LEU	CA-CB-CG	5.63	128.24	115.30
1	A	1000	U	C2'-C3'-O3'	5.62	122.70	113.70
14	N	44	LEU	CA-CB-CG	5.59	128.16	115.30
19	S	15	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	509	A	C4'-C3'-O3'	5.56	124.12	113.00
9	I	96	LEU	CA-CB-CG	5.49	127.94	115.30
2	B	51	LEU	CA-CB-CG	5.46	127.86	115.30
3	C	28	GLN	N-CA-C	5.35	125.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	G	C4'-C3'-O3'	5.28	123.56	113.00
2	B	24	TRP	N-CA-C	5.27	125.23	111.00
1	A	960	U	C2'-C3'-O3'	5.23	122.06	113.70
1	A	748	C	C2'-C3'-O3'	5.19	122.00	113.70
3	C	14	ILE	N-CA-C	5.11	124.78	111.00
19	S	20	LEU	CA-CB-CG	5.07	126.96	115.30
3	C	29	TYR	N-CA-C	5.06	124.67	111.00
1	A	965	A	C2'-C3'-O3'	5.04	121.76	113.70
13	M	81	LEU	CA-CB-CG	5.01	126.83	115.30
9	I	85	LEU	CA-CB-CG	5.01	126.81	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	21	ALA	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	89	ARG	Peptide
16	P	67	THR	Peptide
23	X	53	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32525	0	16435	1137	0
2	B	1900	0	1951	36	0
3	C	1612	0	1677	95	0
4	D	1703	0	1764	81	0
5	E	1146	0	1207	62	0
6	F	843	0	857	20	0
7	G	1257	0	1296	21	0
8	H	1116	0	1177	36	0
9	I	1010	0	1035	25	0
10	J	792	0	832	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	885	0	903	41	0
12	L	970	0	1057	23	0
13	M	933	0	992	15	0
14	N	492	0	533	35	0
15	O	734	0	771	15	0
16	P	700	0	720	20	0
17	Q	823	0	891	32	0
18	R	598	0	670	24	0
19	S	647	0	673	12	0
20	T	763	0	861	35	0
21	V	208	0	221	1	0
22	W	570	0	599	33	0
23	X	1356	0	1399	20	0
24	Y	288	0	143	8	0
25	A	107	0	0	1	0
25	W	1	0	0	0	0
26	A	44	0	22	0	0
26	X	22	0	11	1	0
27	A	23	0	11	2	0
28	D	1	0	0	3	0
28	N	1	0	0	1	0
29	W	20	0	11	0	0
29	X	20	0	10	0	0
All	All	54110	0	38729	1694	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 (1694) 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)
20:T:72:LEU:CD2	20:T:77:ALA:HB2	1.20	1.68
1:A:1080:A:C5'	5:E:16:THR:HG21	1.11	1.57
20:T:72:LEU:HD21	20:T:77:ALA:CA	1.35	1.54
20:T:72:LEU:HD21	20:T:77:ALA:CB	1.33	1.53
1:A:1080:A:C5'	5:E:16:THR:CG2	1.84	1.53
1:A:1080:A:H5''	5:E:16:THR:CG2	1.45	1.44
20:T:72:LEU:CD2	20:T:77:ALA:CB	1.91	1.41
10:J:38:ILE:CG2	10:J:71:LEU:O	1.71	1.38
1:A:279:A:C4	17:Q:98:LEU:HD23	1.59	1.35
1:A:279:A:C4	17:Q:98:LEU:CD2	2.12	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:ARG:CG	3:C:64:VAL:CG2	2.11	1.29
3:C:57:ILE:CG1	3:C:66:VAL:HG22	1.60	1.28
1:A:247:G:OP2	17:Q:100:LYS:CE	1.85	1.23
10:J:17:ASP:OD1	10:J:70:ARG:NH2	1.68	1.23
3:C:57:ILE:HG12	3:C:66:VAL:CG2	1.69	1.22
1:A:1113:C:H4'	3:C:14:ILE:CD1	1.67	1.22
4:D:36:ARG:HD2	4:D:38:TYR:CZ	1.73	1.21
10:J:38:ILE:HG23	10:J:71:LEU:O	1.05	1.20
1:A:262:A:C5'	20:T:73:HIS:HE1	1.54	1.20
3:C:59:ARG:HG3	3:C:64:VAL:CG2	1.68	1.18
1:A:1080:A:H5'	5:E:16:THR:CG2	1.58	1.18
1:A:262:A:C5'	20:T:73:HIS:CE1	2.27	1.17
1:A:1398:A:N6	5:E:21:ALA:O	1.75	1.17
3:C:59:ARG:CG	3:C:64:VAL:HG23	1.72	1.15
22:W:21:THR:HG21	22:W:33:LEU:CD1	1.76	1.14
1:A:827:U:N3	1:A:872:A:N6	1.96	1.13
1:A:1081:G:H2'	1:A:1082:G:H8	1.08	1.12
14:N:24:CYS:SG	28:N:101:ZN:ZN	1.40	1.10
3:C:59:ARG:HG3	3:C:64:VAL:HG22	1.32	1.10
10:J:20:ALA:HB2	10:J:70:ARG:CD	1.81	1.10
1:A:1079:G:H5'	5:E:14:ARG:HH22	0.97	1.09
1:A:1113:C:C4'	3:C:14:ILE:HD12	1.82	1.09
4:D:36:ARG:CD	4:D:38:TYR:CZ	2.36	1.09
1:A:262:A:H5'	20:T:73:HIS:CE1	1.84	1.08
1:A:1113:C:H4'	3:C:14:ILE:HD12	1.09	1.08
3:C:59:ARG:NE	3:C:64:VAL:CG2	2.15	1.08
3:C:59:ARG:CG	3:C:64:VAL:HG22	1.79	1.08
1:A:1081:G:H2'	1:A:1082:G:C8	1.89	1.08
3:C:59:ARG:HG2	3:C:64:VAL:HG23	1.36	1.08
20:T:72:LEU:HD21	20:T:77:ALA:HA	1.35	1.07
8:H:54:ASP:O	8:H:56:LYS:HE3	1.51	1.07
3:C:59:ARG:CZ	3:C:64:VAL:HG21	1.84	1.07
10:J:20:ALA:CB	10:J:70:ARG:CD	2.32	1.07
10:J:20:ALA:HB2	10:J:70:ARG:HD2	1.31	1.07
1:A:1077:G:N2	1:A:1079:G:H3'	1.69	1.06
1:A:1079:G:C5'	5:E:14:ARG:HH22	1.68	1.06
1:A:279:A:C5	17:Q:98:LEU:HD23	1.90	1.05
1:A:864:A:H2'	1:A:865:A:C8	1.92	1.05
22:W:21:THR:HG21	22:W:33:LEU:HD11	1.38	1.03
10:J:50:ILE:HG12	10:J:60:ARG:HH21	1.24	1.03
1:A:1219:U:H2'	1:A:1220:G:H8	1.24	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:U:H3	1:A:872:A:N6	1.52	1.02
3:C:24:ALA:HB1	3:C:28:GLN:HG2	1.38	1.02
1:A:664:G:H22	1:A:741:G:H1	1.05	1.01
10:J:48:THR:HG22	10:J:60:ARG:HG2	1.42	1.01
1:A:920:U:H2'	1:A:921:U:C6	1.95	1.01
20:T:72:LEU:CD2	20:T:77:ALA:CA	2.31	1.01
1:A:279:A:N3	17:Q:98:LEU:CD2	2.24	1.01
3:C:59:ARG:CD	3:C:64:VAL:HG22	1.91	1.00
10:J:50:ILE:HG13	10:J:60:ARG:NE	1.77	1.00
10:J:37:PRO:HA	10:J:72:VAL:HG22	1.42	1.00
1:A:920:U:H2'	1:A:921:U:H6	1.21	1.00
1:A:247:G:OP2	17:Q:100:LYS:HE3	1.58	0.99
1:A:80:G:H3'	1:A:81:U:H5''	1.44	0.99
1:A:1080:A:C5'	5:E:16:THR:HG23	1.91	0.98
1:A:17:U:H2'	1:A:18:C:C6	1.98	0.98
3:C:59:ARG:NE	3:C:64:VAL:HG22	1.78	0.98
10:J:50:ILE:HG13	10:J:60:ARG:HE	1.26	0.98
1:A:1256:A:H3'	3:C:27:LYS:NZ	1.79	0.97
1:A:279:A:N3	17:Q:98:LEU:HD23	1.79	0.97
1:A:1070:U:H2'	1:A:1071:C:C6	1.98	0.97
1:A:1103:C:H2'	1:A:1104:G:O4'	1.64	0.97
1:A:1113:C:C4'	3:C:14:ILE:CD1	2.41	0.97
4:D:9:CYS:SG	28:D:300:ZN:ZN	1.53	0.97
1:A:1322:C:H5''	13:M:100:GLY:HA2	1.45	0.96
1:A:45:U:H2'	1:A:46:G:C8	1.99	0.96
1:A:45:U:H2'	1:A:46:G:H8	1.29	0.96
1:A:745:C:H2'	1:A:746:A:C8	2.01	0.96
5:E:107:ARG:HH11	5:E:107:ARG:HB2	1.28	0.96
16:P:59:TRP:O	16:P:62:VAL:HG22	1.65	0.95
1:A:1219:U:H2'	1:A:1220:G:C8	2.01	0.95
3:C:59:ARG:NE	3:C:64:VAL:HG21	1.81	0.94
1:A:266:G:H3'	17:Q:67:LYS:HB2	1.48	0.94
3:C:64:VAL:O	3:C:99:VAL:HG23	1.67	0.94
1:A:1077:G:H22	1:A:1079:G:H3'	1.26	0.94
1:A:279:A:C2	17:Q:98:LEU:HD23	2.02	0.94
1:A:1080:A:H5'	5:E:16:THR:HG21	1.13	0.93
10:J:20:ALA:CB	10:J:70:ARG:HD3	1.95	0.93
20:T:72:LEU:HD23	20:T:77:ALA:HB2	0.94	0.93
1:A:1079:G:H5'	5:E:14:ARG:NH2	1.82	0.93
3:C:28:GLN:HE21	3:C:32:LEU:HD11	1.29	0.93
1:A:247:G:OP2	17:Q:100:LYS:CD	2.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:A:H5''	20:T:73:HIS:HE1	1.35	0.92
11:K:91:ARG:NH2	11:K:110:ASP:OD2	2.03	0.92
1:A:1158:C:H4'	2:B:132:LYS:HB2	1.54	0.90
1:A:1356:G:H2'	1:A:1357:A:C8	2.07	0.90
1:A:827:U:O4	1:A:872:A:N1	2.05	0.90
1:A:1101:A:H5''	2:B:99:GLY:HA3	1.54	0.89
10:J:50:ILE:CG1	10:J:60:ARG:HH21	1.85	0.89
10:J:36:GLY:O	10:J:72:VAL:HG13	1.73	0.89
1:A:729:A:H2'	1:A:730:G:H8	1.37	0.89
1:A:1070:U:H2'	1:A:1071:C:H6	1.35	0.88
1:A:1022:G:H2'	1:A:1023:G:H8	1.38	0.88
22:W:33:LEU:HD21	22:W:64:ARG:NH1	1.89	0.88
1:A:662:G:H2'	1:A:663:A:C8	2.09	0.88
1:A:917:G:H2'	1:A:918:A:C8	2.09	0.87
4:D:35:ARG:HB3	4:D:35:ARG:HH21	1.37	0.87
3:C:30:ARG:NH1	3:C:30:ARG:HB2	1.89	0.87
10:J:50:ILE:CG1	10:J:60:ARG:HE	1.87	0.87
14:N:24:CYS:HB3	14:N:29:ARG:H	1.40	0.86
10:J:38:ILE:HG22	10:J:71:LEU:O	1.76	0.86
1:A:247:G:OP2	17:Q:100:LYS:NZ	2.08	0.86
1:A:868:C:H2'	1:A:869:G:O4'	1.75	0.86
1:A:1106:G:H5''	3:C:172:ARG:HG3	1.58	0.86
8:H:45:ILE:HG22	8:H:63:LEU:HA	1.57	0.86
4:D:26:CYS:SG	28:D:300:ZN:ZN	1.64	0.85
22:W:21:THR:CG2	22:W:33:LEU:CD1	2.54	0.85
1:A:247:G:OP2	17:Q:100:LYS:HD2	1.74	0.85
3:C:59:ARG:CD	3:C:64:VAL:CG2	2.53	0.85
1:A:1190:G:H5'	3:C:176:HIS:HE1	1.41	0.85
1:A:17:U:O2'	1:A:1079:G:H1'	1.77	0.85
10:J:20:ALA:HB1	10:J:70:ARG:HD3	1.55	0.85
1:A:15:G:H2'	1:A:16:A:H8	1.41	0.84
1:A:745:C:H2'	1:A:746:A:H8	1.40	0.84
1:A:662:G:H2'	1:A:663:A:H8	1.42	0.83
11:K:91:ARG:HH21	18:R:88:LYS:NZ	1.76	0.83
1:A:1099:G:C6	1:A:1100:C:N3	2.47	0.83
22:W:32:ILE:O	22:W:32:ILE:HD13	1.78	0.82
3:C:30:ARG:CD	14:N:35:ARG:O	2.28	0.82
1:A:170:U:H2'	1:A:171:A:H8	1.44	0.82
1:A:1022:G:H2'	1:A:1023:G:C8	2.14	0.82
4:D:36:ARG:CD	4:D:38:TYR:OH	2.27	0.82
1:A:262:A:C4'	20:T:73:HIS:CE1	2.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:C:H2'	1:A:270:A:C8	2.14	0.82
1:A:279:A:N3	17:Q:98:LEU:HD21	1.93	0.82
1:A:1101:A:H4'	1:A:1102:A:O5'	1.79	0.81
3:C:30:ARG:HG2	14:N:37:PHE:C	2.00	0.81
1:A:777:A:H2'	1:A:778:G:C8	2.14	0.81
1:A:398:C:H2'	1:A:399:G:H8	1.44	0.81
1:A:1256:A:H3'	3:C:27:LYS:CE	2.10	0.81
9:I:13:ALA:HB2	9:I:68:GLY:HA3	1.62	0.81
22:W:33:LEU:CD2	22:W:64:ARG:NH1	2.43	0.81
1:A:124:G:H2'	1:A:125:U:O4'	1.79	0.81
6:F:49:ALA:HB1	18:R:80:PRO:HA	1.62	0.81
1:A:870:U:H4'	1:A:871:U:H5''	1.62	0.81
1:A:16:A:N3	1:A:1080:A:H1'	1.96	0.80
1:A:101:A:H2'	1:A:102:G:H8	1.45	0.80
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.63	0.80
1:A:1096:C:H2'	1:A:1097:C:C6	2.17	0.80
1:A:16:A:C2	1:A:1080:A:H1'	2.18	0.80
1:A:303:A:H2'	1:A:304:U:H6	1.44	0.80
1:A:1073:U:H3	1:A:1102:A:H61	1.30	0.79
1:A:729:A:H2'	1:A:730:G:C8	2.16	0.79
1:A:925:G:H1	1:A:1391:U:H3	1.28	0.79
4:D:36:ARG:HG3	4:D:38:TYR:CE2	2.17	0.79
11:K:87:THR:HG23	11:K:91:ARG:HD3	1.65	0.78
1:A:309:G:H2'	1:A:310:G:H8	1.48	0.78
1:A:299:G:H2'	1:A:300:A:C8	2.18	0.78
1:A:1190:G:H5'	3:C:176:HIS:CE1	2.17	0.78
1:A:1390:U:H2'	1:A:1391:U:C6	2.18	0.78
6:F:49:ALA:CB	18:R:80:PRO:HA	2.13	0.78
1:A:1096:C:H2'	1:A:1097:C:H6	1.49	0.78
1:A:1128:C:H2'	1:A:1139:G:N7	1.99	0.78
11:K:87:THR:HA	11:K:91:ARG:HD2	1.65	0.78
1:A:21:G:H2'	1:A:22:G:C8	2.18	0.78
1:A:1127:G:H21	1:A:1147:C:H41	1.29	0.78
20:T:72:LEU:HD21	20:T:77:ALA:N	1.97	0.77
1:A:1435:G:H2'	1:A:1436:U:C6	2.19	0.77
1:A:728:A:H2'	1:A:729:A:C8	2.19	0.77
3:C:59:ARG:HG3	3:C:64:VAL:HG23	1.46	0.77
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.67	0.77
1:A:1507:A:H2'	1:A:1508:G:C8	2.19	0.77
16:P:59:TRP:O	16:P:62:VAL:CG2	2.31	0.77
4:D:35:ARG:HH21	4:D:35:ARG:CB	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:G:H2'	1:A:303:A:C8	2.19	0.77
1:A:914:A:H2'	1:A:915:A:H8	1.48	0.76
8:H:91:ARG:HD3	12:L:7:ILE:HG21	1.67	0.76
11:K:91:ARG:HH21	18:R:88:LYS:HZ2	1.30	0.76
1:A:1367:C:H4'	10:J:48:THR:HG21	1.66	0.76
1:A:24:U:H2'	1:A:25:C:C6	2.20	0.76
1:A:279:A:C4	17:Q:98:LEU:HD21	2.18	0.76
1:A:303:A:H2'	1:A:304:U:C6	2.21	0.76
10:J:37:PRO:O	10:J:70:ARG:CG	2.34	0.76
4:D:36:ARG:HD3	4:D:38:TYR:OH	1.85	0.76
5:E:107:ARG:HB2	5:E:107:ARG:NH1	2.01	0.76
1:A:728:A:H2'	1:A:729:A:H8	1.48	0.75
10:J:60:ARG:HB2	10:J:60:ARG:CZ	2.14	0.75
1:A:262:A:H4'	20:T:73:HIS:CE1	2.20	0.75
1:A:1080:A:H5'	5:E:16:THR:CB	2.15	0.75
1:A:1080:A:H5''	5:E:16:THR:HG21	0.77	0.75
1:A:1256:A:H3'	3:C:27:LYS:HZ2	1.49	0.75
1:A:1102:A:H2'	1:A:1103:C:C6	2.21	0.75
1:A:56:U:H2'	1:A:57:G:C8	2.21	0.74
1:A:919:A:C2	1:A:1080:A:H2	2.05	0.74
1:A:701:C:H4'	1:A:702:A:O5'	1.87	0.74
10:J:17:ASP:OD1	10:J:70:ARG:CZ	2.35	0.74
1:A:90:U:H2'	1:A:91:C:C6	2.22	0.74
1:A:224:C:H2'	1:A:225:C:C6	2.21	0.74
1:A:398:C:H2'	1:A:399:G:C8	2.23	0.74
1:A:1080:A:C4'	5:E:16:THR:HG23	2.17	0.74
3:C:30:ARG:HD2	14:N:35:ARG:O	1.87	0.74
10:J:50:ILE:CD1	10:J:60:ARG:HE	2.00	0.74
1:A:313:A:H2'	1:A:314:C:C6	2.22	0.74
8:H:54:ASP:O	8:H:56:LYS:CE	2.35	0.74
4:D:36:ARG:HD2	4:D:38:TYR:CE1	2.23	0.73
1:A:1077:G:H2'	1:A:1078:U:H2'	1.71	0.73
1:A:269:C:H2'	1:A:270:A:H8	1.52	0.73
1:A:1113:C:H4'	3:C:14:ILE:HD13	1.69	0.73
1:A:1521:G:H2'	1:A:1522:U:C6	2.22	0.73
10:J:50:ILE:HG13	10:J:60:ARG:CZ	2.18	0.73
22:W:23:ARG:HH21	22:W:33:LEU:HB2	1.53	0.73
1:A:439:A:OP2	1:A:493:G:N1	2.19	0.73
1:A:1348:U:H2'	1:A:1349:A:H8	1.52	0.73
1:A:1390:U:H2'	1:A:1391:U:H6	1.54	0.73
3:C:30:ARG:HD3	14:N:35:ARG:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:A:C6	17:Q:98:LEU:HD23	2.25	0.72
4:D:36:ARG:CD	4:D:38:TYR:CE2	2.72	0.72
1:A:262:A:C4'	20:T:73:HIS:HE1	1.98	0.72
2:B:15:VAL:HG11	2:B:209:ARG:HB3	1.70	0.72
1:A:1287:A:H2'	1:A:1288:A:C8	2.24	0.72
11:K:54:ARG:H	11:K:54:ARG:HD2	1.55	0.72
1:A:973:G:H3'	1:A:974:A:H5''	1.72	0.72
3:C:30:ARG:HG3	14:N:36:PHE:O	1.90	0.72
1:A:1256:A:C3'	3:C:27:LYS:NZ	2.51	0.72
1:A:1386:G:H2'	1:A:1387:G:H8	1.54	0.72
10:J:50:ILE:CG1	10:J:60:ARG:NH2	2.53	0.72
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.54	0.71
1:A:13:U:N3	1:A:915:A:N6	2.38	0.71
1:A:113:G:H2'	1:A:114:U:C6	2.25	0.71
10:J:38:ILE:O	10:J:71:LEU:N	2.23	0.71
10:J:40:LEU:HB2	10:J:69:ASN:HB3	1.73	0.71
1:A:562:C:H41	1:A:884:U:H2'	1.55	0.71
10:J:48:THR:HG22	10:J:60:ARG:CG	2.18	0.71
20:T:72:LEU:CD2	20:T:77:ALA:HA	2.11	0.71
22:W:21:THR:CG2	22:W:33:LEU:HG	2.20	0.71
1:A:1080:A:H4'	5:E:16:THR:HG23	1.70	0.71
1:A:1256:A:C3'	3:C:27:LYS:HZ2	2.03	0.71
1:A:524:G:C6	1:A:525:C:N4	2.58	0.71
1:A:1443:G:C6	1:A:1444:C:N4	2.58	0.71
1:A:403:C:H5''	4:D:136:PRO:HD2	1.71	0.71
1:A:664:G:N2	1:A:741:G:H1	1.87	0.71
1:A:769:G:N2	1:A:770:C:C2	2.59	0.71
1:A:1500:A:H5''	1:A:1508:G:H5''	1.73	0.71
1:A:302:G:H2'	1:A:303:A:H8	1.53	0.70
1:A:316:G:H1	1:A:337:C:H42	1.38	0.70
1:A:1081:G:OP2	5:E:16:THR:HG22	1.91	0.70
1:A:69:G:H1	1:A:100:C:N4	1.89	0.70
10:J:37:PRO:HA	10:J:72:VAL:CG2	2.18	0.70
1:A:69:G:H1	1:A:100:C:H42	1.36	0.70
1:A:18:C:H2'	1:A:19:C:C6	2.27	0.70
1:A:406:G:H4'	4:D:5:ILE:HD11	1.73	0.69
10:J:38:ILE:HG23	10:J:71:LEU:C	2.05	0.69
1:A:24:U:H2'	1:A:25:C:H6	1.56	0.69
1:A:424:G:H2'	1:A:425:G:C8	2.27	0.69
5:E:14:ARG:O	5:E:14:ARG:HG2	1.92	0.69
1:A:10:A:H2'	1:A:11:G:C8	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:A:H2'	1:A:11:G:H8	1.56	0.69
1:A:584:G:H2'	1:A:585:G:H8	1.58	0.69
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.74	0.69
22:W:21:THR:HG21	22:W:33:LEU:HD12	1.71	0.69
22:W:33:LEU:HD23	22:W:64:ARG:HG2	1.72	0.69
1:A:312:C:H2'	1:A:313:A:C8	2.28	0.69
1:A:1095:U:H2'	1:A:1096:C:C6	2.27	0.69
1:A:1445:C:C2	1:A:1458:G:C2	2.81	0.69
1:A:584:G:H2'	1:A:585:G:C8	2.27	0.69
1:A:56:U:H2'	1:A:57:G:H8	1.58	0.68
14:N:41:ARG:HE	14:N:42:ILE:HG13	1.58	0.68
24:Y:28:A:H3'	24:Y:29:G:C8	2.27	0.68
4:D:9:CYS:HG	28:D:300:ZN:ZN	1.07	0.68
1:A:13:U:H3	1:A:915:A:N6	1.91	0.68
1:A:67:C:H2'	1:A:68:G:H8	1.57	0.68
1:A:543:C:H2'	1:A:544:G:C8	2.28	0.68
1:A:1079:G:H2'	1:A:1080:A:C8	2.28	0.68
10:J:40:LEU:HG	10:J:71:LEU:HB2	1.76	0.68
23:X:48:VAL:HG21	23:X:58:ARG:HE	1.58	0.68
1:A:16:A:C2	1:A:17:U:C6	2.82	0.68
1:A:1536:C:H42	24:Y:29:G:H1	1.41	0.68
1:A:67:C:H2'	1:A:68:G:C8	2.28	0.68
1:A:524:G:C2	1:A:525:C:N3	2.61	0.68
1:A:576:G:H3'	1:A:577:G:H5''	1.75	0.68
1:A:1256:A:H3'	3:C:27:LYS:HE3	1.74	0.68
10:J:37:PRO:CA	10:J:72:VAL:HG22	2.21	0.68
1:A:1410:G:H2'	1:A:1411:C:C6	2.29	0.68
3:C:71:ALA:HB2	3:C:115:LEU:HD11	1.75	0.68
1:A:860:A:H3'	1:A:861:G:H8	1.59	0.68
1:A:1264:C:H2'	1:A:1265:G:H8	1.58	0.68
1:A:279:A:C2	17:Q:98:LEU:CD2	2.74	0.67
1:A:521:G:N2	1:A:522:C:C2	2.62	0.67
1:A:1016:A:H2'	1:A:1017:G:O4'	1.95	0.67
11:K:33:THR:HA	11:K:39:PRO:HA	1.76	0.67
1:A:564:C:O2	1:A:564:C:H2'	1.94	0.67
1:A:588:G:N2	1:A:589:C:C2	2.63	0.67
1:A:234:C:H2'	1:A:235:C:C6	2.29	0.67
1:A:690:G:OP2	11:K:27:ASN:HB3	1.94	0.67
23:X:5:TYR:HE2	23:X:65:TRP:CH2	2.12	0.67
22:W:33:LEU:HD21	22:W:64:ARG:HH11	1.59	0.67
1:A:1132:C:H2'	1:A:1133:G:C8	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:29:SER:HB3	8:H:32:LYS:HG3	1.78	0.66
15:O:31:LEU:O	15:O:35:ARG:HG3	1.96	0.66
1:A:610:G:H2'	1:A:611:A:H8	1.59	0.66
3:C:57:ILE:CD1	3:C:66:VAL:HG22	2.25	0.66
16:P:67:THR:HG22	16:P:68:ASP:H	1.59	0.66
1:A:16:A:H1'	1:A:1080:A:H4'	1.77	0.66
1:A:568:G:N2	1:A:883:C:C2	2.63	0.66
20:T:72:LEU:HD23	20:T:77:ALA:CB	1.90	0.66
3:C:24:ALA:CB	3:C:28:GLN:HG2	2.22	0.66
1:A:543:C:H2'	1:A:544:G:H8	1.60	0.66
5:E:139:LEU:HA	5:E:142:LEU:HD12	1.77	0.66
4:D:36:ARG:HD3	4:D:38:TYR:CZ	2.26	0.66
1:A:522:C:H41	12:L:53:ARG:HH21	1.44	0.66
1:A:1079:G:C5'	5:E:14:ARG:NH2	2.51	0.66
3:C:66:VAL:HG12	3:C:68:VAL:HG22	1.77	0.65
1:A:955:U:H1'	1:A:1227:A:H61	1.61	0.65
1:A:1244:C:H2'	1:A:1245:A:H8	1.60	0.65
1:A:19:C:H2'	1:A:20:U:C6	2.32	0.65
4:D:63:LYS:O	4:D:67:ILE:HG13	1.97	0.65
1:A:1328:C:H2'	1:A:1329:A:O4'	1.97	0.65
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.78	0.65
10:J:17:ASP:CG	10:J:70:ARG:NH2	2.49	0.65
1:A:253:U:H2'	1:A:254:G:H8	1.62	0.65
1:A:1163:C:H2'	1:A:1164:G:H8	1.60	0.65
3:C:39:ILE:HG21	3:C:66:VAL:HG21	1.77	0.65
9:I:114:TYR:HD2	10:J:58:ASP:O	1.80	0.65
10:J:37:PRO:O	10:J:70:ARG:HG3	1.97	0.64
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.78	0.64
1:A:1020:U:H2'	1:A:1021:G:H8	1.63	0.64
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.79	0.64
1:A:777:A:H2'	1:A:778:G:H8	1.59	0.64
1:A:1504:G:H5''	1:A:1505:G:O4'	1.98	0.64
24:Y:28:A:H3'	24:Y:29:G:H8	1.62	0.64
1:A:930:C:H2'	1:A:931:C:O4'	1.97	0.64
1:A:172:A:H2'	1:A:174:C:H5	1.62	0.64
1:A:587:G:O2'	1:A:588:G:H5'	1.97	0.64
1:A:1073:U:H3	1:A:1102:A:N6	1.94	0.64
1:A:1264:C:H2'	1:A:1265:G:C8	2.33	0.64
16:P:65:GLN:HE21	16:P:66:PRO:HD2	1.62	0.64
1:A:312:C:H2'	1:A:313:A:H8	1.62	0.63
1:A:1255:G:H2'	1:A:1279:A:N6	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:ARG:HB2	3:C:30:ARG:HH11	1.63	0.63
1:A:335:C:H2'	1:A:336:C:C6	2.33	0.63
1:A:424:G:H2'	1:A:425:G:H8	1.60	0.63
19:S:22:LEU:HD13	19:S:28:LYS:HB3	1.78	0.63
1:A:864:A:O2'	1:A:1078:U:C4	2.52	0.63
1:A:1402:C:H2'	1:A:1403:C:H6	1.62	0.63
12:L:46:LYS:HB3	12:L:48:PRO:HD2	1.80	0.63
1:A:878:G:H5'	8:H:89:PRO:HG2	1.79	0.63
1:A:1071:C:H2'	1:A:1072:G:H8	1.64	0.63
1:A:1536:C:N4	24:Y:29:G:H1	1.96	0.63
1:A:370:C:C2	1:A:392:G:N2	2.66	0.63
1:A:1443:G:C2	1:A:1444:C:N3	2.67	0.63
1:A:914:A:H2'	1:A:915:A:C8	2.32	0.62
3:C:29:TYR:OH	14:N:37:PHE:CE1	2.51	0.62
20:T:34:LYS:HG3	20:T:80:ARG:HH12	1.64	0.62
1:A:1241:G:N2	1:A:1242:C:C2	2.67	0.62
1:A:1515:C:H2'	1:A:1516:G:C8	2.34	0.62
5:E:87:SER:HA	5:E:125:SER:HB3	1.80	0.62
1:A:678:U:H2'	1:A:679:C:C6	2.34	0.62
10:J:37:PRO:O	10:J:70:ARG:HG2	1.98	0.62
15:O:8:LYS:HG2	15:O:31:LEU:HD11	1.80	0.62
1:A:919:A:C2	1:A:1079:G:N2	2.68	0.62
10:J:50:ILE:HG12	10:J:60:ARG:NH2	2.06	0.62
23:X:89:LYS:HD2	26:X:201:A:H61	1.64	0.62
1:A:946:A:H2'	1:A:947:G:C8	2.35	0.62
1:A:1152:A:H5'	10:J:13:HIS:HB2	1.81	0.62
1:A:110:C:H2'	1:A:111:G:O4'	1.98	0.62
16:P:13:HIS:O	16:P:15:PRO:HD3	1.99	0.62
22:W:21:THR:CG2	22:W:33:LEU:HD12	2.27	0.62
1:A:1342:C:H2'	1:A:1343:G:C8	2.35	0.62
1:A:1387:G:O3'	1:A:1388:C:H5'	1.99	0.62
1:A:1505:G:H4'	1:A:1506:U:H5''	1.81	0.62
1:A:610:G:H2'	1:A:611:A:C8	2.35	0.61
1:A:1313:U:H2'	1:A:1314:C:C6	2.35	0.61
4:D:36:ARG:CG	4:D:38:TYR:CE2	2.83	0.61
12:L:102:ARG:HG2	12:L:107:ALA:HB1	1.82	0.61
23:X:5:TYR:HE2	23:X:65:TRP:HH2	1.48	0.61
1:A:671:G:N2	1:A:736:C:C2	2.68	0.61
1:A:911:U:H2'	1:A:912:C:C6	2.35	0.61
1:A:112:G:H21	1:A:354:G:H5'	1.64	0.61
1:A:259:G:H2'	1:A:260:G:C8	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:C:H2'	1:A:443:C:C6	2.35	0.61
1:A:725:G:N2	1:A:726:C:C2	2.69	0.61
4:D:36:ARG:HD2	4:D:38:TYR:OH	1.90	0.61
1:A:123:C:H2'	1:A:124:G:H8	1.64	0.61
1:A:974:A:H4'	1:A:975:A:H3'	1.83	0.61
1:A:1098:C:H1'	1:A:1168:A:H2	1.66	0.61
10:J:49:VAL:O	10:J:60:ARG:HG3	2.00	0.61
3:C:57:ILE:HG12	3:C:66:VAL:HG22	0.72	0.61
22:W:32:ILE:HB	22:W:63:THR:O	2.01	0.61
1:A:1080:A:H5'	5:E:16:THR:OG1	2.01	0.61
1:A:1353:G:N2	1:A:1354:C:C2	2.68	0.61
2:B:111:ARG:HD3	2:B:145:LEU:HD21	1.82	0.61
