



## Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:39 am GMT

PDB ID : 5LMV  
EMDB ID : EMD-4083  
Title : Structure of bacterial 30S-IF1-IF2-IF3-mRNA-tRNA translation pre-initiation complex(state-III)  
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.  
Deposited on : 2016-08-01  
Resolution : 4.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

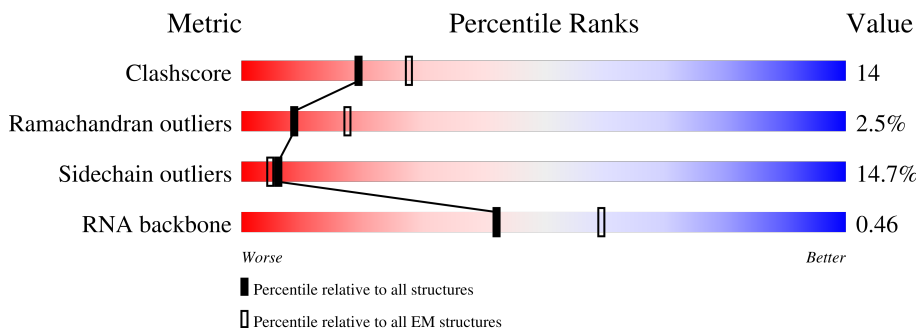
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.90 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.



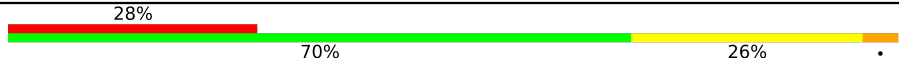

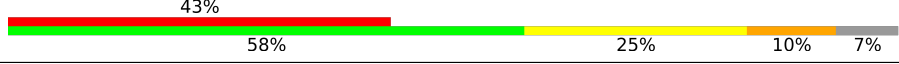
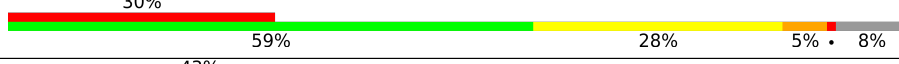

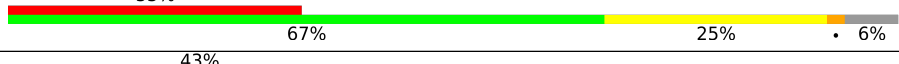


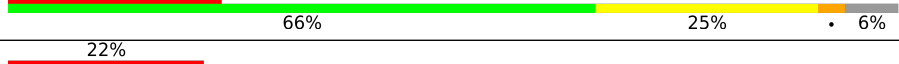


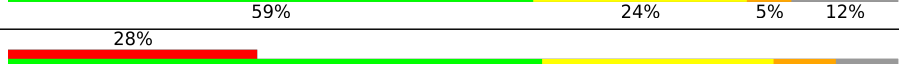



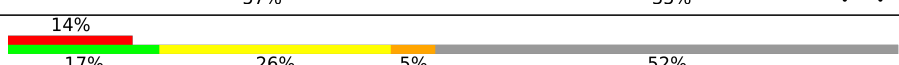
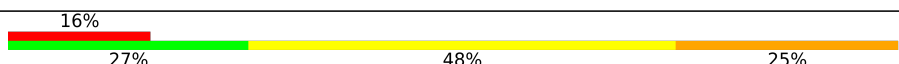


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

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

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Mol	Chain	Length	Quality of chain
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	W	72	
23	X	171	
24	Y	42	
25	Z	77	
26	a	571	

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	-
27	ZN	N	101	-	-	X	-
29	FME	Z	101	-	-	X	-

## 2 Entry composition [i](#)

There are 29 unique types of molecules in this entry. The entry contains 59470 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1515	32548	14490	6022	10523	1513	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	118	937	579	193	163	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	164	Total	C	N	O	S	0	0
			1336	841	245	241	9		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	20	Total	C	N	O	P	0	0
			439	196	89	134	20		

- Molecule 25 is a RNA chain called tRNAi.

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

- Molecule 26 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	502	Total	C	N	O	S	0	0
			3774	2365	679	718	12		

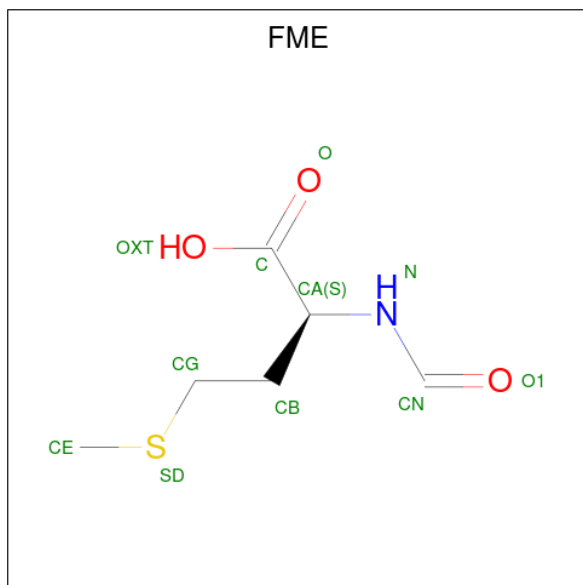
- Molecule 27 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 29 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C<sub>6</sub>H<sub>11</sub>NO<sub>3</sub>S).



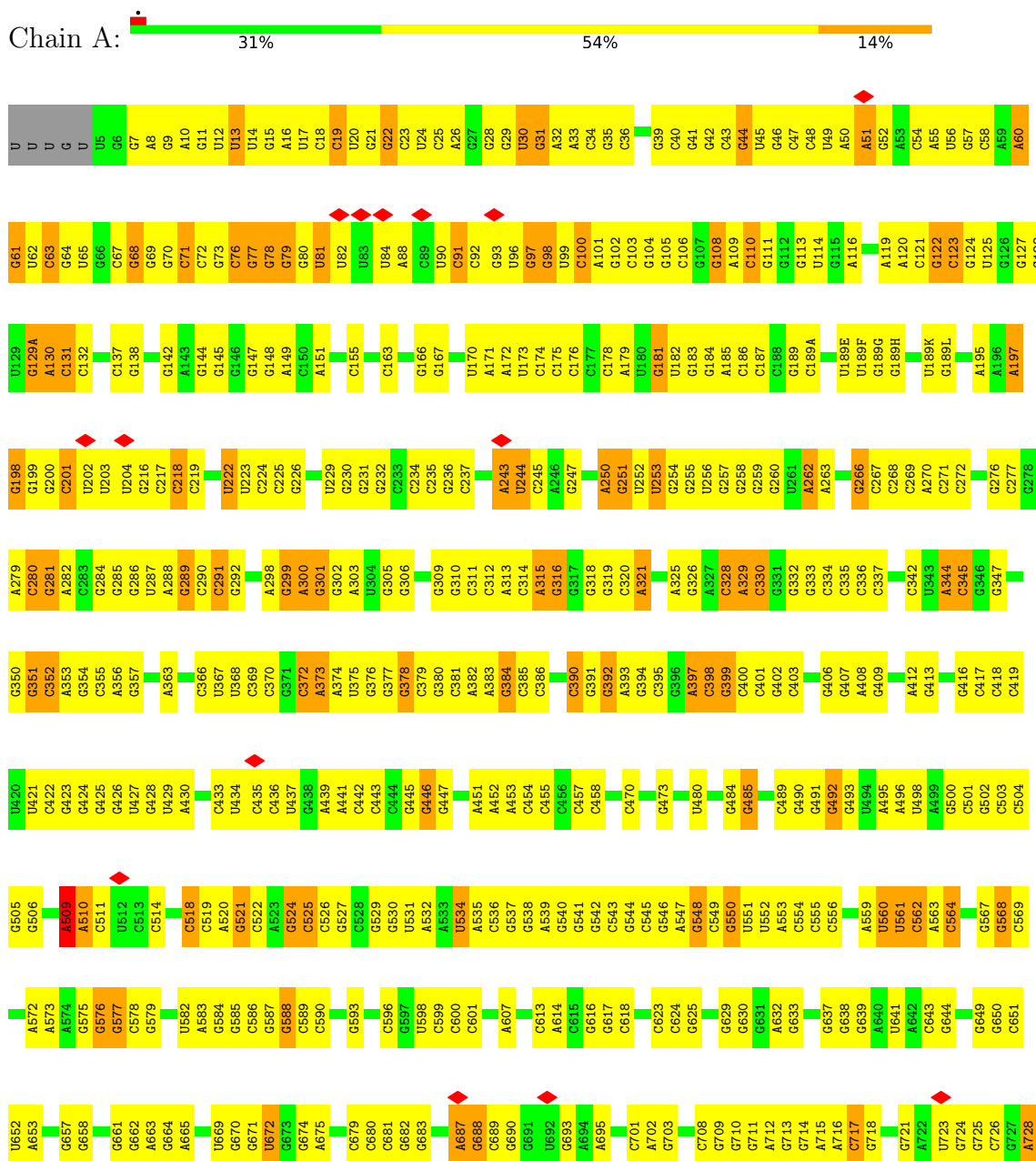
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
29	Z	1	9	6	1	1	1	0

