Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:31 am GMT

PDB ID	:	5LMQ
EMDB ID	:	EMD-4076
Title	:	Structure of bacterial 30S-IF1-IF3-mRNA-tRNA translation pre-initiation complex, open form (state-2A)
Authors	:	Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on	:	2016-08-01
Resolution	:	4.20 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:

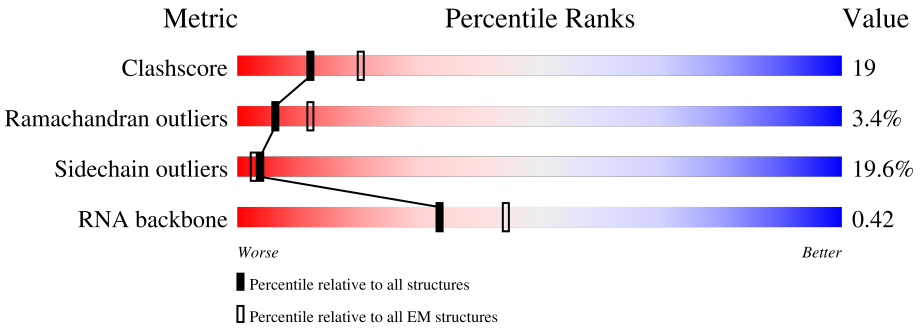
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 4.20 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 <=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	26% 57% 16%
2	B	256	51% 45% 38% 7% 9%
3	C	239	50% 33% 14%
4	D	209	53% 39% 8%
5	E	162	52% 33% 7% 7%
6	F	101	58% 37%
7	G	156	65% 33%

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Mol	Chain	Length	Quality of chain
8	H	138	65% 28% 7%
9	I	128	48% 43% 8%
10	J	105	15% 28% 48% 16% 7%
11	K	129	5% 63% 25% 6% 5%
12	L	132	59% 30% 5% 6%
13	M	126	13% 64% 33%
14	N	61	38% 49% 10%
15	O	89	55% 35% 7%
16	P	88	57% 34% 6%
17	Q	105	69% 20% 6% 6%
18	R	88	8% 42% 30% 11% 17%
19	S	93	6% 48% 32% 6% 12%
20	T	106	58% 25% 8% 7%
21	V	27	56% 33% 11%
22	W	72	11% 58% 33% 7%
23	X	171	22% 61% 29% 8%
24	Y	42	7% 14% 21% 14% 50%
25	Z	77	6% 39% 52% 6%

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
27	ZN	D	300	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 55841 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	32522	14481	6019	10512	1510	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
7	G	155	Total	C	N	O	S	0	0
			1257	781	252	218	6		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	122	Total	C	N	O	S	0	0
			906	563	172	168	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	125	Total	C	N	O	S	0	0
			997	617	207	171	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	21	Total 459	C 205	N 91	O 142	P 21	0	0

- Molecule 25 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	77	Total 1643	C 735	N 297	O 534	P 76	S 1	0	0

- Molecule 26 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
26	A	63	Total 63	Mg 63	0
26	W	1	Total 1	Mg 1	0

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

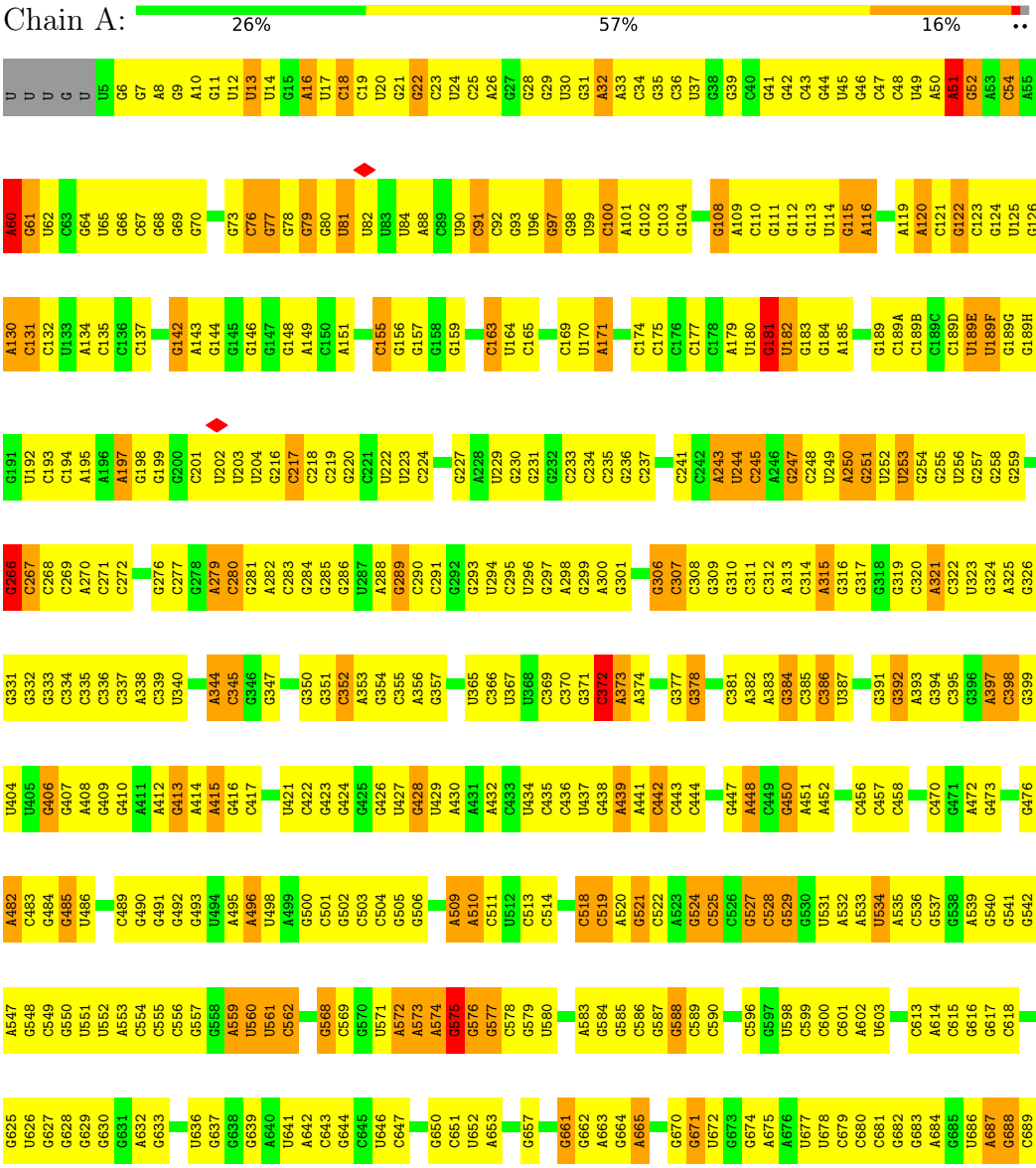
Mol	Chain	Residues	Atoms		AltConf
27	D	1	Total 1	Zn 1	0
27	N	1	Total 1	Zn 1	0

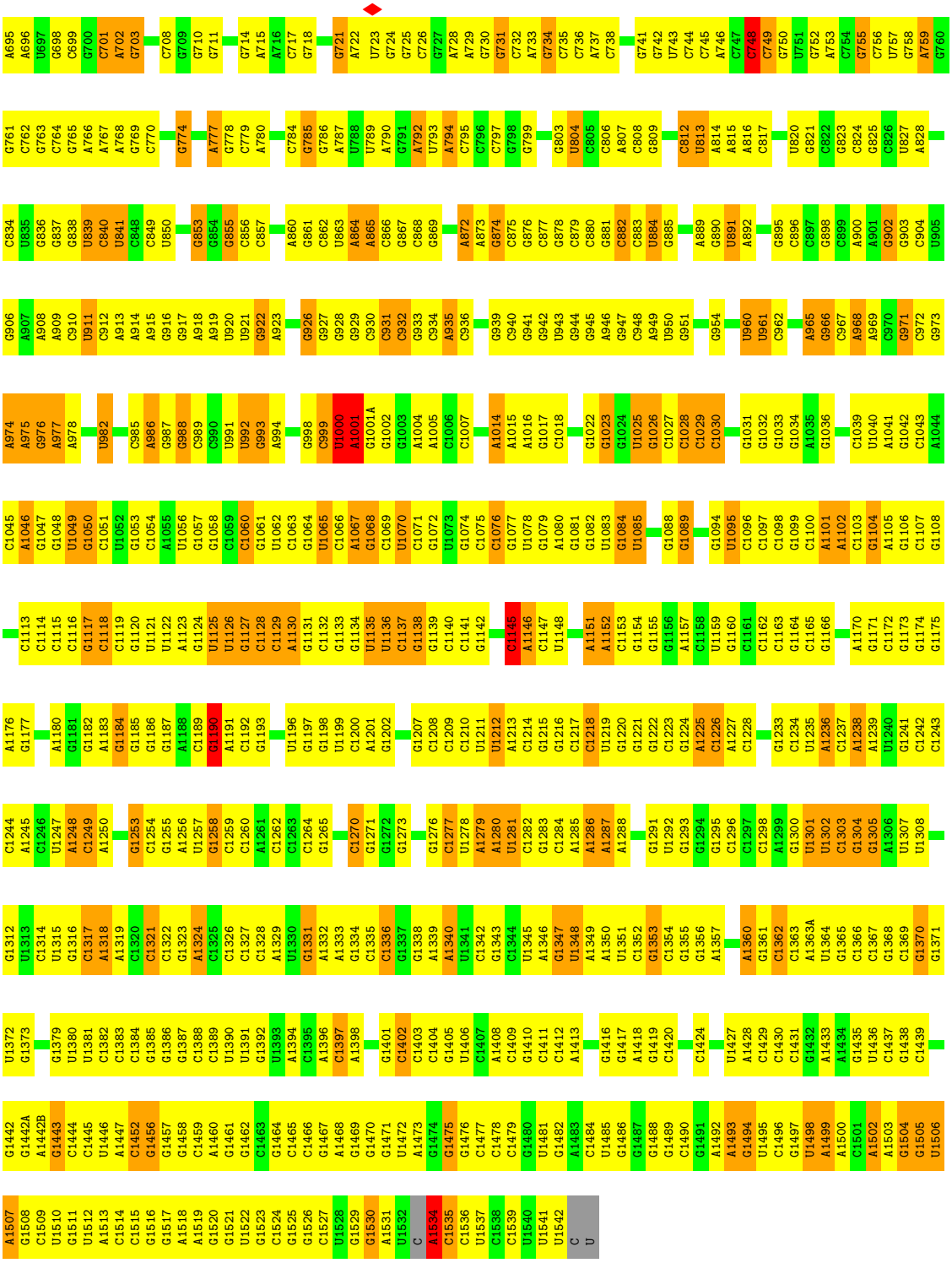
3 Residue-property plots (i)

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

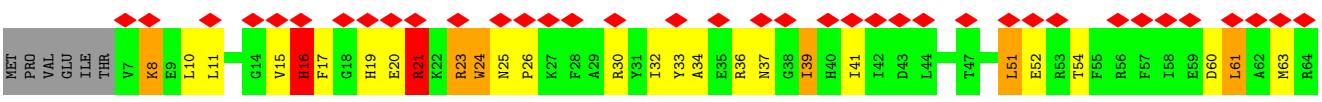
Chain A:





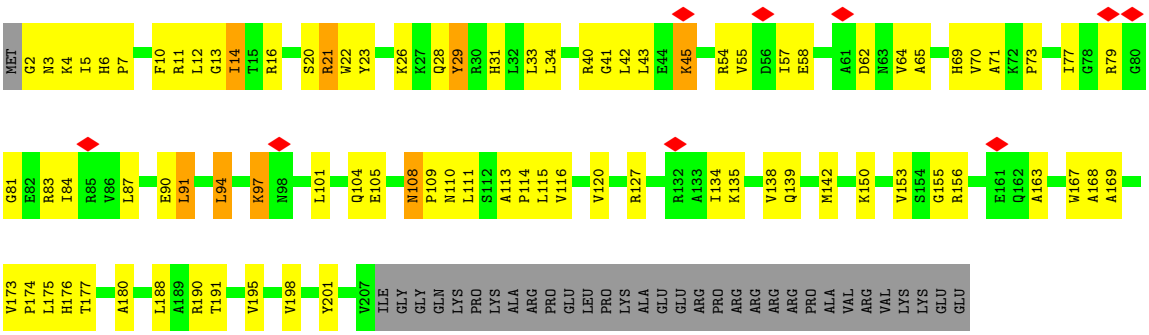
• Molecule 2: 30S ribosomal protein S2

Chain B:



• Molecule 3: 30S ribosomal protein S3

Chain C:

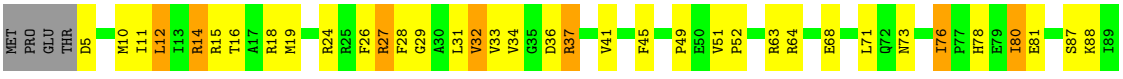


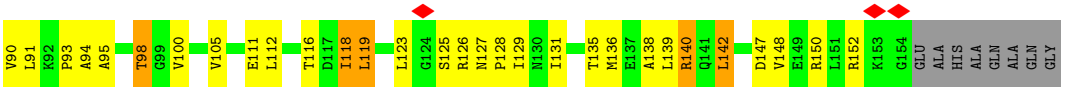
• Molecule 4: 30S ribosomal protein S4

Chain D:

• Molecule 5: 30S ribosomal protein S5

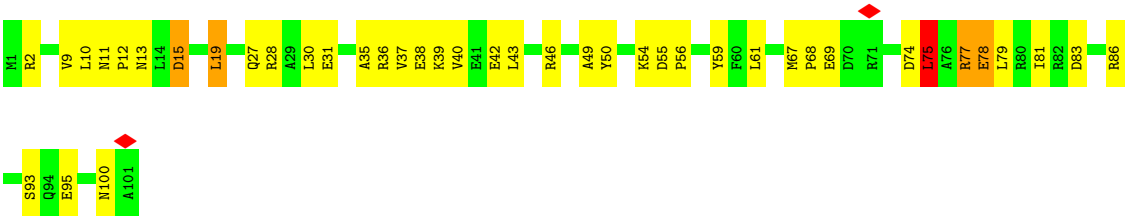
Chain E:





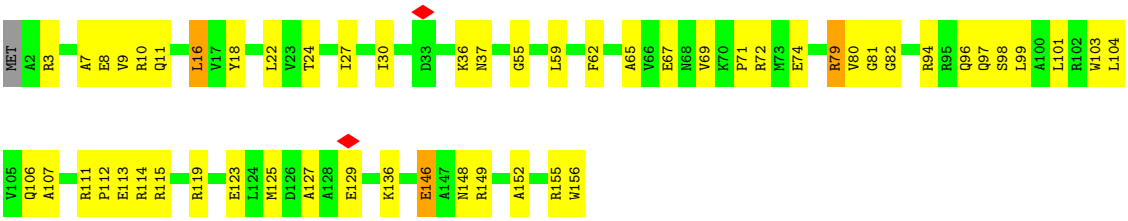
• Molecule 6: 30S ribosomal protein S6

Chain F:



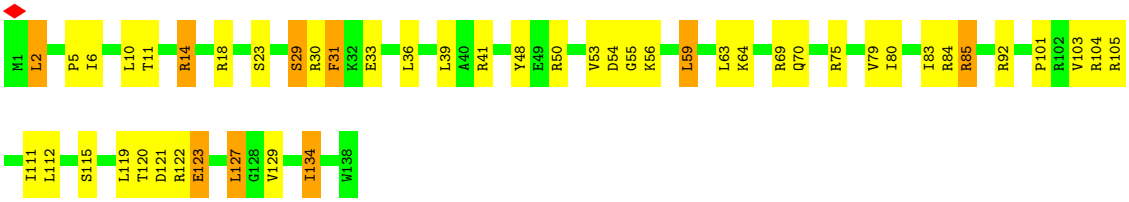
• Molecule 7: 30S ribosomal protein S7

Chain G:



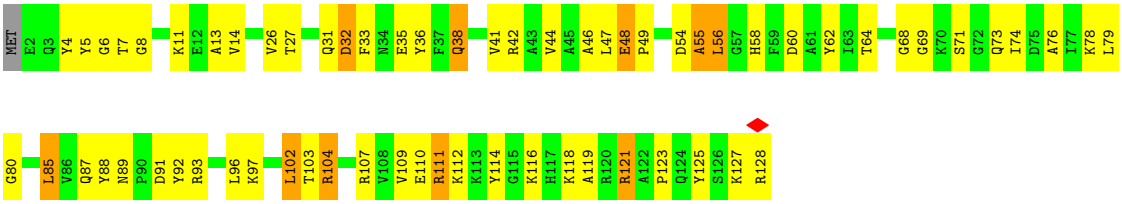
• Molecule 8: 30S ribosomal protein S8

Chain H:



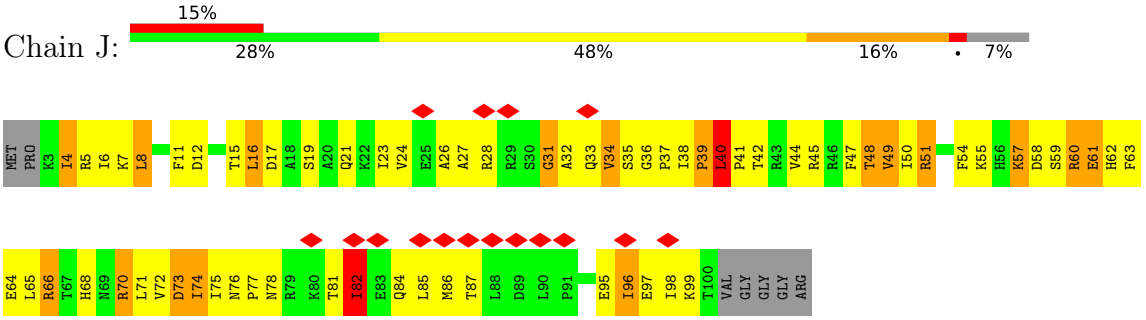
• Molecule 9: 30S ribosomal protein S9

Chain I:



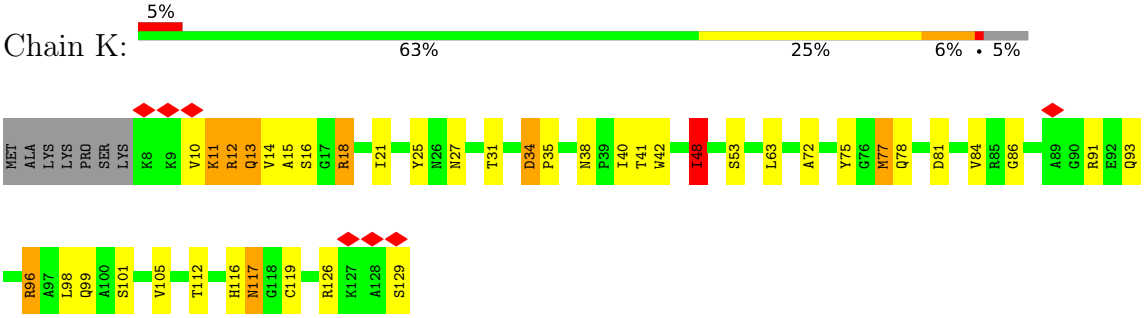
• Molecule 10: 30S ribosomal protein S10

Chain J:



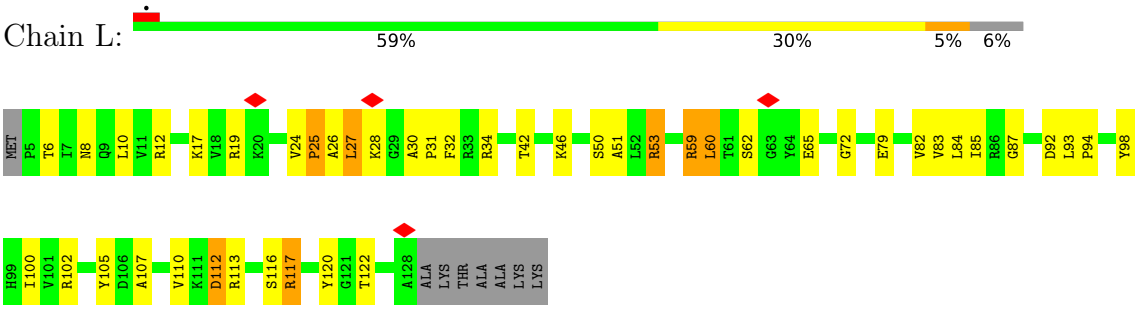
• Molecule 11: 30S ribosomal protein S11

Chain K:



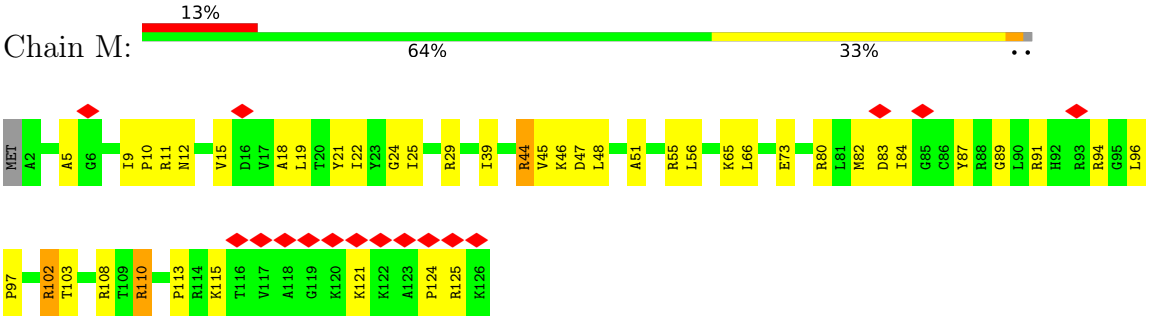
• Molecule 12: 30S ribosomal protein S12

Chain L:



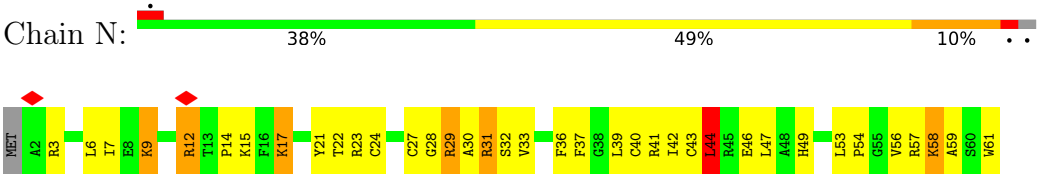
• Molecule 13: 30S ribosomal protein S13

Chain M:



• Molecule 14: 30S ribosomal protein S14 type Z

Chain N:



• Molecule 15: 30S ribosomal protein S15

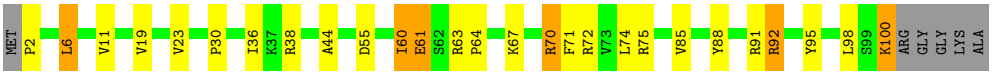
Chain O:

• Molecule 16: 30S ribosomal protein S16

Chain P:

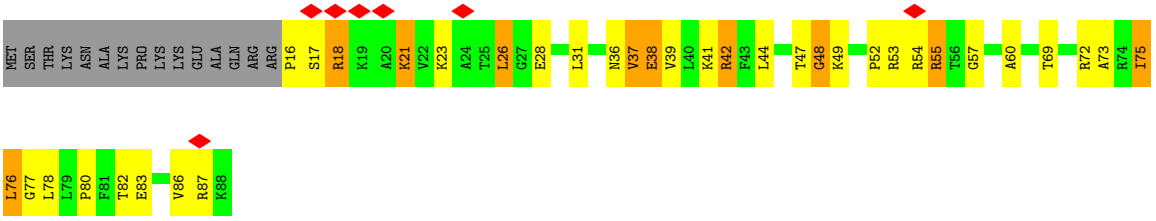
• Molecule 17: 30S ribosomal protein S17

Chain Q:



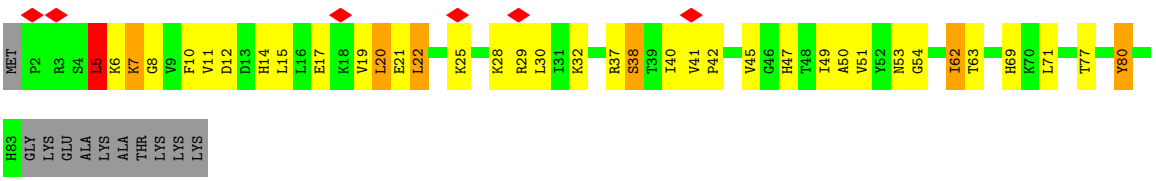
• Molecule 18: 30S ribosomal protein S18

Chain R:



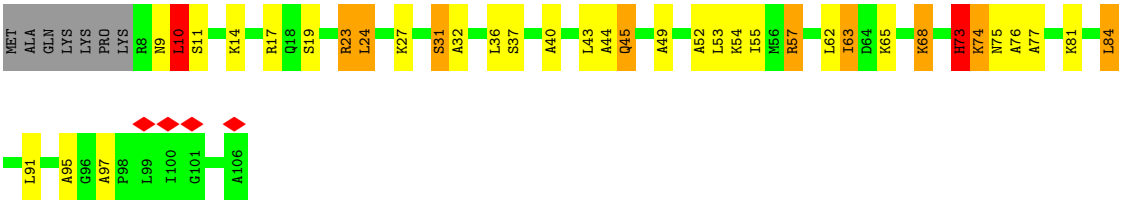
• Molecule 19: 30S ribosomal protein S19

Chain S:



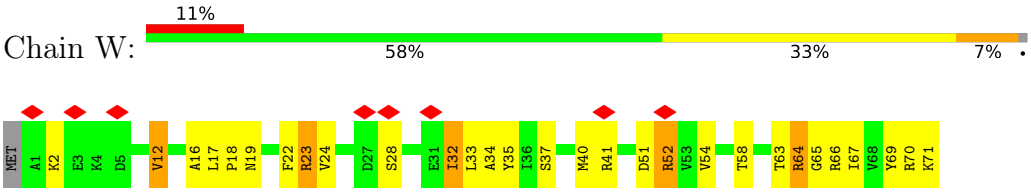
• Molecule 20: 30S ribosomal protein S20

Chain T:

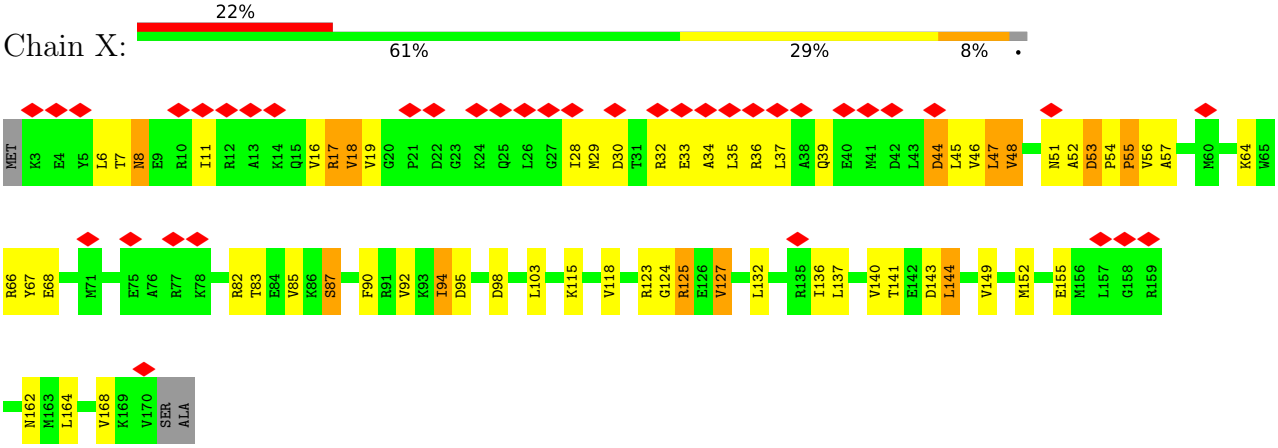


• Molecule 21: 30S ribosomal protein Thx

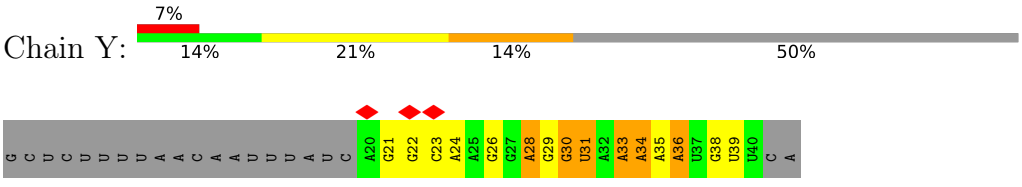
• Molecule 22: Translation initiation factor IF-1



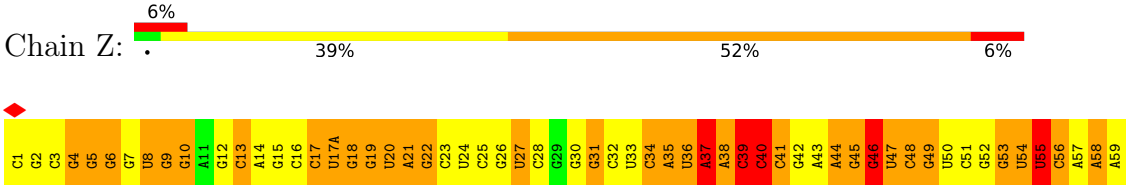
• Molecule 23: Translation initiation factor IF-3