1:A:27:G:H2'	1:A:28:G:C8	2.36	0.61
1:A:827:U:C2	1:A:872:A:N6	2.69	0.61
1:A:1355:G:H2'	1:A:1356:G:H8	1.65	0.61
2:B:71:VAL:HA	2:B:93:VAL:HG12	1.82	0.61
11:K:87:THR:HA	11:K:91:ARG:CD	2.30	0.61
1:A:1111:A:N1	3:C:177:THR:HB	2.16	0.60
1:A:309:G:H2'	1:A:310:G:C8	2.34	0.60
1:A:1065:U:H4'	1:A:1066:C:O5'	2.01	0.60
8:H:121:ASP:CG	8:H:122:ARG:H	2.04	0.60
1:A:376:G:H2'	1:A:377:G:H8	1.67	0.60
1:A:548:G:H2'	1:A:549:C:C6	2.37	0.60
1:A:683:G:N2	1:A:708:C:C2	2.70	0.60
4:D:20:TYR:HA	4:D:26:CYS:HB3	1.83	0.60
1:A:181:G:H4'	1:A:182:U:H5'	1.82	0.60
1:A:407:G:H1'	4:D:119:GLN:HE22	1.67	0.60
1:A:1255:G:H2'	1:A:1279:A:H62	1.67	0.60
6:F:94:GLN:HB3	18:R:32:ARG:HD3	1.82	0.60
1:A:568:G:C2	1:A:883:C:N3	2.70	0.60
1:A:174:C:H2'	1:A:175:C:C6	2.36	0.60
1:A:895:G:H1	1:A:904:C:H42	1.50	0.60
1:A:1355:G:H1	1:A:1367:C:H42	1.50	0.60
1:A:15:G:C5	1:A:16:A:N7	2.69	0.60
1:A:1235:U:H2'	1:A:1236:A:O4'	2.02	0.60
1:A:123:C:H2'	1:A:124:G:C8	2.37	0.60
1:A:255:G:C2	1:A:272:C:C2	2.90	0.60
1:A:279:A:C5	17:Q:98:LEU:CD2	2.67	0.60
1:A:453:A:H2'	1:A:454:C:C6	2.37	0.60
22:W:33:LEU:HD23	22:W:33:LEU:O	2.02	0.60
1:A:266:G:C8	1:A:266:G:H5''	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:21:THR:CG2	22:W:33:LEU:CG	2.80	0.59
1:A:46:G:H2'	1:A:366:C:C5	2.37	0.59
1:A:1001:A:H2'	1:A:1001(A):G:C8	2.36	0.59
3:C:59:ARG:HG2	3:C:64:VAL:CG2	2.03	0.59
4:D:109:GLY:HA3	4:D:165:MET:HG3	1.84	0.59
1:A:1080:A:C4'	5:E:16:THR:CG2	2.70	0.59
1:A:1507:A:H2'	1:A:1508:G:H8	1.67	0.59
4:D:30:LYS:C	4:D:32:ALA:H	2.03	0.59
5:E:18:ARG:HB3	5:E:25:ARG:O	2.02	0.59
11:K:62:GLN:HG2	11:K:97:ALA:HB2	1.83	0.59
23:X:90:PHE:HD1	23:X:94:ILE:HD13	1.67	0.59
1:A:32:A:H2'	1:A:33:A:C8	2.38	0.59
1:A:313:A:H2'	1:A:314:C:H6	1.67	0.59
1:A:521:G:N1	1:A:522:C:C4	2.70	0.59
1:A:1512:U:H2'	1:A:1513:A:C8	2.37	0.59
12:L:24:VAL:HG12	12:L:26:ALA:H	1.67	0.59
1:A:769:G:N1	1:A:770:C:C4	2.71	0.59
1:A:1105:A:H2'	1:A:1106:G:H8	1.68	0.59
10:J:50:ILE:HG13	10:J:60:ARG:NH2	2.18	0.59
1:A:20:U:H2'	1:A:21:G:O4'	2.03	0.59
1:A:183:G:H2'	1:A:184:G:O4'	2.03	0.59
1:A:861:G:O6	1:A:869:G:N2	2.35	0.59
1:A:1416:G:H2'	1:A:1417:G:O4'	2.02	0.59
10:J:50:ILE:CG1	10:J:60:ARG:NE	2.56	0.59
1:A:77:G:H3'	1:A:77:G:C8	2.37	0.59
1:A:170:U:H2'	1:A:171:A:C8	2.33	0.59
1:A:320:C:H2'	1:A:321:A:C8	2.38	0.59
1:A:743:U:H2'	1:A:744:C:C6	2.38	0.59
1:A:1069:C:H42	1:A:1106:G:H1	1.51	0.59
1:A:1162:C:C2	1:A:1175:G:N2	2.70	0.59
1:A:13:U:OP1	25:A:1606:MG:MG	1.45	0.59
1:A:128:G:N2	1:A:234:C:C2	2.71	0.59
4:D:166:LYS:HG3	4:D:178:VAL:HG21	1.85	0.59
7:G:93:PRO:O	7:G:96:GLN:HG2	2.03	0.59
1:A:741:G:H5'	15:O:39:LEU:HD21	1.84	0.59
1:A:920:U:O2'	1:A:1081:G:O2'	2.20	0.59
1:A:1238:A:H5'	1:A:1336:C:H41	1.68	0.59
3:C:66:VAL:CG1	3:C:68:VAL:HG22	2.32	0.59
1:A:926:G:H3'	1:A:1505:G:N2	2.18	0.58
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.85	0.58
1:A:222:U:H2'	1:A:223:U:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:A:C6	12:L:31:PRO:HD2	2.38	0.58
1:A:1074:G:N1	1:A:1075:C:C2	2.72	0.58
1:A:1515:C:H2'	1:A:1516:G:H8	1.68	0.58
1:A:928:G:H2'	1:A:929:G:C8	2.38	0.58
1:A:1099:G:C2	1:A:1100:C:O2	2.56	0.58
1:A:34:C:H2'	1:A:35:G:C8	2.39	0.58
1:A:1128:C:H1'	1:A:1146:A:H61	1.67	0.58
10:J:7:LYS:HB2	10:J:97:GLU:HB2	1.84	0.58
1:A:1456:G:N2	1:A:1457:G:C8	2.72	0.58
22:W:23:ARG:NH2	22:W:33:LEU:HB2	2.19	0.58
1:A:392:G:H2'	1:A:393:A:H8	1.67	0.58
6:F:35:ALA:HA	6:F:67:MET:HB3	1.84	0.58
10:J:60:ARG:HB2	10:J:60:ARG:NH1	2.19	0.58
1:A:1464:G:N2	1:A:1465:C:C2	2.72	0.58
1:A:936:C:H2'	1:A:937:A:H8	1.69	0.58
1:A:1118:C:H2'	1:A:1119:C:C6	2.39	0.58
1:A:1172:C:H2'	1:A:1173:G:H8	1.68	0.58
5:E:81:GLU:HA	5:E:89:ILE:O	2.04	0.58
1:A:1369:C:H2'	1:A:1370:G:C8	2.40	0.57
1:A:397:A:H3'	1:A:397:A:N3	2.18	0.57
1:A:648:A:H2'	1:A:649:G:C8	2.39	0.57
1:A:860:A:H3'	1:A:861:G:C8	2.39	0.57
1:A:1059:C:H2'	1:A:1060:C:C6	2.39	0.57
1:A:128:G:C2	1:A:234:C:C2	2.93	0.57
1:A:1097:C:H2'	1:A:1098:C:C6	2.38	0.57
11:K:15:ALA:HA	11:K:77:MET:HA	1.85	0.57
1:A:689:C:H5''	11:K:27:ASN:ND2	2.20	0.57
1:A:1118:C:H4'	9:I:83:ARG:HH22	1.69	0.57
1:A:883:C:H2'	1:A:884:U:C6	2.38	0.57
10:J:37:PRO:HB2	10:J:70:ARG:HH11	1.68	0.57
22:W:21:THR:HG22	22:W:33:LEU:HG	1.86	0.57
1:A:401:C:H2'	1:A:402:G:H8	1.68	0.57
1:A:540:G:H2'	1:A:541:G:C8	2.39	0.57
1:A:837:G:H8	1:A:837:G:O5'	1.88	0.57
4:D:115:ARG:HB3	4:D:115:ARG:HH11	1.69	0.57
1:A:549:C:H2'	1:A:550:G:H8	1.70	0.57
1:A:681:C:C2	1:A:710:G:N2	2.72	0.57
1:A:392:G:H2'	1:A:393:A:C8	2.40	0.57
1:A:590:C:H42	1:A:649:G:H1	1.53	0.57
1:A:864:A:C2	1:A:865:A:C2	2.92	0.57
1:A:877:C:H2'	1:A:878:G:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:G:H5'	5:E:18:ARG:HD3	1.85	0.57
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.70	0.57
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.87	0.57
14:N:41:ARG:NE	14:N:42:ILE:HG13	2.20	0.57
1:A:78:G:H2'	1:A:79:G:O4'	2.05	0.57
1:A:1132:C:H2'	1:A:1133:G:H8	1.69	0.57
1:A:1225:A:H2'	1:A:1225:A:N3	2.20	0.57
9:I:26:VAL:HG21	9:I:47:LEU:HD21	1.88	0.56
1:A:585:G:H2'	1:A:586:C:O4'	2.04	0.56
1:A:1409:C:H2'	1:A:1410:G:H8	1.70	0.56
1:A:1409:C:H2'	1:A:1410:G:C8	2.40	0.56
1:A:19:C:H2'	1:A:20:U:H6	1.69	0.56
1:A:437:U:H3'	1:A:438:G:C8	2.40	0.56
1:A:1114:C:C2	1:A:1187:G:C2	2.93	0.56
1:A:1300:G:O2'	1:A:1303:C:N4	2.37	0.56
5:E:83:GLU:HA	5:E:87:SER:O	2.04	0.56
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.87	0.56
22:W:22:PHE:HB2	22:W:67:ILE:HD11	1.87	0.56
1:A:579:G:H2'	1:A:580:U:C6	2.41	0.56
1:A:582:U:H2'	1:A:583:A:C8	2.39	0.56
1:A:1104:G:H5''	1:A:1104:G:H8	1.70	0.56
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.86	0.56
12:L:75:HIS:HD2	12:L:77:LEU:H	1.52	0.56
1:A:184:G:H2'	1:A:185:A:H8	1.70	0.56
1:A:1488:G:H2'	1:A:1489:G:H8	1.70	0.56
22:W:32:ILE:H	22:W:32:ILE:CD1	2.18	0.56
1:A:109:A:H2'	1:A:326:G:N2	2.21	0.56
3:C:28:GLN:NE2	3:C:32:LEU:HD11	2.12	0.56
3:C:66:VAL:HG12	3:C:68:VAL:CG2	2.35	0.56
23:X:157:LEU:HB2	23:X:160:ASP:HB2	1.87	0.56
1:A:919:A:N3	1:A:1080:A:H2	2.03	0.56
1:A:434:U:H2'	1:A:435:C:C6	2.41	0.56
1:A:918:A:C2	1:A:1079:G:N2	2.74	0.56
1:A:1121:U:H2'	1:A:1122:U:C6	2.41	0.56
1:A:153:C:N4	1:A:154:C:N4	2.54	0.56
1:A:967:C:H2'	1:A:968:A:C8	2.40	0.56
1:A:1355:G:H2'	1:A:1356:G:C8	2.40	0.56
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.86	0.56
1:A:165:C:H2'	1:A:166:G:H8	1.70	0.55
1:A:409:G:OP1	4:D:24:GLU:HB3	2.06	0.55
1:A:671:G:C2	1:A:736:C:N3	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:C:C2	1:A:853:G:C2	2.94	0.55
1:A:1368:G:N2	1:A:1369:C:C2	2.74	0.55
4:D:101:LEU:HB2	4:D:138:TYR:HB3	1.88	0.55
5:E:106:PRO:HA	5:E:109:ILE:HD12	1.87	0.55
10:J:20:ALA:CB	10:J:70:ARG:NE	2.69	0.55
17:Q:56:VAL:HG13	17:Q:77:VAL:HB	1.87	0.55
1:A:1121:U:H2'	1:A:1122:U:H6	1.71	0.55
1:A:1244:C:H2'	1:A:1245:A:C8	2.40	0.55
1:A:877:C:H2'	1:A:878:G:H8	1.71	0.55
1:A:1163:C:C2	1:A:1174:G:N2	2.75	0.55
10:J:48:THR:O	10:J:60:ARG:HD3	2.05	0.55
1:A:253:U:H2'	1:A:254:G:C8	2.41	0.55
1:A:1071:C:H2'	1:A:1072:G:C8	2.40	0.55
1:A:1106:G:N2	1:A:1107:C:C2	2.74	0.55
1:A:1323:G:H2'	1:A:1324:A:C8	2.41	0.55
3:C:57:ILE:CG1	3:C:66:VAL:CG2	2.54	0.55
5:E:17:ALA:HA	5:E:26:PHE:HA	1.88	0.55
22:W:23:ARG:HH21	22:W:33:LEU:CB	2.18	0.55
1:A:1346:A:C8	1:A:1348:U:C2	2.94	0.55
3:C:30:ARG:HG2	14:N:37:PHE:CA	2.37	0.55
8:H:121:ASP:CG	8:H:122:ARG:N	2.60	0.55
1:A:80:G:H3'	1:A:81:U:C5'	2.26	0.55
1:A:636:U:H5'	17:Q:2:PRO:HG3	1.88	0.55
4:D:32:ALA:O	4:D:36:ARG:N	2.39	0.55
8:H:120:THR:HG22	8:H:121:ASP:H	1.70	0.55
14:N:24:CYS:CB	14:N:29:ARG:H	2.17	0.55
22:W:14:THR:HB	22:W:23:ARG:HB3	1.89	0.55
1:A:558:G:H3'	1:A:559:A:H5''	1.88	0.55
3:C:29:TYR:OH	14:N:37:PHE:HE1	1.89	0.55
3:C:59:ARG:CZ	3:C:64:VAL:CG2	2.64	0.55
1:A:318:G:N2	1:A:336:C:C2	2.75	0.55
1:A:671:G:C2	1:A:736:C:C2	2.95	0.55
1:A:939:G:C6	1:A:940:C:N4	2.75	0.55
1:A:1511:G:H2'	1:A:1512:U:O4'	2.07	0.55
1:A:920:U:C2	1:A:1080:A:C2	2.94	0.55
1:A:927:G:O3'	1:A:928:G:P	2.65	0.55
1:A:1025:U:H2'	1:A:1026:G:C8	2.42	0.55
1:A:383:A:C5	1:A:384:G:H1'	2.42	0.55
1:A:652:U:O4	1:A:752:G:O2'	2.25	0.55
1:A:1233:G:C6	1:A:1234:C:N4	2.75	0.55
9:I:40:LEU:CD2	9:I:74:ILE:HD11	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:G:H5''	1:A:266:G:H8	1.70	0.54
1:A:455:C:H2'	1:A:456:C:C6	2.42	0.54
12:L:25:PRO:C	12:L:27:LEU:H	2.11	0.54
1:A:28:G:H2'	1:A:29:G:O4'	2.06	0.54
1:A:229:U:H2'	1:A:230:G:H8	1.72	0.54
1:A:279:A:N9	17:Q:98:LEU:CD2	2.67	0.54
1:A:659:U:H2'	1:A:660:G:C8	2.42	0.54
1:A:928:G:H2'	1:A:929:G:H8	1.72	0.54
1:A:1512:U:H2'	1:A:1513:A:H8	1.71	0.54
1:A:577:G:N2	1:A:578:C:C2	2.76	0.54
1:A:1020:U:H2'	1:A:1021:G:C8	2.43	0.54
1:A:1162:C:C2	1:A:1175:G:C2	2.96	0.54
1:A:1256:A:H2'	3:C:27:LYS:HZ1	1.72	0.54
6:F:27:GLN:HA	6:F:30:LEU:HD12	1.88	0.54
1:A:761:G:C2	1:A:762:C:C2	2.95	0.54
1:A:1135:U:H4'	1:A:1136:U:H5	1.71	0.54
1:A:1342:C:H2'	1:A:1343:G:H8	1.71	0.54
2:B:61:LEU:HD21	2:B:160:ASP:HB3	1.88	0.54
13:M:34:LEU:HD13	13:M:41:PRO:HG3	1.90	0.54
23:X:6:LEU:HB3	23:X:10:ARG:HB3	1.88	0.54
1:A:333:G:N2	1:A:334:C:C2	2.75	0.54
2:B:61:LEU:HD11	2:B:160:ASP:HB2	1.89	0.54
4:D:24:GLU:HA	4:D:27:TYR:HB2	1.88	0.54
4:D:156:GLU:HA	4:D:159:ARG:HD2	1.90	0.54
11:K:87:THR:HG21	24:Y:29:G:H4'	1.89	0.54
15:O:26:GLU:O	15:O:29:VAL:HG12	2.08	0.54
1:A:101:A:H2'	1:A:102:G:C8	2.34	0.54
1:A:223:U:H5'	20:T:68:LYS:NZ	2.23	0.54
1:A:500:G:C6	1:A:501:C:N4	2.76	0.54
1:A:836:G:H2'	1:A:837:G:C8	2.43	0.54
15:O:82:ILE:HA	15:O:87:ILE:HD12	1.90	0.54
1:A:197:A:C6	1:A:221:C:H4'	2.43	0.54
1:A:262:A:H5''	20:T:73:HIS:CE1	2.21	0.54
1:A:568:G:C2	1:A:883:C:C2	2.95	0.54
1:A:588:G:N1	1:A:589:C:C4	2.75	0.54
1:A:756:C:H2'	1:A:757:U:O4'	2.07	0.54
1:A:927:G:OP2	1:A:927:G:H4'	2.08	0.54
2:B:17:PHE:HB2	2:B:41:ILE:HG12	1.89	0.54
8:H:91:ARG:O	8:H:91:ARG:HG3	2.08	0.54
1:A:661:G:C2	1:A:745:C:N3	2.76	0.54
1:A:669:U:H2'	1:A:670:G:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:C:H2'	1:A:937:A:C8	2.42	0.54
1:A:1008:C:C2	1:A:1022:G:N2	2.76	0.54
10:J:49:VAL:HG11	14:N:44:LEU:HD12	1.90	0.54
20:T:49:ALA:HB3	20:T:99:LEU:HD12	1.89	0.54
1:A:934:C:C5	1:A:1344:C:H2'	2.43	0.54
1:A:972:C:O3'	10:J:57:LYS:HG3	2.07	0.54
1:A:1077:G:N3	1:A:1079:G:C8	2.75	0.54
1:A:166:G:H2'	1:A:167:G:C8	2.43	0.54
1:A:730:G:N2	1:A:765:G:H5''	2.23	0.54
1:A:1098:C:H1'	1:A:1168:A:C2	2.43	0.54
3:C:57:ILE:CD1	3:C:66:VAL:CG2	2.85	0.54
10:J:6:ILE:HG13	10:J:72:VAL:O	2.08	0.54
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.89	0.54
22:W:32:ILE:HD13	22:W:32:ILE:C	2.23	0.54
1:A:184:G:H2'	1:A:185:A:C8	2.42	0.53
1:A:279:A:C4	17:Q:98:LEU:HD22	2.31	0.53
1:A:919:A:N3	1:A:1080:A:C2	2.76	0.53
3:C:30:ARG:CB	3:C:30:ARG:CZ	2.86	0.53
5:E:127:ASN:ND2	5:E:129:ILE:H	2.06	0.53
1:A:994:A:N7	1:A:1216:G:H4'	2.24	0.53
1:A:1513:A:H2'	1:A:1514:C:C6	2.43	0.53
8:H:12:ARG:NH1	8:H:25:ASP:O	2.41	0.53
11:K:84:VAL:CG2	11:K:91:ARG:NH2	2.71	0.53
1:A:504:C:C2	1:A:542:G:N2	2.76	0.53
1:A:589:C:O2	1:A:651:C:O2	2.26	0.53
1:A:872:A:C8	1:A:874:G:C8	2.96	0.53
4:D:43:HIS:HB3	4:D:46:LYS:HD2	1.90	0.53
1:A:114:U:H2'	1:A:115:G:C8	2.43	0.53
1:A:229:U:H2'	1:A:230:G:C8	2.44	0.53
1:A:289:G:N2	1:A:290:C:C2	2.76	0.53
1:A:1118:C:H2'	1:A:1119:C:H6	1.73	0.53
1:A:1526:G:H2'	1:A:1527:C:C6	2.43	0.53
19:S:30:LEU:HD23	19:S:50:ALA:HB2	1.89	0.53
1:A:152:A:OP2	1:A:153:C:N4	2.42	0.53
1:A:939:G:H2'	1:A:940:C:C6	2.44	0.53
1:A:1048:G:H2'	1:A:1050:G:H8	1.73	0.53
1:A:35:G:H2'	1:A:36:C:C6	2.43	0.53
1:A:44:G:H3'	1:A:45:U:C6	2.44	0.53
1:A:509:A:H5'	4:D:55:ALA:HB2	1.89	0.53
1:A:576:G:H3'	1:A:577:G:C5'	2.38	0.53
3:C:77:ILE:HA	3:C:84:ILE:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:C:H1'	14:N:19:ARG:HG2	1.90	0.53
1:A:61:G:H2'	1:A:62:U:O4'	2.08	0.53
1:A:351:G:H4'	1:A:352:C:OP1	2.08	0.53
1:A:669:U:H2'	1:A:670:G:H8	1.74	0.53
1:A:1338:G:H2'	1:A:1339:A:C8	2.44	0.53
1:A:1348:U:H2'	1:A:1349:A:C8	2.41	0.53
1:A:1464:G:N1	1:A:1465:C:C4	2.77	0.53
22:W:21:THR:HG21	22:W:33:LEU:CG	2.37	0.53
1:A:735:C:H5'	18:R:71:LYS:HD3	1.91	0.53
1:A:1088:G:H2'	1:A:1089:G:O4'	2.09	0.53
10:J:48:THR:CG2	10:J:60:ARG:HG2	2.27	0.53
1:A:316:G:H1	1:A:337:C:N4	2.05	0.52
1:A:439:A:C4	1:A:496:A:C2	2.96	0.52
1:A:621:A:H2'	1:A:622:A:C8	2.44	0.52
1:A:1078:U:O2'	1:A:1079:G:O4'	2.27	0.52
1:A:22:G:C6	1:A:23:C:C4	2.96	0.52
1:A:598:U:H2'	1:A:599:C:C6	2.44	0.52
1:A:1321:C:H5'	13:M:87:TYR:CE1	2.45	0.52
4:D:62:GLN:OE1	4:D:62:GLN:HA	2.09	0.52
5:E:110:LEU:HD13	5:E:118:ILE:HG13	1.89	0.52
10:J:17:ASP:HA	10:J:70:ARG:NH2	2.24	0.52
1:A:399:G:C6	1:A:400:C:N4	2.77	0.52
1:A:505:G:H2'	1:A:506:G:H8	1.73	0.52
1:A:643:C:H2'	1:A:644:G:C8	2.43	0.52
1:A:1502:A:H2'	1:A:1504:G:C8	2.44	0.52
2:B:142:LEU:HD23	2:B:146:GLN:HE22	1.74	0.52
3:C:30:ARG:HB2	3:C:30:ARG:CZ	2.37	0.52
1:A:71:C:H2'	1:A:72:C:O4'	2.10	0.52
1:A:122:G:N1	1:A:123:C:C2	2.77	0.52
1:A:598:U:H2'	1:A:599:C:H6	1.74	0.52
1:A:790:A:O2'	23:X:87:SER:O	2.25	0.52
1:A:1151:A:O2'	1:A:1152:A:H8	1.92	0.52
1:A:1291:G:O3'	9:I:39:GLY:HA3	2.09	0.52
1:A:1400:C:N3	27:A:1710:G:O6	2.41	0.52
1:A:189:G:C2	1:A:189(A):C:C2	2.98	0.52
1:A:332:G:C2	1:A:333:G:C8	2.98	0.52
1:A:761:G:C6	1:A:762:C:C4	2.98	0.52
1:A:779:C:H2'	1:A:780:A:O4'	2.09	0.52
1:A:832:C:C2	1:A:855:G:C2	2.97	0.52
1:A:872:A:C4	1:A:874:G:N7	2.77	0.52
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:A:H5'	1:A:110:C:C5	2.44	0.52
1:A:1163:C:N3	1:A:1174:G:C2	2.78	0.52
3:C:174:PRO:HB2	3:C:177:THR:HG23	1.91	0.52
10:J:17:ASP:CB	10:J:70:ARG:NH2	2.73	0.52
1:A:60:A:H4'	1:A:61:G:O5'	2.10	0.52
1:A:122:G:C2	1:A:123:C:C2	2.97	0.52
1:A:1077:G:N2	1:A:1079:G:C3'	2.59	0.52
1:A:1106:G:C6	1:A:1107:C:N4	2.78	0.52
1:A:1127:G:H21	1:A:1147:C:N4	2.02	0.52
1:A:1217:C:N4	1:A:1218:C:N4	2.57	0.52
4:D:200:GLU:OE1	4:D:201:GLN:HG3	2.09	0.52
1:A:504:C:N3	1:A:542:G:C2	2.78	0.52
1:A:643:C:H2'	1:A:644:G:H8	1.75	0.52
1:A:926:G:H3'	1:A:1505:G:H21	1.74	0.52
1:A:1030:C:H42	1:A:1031:G:H1	1.55	0.52
1:A:1518:A:H2'	1:A:1519:A:C8	2.44	0.52
4:D:98:GLU:HA	4:D:103:ASN:ND2	2.25	0.52
1:A:99:U:H2'	1:A:100:C:C6	2.44	0.52
1:A:360:A:H2'	1:A:361:G:O4'	2.09	0.52
1:A:667:G:H2'	1:A:668:G:H8	1.74	0.52
1:A:834:C:O2	1:A:853:G:C2	2.63	0.52
1:A:1488:G:H2'	1:A:1489:G:C8	2.44	0.52
1:A:505:G:H5'	1:A:534:U:H2'	1.92	0.52
1:A:955:U:H1'	1:A:1227:A:N6	2.24	0.52
1:A:1010:G:H1	1:A:1019:C:H42	1.57	0.52
1:A:1068:G:N2	1:A:1069:C:C2	2.78	0.52
4:D:36:ARG:HG3	4:D:38:TYR:CD2	2.44	0.52
15:O:62:GLN:HA	15:O:65:ARG:HH11	1.75	0.52
1:A:558:G:H3'	1:A:559:A:C5'	2.40	0.51
1:A:1048:G:H2'	1:A:1050:G:C8	2.45	0.51
1:A:1223:C:H5''	1:A:1224:G:H5''	1.92	0.51
1:A:1007:C:H42	1:A:1022:G:H1	1.57	0.51
24:Y:27:G:H2'	24:Y:28:A:O4'	2.10	0.51
1:A:44:G:H3'	1:A:45:U:H6	1.75	0.51
1:A:230:G:H2'	1:A:231:G:O4'	2.10	0.51
1:A:766:A:H2'	1:A:767:A:O4'	2.11	0.51
1:A:1014:A:H5''	19:S:14:HIS:HB3	1.92	0.51
1:A:1379:G:HO2'	7:G:156:TRP:HD1	1.57	0.51
15:O:54:ARG:HH21	15:O:58:MET:HG3	1.74	0.51
1:A:755:G:N2	1:A:756:C:C2	2.79	0.51
11:K:21:ILE:HB	11:K:84:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:10:GLU:HG2	22:W:54:VAL:HG22	1.92	0.51
1:A:258:G:N2	1:A:269:C:C2	2.78	0.51
1:A:1148:U:H5''	9:I:7:THR:HG21	1.91	0.51
1:A:1376:U:H5'	7:G:102:ARG:HH22	1.76	0.51
1:A:1434:A:H3'	1:A:1435:G:C8	2.46	0.51
8:H:18:ARG:HH12	8:H:78:GLN:HG3	1.76	0.51
1:A:92:C:H2'	1:A:93:G:H8	1.76	0.51
1:A:262:A:H4'	20:T:73:HIS:HE1	1.66	0.51
1:A:737:A:H2'	1:A:738:C:C6	2.45	0.51
1:A:881:G:OP2	12:L:12:ARG:NH2	2.41	0.51
1:A:1081:G:OP2	5:E:16:THR:CG2	2.58	0.51
3:C:120:VAL:HB	3:C:198:VAL:HG11	1.92	0.51
12:L:41:ARG:HH12	12:L:57:LYS:HG3	1.74	0.51
16:P:33:ILE:HG22	16:P:34:GLU:HB2	1.92	0.51
1:A:827:U:O2'	8:H:19:VAL:HG11	2.11	0.51
1:A:1359:C:H3'	14:N:35:ARG:HH21	1.76	0.51
13:M:2:ALA:O	13:M:9:ILE:HA	2.10	0.51
1:A:437:U:H3'	1:A:438:G:H8	1.76	0.51
1:A:824:C:H2'	1:A:825:G:H8	1.76	0.51
1:A:1226:C:H3'	13:M:96:LEU:HD21	1.92	0.51
1:A:1312:G:C2	1:A:1326:C:C2	2.98	0.51
1:A:1379:G:O2'	7:G:156:TRP:HD1	1.94	0.51
3:C:178:LEU:C	3:C:180:ALA:H	2.14	0.51
4:D:35:ARG:CB	4:D:35:ARG:NH2	2.73	0.51
6:F:45:LEU:HG	6:F:59:TYR:HD2	1.75	0.51
10:J:44:VAL:HG13	10:J:66:ARG:HB3	1.93	0.51
16:P:5:ARG:HH21	16:P:28:ARG:HA	1.75	0.51
16:P:48:TRP:HD1	16:P:48:TRP:H	1.57	0.51
17:Q:19:VAL:HG23	17:Q:44:ALA:HB3	1.91	0.51
1:A:98:G:H2'	1:A:99:U:C6	2.46	0.51
1:A:694:A:H5'	11:K:53:SER:HB2	1.93	0.51
1:A:864:A:O2'	1:A:1078:U:O4	2.28	0.51
1:A:914:A:C4	1:A:915:A:N7	2.78	0.51
1:A:919:A:C2	1:A:1080:A:C2	2.92	0.51
1:A:1086:U:O5'	1:A:1086:U:H6	1.93	0.51
1:A:1466:C:H2'	1:A:1467:G:O4'	2.10	0.51
5:E:50:GLU:HB2	5:E:53:LEU:HB3	1.92	0.51
8:H:28:ALA:HA	8:H:59:LEU:HD12	1.93	0.51
1:A:35:G:C6	1:A:36:C:N4	2.79	0.51
1:A:77:G:C8	1:A:77:G:C3'	2.93	0.51
1:A:122:G:C6	1:A:123:C:C4	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:A:H2'	1:A:664:G:O4'	2.11	0.51
1:A:1281:U:H4'	1:A:1282:C:OP2	2.10	0.51
2:B:124:SER:O	2:B:127:ILE:HG13	2.11	0.51
2:B:163:PHE:HA	2:B:185:ILE:HB	1.93	0.51
7:G:27:ILE:HA	7:G:30:ILE:HD12	1.93	0.51
1:A:251:G:C2	1:A:266:G:C6	3.00	0.50
1:A:270:A:H2'	1:A:271:C:C6	2.46	0.50
1:A:827:U:N3	1:A:872:A:C6	2.67	0.50
1:A:1055:A:H2	3:C:194:GLY:CA	2.24	0.50
1:A:1348:U:OP1	9:I:110:GLU:N	2.31	0.50
5:E:20:GLN:O	5:E:21:ALA:C	2.49	0.50
6:F:78:GLU:HA	6:F:81:ILE:HD12	1.92	0.50
7:G:16:LEU:HD22	9:I:45:ALA:HB2	1.92	0.50
1:A:198:G:H2'	1:A:199:G:C8	2.46	0.50
1:A:769:G:H4'	1:A:1513:A:H4'	1.93	0.50
1:A:1048:G:N2	1:A:1210:C:C2	2.79	0.50
1:A:79:G:H2'	1:A:80:G:H8	1.75	0.50
1:A:661:G:N2	1:A:745:C:C2	2.79	0.50
1:A:1070:U:H2'	1:A:1071:C:C5	2.43	0.50
1:A:1103:C:OP1	2:B:98:LEU:HD22	2.12	0.50
1:A:1323:G:H2'	1:A:1324:A:O4'	2.11	0.50
1:A:1366:C:H2'	1:A:1367:C:C6	2.46	0.50
1:A:1399:C:C2	1:A:1502:A:N6	2.79	0.50
6:F:45:LEU:HG	6:F:59:TYR:CD2	2.46	0.50
6:F:100:ASN:HA	18:R:23:LYS:HE2	1.93	0.50
14:N:24:CYS:HB3	14:N:29:ARG:N	2.19	0.50
1:A:557:G:C6	1:A:558:G:C2	2.99	0.50
1:A:731:G:N2	1:A:732:C:C2	2.79	0.50
1:A:1243:C:C2	1:A:1295:G:N2	2.80	0.50
4:D:24:GLU:O	4:D:25:ARG:HB3	2.12	0.50
9:I:26:VAL:HG22	9:I:61:ALA:HB3	1.92	0.50
15:O:41:GLU:O	15:O:44:LYS:HB2	2.11	0.50
22:W:33:LEU:HD22	22:W:64:ARG:NH1	2.24	0.50
1:A:223:U:H5'	20:T:68:LYS:HZ1	1.77	0.50
1:A:714:G:H2'	1:A:715:A:C8	2.47	0.50
1:A:774:G:N2	1:A:806:C:C2	2.80	0.50
1:A:824:C:H2'	1:A:825:G:C8	2.47	0.50
1:A:932:C:H5'	7:G:3:ARG:CB	2.42	0.50
1:A:13:U:C4	1:A:915:A:N6	2.79	0.50
1:A:90:U:H2'	1:A:91:C:H6	1.71	0.50
1:A:572:A:N1	1:A:864:A:C5	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:C:H2'	1:A:614:A:H8	1.77	0.50
1:A:916:G:C2	1:A:917:G:C5	2.99	0.50
1:A:946:A:H2'	1:A:947:G:H8	1.75	0.50
1:A:1525:G:H2'	1:A:1526:G:H8	1.76	0.50
1:A:30:U:H3'	1:A:31:G:H5''	1.93	0.50
1:A:354:G:N2	1:A:355:C:C2	2.79	0.50