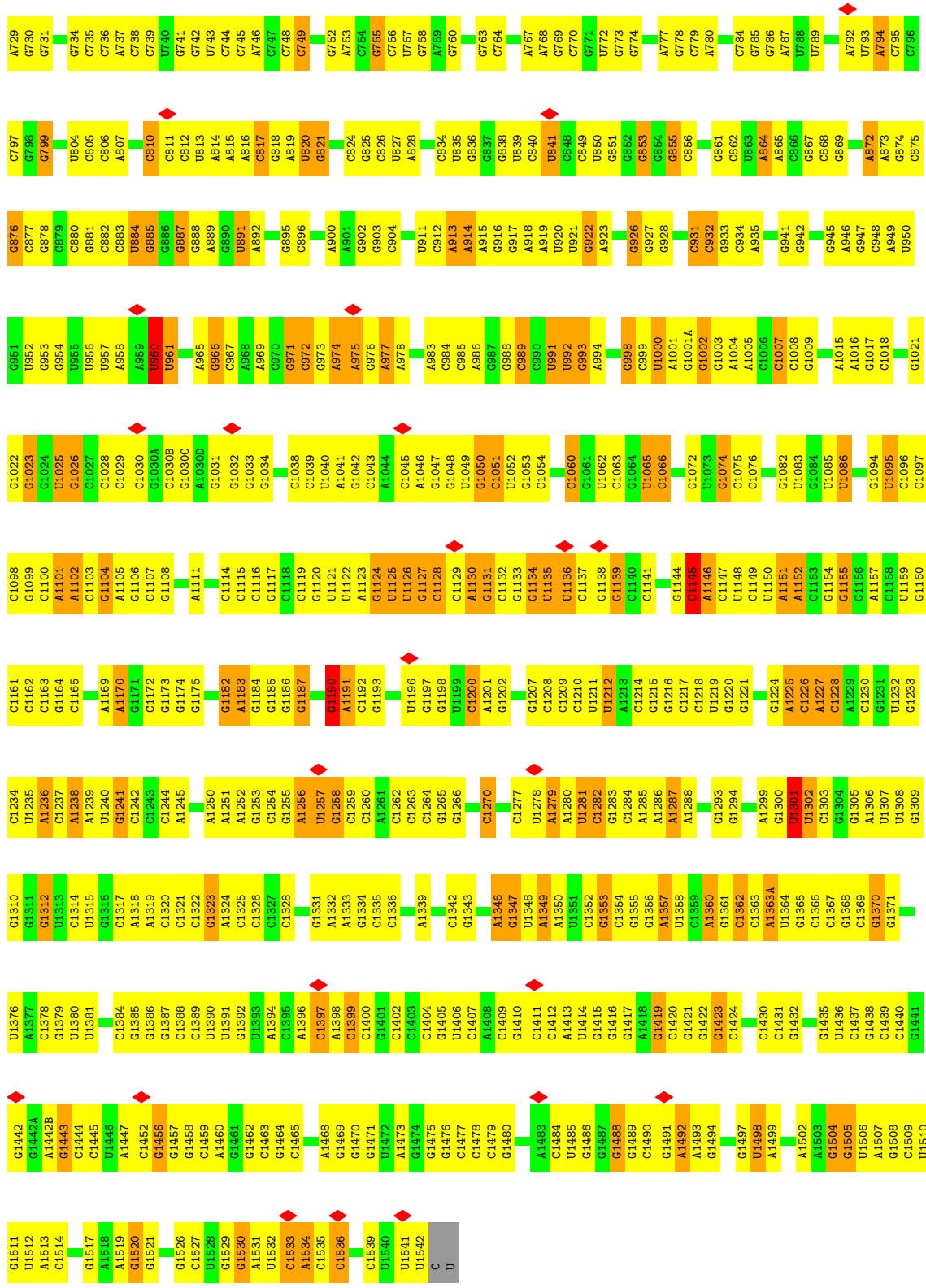


### 3 Residue-property plots

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

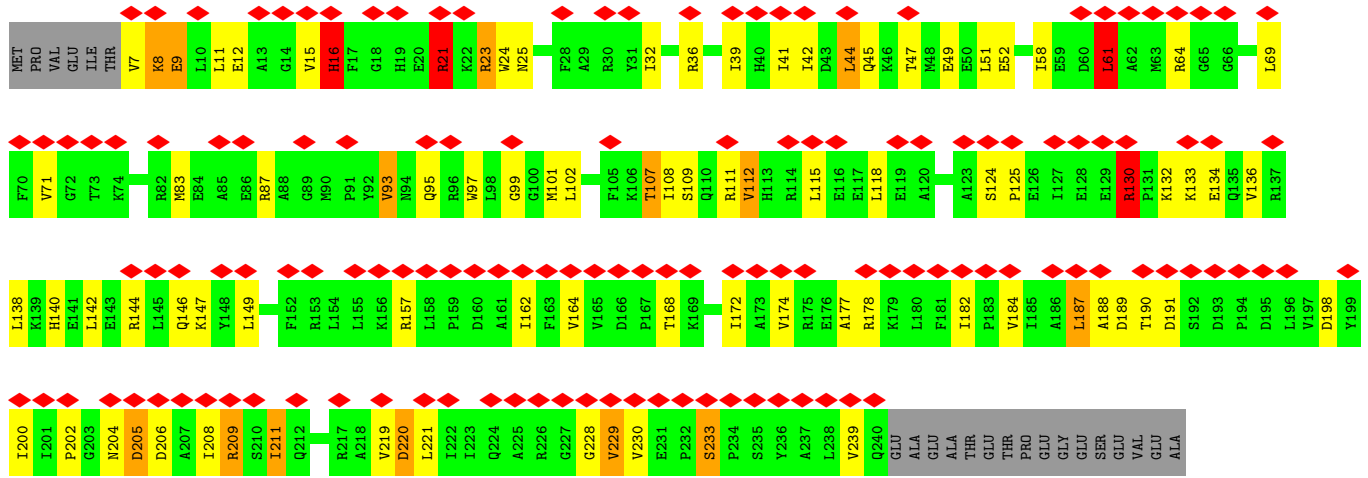
#### • Molecule 1: 16S ribosomal RNA



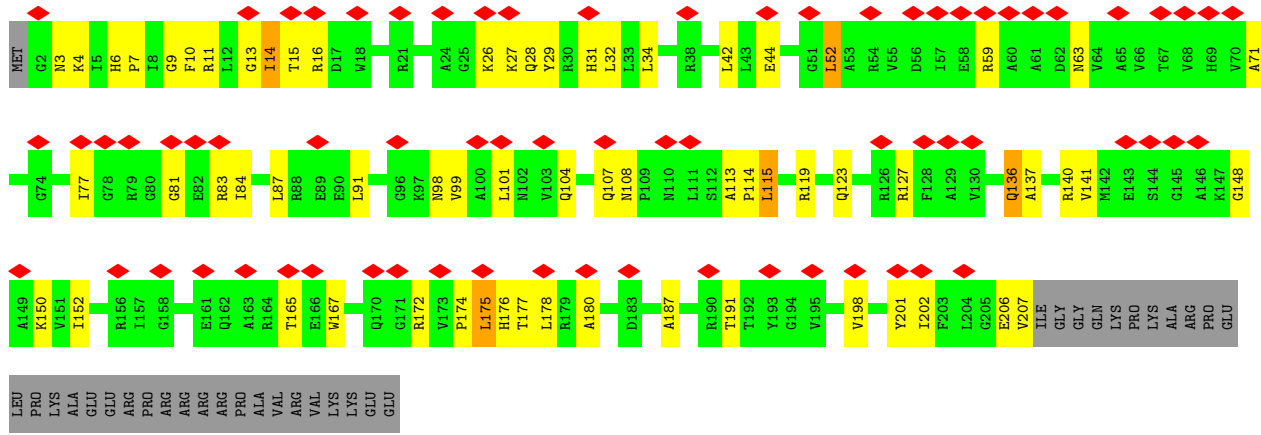


• Molecule 2: 30S ribosomal protein S2

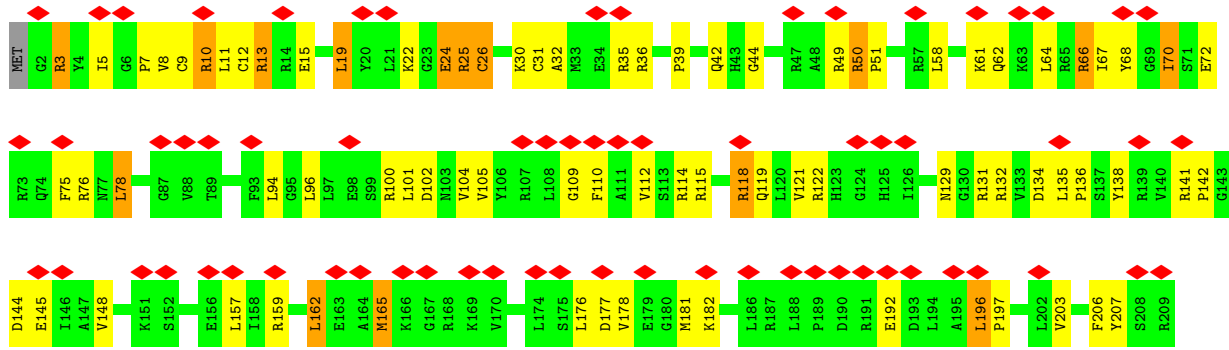




• Molecule 3: 30S ribosomal protein S3

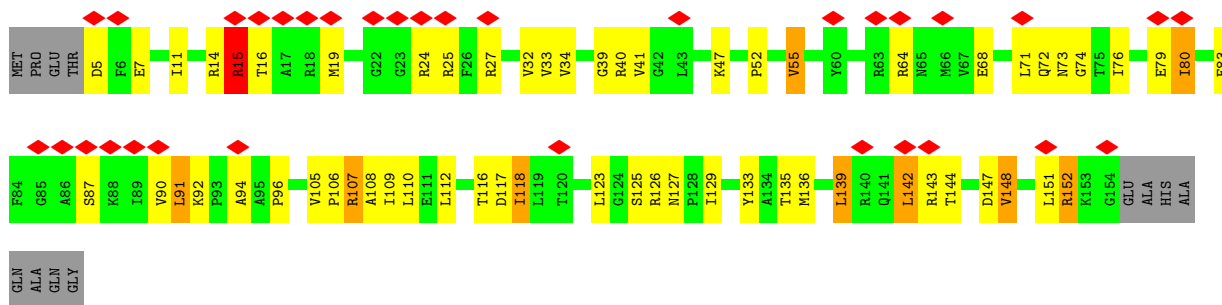


• Molecule 4: 30S ribosomal protein S4

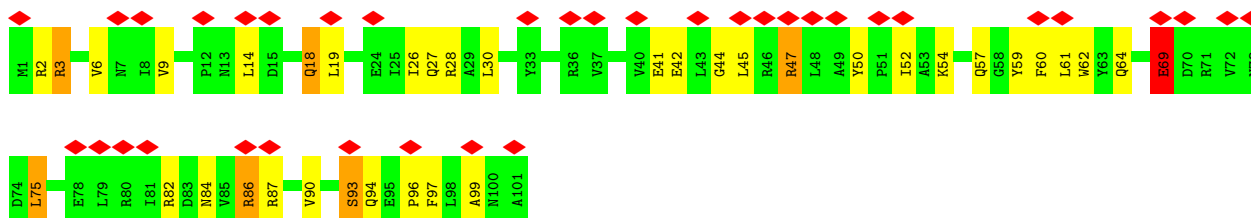


• Molecule 5: 30S ribosomal protein S5

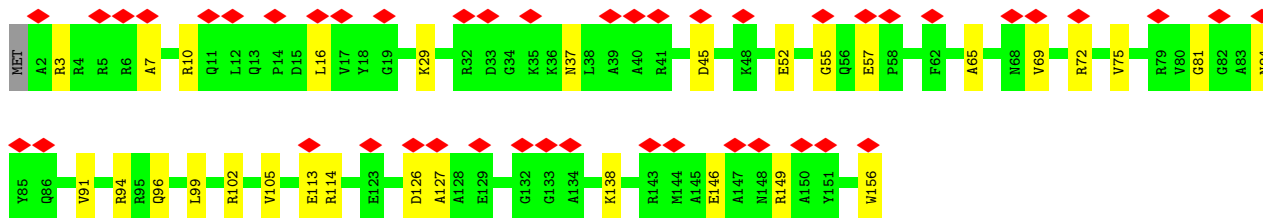
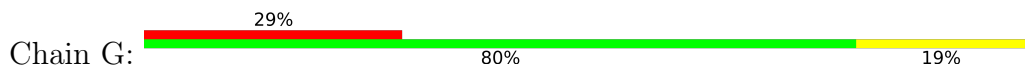