• Molecule 24: mRNA



• Molecule 25: tRNA




U60
C61
C62
G63
G64
C65
C66
C67
C68
C69
G70
C71
A72
A73
C74
C75
A76

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31888	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 ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.532	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.075	Depositor
Map size (Å)	348.4, 348.4, 348.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	2/36394 (0.0%)	0.74	24/56779 (0.0%)
2	B	0.57	0/1935	0.86	1/2609 (0.0%)
3	C	0.48	0/1636	0.85	2/2205 (0.1%)
4	D	0.46	0/1733	0.85	0/2318
5	E	0.47	0/1162	0.82	0/1564
6	F	0.47	0/856	0.88	1/1154 (0.1%)
7	G	0.46	0/1276	0.79	0/1709
8	H	0.43	0/1136	0.82	0/1527
9	I	0.49	0/1029	0.79	1/1379 (0.1%)
10	J	0.51	0/805	0.76	0/1082
11	K	0.49	0/921	0.82	0/1241
12	L	0.44	0/986	0.77	0/1320
13	M	0.53	0/1008	0.82	1/1347 (0.1%)
14	N	0.44	0/501	0.80	1/664 (0.2%)
15	O	0.52	1/745 (0.1%)	0.89	1/992 (0.1%)
16	P	0.44	0/716	0.74	0/963
17	Q	0.43	0/836	0.79	0/1117
18	R	0.51	0/604	0.86	1/801 (0.1%)
19	S	0.55	0/670	0.82	1/903 (0.1%)
20	T	0.50	0/765	0.96	1/1007 (0.1%)
21	V	0.47	0/212	0.77	0/277
22	W	0.51	0/580	0.99	4/782 (0.5%)
23	X	0.56	0/1375	0.86	1/1844 (0.1%)
24	Y	0.56	0/516	0.83	0/804
25	Z	0.55	0/1718	0.90	3/2678 (0.1%)
All	All	0.43	3/60115 (0.0%)	0.78	43/89066 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
8	H	0	1
12	L	0	1
23	X	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	999	C	O3'-P	-6.98	1.52	1.61
1	A	1001	A	O3'-P	-6.75	1.53	1.61
15	O	24	SER	CB-OG	5.23	1.49	1.42

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	W	23	ARG	N-CA-C	-10.10	83.74	111.00
22	W	23	ARG	CB-CA-C	-8.69	93.02	110.40
6	F	75	LEU	CA-CB-CG	8.65	135.20	115.30
1	A	1001	A	O4'-C4'-C3'	-8.10	95.90	104.00
1	A	575	G	C2'-C3'-O3'	7.99	127.07	109.50
22	W	34	ALA	N-CA-CB	-7.90	99.04	110.10
25	Z	37	A	C2'-C3'-O3'	7.40	125.78	109.50
1	A	1001	A	C2'-C3'-O3'	7.33	125.63	109.50
1	A	1534	A	C2'-C3'-O3'	7.32	125.61	109.50
20	T	10	LEU	CA-CB-CG	7.29	132.08	115.30
1	A	1301	U	C2'-C3'-O3'	7.28	125.52	109.50
14	N	44	LEU	CA-CB-CG	7.10	131.63	115.30
1	A	1212	U	C2'-C3'-O3'	6.91	124.75	113.70
3	C	34	LEU	CA-CB-CG	6.90	131.17	115.30
1	A	266	G	C2'-C3'-O3'	6.88	124.70	113.70
1	A	1498	U	C2'-C3'-O3'	6.86	124.67	113.70
3	C	91	LEU	CA-CB-CG	6.63	130.55	115.30
1	A	197	A	C2'-C3'-O3'	6.58	124.23	113.70
1	A	1000	U	C2'-C3'-O3'	6.58	124.22	113.70
1	A	328	C	C2'-C3'-O3'	6.24	123.68	113.70
22	W	24	VAL	N-CA-CB	-6.20	97.85	111.50
1	A	1145	C	C2'-C3'-O3'	6.05	123.38	113.70
15	O	34	LEU	CA-CB-CG	6.05	129.21	115.30
23	X	103	LEU	CA-CB-CG	6.04	129.19	115.30
25	Z	39	C	C4'-C3'-O3'	5.96	124.92	113.00
1	A	748	C	C2'-C3'-O3'	5.95	123.22	113.70
2	B	51	LEU	CA-CB-CG	5.79	128.62	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1190	G	C2'-C3'-O3'	5.71	122.83	113.70
1	A	1067	A	C2'-C3'-O3'	5.69	122.81	113.70
25	Z	40	C	C2'-C3'-O3'	5.67	122.76	113.70
1	A	960	U	C2'-C3'-O3'	5.66	122.76	113.70
19	S	20	LEU	CA-CB-CG	5.60	128.19	115.30
18	R	26	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	428	G	C2'-C3'-O3'	5.37	122.29	113.70
1	A	1065	U	C2'-C3'-O3'	5.32	122.21	113.70
9	I	85	LEU	CA-CB-CG	5.27	127.43	115.30
13	M	56	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	965	A	C2'-C3'-O3'	5.17	121.97	113.70
1	A	792	A	C2'-C3'-O3'	5.16	121.95	113.70
1	A	181	G	C2'-C3'-O3'	5.12	121.90	113.70
1	A	51	A	C4'-C3'-O3'	5.11	123.22	113.00
1	A	372	C	C2'-C3'-O3'	5.10	121.86	113.70
1	A	60	A	C2'-C3'-O3'	5.08	121.82	113.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	11	LEU	Peptide
2	B	130	ARG	Peptide
8	H	2	LEU	Peptide
12	L	112	ASP	Peptide
23	X	53	ASP	Peptide
23	X	55	PRO	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	32522	0	16435	1114	0
2	B	1900	0	1951	55	0
3	C	1612	0	1677	81	0
4	D	1703	0	1765	77	0
5	E	1146	0	1207	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	843	0	857	18	0
7	G	1257	0	1296	25	0
8	H	1116	0	1177	17	0
9	I	1010	0	1037	47	0
10	J	792	0	835	83	0
11	K	906	0	928	21	0
12	L	970	0	1057	23	0
13	M	997	0	1072	27	0
14	N	492	0	530	47	0
15	O	734	0	771	20	0
16	P	700	0	720	18	0
17	Q	823	0	891	20	0
18	R	598	0	670	25	0
19	S	655	0	672	17	0
20	T	763	0	861	20	0
21	V	208	0	221	6	0
22	W	570	0	599	24	0
23	X	1356	0	1401	33	0
24	Y	459	0	228	15	0
25	Z	1643	0	844	128	0
26	A	63	0	0	0	0
26	W	1	0	0	0	0
27	D	1	0	0	4	0
27	N	1	0	0	0	0
All	All	55841	0	39702	1833	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 19.