1:A:525:C:H2'	1:A:526:C:C6	2.46	0.50
1:A:864:A:C2'	1:A:865:A:C8	2.83	0.50
12:L:113:ARG:HH11	12:L:113:ARG:HB3	1.75	0.50
1:A:590:C:N4	1:A:649:G:H1	2.10	0.50
1:A:987:G:O5'	1:A:987:G:H8	1.95	0.50
1:A:1018:C:H2'	1:A:1019:C:C6	2.47	0.50
1:A:1059:C:H2'	1:A:1060:C:H6	1.76	0.50
1:A:1356:G:C2	1:A:1367:C:C2	3.00	0.50
20:T:54:LYS:HA	20:T:57:ARG:HH11	1.77	0.50
23:X:5:TYR:CE2	23:X:65:TRP:CH2	2.96	0.50
1:A:22:G:C2	1:A:23:C:C2	3.00	0.50
1:A:681:C:N3	1:A:710:G:C2	2.79	0.50
1:A:827:U:C4	1:A:872:A:N1	2.79	0.49
1:A:920:U:C2'	1:A:921:U:C6	2.83	0.49
4:D:57:ARG:NE	5:E:107:ARG:HE	2.10	0.49
4:D:133:VAL:HG11	4:D:138:TYR:HD2	1.77	0.49
22:W:32:ILE:CD1	22:W:32:ILE:N	2.73	0.49
1:A:500:G:H2'	1:A:501:C:C6	2.47	0.49
1:A:501:C:H2'	1:A:502:G:H8	1.77	0.49
1:A:717:C:H2'	1:A:734:G:H5'	1.93	0.49
1:A:876:G:C6	1:A:877:C:N4	2.79	0.49
1:A:1365:G:C2	1:A:1366:C:C2	3.00	0.49
1:A:1459:C:H2'	1:A:1460:A:O4'	2.12	0.49
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	1.93	0.49
19:S:22:LEU:CD1	19:S:31:ILE:HD11	2.43	0.49
23:X:71:MET:O	23:X:75:GLU:HG2	2.11	0.49
1:A:130:A:H8	1:A:130:A:OP1	1.94	0.49
1:A:500:G:C2	1:A:501:C:N3	2.80	0.49
1:A:562:C:H2'	1:A:562:C:OP2	2.12	0.49
1:A:648:A:H2'	1:A:649:G:H8	1.76	0.49
1:A:1007:C:O2	1:A:1023:G:C2	2.65	0.49
1:A:1393:U:H2'	1:A:1395:C:C5	2.46	0.49
2:B:61:LEU:HD11	2:B:160:ASP:CB	2.42	0.49
1:A:861:G:N2	1:A:862:C:C2	2.81	0.49
1:A:1135:U:H4'	1:A:1136:U:C5	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:C:H1'	1:A:394:G:H22	1.78	0.49
1:A:725:G:N1	1:A:726:C:C4	2.81	0.49
1:A:1023:G:H2'	1:A:1023:G:N3	2.28	0.49
4:D:133:VAL:HG11	4:D:138:TYR:CD2	2.46	0.49
1:A:92:C:H2'	1:A:93:G:C8	2.47	0.49
1:A:1014:A:C5'	19:S:14:HIS:HB3	2.42	0.49
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.13	0.49
1:A:1354:C:H42	1:A:1368:G:H1	1.60	0.49
4:D:19:LEU:HB3	4:D:21:LEU:HB2	1.93	0.49
4:D:149:ALA:HB3	4:D:152:SER:HB2	1.95	0.49
5:E:82:VAL:O	5:E:89:ILE:HG22	2.12	0.49
1:A:548:G:C6	1:A:549:C:N4	2.80	0.49
1:A:585:G:C2	1:A:586:C:C2	3.00	0.49
1:A:590:C:OP1	8:H:30:ARG:N	2.45	0.49
1:A:623:C:H2'	1:A:624:C:O4'	2.13	0.49
1:A:1127:G:N2	1:A:1145:C:C2	2.81	0.49
1:A:1436:U:H2'	1:A:1437:C:O4'	2.12	0.49
11:K:91:ARG:NH2	18:R:88:LYS:NZ	2.55	0.49
1:A:358:U:H2'	1:A:359:U:O4'	2.12	0.49
1:A:1082:G:H2'	1:A:1083:U:O4'	2.13	0.49
9:I:40:LEU:HD21	9:I:74:ILE:HD11	1.95	0.49
1:A:233:C:H2'	1:A:234:C:H6	1.76	0.49
1:A:505:G:H2'	1:A:506:G:C8	2.47	0.49
1:A:549:C:H2'	1:A:550:G:C8	2.48	0.49
4:D:3:ARG:HA	4:D:3:ARG:CZ	2.43	0.49
17:Q:93:GLN:C	17:Q:93:GLN:HE21	2.15	0.49
18:R:26:LEU:HD21	18:R:39:VAL:HG22	1.95	0.49
1:A:582:U:H2'	1:A:583:A:H8	1.78	0.49
1:A:1106:G:C2	1:A:1107:C:C4	3.01	0.49
1:A:17:U:O2	1:A:1079:G:N3	2.46	0.48
1:A:21:G:C2	1:A:22:G:C5	3.01	0.48
1:A:236:G:C2	1:A:237:C:C2	3.01	0.48
18:R:53:ARG:HE	18:R:60:ALA:HA	1.78	0.48
1:A:46:G:H2'	1:A:366:C:H5	1.76	0.48
1:A:148:G:C2	1:A:175:C:C2	3.02	0.48
1:A:590:C:OP1	8:H:30:ARG:HG2	2.12	0.48
3:C:174:PRO:HD2	3:C:182:ILE:HD11	1.95	0.48
11:K:84:VAL:HG23	11:K:91:ARG:HH22	1.78	0.48
18:R:31:LEU:O	18:R:69:THR:HG21	2.11	0.48
1:A:216:G:C6	1:A:217:C:N4	2.81	0.48
1:A:259:G:H2'	1:A:260:G:H8	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:C:N3	1:A:392:G:C2	2.81	0.48
1:A:557:G:N1	1:A:558:G:C2	2.81	0.48
1:A:707:C:H2'	1:A:708:C:C6	2.48	0.48
1:A:994:A:H8	1:A:1216:G:HO2'	1.56	0.48
1:A:1074:G:H4'	2:B:103:THR:O	2.12	0.48
1:A:1365:G:C6	1:A:1366:C:C4	3.01	0.48
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.48	0.48
5:E:41:VAL:HG13	5:E:113:ALA:HA	1.95	0.48
1:A:29:G:H5''	1:A:30:U:OP2	2.13	0.48
1:A:189:G:C6	1:A:189(A):C:C4	3.01	0.48
1:A:407:G:H2'	1:A:408:A:H8	1.78	0.48
1:A:823:G:H2'	1:A:824:C:C6	2.47	0.48
1:A:972:C:O2	1:A:972:C:H2'	2.12	0.48
1:A:998:G:N2	1:A:999:C:C2	2.80	0.48
1:A:295:C:H2'	1:A:296:U:O4'	2.13	0.48
1:A:1308:U:H2'	1:A:1309:G:C8	2.49	0.48
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.95	0.48
9:I:17:VAL:HG22	9:I:63:ILE:HG12	1.96	0.48
1:A:876:G:H2'	1:A:877:C:C6	2.49	0.48
1:A:1148:U:C5'	9:I:7:THR:HG21	2.43	0.48
2:B:118:LEU:HB3	2:B:142:LEU:HD11	1.95	0.48
9:I:47:LEU:HD22	9:I:50:LEU:HD12	1.96	0.48
1:A:37:U:O2'	1:A:500:G:H4'	2.12	0.48
1:A:165:C:H2'	1:A:166:G:C8	2.48	0.48
1:A:734:G:C2	1:A:735:C:C2	3.01	0.48
1:A:881:G:C2	1:A:882:C:C2	3.02	0.48
1:A:1130:A:H4'	9:I:3:GLN:OE1	2.13	0.48
1:A:1218:C:H2'	1:A:1219:U:C6	2.48	0.48
17:Q:64:PRO:HB3	17:Q:70:ARG:HG3	1.96	0.48
1:A:176:C:H2'	1:A:177:C:C6	2.48	0.48
1:A:675:A:N3	11:K:116:HIS:HB2	2.29	0.48
1:A:1149:C:H2'	1:A:1150:U:C6	2.49	0.48
1:A:1256:A:C2'	3:C:27:LYS:NZ	2.77	0.48
1:A:1267:C:H2'	1:A:1268:A:O4'	2.14	0.48
1:A:1353:G:N1	1:A:1354:C:C4	2.81	0.48
27:A:1710:G:H4'	23:X:123:ARG:HB2	1.94	0.48
8:H:39:LEU:HG	8:H:44:PHE:HB2	1.95	0.48
11:K:91:ARG:NH2	18:R:88:LYS:HZ2	2.06	0.48
14:N:7:ILE:O	14:N:7:ILE:HG22	2.14	0.48
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.96	0.48
1:A:15:G:C4	1:A:16:A:N7	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:C:N4	1:A:154:C:H41	2.12	0.48
1:A:362:G:N2	1:A:364:A:H3'	2.28	0.48
1:A:945:G:H2'	1:A:945:G:N3	2.29	0.48
1:A:1312:G:N2	1:A:1326:C:C2	2.82	0.48
4:D:39:PRO:HB2	4:D:44:GLY:HA2	1.95	0.48
1:A:39:G:N7	1:A:547:A:H2'	2.29	0.48
1:A:218:C:H2'	1:A:219:C:C6	2.49	0.48
1:A:962:C:H1'	1:A:1201:A:N6	2.28	0.48
1:A:974:A:H8	1:A:974:A:OP1	1.97	0.48
1:A:985:C:C2	1:A:1221:G:N2	2.82	0.48
2:B:72:GLY:HA2	2:B:165:VAL:HB	1.96	0.48
4:D:68:TYR:HB2	4:D:70:ILE:HD11	1.96	0.48
8:H:55:GLY:O	8:H:56:LYS:HG3	2.14	0.48
14:N:12:ARG:O	14:N:14:PRO:HD3	2.14	0.48
15:O:26:GLU:HB3	15:O:81:LEU:HD21	1.95	0.48
1:A:718:G:H5'	11:K:117:ASN:HB2	1.96	0.47
1:A:992:U:H4'	1:A:993:G:O5'	2.13	0.47
1:A:1257:U:H4'	1:A:1258:G:O5'	2.14	0.47
1:A:1270:C:H2'	1:A:1271:G:H8	1.78	0.47
8:H:104:ARG:O	8:H:105:ARG:HB2	2.13	0.47
1:A:18:C:C4	1:A:19:C:N4	2.82	0.47
1:A:96:U:H2'	1:A:97:G:H8	1.77	0.47
1:A:504:C:H42	1:A:541:G:H1	1.62	0.47
1:A:585:G:C6	1:A:586:C:C4	3.02	0.47
1:A:1266:G:N2	1:A:1270:C:C2	2.82	0.47
1:A:1504:G:H4'	1:A:1505:G:O5'	2.14	0.47
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.79	0.47
1:A:70:G:C2	1:A:100:C:C2	3.03	0.47
1:A:193:C:H2'	1:A:194:C:C6	2.49	0.47
1:A:262:A:H5''	20:T:76:ALA:HB2	1.95	0.47
1:A:530:G:H8	22:W:38:GLY:HA3	1.79	0.47
1:A:874:G:C2	1:A:875:C:C2	3.03	0.47
1:A:1017:G:C2	1:A:1018:C:C2	3.02	0.47
1:A:1396:A:H4'	1:A:1397:C:H5''	1.96	0.47
1:A:1435:G:H2'	1:A:1436:U:H6	1.71	0.47
1:A:1444:C:H2'	1:A:1445:C:C6	2.50	0.47
6:F:49:ALA:HB2	18:R:80:PRO:HA	1.91	0.47
10:J:37:PRO:HB2	10:J:70:ARG:NH1	2.27	0.47
23:X:89:LYS:HG3	23:X:119:THR:HB	1.96	0.47
1:A:25:C:H2'	1:A:26:A:H8	1.79	0.47
1:A:240:C:H2'	1:A:241:C:H6	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:G:C2	1:A:549:C:C2	3.03	0.47
1:A:613:C:H2'	1:A:614:A:C8	2.49	0.47
1:A:774:G:C2	1:A:806:C:C2	3.02	0.47
1:A:823:G:N2	1:A:824:C:C2	2.82	0.47
1:A:1255:G:O2'	1:A:1258:G:N3	2.46	0.47
1:A:1373:G:H5''	7:G:36:LYS:HB3	1.96	0.47
1:A:1444:C:H2'	1:A:1445:C:H6	1.80	0.47
1:A:1526:G:C6	1:A:1527:C:N4	2.83	0.47
2:B:146:GLN:HG2	2:B:153:ARG:HH21	1.79	0.47
4:D:108:LEU:HB3	4:D:110:PHE:CE1	2.49	0.47
16:P:11:SER:HB2	16:P:14:ASN:HD22	1.79	0.47
1:A:542:G:C6	1:A:543:C:N4	2.82	0.47
1:A:910:C:O2'	1:A:911:U:H5'	2.13	0.47
1:A:1274:G:H2'	1:A:1275:A:H8	1.79	0.47
2:B:25:ASN:HA	2:B:26:PRO:HD3	1.66	0.47
4:D:133:VAL:HG13	4:D:135:LEU:HD12	1.96	0.47
11:K:54:ARG:H	11:K:54:ARG:CD	2.24	0.47
1:A:17:U:H1'	1:A:1079:G:O2'	2.14	0.47
1:A:18:C:H2'	1:A:19:C:H6	1.79	0.47
1:A:63:C:H42	1:A:104:G:H1	1.62	0.47
1:A:69:G:C2	1:A:101:A:N1	2.83	0.47
1:A:246:A:C4	1:A:279:A:C6	3.03	0.47
1:A:399:G:N2	1:A:400:C:C2	2.82	0.47
1:A:1443:G:C2	1:A:1444:C:C4	3.02	0.47
12:L:9:GLN:HG2	12:L:12:ARG:HH21	1.80	0.47
1:A:73:G:H5''	1:A:76:C:OP2	2.15	0.47
1:A:827:U:O3'	8:H:19:VAL:HG21	2.15	0.47
1:A:975:A:H4'	1:A:976:G:H5'	1.97	0.47
1:A:1089:G:N2	1:A:1097:C:C2	2.83	0.47
1:A:1349:A:H5''	9:I:121:ARG:HB2	1.97	0.47
1:A:1365:G:C5	1:A:1366:C:C4	3.03	0.47
1:A:1418:A:H2'	1:A:1418:A:N3	2.29	0.47
1:A:1497:G:H2'	1:A:1498:U:O4'	2.13	0.47
3:C:140:ARG:O	3:C:143:GLU:HB2	2.14	0.47
4:D:25:ARG:CZ	4:D:30:LYS:HB3	2.45	0.47
4:D:64:LEU:HD12	4:D:203:VAL:HG21	1.95	0.47
4:D:150:GLU:HA	4:D:153:ARG:HE	1.79	0.47
11:K:84:VAL:HG21	11:K:91:ARG:NH2	2.30	0.47
12:L:30:ALA:CB	12:L:33:ARG:HE	2.27	0.47
13:M:23:TYR:HE1	13:M:70:LEU:HB3	1.80	0.47
1:A:540:G:H2'	1:A:541:G:H8	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:G:C2	1:A:849:C:C2	3.02	0.47
1:A:944:G:H2'	1:A:945:G:H5'	1.97	0.47
1:A:1008:C:N3	1:A:1022:G:N2	2.63	0.47
1:A:1508:G:C2	1:A:1509:C:C2	3.03	0.47
16:P:53:VAL:O	16:P:57:ARG:HD2	2.15	0.47
1:A:1287:A:H5'	1:A:1287:A:H8	1.80	0.47
7:G:125:MET:O	7:G:129:GLU:HG2	2.14	0.47
10:J:6:ILE:HA	10:J:97:GLU:O	2.14	0.47
1:A:25:C:H2'	1:A:26:A:C8	2.50	0.47
1:A:903:G:H2'	1:A:904:C:C6	2.50	0.47
1:A:1106:G:N1	1:A:1107:C:C4	2.83	0.47
1:A:1171:G:N2	1:A:1172:C:C2	2.83	0.47
1:A:1246:C:H2'	1:A:1247:U:C6	2.49	0.47
1:A:1445:C:N3	1:A:1458:G:C2	2.83	0.47
1:A:1527:C:H2'	1:A:1528:U:C6	2.50	0.47
11:K:100:ALA:O	11:K:102:GLY:N	2.47	0.47
13:M:23:TYR:CE1	13:M:70:LEU:HB3	2.50	0.47
1:A:115:G:O2'	1:A:289:G:H5''	2.15	0.46
1:A:132:C:C2	1:A:231:G:N2	2.83	0.46
1:A:172:A:H2'	1:A:174:C:C5	2.46	0.46
1:A:321:A:H61	1:A:332:G:H1	1.63	0.46
1:A:457:C:H2'	1:A:458:C:C6	2.50	0.46
1:A:715:A:H2'	1:A:716:A:C8	2.50	0.46
1:A:948:C:OP1	13:M:108:ARG:N	2.47	0.46
1:A:1070:U:OP1	5:E:20:GLN:HG3	2.16	0.46
1:A:1103:C:H5''	2:B:98:LEU:HD13	1.97	0.46
1:A:1241:G:N1	1:A:1242:C:C4	2.83	0.46
11:K:91:ARG:HH21	18:R:88:LYS:HZ1	1.59	0.46
1:A:861:G:C2	1:A:862:C:C2	3.03	0.46
1:A:881:G:C6	1:A:882:C:C4	3.03	0.46
1:A:895:G:H1	1:A:904:C:N4	2.11	0.46
1:A:1137:C:H4'	1:A:1138:G:C2	2.49	0.46
4:D:140:VAL:HG11	4:D:146:ILE:HD11	1.98	0.46
13:M:19:LEU:HB3	13:M:25:ILE:HG21	1.97	0.46
20:T:72:LEU:O	20:T:72:LEU:HG	2.15	0.46
23:X:16:VAL:HG12	23:X:55:PRO:HB2	1.96	0.46
1:A:109:A:H5'	1:A:110:C:H5	1.79	0.46
1:A:363:A:OP2	12:L:34:ARG:HG2	2.15	0.46
1:A:443:C:C2	1:A:492:G:N2	2.84	0.46
1:A:827:U:H5''	8:H:21:LYS:HE2	1.96	0.46
4:D:9:CYS:SG	4:D:26:CYS:SG	3.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:14:LEU:HD13	6:F:18:GLN:HB3	1.97	0.46
7:G:12:LEU:H	7:G:12:LEU:HD12	1.80	0.46
1:A:96:U:H2'	1:A:97:G:C8	2.50	0.46
1:A:251:G:N1	1:A:266:G:C6	2.83	0.46
1:A:377:G:H1	1:A:386:C:H42	1.62	0.46
1:A:789:U:H2'	1:A:791:G:OP2	2.14	0.46
1:A:868:C:H5'	1:A:873:A:N6	2.31	0.46
1:A:1355:G:H1	1:A:1367:C:N4	2.12	0.46
1:A:1384:C:H2'	1:A:1385:G:C8	2.50	0.46
1:A:1432:G:O2'	1:A:1468:A:N6	2.49	0.46
1:A:1464:G:C2	1:A:1465:C:C4	3.03	0.46
9:I:71:SER:HA	9:I:74:ILE:HD12	1.96	0.46
1:A:11:G:H2'	1:A:12:U:O4'	2.15	0.46
1:A:334:C:H2'	1:A:335:C:H6	1.80	0.46
1:A:369:C:H2'	1:A:370:C:C6	2.50	0.46
1:A:1493:A:H4'	1:A:1494:G:OP1	2.15	0.46
9:I:16:ARG:HH21	9:I:64:THR:HG21	1.81	0.46
11:K:83:ILE:HG12	11:K:109:VAL:HG12	1.97	0.46
1:A:778:G:C6	1:A:779:C:C4	3.04	0.46
1:A:1127:G:H5''	1:A:1128:C:OP2	2.16	0.46
9:I:26:VAL:HG13	9:I:63:ILE:HD12	1.97	0.46
1:A:240:C:H2'	1:A:241:C:C6	2.50	0.46
1:A:370:C:O2	1:A:482:A:O2'	2.34	0.46
1:A:542:G:C2	1:A:543:C:C2	3.04	0.46
1:A:564:C:O2	1:A:564:C:C2'	2.61	0.46
1:A:577:G:C2	1:A:578:C:C2	3.03	0.46
1:A:675:A:H2'	1:A:676:A:H8	1.81	0.46
1:A:814:A:H2'	1:A:816:A:H5''	1.98	0.46
1:A:1077:G:N3	1:A:1079:G:H8	2.12	0.46
1:A:1537:U:H6	1:A:1537:U:O5'	1.99	0.46
5:E:127:ASN:HD21	5:E:129:ILE:H	1.63	0.46
18:R:58:LEU:HB3	18:R:62:GLU:HB3	1.97	0.46
1:A:17:U:C2	1:A:18:C:C4	3.04	0.46
1:A:266:G:C3'	17:Q:67:LYS:HB2	2.34	0.46
4:D:19:LEU:HD13	4:D:21:LEU:HD22	1.98	0.46
22:W:32:ILE:HD13	22:W:32:ILE:H	1.81	0.46
1:A:244:U:O4	1:A:906:G:H1'	2.16	0.46
1:A:378:G:C6	1:A:379:C:N4	2.83	0.46
1:A:1445:C:C2	1:A:1458:G:N2	2.84	0.46
1:A:1484:C:H2'	1:A:1485:U:O4'	2.16	0.46
4:D:119:GLN:O	4:D:123:HIS:CD2	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:18:ARG:HB2	11:K:33:THR:HG23	1.97	0.46
19:S:22:LEU:HD11	19:S:31:ILE:HD11	1.98	0.46
19:S:40:ILE:HG21	19:S:62:ILE:HD11	1.98	0.46
1:A:21:G:C2	1:A:22:G:C6	3.04	0.46
1:A:39:G:C6	1:A:40:C:C4	3.04	0.46
1:A:155:C:H42	1:A:166:G:H1	1.64	0.46
1:A:246:A:O2'	17:Q:99:SER:HA	2.16	0.46
1:A:614:A:H2'	1:A:615:C:C6	2.51	0.46
1:A:938:A:H8	1:A:938:A:O5'	1.99	0.46
1:A:1459:C:OP1	20:T:28:ALA:HA	2.16	0.46
18:R:37:VAL:O	18:R:40:LEU:HB2	2.15	0.46
1:A:132:C:N3	1:A:231:G:C2	2.84	0.45
1:A:639:G:H2'	1:A:640:A:C8	2.51	0.45
1:A:1074:G:H1'	1:A:1102:A:C2	2.51	0.45
1:A:1315:U:O2'	1:A:1360:A:N3	2.48	0.45
4:D:42:GLN:C	4:D:44:GLY:H	2.18	0.45
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.50	0.45
13:M:3:ARG:H	13:M:57:ARG:HH22	1.63	0.45
23:X:5:TYR:CE2	23:X:65:TRP:HH2	2.30	0.45
1:A:289:G:C2	1:A:290:C:C2	3.04	0.45
1:A:678:U:H2'	1:A:679:C:H6	1.76	0.45
1:A:708:C:H2'	1:A:709:G:H8	1.82	0.45
1:A:951:G:C6	1:A:1231:G:C6	3.04	0.45
1:A:1102:A:H2'	1:A:1103:C:H6	1.76	0.45
1:A:1386:G:H2'	1:A:1387:G:C8	2.41	0.45
4:D:64:LEU:HA	4:D:67:ILE:HD12	1.98	0.45
5:E:10:MET:HA	5:E:32:VAL:HG23	1.97	0.45
6:F:12:PRO:HD3	6:F:58:GLY:HA2	1.97	0.45
6:F:33:TYR:HD1	6:F:71:ARG:HD2	1.81	0.45
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.98	0.45
1:A:15:G:H2'	1:A:16:A:C8	2.32	0.45
1:A:327:A:N3	1:A:329:A:H1'	2.31	0.45
1:A:524:G:C2	1:A:525:C:C4	3.05	0.45
1:A:974:A:OP2	14:N:32:SER:HB2	2.17	0.45
1:A:1007:C:C2	1:A:1023:G:N1	2.84	0.45
1:A:1220:G:H2'	1:A:1221:G:O4'	2.17	0.45
1:A:1241:G:C6	1:A:1242:C:N4	2.84	0.45
1:A:1493:A:C2	22:W:46:ARG:HA	2.52	0.45
4:D:98:GLU:HA	4:D:103:ASN:HD22	1.80	0.45
8:H:39:LEU:HD23	8:H:45:ILE:HG12	1.99	0.45
11:K:18:ARG:HB2	11:K:33:THR:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:43:SER:HB3	11:K:68:ALA:HB2	1.98	0.45
23:X:102:LYS:HD3	23:X:102:LYS:HA	1.78	0.45
1:A:15:G:H21	5:E:19:MET:HB2	1.80	0.45
1:A:79:G:H2'	1:A:80:G:C8	2.52	0.45
1:A:1138:G:H2'	1:A:1140:C:H5''	1.98	0.45
1:A:1162:C:N3	1:A:1175:G:C2	2.85	0.45
1:A:27:G:H2'	1:A:28:G:O4'	2.17	0.45
1:A:317:G:C2	1:A:337:C:C2	3.04	0.45
1:A:568:G:C6	1:A:569:C:N4	2.85	0.45
1:A:823:G:C6	1:A:824:C:N4	2.84	0.45
1:A:1050:G:C6	1:A:1051:C:N4	2.84	0.45
1:A:1105:A:H2'	1:A:1106:G:C8	2.49	0.45
1:A:1525:G:H2'	1:A:1526:G:C8	2.51	0.45
2:B:131:PRO:HA	2:B:135:GLN:OE1	2.17	0.45
1:A:284:G:H2'	1:A:285:G:H8	1.82	0.45
1:A:501:C:H2'	1:A:502:G:C8	2.51	0.45
1:A:524:G:H2'	1:A:525:C:C6	2.51	0.45
1:A:639:G:H2'	1:A:640:A:H8	1.82	0.45
1:A:1313:U:H2'	1:A:1314:C:H6	1.81	0.45
1:A:1351:U:H2'	1:A:1352:C:H6	1.81	0.45
1:A:1391:U:H2'	1:A:1392:G:C8	2.51	0.45
1:A:1408:A:H2'	1:A:1409:C:C6	2.51	0.45
14:N:37:PHE:HB3	14:N:39:LEU:HG	1.98	0.45
23:X:102:LYS:O	23:X:106:ILE:HG13	2.17	0.45
1:A:287:U:C2'	1:A:288:A:H5'	2.47	0.45
1:A:895:G:C2	1:A:896:C:C2	3.05	0.45
1:A:931:C:H2'	1:A:932:C:O4'	2.17	0.45
1:A:1422:G:H1	1:A:1478:C:H42	1.63	0.45
3:C:29:TYR:CE1	14:N:37:PHE:CD1	3.04	0.45
14:N:49:HIS:HE1	14:N:58:LYS:HE2	1.81	0.45
15:O:7:GLU:O	15:O:11:VAL:HG23	2.16	0.45
20:T:42:GLN:O	20:T:45:GLN:HB2	2.17	0.45
1:A:202:U:OP2	1:A:203:U:H5	2.00	0.45
1:A:285:G:H2'	1:A:286:G:O4'	2.16	0.45
1:A:391:G:H2'	1:A:392:G:O4'	2.17	0.45
1:A:439:A:H3'	1:A:441:A:H5''	1.98	0.45
1:A:544:G:OP1	4:D:62:GLN:HG3	2.17	0.45
1:A:573:A:H2'	1:A:574:A:O4'	2.17	0.45
1:A:916:G:H2'	1:A:917:G:C8	2.52	0.45
1:A:1116:C:H2'	1:A:1117:G:O4'	2.17	0.45
1:A:1420:C:H2'	1:A:1421:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:HIS:HD2	3:C:9:GLY:H	1.65	0.45
9:I:48:GLU:N	9:I:49:PRO:HD2	2.32	0.45
11:K:24:SER:C	11:K:26:ASN:H	2.20	0.45
19:S:49:ILE:HD12	19:S:62:ILE:HG21	1.98	0.45
1:A:319:G:C2	1:A:320:C:C2	3.05	0.45
1:A:335:C:H2'	1:A:336:C:H6	1.77	0.45
1:A:613:C:C2	1:A:628:G:N2	2.85	0.45
1:A:985:C:C2	1:A:1221:G:C2	3.05	0.45
1:A:1046:A:H3'	1:A:1047:G:H8	1.82	0.45
7:G:71:PRO:HD2	7:G:96:GLN:HB2	1.99	0.45
10:J:37:PRO:CB	10:J:70:ARG:HH11	2.30	0.45
1:A:233:C:H2'	1:A:234:C:C6	2.52	0.45
1:A:370:C:H42	1:A:391:G:H1	1.65	0.45
1:A:674:G:H2'	1:A:675:A:H8	1.82	0.45
1:A:928:G:H1	1:A:1389:C:N4	2.15	0.45
1:A:1055:A:H2	3:C:194:GLY:HA2	1.81	0.45
1:A:1246:C:H2'	1:A:1247:U:H6	1.82	0.45
1:A:1526:G:C2	1:A:1527:C:C2	3.05	0.45
16:P:67:THR:CG2	16:P:68:ASP:H	2.28	0.45
23:X:117:LYS:HE2	23:X:162:ASN:HB2	1.99	0.45
1:A:79:G:N1	1:A:91:C:C2	2.85	0.44
1:A:189:G:H2'	1:A:189(A):C:C6	2.52	0.44
1:A:444:C:H42	1:A:490:G:H1	1.65	0.44
1:A:502:G:OP1	12:L:118:SER:N	2.46	0.44
1:A:516:U:H4'	22:W:2:LYS:HD2	1.99	0.44
1:A:939:G:C2	1:A:940:C:N3	2.85	0.44
2:B:211:ILE:H	2:B:211:ILE:HG13	1.58	0.44
21:V:3:LYS:O	21:V:11:GLY:HA2	2.17	0.44
1:A:33:A:H2'	1:A:34:C:C6	2.52	0.44
1:A:279:A:N1	17:Q:98:LEU:HD23	2.30	0.44
1:A:542:G:H2'	1:A:543:C:C6	2.52	0.44
1:A:1015:A:H2'	1:A:1016:A:C8	2.52	0.44
1:A:1101:A:H61	2:B:103:THR:HG21	1.82	0.44
1:A:1430:C:C2	1:A:1471:G:N2	2.84	0.44
1:A:1487:G:H5''	1:A:1488:G:OP1	2.17	0.44
1:A:1509:C:H2'	1:A:1510:U:O4'	2.18	0.44
3:C:29:TYR:CD1	14:N:36:PHE:CE2	3.06	0.44
11:K:84:VAL:HG11	11:K:95:ILE:HD11	1.98	0.44
1:A:551:U:H2'	1:A:552:U:C6	2.51	0.44
1:A:763:G:C2	1:A:764:C:C2	3.06	0.44
1:A:903:G:C2	1:A:904:C:C2	3.04	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:G:C8	1:A:1066:C:C2	3.06	0.44
1:A:1251:A:H2'	1:A:1252:A:O4'	2.17	0.44
1:A:1283:G:C6	1:A:1284:C:N4	2.85	0.44
1:A:1329:A:H5''	13:M:26:GLY:N	2.31	0.44
1:A:1391:U:H2'	1:A:1392:G:H8	1.81	0.44
1:A:1541:U:O3'	18:R:19:LYS:HB3	2.16	0.44
2:B:18:GLY:HA2	2:B:42:ILE:HD12	1.98	0.44
2:B:166:ASP:C	2:B:168:THR:H	2.21	0.44
4:D:13:ARG:HH12	4:D:40:PRO:HA	1.81	0.44
4:D:43:HIS:CD2	4:D:43:HIS:H	2.36	0.44
4:D:158:ILE:H	4:D:158:ILE:HG13	1.55	0.44
19:S:30:LEU:H	19:S:48:THR:HB	1.82	0.44
1:A:625:G:OP1	16:P:9:PHE:HB3	2.18	0.44
1:A:1082:G:C8	1:A:1082:G:O5'	2.69	0.44
1:A:1144:G:N2	1:A:1146:A:H62	2.15	0.44
1:A:1151:A:H5'	10:J:41:PRO:HA	1.99	0.44
3:C:24:ALA:HB2	3:C:32:LEU:HD12	2.00	0.44
4:D:173:TRP:HB2	4:D:187:ARG:O	2.18	0.44
7:G:24:THR:HA	7:G:27:ILE:HD12	1.99	0.44
7:G:29:LYS:HB3	7:G:105:VAL:HG21	1.99	0.44
1:A:51:A:C6	1:A:353:A:C2	3.05	0.44
1:A:188:C:H5'	20:T:89:ARG:HD3	2.00	0.44
1:A:455:C:H2'	1:A:456:C:H6	1.81	0.44
1:A:571:U:H5''	1:A:819:A:C5	2.53	0.44
1:A:601:C:C2	1:A:638:G:N2	2.85	0.44
1:A:604:G:H2'	1:A:605:U:O4'	2.17	0.44
1:A:827:U:C4	1:A:872:A:N6	2.73	0.44
1:A:942:G:C6	1:A:1342:C:N3	2.84	0.44
1:A:1017:G:C6	1:A:1018:C:C4	3.06	0.44
1:A:1106:G:H2'	1:A:1107:C:C6	2.53	0.44
1:A:1163:C:H2'	1:A:1164:G:C8	2.45	0.44
1:A:1304:G:H21	1:A:1333:A:H62	1.65	0.44
1:A:1438:G:N2	1:A:1439:C:C2	2.85	0.44
3:C:14:ILE:H	3:C:14:ILE:HG12	1.40	0.44
3:C:116:VAL:O	3:C:120:VAL:HG23	2.18	0.44
4:D:108:LEU:HB3	4:D:110:PHE:HE1	1.83	0.44
5:E:33:VAL:HG12	5:E:112:LEU:HD22	2.00	0.44
1:A:344:A:H4'	1:A:345:C:OP2	2.18	0.44