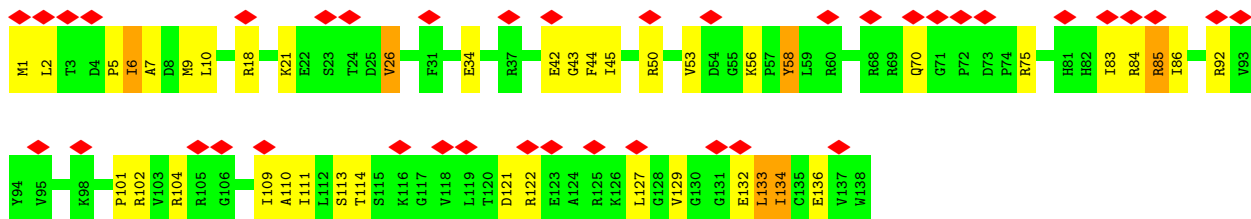
• Molecule 6: 30S ribosomal protein S6



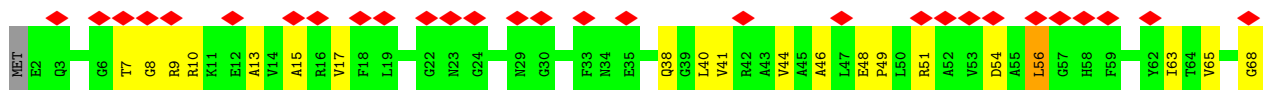
• Molecule 7: 30S ribosomal protein S7

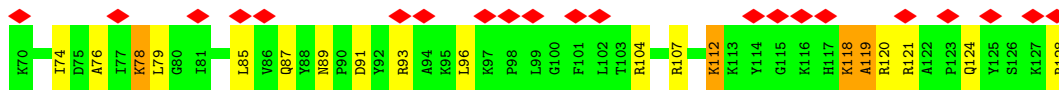


• Molecule 8: 30S ribosomal protein S8

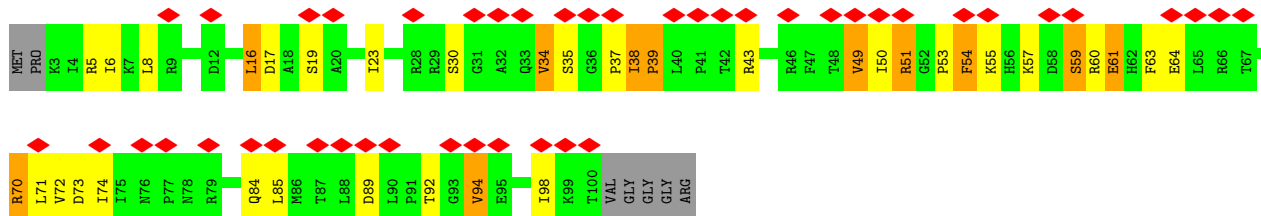
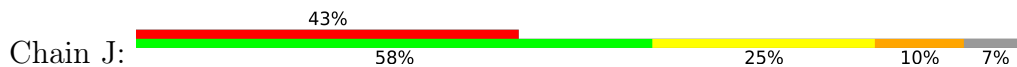


• Molecule 9: 30S ribosomal protein S9

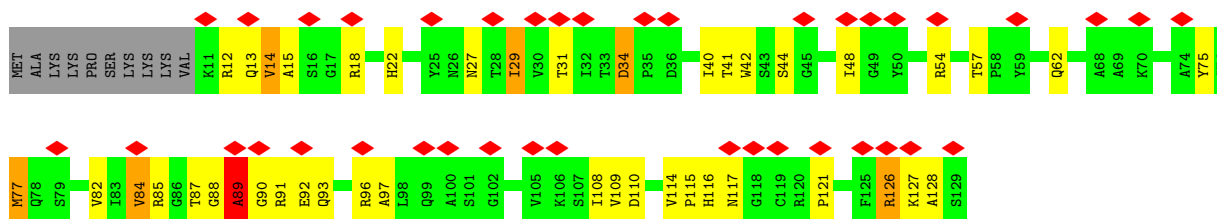




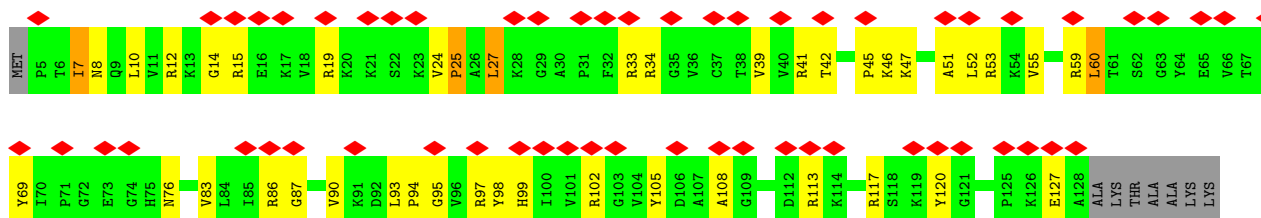
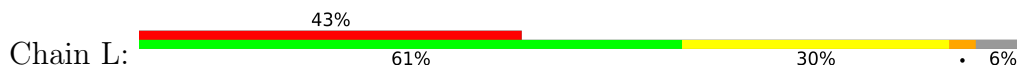
• Molecule 10: 30S ribosomal protein S10



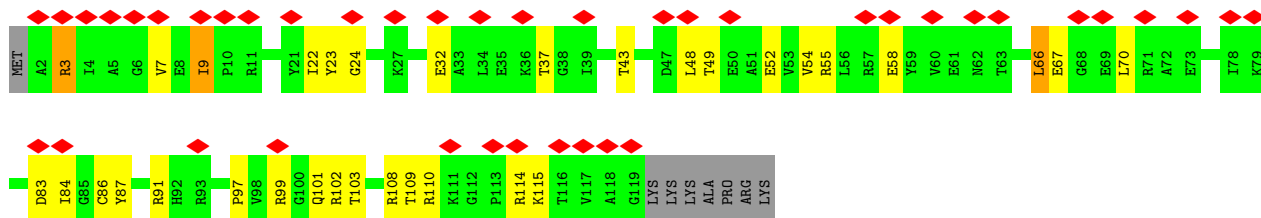
• Molecule 11: 30S ribosomal protein S11



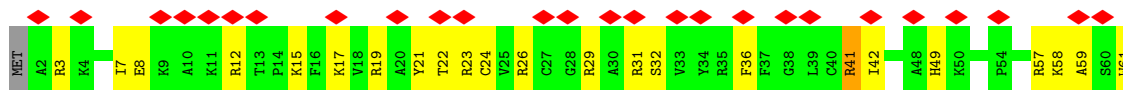
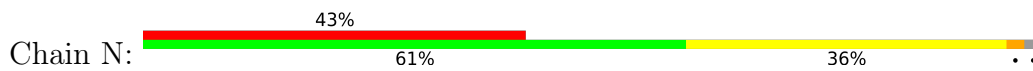
• Molecule 12: 30S ribosomal protein S12



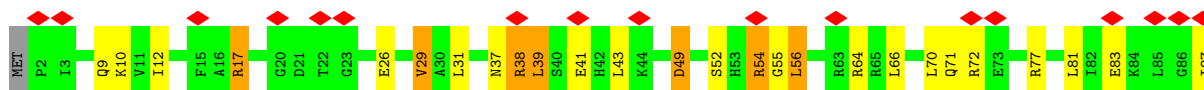
• Molecule 13: 30S ribosomal protein S13



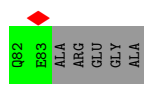
• Molecule 14: 30S ribosomal protein S14 type Z



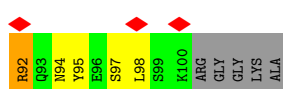
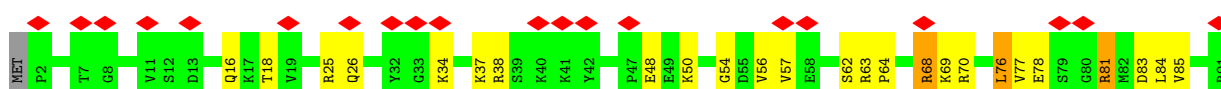
• Molecule 15: 30S ribosomal protein S15



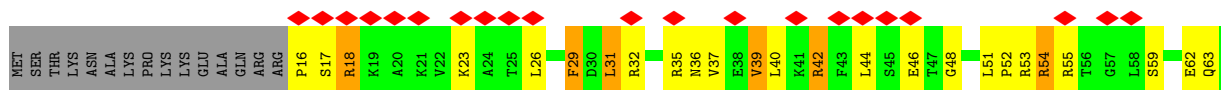
• Molecule 16: 30S ribosomal protein S16



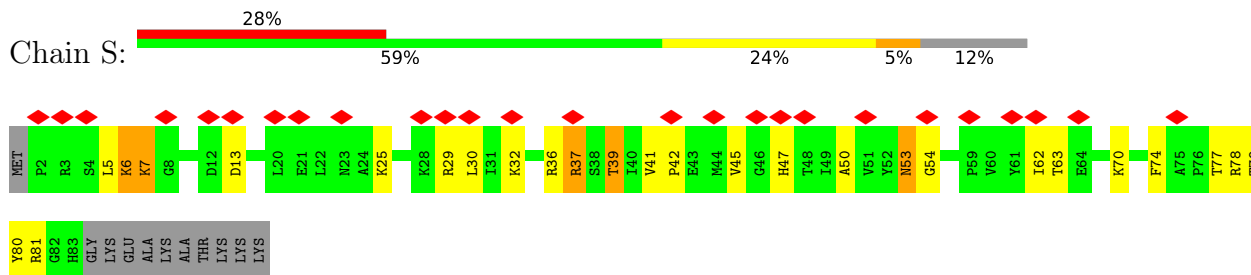
• Molecule 17: 30S ribosomal protein S17



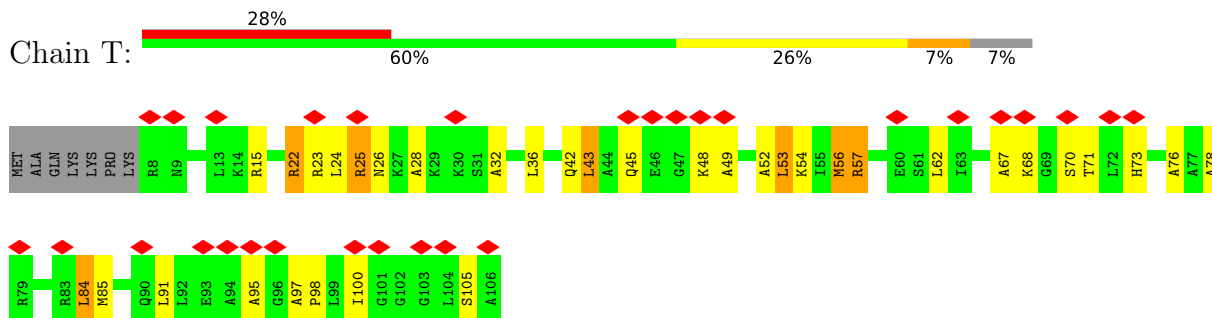
• Molecule 18: 30S ribosomal protein S18



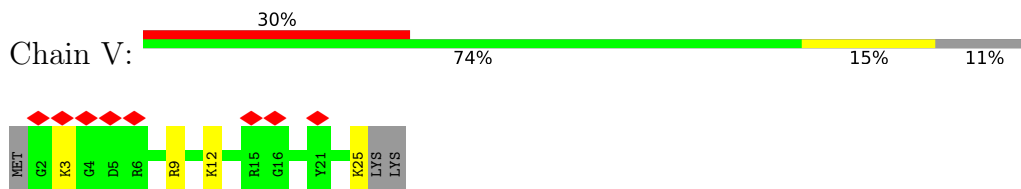
• Molecule 19: 30S ribosomal protein S19