All (1833) 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)
1:A:1080:A:H4'	5:E:16:THR:CG2	1.32	1.59
1:A:1080:A:C5'	5:E:16:THR:HG21	1.42	1.46
1:A:247:G:OP2	17:Q:100:LYS:CG	1.64	1.44
1:A:1080:A:C4'	5:E:16:THR:CG2	2.00	1.40
10:J:61:GLU:CD	14:N:58:LYS:HD3	1.39	1.39
10:J:38:ILE:CG2	10:J:71:LEU:O	1.81	1.29
10:J:36:GLY:O	10:J:72:VAL:HG22	1.10	1.28
10:J:61:GLU:OE2	14:N:58:LYS:HD3	1.25	1.28
1:A:413:G:O6	4:D:35:ARG:NH1	1.67	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:U:H3	1:A:872:A:N6	1.33	1.26
1:A:1080:A:C5'	5:E:16:THR:CG2	2.12	1.23
22:W:23:ARG:NH2	22:W:33:LEU:HD11	1.54	1.22
5:E:15:ARG:HG3	5:E:28:PHE:CE1	1.77	1.20
1:A:1113:C:H4'	3:C:14:ILE:CD1	1.70	1.20
10:J:38:ILE:HG23	10:J:71:LEU:O	1.32	1.18
5:E:15:ARG:CG	5:E:28:PHE:HE1	1.57	1.17
1:A:961:U:O4	1:A:974:A:N1	1.77	1.16
3:C:29:TYR:OH	14:N:54:PRO:HD2	1.44	1.16
1:A:92:C:H2'	1:A:93:G:C8	1.78	1.16
1:A:827:U:N3	1:A:872:A:N6	1.90	1.15
1:A:1080:A:H5"	5:E:16:THR:CG2	1.74	1.15
3:C:29:TYR:OH	14:N:54:PRO:CG	1.96	1.14
1:A:1125:U:C5	10:J:73:ASP:OD2	2.02	1.13
3:C:62:ASP:C	3:C:97:LYS:HD3	1.67	1.13
10:J:37:PRO:HA	10:J:72:VAL:CG2	1.78	1.13
10:J:37:PRO:HA	10:J:72:VAL:HG23	1.30	1.13
3:C:29:TYR:OH	14:N:54:PRO:CD	1.95	1.13
1:A:1080:A:H4'	5:E:16:THR:HG22	1.27	1.12
1:A:1081:G:OP2	5:E:27:ARG:NE	1.81	1.12
3:C:29:TYR:OH	14:N:54:PRO:HG2	1.45	1.11
3:C:64:VAL:HG23	3:C:97:LYS:CD	1.80	1.11
1:A:1113:C:H4'	3:C:14:ILE:HD13	1.30	1.11
3:C:62:ASP:O	3:C:97:LYS:HD3	1.48	1.11
1:A:413:G:C6	4:D:35:ARG:NH1	2.15	1.11
22:W:23:ARG:HH21	22:W:33:LEU:CD1	1.64	1.10
4:D:29:PRO:O	4:D:35:ARG:HD3	1.51	1.10
3:C:64:VAL:CG2	3:C:97:LYS:CE	2.31	1.09
1:A:1080:A:H4'	5:E:16:THR:HG23	1.12	1.08
3:C:64:VAL:HG21	3:C:97:LYS:HE2	1.31	1.07
1:A:247:G:OP2	17:Q:100:LYS:HG3	1.33	1.07
3:C:64:VAL:HG23	3:C:97:LYS:HD2	1.30	1.07
3:C:64:VAL:CG2	3:C:97:LYS:HE2	1.86	1.06
25:Z:5:G:H1	25:Z:68:C:N4	1.52	1.05
1:A:247:G:OP2	17:Q:100:LYS:HG2	1.47	1.05
1:A:1081:G:OP1	5:E:27:ARG:HD2	1.55	1.05
3:C:29:TYR:HE1	3:C:33:LEU:HD12	1.19	1.05
10:J:61:GLU:OE1	14:N:58:LYS:HD3	1.54	1.04
10:J:36:GLY:O	10:J:72:VAL:CG2	2.06	1.04
3:C:29:TYR:CE1	3:C:33:LEU:HD12	1.92	1.03
10:J:61:GLU:CD	14:N:58:LYS:CD	2.26	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:61:GLU:OE2	14:N:58:LYS:CD	2.09	1.01
4:D:201:GLN:NE2	5:E:116:THR:OG1	1.93	1.00
1:A:664:G:H22	1:A:741:G:H1	1.04	1.00
1:A:827:U:O4	1:A:872:A:N1	1.95	1.00
22:W:23:ARG:NH2	22:W:33:LEU:CD1	2.23	0.99
5:E:15:ARG:HG3	5:E:28:PHE:HE1	1.11	0.99
23:X:52:ALA:HB2	25:Z:19:G:N2	1.77	0.99
25:Z:44:A:O2'	25:Z:45:G:H5'	1.62	0.98
1:A:92:C:H2'	1:A:93:G:H8	1.16	0.98
1:A:80:G:H3'	1:A:81:U:H5"	1.45	0.98
4:D:29:PRO:O	4:D:35:ARG:CD	2.12	0.98
1:A:864:A:H2'	1:A:865:A:C8	1.98	0.97
1:A:1081:G:P	5:E:27:ARG:CD	2.52	0.97
25:Z:72:A:H3'	25:Z:73:A:H5"	1.41	0.97
10:J:61:GLU:OE1	14:N:58:LYS:CD	2.13	0.96
1:A:413:G:C5	4:D:35:ARG:NH1	2.33	0.96
10:J:38:ILE:HG22	10:J:71:LEU:O	1.64	0.95
4:D:31:CYS:SG	27:D:300:ZN:ZN	1.56	0.94
1:A:413:G:N7	4:D:35:ARG:NH1	2.17	0.93
25:Z:7:G:H2'	25:Z:49:G:H5'	1.50	0.93
1:A:1081:G:OP2	5:E:27:ARG:CD	2.15	0.93
1:A:1219:U:H2'	1:A:1220:G:C8	2.04	0.93
1:A:1458:G:OP1	20:T:32:ALA:HA	1.67	0.93
1:A:1219:U:H2'	1:A:1220:G:H8	1.33	0.93
1:A:1125:U:H5'	1:A:1126:U:H5	1.34	0.92
2:B:186:ALA:HB2	2:B:197:VAL:HG11	1.52	0.92
5:E:15:ARG:CG	5:E:28:PHE:CE1	2.44	0.92
1:A:1080:A:C4'	5:E:16:THR:HG21	1.86	0.91
1:A:736:C:H2'	1:A:737:A:C8	2.06	0.91
25:Z:5:G:N2	25:Z:68:C:N3	2.20	0.90
3:C:64:VAL:HG23	3:C:97:LYS:CE	2.00	0.90
1:A:1113:C:C4'	3:C:14:ILE:CD1	2.48	0.90
4:D:26:CYS:SG	27:D:300:ZN:ZN	1.60	0.89
1:A:1001:A:H2'	1:A:1001(A):G:C8	2.06	0.89
3:C:62:ASP:O	3:C:97:LYS:CD	2.20	0.89
4:D:35:ARG:NH2	4:D:35:ARG:HB3	1.88	0.89
9:I:125:TYR:CE1	9:I:128:ARG:HB3	2.07	0.89
23:X:52:ALA:HB2	25:Z:19:G:H22	1.33	0.88
1:A:1348:U:H2'	1:A:1349:A:H8	1.37	0.88
1:A:1080:A:C4'	5:E:16:THR:HG23	1.88	0.87
25:Z:4:G:H1	25:Z:69:C:H42	1.23	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1386:G:H2'	1:A:1387:G:H8	1.40	0.86
5:E:15:ARG:HH21	5:E:15:ARG:HG2	1.38	0.86
5:E:15:ARG:NH2	5:E:26:PHE:CG	2.42	0.86
25:Z:9:G:O2'	25:Z:45:G:H1'	1.75	0.86
1:A:18:C:H2'	1:A:19:C:O4'	1.74	0.86
1:A:1403:C:O2	1:A:1499:A:N6	2.08	0.85
1:A:729:A:H2'	1:A:730:G:H8	1.41	0.85
1:A:1079:G:H2'	1:A:1080:A:C8	2.12	0.85
4:D:36:ARG:HD2	4:D:38:TYR:CZ	2.11	0.85
5:E:15:ARG:HA	5:E:28:PHE:CD1	2.12	0.84
10:J:24:VAL:HG13	10:J:28:ARG:HE	1.42	0.84
24:Y:34:A:H2'	24:Y:35:A:C8	2.12	0.84
1:A:1280:A:H3'	1:A:1281:U:H5"	1.58	0.84
1:A:920:U:H2'	1:A:921:U:C6	2.12	0.84
1:A:312:C:H2'	1:A:313:A:C8	2.13	0.84
5:E:27:ARG:CB	5:E:27:ARG:HH11	1.89	0.84
1:A:1488:G:H2'	1:A:1489:G:H8	1.43	0.83
10:J:36:GLY:C	10:J:72:VAL:HG22	1.97	0.83
9:I:5:TYR:CE2	9:I:7:THR:OG1	2.31	0.83
1:A:1125:U:H5	10:J:73:ASP:OD2	1.59	0.83
3:C:29:TYR:CE1	3:C:33:LEU:CD1	2.61	0.83
5:E:15:ARG:HA	5:E:28:PHE:CE1	2.14	0.83
1:A:1081:G:OP1	5:E:27:ARG:CD	2.27	0.82
4:D:18:LYS:NZ	4:D:34:GLU:HG3	1.94	0.82
1:A:1081:G:P	5:E:27:ARG:HD3	2.19	0.81
24:Y:33:A:O2'	24:Y:34:A:C8	2.34	0.81
9:I:97:LYS:HG3	9:I:102:LEU:HD13	1.62	0.81
1:A:662:G:H2'	1:A:663:A:C8	2.17	0.80
1:A:1113:C:O2'	3:C:14:ILE:HD11	1.81	0.80
25:Z:37:A:H3'	25:Z:38:A:H8	1.46	0.80
1:A:917:G:H2'	1:A:918:A:C8	2.16	0.80
3:C:29:TYR:HH	14:N:54:PRO:HG2	1.46	0.80
1:A:1123:A:H4'	10:J:36:GLY:HA3	1.64	0.80
1:A:1080:A:H5"	5:E:16:THR:HG21	0.81	0.79
25:Z:40:C:H2'	25:Z:41:C:H6	1.45	0.79
1:A:76:C:C2'	1:A:77:G:H5'	2.12	0.79
1:A:312:C:H2'	1:A:313:A:H8	1.46	0.79
22:W:23:ARG:HH21	22:W:33:LEU:HD13	1.45	0.79
25:Z:10:G:O6	25:Z:45:G:N2	2.14	0.79
1:A:501:C:H2'	1:A:502:G:C8	2.18	0.79
1:A:1071:C:H2'	1:A:1072:G:H8	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:33:A:O2'	24:Y:34:A:H8	1.66	0.79
25:Z:21:A:N6	25:Z:46:G7M:H2'	1.98	0.78
1:A:1256:A:N6	1:A:1278:U:O2	2.15	0.78
1:A:439:A:P	1:A:493:G:H1	2.06	0.78
1:A:1127:G:H21	1:A:1147:C:N4	1.81	0.78
4:D:36:ARG:HD2	4:D:38:TYR:OH	1.82	0.78
25:Z:68:C:H2'	25:Z:69:C:C6	2.18	0.78
18:R:47:THR:HA	18:R:83:GLU:HB2	1.65	0.78
1:A:1080:A:O3'	5:E:16:THR:HG22	1.83	0.78
1:A:1542:U:H4'	18:R:18:ARG:H	1.46	0.78
10:J:60:ARG:HH11	10:J:60:ARG:HG3	1.49	0.78
1:A:714:G:H2'	1:A:715:A:C8	2.20	0.77
3:C:62:ASP:CA	3:C:97:LYS:HD3	2.13	0.77
25:Z:21:A:H61	25:Z:46:G7M:H2'	1.49	0.77
25:Z:49:G:N2	25:Z:66:C:C2	2.52	0.77
4:D:35:ARG:HB3	4:D:35:ARG:HH21	1.49	0.77
1:A:748:C:H1'	1:A:749:C:H5	1.50	0.76
5:E:15:ARG:HH22	5:E:26:PHE:CB	1.99	0.76
10:J:6:ILE:HA	10:J:97:GLU:O	1.84	0.76
1:A:1113:C:H4'	3:C:14:ILE:HD12	1.65	0.76
2:B:186:ALA:CB	2:B:197:VAL:HG11	2.15	0.76
1:A:1342:C:H2'	1:A:1343:G:H8	1.49	0.76
10:J:5:ARG:HA	10:J:73:ASP:OD1	1.85	0.76
1:A:90:U:H2'	1:A:91:C:C6	2.20	0.76
1:A:736:C:H2'	1:A:737:A:H8	1.49	0.76
1:A:1102:A:H2'	1:A:1103:C:C6	2.20	0.76
3:C:23:TYR:HA	10:J:11:PHE:CE2	2.21	0.76
10:J:60:ARG:HG3	10:J:60:ARG:NH1	2.01	0.76
1:A:247:G:OP2	17:Q:100:LYS:CD	2.34	0.76
3:C:29:TYR:CZ	14:N:54:PRO:HG2	2.20	0.75
1:A:80:G:H3'	1:A:81:U:C5'	2.17	0.75
4:D:68:TYR:HB2	4:D:70:ILE:HD11	1.67	0.75
1:A:918:A:H2'	1:A:919:A:C8	2.22	0.75
3:C:64:VAL:CG2	3:C:97:LYS:HD2	2.14	0.74
4:D:36:ARG:CD	4:D:38:TYR:CZ	2.69	0.74
12:L:117:ARG:HB2	12:L:122:THR:HB	1.68	0.74
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.69	0.74
22:W:33:LEU:O	22:W:64:ARG:HA	1.88	0.74
11:K:18:ARG:HG3	11:K:81:ASP:HB2	1.68	0.74
3:C:64:VAL:CG2	3:C:97:LYS:CD	2.61	0.74
10:J:33:GLN:HB3	10:J:75:ILE:HD12	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1172:C:H2'	1:A:1173:G:H8	1.52	0.74
6:F:49:ALA:HB1	18:R:80:PRO:HA	1.68	0.74
1:A:1342:C:H2'	1:A:1343:G:C8	2.22	0.74
10:J:39:PRO:O	10:J:40:LEU:HB2	1.88	0.73
6:F:100:ASN:HA	18:R:23:LYS:HE2	1.69	0.73
10:J:37:PRO:CA	10:J:72:VAL:CG2	2.63	0.73
23:X:19:VAL:HG21	25:Z:56:C:N4	2.03	0.73
25:Z:6:G:N2	25:Z:68:C:C2	2.56	0.73
1:A:78:G:H2'	1:A:79:G:O4'	1.88	0.73
1:A:880:C:H2'	1:A:881:G:H8	1.52	0.73
9:I:55:ALA:HB1	9:I:58:HIS:HB3	1.71	0.73
20:T:14:LYS:HA	20:T:17:ARG:HD2	1.71	0.73
1:A:24:U:H2'	1:A:25:C:C6	2.24	0.73
1:A:1007:C:H42	1:A:1022:G:H1	1.36	0.73
4:D:29:PRO:O	4:D:35:ARG:CG	2.35	0.73
1:A:664:G:N2	1:A:741:G:H1	1.85	0.73
1:A:973:G:H3'	1:A:974:A:H5"	1.70	0.73
2:B:20:GLU:HB3	2:B:23:ARG:HD2	1.70	0.73
1:A:524:G:C6	1:A:525:C:N4	2.56	0.73
25:Z:49:G:C2	25:Z:66:C:N3	2.57	0.73
25:Z:12:G:H1	25:Z:23:C:H42	1.36	0.72
1:A:814:A:H2'	1:A:816:A:H5"	1.70	0.72
1:A:946:A:H2'	1:A:947:G:C8	2.23	0.72
18:R:37:VAL:HG22	18:R:78:LEU:HD13	1.71	0.72
5:E:27:ARG:HH11	5:E:27:ARG:HB2	1.52	0.72
23:X:64:LYS:O	23:X:68:GLU:HG2	1.89	0.72
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.72	0.72
1:A:1287:A:H2'	1:A:1288:A:C8	2.25	0.72
1:A:76:C:H2'	1:A:77:G:H5'	1.71	0.72
1:A:1384:C:H2'	1:A:1385:G:C8	2.24	0.72
1:A:1105:A:H2'	1:A:1106:G:H8	1.53	0.72
11:K:15:ALA:HA	11:K:77:MET:HA	1.69	0.71
1:A:961:U:C4	1:A:974:A:N1	2.58	0.71
1:A:1427:U:H2'	1:A:1428:A:C8	2.25	0.71
1:A:1081:G:OP2	5:E:27:ARG:HD3	1.88	0.71
1:A:1226:C:H2'	13:M:103:THR:HB	1.72	0.71
3:C:29:TYR:HE1	3:C:33:LEU:CD1	2.00	0.71
25:Z:39:C:H2'	25:Z:40:C:C6	2.26	0.71
1:A:745:C:H2'	1:A:746:A:C8	2.25	0.71
25:Z:48:C:H5"	25:Z:50:U:OP1	1.91	0.71
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:G:C6	1:A:1100:C:N3	2.59	0.70
1:A:868:C:H2'	1:A:869:G:O4'	1.91	0.70
3:C:77:ILE:HA	3:C:84:ILE:HB	1.72	0.70
4:D:18:LYS:HZ2	4:D:34:GLU:HG3	1.56	0.70
1:A:1014:A:H5"	19:S:14:HIS:HB3	1.72	0.70
1:A:1530:G:H2'	1:A:1531:A:C8	2.27	0.70
1:A:1518:A:H2'	1:A:1519:A:C8	2.26	0.70
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.74	0.70
1:A:1128:C:H1'	1:A:1146:A:H61	1.57	0.70
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.74	0.70
11:K:126:ARG:HH12	11:K:129:SER:HA	1.56	0.70
1:A:501:C:H2'	1:A:502:G:H8	1.55	0.69
1:A:1071:C:H2'	1:A:1072:G:C8	2.27	0.69
3:C:73:PRO:O	3:C:77:ILE:HG12	1.92	0.69
25:Z:69:C:H2'	25:Z:70:G:O4'	1.91	0.69
1:A:1022:G:H2'	1:A:1023:G:H8	1.56	0.69
1:A:1513:A:H2'	1:A:1514:C:C6	2.27	0.69
1:A:79:G:H2'	1:A:80:G:H8	1.56	0.69
1:A:834:C:H5"	18:R:60:ALA:CB	2.23	0.69
4:D:36:ARG:CD	4:D:38:TYR:OH	2.39	0.69
5:E:15:ARG:HG3	5:E:28:PHE:CZ	2.28	0.69
1:A:975:A:H4'	1:A:976:G:H5'	1.73	0.69
16:P:59:TRP:O	16:P:62:VAL:HG22	1.92	0.69
1:A:524:G:C2	1:A:525:C:N3	2.61	0.69
1:A:1076:C:H2'	1:A:1077:G:C8	2.28	0.69
1:A:1488:G:H2'	1:A:1489:G:C8	2.26	0.69
1:A:1125:U:H5'	1:A:1126:U:C5	2.25	0.69
1:A:1151:A:O2'	1:A:1152:A:H8	1.76	0.69
1:A:56:U:H2'	1:A:57:G:C8	2.28	0.68
1:A:1348:U:H2'	1:A:1349:A:C8	2.25	0.68
1:A:13:U:H3	1:A:915:A:N6	1.90	0.68
4:D:31:CYS:HG	27:D:300:ZN:ZN	0.40	0.68
1:A:34:C:H2'	1:A:35:G:C8	2.27	0.68
1:A:579:G:H2'	1:A:580:U:C6	2.29	0.68
1:A:778:G:HO2'	11:K:119:CYS:HG	1.32	0.68
1:A:877:C:H2'	1:A:878:G:H8	1.59	0.68
1:A:1218:C:H2'	1:A:1219:U:C6	2.27	0.68
1:A:67:C:H2'	1:A:68:G:C8	2.29	0.68
1:A:1060:C:C5	3:C:2:GLY:HA2	2.29	0.68
25:Z:72:A:H3'	25:Z:73:A:C5'	2.19	0.68
1:A:729:A:H2'	1:A:730:G:C8	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1080:A:C5'	5:E:16:THR:HG23	2.13	0.68
1:A:1080:A:C4'	5:E:16:THR:HG22	1.98	0.68
3:C:116:VAL:O	3:C:120:VAL:HG23	1.94	0.68
4:D:96:LEU:HG	4:D:139:ARG:HE	1.59	0.68
1:A:987:G:H1	1:A:1218:C:H42	1.41	0.67
5:E:100:VAL:HG13	5:E:118:ILE:HD11	1.75	0.67
1:A:269:C:H2'	1:A:270:A:C8	2.28	0.67
1:A:313:A:H2'	1:A:314:C:C6	2.29	0.67
1:A:1386:G:H2'	1:A:1387:G:C8	2.28	0.67
3:C:23:TYR:HA	10:J:11:PHE:HE2	1.58	0.67
5:E:15:ARG:NH2	5:E:26:PHE:CD1	2.62	0.67
1:A:34:C:H2'	1:A:35:G:H8	1.58	0.67
1:A:576:G:H3'	1:A:577:G:H5"	1.76	0.67
25:Z:66:C:H2'	25:Z:67:C:O4'	1.93	0.67
1:A:45:U:H2'	1:A:46:G:C8	2.30	0.67
10:J:51:ARG:HD3	10:J:59:SER:HB3	1.76	0.67
1:A:1113:C:C4'	3:C:14:ILE:HD12	2.24	0.67
1:A:1405:G:H2'	1:A:1406:U:C6	2.30	0.67
10:J:62:HIS:HB2	14:N:59:ALA:HB3	1.76	0.67
1:A:1523:G:H2'	1:A:1524:C:C6	2.30	0.67
1:A:1223:C:H5"	1:A:1224:G:H5"	1.76	0.66
1:A:1384:C:H2'	1:A:1385:G:H8	1.60	0.66
10:J:5:ARG:CA	10:J:73:ASP:OD1	2.42	0.66
1:A:1445:C:C2	1:A:1458:G:C2	2.84	0.66
1:A:1318:A:H1'	19:S:37:ARG:HH11	1.61	0.66
1:A:1353:G:N2	1:A:1354:C:C2	2.64	0.66
25:Z:40:C:H2'	25:Z:41:C:C6	2.29	0.66
1:A:750:G:N3	15:O:23:GLY:HA3	2.11	0.66
25:Z:5:G:H1	25:Z:68:C:H42	0.74	0.66
15:O:26:GLU:O	15:O:29:VAL:HG12	1.95	0.66
16:P:58:TYR:O	16:P:62:VAL:HG13	1.96	0.66
1:A:1404:C:H2'	1:A:1405:G:C8	2.31	0.66
2:B:219:VAL:HA	2:B:222:ILE:HD12	1.76	0.66
15:O:12:ILE:HG21	15:O:22:THR:HG22	1.78	0.66
1:A:398:C:H2'	1:A:399:G:H8	1.59	0.66
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.78	0.66
1:A:92:C:C2'	1:A:93:G:H8	2.02	0.66
1:A:725:G:N2	1:A:726:C:C2	2.64	0.66
1:A:1405:G:H2'	1:A:1406:U:H6	1.60	0.66
1:A:381:C:H2'	1:A:382:A:O4'	1.95	0.65
1:A:457:C:H2'	1:A:458:C:C6	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:8:4SU:H6	25:Z:8:4SU:O5'	1.95	0.65
25:Z:38:A:H3'	25:Z:39:C:H6	1.61	0.65
1:A:774:G:N2	1:A:806:C:C2	2.64	0.65
1:A:243:A:H4'	1:A:244:U:O5'	1.95	0.65
1:A:1281:U:H4'	1:A:1282:C:OP2	1.96	0.65
2:B:21:ARG:HA	2:B:39:ILE:HA	1.78	0.65
8:H:64:LYS:HB3	8:H:79:VAL:HG11	1.77	0.65
1:A:975:A:H4'	1:A:976:G:C5'	2.26	0.65
19:S:47:HIS:O	19:S:62:ILE:HG22	1.97	0.65
25:Z:71:C:H2'	25:Z:72:A:O4'	1.96	0.65
1:A:880:C:H2'	1:A:881:G:C8	2.31	0.65
1:A:910:C:H4'	1:A:1413:A:H4'	1.78	0.65
1:A:1084:G:H5"	1:A:1085:U:H2'	1.77	0.65
1:A:1172:C:H2'	1:A:1173:G:C8	2.31	0.65
25:Z:4:G:H1	25:Z:69:C:N4	1.93	0.65
4:D:11:LEU:HD13	4:D:66:ARG:HG3	1.78	0.65
5:E:15:ARG:HG2	5:E:15:ARG:NH2	2.11	0.65
1:A:289:G:N2	1:A:290:C:C2	2.65	0.65
5:E:140:ARG:HH11	5:E:140:ARG:HB2	1.62	0.65
24:Y:23:C:H2'	24:Y:24:A:O4'	1.97	0.65
1:A:1048:G:N2	1:A:1210:C:C2	2.66	0.64
25:Z:49:G:C2	25:Z:66:C:C2	2.86	0.64
1:A:16:A:H2	1:A:1080:A:N3	1.95	0.64
1:A:1475:G:H2'	1:A:1476:G:H8	1.61	0.64
10:J:5:ARG:HG2	10:J:71:LEU:HD21	1.79	0.64
11:K:99:GLN:HA	11:K:105:VAL:HG21	1.79	0.64
18:R:38:GLU:H	18:R:38:GLU:CD	1.99	0.64
1:A:132:C:C2	1:A:231:G:N2	2.65	0.64
25:Z:10:G:H1	25:Z:25:C:H42	1.45	0.64
1:A:992:U:H1'	1:A:993:G:C2	2.33	0.64
1:A:662:G:H2'	1:A:663:A:H8	1.58	0.64
1:A:737:A:H2'	1:A:738:C:C6	2.33	0.64
1:A:839:U:O2	1:A:839:U:H2'	1.97	0.64
1:A:123:C:H2'	1:A:124:G:H8	1.63	0.64
2:B:72:GLY:HA3	2:B:81:VAL:HG21	1.80	0.64
10:J:82:ILE:HG22	10:J:86:MET:HB2	1.78	0.64
1:A:45:U:H2'	1:A:46:G:H8	1.63	0.64
1:A:254:G:H1	1:A:272:C:H42	1.46	0.63
1:A:999:C:O2	1:A:1043:C:O2	2.15	0.63
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.80	0.63
1:A:354:G:N2	1:A:355:C:C2	2.67	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1507:A:H2'	1:A:1508:G:C8	2.32	0.63
1:A:1523:G:H2'	1:A:1524:C:H6	1.63	0.63
2:B:223:ILE:HG21	2:B:230:VAL:HB	1.79	0.63
4:D:18:LYS:HZ3	4:D:34:GLU:HG3	1.64	0.63
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.80	0.63
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.80	0.63
1:A:748:C:H1'	1:A:749:C:C5	2.33	0.63
17:Q:11:VAL:HG12	17:Q:85:VAL:HG22	1.80	0.63
25:Z:38:A:H3'	25:Z:39:C:C6	2.33	0.63
1:A:1354:C:H2'	1:A:1355:G:H8	1.63	0.63
25:Z:56:C:H2'	25:Z:57:A:C8	2.33	0.63
1:A:695:A:H2'	1:A:696:A:C8	2.34	0.62
1:A:1496:C:H2'	1:A:1497:G:O4'	1.98	0.62
1:A:1125:U:C4	10:J:73:ASP:OD2	2.53	0.62
1:A:1166:G:N2	1:A:1170:A:OP2	2.31	0.62
10:J:6:ILE:CD1	10:J:23:ILE:HG21	2.29	0.62
1:A:24:U:H2'	1:A:25:C:H6	1.63	0.62
5:E:15:ARG:HG2	5:E:28:PHE:HE1	1.57	0.62
6:F:12:PRO:HA	6:F:59:TYR:HB2	1.82	0.62
9:I:5:TYR:HE2	9:I:7:THR:OG1	1.82	0.62
25:Z:67:C:C2	25:Z:68:C:C5	2.87	0.62
1:A:253:U:H2'	1:A:254:G:H8	1.63	0.62
1:A:890:G:O2'	1:A:906:G:O6	2.16	0.62
12:L:25:PRO:C	12:L:27:LEU:H	2.00	0.62
1:A:779:C:H2'	1:A:780:A:O4'	1.99	0.62
1:A:1076:C:H2'	1:A:1077:G:H8	1.65	0.62
1:A:1118:C:P	9:I:104:ARG:HE	2.22	0.62
1:A:258:G:N2	1:A:269:C:C2	2.68	0.62
1:A:1278:U:H5"	1:A:1279:A:O4'	2.00	0.62
1:A:1493:A:H4'	1:A:1494:G:OP1	1.99	0.62
25:Z:37:A:H3'	25:Z:38:A:C8	2.32	0.62
25:Z:52:G:HO2'	25:Z:53:G:H8	1.47	0.62
22:W:17:LEU:HB3	22:W:18:PRO:HD2	1.81	0.62
1:A:911:U:H2'	1:A:912:C:C6	2.35	0.62
1:A:1255:G:H2'	1:A:1279:A:H62	1.65	0.62
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.81	0.62
19:S:11:VAL:HA	19:S:38:SER:HB2	1.82	0.62
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.14	0.62
6:F:75:LEU:O	6:F:79:LEU:HG	2.00	0.62
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.80	0.62
1:A:32:A:H2'	1:A:33:A:C8	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:C:H4'	1:A:841:U:O5'	2.00	0.61
1:A:917:G:H2'	1:A:918:A:H8	1.62	0.61
1:A:961:U:H2'	1:A:962:C:C6	2.35	0.61
3:C:29:TYR:O	3:C:29:TYR:HD1	1.82	0.61
23:X:34:ALA:HA	23:X:37:LEU:HD12	1.81	0.61
1:A:457:C:H2'	1:A:458:C:H6	1.66	0.61
1:A:652:U:O4	1:A:752:G:O2'	2.15	0.61
1:A:1062:U:H2'	1:A:1063:C:C6	2.35	0.61
1:A:132:C:N3	1:A:231:G:C2	2.69	0.61
1:A:992:U:O2	1:A:992:U:H2'	2.00	0.61
1:A:827:U:C2	1:A:872:A:N6	2.65	0.61
10:J:50:ILE:HG13	10:J:60:ARG:HD3	1.82	0.61
11:K:96:ARG:HG2	11:K:96:ARG:HH11	1.65	0.61
21:V:24:ARG:O	21:V:25:LYS:HB2	1.99	0.61
1:A:1264:C:H2'	1:A:1265:G:H8	1.64	0.61
10:J:21:GLN:HA	10:J:24:VAL:HB	1.83	0.61
25:Z:56:C:H2'	25:Z:57:A:H8	1.64	0.61
1:A:718:G:H21	18:R:49:LYS:HE3	1.65	0.61
1:A:1105:A:H2'	1:A:1106:G:C8	2.33	0.61
5:E:27:ARG:HH11	5:E:27:ARG:CG	2.14	0.61
8:H:119:LEU:HD13	8:H:123:GLU:HB3	1.81	0.61
1:A:69:G:H1	1:A:100:C:H42	1.49	0.61
1:A:1189:C:H5'	14:N:58:LYS:HZ1	1.65	0.61
23:X:11:ILE:HG12	23:X:47:LEU:HB2	1.82	0.61
1:A:755:G:N2	1:A:756:C:C2	2.69	0.60
1:A:1539:C:H42	24:Y:26:G:H1	1.50	0.60
25:Z:44:A:C2'	25:Z:45:G:H5'	2.31	0.60
1:A:1255:G:H2'	1:A:1279:A:N6	2.17	0.60
1:A:1356:G:H2'	1:A:1357:A:C8	2.36	0.60
1:A:1514:C:H2'	1:A:1515:C:C6	2.36	0.60
1:A:17:U:O2	1:A:1079:G:N2	2.35	0.60
1:A:170:U:H2'	1:A:171:A:H8	1.66	0.60
1:A:513:C:H2'	1:A:514:C:C6	2.37	0.60
7:G:65:ALA:O	7:G:69:VAL:HG23	2.00	0.60
1:A:56:U:H2'	1:A:57:G:H8	1.67	0.60
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.84	0.60
12:L:32:PHE:HB3	12:L:84:LEU:HD11	1.84	0.60
24:Y:21:G:H2'	24:Y:22:G:C8	2.37	0.60
1:A:413:G:O6	4:D:35:ARG:CZ	2.48	0.60
25:Z:9:G:N3	25:Z:45:G:H2'	2.16	0.60
1:A:1025:U:H2'	1:A:1026:G:C8	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:VAL:CG2	3:C:97:LYS:HE3	2.29	0.60
1:A:537:G:H5"	12:L:113:ARG:HH12	1.66	0.60
22:W:23:ARG:HH22	22:W:33:LEU:HD11	1.62	0.60
23:X:7:THR:HG22	23:X:46:VAL:HG22	1.84	0.60
1:A:17:U:H2'	1:A:18:C:C6	2.37	0.60
1:A:129(A):G:H4'	1:A:130:A:O5'	2.02	0.60
1:A:902:G:H2'	1:A:903:G:H8	1.66	0.60
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.84	0.60
22:W:32:ILE:HB	22:W:63:THR:O	2.02	0.60
25:Z:21:A:H61	25:Z:46:G7M:C2'	2.15	0.60
25:Z:58:A:O3'	25:Z:60:U:H5	1.84	0.60
1:A:613:C:H2'	1:A:614:A:H8	1.66	0.59
1:A:1283:G:N2	1:A:1284:C:C2	2.70	0.59
1:A:1458:G:OP1	20:T:32:ALA:CA	2.49	0.59
10:J:50:ILE:HG13	10:J:60:ARG:CD	2.32	0.59
25:Z:62:C:H2'	25:Z:63:G:O4'	2.02	0.59
1:A:439:A:C4	1:A:496:A:C2	2.90	0.59
12:L:72:GLY:HA3	12:L:102:ARG:HH11	1.67	0.59
18:R:48:GLY:HA3	18:R:82:THR:HA	1.84	0.59
1:A:229:U:H2'	1:A:230:G:C8	2.37	0.59
2:B:19:HIS:CD2	2:B:20:GLU:HG2	2.37	0.59
4:D:25:ARG:C	4:D:27:TYR:H	2.03	0.59
25:Z:35:A:H2'	25:Z:36:U:C6	2.37	0.59
1:A:643:C:H4'	8:H:31:PHE:CE2	2.37	0.59
1:A:948:C:H2'	1:A:949:A:H8	1.67	0.59
1:A:1070:U:H2'	1:A:1071:C:C6	2.37	0.59
4:D:36:ARG:HD2	4:D:38:TYR:CE1	2.38	0.59
15:O:82:ILE:HA	15:O:87:ILE:HD12	1.83	0.59
14:N:41:ARG:HG3	14:N:42:ILE:N	2.18	0.59
1:A:266:G:O2'	17:Q:67:LYS:HD2	2.03	0.59
1:A:1192:C:H2'	1:A:1193:G:O4'	2.03	0.59
1:A:313:A:H2'	1:A:314:C:H6	1.64	0.59
1:A:546:G:OP2	4:D:72:GLU:HB3	2.03	0.59
1:A:975:A:N7	10:J:60:ARG:NH2	2.51	0.59
25:Z:20:U:H5'	25:Z:21:A:OP2	2.03	0.59
1:A:588:G:N2	1:A:589:C:C2	2.71	0.59
1:A:926:G:H3'	1:A:1505:G:H21	1.68	0.59
3:C:156:ARG:H	3:C:163:ALA:HA	1.68	0.59
1:A:636:U:H2'	1:A:637:G:C8	2.38	0.58
10:J:50:ILE:H	10:J:50:ILE:HD12	1.68	0.58
25:Z:50:U:O2	25:Z:64:G:O6	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:G:H5'	4:D:41:GLY:HA3	1.85	0.58
8:H:33:GLU:HA	8:H:36:LEU:HD12	1.85	0.58
12:L:24:VAL:HG12	12:L:26:ALA:H	1.67	0.58
1:A:222:U:H2'	1:A:223:U:C6	2.38	0.58
12:L:83:VAL:HG23	12:L:107:ALA:HB2	1.85	0.58
1:A:69:G:H1	1:A:100:C:N4	2.01	0.58
1:A:671:G:C2	1:A:736:C:N3	2.71	0.58
1:A:500:G:C6	1:A:501:C:N4	2.71	0.58
1:A:757:U:H2'	1:A:758:G:O4'	2.02	0.58
1:A:926:G:H2'	1:A:1505:G:N3	2.18	0.58
1:A:1411:C:H2'	1:A:1412:C:O4'	2.03	0.58
7:G:125:MET:O	7:G:129:GLU:HG2	2.03	0.58
11:K:11:LYS:O	11:K:13:GLN:N	2.34	0.58
25:Z:18:G:N2	25:Z:57:A:H2'	2.19	0.58
1:A:1225:A:H2'	1:A:1225:A:N3	2.18	0.58
1:A:520:A:H62	1:A:529:G:H21	1.52	0.58
1:A:1287:A:H2'	1:A:1288:A:H8	1.67	0.58
10:J:60:ARG:HH11	10:J:60:ARG:CG	2.14	0.58
1:A:110:C:H2'	1:A:111:G:O4'	2.03	0.58
1:A:521:G:N2	1:A:522:C:C2	2.71	0.58
1:A:617:G:N1	1:A:618:C:C4	2.72	0.58
1:A:1418:A:N6	1:A:1482:G:O2'	2.37	0.58
2:B:105:PHE:HA	2:B:108:ILE:HG22	1.85	0.58
2:B:222:ILE:O	2:B:226:ARG:HG3	2.03	0.58
4:D:129:ASN:HD21	4:D:145:GLU:H	1.50	0.58
24:Y:21:G:H2'	24:Y:22:G:H8	1.69	0.58
1:A:1225:A:OP1	13:M:102:ARG:HA	2.03	0.58
1:A:335:C:H2'	1:A:336:C:C6	2.39	0.57
1:A:441:A:H5"	1:A:441:A:H8	1.69	0.57
1:A:522:C:H41	12:L:53:ARG:NH2	2.01	0.57
1:A:734:G:H21	18:R:75:ILE:HD11	1.69	0.57
1:A:1127:G:H21	1:A:1147:C:H41	1.49	0.57
1:A:1427:U:H2'	1:A:1428:A:H8	1.69	0.57
1:A:114:U:H2'	1:A:115:G:C8	2.39	0.57
1:A:575:G:H4'	1:A:576:G:H5'	1.85	0.57
1:A:1141:C:H2'	1:A:1142:G:H8	1.68	0.57
1:A:1221:G:H2'	1:A:1222:G:H8	1.68	0.57
1:A:1443:G:C6	1:A:1444:C:N4	2.72	0.57
1:A:1443:G:N2	1:A:1444:C:C2	2.72	0.57
9:I:114:TYR:CE2	10:J:58:ASP:O	2.57	0.57
1:A:61:G:H2'	1:A:62:U:O4'	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:A:H2'	1:A:795:C:C6	2.39	0.57
4:D:101:LEU:HB2	4:D:138:TYR:HB3	1.85	0.57
5:E:15:ARG:HA	5:E:28:PHE:HD1	1.65	0.57
14:N:24:CYS:HB3	14:N:29:ARG:H	1.68	0.57
1:A:262:A:H5"	20:T:76:ALA:HB2	1.86	0.57
1:A:1530:G:H2'	1:A:1531:A:H8	1.66	0.57
3:C:40:ARG:HG2	3:C:55:VAL:HG11	1.86	0.57
9:I:114:TYR:CD2	10:J:58:ASP:O	2.58	0.57
1:A:67:C:H2'	1:A:68:G:H8	1.69	0.57
1:A:142:G:H2'	1:A:143:A:C8	2.39	0.57
1:A:1069:C:H42	1:A:1106:G:H1	1.51	0.57
1:A:1258:G:C6	1:A:1259:C:N4	2.72	0.57
1:A:1495:U:H1'	23:X:95:ASP:HB2	1.87	0.57
3:C:134:ILE:O	3:C:138:VAL:HG23	2.05	0.57
1:A:684:A:H4'	11:K:12:ARG:CZ	2.34	0.57
1:A:874:G:N2	1:A:875:C:C2	2.73	0.57
1:A:1075:C:H5'	1:A:1101:A:N6	2.20	0.57
25:Z:65:C:C2	25:Z:66:C:C5	2.93	0.57
1:A:434:U:H2'	1:A:435:C:C6	2.39	0.57
1:A:1005:A:O4'	1:A:1036:G:N2	2.38	0.57
1:A:1438:G:N2	1:A:1439:C:C2	2.73	0.57
20:T:37:SER:HB3	20:T:84:LEU:HD21	1.86	0.57
1:A:70:G:C2	1:A:100:C:O2	2.58	0.57
1:A:1391:U:H2'	1:A:1392:G:C8	2.40	0.57
25:Z:9:G:H2'	25:Z:10:G:N7	2.20	0.57
1:A:256:U:H2'	1:A:257:G:C8	2.40	0.57
1:A:1509:C:H2'	1:A:1510:U:O4'	2.04	0.57
13:M:121:LYS:HG2	13:M:125:ARG:HG2	1.87	0.57
18:R:48:GLY:H	18:R:83:GLU:H	1.51	0.57
20:T:54:LYS:HA	20:T:57:ARG:HD3	1.87	0.57
1:A:10:A:H2'	1:A:11:G:C8	2.40	0.56
1:A:598:U:H2'	1:A:599:C:C6	2.39	0.56
1:A:1001:A:H2'	1:A:1001(A):G:H8	1.67	0.56
1:A:1296:C:H5"	13:M:44:ARG:HH22	1.70	0.56
3:C:57:ILE:HA	3:C:65:ALA:O	2.05	0.56
4:D:26:CYS:HG	27:D:300:ZN:ZN	1.17	0.56
10:J:61:GLU:OE2	14:N:58:LYS:CG	2.53	0.56
13:M:97:PRO:HA	13:M:110:ARG:HH11	1.70	0.56
1:A:84:U:H2'	1:A:88:A:O4'	2.04	0.56
1:A:674:G:H2'	1:A:675:A:H8	1.70	0.56
23:X:16:VAL:HG23	23:X:18:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:140:VAL:O	23:X:144:LEU:HG	2.06	0.56
1:A:509:A:H4'	1:A:510:A:OP1	2.05	0.56
1:A:769:G:N2	1:A:770:C:C2	2.73	0.56
1:A:1314:C:H2'	1:A:1315:U:C6	2.40	0.56
3:C:41:GLY:O	3:C:45:LYS:HG2	2.05	0.56
3:C:62:ASP:HA	3:C:97:LYS:HD3	1.87	0.56
23:X:90:PHE:HD2	23:X:94:ILE:HD13	1.70	0.56
1:A:1371:G:OP1	9:I:11:LYS:O	2.24	0.56
1:A:122:G:C6	1:A:123:C:C4	2.94	0.56
1:A:663:A:H2'	1:A:664:G:O4'	2.05	0.56
1:A:1068:G:N2	1:A:1069:C:C2	2.74	0.56
1:A:1354:C:H2'	1:A:1355:G:C8	2.41	0.56
7:G:115:ARG:O	7:G:119:ARG:HG3	2.06	0.56
10:J:47:PHE:HB2	10:J:63:PHE:HB2	1.87	0.56
1:A:247:G:N2	1:A:248:C:C2	2.74	0.56
5:E:14:ARG:HG2	5:E:29:GLY:HA3	1.86	0.56
12:L:60:LEU:HD11	12:L:85:ILE:CD1	2.35	0.56
12:L:110:VAL:HG23	12:L:120:TYR:HB3	1.88	0.56
25:Z:74:C:H2'	25:Z:75:C:H5'	1.86	0.56
1:A:352:C:H4'	1:A:354:G:OP1	2.05	0.56
1:A:827:U:C4	1:A:872:A:N1	2.73	0.56
1:A:1409:C:H2'	1:A:1410:G:C8	2.41	0.56
4:D:64:LEU:HA	4:D:67:ILE:HD12	1.86	0.56
1:A:447:G:H3'	1:A:485:G:H22	1.70	0.56
1:A:725:G:N1	1:A:726:C:C4	2.74	0.56
1:A:1080:A:C3'	5:E:16:THR:HG22	2.35	0.56
4:D:67:ILE:HD13	4:D:196:LEU:HD22	1.87	0.56
14:N:37:PHE:HB3	14:N:39:LEU:HD12	1.86	0.56
1:A:397:A:H3'	1:A:397:A:N3	2.20	0.56
1:A:695:A:H2'	1:A:696:A:H8	1.71	0.56
1:A:701:C:H4'	1:A:702:A:O5'	2.05	0.56
1:A:935:A:H2'	1:A:936:C:C6	2.41	0.56
1:A:1180:A:H5'	9:I:103:THR:HG23	1.88	0.56
13:M:19:LEU:HA	13:M:22:ILE:HD12	1.86	0.56
22:W:32:ILE:HD13	22:W:32:ILE:H	1.70	0.56
1:A:448:A:OP2	1:A:485:G:N2	2.39	0.55
1:A:1016:A:H2'	1:A:1017:G:O4'	2.05	0.55
1:A:1125:U:C5'	1:A:1126:U:H5	2.13	0.55
1:A:264:U:H2'	1:A:265:G:O4'	2.07	0.55
1:A:299:G:H2'	1:A:300:A:C8	2.41	0.55
1:A:560:U:O2'	1:A:561:U:OP2	2.16	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:C:H2'	1:A:1367:C:C6	2.41	0.55
23:X:149:VAL:HG13	23:X:168:VAL:HG22	1.88	0.55
25:Z:48:C:C5'	25:Z:50:U:OP1	2.54	0.55
1:A:235:C:H2'	1:A:236:G:H8	1.71	0.55
1:A:337:C:H2'	1:A:338:A:H8	1.71	0.55
1:A:370:C:C2	1:A:392:G:N2	2.75	0.55
25:Z:64:G:H2'	25:Z:65:C:O4'	2.07	0.55
1:A:414:A:H2'	1:A:415:A:O4'	2.07	0.55
1:A:877:C:H2'	1:A:878:G:C8	2.41	0.55
1:A:60:A:H4'	1:A:61:G:O5'	2.07	0.55
1:A:1409:C:H2'	1:A:1410:G:H8	1.71	0.55
6:F:27:GLN:HA	6:F:30:LEU:HD12	1.88	0.55
1:A:519:C:OP1	22:W:66:ARG:HD3	2.07	0.55
1:A:590:C:N3	1:A:650:G:C2	2.74	0.55
1:A:1323:G:H2'	1:A:1324:A:C8	2.42	0.55
1:A:1339:A:H2'	1:A:1340:A:O4'	2.07	0.55
15:O:18:PHE:O	15:O:21:ASP:HB3	2.06	0.55
17:Q:88:TYR:O	17:Q:92:ARG:HG2	2.06	0.55
1:A:216:G:C6	1:A:217:C:N4	2.74	0.55
1:A:671:G:N2	1:A:736:C:C2	2.75	0.55
1:A:743:U:H2'	1:A:744:C:C6	2.42	0.55
1:A:1022:G:H2'	1:A:1023:G:C8	2.39	0.55
1:A:1485:U:H2'	1:A:1486:G:H8	1.71	0.55
3:C:43:LEU:HD12	3:C:55:VAL:HG13	1.89	0.55
13:M:10:PRO:HG2	13:M:18:ALA:HB1	1.89	0.55
1:A:16:A:C2	1:A:1080:A:N3	2.74	0.55
1:A:613:C:H2'	1:A:614:A:C8	2.41	0.55
1:A:987:G:H1	1:A:1218:C:N4	2.05	0.55
1:A:1241:G:N2	1:A:1242:C:C2	2.75	0.55
20:T:40:ALA:HB2	20:T:55:ILE:HG22	1.87	0.55
1:A:182:U:OP2	1:A:183:G:C8	2.60	0.55
1:A:333:G:N2	1:A:334:C:C2	2.74	0.55