1:A:624:C:O3'	16:P:10:GLY:HA2	2.18	0.44
1:A:751:U:C5	1:A:752:G:C5	3.05	0.44
1:A:761:G:C5	1:A:762:C:C4	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:A:O2'	1:A:865:A:O4'	2.35	0.44
1:A:920:U:C2	1:A:921:U:C5	3.05	0.44
1:A:1001(A):G:N2	1:A:1040:U:C2	2.86	0.44
1:A:1007:C:N3	1:A:1023:G:C6	2.85	0.44
3:C:50:ALA:HA	3:C:72:LYS:HB2	1.98	0.44
3:C:153:VAL:HG22	3:C:198:VAL:HA	2.00	0.44
15:O:54:ARG:HG3	15:O:55:GLY:N	2.32	0.44
1:A:18:C:H4'	1:A:1078:U:H1'	1.99	0.44
1:A:105:G:C2	1:A:106:C:C2	3.06	0.44
1:A:1110:A:H2'	1:A:1111:A:O4'	2.18	0.44
1:A:1276:G:H2'	1:A:1277:C:O4'	2.18	0.44
10:J:7:LYS:HG2	10:J:71:LEU:CD2	2.48	0.44
23:X:17:ARG:HB2	23:X:54:PRO:O	2.18	0.44
1:A:291:C:O2	1:A:310:G:C2	2.71	0.44
1:A:334:C:H2'	1:A:335:C:C6	2.52	0.44
1:A:1419:G:C2	1:A:1420:C:C2	3.05	0.44
11:K:50:TYR:CD2	11:K:54:ARG:HB2	2.52	0.44
12:L:75:HIS:HB2	12:L:77:LEU:HD13	2.00	0.44
1:A:6:G:N2	5:E:98:THR:OG1	2.51	0.44
1:A:236:G:C6	1:A:237:C:C4	3.06	0.44
1:A:307:C:C6	1:A:308:C:C5	3.05	0.44
1:A:926:G:C8	1:A:926:G:O5'	2.71	0.44
1:A:1518:A:H2'	1:A:1519:A:H8	1.83	0.44
12:L:60:LEU:HD11	12:L:85:ILE:HD13	2.00	0.44
1:A:237:C:H2'	1:A:238:G:H8	1.83	0.43
1:A:836:G:C6	1:A:851:G:C6	3.06	0.43
1:A:1134:G:N2	1:A:1141:C:C2	2.85	0.43
1:A:1401:G:O6	1:A:1504:G:N2	2.51	0.43
3:C:55:VAL:HG22	3:C:68:VAL:HG13	1.98	0.43
1:A:674:G:H2'	1:A:675:A:C8	2.53	0.43
1:A:1081:G:C2'	1:A:1082:G:H8	2.00	0.43
1:A:1253:G:C2	1:A:1254:C:C2	3.06	0.43
3:C:91:LEU:HG	3:C:99:VAL:HG11	1.99	0.43
10:J:37:PRO:C	10:J:72:VAL:HG22	2.38	0.43
10:J:38:ILE:HA	10:J:39:PRO:HD3	1.87	0.43
16:P:21:VAL:HG12	16:P:34:GLU:HB3	2.00	0.43
1:A:60:A:H8	1:A:60:A:OP1	2.01	0.43
1:A:158:G:H8	1:A:158:G:O5'	2.01	0.43
1:A:276:G:C2	1:A:277:C:C2	3.06	0.43
1:A:792:A:H4'	1:A:793:U:C5'	2.49	0.43
1:A:942:G:C2	1:A:1342:C:O2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:C:C1'	1:A:1168:A:H2	2.31	0.43
1:A:1241:G:C2	1:A:1242:C:C4	3.06	0.43
1:A:1462:G:N2	1:A:1463:C:C2	2.87	0.43
16:P:48:TRP:CD1	16:P:48:TRP:N	2.86	0.43
17:Q:92:ARG:O	17:Q:95:TYR:HB2	2.18	0.43
18:R:25:THR:HB	18:R:42:ARG:HH22	1.83	0.43
1:A:767:A:H2'	1:A:768:A:O4'	2.17	0.43
1:A:778:G:C2	1:A:779:C:C2	3.07	0.43
1:A:1343:G:C6	1:A:1344:C:N3	2.87	0.43
1:A:1381:U:H1'	7:G:78:ARG:HE	1.84	0.43
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.99	0.43
4:D:119:GLN:HG2	4:D:120:LEU:N	2.33	0.43
12:L:102:ARG:CZ	12:L:110:VAL:HG22	2.48	0.43
1:A:29:G:N2	1:A:555:C:C2	2.86	0.43
1:A:70:G:C2	1:A:100:C:O2	2.71	0.43
1:A:174:C:H2'	1:A:175:C:H6	1.83	0.43
1:A:291:C:H2'	1:A:292:G:C8	2.53	0.43
1:A:321:A:H2'	1:A:322:C:C6	2.53	0.43
1:A:457:C:H2'	1:A:458:C:H6	1.84	0.43
1:A:602:A:H2'	1:A:603:U:O4'	2.17	0.43
1:A:667:G:H2'	1:A:668:G:C8	2.51	0.43
1:A:828:A:H2'	1:A:829:G:O4'	2.18	0.43
1:A:886:G:N1	1:A:912:C:C2	2.86	0.43
8:H:53:VAL:HG23	8:H:58:TYR:CD2	2.54	0.43
11:K:84:VAL:CG2	11:K:91:ARG:HH22	2.30	0.43
12:L:90:VAL:HG11	12:L:93:LEU:HD12	2.00	0.43
1:A:245:C:C2	1:A:284:G:C2	3.06	0.43
1:A:662:G:C2	1:A:744:C:O2	2.71	0.43
1:A:734:G:C6	1:A:735:C:C4	3.07	0.43
1:A:794:A:H2'	1:A:795:C:H6	1.84	0.43
1:A:1081:G:OP1	5:E:18:ARG:HA	2.18	0.43
1:A:1373:G:H5''	7:G:36:LYS:CB	2.49	0.43
3:C:29:TYR:HE1	14:N:37:PHE:CD1	2.36	0.43
3:C:30:ARG:HG2	14:N:37:PHE:O	2.17	0.43
12:L:93:LEU:HA	12:L:94:PRO:HD3	1.68	0.43
17:Q:51:TYR:HE2	17:Q:76:LEU:HB2	1.83	0.43
1:A:115:G:C2	1:A:289:G:N7	2.87	0.43
1:A:137:C:C2	1:A:227:G:C2	3.06	0.43
1:A:166:G:H2'	1:A:167:G:H8	1.83	0.43
1:A:407:G:H2'	1:A:408:A:C8	2.53	0.43
1:A:677:U:H3	1:A:713:G:H1	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:HIS:HB2	8:H:104:ARG:HD2	2.01	0.43
5:E:88:LYS:HB3	5:E:123:LEU:HB2	2.00	0.43
7:G:16:LEU:H	7:G:16:LEU:HG	1.54	0.43
10:J:60:ARG:NH1	10:J:60:ARG:CB	2.81	0.43
18:R:26:LEU:HD13	18:R:42:ARG:HE	1.84	0.43
1:A:237:C:H2'	1:A:238:G:C8	2.54	0.43
1:A:250:A:H1'	1:A:252:U:C4	2.54	0.43
1:A:430:A:P	4:D:8:VAL:H	2.41	0.43
1:A:529:G:H5'	1:A:530:G:OP2	2.19	0.43
1:A:651:C:H2'	1:A:652:U:C6	2.53	0.43
1:A:668:G:H2'	1:A:669:U:C6	2.54	0.43
1:A:698:G:C6	1:A:699:C:N4	2.87	0.43
1:A:861:G:C6	1:A:862:C:C4	3.07	0.43
1:A:922:G:C2	1:A:923:A:C4	3.06	0.43
1:A:1081:G:P	5:E:18:ARG:HA	2.58	0.43
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.33	0.43
9:I:26:VAL:HB	9:I:33:PHE:HB2	2.01	0.43
10:J:57:LYS:HA	10:J:60:ARG:HH22	1.84	0.43
22:W:55:VAL:HG13	22:W:66:ARG:H	1.82	0.43
1:A:39:G:C2	1:A:40:C:C2	3.07	0.43
1:A:444:C:C2	1:A:491:G:N2	2.87	0.43
1:A:502:G:H2'	1:A:503:C:O4'	2.19	0.43
1:A:560:U:H2'	5:E:123:LEU:HD22	2.01	0.43
1:A:740:U:H2'	1:A:741:G:H8	1.84	0.43
1:A:1192:C:H2'	1:A:1193:G:O4'	2.18	0.43
1:A:1419:G:C6	1:A:1420:C:C4	3.07	0.43
1:A:1542:U:O2	1:A:1542:U:H2'	2.18	0.43
14:N:15:LYS:HD3	14:N:19:ARG:HH12	1.83	0.43
1:A:15:G:N1	1:A:921:U:C2	2.87	0.43
1:A:73:G:N1	1:A:76:C:C2	2.87	0.43
1:A:250:A:H4'	1:A:251:G:O5'	2.19	0.43
1:A:276:G:O2'	17:Q:68:ARG:NH2	2.49	0.43
1:A:442:C:H2'	1:A:443:C:H6	1.79	0.43
1:A:476:G:H2'	1:A:477:A:C8	2.54	0.43
1:A:769:G:C2	1:A:770:C:C4	3.07	0.43
1:A:836:G:C6	1:A:837:G:C6	3.07	0.43
1:A:1050:G:N2	1:A:1051:C:C2	2.87	0.43
3:C:6:HIS:HA	3:C:7:PRO:HD3	1.85	0.43
3:C:62:ASP:HA	3:C:97:LYS:HE3	2.00	0.43
4:D:3:ARG:HD2	4:D:118:ARG:HD3	2.01	0.43
4:D:30:LYS:C	4:D:32:ALA:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:ARG:HD3	5:E:28:PHE:CE1	2.54	0.43
1:A:157:G:C6	1:A:165:C:N3	2.87	0.42
1:A:399:G:H2'	1:A:400:C:C6	2.53	0.42
1:A:416:G:C6	1:A:417:C:C4	3.07	0.42
1:A:806:C:H2'	1:A:807:A:C8	2.54	0.42
1:A:1141:C:H2'	1:A:1142:G:H8	1.84	0.42
1:A:1256:A:C2'	3:C:27:LYS:HZ1	2.32	0.42
1:A:1484:C:H6	1:A:1484:C:O5'	2.01	0.42
1:A:1508:G:C6	1:A:1509:C:C4	3.07	0.42
2:B:33:TYR:HB3	2:B:41:ILE:HG22	2.01	0.42
8:H:25:ASP:OD2	8:H:53:VAL:HG21	2.18	0.42
1:A:115:G:C2	1:A:289:G:C5	3.07	0.42
1:A:621:A:H2'	1:A:622:A:H8	1.84	0.42
1:A:1189:C:H5''	3:C:5:ILE:HG12	2.00	0.42
1:A:1393:U:H2'	1:A:1395:C:H5	1.83	0.42
2:B:55:PHE:HD1	2:B:55:PHE:HA	1.74	0.42
8:H:6:ILE:HD12	8:H:35:ILE:HD12	2.00	0.42
1:A:258:G:H2'	1:A:259:G:H8	1.84	0.42
1:A:456:C:C2	1:A:476:G:C2	3.07	0.42
1:A:976:G:N2	1:A:1363:C:H5''	2.34	0.42
1:A:1253:G:C6	1:A:1254:C:C4	3.07	0.42
3:C:135:LYS:O	3:C:139:GLN:HG2	2.19	0.42
4:D:150:GLU:O	4:D:153:ARG:HB2	2.19	0.42
8:H:3:THR:HG23	8:H:4:ASP:H	1.83	0.42
9:I:114:TYR:CD2	10:J:58:ASP:O	2.66	0.42
11:K:21:ILE:HG23	11:K:30:VAL:HG22	2.01	0.42
1:A:104:G:C2	1:A:105:G:C5	3.07	0.42
1:A:333:G:C2	1:A:334:C:C2	3.08	0.42
1:A:502:G:C2	1:A:503:C:C2	3.07	0.42
1:A:786:G:N2	1:A:797:C:C2	2.88	0.42
1:A:895:G:C6	1:A:896:C:C4	3.07	0.42
1:A:1172:C:H2'	1:A:1173:G:C8	2.51	0.42
1:A:1368:G:N1	1:A:1369:C:C4	2.88	0.42
2:B:115:LEU:HD11	2:B:146:GLN:HG3	2.01	0.42
8:H:134:ILE:H	8:H:134:ILE:HG13	1.62	0.42
1:A:27:G:H2'	1:A:28:G:H8	1.83	0.42
1:A:41:G:C6	1:A:402:G:C6	3.07	0.42
1:A:293:G:C4	1:A:305:G:N2	2.88	0.42
1:A:333:G:N1	1:A:334:C:C4	2.87	0.42
1:A:357:G:OP1	1:A:367:U:H5''	2.20	0.42
1:A:399:G:C2	1:A:400:C:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:G:OP1	4:D:74:GLN:HG3	2.19	0.42
1:A:580:U:O4	1:A:581:G:C6	2.73	0.42
1:A:810:C:H2'	1:A:811:C:O4'	2.19	0.42
1:A:1119:C:C2	1:A:1155:G:N2	2.87	0.42
20:T:61:SER:O	20:T:65:LYS:HG2	2.18	0.42
1:A:112:G:C2	1:A:113:G:C8	3.08	0.42
1:A:396:G:O2'	1:A:398:C:OP1	2.24	0.42
1:A:577:G:N1	1:A:578:C:C4	2.87	0.42
1:A:829:G:O4'	2:B:26:PRO:HG2	2.18	0.42
1:A:874:G:C6	1:A:875:C:C4	3.07	0.42
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.54	0.42
4:D:36:ARG:HD3	4:D:38:TYR:CE2	2.49	0.42
11:K:92:GLU:HA	11:K:95:ILE:HD12	2.01	0.42
1:A:310:G:C6	1:A:311:C:C4	3.07	0.42
1:A:617:G:C6	1:A:618:C:N4	2.87	0.42
1:A:768:A:C5	1:A:769:G:C8	3.08	0.42
1:A:823:G:C2	1:A:824:C:C2	3.08	0.42
1:A:939:G:H1'	1:A:1375:A:C2	2.54	0.42
1:A:966:G:C6	1:A:967:C:C4	3.07	0.42
1:A:998:G:N1	1:A:999:C:C4	2.88	0.42
1:A:1081:G:OP1	5:E:18:ARG:CA	2.68	0.42
1:A:1095:U:C4	1:A:1096:C:N4	2.87	0.42
1:A:1270:C:H2'	1:A:1271:G:C8	2.54	0.42
1:A:1286:A:H2'	1:A:1287:A:H4'	2.02	0.42
1:A:1361:G:C6	1:A:1362:C:N3	2.87	0.42
4:D:89:THR:HA	4:D:92:VAL:HG12	2.02	0.42
7:G:26:PHE:O	7:G:30:ILE:HG13	2.20	0.42
8:H:29:SER:HB3	8:H:32:LYS:CG	2.48	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	3.08	0.42
1:A:590:C:N3	1:A:650:G:C2	2.87	0.42
1:A:1123:A:H4'	10:J:36:GLY:HA3	2.02	0.42
1:A:1158:C:O2	1:A:1158:C:H2'	2.20	0.42
3:C:29:TYR:CE1	14:N:37:PHE:CE1	3.07	0.42
3:C:34:LEU:HD11	14:N:25:VAL:HG21	2.01	0.42
8:H:51:VAL:HB	8:H:52:ASP:H	1.73	0.42
13:M:22:ILE:HG22	13:M:24:GLY:H	1.85	0.42
1:A:187:C:N3	20:T:105:SER:HB2	2.35	0.42
1:A:189(C):C:C2	1:A:189(I):G:C2	3.08	0.42
1:A:200:G:C2	1:A:218:C:C2	3.08	0.42
1:A:310:G:C2	1:A:311:C:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:G:C6	1:A:403:C:C4	3.08	0.42
1:A:617:G:N1	1:A:618:C:C4	2.88	0.42
1:A:1063:C:O5'	1:A:1064:G:H2'	2.19	0.42
1:A:1356:G:N2	1:A:1367:C:C2	2.88	0.42
3:C:113:ALA:N	3:C:114:PRO:CD	2.83	0.42
5:E:41:VAL:HG23	5:E:67:VAL:HG12	2.02	0.42
6:F:30:LEU:HD22	6:F:65:VAL:HG11	2.01	0.42
16:P:67:THR:HG22	16:P:68:ASP:N	2.29	0.42
1:A:17:U:H2'	1:A:18:C:C5	2.49	0.42
1:A:35:G:C5	1:A:36:C:C4	3.07	0.42
1:A:377:G:H1	1:A:386:C:N4	2.17	0.42
1:A:495:A:H4'	1:A:496:A:OP1	2.19	0.42
1:A:891:U:H2'	1:A:892:A:H8	1.84	0.42
1:A:1405:G:H2'	1:A:1406:U:C6	2.55	0.42
1:A:1411:C:H2'	1:A:1412:C:O4'	2.20	0.42
1:A:1478:C:H2'	1:A:1479:C:C6	2.55	0.42
5:E:48:ALA:HB1	5:E:53:LEU:HD23	2.02	0.42
8:H:96:GLY:HA2	8:H:130:GLY:HA3	2.01	0.42
11:K:86:GLY:O	11:K:91:ARG:HD2	2.20	0.42
18:R:51:LEU:HB3	18:R:55:ARG:HB2	2.02	0.42
1:A:90:U:O2'	1:A:91:C:H5'	2.20	0.41
1:A:178:C:H2'	1:A:179:A:H8	1.85	0.41
1:A:306:G:C6	1:A:307:C:C4	3.08	0.41
1:A:488:C:H2'	1:A:489:C:C6	2.55	0.41
1:A:509:A:H4'	1:A:510:A:OP1	2.19	0.41
1:A:942:G:N2	1:A:943:U:H1'	2.35	0.41
1:A:947:G:C2	1:A:948:C:C2	3.08	0.41
1:A:985:C:H2'	1:A:986:A:C8	2.55	0.41
1:A:1050:G:C2	1:A:1051:C:C2	3.07	0.41
1:A:1510:U:H2'	1:A:1511:G:C8	2.55	0.41
1:A:1537:U:H3	24:Y:28:A:H61	1.68	0.41
5:E:11:ILE:HB	5:E:31:LEU:HD12	2.02	0.41
6:F:41:GLU:HB2	6:F:62:TRP:HE3	1.85	0.41
1:A:289:G:C6	1:A:290:C:C4	3.08	0.41
1:A:502:G:C6	1:A:503:C:C4	3.08	0.41
1:A:1198:G:C5	1:A:1199:U:C4	3.08	0.41
4:D:67:ILE:O	4:D:114:ARG:HD2	2.19	0.41
1:A:241:C:C2	1:A:286:G:N2	2.89	0.41
1:A:276:G:H2'	1:A:277:C:C6	2.55	0.41
1:A:613:C:H42	1:A:627:G:H1	1.68	0.41
1:A:673:G:H1	1:A:717:C:H42	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:874:G:N2	1:A:875:C:C2	2.88	0.41
1:A:942:G:N1	1:A:1342:C:C2	2.88	0.41
1:A:966:G:C2	1:A:967:C:C2	3.08	0.41
1:A:1106:G:C2	1:A:1107:C:C2	3.08	0.41
1:A:1423:G:C2	1:A:1424:C:C2	3.09	0.41
6:F:2:ARG:HB2	6:F:4:TYR:CE2	2.55	0.41
11:K:27:ASN:HA	11:K:56:GLY:HA2	2.02	0.41
15:O:9:GLN:HA	15:O:12:ILE:HD12	2.01	0.41
18:R:25:THR:HB	18:R:42:ARG:NH2	2.35	0.41
1:A:129(A):G:O2'	1:A:189(F):U:H2'	2.20	0.41
1:A:324:G:H8	1:A:324:G:OP2	2.03	0.41
1:A:352:C:N3	1:A:356:A:N6	2.67	0.41
1:A:568:G:N1	1:A:883:C:C4	2.89	0.41
1:A:590:C:C2	1:A:650:G:N2	2.88	0.41
1:A:681:C:H42	1:A:709:G:H1	1.67	0.41
1:A:725:G:C2	1:A:726:C:C2	3.09	0.41
1:A:1216:G:N2	1:A:1217:C:C2	2.88	0.41
1:A:1526:G:C6	1:A:1527:C:C4	3.08	0.41
2:B:105:PHE:HA	2:B:108:ILE:HG22	2.03	0.41
3:C:148:GLY:HA3	3:C:172:ARG:O	2.20	0.41
4:D:173:TRP:CD1	4:D:174:LEU:HG	2.56	0.41
5:E:80:ILE:CD1	5:E:138:ALA:HB1	2.49	0.41
7:G:71:PRO:HD3	7:G:103:TRP:HZ3	1.85	0.41
10:J:20:ALA:HB1	10:J:37:PRO:HB3	2.02	0.41
1:A:130:A:OP1	1:A:130:A:C8	2.72	0.41
1:A:197:A:H4'	1:A:198:G:O5'	2.20	0.41
1:A:333:G:C6	1:A:334:C:N4	2.88	0.41
1:A:381:C:H2'	1:A:382:A:O4'	2.20	0.41
1:A:841:U:H6	1:A:841:U:H5''	1.86	0.41
1:A:886:G:C2	1:A:912:C:O2	2.73	0.41
1:A:937:A:H1'	1:A:1379:G:N2	2.36	0.41
1:A:1005:A:O4'	1:A:1036:G:N2	2.53	0.41
1:A:1068:G:C2	1:A:1069:C:C2	3.09	0.41
1:A:1171:G:C2	1:A:1172:C:C2	3.09	0.41
1:A:1464:G:C2	1:A:1465:C:N3	2.88	0.41
10:J:17:ASP:CG	10:J:70:ARG:HH22	2.06	0.41
1:A:417:C:N4	1:A:418:C:N4	2.69	0.41
1:A:521:G:C2	1:A:522:C:C4	3.08	0.41
1:A:675:A:H2'	1:A:676:A:C8	2.56	0.41
1:A:916:G:H2'	1:A:917:G:H8	1.83	0.41
1:A:1158:C:O2	1:A:1158:C:C2'	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1458:G:OP1	20:T:32:ALA:HA	2.21	0.41
1:A:1464:G:C6	1:A:1465:C:N4	2.88	0.41
2:B:77:ALA:HB2	2:B:211:ILE:HG21	2.01	0.41
5:E:79:GLU:HA	5:E:91:LEU:O	2.21	0.41
8:H:36:LEU:HD12	8:H:59:LEU:HD22	2.02	0.41
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.55	0.41
1:A:216:G:C2	1:A:217:C:N3	2.88	0.41
1:A:306:G:C2	1:A:307:C:C2	3.08	0.41
1:A:376:G:H2'	1:A:377:G:C8	2.52	0.41
1:A:695:A:OP2	11:K:53:SER:N	2.53	0.41
1:A:830:G:H2'	1:A:831:U:O4'	2.20	0.41
1:A:1004:A:N7	1:A:1037:C:N3	2.68	0.41
1:A:1096:C:C2	1:A:1097:C:C5	3.08	0.41
1:A:1171:G:N1	1:A:1172:C:C4	2.89	0.41
1:A:1413:A:H2'	1:A:1414:U:O4'	2.21	0.41
1:A:1523:G:H2'	1:A:1524:C:C6	2.56	0.41
12:L:93:LEU:O	12:L:96:VAL:HB	2.20	0.41
14:N:3:ARG:CZ	14:N:6:LEU:HD11	2.51	0.41
16:P:59:TRP:C	16:P:62:VAL:HG22	2.39	0.41
19:S:17:GLU:HA	19:S:20:LEU:HG	2.02	0.41
1:A:265:G:H2'	1:A:267:C:H5	1.85	0.41
1:A:427:U:H4'	1:A:541:G:H5''	2.03	0.41
1:A:691:G:C8	11:K:26:ASN:HB3	2.56	0.41
1:A:769:G:N3	1:A:769:G:H2'	2.36	0.41
1:A:903:G:C6	1:A:904:C:C4	3.09	0.41
1:A:1468:A:H2'	1:A:1469:G:O4'	2.21	0.41
4:D:69:GLY:C	4:D:70:ILE:HG13	2.41	0.41
13:M:16:ASP:HB3	13:M:34:LEU:HD11	2.03	0.41
1:A:197:A:N6	1:A:221:C:H4'	2.35	0.41
1:A:299:G:C6	1:A:300:A:C6	3.09	0.41
1:A:500:G:C2	1:A:501:C:C2	3.09	0.41
1:A:563:A:N3	1:A:563:A:H2'	2.35	0.41
1:A:577:G:C6	1:A:578:C:C4	3.08	0.41
1:A:1048:G:C2	1:A:1210:C:C2	3.08	0.41
1:A:1119:C:H2'	1:A:1120:G:O4'	2.21	0.41
1:A:1283:G:N2	1:A:1284:C:C2	2.89	0.41
1:A:1288:A:H2'	1:A:1289:A:H8	1.86	0.41
1:A:1444:C:H6	1:A:1444:C:O5'	2.04	0.41
2:B:54:THR:HG21	2:B:185:ILE:HG23	2.02	0.41
2:B:215:LEU:O	2:B:219:VAL:HG23	2.21	0.41
3:C:29:TYR:CD2	3:C:29:TYR:O	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:ALA:HA	3:C:100:ALA:O	2.21	0.41
5:E:127:ASN:HA	5:E:128:PRO:HD2	1.83	0.41
10:J:60:ARG:CZ	10:J:60:ARG:CB	2.95	0.41
20:T:43:LEU:HD11	20:T:55:ILE:HD13	2.03	0.41
1:A:666:G:C6	1:A:741:G:C5	3.09	0.41
1:A:716:A:C6	1:A:717:C:C4	3.10	0.41
1:A:763:G:C6	1:A:764:C:C4	3.09	0.41
1:A:794:A:H2'	1:A:795:C:C6	2.55	0.41
1:A:861:G:H2'	1:A:862:C:C6	2.56	0.41
1:A:1106:G:C2	1:A:1107:C:N3	2.89	0.41
1:A:1323:G:H4'	1:A:1363:C:C2	2.56	0.41
1:A:1341:U:H2'	1:A:1342:C:C6	2.55	0.41
1:A:1374:A:O2'	7:G:28:ASN:HB3	2.21	0.41
1:A:1514:C:H2'	1:A:1515:C:C6	2.56	0.41
15:O:67:LEU:HD11	15:O:87:ILE:HG21	2.02	0.41
16:P:12:LYS:C	16:P:14:ASN:H	2.24	0.41
1:A:673:G:H2'	1:A:674:G:C8	2.56	0.40
1:A:749:C:H2'	1:A:750:G:H8	1.86	0.40
1:A:784:C:C2	1:A:799:G:N2	2.89	0.40
1:A:886:G:C4	1:A:887:G:C8	3.08	0.40
1:A:1423:G:C6	1:A:1424:C:C4	3.09	0.40
1:A:1425:U:H2'	1:A:1426:C:C6	2.56	0.40
1:A:1495:U:O2'	23:X:98:ASP:OD2	2.31	0.40
1:A:1522:U:H2'	1:A:1523:G:H8	1.85	0.40
1:A:1534:A:H2'	1:A:1535:C:C6	2.56	0.40
3:C:13:GLY:HA2	14:N:57:ARG:HE	1.85	0.40
7:G:39:ALA:HA	7:G:42:ILE:HD12	2.03	0.40
15:O:75:PRO:O	15:O:78:TYR:HB3	2.22	0.40
1:A:977:A:H1'	1:A:982:U:O4	2.21	0.40
1:A:1274:G:H2'	1:A:1275:A:C8	2.57	0.40
1:A:1300:G:HO2'	1:A:1303:C:H41	1.65	0.40
4:D:61:LYS:HD2	4:D:207:TYR:HE1	1.86	0.40
5:E:13:ILE:HA	5:E:29:GLY:O	2.22	0.40
10:J:17:ASP:OD1	10:J:70:ARG:NH1	2.54	0.40
14:N:6:LEU:C	14:N:8:GLU:H	2.23	0.40
18:R:61:LYS:HG2	18:R:62:GLU:N	2.37	0.40
22:W:55:VAL:HA	22:W:66:ARG:O	2.19	0.40
1:A:289:G:N1	1:A:290:C:C4	2.89	0.40
1:A:394:G:C2	1:A:395:C:C2	3.10	0.40
1:A:832:C:O2	1:A:855:G:C2	2.74	0.40
1:A:1198:G:H2'	1:A:1199:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1540:U:H3	24:Y:25:A:H61	1.67	0.40
2:B:130:ARG:HD2	2:B:130:ARG:N	2.36	0.40
3:C:30:ARG:NH1	3:C:30:ARG:CB	2.73	0.40
5:E:127:ASN:O	5:E:131:ILE:HG12	2.20	0.40
6:F:3:ARG:HB3	6:F:93:SER:HB2	2.04	0.40
7:G:50:ILE:HD11	7:G:124:LEU:HB3	2.03	0.40
10:J:17:ASP:CA	10:J:70:ARG:NH2	2.85	0.40
10:J:90:LEU:HA	10:J:91:PRO:HD3	1.76	0.40
13:M:16:ASP:HB3	13:M:34:LEU:CD1	2.52	0.40
14:N:53:LEU:HA	14:N:54:PRO:HD2	1.85	0.40
15:O:87:ILE:HG22	15:O:88:ARG:H	1.87	0.40
16:P:70:ALA:O	16:P:74:LEU:HD12	2.21	0.40
19:S:53:ASN:ND2	19:S:75:ALA:HB1	2.37	0.40
20:T:43:LEU:HB3	20:T:52:ALA:HB2	2.03	0.40
1:A:102:G:C2	1:A:103:C:C2	3.09	0.40
1:A:319:G:C6	1:A:320:C:C4	3.09	0.40
1:A:407:G:H1'	4:D:119:GLN:NE2	2.33	0.40
1:A:926:G:O5'	1:A:926:G:H8	2.04	0.40
1:A:975:A:H4'	1:A:976:G:C5'	2.51	0.40
1:A:1099:G:C6	1:A:1100:C:C2	3.08	0.40
1:A:1169:A:H2'	1:A:1170:A:O4'	2.21	0.40
1:A:1241:G:C2	1:A:1242:C:C2	3.09	0.40
1:A:1342:C:H5''	9:I:125:TYR:CE1	2.57	0.40
2:B:201:ILE:HG21	2:B:214:ILE:HG21	2.02	0.40
5:E:18:ARG:H	5:E:25:ARG:H	1.69	0.40
10:J:47:PHE:CZ	14:N:37:PHE:HE2	2.40	0.40
12:L:42:THR:CG2	12:L:52:LEU:HB3	2.51	0.40
18:R:37:VAL:HG21	18:R:78:LEU:HB3	2.03	0.40
23:X:90:PHE:HB2	23:X:120:ILE:HG12	2.03	0.40
1:A:289:G:C6	1:A:290:C:N4	2.90	0.40
1:A:434:U:H2'	1:A:435:C:H6	1.84	0.40
1:A:725:G:C2	1:A:726:C:C4	3.10	0.40
1:A:895:G:H2'	1:A:896:C:C6	2.55	0.40
1:A:948:C:OP2	13:M:108:ARG:HG2	2.22	0.40
1:A:1069:C:N4	1:A:1106:G:H1	2.18	0.40
1:A:1113:C:O4'	3:C:14:ILE:CD1	2.68	0.40
1:A:1356:G:N2	1:A:1357:A:C2	2.90	0.40
1:A:1395:C:H2'	1:A:1396:A:C8	2.57	0.40
4:D:52:SER:O	4:D:55:ALA:HB3	2.21	0.40
4:D:138:TYR:CD1	4:D:138:TYR:C	2.95	0.40
11:K:86:GLY:HA2	11:K:112:THR:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:120:ARG:HH11	11:K:120:ARG:HG3	1.86	0.40
16:P:19:ILE:H	16:P:19:ILE:HG13	1.72	0.40
22:W:32:ILE:HD11	22:W:34:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	186 (80%)	26 (11%)	20 (9%)	1	13
3	C	204/239 (85%)	181 (89%)	17 (8%)	6 (3%)	4	32
4	D	206/209 (99%)	181 (88%)	18 (9%)	7 (3%)	3	29
5	E	148/162 (91%)	130 (88%)	13 (9%)	5 (3%)	3	29
6	F	99/101 (98%)	90 (91%)	6 (6%)	3 (3%)	4	32
7	G	153/156 (98%)	139 (91%)	10 (6%)	4 (3%)	5	35
8	H	136/138 (99%)	124 (91%)	9 (7%)	3 (2%)	6	38
9	I	125/128 (98%)	103 (82%)	17 (14%)	5 (4%)	3	26
10	J	96/105 (91%)	81 (84%)	10 (10%)	5 (5%)	2	22
11	K	117/129 (91%)	98 (84%)	14 (12%)	5 (4%)	2	25
12	L	122/132 (92%)	93 (76%)	26 (21%)	3 (2%)	5	35
13	M	115/126 (91%)	93 (81%)	20 (17%)	2 (2%)	9	43
14	N	58/61 (95%)	45 (78%)	11 (19%)	2 (3%)	3	29
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	P	81/88 (92%)	68 (84%)	13 (16%)	0	100	100
17	Q	97/105 (92%)	82 (84%)	14 (14%)	1 (1%)	15	54
18	R	71/88 (81%)	60 (84%)	7 (10%)	4 (6%)	2	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	78/93 (84%)	64 (82%)	10 (13%)	4 (5%)	2	22
20	T	97/106 (92%)	87 (90%)	5 (5%)	5 (5%)	2	22
21	V	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
22	W	69/72 (96%)	63 (91%)	4 (6%)	2 (3%)	4	32
23	X	162/171 (95%)	141 (87%)	14 (9%)	7 (4%)	2	25
All	All	2574/2781 (93%)	2209 (86%)	272 (11%)	93 (4%)	6	28