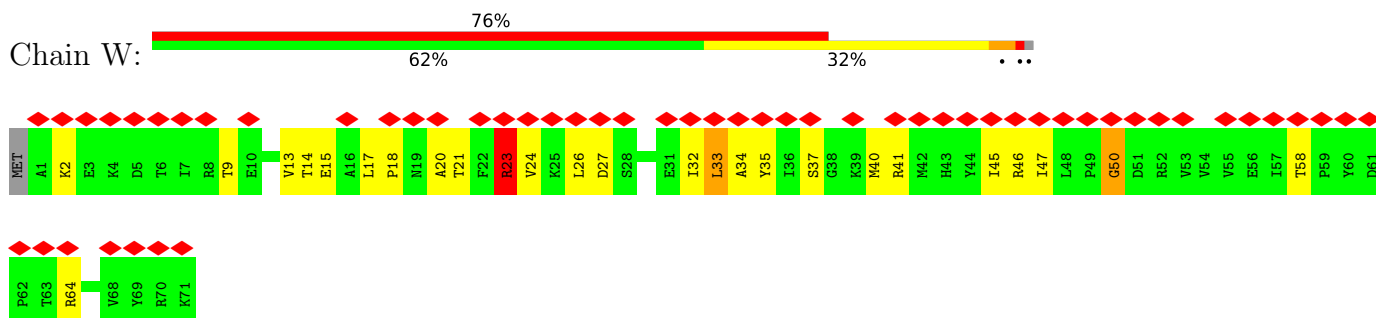
• Molecule 20: 30S ribosomal protein S20



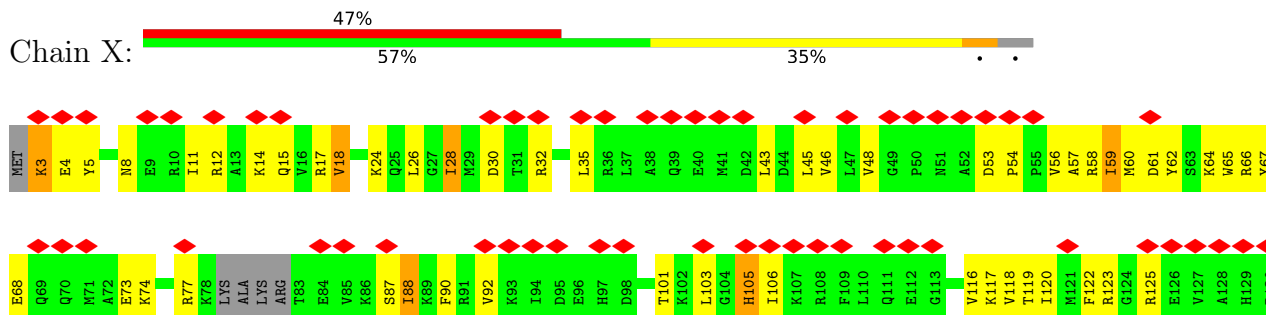
• Molecule 21: 30S ribosomal protein Thx

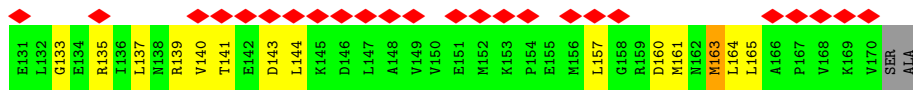


• Molecule 22: Translation initiation factor IF-1

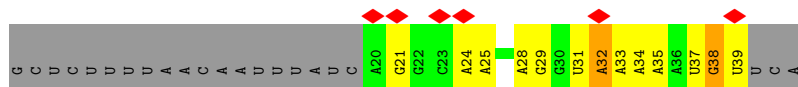
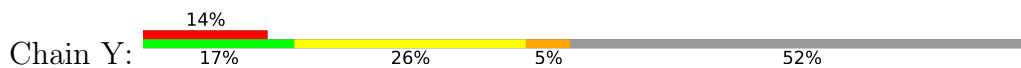


• Molecule 23: Translation initiation factor IF-3

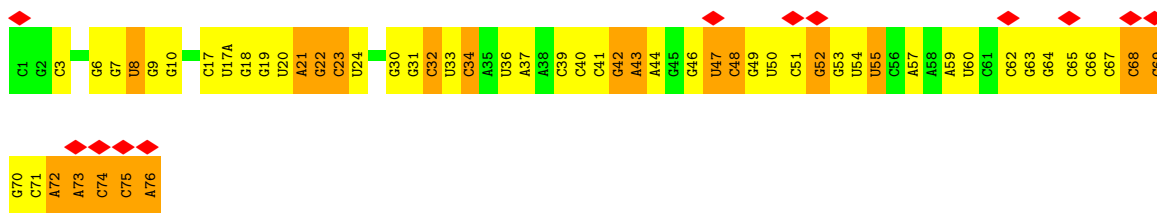




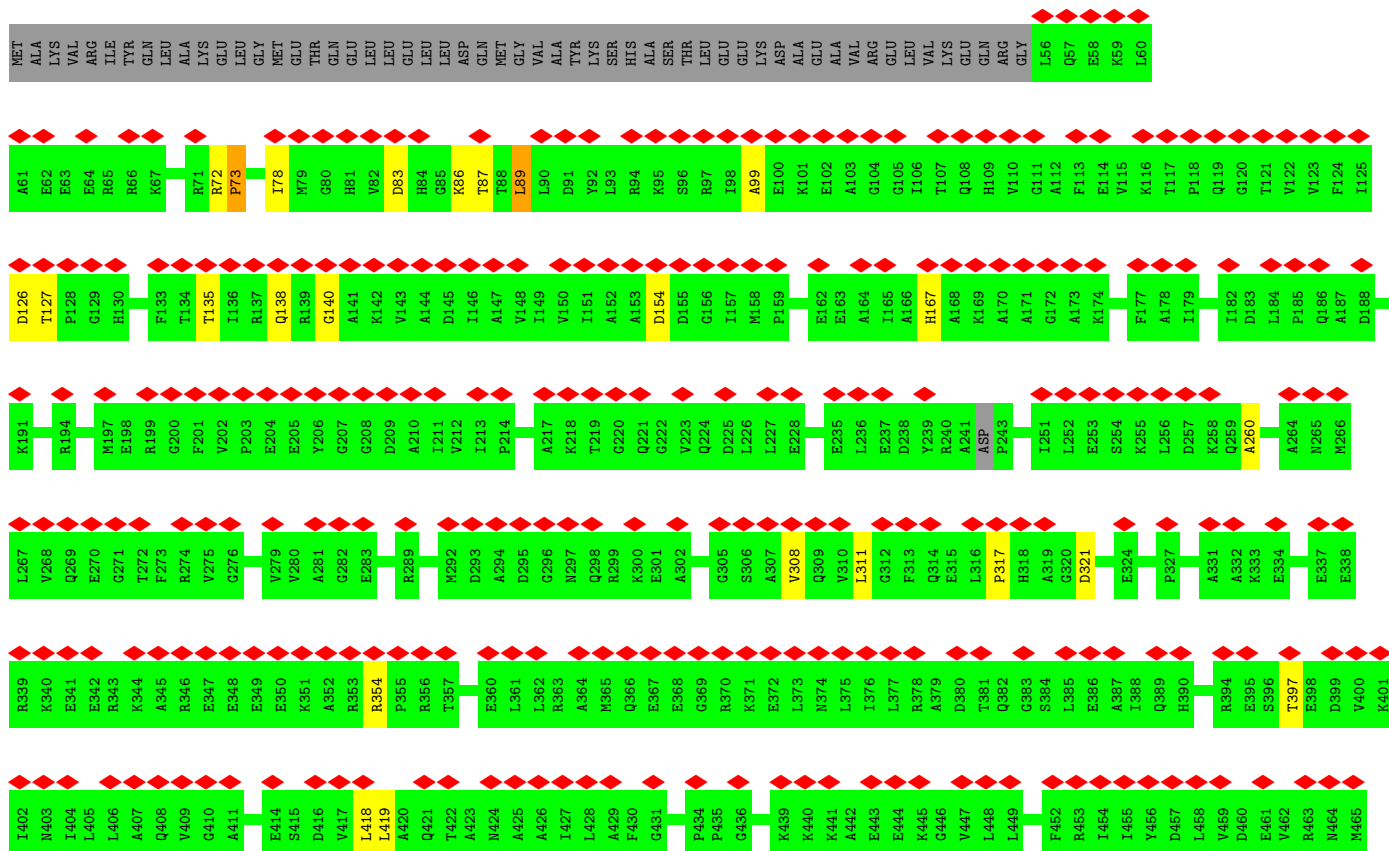
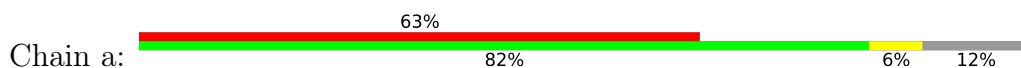
• Molecule 24: mRNA



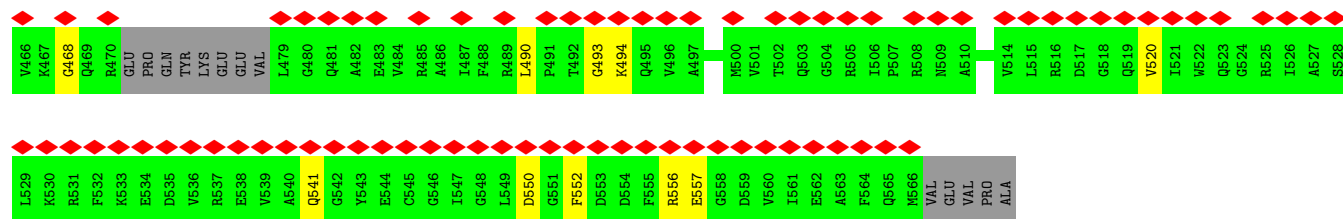
• Molecule 25: tRNAi



• Molecule 26: Translation initiation factor IF-2







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26324	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.308	Depositor
Minimum map value	-0.164	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.08	Depositor
Map size ( $\text{\AA}$ )	348.4, 348.4, 348.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.34, 1.34, 1.34	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.29	1/36426 (0.0%)	0.70	10/56837 (0.0%)
2	B	0.44	0/1935	0.79	1/2609 (0.0%)
3	C	0.39	0/1636	0.75	2/2205 (0.1%)
4	D	0.41	0/1733	0.80	1/2318 (0.0%)
5	E	0.41	0/1162	0.88	2/1564 (0.1%)
6	F	0.39	0/856	0.78	1/1154 (0.1%)
7	G	0.41	0/1276	0.73	0/1709
8	H	0.38	0/1136	0.76	0/1527
9	I	0.41	0/1029	0.78	1/1379 (0.1%)
10	J	0.39	0/805	0.74	1/1082 (0.1%)
11	K	0.41	0/900	0.90	2/1213 (0.2%)
12	L	0.35	0/986	0.76	0/1320
13	M	0.41	0/947	0.74	0/1270
14	N	0.40	0/501	0.78	0/664
15	O	0.41	0/745	0.83	0/992
16	P	0.39	0/716	0.73	0/963
17	Q	0.38	0/836	0.75	0/1117
18	R	0.40	0/604	0.85	0/801
19	S	0.42	0/670	0.70	0/903
20	T	0.42	0/765	0.87	0/1007
21	V	0.43	0/212	0.69	0/277
22	W	0.48	0/580	1.07	5/782 (0.6%)
23	X	0.49	0/1354	0.74	1/1813 (0.1%)
24	Y	0.36	0/494	0.67	0/770
25	Z	0.34	0/1721	0.71	1/2682 (0.0%)
26	a	0.46	0/3824	0.70	2/5169 (0.0%)
All	All	0.35	1/63849 (0.0%)	0.73	30/94127 (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
1	A	0	1
11	K	1	0
23	X	0	1
26	a	0	1
All	All	1	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	C	O3'-P	-5.32	1.54	1.61