1:A:571:U:H3'	1:A:572:A:H5"	1.88	0.55
1:A:1221:G:H2'	1:A:1222:G:C8	2.41	0.55
5:E:139:LEU:HA	5:E:142:LEU:HD12	1.87	0.55
10:J:81:THR:HG22	10:J:85:LEU:HD12	1.89	0.55
25:Z:69:C:H2'	25:Z:70:G:C1'	2.36	0.55
1:A:325:A:H2'	1:A:326:G:C8	2.42	0.55
1:A:761:G:C2	1:A:762:C:C2	2.95	0.55
9:I:48:GLU:N	9:I:49:PRO:HD2	2.21	0.55
9:I:125:TYR:HE1	9:I:128:ARG:HB3	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:6:LYS:HG3	19:S:8:GLY:H	1.71	0.55
1:A:1353:G:N1	1:A:1354:C:C4	2.74	0.54
2:B:61:LEU:HD13	2:B:66:GLY:HA3	1.88	0.54
7:G:65:ALA:HB1	7:G:127:ALA:CB	2.37	0.54
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.24	0.54
10:J:16:LEU:HD13	10:J:68:HIS:HB2	1.88	0.54
25:Z:6:G:H2'	25:Z:7:G:C8	2.42	0.54
1:A:753:A:H5"	15:O:69:TYR:HE1	1.71	0.54
22:W:16:ALA:HA	22:W:22:PHE:HD1	1.71	0.54
23:X:56:VAL:HG21	25:Z:56:C:C2	2.42	0.54
25:Z:30:G:C2	25:Z:41:C:C2	2.95	0.54
1:A:1521:G:H2'	1:A:1522:U:C6	2.43	0.54
1:A:181:G:H4'	1:A:182:U:H5'	1.88	0.54
1:A:824:C:H2'	1:A:825:G:H8	1.72	0.54
1:A:838:G:C2	1:A:849:C:C2	2.95	0.54
18:R:42:ARG:HB3	18:R:42:ARG:HH11	1.70	0.54
6:F:35:ALA:HA	6:F:67:MET:HB3	1.89	0.54
20:T:65:LYS:O	20:T:68:LYS:HB3	2.06	0.54
1:A:170:U:H2'	1:A:171:A:C8	2.42	0.54
1:A:961:U:H3	1:A:974:A:H61	1.56	0.54
1:A:1074:G:O2'	1:A:1101:A:N1	2.37	0.54
1:A:1262:C:H42	1:A:1273:G:H1	1.55	0.54
1:A:1542:U:H4'	18:R:18:ARG:N	2.21	0.54
4:D:33:MET:HA	4:D:36:ARG:O	2.08	0.54
9:I:6:GLY:HA3	9:I:80:GLY:O	2.07	0.54
23:X:52:ALA:CB	25:Z:19:G:H22	2.13	0.54
25:Z:27:U:H2'	25:Z:28:C:C6	2.43	0.54
1:A:1234:C:H2'	1:A:1235:U:C6	2.42	0.54
8:H:6:ILE:O	8:H:10:LEU:HG	2.07	0.54
24:Y:35:A:O3'	24:Y:36:A:H8	1.89	0.54
1:A:373:A:H2'	1:A:374:A:H8	1.73	0.54
2:B:215:LEU:O	2:B:219:VAL:HG23	2.07	0.54
25:Z:6:G:C2	25:Z:68:C:C2	2.96	0.54
1:A:914:A:H2'	1:A:915:A:H8	1.72	0.54
10:J:5:ARG:CG	10:J:71:LEU:HD21	2.38	0.54
11:K:11:LYS:O	11:K:75:TYR:CD2	2.61	0.54
1:A:559:A:O2'	1:A:560:U:OP2	2.24	0.54
1:A:575:G:H4'	1:A:576:G:C5'	2.38	0.54
1:A:1431:C:C2	1:A:1470:G:N2	2.76	0.54
5:E:27:ARG:O	5:E:27:ARG:HG2	2.05	0.54
7:G:24:THR:HA	7:G:27:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189(D):C:H3'	1:A:189(E):U:C6	2.43	0.53
1:A:437:U:H3'	1:A:438:G:H8	1.71	0.53
1:A:864:A:C2	1:A:865:A:C2	2.96	0.53
1:A:1534:A:H2'	1:A:1535:C:C6	2.43	0.53
1:A:391:G:H2'	1:A:392:G:O4'	2.08	0.53
1:A:922:G:H3'	1:A:923:A:H8	1.72	0.53
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.90	0.53
1:A:752:G:H4'	15:O:69:TYR:OH	2.07	0.53
1:A:947:G:H2'	1:A:948:C:O4'	2.08	0.53
1:A:1342:C:H5"	9:I:125:TYR:CZ	2.43	0.53
1:A:450:G:H5"	1:A:451:A:H3'	1.90	0.53
1:A:621:A:H2'	1:A:622:A:O4'	2.09	0.53
1:A:1537:U:N3	24:Y:28:A:N6	2.57	0.53
25:Z:47:U:O5'	25:Z:47:U:H6	1.91	0.53
1:A:122:G:C2	1:A:123:C:C2	2.96	0.53
1:A:289:G:N1	1:A:290:C:C4	2.76	0.53
16:P:42:ARG:HB3	16:P:44:THR:HG23	1.89	0.53
1:A:19:C:O2	1:A:917:G:C2	2.62	0.53
1:A:100:C:H2'	1:A:101:A:C8	2.43	0.53
1:A:553:A:H2'	1:A:554:C:C6	2.43	0.53
1:A:1361:G:C6	1:A:1362:C:N3	2.76	0.53
10:J:31:GLY:HA3	10:J:78:ASN:HD22	1.71	0.53
1:A:137:C:C2	1:A:227:G:C2	2.96	0.53
1:A:253:U:H2'	1:A:254:G:C8	2.42	0.53
1:A:522:C:H41	12:L:53:ARG:HH21	1.54	0.53
1:A:615:C:H2'	1:A:616:G:H8	1.73	0.53
1:A:1347:G:N2	1:A:1373:G:H2'	2.23	0.53
1:A:1541:U:H3	24:Y:24:A:H61	1.57	0.53
14:N:3:ARG:H	14:N:6:LEU:HD12	1.74	0.53
1:A:1264:C:H2'	1:A:1265:G:C8	2.44	0.53
1:A:1464:G:C2	1:A:1465:C:N3	2.77	0.53
10:J:6:ILE:HD11	10:J:23:ILE:HG21	1.90	0.53
1:A:767:A:H2'	1:A:768:A:O4'	2.09	0.53
1:A:777:A:H2'	1:A:778:G:C8	2.44	0.53
1:A:1248:A:H2'	1:A:1249:C:C6	2.44	0.53
1:A:1456:G:N2	1:A:1457:G:C8	2.76	0.53
2:B:69:LEU:HD13	2:B:155:LEU:HD11	1.90	0.53
1:A:112:G:OP2	16:P:27:LYS:HE3	2.09	0.53
1:A:774:G:C2	1:A:806:C:N3	2.77	0.53
1:A:976:G:H4'	1:A:977:A:OP1	2.08	0.53
1:A:66:G:N2	1:A:67:C:C2	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:A:H5”	1:A:280:C:H3’	1.91	0.52
1:A:333:G:C6	1:A:334:C:N4	2.78	0.52
1:A:456:C:C2	1:A:476:G:N2	2.77	0.52
1:A:1106:G:C6	1:A:1107:C:N4	2.78	0.52
1:A:1327:C:H5”	21:V:20:LYS:HB2	1.91	0.52
12:L:60:LEU:HD11	12:L:85:ILE:HD11	1.90	0.52
17:Q:92:ARG:O	17:Q:95:TYR:HB2	2.09	0.52
1:A:1101:A:H5’	2:B:172:ILE:HG21	1.92	0.52
1:A:1137:C:H4’	1:A:1138:G:C2	2.44	0.52
22:W:37:SER:HB3	22:W:40:MET:HG3	1.90	0.52
23:X:137:LEU:O	23:X:141:THR:HG23	2.08	0.52
25:Z:58:A:C2	25:Z:60:U:H2’	2.44	0.52
1:A:20:U:H2’	1:A:21:G:O4’	2.09	0.52
1:A:159:G:N2	1:A:163:C:C2	2.77	0.52
1:A:577:G:N2	1:A:578:C:C2	2.77	0.52
1:A:636:U:H5’	17:Q:2:PRO:HG3	1.90	0.52
1:A:1404:C:H2’	1:A:1405:G:H8	1.75	0.52
1:A:1475:G:H2’	1:A:1476:G:C8	2.43	0.52
1:A:124:G:H2’	1:A:125:U:O4’	2.09	0.52
1:A:628:G:H2’	1:A:629:G:C8	2.45	0.52
1:A:1437:C:H2’	1:A:1438:G:H8	1.74	0.52
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.91	0.52
25:Z:12:G:H1	25:Z:23:C:N4	2.06	0.52
1:A:97:G:H2’	1:A:98:G:C8	2.44	0.52
1:A:216:G:C2	1:A:217:C:N3	2.77	0.52
1:A:236:G:C2	1:A:237:C:C2	2.98	0.52
1:A:403:C:H2’	1:A:404:U:H6	1.75	0.52
1:A:1382:C:H2’	1:A:1383:C:C6	2.44	0.52
2:B:91:PRO:HB3	2:B:154:LEU:HB2	1.92	0.52
24:Y:30:G:H2’	24:Y:31:U:H5”	1.91	0.52
1:A:1000:U:H3’	1:A:1000:U:H6	1.75	0.52
1:A:1464:G:C6	1:A:1465:C:N4	2.77	0.52
1:A:21:G:H2’	1:A:22:G:C8	2.45	0.52
1:A:217:C:H2’	1:A:218:C:C6	2.45	0.52
1:A:571:U:C3’	1:A:572:A:H5”	2.40	0.52
1:A:722:A:H2’	1:A:724:G:C8	2.45	0.52
1:A:1048:G:C2	1:A:1210:C:C2	2.98	0.52
1:A:1258:G:C2	1:A:1259:C:N3	2.78	0.52
4:D:63:LYS:HD3	4:D:197:PRO:HB2	1.91	0.52
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.92	0.52
10:J:50:ILE:HA	10:J:59:SER:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:67:LEU:HD11	15:O:87:ILE:HG21	1.92	0.52
25:Z:30:G:N2	25:Z:41:C:C2	2.77	0.52
1:A:823:G:H2'	1:A:824:C:C6	2.45	0.52
2:B:71:VAL:HB	2:B:164:VAL:HA	1.92	0.52
10:J:61:GLU:OE1	14:N:58:LYS:HD2	2.04	0.52
15:O:75:PRO:O	15:O:79:ARG:HG3	2.10	0.52
1:A:233:C:H2'	1:A:234:C:C6	2.45	0.52
1:A:590:C:C2	1:A:650:G:C2	2.97	0.52
1:A:601:C:H42	1:A:637:G:H1	1.57	0.52
1:A:1500:A:H5"	1:A:1508:G:H5"	1.92	0.52
4:D:209:ARG:HG2	4:D:209:ARG:HH11	1.74	0.52
25:Z:67:C:H2'	25:Z:68:C:C6	2.45	0.52
1:A:70:G:C6	1:A:100:C:N3	2.78	0.52
1:A:321:A:H2'	1:A:322:C:C6	2.45	0.52
1:A:504:C:C2	1:A:542:G:C2	2.98	0.52
1:A:657:G:H4'	15:O:28:GLN:HG3	1.91	0.52
1:A:761:G:C6	1:A:762:C:C4	2.98	0.52
1:A:1082:G:H2'	1:A:1083:U:O4'	2.10	0.52
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.45	0.51
1:A:674:G:H5'	6:F:50:TYR:CE2	2.45	0.51
1:A:939:G:C6	1:A:940:C:N4	2.78	0.51
1:A:1000:U:H3'	1:A:1000:U:C6	2.44	0.51
4:D:196:LEU:HB3	4:D:198:VAL:HG12	1.91	0.51
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.90	0.51
1:A:309:G:H2'	1:A:310:G:H8	1.75	0.51
1:A:599:C:O2'	8:H:129:VAL:HG23	2.09	0.51
1:A:1190:G:H5'	3:C:176:HIS:CE1	2.45	0.51
4:D:60:GLU:HG3	4:D:198:VAL:HG23	1.91	0.51
1:A:22:G:C6	1:A:23:C:C4	2.98	0.51
1:A:257:G:H1	1:A:269:C:H42	1.58	0.51
1:A:339:C:H2'	1:A:340:U:C6	2.45	0.51
1:A:441:A:H5"	1:A:441:A:C8	2.45	0.51
1:A:617:G:N2	1:A:618:C:C2	2.78	0.51
1:A:1103:C:H2'	1:A:1104:G:O4'	2.10	0.51
9:I:89:ASN:HB3	9:I:92:TYR:CD2	2.45	0.51
1:A:598:U:H2'	1:A:599:C:H6	1.74	0.51
1:A:1106:G:H2'	1:A:1107:C:C6	2.46	0.51
1:A:1466:C:H2'	1:A:1467:G:O4'	2.11	0.51
4:D:64:LEU:HD12	4:D:198:VAL:HG21	1.93	0.51
7:G:97:GLN:O	7:G:101:LEU:HG	2.10	0.51
25:Z:2:G:C2	25:Z:3:C:C2	2.98	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:C:H2'	1:A:338:A:C8	2.46	0.51
1:A:568:G:C6	1:A:569:C:N4	2.78	0.51
1:A:1125:U:O4	10:J:5:ARG:HB2	2.11	0.51
3:C:29:TYR:HD1	3:C:29:TYR:C	2.14	0.51
25:Z:49:G:C2	25:Z:50:U:H1'	2.45	0.51
1:A:250:A:H4'	1:A:251:G:O5'	2.10	0.51
1:A:785:G:H1	1:A:797:C:H42	1.59	0.51
1:A:1050:G:C6	1:A:1051:C:N4	2.79	0.51
1:A:1164:G:N2	1:A:1165:C:C2	2.79	0.51
3:C:42:LEU:HD11	3:C:94:LEU:HG	1.93	0.51
9:I:8:GLY:HA3	9:I:76:ALA:O	2.10	0.51
1:A:520:A:N1	1:A:536:C:H1'	2.26	0.51
1:A:823:G:N2	1:A:824:C:C2	2.79	0.51
5:E:127:ASN:O	5:E:131:ILE:HG12	2.10	0.51
7:G:71:PRO:HD2	7:G:96:GLN:HG3	1.93	0.51
9:I:41:VAL:O	9:I:44:VAL:HG22	2.10	0.51
10:J:7:LYS:HB3	10:J:97:GLU:HB2	1.92	0.51
20:T:63:ILE:HG23	20:T:77:ALA:HB1	1.93	0.51
1:A:794:A:H2'	1:A:795:C:H6	1.75	0.51
1:A:834:C:C2	1:A:853:G:C2	2.99	0.51
2:B:158:LEU:HD21	2:B:180:LEU:HD22	1.93	0.51
3:C:21:ARG:HG2	3:C:58:GLU:HG2	1.93	0.51
1:A:1424:C:H42	1:A:1476:G:H1	1.59	0.51
6:F:2:ARG:HG3	6:F:69:GLU:HG3	1.92	0.51
14:N:41:ARG:HG3	14:N:42:ILE:H	1.76	0.51
25:Z:6:G:H2'	25:Z:7:G:H8	1.74	0.51
25:Z:18:G:C2	25:Z:58:A:C5	2.99	0.51
1:A:255:G:H2'	1:A:256:U:C6	2.46	0.51
1:A:320:C:H2'	1:A:321:A:C8	2.46	0.51
1:A:444:C:H42	1:A:490:G:H1	1.57	0.51
1:A:540:G:H2'	1:A:541:G:C8	2.46	0.51
1:A:756:C:H2'	1:A:757:U:O4'	2.11	0.51
1:A:1235:U:H2'	1:A:1236:A:O4'	2.11	0.51
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.76	0.51
10:J:28:ARG:HH22	10:J:36:GLY:HA2	1.74	0.51
23:X:90:PHE:CD2	23:X:94:ILE:HD13	2.46	0.51
25:Z:12:G:N1	25:Z:13:C:C2	2.79	0.51
1:A:521:G:N1	1:A:522:C:C4	2.80	0.50
1:A:1077:G:N1	1:A:1081:G:C6	2.78	0.50
1:A:1416:G:H2'	1:A:1417:G:O4'	2.12	0.50
1:A:1512:U:H2'	1:A:1513:A:H8	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:29:PRO:O	4:D:35:ARG:HG2	2.11	0.50
1:A:217:C:H2'	1:A:218:C:H6	1.75	0.50
1:A:289:G:C2	1:A:290:C:C4	2.99	0.50
1:A:385:C:N4	1:A:386:C:N4	2.59	0.50
1:A:444:C:C2	1:A:491:G:N2	2.80	0.50
1:A:784:C:C2	1:A:799:G:N2	2.79	0.50
1:A:908:A:H2'	1:A:909:A:C8	2.46	0.50
1:A:1151:A:O2'	1:A:1152:A:C8	2.61	0.50
1:A:1312:G:C2	1:A:1326:C:C2	2.99	0.50
3:C:26:LYS:HD3	14:N:36:PHE:CE1	2.47	0.50
18:R:26:LEU:HD21	18:R:39:VAL:HG22	1.94	0.50
25:Z:51:C:N3	25:Z:63:G:O6	2.44	0.50
1:A:946:A:H2'	1:A:947:G:H8	1.73	0.50
1:A:1148:U:H5'	9:I:7:THR:HG21	1.94	0.50
7:G:71:PRO:HG3	7:G:103:TRP:HH2	1.74	0.50
11:K:16:SER:O	11:K:35:PRO:HD3	2.11	0.50
15:O:63:ARG:HA	15:O:66:LEU:HD12	1.93	0.50
1:A:270:A:H2'	1:A:271:C:C6	2.46	0.50
1:A:410:G:H21	1:A:432:A:H62	1.58	0.50
1:A:500:G:C2	1:A:501:C:N3	2.79	0.50
1:A:579:G:H5'	1:A:728:A:H1'	1.92	0.50
1:A:971:G:C8	1:A:1365:G:H4'	2.47	0.50
1:A:1132:C:H2'	1:A:1133:G:C8	2.47	0.50
2:B:68:ILE:HG12	2:B:161:ALA:HB3	1.92	0.50
2:B:96:ARG:HB3	2:B:148:TYR:CE2	2.46	0.50
3:C:28:GLN:HA	3:C:31:HIS:CD2	2.46	0.50
3:C:108:ASN:HD21	3:C:110:ASN:HB2	1.76	0.50
25:Z:52:G:O2'	25:Z:53:G:H8	1.94	0.50
1:A:64:G:H4'	1:A:65:U:H5"	1.94	0.50
1:A:369:C:H2'	1:A:370:C:C6	2.47	0.50
1:A:392:G:H2'	1:A:393:A:C8	2.46	0.50
1:A:576:G:H3'	1:A:577:G:C5'	2.41	0.50
1:A:670:G:H1	1:A:736:C:H42	1.59	0.50
1:A:908:A:H2'	1:A:909:A:H8	1.77	0.50
1:A:1050:G:N2	1:A:1051:C:C2	2.79	0.50
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.94	0.50
3:C:150:LYS:HD2	3:C:173:VAL:HG11	1.94	0.50
13:M:18:ALA:HA	13:M:21:TYR:HD2	1.77	0.50
1:A:629:G:H2'	1:A:630:G:O4'	2.11	0.50
1:A:902:G:H2'	1:A:903:G:C8	2.45	0.50
1:A:1280:A:C3'	1:A:1281:U:H5"	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:129:ASN:HD21	4:D:145:GLU:N	2.09	0.50
10:J:32:ALA:CB	10:J:74:ILE:HG22	2.41	0.50
19:S:22:LEU:HD22	19:S:28:LYS:HB2	1.93	0.50
1:A:544:G:OP1	4:D:62:GLN:HG3	2.11	0.50
1:A:665:A:N3	1:A:732:C:H2'	2.27	0.50
4:D:108:LEU:HG	4:D:174:LEU:HD22	1.94	0.50
1:A:192:U:H2'	1:A:193:C:C6	2.47	0.50
1:A:542:G:N2	1:A:543:C:C2	2.80	0.50
1:A:1537:U:C4	24:Y:28:A:N6	2.80	0.50
4:D:121:VAL:O	4:D:134:ASP:HA	2.12	0.50
6:F:30:LEU:HD13	6:F:37:VAL:HG21	1.94	0.50
10:J:44:VAL:HG22	10:J:66:ARG:HB3	1.93	0.50
14:N:24:CYS:HB3	14:N:28:GLY:H	1.77	0.50
25:Z:2:G:H3'	25:Z:3:C:H6	1.75	0.50
1:A:584:G:H2'	1:A:585:G:H8	1.76	0.50
1:A:745:C:H2'	1:A:746:A:H8	1.73	0.50
1:A:945:G:H2'	1:A:945:G:N3	2.27	0.50
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.94	0.50
1:A:602:A:H2'	1:A:603:U:O4'	2.12	0.49
1:A:1216:G:N2	1:A:1217:C:C2	2.80	0.49
3:C:29:TYR:HH	14:N:54:PRO:CG	2.13	0.49
10:J:5:ARG:O	10:J:98:ILE:HA	2.11	0.49
25:Z:36:U:H2'	25:Z:37:A:O4'	2.12	0.49
1:A:573:A:H2'	1:A:574:A:O4'	2.12	0.49
16:P:57:ARG:NE	16:P:79:VAL:O	2.45	0.49
25:Z:6:G:C2	25:Z:68:C:N3	2.79	0.49
3:C:71:ALA:HB2	3:C:115:LEU:HD13	1.94	0.49
5:E:27:ARG:CG	5:E:27:ARG:NH1	2.73	0.49
17:Q:60:ILE:HG22	17:Q:72:ARG:HB2	1.94	0.49
25:Z:2:G:N2	25:Z:3:C:C2	2.81	0.49
1:A:559:A:H4'	1:A:560:U:H5"	1.93	0.49
1:A:731:G:N2	1:A:732:C:C2	2.80	0.49
1:A:988:G:N1	1:A:989:C:C2	2.80	0.49
1:A:1127:G:N2	1:A:1147:C:N4	2.57	0.49
1:A:1129:C:H1'	1:A:1132:C:H5	1.77	0.49
1:A:1220:G:H2'	1:A:1221:G:O4'	2.12	0.49
1:A:1353:G:C2	1:A:1354:C:C4	3.00	0.49
3:C:135:LYS:O	3:C:139:GLN:HG2	2.11	0.49
11:K:86:GLY:HA2	11:K:112:THR:HG23	1.94	0.49
25:Z:35:A:H4'	25:Z:36:U:OP1	2.12	0.49
1:A:123:C:H2'	1:A:124:G:C8	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:U:H2'	1:A:193:C:H6	1.77	0.49
1:A:861:G:N2	1:A:862:C:C2	2.81	0.49
1:A:1338:G:H2'	1:A:1339:A:C8	2.47	0.49
3:C:29:TYR:C	3:C:29:TYR:CD1	2.86	0.49
1:A:28:G:H2'	1:A:29:G:O4'	2.13	0.49
1:A:623:C:H2'	1:A:624:C:O4'	2.12	0.49
1:A:1435:G:H2'	1:A:1436:U:C6	2.47	0.49
3:C:70:VAL:O	3:C:105:GLU:HA	2.12	0.49
9:I:32:ASP:HB3	9:I:35:GLU:HB2	1.95	0.49
1:A:524:G:C2	1:A:525:C:C4	3.01	0.49
1:A:967:C:H2'	1:A:968:A:C8	2.48	0.49
1:A:1525:G:H2'	1:A:1526:G:H8	1.77	0.49
2:B:115:LEU:HD21	2:B:153:ARG:HE	1.78	0.49
18:R:17:SER:HB3	18:R:55:ARG:HD3	1.94	0.49
22:W:12:VAL:HG22	22:W:52:ARG:HD3	1.94	0.49
1:A:137:C:C2	1:A:227:G:N2	2.80	0.49
1:A:233:C:H2'	1:A:234:C:H6	1.78	0.49
1:A:601:C:H2'	1:A:602:A:H8	1.77	0.49
1:A:914:A:C4	1:A:915:A:N7	2.81	0.49
1:A:945:G:C2	1:A:946:A:C8	3.01	0.49
1:A:1392:G:H21	1:A:1502:A:H8	1.61	0.49
1:A:109:A:C6	1:A:326:G:C6	3.00	0.49
1:A:258:G:C2	1:A:269:C:N3	2.81	0.49
1:A:354:G:N1	1:A:355:C:C4	2.80	0.49
1:A:382:A:H2'	1:A:383:A:C8	2.48	0.49
1:A:753:A:H5"	15:O:69:TYR:CE1	2.46	0.49
1:A:1015:A:H2'	1:A:1016:A:C8	2.47	0.49
1:A:1027:C:H2'	1:A:1028:C:H5'	1.94	0.49
1:A:1347:G:O2'	1:A:1348:U:OP2	2.22	0.49
3:C:177:THR:HG23	3:C:180:ALA:HB2	1.95	0.49
7:G:16:LEU:HD12	9:I:41:VAL:HG12	1.95	0.49
9:I:93:ARG:HH21	9:I:97:LYS:HE3	1.77	0.49
9:I:96:LEU:HB3	9:I:102:LEU:HD12	1.95	0.49
11:K:34:ASP:OD1	11:K:38:ASN:N	2.42	0.49
25:Z:10:G:H1	25:Z:25:C:N4	2.11	0.49
1:A:19:C:N3	1:A:917:G:C6	2.81	0.49
1:A:22:G:C2	1:A:23:C:C2	3.01	0.49
1:A:971:G:OP1	1:A:971:G:H3'	2.13	0.49
1:A:1349:A:H5"	9:I:121:ARG:HB2	1.95	0.49
10:J:5:ARG:N	10:J:73:ASP:OD1	2.45	0.49
16:P:2:VAL:HG13	16:P:64:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:U:H2'	1:A:678:U:O4'	2.12	0.48
1:A:1049:U:H4'	1:A:1050:G:OP2	2.13	0.48
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.95	0.48
25:Z:52:G:C4	25:Z:53:G:C8	3.00	0.48
1:A:17:U:H2'	1:A:18:C:C5	2.47	0.48
1:A:1283:G:N1	1:A:1284:C:C4	2.81	0.48
1:A:1347:G:HO2'	1:A:1348:U:P	2.36	0.48
1:A:1468:A:H2'	1:A:1469:G:O4'	2.12	0.48
2:B:19:HIS:CG	2:B:20:GLU:HG2	2.47	0.48
9:I:31:GLN:HB3	9:I:35:GLU:HB3	1.95	0.48
1:A:42:G:C2	1:A:43:C:C2	3.01	0.48
1:A:838:G:N2	1:A:849:C:C2	2.81	0.48
1:A:898:G:C2	1:A:902:G:C6	3.01	0.48
1:A:961:U:O4	1:A:974:A:C2	2.59	0.48
1:A:1347:G:O2'	1:A:1373:G:N1	2.43	0.48
1:A:1443:G:C2	1:A:1444:C:C4	3.01	0.48
5:E:76:ILE:HG22	5:E:93:PRO:HB3	1.93	0.48
19:S:40:ILE:HD12	19:S:69:HIS:HB2	1.94	0.48
25:Z:34:C:H2'	25:Z:35:A:C8	2.48	0.48
1:A:504:C:C2	1:A:542:G:N2	2.82	0.48
1:A:540:G:H2'	1:A:541:G:H8	1.78	0.48
1:A:579:G:H2'	1:A:580:U:H6	1.74	0.48
1:A:947:G:C2	1:A:948:C:C2	3.02	0.48
1:A:148:G:H2'	1:A:149:A:C8	2.48	0.48
1:A:518:C:O2'	1:A:519:C:OP2	2.28	0.48
1:A:872:A:C8	1:A:874:G:C8	3.01	0.48
1:A:992:U:H4'	1:A:993:G:O5'	2.13	0.48
1:A:1134:G:N2	1:A:1141:C:C2	2.81	0.48
1:A:1281:U:H3'	1:A:1282:C:C6	2.48	0.48
1:A:1438:G:N1	1:A:1439:C:C4	2.80	0.48
7:G:107:ALA:HB3	7:G:123:GLU:HG2	1.95	0.48
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.94	0.48
22:W:33:LEU:O	22:W:65:GLY:N	2.44	0.48
1:A:344:A:H4'	1:A:345:C:OP2	2.13	0.48
1:A:939:G:H2'	1:A:940:C:C6	2.48	0.48
1:A:1163:C:C2	1:A:1174:G:N2	2.82	0.48
1:A:1233:G:C6	1:A:1234:C:N4	2.82	0.48
2:B:15:VAL:HG11	2:B:209:ARG:HB3	1.95	0.48
3:C:26:LYS:HA	14:N:36:PHE:HE1	1.78	0.48
10:J:24:VAL:HG13	10:J:28:ARG:NE	2.21	0.48
11:K:11:LYS:O	11:K:75:TYR:HD2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:1:C:H2'	25:Z:2:G:C8	2.49	0.48
1:A:189(A):C:H2'	1:A:189(B):C:C6	2.49	0.48
1:A:189(K):U:H2'	1:A:189(L):G:H8	1.79	0.48
1:A:504:C:N3	1:A:542:G:C2	2.81	0.48
1:A:928:G:H1	1:A:1389:C:H42	1.60	0.48
1:A:977:A:H2'	1:A:978:A:H5"	1.94	0.48
1:A:1106:G:N2	1:A:1107:C:C2	2.82	0.48
13:M:10:PRO:HB3	13:M:21:TYR:CD2	2.48	0.48
1:A:505:G:H5'	1:A:534:U:H2'	1.95	0.48
1:A:734:G:C2	1:A:735:C:C2	3.01	0.48
1:A:1074:G:C6	1:A:1075:C:C4	3.01	0.48
1:A:1080:A:C3'	5:E:16:THR:CG2	2.84	0.48
7:G:71:PRO:HG3	7:G:103:TRP:CH2	2.48	0.48
15:O:87:ILE:C	15:O:89:GLY:H	2.16	0.48
1:A:755:G:OP2	15:O:65:ARG:HG2	2.14	0.48
1:A:1119:C:H2'	1:A:1120:G:H8	1.79	0.48
1:A:1133:G:H1	1:A:1141:C:H42	1.61	0.48
1:A:1233:G:N2	1:A:1234:C:C2	2.82	0.48
1:A:1352:C:H2'	1:A:1353:G:C8	2.49	0.48
2:B:93:VAL:HG11	2:B:97:TRP:CD1	2.47	0.48
3:C:91:LEU:HD22	3:C:101:LEU:HD12	1.96	0.48
3:C:153:VAL:HG13	3:C:198:VAL:HG22	1.96	0.48
19:S:42:PRO:HA	19:S:45:VAL:HG23	1.95	0.48
20:T:73:HIS:HB3	20:T:74:LYS:HZ1	1.79	0.48
1:A:90:U:H2'	1:A:91:C:H6	1.76	0.48
1:A:588:G:N1	1:A:589:C:C4	2.82	0.48
1:A:734:G:C6	1:A:735:C:C4	3.02	0.48
2:B:76:GLN:H	2:B:76:GLN:HG2	1.51	0.48
2:B:167:PRO:HB3	2:B:174:VAL:HG21	1.95	0.48
19:S:32:LYS:HA	19:S:50:ALA:O	2.14	0.48
1:A:1050:G:N1	1:A:1051:C:C4	2.82	0.47
1:A:1135:U:H4'	1:A:1136:U:C5	2.49	0.47
1:A:1298:C:C4	7:G:114:ARG:HD3	2.49	0.47
2:B:80:ILE:HG21	2:B:212:GLN:HA	1.95	0.47
4:D:157:LEU:HA	4:D:160:GLN:HE21	1.78	0.47
10:J:12:ASP:HB3	10:J:15:THR:HG22	1.95	0.47
1:A:1237:C:H3'	1:A:1336:C:H41	1.79	0.47
11:K:72:ALA:O	11:K:77:MET:HB2	2.13	0.47
15:O:3:ILE:HG21	15:O:34:LEU:HD11	1.95	0.47
15:O:21:ASP:OD1	15:O:24:SER:HB2	2.14	0.47
15:O:87:ILE:O	15:O:88:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:U:H2'	1:A:97:G:C8	2.50	0.47
1:A:127:G:C2	1:A:235:C:N3	2.82	0.47
1:A:189:G:C2	1:A:189(A):C:C2	3.02	0.47
1:A:533:A:O2'	1:A:535:A:OP2	2.28	0.47
1:A:551:U:H2'	1:A:552:U:C6	2.50	0.47
1:A:688:G:H1	1:A:699:C:H42	1.63	0.47
14:N:9:LYS:O	14:N:12:ARG:NH2	2.46	0.47
1:A:439:A:P	1:A:493:G:N1	2.77	0.47
1:A:443:C:C2	1:A:492:G:N2	2.82	0.47
1:A:502:G:H2'	1:A:503:C:O4'	2.14	0.47
1:A:827:U:N3	1:A:872:A:C6	2.69	0.47
1:A:922:G:H3'	1:A:923:A:C8	2.49	0.47
1:A:1371:G:H2'	1:A:1372:U:C6	2.50	0.47
6:F:67:MET:HB2	6:F:68:PRO:CD	2.44	0.47
9:I:71:SER:HA	9:I:74:ILE:HD12	1.97	0.47
17:Q:64:PRO:HB3	17:Q:70:ARG:HG3	1.95	0.47
1:A:643:C:H2'	1:A:644:G:H8	1.79	0.47
1:A:1515:C:H2'	1:A:1516:G:C8	2.50	0.47
9:I:5:TYR:OH	9:I:7:THR:HG23	2.14	0.47
13:M:45:VAL:HA	13:M:48:LEU:HD12	1.95	0.47
13:M:51:ALA:O	13:M:55:ARG:HG3	2.13	0.47
1:A:13:U:H3	1:A:915:A:H62	1.59	0.47
1:A:1355:G:H2'	1:A:1356:G:H8	1.79	0.47
5:E:10:MET:HA	5:E:32:VAL:HG23	1.95	0.47
7:G:146:GLU:C	7:G:148:ASN:H	2.16	0.47
1:A:42:G:C6	1:A:43:C:C4	3.03	0.47
1:A:132:C:N4	1:A:231:G:C6	2.83	0.47
1:A:585:G:C2	1:A:586:C:C2	3.03	0.47
1:A:778:G:C6	1:A:779:C:C4	3.02	0.47
1:A:803:G:H2'	1:A:804:U:O4'	2.14	0.47
1:A:860:A:H2'	1:A:861:G:O4'	2.15	0.47
1:A:1114:C:C2	1:A:1187:G:C2	3.02	0.47
1:A:1117:G:H5'	1:A:1118:C:OP2	2.15	0.47
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.48	0.47
1:A:1412:C:H2'	1:A:1413:A:O4'	2.14	0.47
1:A:1430:C:C2	1:A:1471:G:N2	2.82	0.47
4:D:24:GLU:O	4:D:25:ARG:HB3	2.14	0.47
23:X:18:VAL:HB	23:X:29:MET:HG2	1.96	0.47
23:X:33:GLU:HA	23:X:36:ARG:HD2	1.97	0.47
25:Z:2:G:H1	25:Z:71:C:H42	1.62	0.47
1:A:123:C:H5"	1:A:311:C:O2'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:C:H2'	1:A:132:C:C6	2.50	0.47
1:A:646:U:H2'	1:A:647:C:C6	2.50	0.47
1:A:731:G:OP1	1:A:766:A:H1'	2.15	0.47
1:A:1171:G:N2	1:A:1172:C:C2	2.83	0.47
1:A:1305:G:N2	1:A:1331:G:H1'	2.30	0.47
1:A:1367:C:H5'	10:J:60:ARG:HH12	1.78	0.47
1:A:1472:U:H2'	1:A:1473:A:C8	2.50	0.47
1:A:1506:U:N3	1:A:1522:U:OP1	2.43	0.47
4:D:97:LEU:O	4:D:100:ARG:HG3	2.14	0.47
6:F:43:LEU:HB3	6:F:46:ARG:HD2	1.95	0.47
22:W:32:ILE:HD13	22:W:32:ILE:O	2.14	0.47
1:A:81:U:H4'	1:A:81:U:OP1	2.15	0.47
1:A:836:G:H1	1:A:850:U:H3	1.63	0.47
1:A:1033:G:H2'	1:A:1034:G:C8	2.50	0.47
1:A:1312:G:N2	1:A:1326:C:C2	2.83	0.47
4:D:176:LEU:HA	4:D:183:GLY:HA2	1.97	0.47
5:E:15:ARG:HG2	5:E:28:PHE:CE1	2.39	0.47
8:H:11:THR:HA	8:H:14:ARG:NH1	2.30	0.47
1:A:765:G:N1	1:A:812:C:H2'	2.30	0.47
1:A:920:U:H2'	1:A:921:U:H6	1.70	0.47
1:A:1095:U:H2'	1:A:1096:C:C6	2.49	0.47
8:H:48:TYR:HD2	8:H:59:LEU:HD21	1.81	0.47
8:H:79:VAL:HG13	8:H:80:ILE:HG13	1.97	0.47
1:A:128:G:C2	1:A:234:C:C2	3.03	0.46
1:A:399:G:H2'	1:A:400:C:C6	2.50	0.46
1:A:524:G:H2'	1:A:525:C:C6	2.50	0.46
1:A:615:C:H2'	1:A:616:G:C8	2.50	0.46
1:A:680:C:C2	1:A:711:G:N2	2.83	0.46
1:A:769:G:N1	1:A:770:C:C4	2.82	0.46
1:A:943:U:H2'	1:A:944:G:H8	1.80	0.46
1:A:1508:G:C2	1:A:1509:C:C2	3.03	0.46
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.97	0.46
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.97	0.46
25:Z:2:G:C4	25:Z:3:C:C5	3.03	0.46
25:Z:22:G:N2	25:Z:23:C:C2	2.83	0.46
25:Z:55:PSU:O2'	25:Z:57:A:N7	2.30	0.46
1:A:70:G:C2	1:A:100:C:C2	3.04	0.46
1:A:308:C:H2'	1:A:309:G:H8	1.80	0.46
1:A:519:C:H2'	1:A:520:A:C8	2.50	0.46
1:A:1116:C:H2'	1:A:1117:G:O4'	2.15	0.46
1:A:1242:C:H2'	1:A:1243:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:HO2'	1:A:1373:G:H1	1.61	0.46
1:A:1511:G:H2'	1:A:1512:U:O4'	2.15	0.46
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.50	0.46
2:B:98:LEU:O	2:B:101:MET:HG3	2.15	0.46
3:C:113:ALA:N	3:C:114:PRO:CD	2.78	0.46
10:J:76:ASN:HA	10:J:77:PRO:HD3	1.72	0.46
1:A:590:C:C2	1:A:650:G:N2	2.84	0.46
1:A:601:C:H2'	1:A:602:A:C8	2.50	0.46
1:A:786:G:N2	1:A:797:C:C2	2.83	0.46
1:A:1060:C:H5'	10:J:51:ARG:HB3	1.97	0.46
2:B:93:VAL:HG11	2:B:97:TRP:HD1	1.80	0.46
3:C:108:ASN:HA	3:C:109:PRO:HD2	1.83	0.46
10:J:70:ARG:HA	10:J:70:ARG:HD3	1.35	0.46
25:Z:2:G:C6	25:Z:3:C:C4	3.04	0.46
25:Z:35:A:O2'	25:Z:36:U:H5'	2.16	0.46
1:A:41:G:H2'	1:A:42:G:H8	1.80	0.46
1:A:135:C:O2	16:P:1:MET:HB2	2.15	0.46
1:A:184:G:H2'	1:A:185:A:H8	1.79	0.46
1:A:219:C:H2'	1:A:220:G:O4'	2.14	0.46
1:A:310:G:C2	1:A:311:C:C2	3.03	0.46
1:A:406:G:H2'	1:A:407:G:H8	1.81	0.46
1:A:589:C:O2	1:A:651:C:O2	2.33	0.46
1:A:935:A:H2'	1:A:936:C:H6	1.80	0.46
1:A:1176:A:H2'	1:A:1177:G:C8	2.51	0.46
1:A:1238:A:H5'	1:A:1336:C:H41	1.79	0.46
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.96	0.46
5:E:94:ALA:HB2	5:E:119:LEU:HD12	1.97	0.46
1:A:13:U:H5'	1:A:14:U:C5	2.51	0.46
1:A:54:C:H41	1:A:352:C:H2'	1.81	0.46
1:A:437:U:H3'	1:A:438:G:C8	2.49	0.46
1:A:948:C:P	13:M:108:ARG:H	2.38	0.46
1:A:1321:C:H5'	13:M:87:TYR:CE2	2.50	0.46
5:E:15:ARG:HH22	5:E:26:PHE:HB3	1.75	0.46
25:Z:47:U:C6	25:Z:50:U:OP1	2.69	0.46
1:A:738:C:H5"	6:F:69:GLU:HB3	1.96	0.46
1:A:974:A:H1'	14:N:31:ARG:NH2	2.31	0.46
1:A:1373:G:H5'	7:G:36:LYS:HB2	1.97	0.46
22:W:16:ALA:HA	22:W:22:PHE:CD1	2.49	0.46
22:W:32:ILE:H	22:W:32:ILE:CD1	2.27	0.46
23:X:19:VAL:HG21	25:Z:56:C:H41	1.80	0.46
1:A:13:U:N3	1:A:915:A:N6	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:G:H2'	1:A:99:U:O4'	2.16	0.46
1:A:236:G:C6	1:A:237:C:C4	3.03	0.46
1:A:245:C:C2	1:A:284:G:C2	3.03	0.46
1:A:276:G:C2	1:A:277:C:C2	3.04	0.46
1:A:333:G:C2	1:A:334:C:C4	3.03	0.46
1:A:1017:G:C2	1:A:1018:C:C2	3.03	0.46
1:A:1367:C:H4'	10:J:48:THR:HG21	1.98	0.46
1:A:1368:G:H5"	14:N:61:TRP:HZ2	1.80	0.46
1:A:1537:U:O2	1:A:1537:U:H2'	2.16	0.46
2:B:204:ASN:C	2:B:204:ASN:HD22	2.19	0.46
10:J:26:ALA:HB1	10:J:84:GLN:HB3	1.98	0.46
1:A:59:A:H3'	1:A:331:G:H22	1.80	0.46
1:A:786:G:H2'	1:A:787:A:O4'	2.16	0.46
1:A:1102:A:H2'	1:A:1103:C:H6	1.77	0.46
1:A:1350:A:P	9:I:121:ARG:HG3	2.55	0.46
2:B:97:TRP:CH2	2:B:101:MET:HB2	2.51	0.46
4:D:67:ILE:HD11	4:D:197:PRO:HG2	1.98	0.46
23:X:17:ARG:HB2	23:X:56:VAL:HG22	1.97	0.46
25:Z:49:G:C2	25:Z:66:C:C4	3.04	0.46
1:A:855:G:C6	1:A:856:C:C4	3.04	0.46
1:A:862:C:H2'	1:A:863:U:O4'	2.15	0.46
1:A:1080:A:O3'	5:E:16:THR:CG2	2.60	0.46
1:A:1304:G:H21	1:A:1333:A:H62	1.63	0.46
1:A:1307:U:H2'	1:A:1308:U:C6	2.51	0.46
1:A:1504:G:H5"	1:A:1505:G:O4'	2.16	0.46
3:C:6:HIS:HB3	14:N:49:HIS:HB3	1.97	0.46
10:J:8:LEU:HB2	10:J:70:ARG:HB3	1.97	0.46
12:L:25:PRO:C	12:L:27:LEU:N	2.69	0.46
14:N:37:PHE:HB3	14:N:39:LEU:HB2	1.96	0.46
1:A:102:G:C2	1:A:103:C:C2	3.04	0.46
1:A:127:G:N2	1:A:235:C:C2	2.83	0.46
1:A:399:G:C2	1:A:400:C:C2	3.05	0.46
1:A:427:U:O2'	1:A:541:G:OP1	2.28	0.46
1:A:548:G:C2	1:A:549:C:C2	3.03	0.46
1:A:562:C:H41	1:A:884:U:H2'	1.81	0.46
1:A:584:G:C4	1:A:585:G:C8	3.04	0.46
1:A:585:G:C6	1:A:586:C:C4	3.04	0.46
1:A:1057:G:H2'	1:A:1058:G:C8	2.50	0.46
1:A:1097:C:H2'	1:A:1098:C:C6	2.51	0.46
1:A:1117:G:O3'	9:I:104:ARG:NE	2.49	0.46
1:A:1446:U:O2'	1:A:1456:G:O6	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:LEU:HD21	2:B:214:ILE:HD13	1.98	0.46
6:F:19:LEU:HD21	6:F:59:TYR:CZ	2.51	0.46
7:G:101:LEU:HA	7:G:104:LEU:HD12	1.98	0.46
25:Z:2:G:H3'	25:Z:3:C:C6	2.51	0.46
1:A:17:U:C2	1:A:1079:G:N2	2.83	0.45
1:A:356:A:H2'	1:A:357:G:C8	2.50	0.45
1:A:477:A:H2'	1:A:479:C:C6	2.51	0.45
1:A:527:G:N2	1:A:528:C:C2	2.84	0.45
1:A:542:G:N1	1:A:543:C:C4	2.84	0.45
1:A:883:C:H2'	1:A:884:U:C6	2.51	0.45
1:A:1046:A:H3'	1:A:1047:G:H8	1.81	0.45
1:A:1361:G:C2	1:A:1362:C:O2	2.69	0.45
4:D:6:GLY:O	4:D:8:VAL:HG23	2.16	0.45
4:D:35:ARG:HB3	4:D:35:ARG:CZ	2.45	0.45
20:T:32:ALA:O	20:T:36:LEU:HB2	2.16	0.45
25:Z:9:G:C2'	25:Z:10:G:N7	2.79	0.45
25:Z:44:A:H2'	25:Z:45:G:C8	2.51	0.45
25:Z:64:G:C2	25:Z:65:C:H1'	2.50	0.45
1:A:865:A:O5'	1:A:865:A:H8	1.98	0.45
1:A:1007:C:N3	1:A:1022:G:N2	2.64	0.45
18:R:73:ALA:HA	18:R:76:LEU:HD12	1.98	0.45
25:Z:49:G:N1	25:Z:66:C:C4	2.84	0.45
1:A:269:C:H2'	1:A:270:A:H8	1.76	0.45
1:A:289:G:C6	1:A:290:C:N4	2.84	0.45
1:A:344:A:H5"	1:A:345:C:H5	1.81	0.45
1:A:688:G:C6	1:A:689:C:N4	2.85	0.45
1:A:1186:G:H4'	9:I:110:GLU:CD	2.37	0.45
1:A:1464:G:C2	1:A:1465:C:C4	3.04	0.45
1:A:91:C:N4	1:A:92:C:N4	2.64	0.45
1:A:247:G:N1	1:A:248:C:C4	2.84	0.45
1:A:254:G:H1	1:A:272:C:N4	2.12	0.45
1:A:434:U:H2'	1:A:435:C:H6	1.79	0.45
1:A:537:G:H5"	12:L:113:ARG:NH1	2.28	0.45
1:A:568:G:N2	1:A:569:C:C2	2.85	0.45
1:A:571:U:H3'	1:A:572:A:C5'	2.47	0.45
1:A:632:A:H2'	1:A:633:G:O4'	2.16	0.45
1:A:1027:C:C2'	1:A:1028:C:H5'	2.45	0.45
1:A:1074:G:C2	1:A:1075:C:C2	3.05	0.45
1:A:1135:U:H4'	1:A:1136:U:H5	1.81	0.45
1:A:1164:G:N1	1:A:1165:C:C4	2.84	0.45