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	PHE
2	B	20	GLU
2	B	24	TRP
2	B	208	ILE
4	D	37	PRO
5	E	17	ALA
5	E	21	ALA
9	I	11	LYS
12	L	27	LEU
12	L	45	PRO
13	M	113	PRO
19	S	71	LEU
23	X	54	PRO
2	B	16	HIS
2	B	21	ARG
2	B	204	ASN
2	B	228	GLY
2	B	229	VAL
3	C	13	GLY
4	D	5	ILE
4	D	42	GLN
6	F	96	PRO
9	I	56	LEU
11	K	101	SER
17	Q	67	LYS
18	R	18	ARG
18	R	20	ALA
18	R	32	ARG
20	T	49	ALA
20	T	95	ALA

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Mol	Chain	Res	Type
20	T	98	PRO
23	X	83	THR
23	X	92	VAL
3	C	4	LYS
4	D	9	CYS
4	D	43	HIS
7	G	4	ARG
7	G	53	LYS
10	J	34	VAL
10	J	38	ILE
10	J	54	PHE
10	J	55	LYS
11	K	55	LYS
13	M	67	GLU
19	S	42	PRO
2	B	9	GLU
2	B	78	GLN
2	B	123	ALA
3	C	108	ASN
4	D	31	CYS
7	G	7	ALA
7	G	55	GLY
8	H	5	PRO
8	H	102	ARG
10	J	56	HIS
11	K	14	VAL
14	N	23	ARG
18	R	17	SER
19	S	9	VAL
20	T	97	ALA
22	W	50	GLY
23	X	8	ASN
23	X	96	GLU
23	X	154	PRO
2	B	8	LYS
2	B	130	ARG
2	B	194	PRO
2	B	233	SER
3	C	156	ARG
3	C	179	ARG
8	H	75	ARG
9	I	54	ASP