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	89	ALA	CB-CA-C	18.64	138.06	110.10
9	I	7	THR	CB-CA-C	-13.26	75.81	111.60
5	E	15	ARG	N-CA-C	-12.58	77.04	111.00
22	W	33	LEU	CB-CA-C	-12.05	87.30	110.20
22	W	23	ARG	N-CA-C	-10.10	83.72	111.00
5	E	16	THR	N-CA-CB	-9.31	92.61	110.30
22	W	33	LEU	N-CA-C	-7.86	89.78	111.00
11	K	90	GLY	N-CA-C	7.75	132.49	113.10
3	C	29	TYR	N-CA-CB	-6.71	98.52	110.60
1	A	1190	G	C2'-C3'-O3'	6.55	124.19	113.70
1	A	1301	U	C2'-C3'-O3'	6.51	124.12	113.70
10	J	38	ILE	C-N-CD	-6.50	106.30	120.60
1	A	1498	U	C2'-C3'-O3'	6.24	123.68	113.70
1	A	1145	C	C2'-C3'-O3'	6.15	123.55	113.70
26	a	89	LEU	CA-CB-CG	6.12	129.38	115.30
22	W	23	ARG	CB-CA-C	-6.00	98.40	110.40
22	W	34	ALA	N-CA-CB	-5.96	101.76	110.10
1	A	266	G	C2'-C3'-O3'	5.91	123.16	113.70
1	A	281	G	C2'-C3'-O3'	5.86	123.08	113.70
26	a	418	LEU	CA-CB-CG	5.82	128.68	115.30
6	F	75	LEU	CA-CB-CG	5.82	128.68	115.30
3	C	34	LEU	CA-CB-CG	5.79	128.61	115.30
2	B	61	LEU	CA-CB-CG	5.78	128.60	115.30
25	Z	47	U	C2'-C3'-O3'	5.75	122.90	113.70
4	D	58	LEU	CA-CB-CG	5.43	127.78	115.30
23	X	35	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	509	A	C4'-C3'-O3'	5.17	123.34	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	960	U	C2'-C3'-O3'	5.13	121.91	113.70
1	A	1257	U	C2'-C3'-O3'	5.09	121.85	113.70
1	A	181	G	C2'-C3'-O3'	5.09	121.84	113.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	K	89	ALA	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	C	Sidechain
23	X	53	ASP	Peptide
26	a	73	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	32548	0	16440	867	0
2	B	1900	0	1951	40	0
3	C	1612	0	1677	41	0
4	D	1703	0	1766	46	0
5	E	1146	0	1207	23	0
6	F	843	0	857	19	0
7	G	1257	0	1296	13	0
8	H	1116	0	1177	16	0
9	I	1010	0	1037	22	0
10	J	792	0	835	30	0
11	K	885	0	904	20	0
12	L	970	0	1057	24	0
13	M	937	0	995	18	0
14	N	492	0	530	18	0
15	O	734	0	771	11	0
16	P	700	0	720	13	0
17	Q	823	0	891	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	598	0	670	26	0
19	S	655	0	672	14	0
20	T	763	0	861	22	0
21	V	208	0	221	2	0
22	W	570	0	599	24	0
23	X	1336	0	1389	45	0
24	Y	439	0	218	10	0
25	Z	1646	0	843	71	0
26	a	3774	0	3747	0	0
27	D	1	0	0	2	0
27	N	1	0	0	2	0
28	W	1	0	0	0	0
28	Z	1	0	0	0	0
29	Z	9	0	10	6	0
All	All	59470	0	43341	1342	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 14.