1:A:1382:C:H2'	1:A:1383:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1419:G:C2	1:A:1420:C:C2	3.05	0.45
1:A:1436:U:H2'	1:A:1437:C:O4'	2.16	0.45
3:C:28:GLN:OE1	3:C:28:GLN:N	2.49	0.45
3:C:33:LEU:HD11	14:N:53:LEU:CD2	2.47	0.45
7:G:152:ALA:HB1	7:G:155:ARG:NH2	2.31	0.45
20:T:43:LEU:HB3	20:T:52:ALA:HB2	1.98	0.45
1:A:115:G:H1'	1:A:116:A:N7	2.31	0.45
1:A:125:U:H2'	1:A:126:G:C8	2.52	0.45
1:A:437:U:H2'	1:A:438:G:O4'	2.17	0.45
1:A:678:U:H2'	1:A:679:C:C6	2.51	0.45
1:A:941:G:H2'	1:A:942:G:O4'	2.17	0.45
1:A:1077:G:N2	1:A:1079:G:H3'	2.31	0.45
1:A:1127:G:N2	1:A:1145:C:C2	2.71	0.45
1:A:1241:G:C6	1:A:1242:C:N4	2.85	0.45
1:A:1328:C:H2'	1:A:1329:A:H8	1.81	0.45
3:C:11:ARG:NH1	3:C:177:THR:O	2.49	0.45
4:D:36:ARG:HD3	4:D:38:TYR:OH	2.15	0.45
4:D:196:LEU:C	4:D:198:VAL:H	2.20	0.45
1:A:293:G:C6	1:A:294:U:C4	3.05	0.45
1:A:823:G:C2	1:A:824:C:C2	3.05	0.45
1:A:834:C:H5"	18:R:60:ALA:HB2	1.97	0.45
1:A:961:U:O4	1:A:974:A:C6	2.62	0.45
1:A:1207:G:C2	1:A:1208:C:C2	3.05	0.45
1:A:1253:G:C2	1:A:1254:C:C2	3.04	0.45
1:A:1368:G:N2	1:A:1369:C:C2	2.84	0.45
1:A:1512:U:H2'	1:A:1513:A:C8	2.52	0.45
6:F:78:GLU:HA	6:F:81:ILE:HD12	1.97	0.45
10:J:45:ARG:O	10:J:64:GLU:HA	2.16	0.45
20:T:73:HIS:HB3	20:T:74:LYS:NZ	2.31	0.45
1:A:120:A:C5	1:A:122:G:C5	3.05	0.45
1:A:259:G:C2	1:A:268:C:C2	3.05	0.45
1:A:271:C:H2'	1:A:272:C:C6	2.52	0.45
1:A:583:A:O2'	17:Q:91:ARG:HG3	2.17	0.45
1:A:1366:C:H2'	1:A:1367:C:H6	1.80	0.45
1:A:1464:G:N2	1:A:1465:C:C2	2.84	0.45
2:B:146:GLN:HG2	2:B:153:ARG:HH21	1.81	0.45
9:I:13:ALA:HB2	9:I:68:GLY:HA3	1.98	0.45
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.99	0.45
1:A:59:A:H5"	1:A:387:U:H5"	1.97	0.45
1:A:314:C:H2'	1:A:315:A:C8	2.52	0.45
1:A:1127:G:H1	1:A:1145:C:N4	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1408:A:H2'	1:A:1409:C:C6	2.52	0.45
1:A:1484:C:H6	1:A:1484:C:O5'	2.00	0.45
4:D:25:ARG:C	4:D:27:TYR:N	2.69	0.45
10:J:65:LEU:HD23	14:N:56:VAL:HG22	1.98	0.45
17:Q:61:GLU:HA	17:Q:71:PHE:CD1	2.52	0.45
22:W:17:LEU:HB3	22:W:18:PRO:CD	2.46	0.45
1:A:104:G:H4'	1:A:174:C:H5'	1.98	0.45
1:A:577:G:C2	1:A:578:C:C2	3.05	0.45
1:A:1079:G:C6	1:A:1080:A:N6	2.85	0.45
1:A:1355:G:H2'	1:A:1356:G:C8	2.51	0.45
2:B:54:THR:CG2	2:B:185:ILE:HG23	2.46	0.45
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.99	0.45
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.98	0.45
25:Z:10:G:N3	25:Z:10:G:H2'	2.32	0.45
1:A:249:U:O2'	1:A:252:U:H4'	2.17	0.45
1:A:333:G:N1	1:A:334:C:C4	2.85	0.45
1:A:377:G:H2'	1:A:378:G:C8	2.52	0.45
1:A:416:G:C6	1:A:417:C:C4	3.06	0.45
1:A:684:A:H4'	11:K:12:ARG:NH2	2.32	0.45
1:A:874:G:N1	1:A:875:C:C4	2.85	0.45
1:A:1129:C:OP1	1:A:1130:A:H5'	2.17	0.45
4:D:173:TRP:O	4:D:186:LEU:HB2	2.16	0.45
5:E:148:VAL:O	5:E:152:ARG:HG2	2.17	0.45
6:F:69:GLU:H	6:F:69:GLU:CD	2.19	0.45
9:I:118:LYS:O	9:I:119:ALA:HB3	2.17	0.45
1:A:229:U:H2'	1:A:230:G:H8	1.82	0.44
1:A:539:A:H2'	1:A:540:G:C8	2.52	0.44
1:A:689:C:H2'	1:A:690:G:O4'	2.17	0.44
1:A:755:G:N1	1:A:756:C:C4	2.85	0.44
1:A:761:G:H2'	1:A:762:C:C6	2.52	0.44
1:A:823:G:C6	1:A:824:C:N4	2.84	0.44
1:A:1244:C:H2'	1:A:1245:A:C8	2.52	0.44
2:B:212:GLN:HG3	2:B:239:VAL:CG2	2.47	0.44
5:E:87:SER:HA	5:E:125:SER:HB3	1.99	0.44
16:P:57:ARG:CZ	16:P:79:VAL:O	2.66	0.44
23:X:11:ILE:HG23	23:X:47:LEU:HD22	1.98	0.44
25:Z:6:G:C2	25:Z:7:G:C5	3.05	0.44
25:Z:37:A:C4	25:Z:38:A:C8	3.05	0.44
1:A:189:G:C6	1:A:189(A):C:C4	3.05	0.44
1:A:266:G:O2'	1:A:267:C:OP2	2.21	0.44
1:A:310:G:C6	1:A:311:C:C4	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:U:H1'	12:L:32:PHE:CE1	2.52	0.44
1:A:584:G:C5	1:A:585:G:N7	2.85	0.44
1:A:891:U:H2'	1:A:892:A:H8	1.83	0.44
1:A:1401:G:C6	1:A:1402:C:C2	3.05	0.44
4:D:31:CYS:C	4:D:33:MET:H	2.20	0.44
1:A:372:C:H1'	1:A:373:A:OP2	2.17	0.44
1:A:674:G:H2'	1:A:675:A:C8	2.51	0.44
1:A:778:G:C2	1:A:779:C:C2	3.06	0.44
1:A:824:C:H2'	1:A:825:G:C8	2.51	0.44
1:A:1115:C:C2	1:A:1186:G:C2	3.05	0.44
4:D:162:LEU:HD12	4:D:178:VAL:HG23	1.98	0.44
5:E:15:ARG:CG	5:E:15:ARG:NH2	2.73	0.44
13:M:22:ILE:HG22	13:M:24:GLY:H	1.82	0.44
18:R:37:VAL:HG13	18:R:78:LEU:HB3	2.00	0.44
22:W:51:ASP:OD2	23:X:125:ARG:HD3	2.18	0.44
1:A:407:G:H5"	4:D:115:ARG:HB2	2.00	0.44
1:A:407:G:H2'	1:A:408:A:C8	2.52	0.44
1:A:502:G:C2	1:A:503:C:C2	3.05	0.44
1:A:681:C:C2	1:A:710:G:N2	2.84	0.44
1:A:834:C:H5"	18:R:60:ALA:HB3	1.99	0.44
1:A:1207:G:C6	1:A:1208:C:C4	3.06	0.44
1:A:1277:C:HO2'	1:A:1279:A:H8	1.64	0.44
16:P:67:THR:HG22	16:P:68:ASP:H	1.82	0.44
19:S:6:LYS:HE3	19:S:7:LYS:HE3	2.00	0.44
25:Z:38:A:H2'	25:Z:39:C:O4'	2.18	0.44
1:A:861:G:C2	1:A:862:C:C2	3.05	0.44
1:A:1064:G:H8	1:A:1064:G:OP1	2.01	0.44
1:A:1133:G:H1	1:A:1141:C:N4	2.16	0.44
1:A:1148:U:C5'	9:I:7:THR:HG21	2.47	0.44
1:A:1305:G:H5"	21:V:5:ASP:HB2	2.00	0.44
1:A:1351:U:H2'	1:A:1352:C:H6	1.81	0.44
1:A:1390:U:H2'	1:A:1391:U:C6	2.51	0.44
1:A:1504:G:H4'	1:A:1505:G:O5'	2.17	0.44
6:F:11:ASN:HD21	6:F:13:ASN:HD22	1.65	0.44
6:F:74:ASP:HA	6:F:77:ARG:HD2	2.00	0.44
9:I:36:TYR:HE2	9:I:73:GLN:OE1	2.00	0.44
18:R:31:LEU:O	18:R:69:THR:HG21	2.18	0.44
25:Z:17:C:H4'	25:Z:17(A):U:OP2	2.17	0.44
1:A:43:C:H2'	1:A:44:G:O4'	2.17	0.44
1:A:1004:A:H5"	1:A:1025:U:C5	2.53	0.44
1:A:1048:G:H5"	14:N:3:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:98:SER:HA	7:G:101:LEU:HD12	2.00	0.44
13:M:125:ARG:NH2	25:Z:30:G:OP2	2.50	0.44
20:T:74:LYS:HB2	20:T:75:ASN:H	1.31	0.44
25:Z:27:U:H2'	25:Z:28:C:H6	1.83	0.44
25:Z:49:G:C6	25:Z:66:C:N4	2.86	0.44
1:A:41:G:H2'	1:A:42:G:C8	2.53	0.44
1:A:223:U:H2'	1:A:224:C:C6	2.53	0.44
1:A:382:A:H2'	1:A:383:A:H8	1.81	0.44
1:A:399:G:C6	1:A:400:C:N4	2.86	0.44
1:A:568:G:C2	1:A:569:C:N3	2.86	0.44
1:A:807:A:H2'	1:A:808:C:C6	2.53	0.44
1:A:1048:G:H2'	1:A:1050:G:H8	1.83	0.44
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.50	0.44
1:A:1226:C:H2'	13:M:103:THR:CB	2.43	0.44
1:A:1237:C:H5"	1:A:1238:A:O4'	2.18	0.44
1:A:1411:C:H5"	22:W:64:ARG:HH22	1.82	0.44
8:H:101:PRO:HB2	8:H:103:VAL:HG23	1.98	0.44
9:I:27:THR:HB	9:I:62:TYR:HD1	1.82	0.44
20:T:10:LEU:HD12	20:T:11:SER:N	2.32	0.44
22:W:33:LEU:HD22	22:W:33:LEU:H	1.83	0.44
25:Z:23:C:H2'	25:Z:24:U:C6	2.53	0.44
1:A:108:G:H5'	1:A:109:A:H5"	2.00	0.44
1:A:296:U:H2'	1:A:297:G:C8	2.53	0.44
1:A:317:G:C2	1:A:337:C:C2	3.05	0.44
1:A:579:G:H1	1:A:762:C:H42	1.65	0.44
1:A:778:G:C6	1:A:779:C:N3	2.86	0.44
1:A:881:G:C2	1:A:882:C:C2	3.05	0.44
1:A:1171:G:C6	1:A:1172:C:N4	2.86	0.44
1:A:1280:A:H3'	1:A:1281:U:C5'	2.41	0.44
1:A:1305:G:H22	1:A:1331:G:H1'	1.83	0.44
1:A:1392:G:N2	1:A:1502:A:H8	2.16	0.44
1:A:1446:U:H1'	1:A:1457:G:C2	2.53	0.44
4:D:104:VAL:O	4:D:108:LEU:HD12	2.18	0.44
13:M:18:ALA:O	13:M:21:TYR:HB2	2.18	0.44
17:Q:74:LEU:HG	17:Q:75:ARG:HG2	2.00	0.44
25:Z:64:G:C6	25:Z:65:C:C2	3.05	0.44
1:A:129(A):G:O2'	1:A:189(F):U:H2'	2.18	0.44
1:A:255:G:C2	1:A:272:C:C2	3.06	0.44
1:A:721:G:H4'	1:A:722:A:O4'	2.18	0.44
1:A:867:G:N2	1:A:868:C:C2	2.85	0.44
1:A:947:G:C6	1:A:948:C:C4	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:U:H2'	1:A:1041:A:C8	2.53	0.44
1:A:1145:C:H1'	1:A:1146:A:C8	2.53	0.44
1:A:1387:G:C2	1:A:1388:C:C2	3.06	0.44
13:M:65:LYS:NZ	13:M:73:GLU:HB2	2.32	0.44
1:A:625:G:H2'	1:A:626:U:C6	2.52	0.43
1:A:741:G:H2'	1:A:742:G:O4'	2.18	0.43
1:A:758:G:O2'	1:A:759:A:H5'	2.17	0.43
1:A:763:G:C2	1:A:764:C:C2	3.06	0.43
1:A:966:G:C6	25:Z:34:C:H5'	2.52	0.43
1:A:985:C:C2	1:A:1221:G:N2	2.86	0.43
1:A:998:G:N2	1:A:999:C:C2	2.86	0.43
1:A:1041:A:H2'	1:A:1042:G:C8	2.52	0.43
4:D:30:LYS:C	4:D:32:ALA:H	2.20	0.43
12:L:30:ALA:HA	12:L:31:PRO:HD3	1.85	0.43
13:M:11:ARG:HH11	13:M:45:VAL:HG12	1.82	0.43
14:N:43:CYS:O	14:N:47:LEU:HG	2.18	0.43
1:A:174:C:H2'	1:A:175:C:C6	2.53	0.43
1:A:243:A:H4'	1:A:244:U:C5'	2.47	0.43
1:A:322:C:H2'	1:A:323:U:C6	2.53	0.43
1:A:1508:G:C6	1:A:1509:C:C4	3.07	0.43
5:E:16:THR:HB	5:E:27:ARG:O	2.19	0.43
19:S:22:LEU:HA	19:S:25:LYS:HB3	2.00	0.43
1:A:295:C:H2'	1:A:296:U:O4'	2.18	0.43
1:A:355:C:C4	1:A:356:A:N7	2.86	0.43
1:A:403:C:H2'	1:A:404:U:C6	2.53	0.43
1:A:856:C:N4	1:A:857:C:N4	2.66	0.43
1:A:966:G:C5	25:Z:34:C:H5'	2.53	0.43
1:A:1328:C:H2'	1:A:1329:A:C8	2.54	0.43
1:A:1445:C:O2	1:A:1458:G:C2	2.70	0.43
1:A:1525:G:H2'	1:A:1526:G:C8	2.53	0.43
3:C:29:TYR:CZ	14:N:54:PRO:CG	2.90	0.43
5:E:12:LEU:HB3	5:E:31:LEU:HB3	2.00	0.43
10:J:40:LEU:HD23	10:J:41:PRO:HD2	2.00	0.43
19:S:20:LEU:HD12	19:S:21:GLU:HG3	2.00	0.43
1:A:10:A:H2'	1:A:11:G:H8	1.80	0.43
1:A:120:A:C5	1:A:122:G:C6	3.06	0.43
1:A:132:C:C4	1:A:231:G:N1	2.86	0.43
1:A:189:G:H2'	1:A:189(A):C:C6	2.54	0.43
1:A:289:G:C2	1:A:290:C:C2	3.07	0.43
1:A:451:A:N6	1:A:480:U:H2'	2.34	0.43
1:A:683:G:N2	1:A:708:C:C2	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:G:H2'	1:A:879:C:C6	2.54	0.43
1:A:1001:A:C6	1:A:1001(A):G:C6	3.07	0.43
1:A:1081:G:H2'	1:A:1082:G:O4'	2.18	0.43
13:M:80:ARG:O	13:M:84:ILE:HG12	2.19	0.43
23:X:152:MET:HG2	23:X:164:LEU:HB3	2.01	0.43
1:A:179:A:C2	1:A:180:U:C2	3.07	0.43
1:A:407:G:H2'	1:A:408:A:H8	1.83	0.43
1:A:577:G:C6	1:A:578:C:C4	3.06	0.43
1:A:682:G:H2'	1:A:683:G:O4'	2.19	0.43
1:A:872:A:H2'	1:A:872:A:N3	2.32	0.43
1:A:1429:C:H2'	1:A:1430:C:C6	2.52	0.43
2:B:188:ALA:HB3	2:B:200:ILE:HG23	2.00	0.43
4:D:35:ARG:CZ	4:D:35:ARG:CB	2.97	0.43
4:D:109:GLY:HA3	4:D:165:MET:HG3	2.00	0.43
5:E:127:ASN:HD21	5:E:129:ILE:HD12	1.83	0.43
6:F:55:ASP:HA	6:F:56:PRO:HD2	1.85	0.43
13:M:91:ARG:HH21	13:M:96:LEU:HB3	1.84	0.43
23:X:8:ASN:HD21	23:X:44:ASP:HA	1.82	0.43
25:Z:39:C:O2'	25:Z:40:C:H5'	2.19	0.43
1:A:812:C:HO2'	1:A:813:U:P	2.41	0.43
1:A:916:G:H2'	1:A:917:G:H8	1.83	0.43
1:A:1048:G:C2	1:A:1210:C:N3	2.87	0.43
1:A:1061:G:H2'	1:A:1062:U:O4'	2.18	0.43
1:A:1279:A:H5'	10:J:7:LYS:HE2	2.00	0.43
1:A:1360:A:H2'	1:A:1361:G:C8	2.53	0.43
2:B:61:LEU:HD11	2:B:160:ASP:HB2	2.01	0.43
11:K:48:ILE:H	11:K:48:ILE:HG13	1.48	0.43
15:O:41:GLU:HA	15:O:44:LYS:HD2	2.00	0.43
23:X:132:LEU:O	23:X:136:ILE:HG13	2.18	0.43
25:Z:22:G:N1	25:Z:23:C:C4	2.86	0.43
1:A:29:G:N2	1:A:555:C:C2	2.87	0.43
1:A:448:A:H62	1:A:486:U:H3	1.67	0.43
1:A:903:G:C2	1:A:904:C:C2	3.06	0.43
1:A:1088:G:H2'	1:A:1089:G:O4'	2.18	0.43
1:A:1133:G:H2'	1:A:1134:G:C8	2.53	0.43
2:B:96:ARG:HB3	2:B:148:TYR:HE2	1.83	0.43
4:D:18:LYS:HE3	4:D:31:CYS:HB3	2.01	0.43
10:J:8:LEU:HA	10:J:95:GLU:O	2.19	0.43
17:Q:6:LEU:HD23	17:Q:23:VAL:HG11	1.99	0.43
1:A:134:A:H2'	1:A:135:C:O4'	2.19	0.43
1:A:184:G:H2'	1:A:185:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:C:N4	17:Q:91:ARG:NH2	2.67	0.43
1:A:426:G:H2'	1:A:427:U:O4'	2.18	0.43
1:A:1114:C:H2'	1:A:1115:C:C6	2.53	0.43
1:A:1114:C:H2'	1:A:1115:C:H6	1.83	0.43
1:A:1162:C:C2	1:A:1175:G:N2	2.87	0.43
1:A:1244:C:H42	1:A:1293:G:H1	1.65	0.43
1:A:1253:G:C6	1:A:1254:C:C4	3.07	0.43
1:A:1369:C:H2'	1:A:1370:G:O4'	2.19	0.43
9:I:116:LYS:HA	9:I:123:PRO:HD3	1.99	0.43
13:M:25:ILE:HG12	13:M:29:ARG:HB3	2.00	0.43
25:Z:67:C:H2'	25:Z:68:C:H6	1.83	0.43
1:A:23:C:C4	1:A:24:U:C4	3.07	0.43
1:A:109:A:H5'	1:A:110:C:H5	1.84	0.43
1:A:193:C:H2'	1:A:194:C:C6	2.54	0.43
1:A:384:G:C2	1:A:385:C:C2	3.07	0.43
1:A:439:A:C6	1:A:496:A:C4	3.07	0.43
1:A:444:C:N4	1:A:490:G:H1	2.17	0.43
1:A:617:G:C2	1:A:618:C:C4	3.06	0.43
1:A:698:G:C2	1:A:699:C:C2	3.06	0.43
1:A:725:G:C2	1:A:726:C:C4	3.07	0.43
1:A:769:G:H4'	1:A:1513:A:H4'	2.01	0.43
1:A:855:G:C2	1:A:856:C:C2	3.07	0.43
1:A:874:G:C2	1:A:875:C:C2	3.07	0.43
1:A:1081:G:P	5:E:27:ARG:NE	2.80	0.43
1:A:1292:U:H2'	1:A:1293:G:C8	2.54	0.43
1:A:1371:G:H2'	1:A:1372:U:H6	1.83	0.43
7:G:27:ILE:HA	7:G:30:ILE:HD12	2.00	0.43
7:G:79:ARG:NH2	7:G:82:GLY:H	2.17	0.43
13:M:44:ARG:H	13:M:47:ASP:HB2	1.84	0.43
18:R:16:PRO:HB2	18:R:18:ARG:HB2	2.00	0.43
1:A:137:C:H1'	16:P:62:VAL:O	2.19	0.43
1:A:280:C:O2	17:Q:38:ARG:HA	2.19	0.43
1:A:392:G:H5'	16:P:12:LYS:HG2	2.01	0.43
1:A:714:G:H2'	1:A:715:A:H8	1.75	0.43
1:A:975:A:H4'	1:A:976:G:O5'	2.19	0.43
1:A:1068:G:N1	1:A:1069:C:C4	2.87	0.43
1:A:1333:A:H3'	1:A:1334:G:H8	1.83	0.43
2:B:84:GLU:HB2	2:B:215:LEU:HD22	2.01	0.43
9:I:92:TYR:O	9:I:96:LEU:HB2	2.19	0.43
12:L:8:ASN:O	12:L:12:ARG:HG3	2.19	0.43
25:Z:53:G:N2	25:Z:61:C:C2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:G:C2	1:A:269:C:C2	3.07	0.42
1:A:584:G:H2'	1:A:585:G:C8	2.53	0.42
1:A:1347:G:O2'	1:A:1348:U:P	2.77	0.42
1:A:1419:G:C6	1:A:1420:C:C4	3.06	0.42
1:A:1481:U:H2'	1:A:1482:G:C8	2.53	0.42
4:D:36:ARG:CG	4:D:38:TYR:CZ	3.02	0.42
5:E:11:ILE:HG22	5:E:12:LEU:HB2	2.01	0.42
8:H:29:SER:O	8:H:33:GLU:HB2	2.19	0.42
8:H:127:LEU:HB3	8:H:129:VAL:HG12	2.01	0.42
25:Z:22:G:C2	25:Z:23:C:C2	3.07	0.42
25:Z:31:G:C2	25:Z:40:C:N3	2.87	0.42
1:A:35:G:C6	1:A:36:C:N4	2.87	0.42
1:A:247:G:P	17:Q:100:LYS:HD2	2.59	0.42
1:A:416:G:C2	1:A:417:C:C2	3.08	0.42
1:A:823:G:N1	1:A:824:C:C4	2.87	0.42
1:A:1002:G:N1	1:A:1039:C:C2	2.81	0.42
1:A:1189:C:H5'	14:N:58:LYS:NZ	2.34	0.42
1:A:1352:C:P	21:V:3:LYS:HZ1	2.42	0.42
2:B:172:ILE:H	2:B:172:ILE:HG13	1.56	0.42
4:D:33:MET:CA	4:D:36:ARG:O	2.67	0.42
22:W:32:ILE:CD1	22:W:32:ILE:N	2.82	0.42
22:W:35:TYR:CZ	22:W:66:ARG:HG3	2.54	0.42
25:Z:71:C:C2'	25:Z:72:A:O4'	2.66	0.42
1:A:102:G:C6	1:A:103:C:C4	3.07	0.42
1:A:279:A:OP2	17:Q:95:TYR:OH	2.35	0.42
1:A:505:G:H2'	1:A:506:G:H8	1.84	0.42
1:A:542:G:C2	1:A:543:C:C2	3.07	0.42
1:A:741:G:H5"	15:O:39:LEU:HD11	2.01	0.42
18:R:52:PRO:HB2	18:R:54:ARG:HG3	2.01	0.42
19:S:49:ILE:HG22	19:S:51:VAL:HG23	2.01	0.42
1:A:241:C:C2	1:A:286:G:C2	3.07	0.42
1:A:544:G:H2'	1:A:545:C:O4'	2.19	0.42
1:A:1353:G:C6	1:A:1354:C:N4	2.87	0.42
1:A:1511:G:H2'	1:A:1512:U:C6	2.54	0.42
3:C:13:GLY:HA3	14:N:57:ARG:HE	1.84	0.42
4:D:185:PHE:HZ	4:D:189:PRO:HD3	1.84	0.42
11:K:21:ILE:HD11	11:K:98:LEU:HD12	2.00	0.42
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.34	0.42
23:X:85:VAL:HA	23:X:115:LYS:O	2.20	0.42
25:Z:12:G:C6	25:Z:13:C:C4	3.07	0.42
1:A:79:G:H2'	1:A:80:G:C8	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:G:C6	1:A:277:C:C4	3.07	0.42
1:A:687:A:H4'	1:A:688:G:O5'	2.19	0.42
1:A:1233:G:C2	1:A:1234:C:C2	3.07	0.42
1:A:1387:G:C6	1:A:1388:C:C4	3.07	0.42
1:A:1514:C:H2'	1:A:1515:C:H6	1.82	0.42
1:A:1526:G:C2	1:A:1527:C:C2	3.07	0.42
11:K:18:ARG:HD3	11:K:35:PRO:HA	2.00	0.42
20:T:23:ARG:HG3	20:T:24:LEU:N	2.35	0.42
1:A:51:A:H4'	1:A:52:G:C5'	2.50	0.42
1:A:164:U:H2'	1:A:165:C:C6	2.54	0.42
1:A:329:A:H4'	1:A:330:C:OP1	2.18	0.42
1:A:333:G:C2	1:A:334:C:C2	3.07	0.42
1:A:556:C:H2'	1:A:557:G:O4'	2.20	0.42
1:A:670:G:H1	1:A:736:C:N4	2.16	0.42
1:A:1152:A:H2'	1:A:1153:C:C6	2.54	0.42
1:A:1154:G:H2'	1:A:1155:G:H8	1.83	0.42
1:A:1198:G:H2'	1:A:1199:U:C6	2.54	0.42
1:A:1270:C:H2'	1:A:1271:G:H8	1.85	0.42
1:A:1353:G:OP2	21:V:3:LYS:NZ	2.51	0.42
2:B:34:ALA:HB3	2:B:36:ARG:NH1	2.35	0.42
2:B:118:LEU:O	2:B:122:PHE:HB2	2.18	0.42
2:B:122:PHE:HA	2:B:127:ILE:HG12	2.00	0.42
12:L:59:ARG:HB2	12:L:59:ARG:NH1	2.35	0.42
25:Z:21:A:N6	25:Z:46:G7M:C2'	2.76	0.42
25:Z:31:G:C2	25:Z:40:C:C2	3.07	0.42
1:A:36:C:H2'	1:A:37:U:O4'	2.20	0.42
1:A:325:A:H2'	1:A:326:G:O4'	2.20	0.42
1:A:559:A:H4'	1:A:560:U:C5'	2.49	0.42
1:A:929:G:C2	1:A:930:C:C2	3.07	0.42
1:A:932:C:H5'	7:G:3:ARG:HB2	2.02	0.42
1:A:939:G:C2	1:A:940:C:C2	3.07	0.42
1:A:1106:G:C2	1:A:1107:C:C2	3.07	0.42
1:A:1106:G:C2	1:A:1107:C:C4	3.08	0.42
1:A:1459:C:H2'	1:A:1460:A:H8	1.84	0.42
1:A:1502:A:H2'	1:A:1504:G:C8	2.54	0.42
5:E:15:ARG:NH2	5:E:26:PHE:HB3	2.35	0.42
25:Z:7:G:C5	25:Z:49:G:C8	3.08	0.42
25:Z:31:G:N2	25:Z:40:C:C2	2.88	0.42
1:A:11:G:H2'	1:A:12:U:O4'	2.19	0.42
1:A:338:A:C6	1:A:339:C:C4	3.08	0.42
1:A:501:C:OP1	12:L:117:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:G:N2	1:A:651:C:C2	2.88	0.42
1:A:661:G:C2	1:A:745:C:N3	2.88	0.42
1:A:806:C:H2'	1:A:807:A:H8	1.84	0.42
1:A:825:G:H1	1:A:875:C:H42	1.68	0.42
1:A:1115:C:C2	1:A:1186:G:N2	2.87	0.42
2:B:77:ALA:C	2:B:79:ASP:H	2.23	0.42
5:E:11:ILE:HD13	5:E:33:VAL:HG23	2.02	0.42
14:N:17:LYS:H	14:N:17:LYS:HG3	1.64	0.42
1:A:155:C:H2'	1:A:156:G:H8	1.85	0.42
1:A:394:G:C2	1:A:395:C:C2	3.07	0.42
1:A:447:G:C3'	1:A:485:G:H22	2.33	0.42
1:A:1002:G:O6	1:A:1039:C:N3	2.53	0.42
1:A:1050:G:C2	1:A:1051:C:C4	3.08	0.42
3:C:62:ASP:HA	3:C:97:LYS:CE	2.50	0.42
4:D:129:ASN:ND2	4:D:145:GLU:H	2.16	0.42
23:X:152:MET:HB3	23:X:155:GLU:OE1	2.20	0.42
25:Z:70:G:C6	25:Z:71:C:N3	2.88	0.42
1:A:252:U:H2'	1:A:253:U:C6	2.55	0.42
1:A:319:G:C2	1:A:320:C:C2	3.08	0.42
1:A:774:G:C2	1:A:806:C:C2	3.07	0.42
1:A:903:G:C6	1:A:904:C:C4	3.08	0.42
1:A:1001(A):G:N1	1:A:1002:G:C6	2.88	0.42
1:A:1029:C:H2'	1:A:1030:C:C6	2.55	0.42
1:A:1283:G:C6	1:A:1284:C:N4	2.87	0.42
2:B:25:ASN:HA	2:B:26:PRO:HD3	1.83	0.42
3:C:6:HIS:HA	3:C:7:PRO:HD3	1.88	0.42
5:E:76:ILE:HG23	5:E:78:HIS:H	1.85	0.42
1:A:169:C:H2'	1:A:170:U:C6	2.55	0.41
1:A:436:C:O2'	4:D:155:LEU:HD21	2.19	0.41
1:A:590:C:OP1	8:H:30:ARG:N	2.49	0.41
1:A:718:G:H5'	11:K:117:ASN:HB2	2.01	0.41
1:A:731:G:C6	1:A:732:C:C4	3.08	0.41
1:A:836:G:H2'	1:A:837:G:C8	2.54	0.41
5:E:15:ARG:NH2	5:E:26:PHE:CB	2.76	0.41
9:I:111:ARG:NH1	14:N:61:TRP:OXT	2.52	0.41
20:T:44:ALA:HB1	20:T:91:LEU:HB2	2.02	0.41
25:Z:38:A:C8	25:Z:39:C:C5	3.08	0.41
1:A:442:C:H2'	1:A:443:C:C6	2.55	0.41
1:A:450:G:N7	1:A:481:G:C6	2.88	0.41
1:A:481:G:O2'	1:A:483:C:N4	2.53	0.41
1:A:977:A:H1'	1:A:982:U:O4	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:G:C2	1:A:1069:C:C2	3.09	0.41
1:A:1095:U:OP1	1:A:1108:G:N1	2.53	0.41
1:A:1116:C:C2	1:A:1185:G:C2	3.07	0.41
1:A:1241:G:N1	1:A:1242:C:C4	2.89	0.41
1:A:1347:G:C8	9:I:107:ARG:HB3	2.55	0.41
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.54	0.41
3:C:29:TYR:CD1	3:C:33:LEU:HB2	2.55	0.41
5:E:31:LEU:HD23	5:E:45:PHE:HD1	1.84	0.41
19:S:5:LEU:HB3	19:S:6:LYS:H	1.46	0.41
23:X:19:VAL:HG21	25:Z:56:C:C4	2.55	0.41
1:A:142:G:H2'	1:A:143:A:H8	1.85	0.41
1:A:183:G:H2'	1:A:184:G:O4'	2.21	0.41
1:A:189(L):G:H2'	1:A:190:U:C6	2.55	0.41
1:A:321:A:H2'	1:A:322:C:H6	1.85	0.41
1:A:542:G:C6	1:A:543:C:N4	2.89	0.41
1:A:881:G:C6	1:A:882:C:C4	3.08	0.41
1:A:1459:C:H2'	1:A:1460:A:O4'	2.20	0.41
1:A:1502:A:H2	1:A:1505:G:N1	2.18	0.41
1:A:1541:U:H3	24:Y:24:A:N6	2.18	0.41
7:G:111:ARG:HA	7:G:112:PRO:HD3	1.80	0.41
13:M:82:MET:HA	13:M:89:GLY:HA3	2.02	0.41
14:N:12:ARG:H	14:N:12:ARG:HG2	1.71	0.41
16:P:9:PHE:CD2	16:P:18:ARG:HG3	2.55	0.41
16:P:73:LEU:HD23	16:P:73:LEU:HA	1.97	0.41
23:X:45:LEU:HG	23:X:57:ALA:HB1	2.02	0.41
1:A:778:G:N1	1:A:779:C:C2	2.88	0.41
1:A:861:G:C6	1:A:862:C:C4	3.09	0.41
1:A:914:A:C5	1:A:915:A:N7	2.89	0.41
1:A:986:A:H1'	19:S:54:GLY:O	2.21	0.41
1:A:1226:C:H5"	13:M:96:LEU:HD13	2.01	0.41
1:A:1478:C:H2'	1:A:1479:C:C6	2.55	0.41
12:L:93:LEU:HA	12:L:94:PRO:HD3	1.78	0.41
1:A:489:C:H2'	1:A:490:G:H8	1.85	0.41
1:A:916:G:C2	1:A:917:G:N7	2.88	0.41
1:A:921:U:H2'	1:A:922:G:O4'	2.20	0.41
1:A:1050:G:C2	1:A:1209:C:C2	3.08	0.41
1:A:1258:G:H2'	1:A:1259:C:C6	2.55	0.41
1:A:1283:G:C2	1:A:1284:C:C4	3.08	0.41
1:A:1452:C:H4'	1:A:1456:G:O4'	2.21	0.41
4:D:3:ARG:HB3	4:D:4:TYR:H	1.69	0.41
4:D:90:GLY:O	4:D:93:PHE:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:85:ILE:HG22	12:L:87:GLY:H	1.85	0.41
14:N:21:TYR:O	14:N:23:ARG:N	2.53	0.41
1:A:113:G:H1'	1:A:354:G:H5'	2.02	0.41
1:A:502:G:C6	1:A:503:C:C4	3.09	0.41
1:A:1106:G:C2	1:A:1107:C:N3	2.89	0.41
1:A:1171:G:C2	1:A:1172:C:C2	3.08	0.41
1:A:1171:G:N1	1:A:1172:C:C4	2.88	0.41
2:B:33:TYR:HB3	2:B:41:ILE:HG22	2.02	0.41
2:B:84:GLU:HA	2:B:87:ARG:HB2	2.01	0.41
7:G:18:TYR:CE1	7:G:59:LEU:HB2	2.55	0.41
10:J:34:VAL:HG13	10:J:72:VAL:CG1	2.50	0.41
20:T:63:ILE:HG21	20:T:81:LYS:HG3	2.01	0.41
23:X:46:VAL:O	23:X:48:VAL:HG22	2.20	0.41
1:A:365:U:O2	1:A:365:U:H2'	2.20	0.41
1:A:399:G:N2	1:A:400:C:C2	2.89	0.41
1:A:626:U:H2'	1:A:627:G:C8	2.56	0.41
1:A:785:G:H1	1:A:797:C:N4	2.19	0.41
1:A:790:A:H4'	23:X:87:SER:OG	2.20	0.41
1:A:1126:U:O2	1:A:1126:U:H2'	2.20	0.41
1:A:1128:C:O2'	1:A:1130:A:N7	2.42	0.41
1:A:1329:A:H5"	13:M:25:ILE:HA	2.02	0.41
7:G:9:VAL:HB	7:G:11:GLN:HE22	1.86	0.41
8:H:79:VAL:HG13	8:H:80:ILE:N	2.35	0.41
15:O:41:GLU:O	15:O:44:LYS:HB2	2.20	0.41
17:Q:19:VAL:HG23	17:Q:44:ALA:HB3	2.03	0.41
21:V:3:LYS:HD3	21:V:14:TRP:CD1	2.56	0.41
1:A:284:G:C2	1:A:285:G:C5	3.08	0.41
1:A:354:G:C2	1:A:355:C:C4	3.09	0.41
1:A:402:G:C2	1:A:403:C:C2	3.09	0.41
1:A:767:A:H2'	1:A:768:A:C8	2.56	0.41
1:A:1292:U:H2'	1:A:1293:G:H8	1.86	0.41
1:A:1302:U:H3'	1:A:1303:C:C5'	2.51	0.41
1:A:1443:G:C2	1:A:1444:C:N3	2.89	0.41
1:A:1458:G:H5"	20:T:31:SER:HB3	2.02	0.41
1:A:1507:A:C8	1:A:1530:G:N2	2.88	0.41
10:J:4:ILE:HD12	10:J:74:ILE:HD13	2.01	0.41
1:A:76:C:O2'	1:A:77:G:H5'	2.21	0.41
1:A:146:G:N2	1:A:177:C:C2	2.89	0.41
1:A:291:C:O2	1:A:310:G:C2	2.74	0.41
1:A:310:G:OP1	16:P:27:LYS:HD2	2.21	0.41
1:A:472:A:OP1	16:P:75:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:G:O3'	4:D:14:ARG:NH2	2.53	0.41
1:A:662:G:C2	1:A:744:C:O2	2.74	0.41
1:A:1017:G:C6	1:A:1018:C:C4	3.09	0.41
1:A:1069:C:H2'	1:A:1070:U:O4'	2.21	0.41
1:A:1217:C:N4	1:A:1218:C:N4	2.68	0.41
1:A:1286:A:C8	1:A:1286:A:H3'	2.56	0.41
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.20	0.41
1:A:1396:A:O3'	1:A:1397:C:H5"	2.21	0.41
3:C:33:LEU:HD11	14:N:53:LEU:HD22	2.02	0.41
4:D:185:PHE:CZ	4:D:189:PRO:HD3	2.56	0.41
5:E:37:ARG:HH12	5:E:111:GLU:HB3	1.86	0.41
9:I:89:ASN:ND2	9:I:91:ASP:HB2	2.35	0.41
10:J:49:VAL:HG11	14:N:44:LEU:HD12	2.03	0.41
14:N:24:CYS:HB3	14:N:29:ARG:N	2.35	0.41
18:R:72:ARG:O	18:R:75:ILE:HG22	2.20	0.41
25:Z:2:G:H1	25:Z:71:C:N4	2.19	0.41
25:Z:53:G:H2'	25:Z:54:5MU:C6	2.56	0.41
1:A:333:G:H2'	1:A:334:C:C6	2.56	0.41
1:A:399:G:C6	1:A:400:C:C4	3.08	0.41
1:A:701:C:H1'	1:A:703:G:C5	2.56	0.41
1:A:786:G:C2	1:A:797:C:N3	2.89	0.41
1:A:895:G:C2	1:A:896:C:C2	3.09	0.41
1:A:1096:C:H2'	1:A:1097:C:C6	2.56	0.41
1:A:1162:C:C2	1:A:1175:G:C2	3.09	0.41
2:B:16:HIS:HB3	2:B:17:PHE:H	1.76	0.41
3:C:83:ARG:O	3:C:87:LEU:HG	2.21	0.41
5:E:95:ALA:O	5:E:98:THR:OG1	2.39	0.41
11:K:10:VAL:C	11:K:12:ARG:H	2.23	0.41
11:K:31:THR:HG23	11:K:42:TRP:HB3	2.02	0.41
14:N:27:CYS:SG	14:N:28:GLY:N	2.94	0.41
22:W:37:SER:HB2	22:W:67:ILE:O	2.20	0.41
23:X:123:ARG:HB3	23:X:124:GLY:H	1.69	0.41
25:Z:2:G:N3	25:Z:3:C:C6	2.89	0.41
1:A:13:U:H5'	1:A:14:U:H5	1.85	0.40
1:A:865:A:H2'	1:A:866:C:C6	2.56	0.40
1:A:1243:C:C2	1:A:1295:G:C2	3.09	0.40
1:A:1247:U:H1'	1:A:1291:G:N2	2.36	0.40
1:A:1291:G:H4'	9:I:38:GLN:O	2.21	0.40
3:C:29:TYR:CE1	3:C:33:LEU:HD13	2.51	0.40
4:D:117:ALA:O	4:D:121:VAL:HG23	2.22	0.40
9:I:33:PHE:CZ	9:I:47:LEU:HG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:U:O2'	1:A:500:G:H4'	2.20	0.40
1:A:146:G:C2	1:A:177:C:C2	3.10	0.40
1:A:599:C:H2'	1:A:600:C:C6	2.56	0.40
1:A:943:U:H2'	1:A:944:G:C8	2.56	0.40
1:A:1119:C:H2'	1:A:1120:G:C8	2.56	0.40
1:A:1431:C:N3	1:A:1470:G:C2	2.90	0.40
2:B:212:GLN:HG3	2:B:239:VAL:HG23	2.03	0.40
4:D:33:MET:O	4:D:36:ARG:O	2.37	0.40
12:L:82:VAL:HG12	12:L:105:TYR:HB3	2.02	0.40
16:P:33:ILE:H	16:P:33:ILE:HG13	1.76	0.40
18:R:42:ARG:HB3	18:R:42:ARG:NH1	2.36	0.40
19:S:5:LEU:HD13	19:S:10:PHE:H	1.85	0.40
25:Z:58:A:H2	25:Z:60:U:H2'	1.85	0.40
1:A:148:G:C2	1:A:175:C:C2	3.09	0.40
1:A:482:A:C2	1:A:483:C:H1'	2.56	0.40
1:A:548:G:C6	1:A:549:C:C4	3.10	0.40
1:A:922:G:C2	1:A:923:A:C4	3.09	0.40
1:A:929:G:C6	1:A:930:C:C4	3.10	0.40
1:A:931:C:O2	1:A:1387:G:C2	2.75	0.40
1:A:939:G:C2	1:A:940:C:N3	2.89	0.40
1:A:1000:U:C6	1:A:1000:U:C3'	3.04	0.40
1:A:1145:C:HO2'	1:A:1146:A:C5'	2.34	0.40
1:A:1518:A:H2'	1:A:1519:A:H8	1.83	0.40
1:A:1526:G:C6	1:A:1527:C:C4	3.09	0.40
3:C:20:SER:HB3	3:C:22:TRP:NE1	2.36	0.40
3:C:54:ARG:HB2	3:C:69:HIS:HB2	2.02	0.40
4:D:196:LEU:HA	4:D:197:PRO:HD2	1.84	0.40
10:J:61:GLU:OE2	14:N:58:LYS:HG2	2.20	0.40
23:X:11:ILE:HG12	23:X:47:LEU:CB	2.51	0.40
1:A:76:C:C3'	1:A:77:G:H5'	2.51	0.40
1:A:112:G:P	16:P:27:LYS:HG2	2.62	0.40
1:A:489:C:H2'	1:A:490:G:C8	2.56	0.40
1:A:778:G:H2'	1:A:779:C:O4'	2.20	0.40
1:A:966:G:C6	1:A:967:C:N3	2.89	0.40
1:A:1023:G:N3	1:A:1023:G:H2'	2.35	0.40
1:A:1121:U:H2'	1:A:1122:U:C6	2.57	0.40
1:A:1242:C:H4'	1:A:1304:G:OP1	2.22	0.40
1:A:1317:C:H42	19:S:37:ARG:HH22	1.69	0.40
1:A:1489:G:C2	1:A:1490:C:C2	3.10	0.40
5:E:127:ASN:O	5:E:128:PRO:C	2.59	0.40
8:H:10:LEU:HD12	8:H:85:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:8:LEU:HG	10:J:96:ILE:HG23	2.03	0.40
10:J:51:ARG:CD	10:J:59:SER:HB3	2.48	0.40
16:P:49:LEU:HD13	16:P:73:LEU:HD22	2.04	0.40
18:R:21:LYS:HG2	18:R:57:GLY:HA3	2.04	0.40
25:Z:7:G:C6	25:Z:49:G:C8	3.09	0.40
1:A:230:G:H2'	1:A:231:G:O4'	2.21	0.40
1:A:306:G:N2	1:A:307:C:C2	2.89	0.40
1:A:369:C:C2	1:A:393:A:C2	3.10	0.40
1:A:577:G:N1	1:A:578:C:C4	2.89	0.40
1:A:761:G:C5	1:A:762:C:C4	3.09	0.40
1:A:914:A:H2'	1:A:915:A:C8	2.55	0.40
1:A:1184:G:H2'	1:A:1185:G:H8	1.87	0.40
1:A:1276:G:H2'	1:A:1277:C:O4'	2.22	0.40
1:A:1389:C:H2'	1:A:1390:U:O4'	2.21	0.40
1:A:1461:G:H2'	1:A:1462:G:C8	2.57	0.40
1:A:1536:C:H42	24:Y:29:G:H1	1.69	0.40
1:A:1539:C:N4	24:Y:26:G:H1	2.15	0.40
2:B:208:ILE:H	2:B:208:ILE:HG13	1.45	0.40
13:M:94:ARG:HB3	13:M:96:LEU:HD12	2.04	0.40
25:Z:53:G:H2'	25:Z:54:5MU:H6	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	232/256 (91%)	187 (81%)	33 (14%)	12 (5%)	2 22
3	C	204/239 (85%)	176 (86%)	20 (10%)	8 (4%)	3 27
4	D	206/209 (99%)	185 (90%)	14 (7%)	7 (3%)	3 30
5	E	148/162 (91%)	134 (90%)	12 (8%)	2 (1%)	11 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	F	99/101 (98%)	90 (91%)	7 (7%)	2 (2%)	7 40
7	G	153/156 (98%)	134 (88%)	15 (10%)	4 (3%)	5 35
8	H	136/138 (99%)	122 (90%)	11 (8%)	3 (2%)	6 38
9	I	125/128 (98%)	106 (85%)	16 (13%)	3 (2%)	6 36
10	J	96/105 (91%)	74 (77%)	14 (15%)	8 (8%)	1 13
11	K	120/129 (93%)	100 (83%)	14 (12%)	6 (5%)	2 23
12	L	122/132 (92%)	99 (81%)	19 (16%)	4 (3%)	4 30
13	M	123/126 (98%)	105 (85%)	15 (12%)	3 (2%)	6 36
14	N	58/61 (95%)	49 (84%)	6 (10%)	3 (5%)	2 22
15	O	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	13 50
16	P	81/88 (92%)	73 (90%)	8 (10%)	0	100 100
17	Q	97/105 (92%)	87 (90%)	9 (9%)	1 (1%)	15 54
18	R	71/88 (81%)	64 (90%)	4 (6%)	3 (4%)	3 26
19	S	80/93 (86%)	59 (74%)	17 (21%)	4 (5%)	2 23
20	T	97/106 (92%)	84 (87%)	8 (8%)	5 (5%)	2 22
21	V	22/27 (82%)	19 (86%)	3 (14%)	0	100 100
22	W	69/72 (96%)	61 (88%)	6 (9%)	2 (3%)	4 32
23	X	166/171 (97%)	143 (86%)	15 (9%)	8 (5%)	2 24
All	All	2591/2781 (93%)	2230 (86%)	272 (10%)	89 (3%)	6 30