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Mol	Chain	Res	Type
11	K	74	ALA
2	B	75	LYS
2	B	125	PRO
3	C	3	ASN
5	E	85	GLY
6	F	15	ASP
6	F	35	ALA
9	I	24	GLY
9	I	119	ALA
12	L	79	GLU
14	N	7	ILE
22	W	2	LYS
2	B	167	PRO
4	D	69	GLY
5	E	77	PRO
19	S	8	GLY
2	B	131	PRO
5	E	105	VAL
11	K	48	ILE
20	T	96	GLY
23	X	55	PRO

5.3.2 Protein sidechains [i](#)

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%)	153 (76%)	49 (24%)	0 4
3	C	160/188 (85%)	137 (86%)	23 (14%)	3 18
4	D	180/181 (99%)	125 (69%)	55 (31%)	0 2
5	E	115/123 (94%)	83 (72%)	32 (28%)	0 3
6	F	90/90 (100%)	75 (83%)	15 (17%)	2 14
7	G	126/127 (99%)	117 (93%)	9 (7%)	14 41
8	H	119/119 (100%)	99 (83%)	20 (17%)	2 14
9	I	98/99 (99%)	84 (86%)	14 (14%)	3 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	87/92 (95%)	72 (83%)	15 (17%)	2	13
11	K	90/99 (91%)	70 (78%)	20 (22%)	1	6
12	L	104/109 (95%)	85 (82%)	19 (18%)	1	11
13	M	94/101 (93%)	80 (85%)	14 (15%)	3	17
14	N	49/50 (98%)	44 (90%)	5 (10%)	7	28
15	O	79/80 (99%)	52 (66%)	27 (34%)	0	1
16	P	72/74 (97%)	58 (81%)	14 (19%)	1	9
17	Q	94/97 (97%)	84 (89%)	10 (11%)	6	27
18	R	64/77 (83%)	50 (78%)	14 (22%)	1	6
19	S	71/80 (89%)	59 (83%)	12 (17%)	2	13
20	T	76/82 (93%)	60 (79%)	16 (21%)	1	7
21	V	19/22 (86%)	17 (90%)	2 (10%)	7	27
22	W	62/63 (98%)	56 (90%)	6 (10%)	8	29
23	X	145/150 (97%)	126 (87%)	19 (13%)	4	21
All	All	2196/2323 (94%)	1786 (81%)	410 (19%)	4	10

All (410) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	10	LEU
2	B	15	VAL
2	B	16	HIS
2	B	21	ARG
2	B	23	ARG
2	B	28	PHE
2	B	40	HIS
2	B	44	LEU
2	B	45	GLN
2	B	61	LEU
2	B	73	THR
2	B	82	ARG
2	B	83	MET
2	B	87	ARG
2	B	95	GLN
2	B	96	ARG
2	B	102	LEU

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Mol	Chain	Res	Type
2	B	107	THR
2	B	111	ARG
2	B	112	VAL
2	B	114	ARG
2	B	117	GLU
2	B	126	GLU
2	B	127	ILE
2	B	130	ARG
2	B	137	ARG
2	B	144	ARG
2	B	146	GLN
2	B	154	LEU
2	B	155	LEU
2	B	157	ARG
2	B	163	PHE
2	B	165	VAL
2	B	168	THR
2	B	172	ILE
2	B	178	ARG
2	B	180	LEU
2	B	187	LEU
2	B	190	THR
2	B	195	ASP
2	B	198	ASP
2	B	200	ILE
2	B	205	ASP
2	B	208	ILE
2	B	211	ILE
2	B	213	LEU
2	B	221	LEU
2	B	229	VAL
3	C	3	ASN
3	C	4	LYS
3	C	14	ILE
3	C	21	ARG
3	C	33	LEU
3	C	40	ARG
3	C	52	LEU
3	C	82	GLU
3	C	87	LEU
3	C	90	GLU
3	C	91	LEU

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Mol	Chain	Res	Type
3	C	94	LEU
3	C	98	ASN
3	C	101	LEU
3	C	102	ASN
3	C	115	LEU
3	C	119	ARG
3	C	157	ILE
3	C	177	THR
3	C	188	LEU
3	C	190	ARG
3	C	191	THR
3	C	204	LEU
4	D	5	ILE
4	D	11	LEU
4	D	13	ARG
4	D	14	ARG
4	D	15	GLU
4	D	20	TYR
4	D	21	LEU
4	D	25	ARG
4	D	27	TYR
4	D	35	ARG
4	D	45	GLN
4	D	46	LYS
4	D	49	ARG
4	D	50	ARG
4	D	53	ASP
4	D	59	ARG
4	D	64	LEU
4	D	65	ARG
4	D	70	ILE
4	D	74	GLN
4	D	76	ARG
4	D	78	LEU
4	D	83	SER
4	D	97	LEU
4	D	112	VAL
4	D	115	ARG
4	D	119	GLN
4	D	122	ARG
4	D	132	ARG
4	D	135	LEU

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Mol	Chain	Res	Type
4	D	137	SER
4	D	138	TYR
4	D	141	ARG
4	D	144	ASP
4	D	153	ARG
4	D	154	ASN
4	D	155	LEU
4	D	157	LEU
4	D	158	ILE
4	D	162	LEU
4	D	163	GLU
4	D	168	ARG
4	D	174	LEU
4	D	176	LEU
4	D	178	VAL
4	D	181	MET
4	D	186	LEU
4	D	187	ARG
4	D	190	ASP
4	D	192	GLU
4	D	193	ASP
4	D	196	LEU
4	D	200	GLU
4	D	207	TYR
4	D	209	ARG
5	E	5	ASP
5	E	7	GLU
5	E	12	LEU
5	E	14	ARG
5	E	19	MET
5	E	27	ARG
5	E	32	VAL
5	E	34	VAL
5	E	36	ASP
5	E	37	ARG
5	E	38	GLN
5	E	40	ARG
5	E	41	VAL
5	E	47	LYS
5	E	63	ARG
5	E	67	VAL
5	E	71	LEU

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Mol	Chain	Res	Type
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	91	LEU
5	E	98	THR
5	E	107	ARG
5	E	116	THR
5	E	118	ILE
5	E	127	ASN
5	E	135	THR
5	E	136	MET
5	E	141	GLN
5	E	144	THR
5	E	147	ASP
5	E	148	VAL
6	F	5	GLU
6	F	18	GLN
6	F	19	LEU
6	F	27	GLN
6	F	28	ARG
6	F	31	GLU
6	F	32	ASN
6	F	36	ARG
6	F	40	VAL
6	F	61	LEU
6	F	69	GLU
6	F	75	LEU
6	F	77	ARG
6	F	82	ARG
6	F	86	ARG
7	G	16	LEU
7	G	60	LYS
7	G	72	ARG
7	G	74	GLU
7	G	91	VAL
7	G	136	LYS
7	G	137	LYS
7	G	142	GLU
7	G	156	TRP
8	H	8	ASP
8	H	11	THR
8	H	18	ARG

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Mol	Chain	Res	Type
8	H	21	LYS
8	H	31	PHE
8	H	45	ILE
8	H	50	ARG
8	H	59	LEU
8	H	63	LEU
8	H	78	GLN
8	H	82	HIS
8	H	85	ARG
8	H	87	SER
8	H	92	ARG
8	H	93	VAL
8	H	102	ARG
8	H	104	ARG
8	H	120	THR
8	H	127	LEU
8	H	135	CYS
9	I	3	GLN
9	I	12	GLU
9	I	38	GLN
9	I	56	LEU
9	I	65	VAL
9	I	78	LYS
9	I	79	LEU
9	I	85	LEU
9	I	95	LYS
9	I	102	LEU
9	I	111	ARG
9	I	112	LYS
9	I	121	ARG
9	I	127	LYS
10	J	4	ILE
10	J	8	LEU
10	J	23	ILE
10	J	44	VAL
10	J	46	ARG
10	J	49	VAL
10	J	61	GLU
10	J	62	HIS
10	J	66	ARG
10	J	71	LEU
10	J	74	ILE

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Mol	Chain	Res	Type
10	J	82	ILE
10	J	83	GLU
10	J	86	MET
10	J	87	THR
11	K	18	ARG
11	K	25	TYR
11	K	29	ILE
11	K	34	ASP
11	K	41	THR
11	K	47	VAL
11	K	48	ILE
11	K	54	ARG
11	K	57	THR
11	K	62	GLN
11	K	63	LEU
11	K	77	MET
11	K	92	GLU
11	K	93	GLN
11	K	96	ARG
11	K	103	LEU
11	K	109	VAL
11	K	111	ASP
11	K	116	HIS
11	K	123	LYS
12	L	6	THR
12	L	7	ILE
12	L	17	LYS
12	L	33	ARG
12	L	36	VAL
12	L	39	VAL
12	L	41	ARG
12	L	46	LYS
12	L	50	SER
12	L	53	ARG
12	L	59	ARG
12	L	81	SER
12	L	83	VAL
12	L	89	ARG
12	L	90	VAL
12	L	104	VAL
12	L	110	VAL
12	L	113	ARG

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Mol	Chain	Res	Type
12	L	122	THR
13	M	12	ASN
13	M	32	GLU
13	M	37	THR
13	M	44	ARG
13	M	45	VAL
13	M	66	LEU
13	M	67	GLU
13	M	73	GLU
13	M	87	TYR
13	M	90	LEU
13	M	102	ARG
13	M	110	ARG
13	M	115	LYS
13	M	116	THR
14	N	3	ARG
14	N	4	LYS
14	N	12	ARG
14	N	17	LYS
14	N	41	ARG
15	O	10	LYS
15	O	17	ARG
15	O	21	ASP
15	O	22	THR
15	O	25	THR
15	O	27	VAL
15	O	28	GLN
15	O	29	VAL
15	O	39	LEU
15	O	40	SER
15	O	41	GLU
15	O	43	LEU
15	O	45	VAL
15	O	48	LYS
15	O	49	ASP
15	O	52	SER
15	O	54	ARG
15	O	56	LEU
15	O	64	ARG
15	O	67	LEU
15	O	68	ARG
15	O	70	LEU

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Mol	Chain	Res	Type
15	O	71	GLN
15	O	72	ARG
15	O	77	ARG
15	O	84	LYS
15	O	88	ARG
16	P	8	ARG
16	P	20	VAL
16	P	23	ASP
16	P	28	ARG
16	P	29	ASP
16	P	39	TYR
16	P	42	ARG
16	P	44	THR
16	P	45	THR
16	P	48	TRP
16	P	54	GLU
16	P	55	ARG
16	P	57	ARG
16	P	60	LEU
17	Q	27	PHE
17	Q	38	ARG
17	Q	52	LYS
17	Q	63	ARG
17	Q	68	ARG
17	Q	70	ARG
17	Q	81	ARG
17	Q	89	LEU
17	Q	93	GLN
17	Q	100	LYS
18	R	35	ARG
18	R	38	GLU
18	R	41	LYS
18	R	44	LEU
18	R	46	GLU
18	R	47	THR
18	R	53	ARG
18	R	54	ARG
18	R	61	LYS
18	R	66	LEU
18	R	75	ILE
18	R	76	LEU
18	R	82	THR

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Mol	Chain	Res	Type
18	R	87	ARG
19	S	6	LYS
19	S	7	LYS
19	S	13	ASP
19	S	15	LEU
19	S	19	VAL
19	S	25	LYS
19	S	29	ARG
19	S	30	LEU
19	S	37	ARG
19	S	41	VAL
19	S	52	TYR
19	S	63	THR
20	T	10	LEU
20	T	15	ARG
20	T	19	SER
20	T	22	ARG
20	T	23	ARG
20	T	24	LEU
20	T	46	GLU
20	T	62	LEU
20	T	64	ASP
20	T	68	LYS
20	T	72	LEU
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
20	T	89	ARG
21	V	7	ARG
21	V	12	LYS
22	W	8	ARG
22	W	19	ASN
22	W	32	ILE
22	W	33	LEU
22	W	47	ILE
22	W	48	LEU
23	X	31	THR
23	X	35	LEU
23	X	73	GLU
23	X	74	LYS
23	X	78	LYS

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Mol	Chain	Res	Type
23	X	91	ARG
23	X	98	ASP
23	X	118	VAL
23	X	123	ARG
23	X	125	ARG
23	X	132	LEU
23	X	134	GLU
23	X	135	ARG
23	X	143	ASP
23	X	144	LEU
23	X	152	MET
23	X	162	ASN
23	X	163	MET
23	X	164	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	16	HIS
2	B	19	HIS
2	B	25	ASN
2	B	95	GLN
2	B	146	GLN
2	B	204	ASN
3	C	3	ASN
3	C	6	HIS
3	C	28	GLN
3	C	108	ASN
3	C	123	GLN
3	C	176	HIS
4	D	119	GLN
4	D	123	HIS
4	D	125	HIS
4	D	129	ASN
6	F	7	ASN
7	G	37	ASN
7	G	97	GLN
8	H	82	HIS
10	J	68	HIS
12	L	8	ASN
12	L	75	HIS
15	O	28	GLN

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Mol	Chain	Res	Type
15	O	62	GLN
16	P	14	ASN
16	P	65	GLN
17	Q	93	GLN
17	Q	94	ASN
18	R	36	ASN
18	R	63	GLN
19	S	47	HIS
19	S	53	ASN
20	T	73	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1522 (98%)	468 (31%)	114 (7%)
24	Y	12/39 (30%)	4 (33%)	0
All	All	1517/1561 (97%)	472 (31%)	114 (7%)

All (472) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	13	U
1	A	14	U
1	A	18	C
1	A	19	C
1	A	22	G
1	A	29	G
1	A	30	U
1	A	31	G
1	A	32	A
1	A	35	G
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

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Mol	Chain	Res	Type
1	A	52	G
1	A	54	C
1	A	59	A
1	A	60	A
1	A	61	G
1	A	62	U
1	A	66	G
1	A	68	G
1	A	73	G
1	A	76	C
1	A	77	G
1	A	79	G
1	A	81	U
1	A	83	U
1	A	91	C
1	A	97	G
1	A	101	A
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	142	G
1	A	144	G
1	A	151	A
1	A	153	C
1	A	157	G
1	A	163	C
1	A	167	G
1	A	173	U
1	A	174	C
1	A	175	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

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Mol	Chain	Res	Type
1	A	195	A
1	A	196	A
1	A	197	A
1	A	198	G
1	A	199	G
1	A	201	C
1	A	203	U
1	A	204	U
1	A	217	C
1	A	220	G
1	A	243	A
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
1	A	252	U
1	A	253	U
1	A	266	G
1	A	267	C
1	A	279	A
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	299	G
1	A	300	A
1	A	301	G
1	A	306	G
1	A	309	G
1	A	315	A
1	A	316	G
1	A	321	A
1	A	324	G
1	A	325	A
1	A	327	A
1	A	328	C
1	A	329	A
1	A	330	C

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Mol	Chain	Res	Type
1	A	332	G
1	A	339	C
1	A	340	U
1	A	342	C
1	A	344	A
1	A	345	C
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	357	G
1	A	366	C
1	A	367	U
1	A	368	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	395	C
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	438	G
1	A	439	A
1	A	441	A
1	A	444	C

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Mol	Chain	Res	Type
1	A	446	G
1	A	450	G
1	A	451	A
1	A	452	A
1	A	470	C
1	A	484	G
1	A	485	G
1	A	492	G
1	A	495	A
1	A	496	A
1	A	498	U
1	A	510	A
1	A	511	C
1	A	517	G
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	545	C
1	A	547	A
1	A	548	G
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	565	U
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	578	C

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Mol	Chain	Res	Type
1	A	587	G
1	A	588	G
1	A	596	C
1	A	597	G
1	A	607	A
1	A	619	U
1	A	620	C
1	A	641	U
1	A	642	A
1	A	644	G
1	A	650	G
1	A	652	U
1	A	653	A
1	A	654	G
1	A	665	A
1	A	666	G
1	A	671	G
1	A	672	U
1	A	677	U
1	A	687	A
1	A	688	G
1	A	697	U
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	731	G
1	A	737	A
1	A	740	U
1	A	748	C
1	A	749	C
1	A	755	G
1	A	760	G
1	A	764	C
1	A	777	A
1	A	784	C
1	A	785	G

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Mol	Chain	Res	Type
1	A	787	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	802	A
1	A	812	C
1	A	815	A
1	A	817	C
1	A	819	A
1	A	821	G
1	A	828	A
1	A	835	U
1	A	839	U
1	A	841	U
1	A	851	G
1	A	853	G
1	A	855	G
1	A	859	A
1	A	864	A
1	A	865	A
1	A	866	C
1	A	869	G
1	A	871	U
1	A	872	A
1	A	873	A
1	A	874	G
1	A	876	G
1	A	882	C
1	A	885	G
1	A	889	A
1	A	900	A
1	A	902	G
1	A	911	U
1	A	920	U
1	A	922	G
1	A	927	G
1	A	930	C
1	A	932	C
1	A	933	G
1	A	934	C
1	A	935	A
1	A	937	A

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Mol	Chain	Res	Type
1	A	942	G
1	A	943	U
1	A	945	G
1	A	950	U
1	A	960	U
1	A	961	U
1	A	965	A
1	A	966	G
1	A	968	A
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	989	C
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	1005	A
1	A	1007	C
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1026	G
1	A	1028	C
1	A	1029	C
1	A	1030(C)	G
1	A	1031	G
1	A	1045	C
1	A	1046	A
1	A	1049	U
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1054	C
1	A	1055	A

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Mol	Chain	Res	Type
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1067	A
1	A	1070	U
1	A	1074	G
1	A	1078	U
1	A	1079	G
1	A	1081	G
1	A	1085	U
1	A	1086	U
1	A	1092	A
1	A	1093	A
1	A	1094	G
1	A	1095	U
1	A	1097	C
1	A	1098	C
1	A	1100	C
1	A	1101	A
1	A	1102	A
1	A	1104	G
1	A	1117	G
1	A	1118	C
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1145	C
1	A	1146	A
1	A	1150	U
1	A	1152	A
1	A	1157	A
1	A	1158	C

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Mol	Chain	Res	Type
1	A	1159	U
1	A	1170	A
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	1205	U
1	A	1212	U
1	A	1213	A
1	A	1215	G
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1239	A
1	A	1240	U
1	A	1249	C
1	A	1250	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1266	G
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1295	G
1	A	1297	C

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Mol	Chain	Res	Type
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1306	A
1	A	1312	G
1	A	1317	C
1	A	1318	A
1	A	1319	A
1	A	1321	C
1	A	1322	C
1	A	1323	G
1	A	1331	G
1	A	1332	A
1	A	1336	C
1	A	1338	G
1	A	1342	C
1	A	1346	A
1	A	1347	G
1	A	1351	U
1	A	1353	G
1	A	1357	A
1	A	1362	C
1	A	1363	C
1	A	1363(A)	A
1	A	1364	U
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	1409	C
1	A	1412	C
1	A	1418	A
1	A	1419	G
1	A	1433	A
1	A	1440	C
1	A	1442	G
1	A	1442(A)	G
1	A	1443	G

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Mol	Chain	Res	Type
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1457	G
1	A	1485	U
1	A	1486	G
1	A	1488	G
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1499	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	1519	A
1	A	1520	G
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1535	C
1	A	1536	C
1	A	1539	C
1	A	1541	U
1	A	1542	U
24	Y	28	A
24	Y	30	G
24	Y	31	U
24	Y	32	A

All (114) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	A
1	A	13	U
1	A	30	U
1	A	31	G
1	A	48	C

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Mol	Chain	Res	Type
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	145	G
1	A	156	G
1	A	173	U
1	A	181	G
1	A	195	A
1	A	197	A
1	A	202	U
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	274	A
1	A	279	A
1	A	281	G
1	A	289	G
1	A	327	A
1	A	328	C
1	A	329	A
1	A	344	A
1	A	350	G
1	A	351	G
1	A	366	C
1	A	372	C
1	A	389	A
1	A	421	U
1	A	428	G
1	A	484	G
1	A	495	A
1	A	496	A
1	A	509	A
1	A	518	C
1	A	535	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	576	G

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Mol	Chain	Res	Type
1	A	577	G
1	A	595	G
1	A	641	U
1	A	653	A
1	A	687	A
1	A	701	C
1	A	702	A
1	A	748	C
1	A	777	A
1	A	792	A
1	A	840	C
1	A	864	A
1	A	872	A
1	A	884	U
1	A	932	C
1	A	933	G
1	A	960	U
1	A	965	A
1	A	975	A
1	A	992	U
1	A	993	G
1	A	1000	U
1	A	1050	G
1	A	1065	U
1	A	1077	G
1	A	1078	U
1	A	1082	G
1	A	1092	A
1	A	1101	A
1	A	1145	C
1	A	1151	A
1	A	1182	G
1	A	1187	G
1	A	1190	G
1	A	1196	U
1	A	1200	C
1	A	1201	A
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1226	C
1	A	1239	A