All (1342) 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)
25:Z:76:A:O3'	29:Z:101:FME:C	1.70	1.37
1:A:1358:U:H3	1:A:1363(A):A:N6	1.21	1.33
25:Z:76:A:C3'	29:Z:101:FME:C	2.09	1.28
3:C:28:GLN:O	3:C:32:LEU:HG	1.32	1.27
23:X:3:LYS:CB	23:X:66:ARG:NH2	2.02	1.20
23:X:3:LYS:HB3	23:X:66:ARG:NH2	1.54	1.19
1:A:1358:U:O4	1:A:1363(A):A:N1	1.77	1.17
3:C:14:ILE:CG2	3:C:15:THR:H	1.56	1.17
16:P:59:TRP:O	16:P:62:VAL:HG22	1.50	1.09
1:A:473:G:OP1	16:P:81:ARG:HB3	1.58	1.04
3:C:14:ILE:HG22	3:C:15:THR:N	1.56	1.03
1:A:827:U:O4	1:A:872:A:N1	1.95	1.00
1:A:827:U:N3	1:A:872:A:N6	2.08	1.00
1:A:92:C:H2'	1:A:93:G:C8	1.97	1.00
3:C:14:ILE:HG22	3:C:15:THR:H	0.82	0.98
1:A:92:C:H2'	1:A:93:G:H8	1.28	0.97
14:N:24:CYS:HG	27:N:101:ZN:ZN	0.64	0.96
4:D:32:ALA:O	4:D:36:ARG:O	1.84	0.95
25:Z:76:A:O2'	29:Z:101:FME:C	2.14	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:58:TYR:O	16:P:62:VAL:HG13	1.69	0.93
23:X:3:LYS:HB3	23:X:66:ARG:HH22	1.10	0.93
1:A:1458:G:H5'	20:T:32:ALA:HB2	1.51	0.93
25:Z:76:A:C2'	29:Z:101:FME:C	2.48	0.92
1:A:80:G:H3'	1:A:81:U:H5''	1.50	0.92
1:A:827:U:H3	1:A:872:A:N6	1.65	0.92
3:C:14:ILE:CD1	3:C:178:LEU:HB3	1.99	0.92
25:Z:71:C:H2'	25:Z:72:A:H5'	1.52	0.91
1:A:1505:G:H2'	24:Y:35:A:OP2	1.71	0.90
1:A:1358:U:N3	1:A:1363(A):A:N6	1.93	0.90
23:X:3:LYS:HB2	23:X:66:ARG:NH2	1.87	0.89
1:A:664:G:H22	1:A:741:G:H1	1.18	0.88
1:A:1124:G:OP1	10:J:35:SER:O	1.91	0.88
25:Z:74:C:H2'	25:Z:75:C:C2	2.08	0.88
1:A:1536:C:H42	24:Y:29:G:H1	1.21	0.88
1:A:45:U:H2'	1:A:46:G:C8	2.12	0.85
25:Z:76:A:H3'	29:Z:101:FME:C	2.05	0.84
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.11	0.83
10:J:51:ARG:HB2	10:J:59:SER:O	1.81	0.81
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.60	0.81
10:J:49:VAL:O	10:J:60:ARG:HG2	1.80	0.81
1:A:973:G:H3'	1:A:974:A:H5''	1.61	0.80
1:A:920:U:H2'	1:A:921:U:C6	2.17	0.80
1:A:96:U:H2'	1:A:97:G:C8	2.17	0.79
1:A:718:G:H5'	11:K:117:ASN:HB2	1.63	0.79
24:Y:38:G:H1	25:Z:34:C:H42	1.31	0.79
1:A:1123:A:O2'	10:J:37:PRO:O	1.99	0.78
25:Z:76:A:HO3'	29:Z:101:FME:C	1.94	0.78
2:B:8:LYS:HD2	2:B:9:GLU:H	1.47	0.77
1:A:1493:A:C4	22:W:18:PRO:HA	2.19	0.77
3:C:14:ILE:HD13	3:C:178:LEU:HB3	1.66	0.77
1:A:1475:G:H2'	1:A:1476:G:C8	2.20	0.76
25:Z:71:C:C2'	25:Z:72:A:H5'	2.16	0.76
18:R:42:ARG:HH11	18:R:42:ARG:HB3	1.49	0.76
25:Z:74:C:H3'	25:Z:74:C:H6	1.50	0.76
4:D:9:CYS:SG	27:D:300:ZN:ZN	1.73	0.76
1:A:1264:C:H2'	1:A:1265:G:H8	1.51	0.75
10:J:50:ILE:HG13	10:J:60:ARG:HG2	1.66	0.75
1:A:1458:G:OP1	20:T:32:ALA:HA	1.87	0.75
1:A:1048:G:H5''	14:N:3:ARG:HG2	1.69	0.74
1:A:518:C:H2'	1:A:530:G:C8	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:G:C6	1:A:1100:C:N3	2.56	0.74
8:H:86:ILE:HD11	8:H:136:GLU:HB2	1.70	0.74
1:A:79:G:H2'	1:A:80:G:H8	1.51	0.73
3:C:28:GLN:O	3:C:32:LEU:CG	2.26	0.73
1:A:1281:U:H5'	1:A:1282:C:H5	1.53	0.73
1:A:69:G:H1	1:A:100:C:H42	1.37	0.73
14:N:24:CYS:SG	27:N:101:ZN:ZN	1.77	0.73
1:A:1347:G:C8	9:I:107:ARG:HB3	2.23	0.72
11:K:15:ALA:HA	11:K:77:MET:HA	1.71	0.72
1:A:524:G:C6	1:A:525:C:N4	2.57	0.72
22:W:33:LEU:O	22:W:64:ARG:HA	1.89	0.72
1:A:45:U:H2'	1:A:46:G:H8	1.52	0.72
2:B:21:ARG:HA	2:B:39:ILE:HA	1.71	0.72
1:A:1323:G:H2'	1:A:1324:A:C8	2.25	0.72
1:A:1356:G:H2'	1:A:1357:A:C8	2.26	0.71
1:A:21:G:H2'	1:A:22:G:C8	2.25	0.71
1:A:864:A:H2'	1:A:865:A:C8	2.25	0.71
1:A:55:A:H2'	1:A:56:U:C6	2.24	0.71
6:F:52:ILE:HD11	18:R:77:GLY:HA3	1.73	0.71
1:A:1264:C:H2'	1:A:1265:G:C8	2.26	0.71
4:D:13:ARG:HH21	4:D:36:ARG:NH2	1.88	0.70
1:A:398:C:H2'	1:A:399:G:H8	1.57	0.70
1:A:1219:U:H2'	1:A:1220:G:C8	2.27	0.70
3:C:71:ALA:HB2	3:C:115:LEU:HD11	1.72	0.70
10:J:50:ILE:HG13	10:J:60:ARG:CG	2.21	0.70
25:Z:75:C:C3'	25:Z:76:A:H8	2.04	0.70
1:A:1533:C:H4'	1:A:1533:C:OP1	1.92	0.70
1:A:17:U:H2'	1:A:18:C:C6	2.26	0.70
22:W:17:LEU:HB3	22:W:18:PRO:HD2	1.73	0.69
1:A:34:C:H2'	1:A:35:G:H8	1.57	0.69
1:A:658:G:C2	1:A:749:C:N3	2.60	0.69
3:C:14:ILE:HD11	3:C:178:LEU:HB3	1.74	0.69
1:A:224:C:H2'	1:A:225:C:C6	2.28	0.69
1:A:79:G:H2'	1:A:80:G:C8	2.26	0.69
1:A:269:C:H2'	1:A:270:A:C8	2.27	0.69
1:A:505:G:H5'	1:A:534:U:H2'	1.75	0.69
1:A:1391:U:H2'	1:A:1392:G:C8	2.28	0.68
23:X:48:VAL:HG21	23:X:58:ARG:HE	1.57	0.68
25:Z:69:C:H2'	25:Z:70:G:C8	2.27	0.68
23:X:141:THR:HG22	23:X:165:LEU:HD21	1.74	0.68
1:A:524:G:C2	1:A:525:C:N3	2.61	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:75:C:H3'	25:Z:76:A:H8	1.57	0.68
1:A:553:A:H2'	1:A:554:C:C6	2.28	0.68
4:D:26:CYS:SG	27:D:300:ZN:ZN	1.81	0.68
1:A:914:A:H2'	1:A:915:A:H8	1.59	0.68
23:X:15:GLN:HB3	23:X:28:ILE:HG22	1.76	0.68
6:F:6:VAL:HG22	6:F:90:VAL:HG22	1.75	0.68
13:M:22:ILE:HG22	13:M:24:GLY:H	1.59	0.68
1:A:736:C:H2'	1:A:737:A:C8	2.29	0.68
1:A:1219:U:H2'	1:A:1220:G:H8	1.58	0.68
1:A:1391:U:H2'	1:A:1392:G:H8	1.59	0.67
1:A:880:C:H2'	1:A:881:G:H8	1.59	0.67
22:W:21:THR:HA	22:W:35:TYR:HA	1.76	0.67
1:A:662:G:H2'	1:A:663:A:C8	2.30	0.67
1:A:737:A:H2'	1:A:738:C:C6	2.30	0.67
1:A:588:G:N2	1:A:589:C:C2	2.63	0.67
4:D:101:LEU:O	4:D:104:VAL:HG12	1.95	0.67
10:J:61:GLU:OE1	10:J:63:PHE:CE1	2.47	0.67
1:A:521:G:N2	1:A:522:C:C2	2.63	0.67
1:A:124:G:H2'	1:A:125:U:O4'	1.94	0.66
25:Z:75:C:H3'	25:Z:76:A:C8	2.31	0.66
1:A:1025:U:H2'	1:A:1026:G:C8	2.30	0.66
1:A:80:G:H3'	1:A:81:U:C5'	2.25	0.66
1:A:1437:C:H2'	1:A:1438:G:H8	1.60	0.66
25:Z:63:G:H2'	25:Z:64:G:H8	1.60	0.66
3:C:14:ILE:CG2	3:C:15:THR:N	2.28	0.66
25:Z:75:C:H4'	25:Z:76:A:OP1	1.95	0.66
1:A:1409:C:H2'	1:A:1410:G:H8	1.61	0.66
3:C:150:LYS:HE2	3:C:167:TRP:HE1	1.61	0.66
1:A:1358:U:C4	1:A:1363(A):A:N1	2.63	0.65
1:A:1218:C:H2'	1:A:1219:U:C6	2.31	0.65
1:A:24:U:H2'	1:A:25:C:C6	2.32	0.65
1:A:30:U:H3'	1:A:31:G:H5''	1.77	0.65
1:A:1016:A:H2'	1:A:1017:G:O4'	1.97	0.65
1:A:1535:C:H2'	1:A:1536:C:C6	2.31	0.65
1:A:34:C:H2'	1:A:35:G:C8	2.31	0.65
1:A:78:G:H2'	1:A:79:G:O4'	1.95	0.65
1:A:917:G:H2'	1:A:918:A:C8	2.32	0.65
1:A:868:C:H2'	1:A:869:G:O4'	1.95	0.65
1:A:1348:U:H2'	1:A:1349:A:H8	1.62	0.65
25:Z:74:C:H2'	25:Z:75:C:N3	2.11	0.64
1:A:1349:A:H3'	1:A:1350:A:H8	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:27:GLN:HA	6:F:30:LEU:HD12	1.79	0.64
1:A:269:C:H2'	1:A:270:A:H8	1.60	0.64
1:A:1520:G:H2'	1:A:1521:G:C8	2.33	0.64
2:B:71:VAL:HA	2:B:93:VAL:HG12	1.80	0.64
23:X:106:ILE:HG12	23:X:116:VAL:HG11	1.78	0.64
1:A:1513:A:H2'	1:A:1514:C:C6	2.33	0.64
23:X:90:PHE:HB2	23:X:120:ILE:HG12	1.77	0.64
1:A:71:C:H2'	1:A:72:C:O4'	1.98	0.64
1:A:1342:C:H2'	1:A:1343:G:H8	1.63	0.64
22:W:17:LEU:CB	22:W:18:PRO:HD2	2.27	0.64
2:B:95:GLN:HG3	2:B:147:LYS:HG2	1.80	0.63
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.80	0.63
8:H:101:PRO:HG2	8:H:133:LEU:HD11	1.80	0.63
11:K:62:GLN:HG2	11:K:97:ALA:HB2	1.81	0.63
8:H:84:ARG:HD2	8:H:86:ILE:HG12	1.80	0.63
1:A:1126:U:O2	1:A:1126:U:H2'	1.97	0.63
23:X:5:TYR:HD2	23:X:65:TRP:HH2	1.45	0.63
1:A:10:A:H2'	1:A:11:G:H8	1.63	0.63
1:A:1443:G:C6	1:A:1444:C:N4	2.66	0.63
1:A:316:G:H1	1:A:337:C:H42	1.44	0.63
1:A:1536:C:N4	24:Y:29:G:H1	1.95	0.63
2:B:115:LEU:HD11	2:B:146:GLN:HG3	1.79	0.63
9:I:13:ALA:HB2	9:I:68:GLY:HA3	1.79	0.63
1:A:1255:G:H2'	1:A:1279:A:N6	2.14	0.63
9:I:48:GLU:N	9:I:49:PRO:HD2	2.14	0.63
25:Z:75:C:O3'	25:Z:76:A:O4'	2.16	0.63
1:A:19:C:H2'	1:A:20:U:C6	2.34	0.63
1:A:262:A:H5''	20:T:76:ALA:HB2	1.81	0.63
1:A:914:A:H2'	1:A:915:A:C8	2.34	0.63
24:Y:38:G:H1	25:Z:34:C:N4	1.95	0.63
1:A:741:G:H5'	15:O:39:LEU:HD21	1.81	0.62
4:D:13:ARG:NH2	4:D:36:ARG:NH2	2.46	0.62
1:A:128:G:N2	1:A:234:C:C2	2.67	0.62
1:A:1342:C:H2'	1:A:1343:G:C8	2.34	0.62
1:A:1354:C:H2'	1:A:1355:G:H8	1.63	0.62
10:J:6:ILE:HG13	10:J:72:VAL:O	2.00	0.62
1:A:1445:C:C2	1:A:1458:G:C2	2.87	0.62
1:A:745:C:H2'	1:A:746:A:C8	2.34	0.62
5:E:33:VAL:HG12	5:E:112:LEU:HD22	1.81	0.62
22:W:18:PRO:O	22:W:21:THR:HB	2.00	0.62