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
2	B	24	TRP
4	D	37	PRO
9	I	56	LEU
13	M	113	PRO
14	N	22	THR
20	T	49	ALA
22	W	70	ARG
23	X	8	ASN
23	X	54	PRO
23	X	94	ILE
4	D	5	ILE
4	D	26	CYS

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Mol	Chain	Res	Type
5	E	37	ARG
6	F	15	ASP
6	F	93	SER
10	J	39	PRO
10	J	55	LYS
11	K	11	LYS
11	K	12	ARG
13	M	124	PRO
14	N	14	PRO
18	R	76	LEU
19	S	5	LEU
22	W	2	LYS
23	X	47	LEU
23	X	82	ARG
23	X	83	THR
3	C	12	LEU
3	C	16	ARG
3	C	108	ASN
7	G	7	ALA
8	H	5	PRO
10	J	31	GLY
10	J	34	VAL
10	J	57	LYS
12	L	27	LEU
13	M	5	ALA
15	O	88	ARG
19	S	71	LEU
20	T	9	ASN
20	T	95	ALA
2	B	8	LYS
2	B	65	GLY
3	C	4	LYS
4	D	3	ARG
4	D	39	PRO
4	D	208	SER
7	G	149	ARG
8	H	55	GLY
9	I	54	ASP
10	J	40	LEU
10	J	54	PHE
10	J	82	ILE
11	K	14	VAL