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Mol	Chain	Res	Type
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	1322	C
1	A	1331	G
1	A	1335	C
1	A	1337	G
1	A	1346	A
1	A	1364	U
1	A	1380	U
1	A	1398	A
1	A	1442(B)	A
1	A	1447	A
1	A	1452	C
1	A	1493	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1529	G
1	A	1534	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 116 ligands modelled in this entry, 110 are monoatomic - leaving 6 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	A	A	1708	-	18,24,25	0.60	0	18,35,38	0.90	1 (5%)
26	A	A	1709	-	18,24,25	0.62	0	18,35,38	0.87	1 (5%)
29	U	X	202	-	18,21,22	0.32	0	26,30,33	0.50	0
26	A	X	201	-	18,24,25	0.62	0	18,35,38	0.77	1 (5%)
29	U	W	102	-	18,21,22	0.24	0	26,30,33	0.46	0
27	G	A	1710	-	18,25,26	1.02	2 (11%)	19,37,40	0.72	1 (5%)

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
26	A	A	1708	-	-	2/3/25/26	0/3/3/3
26	A	A	1709	-	-	2/3/25/26	0/3/3/3
29	U	X	202	-	-	3/7/25/26	0/2/2/2
26	A	X	201	-	-	3/3/25/26	0/3/3/3
29	U	W	102	-	-	6/7/25/26	0/2/2/2
27	G	A	1710	-	-	2/3/25/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1710	G	C8-N7	-2.35	1.31	1.35
27	A	1710	G	C5-C6	-2.24	1.42	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1708	A	C5-C6-N6	2.24	123.76	120.35
26	A	1709	A	C5-C6-N6	2.22	123.72	120.35
27	A	1710	G	O6-C6-C5	2.19	128.64	124.37
26	X	201	A	C5-C6-N6	2.16	123.64	120.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

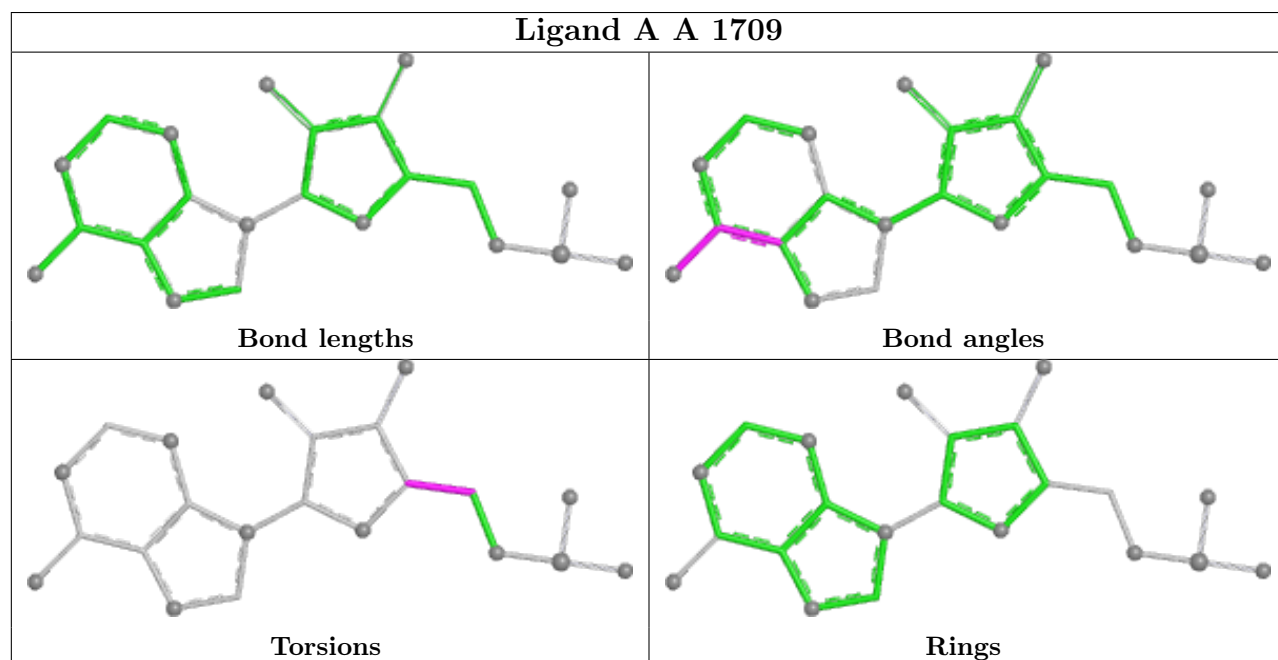
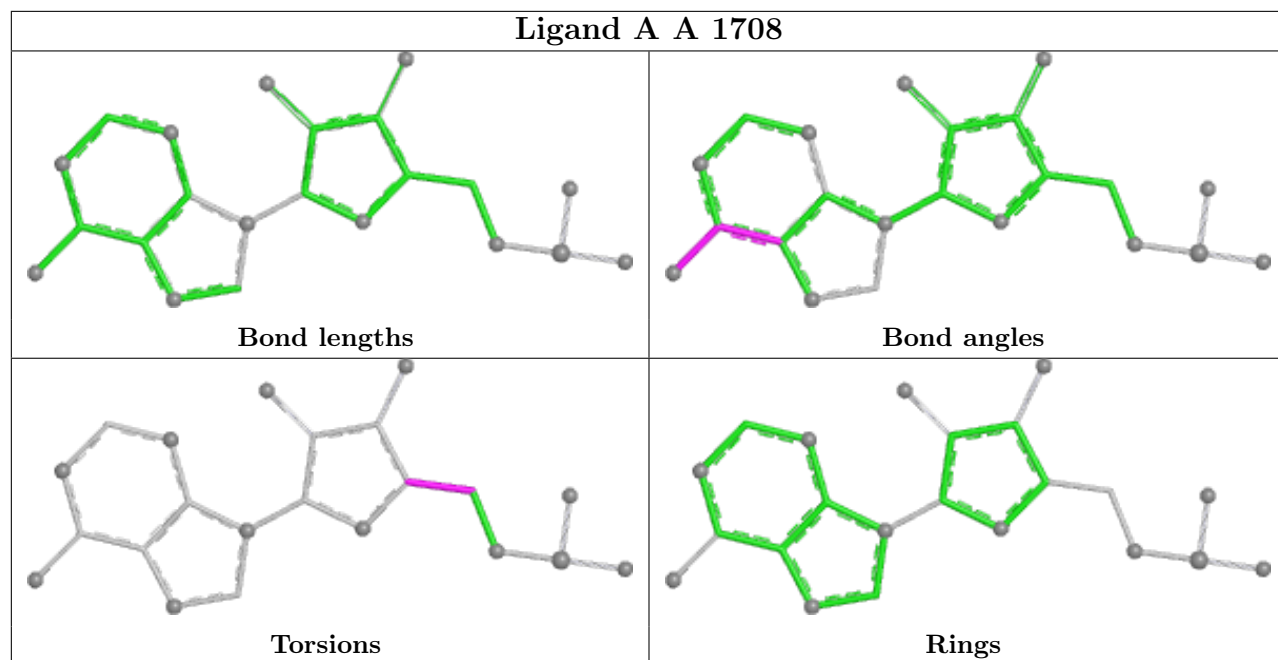
Mol	Chain	Res	Type	Atoms
26	A	1708	A	O4'-C4'-C5'-O5'
26	A	1708	A	C3'-C4'-C5'-O5'
29	X	202	U	O4'-C4'-C5'-O5'
29	X	202	U	C3'-C4'-C5'-O5'
29	W	102	U	O4'-C4'-C5'-O5'
29	W	102	U	C3'-C4'-C5'-O5'
26	X	201	A	C3'-C4'-C5'-O5'
26	A	1709	A	O4'-C4'-C5'-O5'
26	A	1709	A	C3'-C4'-C5'-O5'
26	X	201	A	O4'-C4'-C5'-O5'
29	W	102	U	O4'-C1'-N1-C6
29	W	102	U	C2'-C1'-N1-C6
26	X	201	A	C4'-C5'-O5'-P
27	A	1710	G	C3'-C4'-C5'-O5'
29	W	102	U	O4'-C1'-N1-C2
27	A	1710	G	O4'-C4'-C5'-O5'
29	W	102	U	C2'-C1'-N1-C2
29	X	202	U	C2'-C1'-N1-C2

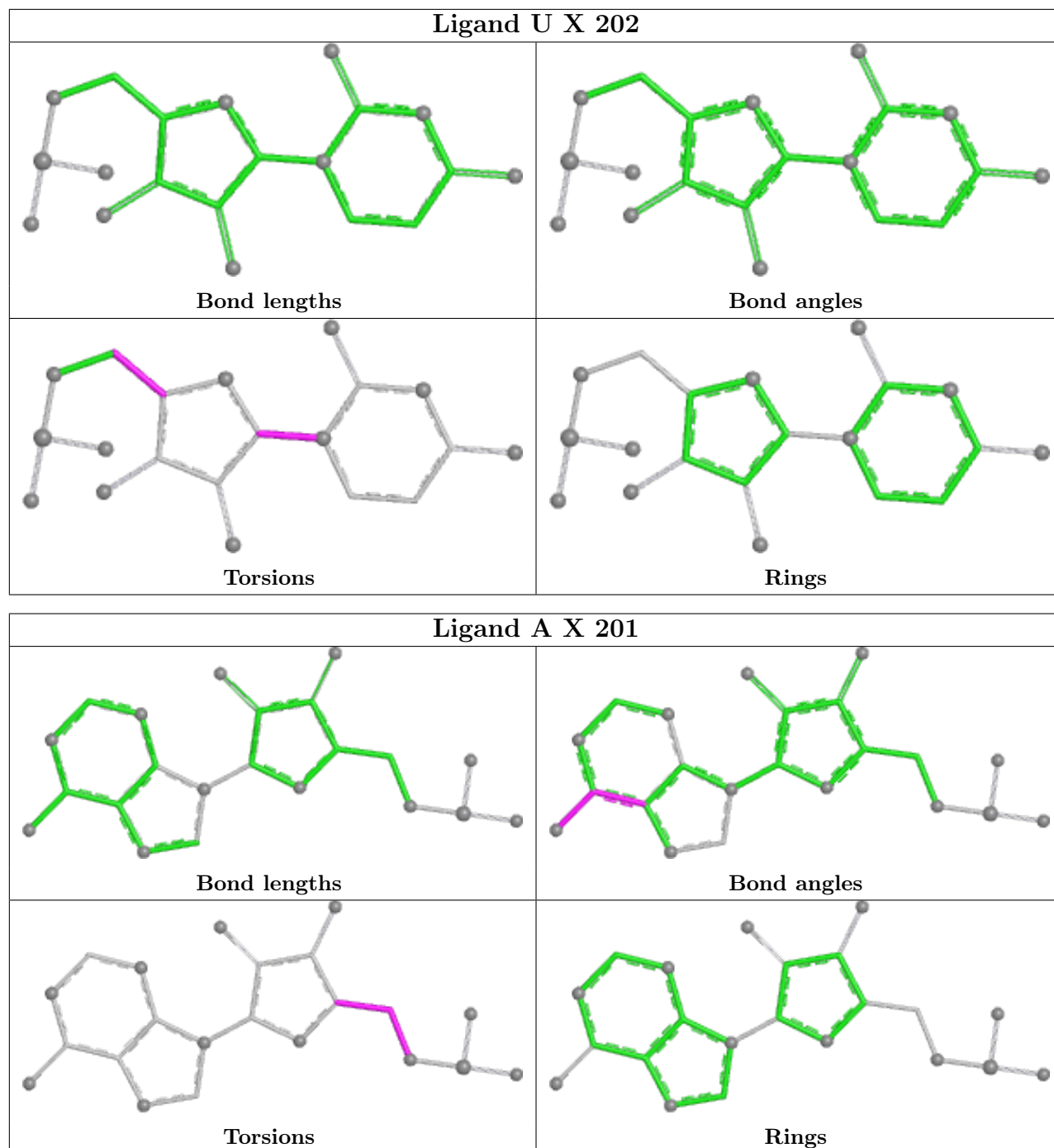
There are no ring outliers.

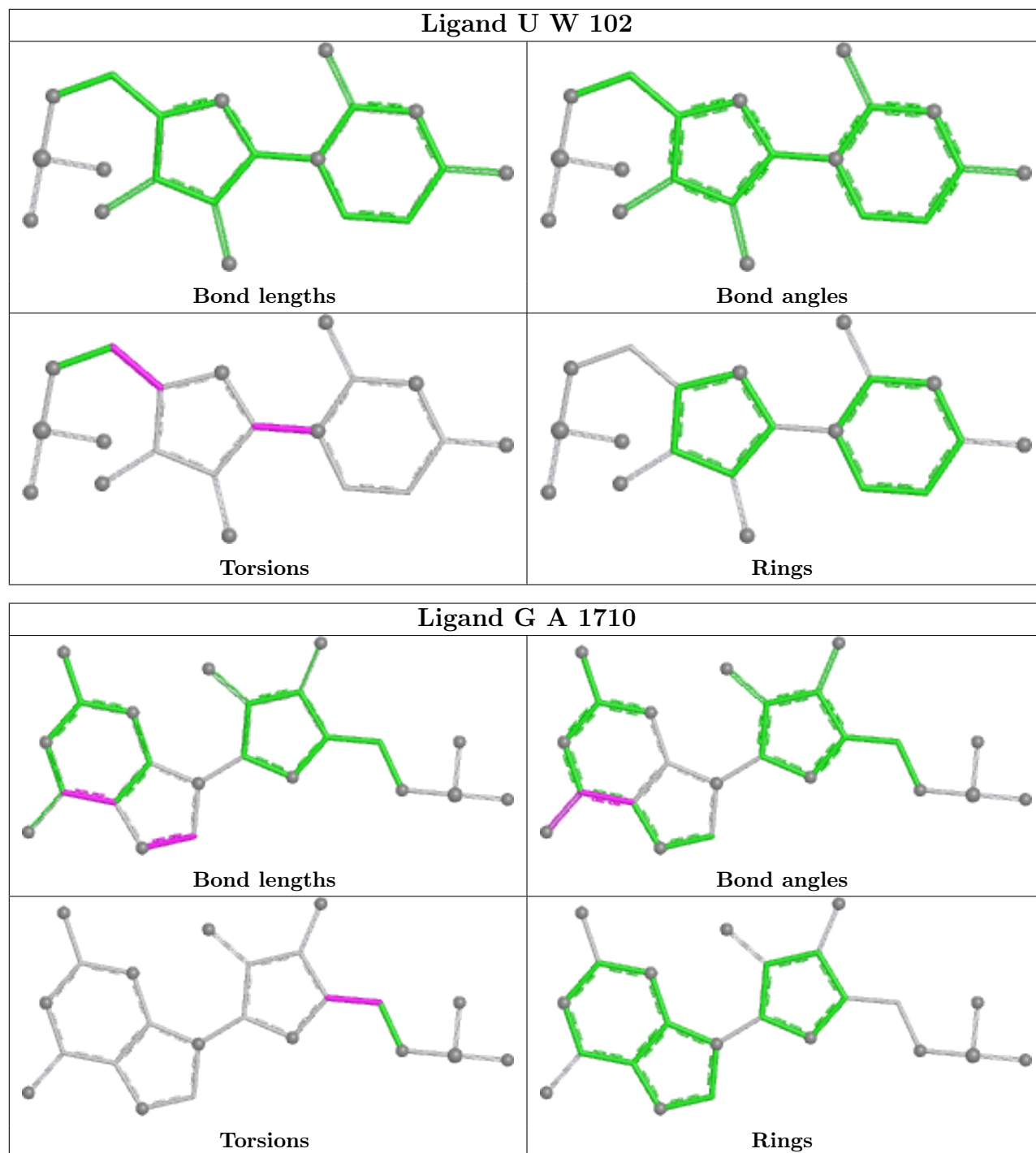
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	X	201	A	1	0
27	A	1710	G	2	0

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







5.7 Other polymers [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
23	X	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	84:U	O3'	88:A	P	5.27
1	A	93:G	O3'	96:U	P	4.63
1	A	204:U	O3'	216:G	P	4.48
1	A	841:U	O3'	848:C	P	4.32
1	A	1442(A):G	O3'	1442(B):A	P	3.82
1	X	81:LYS	C	82:ARG	N	3.73
1	X	79:LYS	C	80:ALA	N	3.54
1	A	1387:G	O3'	1388:C	P	3.33
1	A	927:G	O3'	928:G	P	2.65

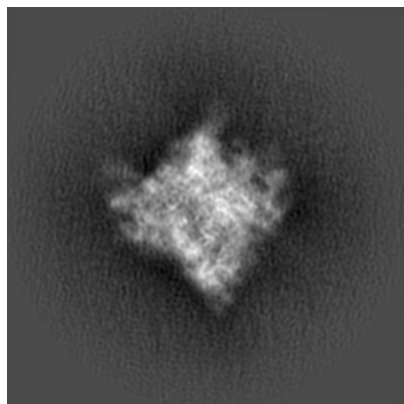
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4074. These allow visual inspection of the internal detail of the map and identification of artifacts.

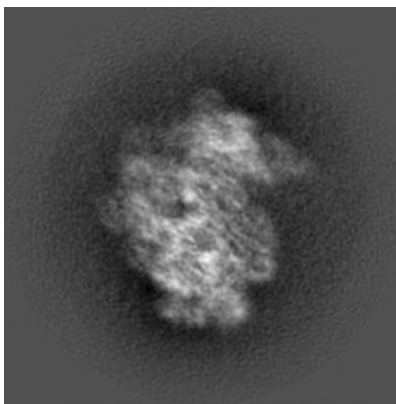
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

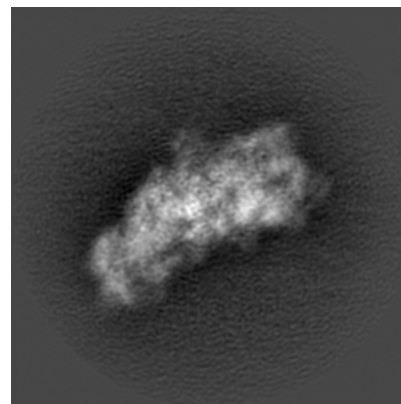
6.1.1 Primary map



X

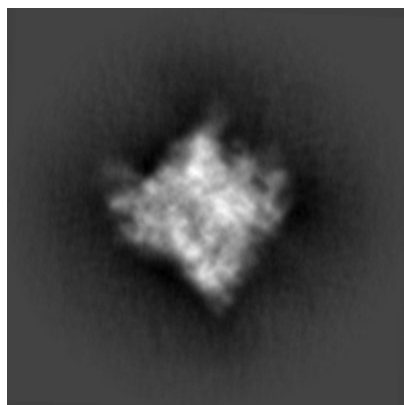


Y

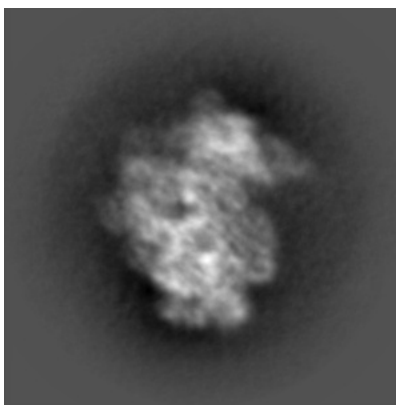


Z

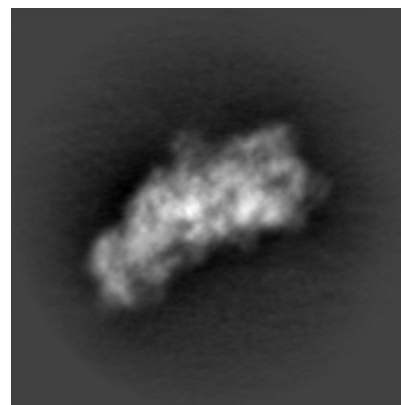
6.1.2 Raw map



X



Y

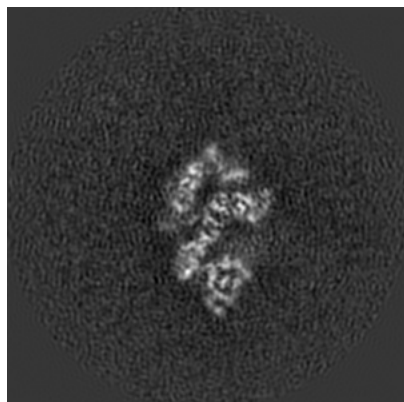


Z

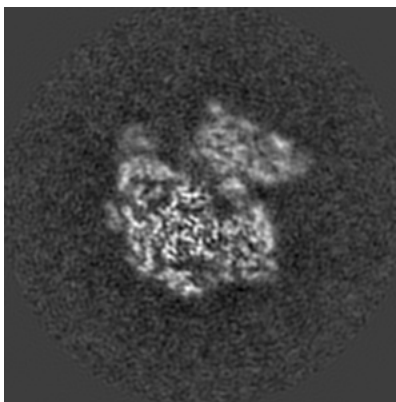
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

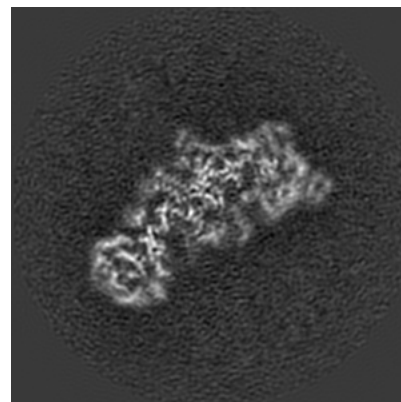
6.2.1 Primary map



X Index: 130

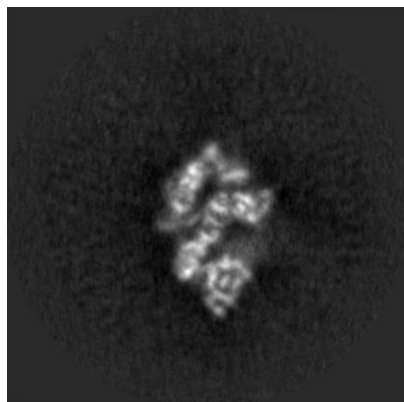


Y Index: 130

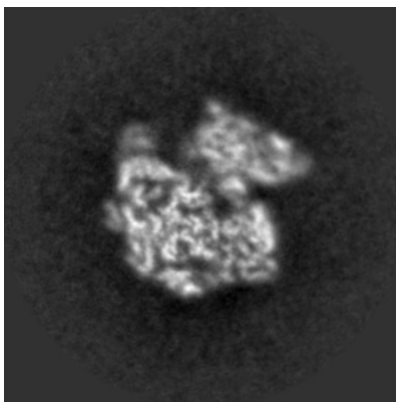


Z Index: 130

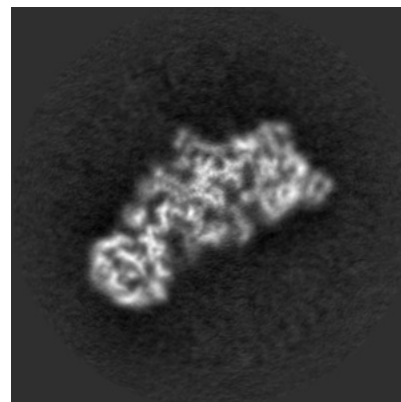
6.2.2 Raw map



X Index: 130



Y Index: 130

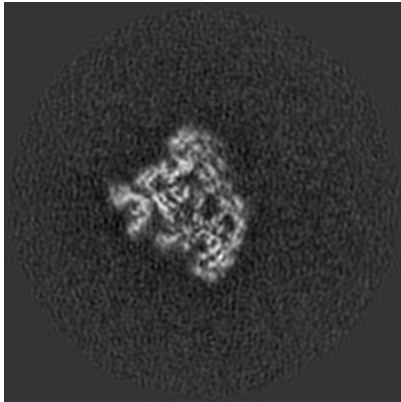


Z Index: 130

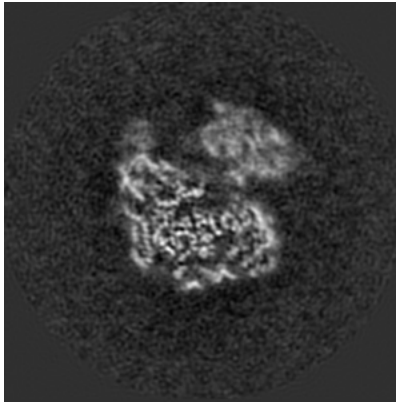
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

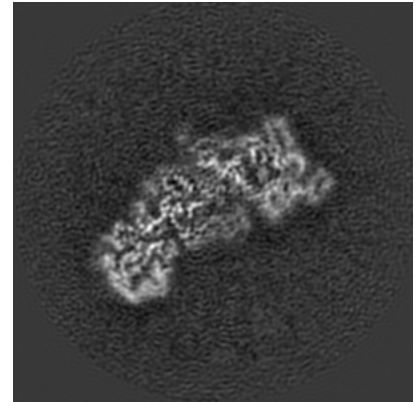
6.3.1 Primary map



X Index: 95

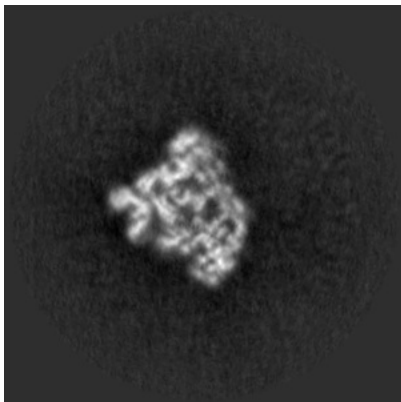


Y Index: 127

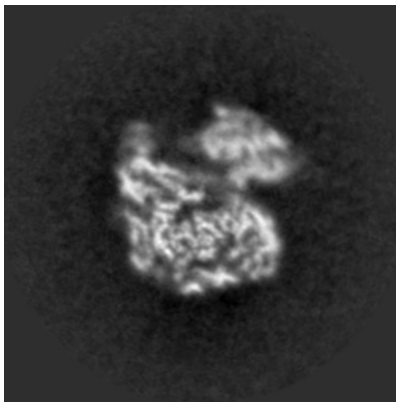


Z Index: 134

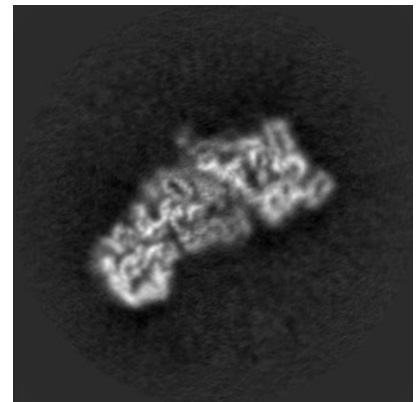
6.3.2 Raw map



X Index: 96



Y Index: 126



Z Index: 134

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



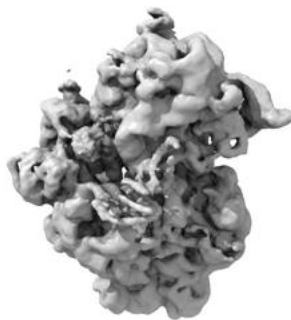
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