9:I:46:ALA:HA	9:I:78:LYS:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:G:N1	1:A:522:C:C4	2.68	0.62
1:A:1106:G:N2	1:A:1107:C:C2	2.68	0.61
1:A:1151:A:O2'	1:A:1152:A:H8	1.83	0.61
1:A:736:C:H2'	1:A:737:A:H8	1.64	0.61
1:A:1504:G:H4'	1:A:1505:G:O5'	1.99	0.61
25:Z:73:A:H8	25:Z:73:A:C5'	2.13	0.61
1:A:243:A:H4'	1:A:244:U:O5'	2.00	0.61
1:A:874:G:N2	1:A:875:C:C2	2.69	0.61
12:L:86:ARG:HB3	12:L:99:HIS:HB2	1.82	0.61
1:A:662:G:C2	1:A:744:C:O2	2.54	0.61
1:A:576:G:H3'	1:A:577:G:H5''	1.81	0.61
1:A:974:A:H4'	1:A:975:A:H3'	1.82	0.61
1:A:1414:U:H2'	1:A:1415:G:C8	2.35	0.61
22:W:20:ALA:HB3	22:W:41:ARG:HH21	1.66	0.61
1:A:320:C:H2'	1:A:321:A:C8	2.35	0.61
1:A:681:C:C2	1:A:710:G:N2	2.69	0.61
1:A:1040:U:H2'	1:A:1041:A:C8	2.36	0.61
1:A:1293:G:H2'	1:A:1294:G:C8	2.36	0.61
1:A:1458:G:C5'	20:T:32:ALA:HB2	2.28	0.61
1:A:302:G:H2'	1:A:303:A:C8	2.36	0.61
1:A:585:G:H4'	12:L:8:ASN:HD21	1.66	0.61
1:A:1475:G:H2'	1:A:1476:G:H8	1.64	0.60
14:N:24:CYS:HB3	14:N:29:ARG:H	1.66	0.60
1:A:769:G:N2	1:A:770:C:C2	2.69	0.60
10:J:23:ILE:HG13	10:J:85:LEU:HD22	1.83	0.60
1:A:97:G:H2'	1:A:98:G:C8	2.36	0.60
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.82	0.60
13:M:80:ARG:O	13:M:84:ILE:HG12	2.01	0.60
1:A:132:C:N3	1:A:231:G:C2	2.70	0.60
1:A:1353:G:N2	1:A:1354:C:C2	2.70	0.60
6:F:50:TYR:CE2	18:R:77:GLY:HA2	2.37	0.60
1:A:598:U:H2'	1:A:599:C:H6	1.66	0.60
1:A:946:A:H2'	1:A:947:G:C8	2.36	0.60
1:A:1127:G:H21	1:A:1147:C:H41	1.48	0.60
1:A:1438:G:N2	1:A:1439:C:C2	2.70	0.60
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.83	0.60
10:J:53:PRO:HB3	14:N:42:ILE:HG12	1.84	0.60
2:B:87:ARG:HH22	2:B:233:SER:H	1.48	0.60
18:R:37:VAL:HG21	18:R:78:LEU:HB3	1.84	0.60
1:A:56:U:H2'	1:A:57:G:C8	2.37	0.60
1:A:1283:G:N2	1:A:1284:C:C2	2.70	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:G:H2'	1:A:1294:G:H8	1.65	0.60
25:Z:63:G:H2'	25:Z:64:G:C8	2.37	0.60
1:A:1509:C:H2'	1:A:1510:U:O4'	2.02	0.60
1:A:335:C:H2'	1:A:336:C:C6	2.37	0.59
1:A:598:U:H2'	1:A:599:C:C6	2.37	0.59
1:A:1000:U:H2'	1:A:1001:A:O4'	2.02	0.59
13:M:54:VAL:O	13:M:58:GLU:HG2	2.02	0.59
25:Z:74:C:H3'	25:Z:74:C:C6	2.34	0.59
12:L:7:ILE:H	12:L:7:ILE:HD13	1.67	0.59
1:A:222:U:H2'	1:A:223:U:C6	2.37	0.59
1:A:69:G:H1	1:A:100:C:N4	2.00	0.59
2:B:118:LEU:HD21	2:B:138:LEU:HD22	1.85	0.59
1:A:72:C:H42	1:A:97:G:H1	1.51	0.59
1:A:127:G:N2	1:A:235:C:C2	2.71	0.59
1:A:216:G:H2'	1:A:217:C:C6	2.38	0.59
1:A:390:C:H2'	1:A:391:G:H8	1.67	0.59
25:Z:74:C:C6	25:Z:74:C:C3'	2.85	0.59
1:A:127:G:C2	1:A:235:C:N3	2.71	0.59
1:A:922:G:H2'	1:A:923:A:C8	2.38	0.59
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.84	0.59
23:X:5:TYR:HD2	23:X:65:TRP:CH2	2.20	0.59
1:A:10:A:H2'	1:A:11:G:C8	2.38	0.59
1:A:674:G:H2'	1:A:675:A:H8	1.67	0.58
25:Z:73:A:C8	25:Z:73:A:P	2.96	0.58
1:A:101:A:H2'	1:A:102:G:H8	1.69	0.58
1:A:1232:U:H5''	9:I:124:GLN:O	2.04	0.58
1:A:90:U:H2'	1:A:91:C:C6	2.39	0.58
1:A:1151:A:O2'	1:A:1152:A:C8	2.55	0.58
1:A:1256:A:N6	1:A:1278:U:C2	2.71	0.58
1:A:1392:G:N2	1:A:1502:A:H8	2.00	0.58
1:A:683:G:N2	1:A:708:C:C2	2.71	0.58
1:A:1323:G:H2'	1:A:1324:A:H8	1.68	0.58
1:A:1361:G:C6	1:A:1362:C:N3	2.72	0.58
1:A:1437:C:H2'	1:A:1438:G:C8	2.37	0.58
1:A:985:C:C2	1:A:1221:G:N2	2.72	0.58
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.84	0.58
25:Z:74:C:H5'	25:Z:75:C:OP1	2.03	0.58
1:A:96:U:H2'	1:A:97:G:H8	1.65	0.58
1:A:344:A:H4'	1:A:345:C:OP2	2.01	0.58
1:A:536:C:H2'	1:A:537:G:C8	2.38	0.58
1:A:954:G:H21	1:A:1227:A:H62	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1376:U:H5'	7:G:102:ARG:HH22	1.69	0.58
4:D:70:ILE:HD13	4:D:75:PHE:HD1	1.66	0.58
1:A:20:U:H2'	1:A:21:G:O4'	2.04	0.58
22:W:17:LEU:HD22	22:W:18:PRO:CD	2.33	0.58
25:Z:73:A:O2'	25:Z:74:C:OP1	2.19	0.58
1:A:376:G:H2'	1:A:377:G:H8	1.69	0.58
1:A:397:A:H3'	1:A:397:A:N3	2.18	0.58
1:A:658:G:N2	1:A:749:C:C2	2.72	0.57
1:A:885:G:H1	1:A:912:C:H42	1.52	0.57
1:A:1485:U:H2'	1:A:1486:G:H8	1.69	0.57
9:I:112:LYS:HG2	9:I:119:ALA:H	1.68	0.57
1:A:568:G:N2	1:A:883:C:C2	2.72	0.57
8:H:110:ALA:HB1	8:H:133:LEU:HD21	1.86	0.57
1:A:1507:A:H2'	1:A:1508:G:C8	2.40	0.57
5:E:52:PRO:O	5:E:55:VAL:HG12	2.04	0.57
1:A:525:C:H2'	1:A:526:C:C6	2.40	0.57
25:Z:50:U:H2'	25:Z:51:C:C6	2.38	0.57
1:A:148:G:H2'	1:A:149:A:C8	2.38	0.57
1:A:390:C:H2'	1:A:391:G:C8	2.39	0.57
1:A:1354:C:H2'	1:A:1355:G:C8	2.39	0.57
1:A:728:A:H2'	1:A:729:A:C8	2.40	0.57
1:A:932:C:H5'	7:G:3:ARG:HB3	1.86	0.57
10:J:38:ILE:HG23	10:J:71:LEU:N	2.18	0.57
12:L:76:ASN:HD21	12:L:108:ALA:H	1.52	0.57
1:A:122:G:N1	1:A:123:C:C2	2.73	0.57
1:A:560:U:H5''	1:A:561:U:H5'	1.87	0.57
5:E:79:GLU:HG2	5:E:92:LYS:HG3	1.86	0.57
18:R:51:LEU:HD22	18:R:55:ARG:HG2	1.86	0.57
25:Z:75:C:C3'	25:Z:76:A:C8	2.86	0.57
1:A:1134:G:N2	1:A:1141:C:C2	2.73	0.56
23:X:144:LEU:HD11	23:X:165:LEU:HD13	1.87	0.56
3:C:136:GLN:HB3	3:C:140:ARG:HH21	1.70	0.56
5:E:107:ARG:HH11	5:E:107:ARG:HB2	1.71	0.56
1:A:755:G:N2	1:A:756:C:C2	2.73	0.56
1:A:1102:A:H2'	1:A:1103:C:C6	2.39	0.56
1:A:67:C:H2'	1:A:68:G:C8	2.40	0.56
3:C:148:GLY:HA3	3:C:172:ARG:O	2.05	0.56
4:D:3:ARG:HA	4:D:3:ARG:NH1	2.21	0.56
23:X:5:TYR:CD2	23:X:65:TRP:HH2	2.23	0.56
1:A:588:G:N1	1:A:589:C:C4	2.74	0.56
1:A:1542:U:H4'	18:R:18:ARG:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:13:GLN:HE21	11:K:75:TYR:HA	1.69	0.56
11:K:126:ARG:C	11:K:128:ALA:H	2.09	0.56
1:A:258:G:N2	1:A:269:C:C2	2.73	0.56
1:A:1225:A:H4'	19:S:78:ARG:HD3	1.87	0.56
1:A:1409:C:H2'	1:A:1410:G:C8	2.41	0.56
17:Q:56:VAL:HG13	17:Q:77:VAL:HB	1.88	0.56
1:A:1033:G:H2'	1:A:1034:G:C8	2.41	0.56
2:B:174:VAL:HG13	2:B:184:VAL:HG21	1.87	0.56
1:A:725:G:N2	1:A:726:C:C2	2.74	0.56
23:X:18:VAL:HG12	23:X:59:ILE:HD11	1.86	0.56
25:Z:51:C:H42	25:Z:63:G:H1	1.53	0.56
1:A:29:G:N2	1:A:555:C:C2	2.74	0.56
1:A:128:G:C2	1:A:234:C:C2	2.94	0.56
1:A:442:C:H2'	1:A:443:C:C6	2.41	0.56
1:A:436:C:H2'	1:A:437:U:C6	2.41	0.55
1:A:784:C:C2	1:A:799:G:N2	2.73	0.55
8:H:44:PHE:HE2	8:H:109:ILE:HG12	1.70	0.55
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.87	0.55
22:W:17:LEU:HD22	22:W:18:PRO:HD3	1.89	0.55
25:Z:49:G:C2	25:Z:66:C:C2	2.93	0.55
1:A:35:G:C6	1:A:36:C:N4	2.74	0.55
1:A:1161:C:H2'	1:A:1162:C:C6	2.41	0.55
2:B:8:LYS:HD2	2:B:9:GLU:N	2.20	0.55
23:X:3:LYS:HA	23:X:66:ARG:NH1	2.21	0.55
25:Z:62:C:H2'	25:Z:63:G:C8	2.42	0.55
1:A:1097:C:H2'	1:A:1098:C:C6	2.40	0.55
1:A:1106:G:N1	1:A:1107:C:C4	2.75	0.55
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.87	0.55
1:A:1410:G:C6	1:A:1411:C:N4	2.75	0.55
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.88	0.55
4:D:129:ASN:HD21	4:D:145:GLU:H	1.54	0.55
5:E:152:ARG:HB2	8:H:43:GLY:HA3	1.88	0.55
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.88	0.55
25:Z:32:OMC:HM22	25:Z:33:U:H5'	1.87	0.55
2:B:44:LEU:HA	2:B:47:THR:HB	1.88	0.55
25:Z:49:G:N2	25:Z:66:C:C2	2.74	0.55
1:A:1458:G:H5'	20:T:32:ALA:CB	2.33	0.55
22:W:15:GLU:HB3	22:W:23:ARG:HB2	1.88	0.55
1:A:664:G:N2	1:A:741:G:H1	1.98	0.55
1:A:836:G:H1	1:A:850:U:H3	1.55	0.55
1:A:1233:G:H2'	1:A:1234:C:C6	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:41:GLU:HB2	6:F:62:TRP:HE3	1.70	0.55
1:A:769:G:H4'	1:A:1513:A:H4'	1.89	0.55
1:A:806:C:H2'	1:A:807:A:C8	2.42	0.55
1:A:998:G:N2	1:A:999:C:C2	2.74	0.55
1:A:1032:G:H2'	1:A:1033:G:C8	2.42	0.55
1:A:1228:C:H5'	13:M:108:ARG:HH22	1.70	0.55
1:A:1368:G:N2	1:A:1369:C:C2	2.75	0.55
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.88	0.55
11:K:88:GLY:O	11:K:89:ALA:C	2.44	0.55
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.89	0.55
1:A:1163:C:C2	1:A:1174:G:N2	2.75	0.55
1:A:1281:U:H5'	1:A:1282:C:C5	2.38	0.55
19:S:37:ARG:HB3	19:S:37:ARG:HH11	1.71	0.55
1:A:416:G:C6	1:A:417:C:N3	2.75	0.55