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Mol	Chain	Res	Type
11	K	27	ASN
11	K	101	SER
12	L	28	LYS
12	L	51	ALA
17	Q	30	PRO
20	T	97	ALA
23	X	55	PRO
2	B	16	HIS
2	B	37	ASN
2	B	130	ARG
2	B	229	VAL
3	C	127	ARG
3	C	168	ALA
3	C	175	LEU
8	H	54	ASP
9	I	55	ALA
18	R	48	GLY
18	R	77	GLY
19	S	30	LEU
20	T	73	HIS
2	B	78	GLN
7	G	55	GLY
7	G	81	GLY
12	L	25	PRO
19	S	80	TYR
2	B	194	PRO
5	E	49	PRO
23	X	127	VAL
2	B	232	PRO
3	C	155	GLY
14	N	7	ILE
2	B	131	PRO
4	D	197	PRO
11	K	48	ILE

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%)	148 (73%)	54 (27%)	0 3
3	C	160/188 (85%)	143 (89%)	17 (11%)	6 27
4	D	180/181 (99%)	141 (78%)	39 (22%)	1 6
5	E	115/123 (94%)	85 (74%)	30 (26%)	0 3
6	F	90/90 (100%)	71 (79%)	19 (21%)	1 7
7	G	126/127 (99%)	109 (86%)	17 (14%)	4 20
8	H	119/119 (100%)	90 (76%)	29 (24%)	0 4
9	I	98/99 (99%)	81 (83%)	17 (17%)	2 13
10	J	87/92 (95%)	65 (75%)	22 (25%)	0 4
11	K	92/99 (93%)	75 (82%)	17 (18%)	1 11
12	L	104/109 (95%)	85 (82%)	19 (18%)	1 11
13	M	100/101 (99%)	89 (89%)	11 (11%)	6 26
14	N	49/50 (98%)	37 (76%)	12 (24%)	0 4
15	O	79/80 (99%)	58 (73%)	21 (27%)	0 3
16	P	72/74 (97%)	56 (78%)	16 (22%)	1 6
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%)	56 (79%)	15 (21%)	1 7
20	T	76/82 (93%)	61 (80%)	15 (20%)	1 9
21	V	19/22 (86%)	16 (84%)	3 (16%)	2 16
22	W	62/63 (98%)	51 (82%)	11 (18%)	2 12
23	X	145/150 (97%)	122 (84%)	23 (16%)	2 16
All	All	2204/2323 (95%)	1773 (80%)	431 (20%)	4 9

All (431) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	10	LEU
2	B	16	HIS
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	30	ARG
2	B	32	ILE

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Mol	Chain	Res	Type
2	B	39	ILE
2	B	51	LEU
2	B	52	GLU
2	B	60	ASP
2	B	61	LEU
2	B	63	MET
2	B	67	THR
2	B	75	LYS
2	B	76	GLN
2	B	83	MET
2	B	95	GLN
2	B	96	ARG
2	B	98	LEU
2	B	103	THR
2	B	107	THR
2	B	114	ARG
2	B	121	LEU
2	B	122	PHE
2	B	124	SER
2	B	130	ARG
2	B	137	ARG
2	B	140	HIS
2	B	142	LEU
2	B	144	ARG
2	B	150	SER
2	B	152	PHE
2	B	153	ARG
2	B	156	LYS
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	204	ASN
2	B	205	ASP
2	B	208	ILE
2	B	211	ILE
2	B	215	LEU

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Mol	Chain	Res	Type
2	B	220	ASP
2	B	221	LEU
2	B	233	SER
2	B	235	SER
3	C	3	ASN
3	C	14	ILE
3	C	21	ARG
3	C	29	TYR
3	C	45	LYS
3	C	79	ARG
3	C	90	GLU
3	C	94	LEU
3	C	97	LYS
3	C	104	GLN
3	C	111	LEU
3	C	142	MET
3	C	167	TRP
3	C	188	LEU
3	C	190	ARG
3	C	191	THR
3	C	195	VAL
4	D	10	ARG
4	D	12	CYS
4	D	13	ARG
4	D	19	LEU
4	D	25	ARG
4	D	27	TYR
4	D	35	ARG
4	D	36	ARG
4	D	49	ARG
4	D	50	ARG
4	D	52	SER
4	D	53	ASP
4	D	59	ARG
4	D	61	LYS
4	D	66	ARG
4	D	70	ILE
4	D	72	GLU
4	D	74	GLN
4	D	76	ARG
4	D	78	LEU
4	D	85	LYS

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Mol	Chain	Res	Type
4	D	92	VAL
4	D	94	LEU
4	D	97	LEU
4	D	103	ASN
4	D	104	VAL
4	D	118	ARG
4	D	120	LEU
4	D	122	ARG
4	D	131	ARG
4	D	132	ARG
4	D	141	ARG
4	D	152	SER
4	D	159	ARG
4	D	162	LEU
4	D	165	MET
4	D	174	LEU
4	D	176	LEU
4	D	191	ARG
5	E	5	ASP
5	E	12	LEU
5	E	14	ARG
5	E	18	ARG
5	E	19	MET
5	E	24	ARG
5	E	27	ARG
5	E	32	VAL
5	E	34	VAL
5	E	36	ASP
5	E	41	VAL
5	E	63	ARG
5	E	64	ARG
5	E	68	GLU
5	E	71	LEU
5	E	73	ASN
5	E	76	ILE
5	E	80	ILE
5	E	98	THR
5	E	105	VAL
5	E	112	LEU
5	E	118	ILE
5	E	119	LEU
5	E	126	ARG

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Mol	Chain	Res	Type
5	E	135	THR
5	E	136	MET
5	E	140	ARG
5	E	142	LEU
5	E	147	ASP
5	E	150	ARG
6	F	9	VAL
6	F	10	LEU
6	F	15	ASP
6	F	19	LEU
6	F	28	ARG
6	F	31	GLU
6	F	36	ARG
6	F	38	GLU
6	F	39	LYS
6	F	40	VAL
6	F	42	GLU
6	F	54	LYS
6	F	61	LEU
6	F	75	LEU
6	F	77	ARG
6	F	78	GLU
6	F	83	ASP
6	F	86	ARG
6	F	95	GLU
7	G	8	GLU
7	G	10	ARG
7	G	16	LEU
7	G	22	LEU
7	G	37	ASN
7	G	62	PHE
7	G	67	GLU
7	G	72	ARG
7	G	74	GLU
7	G	79	ARG
7	G	80	VAL
7	G	94	ARG
7	G	99	LEU
7	G	106	GLN
7	G	136	LYS
7	G	146	GLU
7	G	156	TRP

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Mol	Chain	Res	Type
8	H	2	LEU
8	H	14	ARG
8	H	18	ARG
8	H	23	SER
8	H	29	SER
8	H	31	PHE
8	H	39	LEU
8	H	41	ARG
8	H	50	ARG
8	H	53	VAL
8	H	56	LYS
8	H	59	LEU
8	H	63	LEU
8	H	69	ARG
8	H	70	GLN
8	H	75	ARG
8	H	84	ARG
8	H	85	ARG
8	H	92	ARG
8	H	104	ARG
8	H	105	ARG
8	H	112	LEU
8	H	115	SER
8	H	120	THR
8	H	121	ASP
8	H	122	ARG
8	H	123	GLU
8	H	127	LEU
8	H	134	ILE
9	I	14	VAL
9	I	32	ASP
9	I	38	GLN
9	I	42	ARG
9	I	48	GLU
9	I	56	LEU
9	I	60	ASP
9	I	64	THR
9	I	78	LYS
9	I	85	LEU
9	I	87	GLN
9	I	102	LEU
9	I	104	ARG

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Mol	Chain	Res	Type
9	I	109	VAL
9	I	111	ARG
9	I	121	ARG
9	I	127	LYS
10	J	4	ILE
10	J	8	LEU
10	J	16	LEU
10	J	17	ASP
10	J	19	SER
10	J	35	SER
10	J	40	LEU
10	J	42	THR
10	J	48	THR
10	J	49	VAL
10	J	51	ARG
10	J	57	LYS
10	J	60	ARG
10	J	61	GLU
10	J	66	ARG
10	J	70	ARG
10	J	73	ASP
10	J	74	ILE
10	J	82	ILE
10	J	87	THR
10	J	96	ILE
10	J	99	LYS
11	K	13	GLN
11	K	18	ARG
11	K	25	TYR
11	K	34	ASP
11	K	40	ILE
11	K	41	THR
11	K	48	ILE
11	K	53	SER
11	K	63	LEU
11	K	77	MET
11	K	78	GLN
11	K	84	VAL
11	K	91	ARG
11	K	93	GLN
11	K	96	ARG
11	K	116	HIS

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Mol	Chain	Res	Type
11	K	117	ASN
12	L	6	THR
12	L	10	LEU
12	L	17	LYS
12	L	19	ARG
12	L	34	ARG
12	L	42	THR
12	L	46	LYS
12	L	50	SER
12	L	53	ARG
12	L	59	ARG
12	L	60	LEU
12	L	62	SER
12	L	65	GLU
12	L	79	GLU
12	L	92	ASP
12	L	100	ILE
12	L	112	ASP
12	L	116	SER
12	L	117	ARG
13	M	9	ILE
13	M	12	ASN
13	M	15	VAL
13	M	39	ILE
13	M	44	ARG
13	M	46	LYS
13	M	66	LEU
13	M	83	ASP
13	M	102	ARG
13	M	110	ARG
13	M	115	LYS
14	N	9	LYS
14	N	12	ARG
14	N	15	LYS
14	N	17	LYS
14	N	29	ARG
14	N	31	ARG
14	N	32	SER
14	N	33	VAL
14	N	40	CYS
14	N	44	LEU
14	N	46	GLU

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Mol	Chain	Res	Type
14	N	58	LYS
15	O	3	ILE
15	O	4	THR
15	O	9	GLN
15	O	13	GLN
15	O	17	ARG
15	O	21	ASP
15	O	34	LEU
15	O	37	ASN
15	O	43	LEU
15	O	52	SER
15	O	56	LEU
15	O	59	MET
15	O	60	VAL
15	O	63	ARG
15	O	65	ARG
15	O	70	LEU
15	O	71	GLN
15	O	77	ARG
15	O	85	LEU
15	O	87	ILE
15	O	88	ARG
16	P	5	ARG
16	P	28	ARG
16	P	36	ILE
16	P	40	ASP
16	P	44	THR
16	P	45	THR
16	P	51	VAL
16	P	54	GLU
16	P	57	ARG
16	P	60	LEU
16	P	71	ARG
16	P	72	ARG
16	P	76	GLN
16	P	79	VAL
16	P	81	ARG
16	P	82	GLN
17	Q	6	LEU
17	Q	36	ILE
17	Q	55	ASP
17	Q	60	ILE

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Mol	Chain	Res	Type
17	Q	61	GLU
17	Q	63	ARG
17	Q	70	ARG
17	Q	92	ARG
17	Q	98	LEU
17	Q	100	LYS
18	R	18	ARG
18	R	21	LYS
18	R	28	GLU
18	R	36	ASN
18	R	37	VAL
18	R	38	GLU
18	R	41	LYS
18	R	42	ARG
18	R	44	LEU
18	R	53	ARG
18	R	55	ARG
18	R	75	ILE
18	R	86	VAL
18	R	87	ARG
19	S	5	LEU
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
19	S	17	GLU
19	S	19	VAL
19	S	22	LEU
19	S	29	ARG
19	S	38	SER
19	S	41	VAL
19	S	53	ASN
19	S	62	ILE
19	S	63	THR
19	S	77	THR
19	S	80	TYR
20	T	10	LEU
20	T	19	SER
20	T	23	ARG
20	T	24	LEU
20	T	27	LYS
20	T	31	SER
20	T	45	GLN

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Mol	Chain	Res	Type
20	T	53	LEU
20	T	57	ARG
20	T	62	LEU
20	T	63	ILE
20	T	68	LYS
20	T	73	HIS
20	T	74	LYS
20	T	84	LEU
21	V	6	ARG
21	V	8	THR
21	V	9	ARG
22	W	12	VAL
22	W	19	ASN
22	W	28	SER
22	W	32	ILE
22	W	41	ARG
22	W	52	ARG
22	W	54	VAL
22	W	58	THR
22	W	64	ARG
22	W	69	TYR
22	W	71	LYS
23	X	6	LEU
23	X	17	ARG
23	X	18	VAL
23	X	28	ILE
23	X	30	ASP
23	X	32	ARG
23	X	35	LEU
23	X	39	GLN
23	X	44	ASP
23	X	48	VAL
23	X	51	ASN
23	X	53	ASP
23	X	66	ARG
23	X	67	TYR
23	X	87	SER
23	X	92	VAL
23	X	98	ASP
23	X	118	VAL
23	X	125	ARG
23	X	127	VAL

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Mol	Chain	Res	Type
23	X	143	ASP
23	X	144	LEU
23	X	162	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
2	B	212	GLN
3	C	6	HIS
3	C	31	HIS
3	C	108	ASN
4	D	45	GLN
4	D	74	GLN
4	D	129	ASN
4	D	160	GLN
4	D	161	ASN
4	D	201	GLN
6	F	13	ASN
6	F	73	ASN
7	G	11	GLN
7	G	84	ASN
7	G	86	GLN
7	G	97	GLN
8	H	82	HIS
9	I	58	HIS
10	J	56	HIS
10	J	78	ASN
11	K	13	GLN
11	K	117	ASN
13	M	62	ASN
19	S	53	ASN
19	S	69	HIS
19	S	83	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	394 (26%)	107 (7%)
24	Y	20/42 (47%)	8 (40%)	2 (10%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	Z	76/77 (98%)	51 (67%)	9 (11%)
All	All	1602/1641 (97%)	453 (28%)	118 (7%)

All (453) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	16	A
1	A	18	C
1	A	22	G
1	A	26	A
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	54	C
1	A	60	A
1	A	61	G
1	A	76	C
1	A	77	G
1	A	79	G
1	A	81	U
1	A	82	U
1	A	91	C
1	A	97	G
1	A	100	C
1	A	108	G
1	A	115	G
1	A	116	A
1	A	120	A
1	A	121	C
1	A	122	G
1	A	127	G

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Mol	Chain	Res	Type
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	155	C
1	A	163	C
1	A	171	A
1	A	181	G
1	A	182	U
1	A	189(E)	U
1	A	189(F)	U
1	A	189(G)	G
1	A	189(H)	G
1	A	195	A
1	A	197	A
1	A	198	G
1	A	199	G
1	A	201	C
1	A	203	U
1	A	204	U
1	A	217	C
1	A	243	A
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
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	298	A
1	A	301	G
1	A	306	G
1	A	307	C

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Mol	Chain	Res	Type
1	A	315	A
1	A	316	G
1	A	321	A
1	A	324	G
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	344	A
1	A	345	C
1	A	347	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	366	C
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	378	G
1	A	384	G
1	A	386	C
1	A	392	G
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	415	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	442	C
1	A	448	A
1	A	450	G

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Mol	Chain	Res	Type
1	A	452	A
1	A	470	C
1	A	473	G
1	A	481	G
1	A	482	A
1	A	484	G
1	A	485	G
1	A	495	A
1	A	496	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	521	G
1	A	524	G
1	A	525	C
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	545	C
1	A	547	A
1	A	550	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	574	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	587	G
1	A	588	G
1	A	596	C
1	A	639	G

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Mol	Chain	Res	Type
1	A	642	A
1	A	653	A
1	A	661	G
1	A	665	A
1	A	671	G
1	A	672	U
1	A	686	U
1	A	687	A
1	A	688	G
1	A	693	G
1	A	694	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	717	C
1	A	721	G
1	A	723	U
1	A	731	G
1	A	733	A
1	A	734	G
1	A	748	C
1	A	749	C
1	A	755	G
1	A	759	A
1	A	774	G
1	A	777	A
1	A	785	G
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	804	U
1	A	812	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	820	U
1	A	821	G
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U

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Mol	Chain	Res	Type
1	A	853	G
1	A	855	G
1	A	864	A
1	A	865	A
1	A	873	A
1	A	874	G
1	A	876	G
1	A	882	C
1	A	884	U
1	A	885	G
1	A	889	A
1	A	891	U
1	A	900	A
1	A	902	G
1	A	911	U
1	A	913	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	931	C
1	A	932	C
1	A	933	G
1	A	934	C
1	A	935	A
1	A	950	U
1	A	951	G
1	A	954	G
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	982	U
1	A	986	A
1	A	991	U

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Mol	Chain	Res	Type
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1001	A
1	A	1014	A
1	A	1023	G
1	A	1025	U
1	A	1026	G
1	A	1028	C
1	A	1029	C
1	A	1030	C
1	A	1031	G
1	A	1045	C
1	A	1046	A
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1056	U
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1067	A
1	A	1068	G
1	A	1070	U
1	A	1076	C
1	A	1078	U
1	A	1084	G
1	A	1085	U
1	A	1089	G
1	A	1094	G
1	A	1095	U
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

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Mol	Chain	Res	Type
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	1140	C
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1218	C
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1236	A
1	A	1238	A
1	A	1248	A
1	A	1249	C
1	A	1250	A
1	A	1253	G
1	A	1257	U
1	A	1258	G
1	A	1260	C

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Mol	Chain	Res	Type
1	A	1270	C
1	A	1277	C
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1316	G
1	A	1317	C
1	A	1318	A
1	A	1319	A
1	A	1321	C
1	A	1322	C
1	A	1324	A
1	A	1332	A
1	A	1335	C
1	A	1336	C
1	A	1340	A
1	A	1345	U
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1360	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	1381	U
1	A	1394	A
1	A	1398	A
1	A	1402	C
1	A	1433	A

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Mol	Chain	Res	Type
1	A	1442	G
1	A	1442(A)	G
1	A	1443	G
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1475	G
1	A	1477	C
1	A	1492	A
1	A	1494	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1535	C
24	Y	28	A
24	Y	30	G
24	Y	31	U
24	Y	33	A
24	Y	34	A
24	Y	36	A
24	Y	38	G
24	Y	39	U
25	Z	4	G
25	Z	5	G
25	Z	6	G
25	Z	9	G
25	Z	10	G
25	Z	13	C
25	Z	14	A
25	Z	15	G
25	Z	16	C
25	Z	17	C
25	Z	17(A)	U
25	Z	18	G

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Mol	Chain	Res	Type
25	Z	19	G
25	Z	20	U
25	Z	21	A
25	Z	22	G
25	Z	27	U
25	Z	31	G
25	Z	33	U
25	Z	34	C
25	Z	35	A
25	Z	36	U
25	Z	37	A
25	Z	38	A
25	Z	39	C
25	Z	40	C
25	Z	41	C
25	Z	42	G
25	Z	43	A
25	Z	44	A
25	Z	45	G
25	Z	46	G7M
25	Z	47	U
25	Z	48	C
25	Z	49	G
25	Z	53	G
25	Z	55	PSU
25	Z	56	C
25	Z	58	A
25	Z	59	A
25	Z	60	U
25	Z	61	C
25	Z	63	G
25	Z	65	C
25	Z	66	C
25	Z	67	C
25	Z	68	C
25	Z	70	G
25	Z	73	A
25	Z	75	C
25	Z	76	A

All (118) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	48	C
1	A	49	U
1	A	51	A
1	A	60	A
1	A	73	G
1	A	81	U
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	157	G
1	A	181	G
1	A	197	A
1	A	202	U
1	A	243	A
1	A	250	A
1	A	266	G
1	A	279	A
1	A	281	G
1	A	328	C
1	A	329	A
1	A	344	A
1	A	351	G
1	A	366	C
1	A	372	C
1	A	421	U
1	A	422	C
1	A	428	G
1	A	429	U
1	A	481	G
1	A	484	G
1	A	495	A
1	A	496	A
1	A	509	A
1	A	518	C
1	A	532	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	576	G
1	A	587	G
1	A	641	U

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Mol	Chain	Res	Type
1	A	687	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	717	C
1	A	748	C
1	A	792	A
1	A	809	G
1	A	812	C
1	A	840	C
1	A	864	A
1	A	872	A
1	A	884	U
1	A	960	U
1	A	965	A
1	A	974	A
1	A	975	A
1	A	982	U
1	A	988	G
1	A	992	U
1	A	993	G
1	A	1000	U
1	A	1001	A
1	A	1032	G
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1101	A
1	A	1139	G
1	A	1145	C
1	A	1151	A
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1226	C
1	A	1227	A
1	A	1239	A

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Mol	Chain	Res	Type
1	A	1257	U
1	A	1279	A
1	A	1280	A
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1335	C
1	A	1345	U
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1397	C
1	A	1442(B)	A
1	A	1447	A
1	A	1493	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1520	G
1	A	1529	G
1	A	1534	A
24	Y	34	A
24	Y	38	G
25	Z	26	G
25	Z	35	A
25	Z	36	U
25	Z	37	A
25	Z	39	C
25	Z	40	C
25	Z	44	A
25	Z	58	A
25	Z	60	U

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	5MU	Z	54	25	19,22,23	1.57	4 (21%)	28,32,35	1.79	8 (28%)
25	4SU	Z	8	25	18,21,22	1.69	4 (22%)	26,30,33	2.22	8 (30%)
25	G7M	Z	46	25	20,26,27	2.86	4 (20%)	17,39,42	1.57	3 (17%)
25	OMC	Z	32	25	19,22,23	0.97	2 (10%)	26,31,34	1.22	2 (7%)
25	PSU	Z	55	25	18,21,22	1.45	2 (11%)	22,30,33	2.03	5 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	5MU	Z	54	25	-	0/7/25/26	0/2/2/2
25	4SU	Z	8	25	-	0/7/25/26	0/2/2/2
25	G7M	Z	46	25	-	2/3/25/26	0/3/3/3
25	OMC	Z	32	25	-	0/9/27/28	0/2/2/2
25	PSU	Z	55	25	-	3/7/25/26	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	46	G7M	C8-N9	8.34	1.48	1.33
25	Z	46	G7M	C8-N7	6.99	1.45	1.33
25	Z	46	G7M	C5-C4	5.29	1.49	1.39
25	Z	55	PSU	C6-C5	4.76	1.40	1.35
25	Z	8	4SU	C4-S4	-4.08	1.60	1.68
25	Z	8	4SU	C2-N1	3.60	1.44	1.38
25	Z	54	5MU	C2-N1	3.44	1.44	1.38
25	Z	54	5MU	C6-C5	3.20	1.39	1.34
25	Z	54	5MU	C4-C5	2.89	1.49	1.44
25	Z	8	4SU	C6-C5	2.45	1.40	1.35
25	Z	55	PSU	C4-C5	2.40	1.51	1.44
25	Z	32	OMC	C6-C5	2.36	1.40	1.35
25	Z	8	4SU	C4-N3	-2.19	1.35	1.37
25	Z	54	5MU	C4-N3	-2.12	1.34	1.38
25	Z	46	G7M	C2-N3	2.03	1.38	1.33
25	Z	32	OMC	C2-N1	2.02	1.44	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Z	55	PSU	N1-C2-N3	5.49	121.36	115.13
25	Z	8	4SU	C4-N3-C2	-5.23	122.26	127.34
25	Z	8	4SU	N3-C2-N1	4.70	121.13	114.89
25	Z	8	4SU	C5-C4-N3	4.60	118.95	114.69
25	Z	46	G7M	C3'-C2'-C1'	4.33	107.50	100.98
25	Z	8	4SU	C6-N1-C2	-4.10	115.75	120.99
25	Z	54	5MU	N3-C2-N1	3.95	120.13	114.89
25	Z	55	PSU	O2-C2-N1	-3.86	118.54	122.79
25	Z	55	PSU	C6-C5-C4	-3.50	115.75	118.20
25	Z	54	5MU	C5-C4-N3	3.38	118.20	115.31
25	Z	55	PSU	C4-N3-C2	-3.31	121.57	126.34
25	Z	32	OMC	O2-C2-N3	-3.22	117.09	122.33
25	Z	54	5MU	C4-N3-C2	-3.03	123.44	127.35
25	Z	55	PSU	C3'-C2'-C1'	2.95	105.08	101.64
25	Z	8	4SU	C5-C4-S4	-2.93	120.69	124.47
25	Z	54	5MU	C5M-C5-C4	2.85	121.91	118.77
25	Z	46	G7M	CN7-N7-C8	-2.74	112.25	125.43
25	Z	54	5MU	C6-N1-C2	-2.63	118.63	121.30
25	Z	54	5MU	O4-C4-C5	-2.63	121.86	124.90
25	Z	8	4SU	C1'-N1-C2	2.46	122.02	117.57
25	Z	32	OMC	O4'-C1'-N1	2.32	113.67	108.36
25	Z	8	4SU	C3'-C2'-C1'	2.25	105.70	101.43
25	Z	54	5MU	O2-C2-N3	-2.13	117.53	121.50
25	Z	8	4SU	O2-C2-N3	-2.10	117.58	121.50
25	Z	54	5MU	O4'-C4'-C5'	2.09	116.24	109.37
25	Z	46	G7M	O4'-C4'-C3'	2.07	109.22	105.11

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	Z	46	G7M	O4'-C4'-C5'-O5'
25	Z	46	G7M	C3'-C4'-C5'-O5'
25	Z	55	PSU	O4'-C4'-C5'-O5'
25	Z	55	PSU	C3'-C4'-C5'-O5'
25	Z	55	PSU	O4'-C1'-C5-C4

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	54	5MU	2	0
25	Z	8	4SU	1	0
25	Z	46	G7M	4	0
25	Z	55	PSU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 66 ligands modelled in this entry, 66 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6

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	4.82
1	A	93:G	O3'	96:U	P	4.82
1	A	841:U	O3'	848:C	P	4.25
1	A	204:U	O3'	216:G	P	3.81
1	A	1442(A):G	O3'	1442(B):A	P	3.32

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	927:G	O3'	928:G	P	3.10

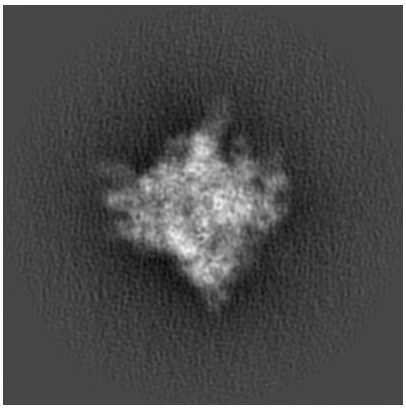
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4076. These allow visual inspection of the internal detail of the map and identification of artifacts.