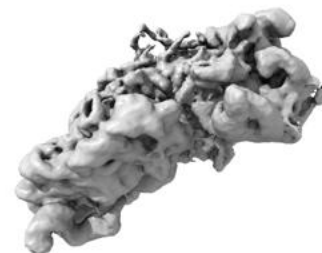
6.4.2 Raw map



X



Y



Z

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

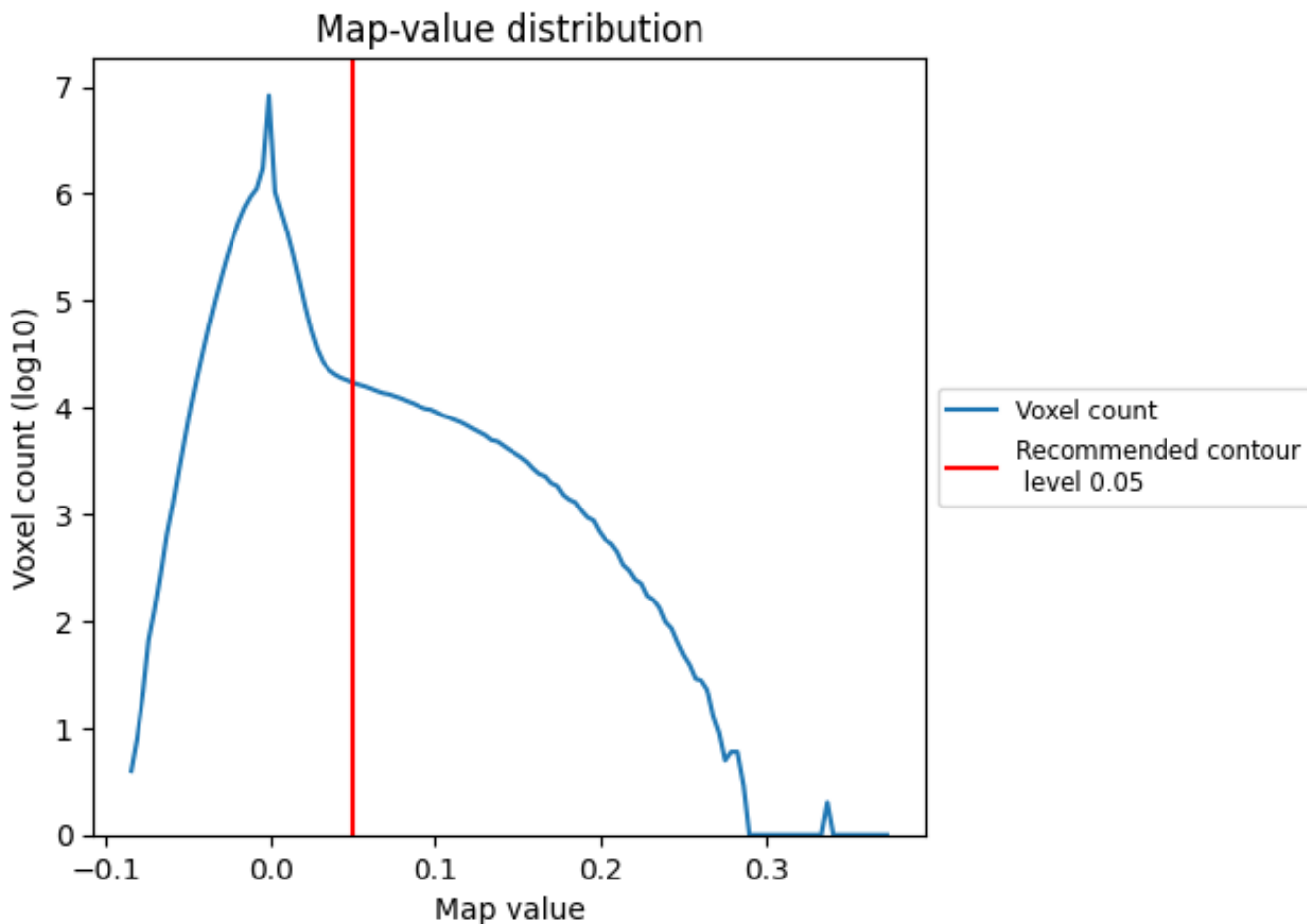
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

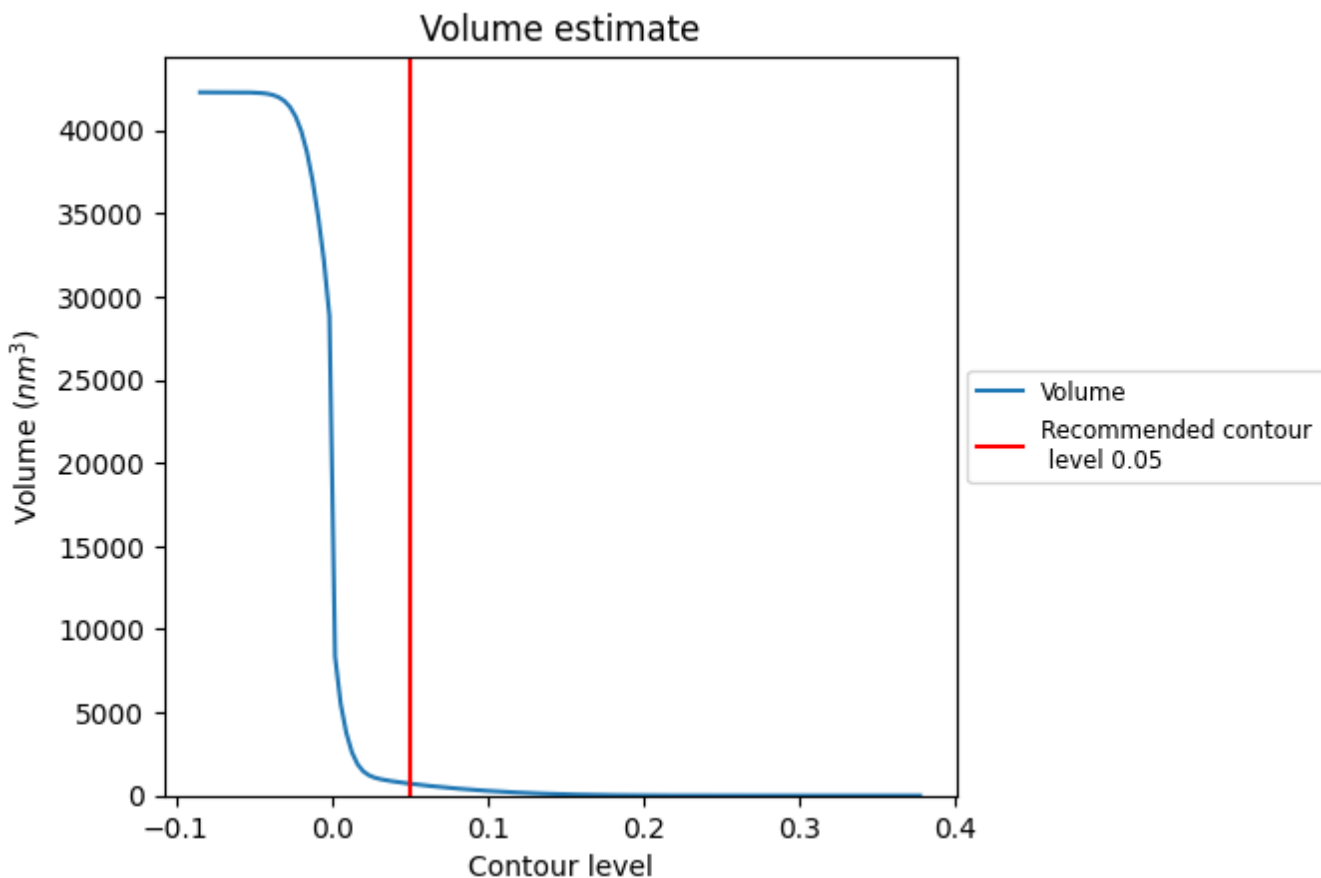
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

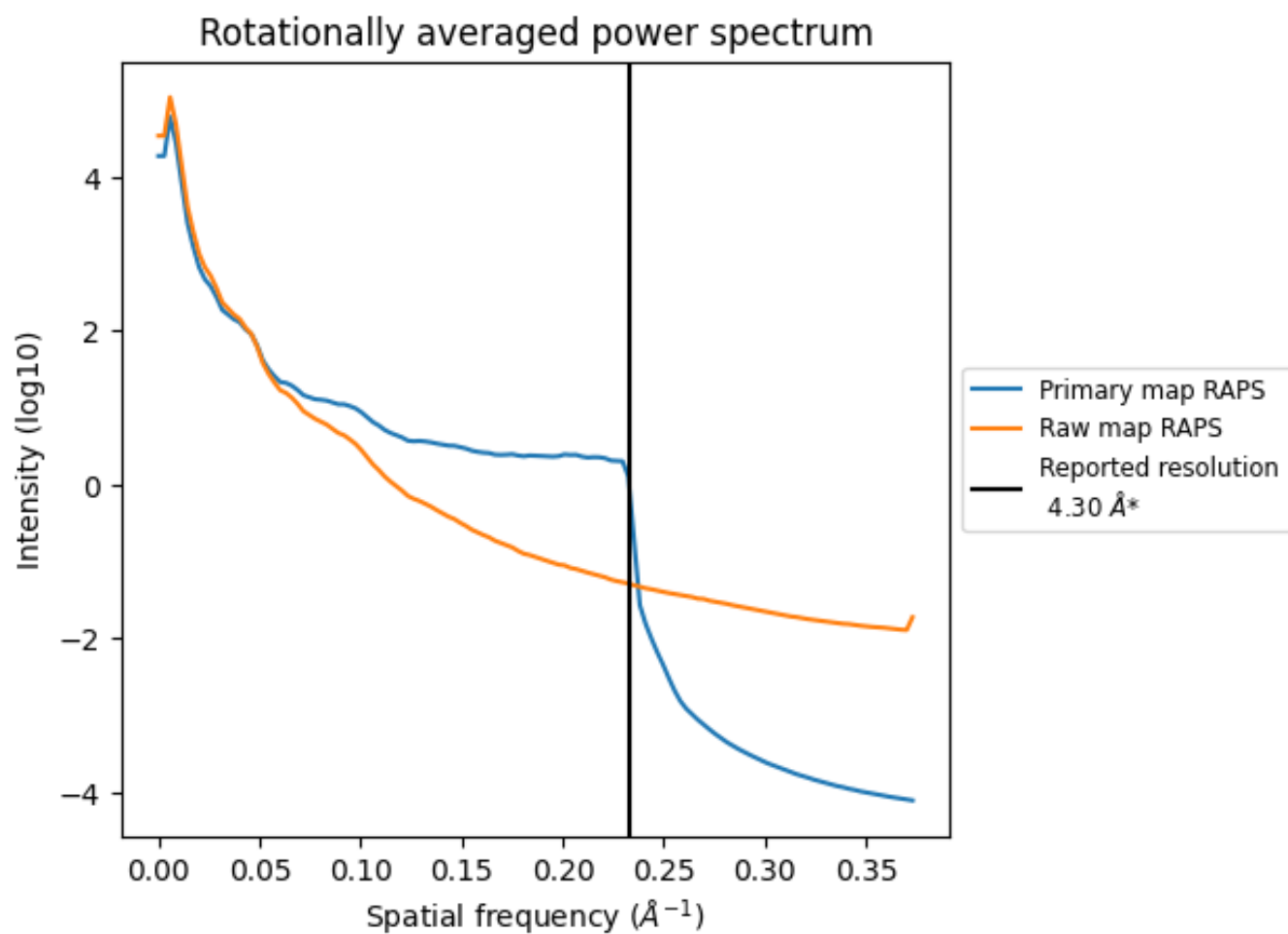
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 718 nm^3 ; this corresponds to an approximate mass of 649 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum i

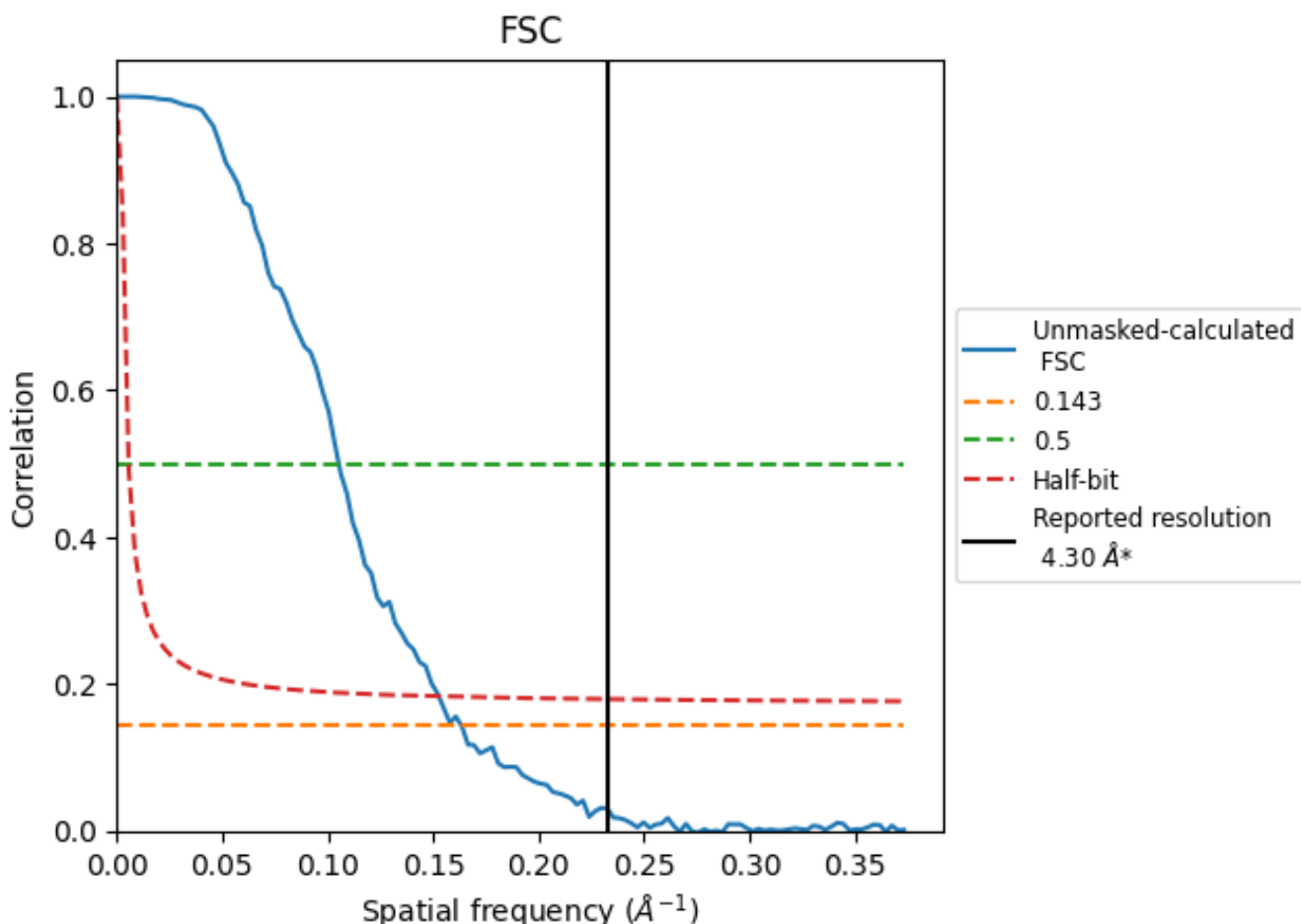


*Reported resolution corresponds to spatial frequency of 0.233 Å⁻¹

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

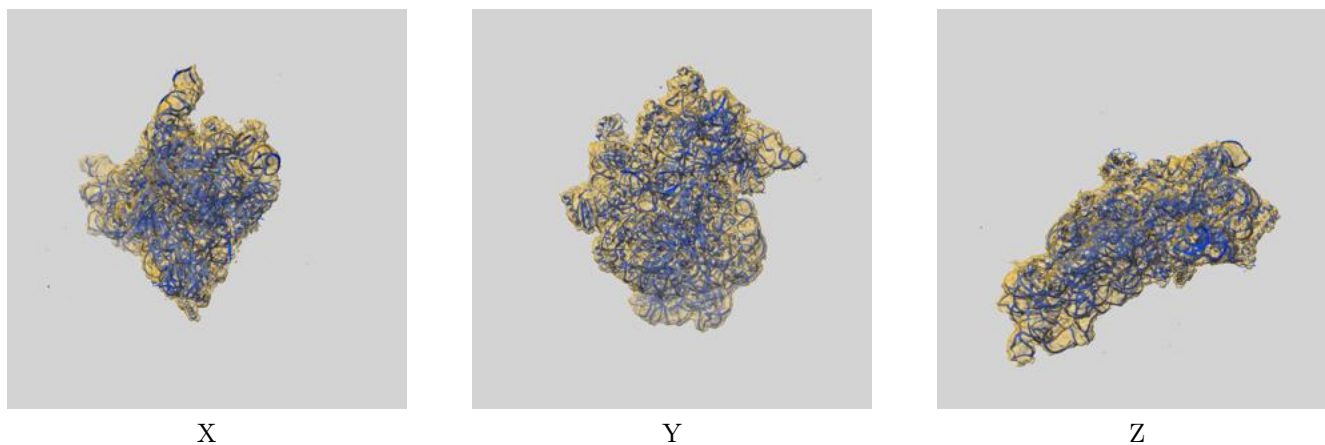
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.12	9.51	6.55

*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 6.12 differs from the reported value 4.3 by more than 10 %

9 Map-model fit [i](#)

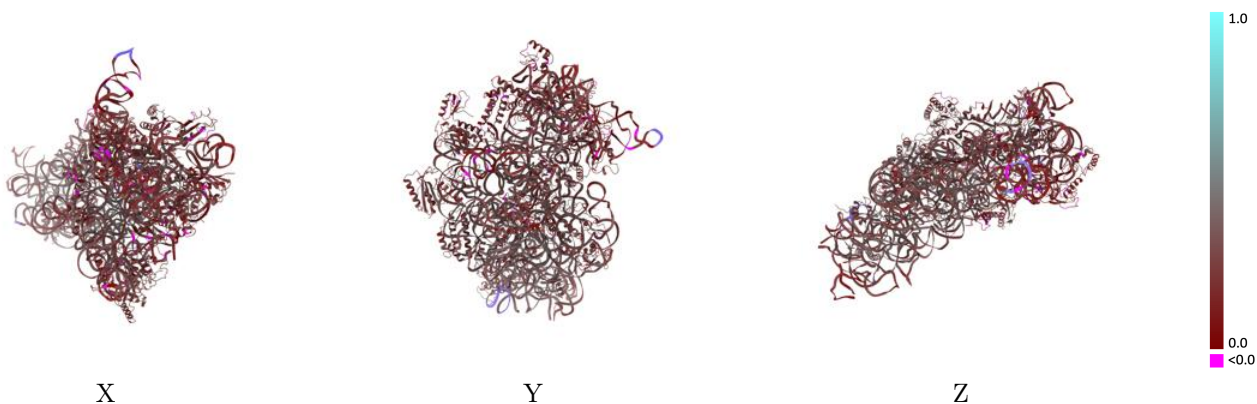
This section contains information regarding the fit between EMDB map EMD-4074 and PDB model 5LMO. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



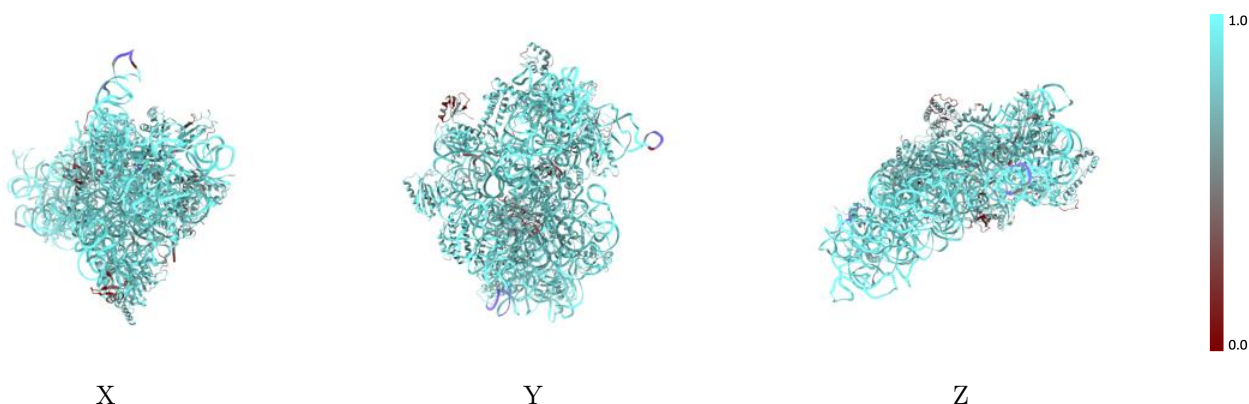
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



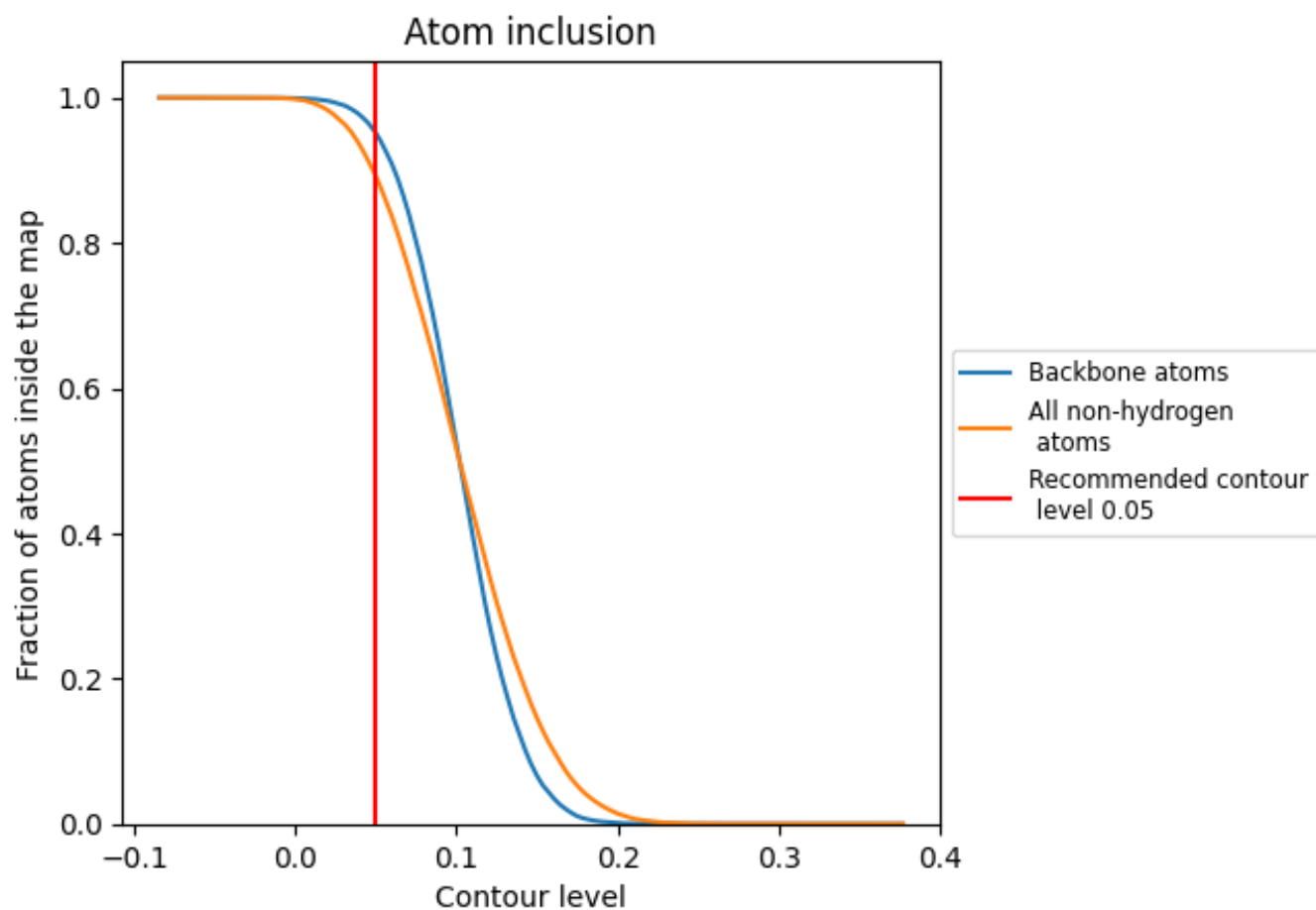
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 89% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8922	 0.2810
A	 0.9696	 0.2960
B	 0.5985	 0.2470
C	 0.8215	 0.2530
D	 0.8110	 0.2790
E	 0.8227	 0.3090
F	 0.8069	 0.2700
G	 0.8113	 0.2100
H	 0.8616	 0.3350
I	 0.7850	 0.2350
J	 0.7344	 0.2470
K	 0.8389	 0.2620
L	 0.8260	 0.3450
M	 0.7697	 0.1780
N	 0.7927	 0.2400
O	 0.8390	 0.2900
P	 0.8741	 0.3290
Q	 0.8584	 0.3270
R	 0.7722	 0.2370
S	 0.7322	 0.1660
T	 0.8295	 0.2720
V	 0.8534	 0.2280
W	 0.4326	 0.2160
X	 0.6368	 0.2290
Y	 0.6424	 0.1210