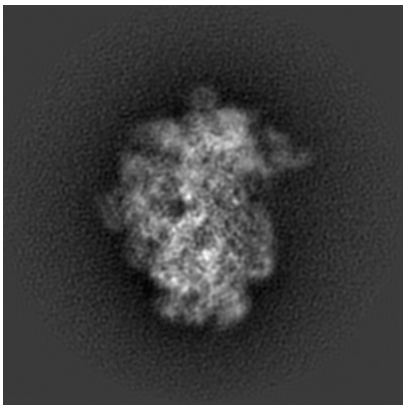
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

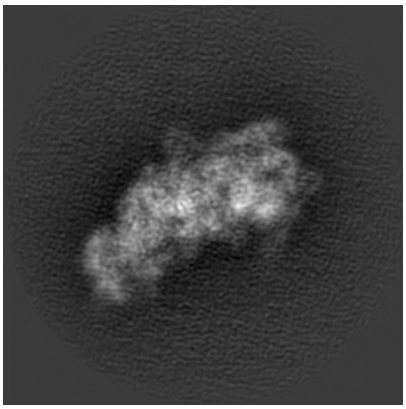
6.1.1 Primary map



X

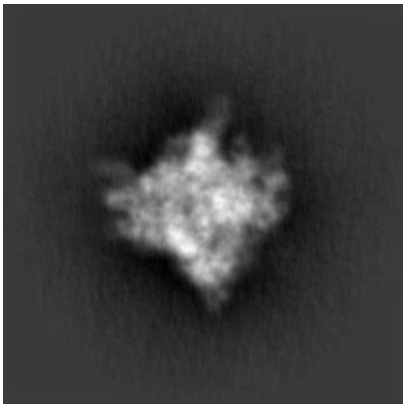


Y

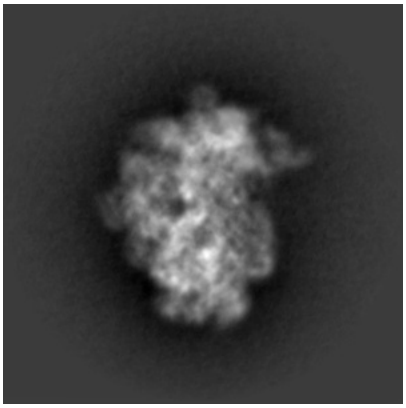


Z

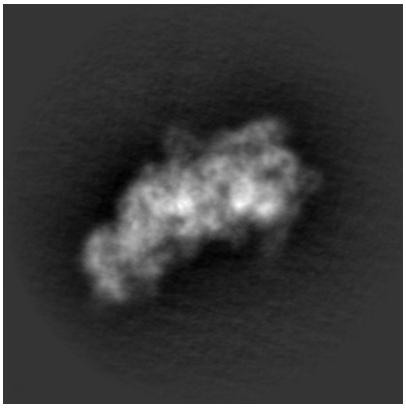
6.1.2 Raw map



X



Y

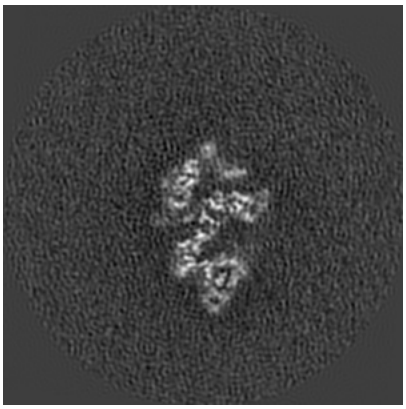


Z

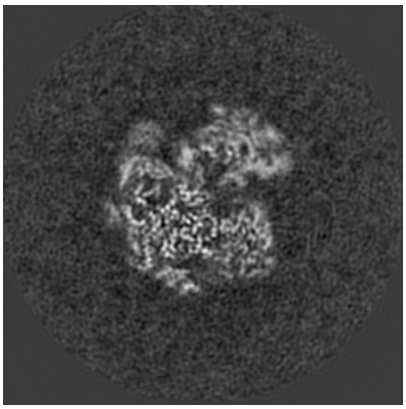
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

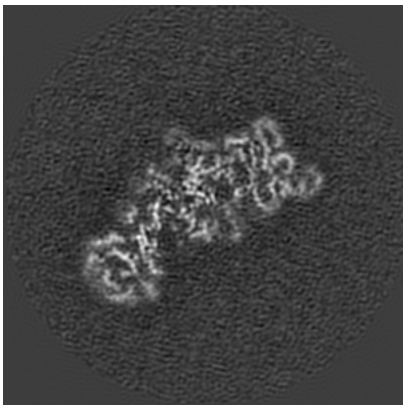
6.2.1 Primary map



X Index: 130

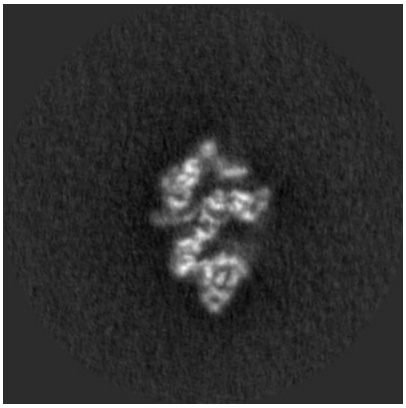


Y Index: 130

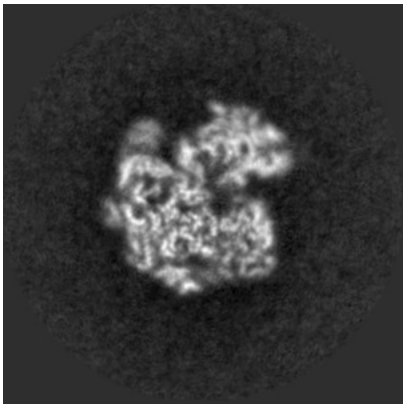


Z Index: 130

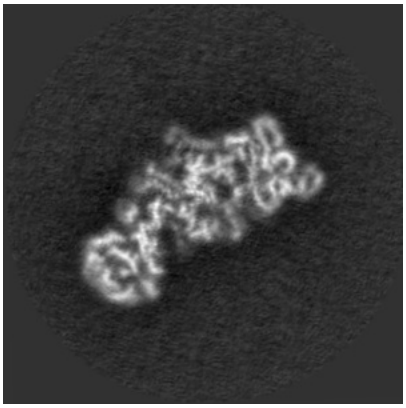
6.2.2 Raw map



X Index: 130



Y Index: 130

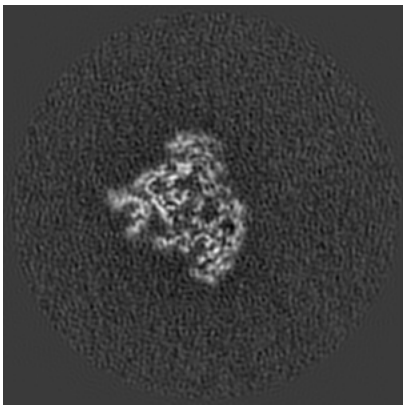


Z Index: 130

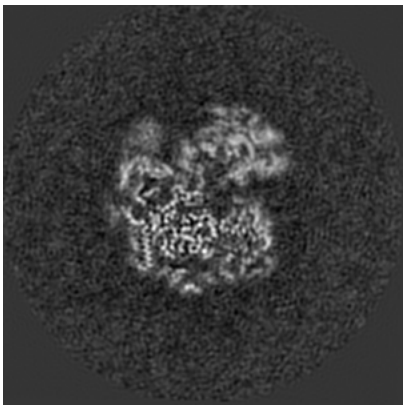
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

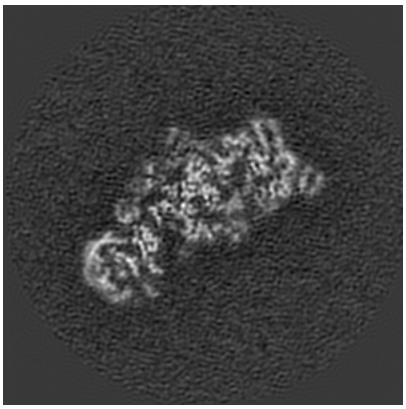
6.3.1 Primary map



X Index: 95

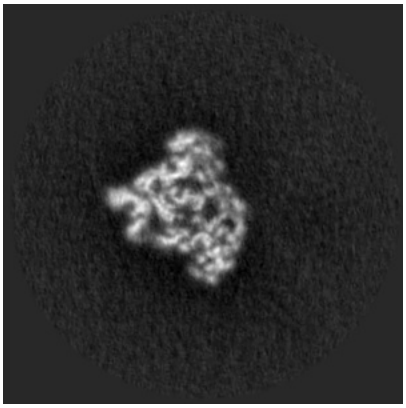


Y Index: 129

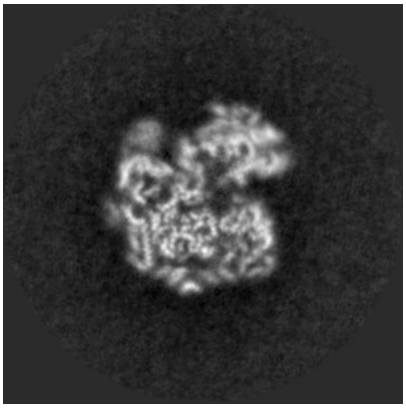


Z Index: 128

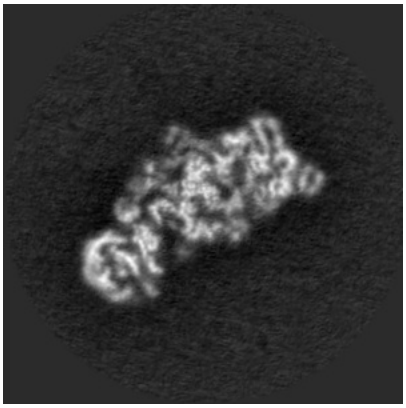
6.3.2 Raw map



X Index: 96



Y Index: 129



Z Index: 128

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

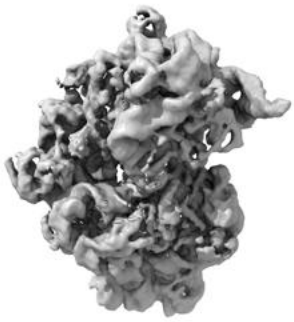
Y

Z

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

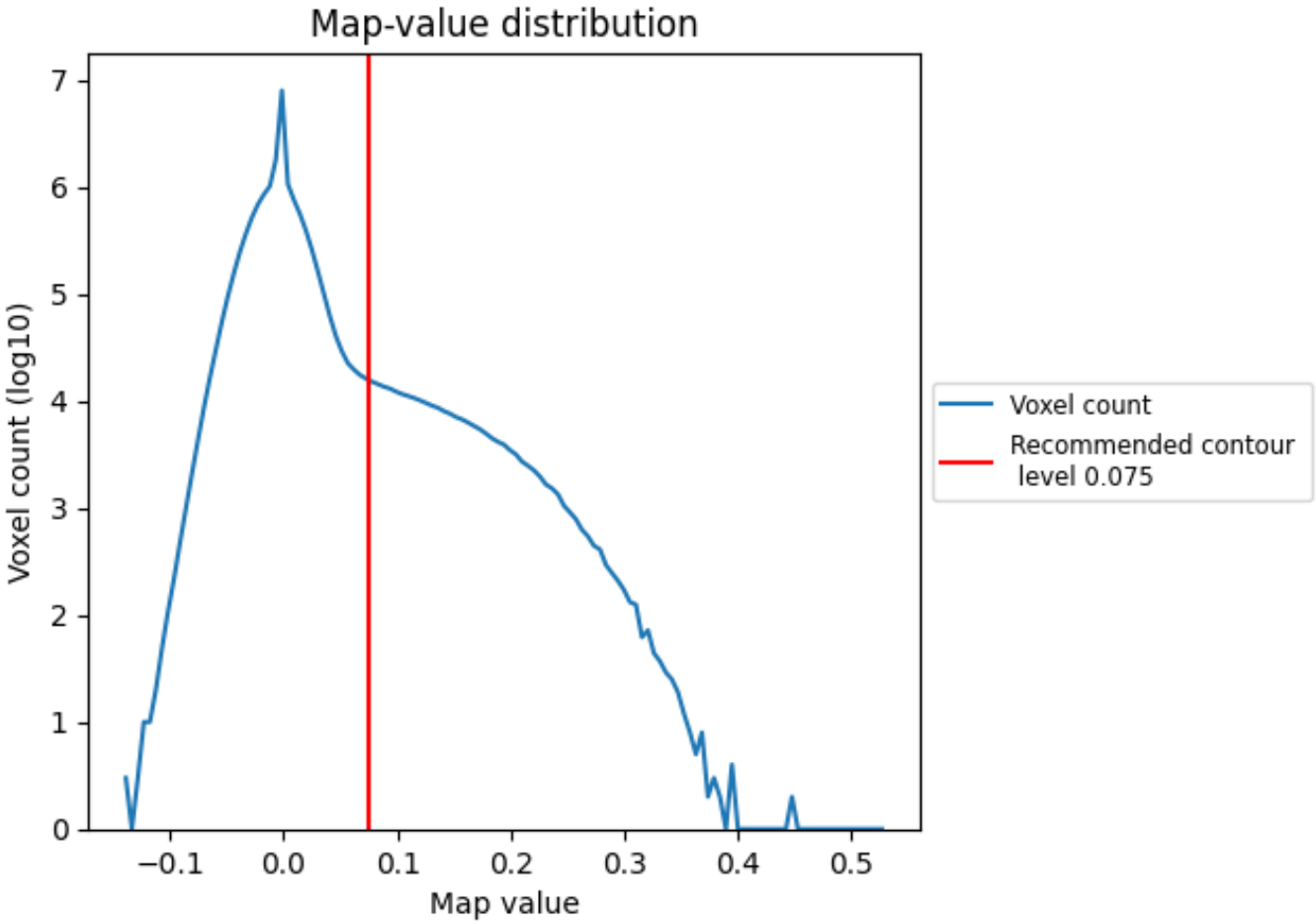
6.5 Mask visualisation (i)

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

7 Map analysis

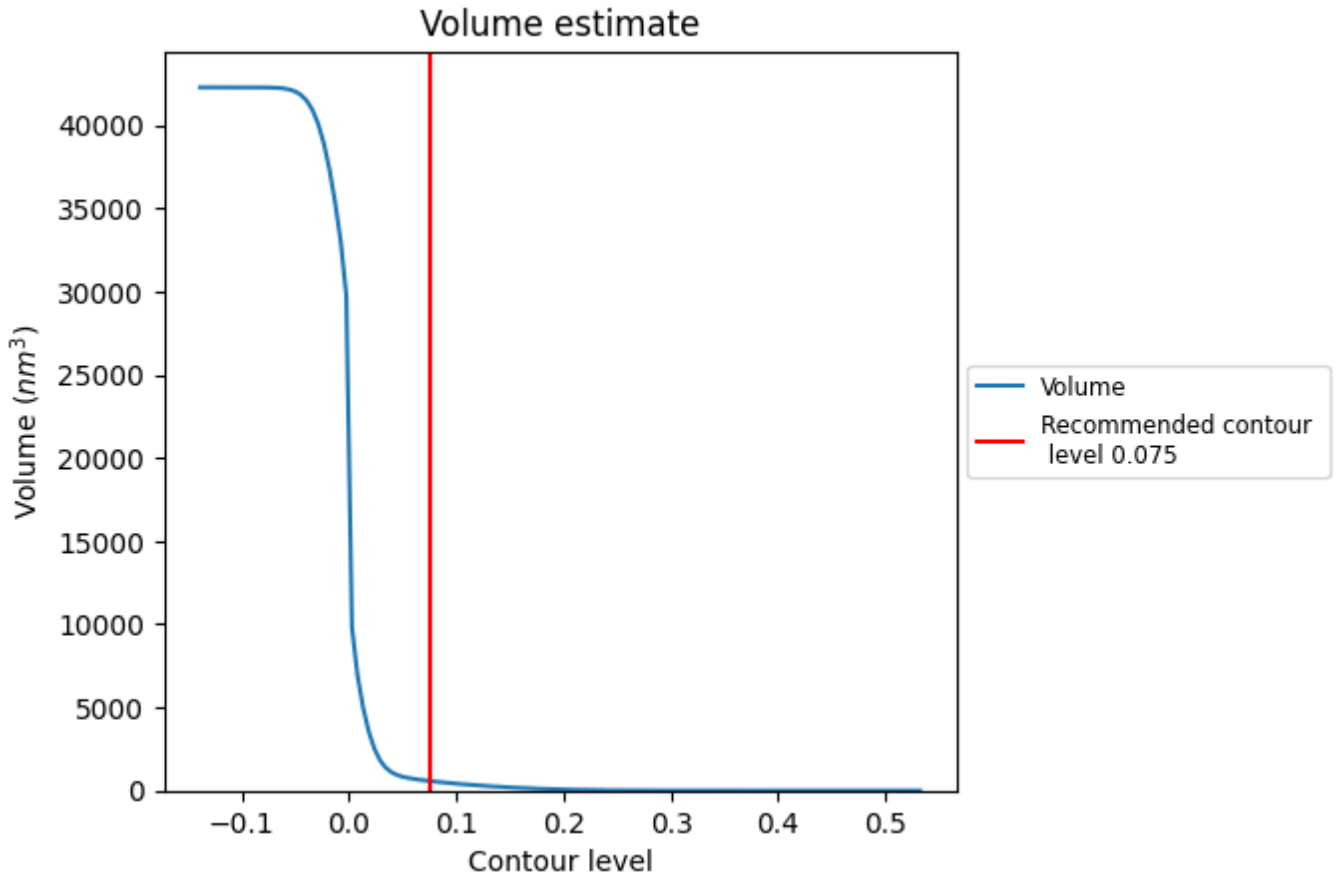
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

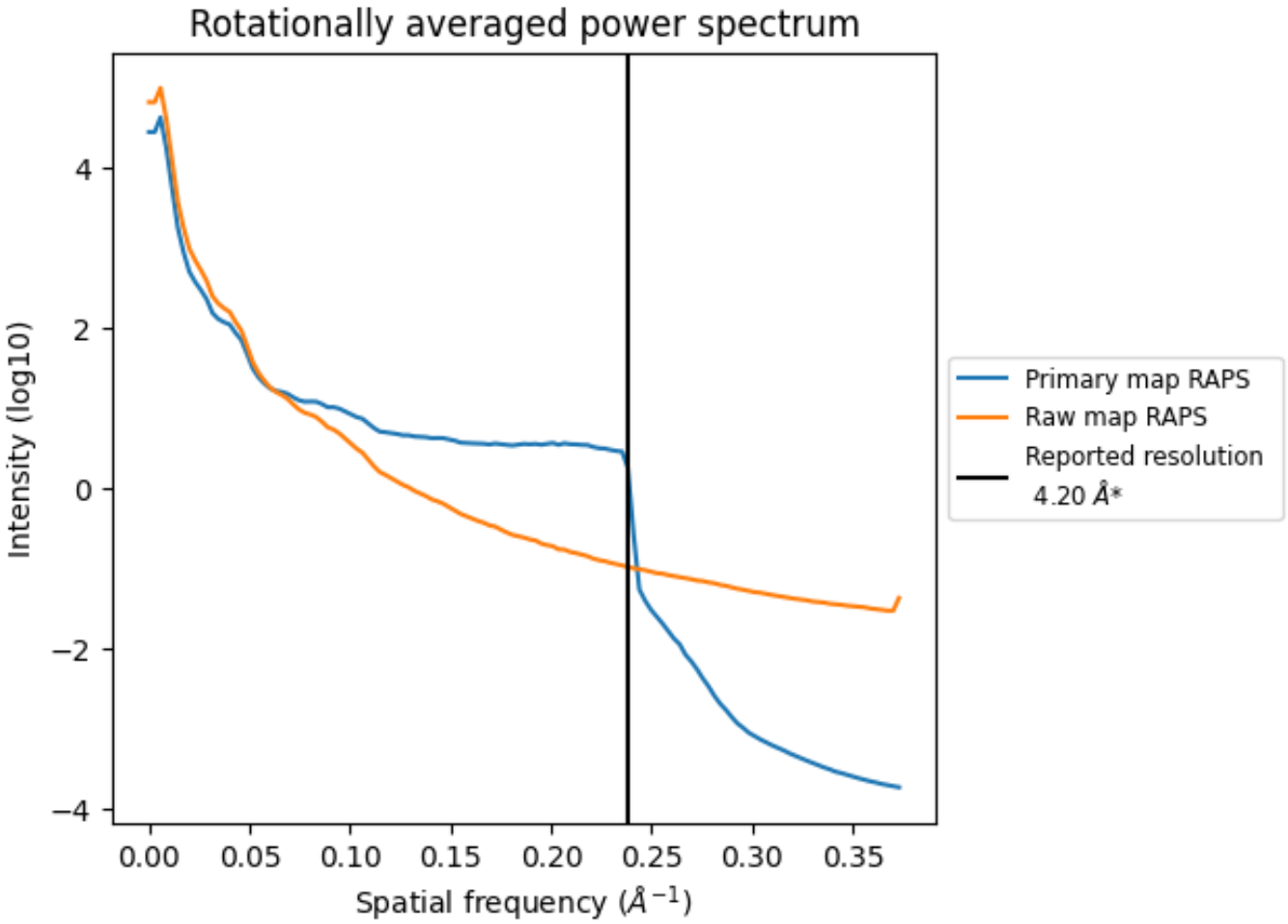
7.2 Volume estimate



The volume at the recommended contour level is 575 nm^3; this corresponds to an approximate mass of 519 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)

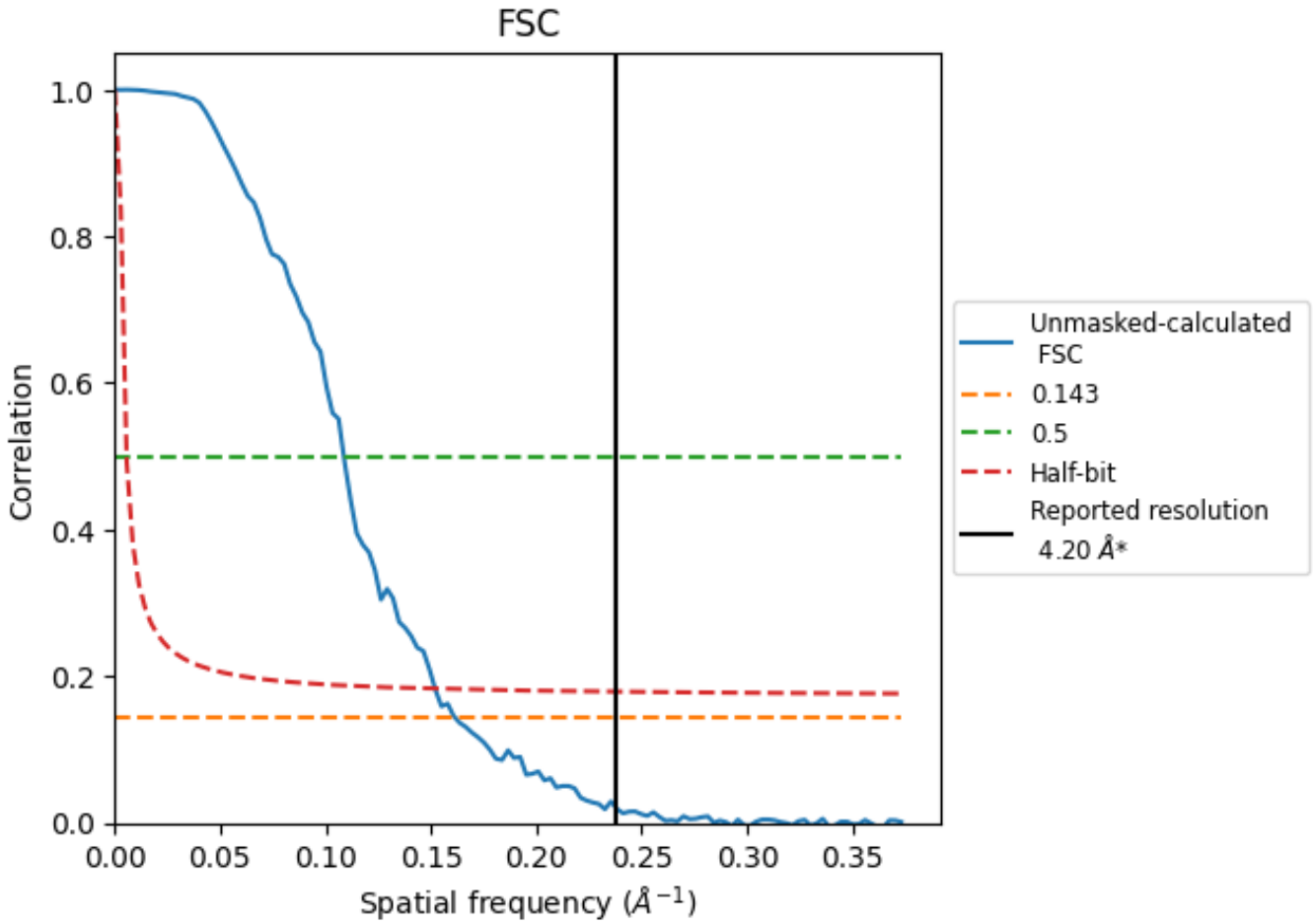


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

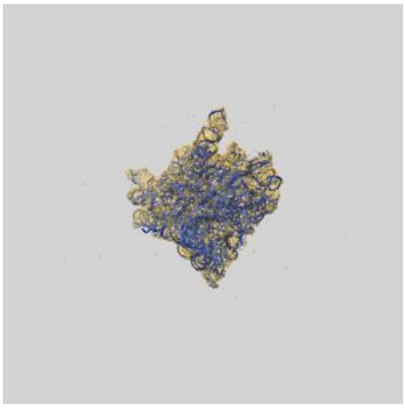
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.19	9.21	6.58

*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 6.19 differs from the reported value 4.2 by more than 10 %

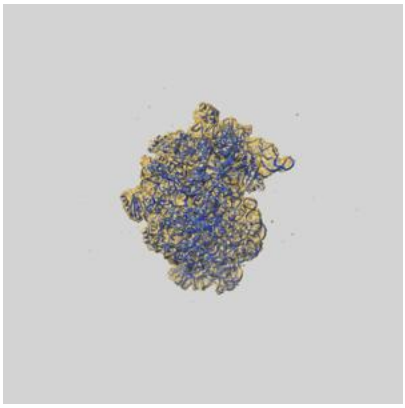
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4076 and PDB model 5LMQ. Per-residue inclusion information can be found in section 3 on page 8.

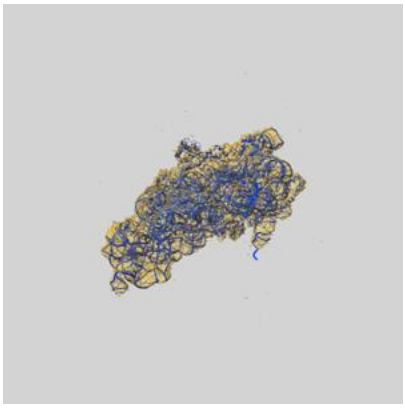
9.1 Map-model overlay



X



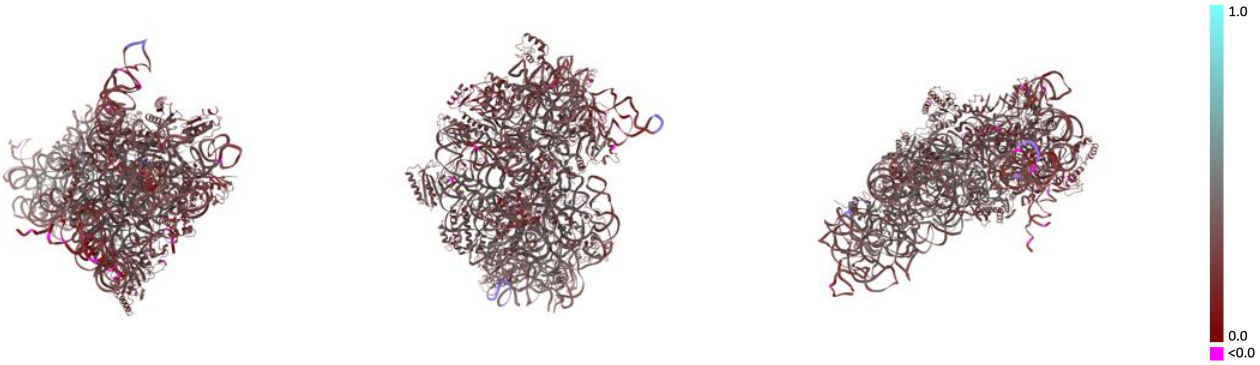
Y



Z

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

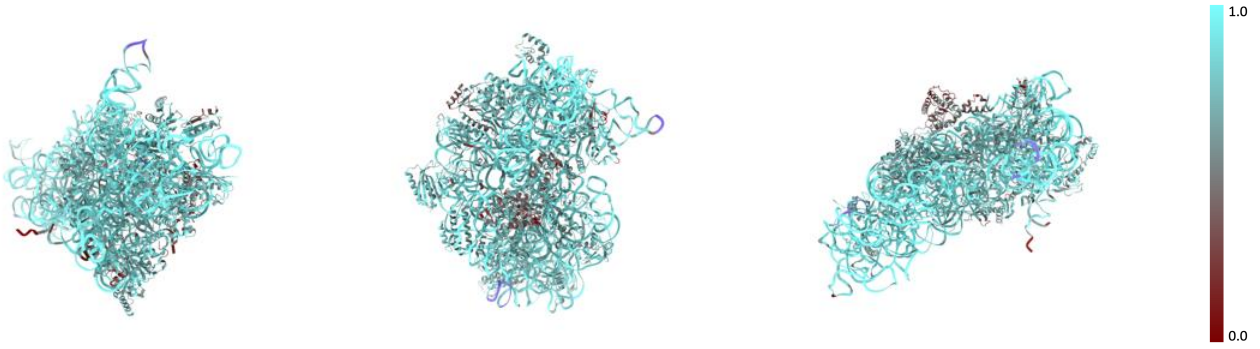
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

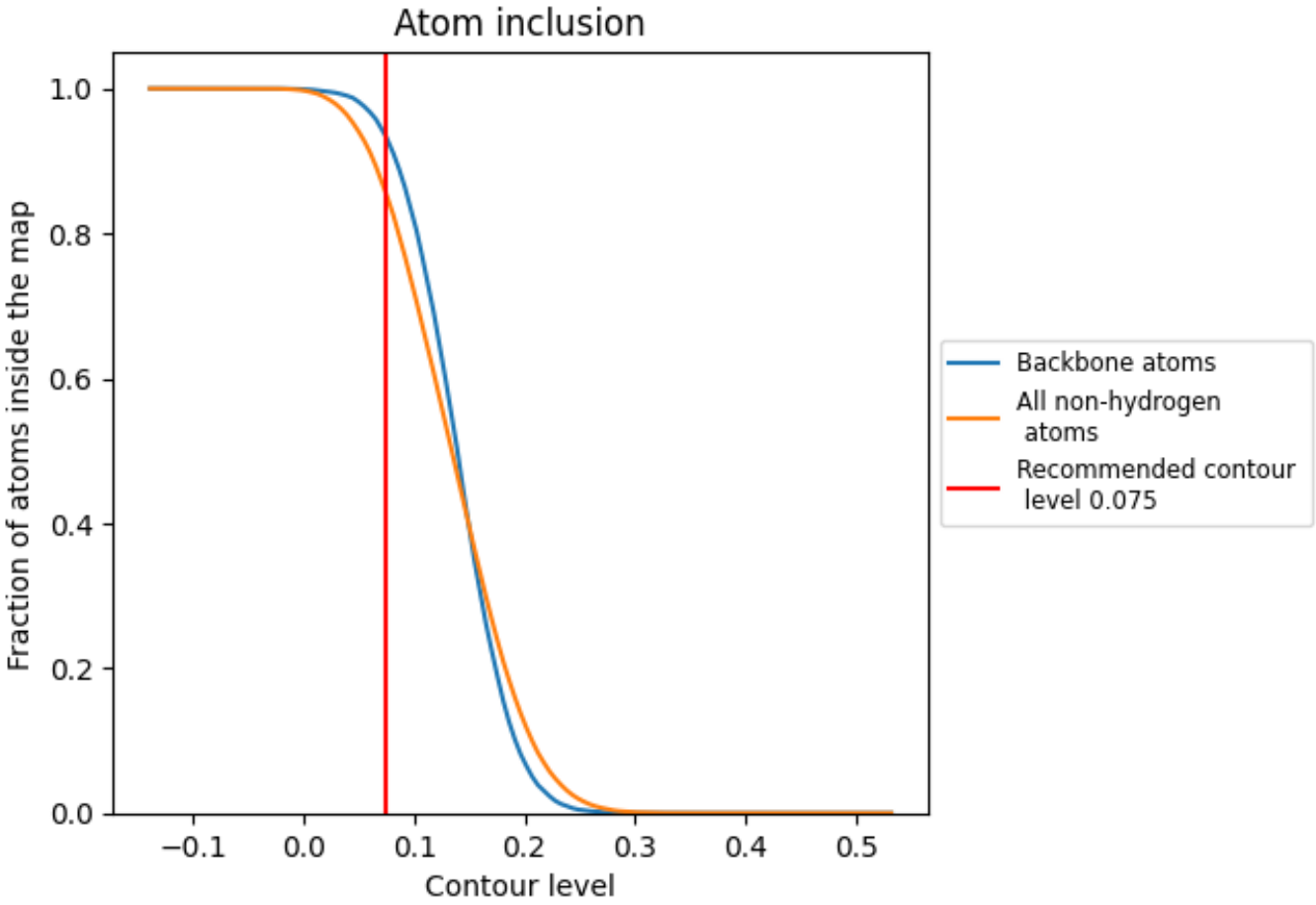
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.075).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8541	0.3260
A	0.9532	0.3410
B	0.3707	0.2650
C	0.7405	0.3250
D	0.7374	0.3160
E	0.7525	0.3670
F	0.7565	0.3170
G	0.7541	0.3120
H	0.7708	0.3670
I	0.7695	0.2990
J	0.6510	0.2930
K	0.7783	0.3420
L	0.7513	0.3830
M	0.6786	0.2580
N	0.7479	0.3250
O	0.7797	0.3380
P	0.8111	0.3620
Q	0.7920	0.3710
R	0.7409	0.3060
S	0.7441	0.2670
T	0.7294	0.2910
V	0.7487	0.2940
W	0.6461	0.3220
X	0.6185	0.2500
Y	0.6754	0.2070
Z	0.8156	0.1910