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.89	0.55
1:A:1258:G:H1	1:A:1277:C:H42	1.55	0.55
1:A:1405:G:H2'	1:A:1406:U:C6	2.42	0.55
2:B:25:ASN:H	2:B:191:ASP:HA	1.72	0.55
1:A:524:G:C2	1:A:525:C:C4	2.95	0.54
1:A:728:A:H2'	1:A:729:A:H8	1.70	0.54
4:D:3:ARG:HA	4:D:3:ARG:HH11	1.71	0.54
1:A:971:G:H4'	1:A:972:C:H5''	1.89	0.54
1:A:1103:C:H2'	1:A:1104:G:O4'	2.07	0.54
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.89	0.54
20:T:56:MET:HG2	20:T:84:LEU:HD21	1.89	0.54
25:Z:23:C:H2'	25:Z:24:U:C6	2.42	0.54
9:I:15:ALA:HA	9:I:65:VAL:HA	1.88	0.54
23:X:43:LEU:HD23	23:X:60:MET:HA	1.90	0.54
25:Z:74:C:C2'	25:Z:75:C:C2	2.88	0.54
1:A:132:C:C2	1:A:231:G:N2	2.75	0.54
1:A:1032:G:H2'	1:A:1033:G:H8	1.73	0.54
1:A:1128:C:H1'	1:A:1146:A:H61	1.73	0.54
1:A:1435:G:H2'	1:A:1436:U:C6	2.42	0.54
9:I:8:GLY:HA3	9:I:76:ALA:O	2.08	0.54
15:O:26:GLU:HG3	15:O:81:LEU:HD11	1.89	0.54
23:X:3:LYS:CA	23:X:66:ARG:NH2	2.68	0.54
1:A:216:G:C6	1:A:217:C:N4	2.75	0.54
3:C:152:ILE:HG12	3:C:167:TRP:HD1	1.72	0.54
25:Z:75:C:O3'	25:Z:76:A:H8	1.90	0.54
25:Z:74:C:H6	25:Z:74:C:C3'	2.17	0.54
1:A:384:G:H2'	1:A:385:C:C6	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:C:H2'	1:A:111:G:O4'	2.08	0.54
1:A:200:G:C2	1:A:218:C:C2	2.95	0.54
25:Z:22:G:N2	25:Z:23:C:C2	2.76	0.54
1:A:806:C:H2'	1:A:807:A:H8	1.73	0.54
1:A:1151:A:HO2'	1:A:1152:A:H8	1.46	0.54
1:A:1233:G:C6	1:A:1234:C:N4	2.76	0.54
1:A:1312:G:N2	1:A:1326:C:C2	2.75	0.54
11:K:88:GLY:O	11:K:89:ALA:O	2.26	0.54
1:A:1104:G:H4'	2:B:111:ARG:HD2	1.90	0.53
25:Z:72:A:O2'	25:Z:73:A:N7	2.36	0.53
1:A:370:C:C2	1:A:392:G:N2	2.76	0.53
1:A:682:G:H1	1:A:708:C:H42	1.56	0.53
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.43	0.53
1:A:794:A:H2'	1:A:795:C:C6	2.43	0.53
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.90	0.53
18:R:42:ARG:HB3	18:R:42:ARG:NH1	2.21	0.53
1:A:514:C:H42	1:A:537:G:H1	1.54	0.53
1:A:687:A:H4'	1:A:688:G:O5'	2.07	0.53
3:C:123:GLN:HE22	3:C:140:ARG:HH22	1.54	0.53
9:I:51:ARG:HG2	9:I:56:LEU:HD11	1.91	0.53
18:R:37:VAL:HG22	18:R:79:LEU:HG	1.90	0.53
18:R:48:GLY:H	18:R:83:GLU:H	1.57	0.53
1:A:1491:G:H21	22:W:18:PRO:HB2	1.74	0.53
8:H:113:SER:HB3	8:H:132:GLU:HB3	1.89	0.53
25:Z:73:A:H8	25:Z:73:A:P	2.31	0.53
1:A:552:U:H4'	12:L:86:ARG:HG3	1.90	0.53
1:A:589:C:O2	1:A:651:C:O2	2.27	0.53
1:A:625:G:OP1	16:P:9:PHE:HB3	2.09	0.53
1:A:827:U:C4	1:A:872:A:N1	2.73	0.53
15:O:49:ASP:OD2	15:O:52:SER:HB2	2.07	0.53
17:Q:64:PRO:HB3	17:Q:70:ARG:HE	1.74	0.53
1:A:35:G:H2'	1:A:36:C:C6	2.43	0.53
1:A:657:G:H1	1:A:749:C:N4	2.07	0.53
1:A:834:C:C2	1:A:853:G:C2	2.96	0.53
1:A:838:G:C2	1:A:849:C:C2	2.97	0.53
1:A:1256:A:H62	1:A:1278:U:H1'	1.74	0.53
1:A:70:G:C2	1:A:100:C:C2	2.96	0.53
1:A:945:G:H2'	1:A:945:G:N3	2.23	0.53
1:A:1114:C:C2	1:A:1187:G:C2	2.97	0.53
16:P:11:SER:HB3	16:P:14:ASN:HB3	1.91	0.53
25:Z:74:C:O3'	25:Z:75:C:O4'	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:U:H3	1:A:734:G:H1	1.57	0.53
1:A:820:U:H3'	1:A:821:G:C5'	2.39	0.53
1:A:1456:G:N2	1:A:1457:G:C5	2.77	0.53
4:D:100:ARG:HH22	4:D:118:ARG:HH22	1.55	0.53
23:X:17:ARG:HE	23:X:56:VAL:HG22	1.74	0.53
1:A:253:U:H2'	1:A:254:G:H8	1.74	0.52
1:A:354:G:N2	1:A:355:C:C2	2.77	0.52
1:A:1386:G:H2'	1:A:1387:G:H8	1.74	0.52
1:A:1530:G:H2'	1:A:1531:A:C8	2.44	0.52
2:B:42:ILE:HD11	2:B:190:THR:HB	1.91	0.52
8:H:6:ILE:HG13	8:H:85:ARG:NH2	2.24	0.52
1:A:662:G:C6	1:A:744:C:N3	2.77	0.52
1:A:1314:C:H2'	1:A:1315:U:C6	2.43	0.52
1:A:1376:U:H5'	7:G:102:ARG:NH2	2.24	0.52
9:I:112:LYS:HG2	9:I:118:LYS:HA	1.89	0.52
13:M:97:PRO:HG2	13:M:103:THR:HG22	1.91	0.52
23:X:3:LYS:CB	23:X:66:ARG:HH21	2.15	0.52
1:A:122:G:C2	1:A:123:C:C2	2.97	0.52
1:A:505:G:H1	1:A:526:C:H42	1.57	0.52
8:H:42:GLU:HG3	8:H:109:ILE:HD13	1.91	0.52
15:O:26:GLU:O	15:O:29:VAL:HG12	2.10	0.52
18:R:53:ARG:HB3	18:R:53:ARG:NH1	2.25	0.52
1:A:22:G:C6	1:A:23:C:C4	2.97	0.52
1:A:841:U:H6	1:A:841:U:H5''	1.73	0.52
1:A:1172:C:H2'	1:A:1173:G:H8	1.74	0.52
7:G:37:ASN:HD21	9:I:41:VAL:H	1.57	0.52
23:X:101:THR:HG22	23:X:105:HIS:CE1	2.44	0.52
1:A:235:C:H2'	1:A:236:G:H8	1.74	0.52
1:A:398:C:H2'	1:A:399:G:C8	2.43	0.52
2:B:112:VAL:HG23	2:B:149:LEU:HB3	1.91	0.52
2:B:208:ILE:HG22	2:B:239:VAL:HG13	1.91	0.52
1:A:543:C:H2'	1:A:544:G:C8	2.45	0.52
1:A:129(A):G:H4'	1:A:130:A:O5'	2.09	0.52
1:A:373:A:H2'	1:A:374:A:H8	1.73	0.52
1:A:824:C:H2'	1:A:825:G:H8	1.74	0.52
1:A:64:G:H4'	1:A:65:U:H5''	1.91	0.52
1:A:100:C:H2'	1:A:101:A:C8	2.45	0.52
1:A:568:G:C2	1:A:883:C:N3	2.77	0.52
1:A:1163:C:N3	1:A:1174:G:C2	2.78	0.52
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.91	0.52
1:A:122:G:C6	1:A:123:C:C4	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:G:H1	1:A:337:C:N4	2.08	0.52
2:B:21:ARG:H	2:B:39:ILE:HG23	1.75	0.52
20:T:43:LEU:HB3	20:T:52:ALA:HB2	1.92	0.52
1:A:255:G:C2	1:A:272:C:C2	2.98	0.52
7:G:69:VAL:O	7:G:138:LYS:HG3	2.10	0.52
25:Z:49:G:C2	25:Z:66:C:N3	2.77	0.52
1:A:543:C:H2'	1:A:544:G:H8	1.75	0.51
1:A:1038:C:H2'	1:A:1039:C:H6	1.74	0.51
2:B:184:VAL:HG13	2:B:198:ASP:H	1.75	0.51
7:G:65:ALA:O	7:G:69:VAL:HG23	2.10	0.51
1:A:24:U:H2'	1:A:25:C:H6	1.74	0.51
1:A:183:G:H2'	1:A:184:G:O4'	2.09	0.51
1:A:1216:G:N2	1:A:1217:C:C2	2.78	0.51
1:A:1512:U:H2'	1:A:1513:A:C8	2.46	0.51
2:B:97:TRP:CH2	2:B:101:MET:HB2	2.45	0.51
6:F:14:LEU:HB3	6:F:18:GLN:HB3	1.92	0.51
9:I:17:VAL:HG22	9:I:63:ILE:HG12	1.91	0.51
19:S:42:PRO:HA	19:S:45:VAL:HG23	1.92	0.51
1:A:302:G:H2'	1:A:303:A:H8	1.74	0.51
1:A:629:G:H2'	1:A:630:G:O4'	2.11	0.51
1:A:658:G:C2	1:A:749:C:C2	2.98	0.51
1:A:1308:U:H2'	1:A:1309:G:H8	1.76	0.51
11:K:27:ASN:HD21	11:K:44:SER:HB2	1.74	0.51
12:L:76:ASN:ND2	12:L:108:ALA:H	2.09	0.51
1:A:391:G:H2'	1:A:392:G:O4'	2.10	0.51
1:A:538:G:H2'	1:A:539:A:C8	2.45	0.51
1:A:681:C:N3	1:A:710:G:C2	2.79	0.51
1:A:988:G:N1	1:A:989:C:C2	2.78	0.51
1:A:1262:C:H2'	1:A:1263:C:C6	2.44	0.51
1:A:197:A:H4'	1:A:198:G:O5'	2.11	0.51
1:A:590:C:N3	1:A:650:G:C2	2.78	0.51
1:A:928:G:H1	1:A:1389:C:H42	1.57	0.51
1:A:1164:G:N2	1:A:1165:C:C2	2.79	0.51
1:A:1405:G:H2'	1:A:1406:U:H6	1.75	0.51
2:B:58:ILE:HA	2:B:61:LEU:HD23	1.92	0.51
23:X:3:LYS:CB	23:X:66:ARG:CZ	2.86	0.51
1:A:131:C:O2	1:A:232:G:C2	2.64	0.51
1:A:184:G:H2'	1:A:185:A:H8	1.74	0.51
1:A:189(K):U:H2'	1:A:189(L):G:H8	1.76	0.51
1:A:424:G:H2'	1:A:425:G:C8	2.45	0.51
1:A:491:G:H2'	1:A:492:G:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1431:C:C2	1:A:1470:G:N2	2.79	0.51
1:A:1438:G:N1	1:A:1439:C:C4	2.79	0.51
1:A:1491:G:H21	22:W:18:PRO:CB	2.23	0.51
6:F:97:PHE:HD2	18:R:31:LEU:HD13	1.76	0.51
11:K:82:VAL:HG13	11:K:108:ILE:HA	1.92	0.51
25:Z:7:G:H1	25:Z:66:C:H42	1.57	0.51
1:A:145:G:N2	1:A:178:C:C2	2.79	0.51
1:A:913:A:H4'	1:A:914:A:O5'	2.10	0.51
1:A:1119:C:H2'	1:A:1120:G:H8	1.76	0.51
1:A:1251:A:H2'	1:A:1252:A:O4'	2.11	0.51
13:M:84:ILE:HD12	19:S:74:PHE:HE1	1.75	0.51
1:A:744:C:H2'	1:A:745:C:C6	2.46	0.51
4:D:196:LEU:HD13	4:D:197:PRO:HD2	1.93	0.51
1:A:76:C:C2'	1:A:77:G:H5'	2.41	0.51
1:A:145:G:C2	1:A:178:C:N3	2.79	0.51
1:A:1312:G:C2	1:A:1326:C:C2	2.99	0.51
1:A:1339:A:H1'	25:Z:41:C:H1'	1.91	0.51
1:A:1396:A:H4'	1:A:1397:C:H5'	1.92	0.51
1:A:1443:G:C2	1:A:1444:C:N3	2.79	0.51
1:A:1542:U:H1'	18:R:16:PRO:HD2	1.93	0.51
23:X:137:LEU:HB3	23:X:163:MET:SD	2.51	0.51
25:Z:72:A:C2'	25:Z:73:A:N7	2.74	0.51
25:Z:73:A:H8	25:Z:73:A:O5'	1.93	0.51
1:A:441:A:H3'	1:A:442:C:H6	1.75	0.51
1:A:546:G:P	4:D:72:GLU:HB3	2.51	0.51
1:A:1017:G:C2	1:A:1018:C:C2	2.99	0.51
1:A:1456:G:N2	1:A:1457:G:N7	2.59	0.51
2:B:36:ARG:HB2	2:B:41:ILE:HD13	1.93	0.51
4:D:121:VAL:O	4:D:134:ASP:HA	2.11	0.51
13:M:24:GLY:HA3	13:M:66:LEU:HB3	1.93	0.51
1:A:363:A:H5'	12:L:34:ARG:HB3	1.93	0.50
1:A:671:G:N2	1:A:736:C:C2	2.79	0.50
3:C:28:GLN:HA	3:C:31:HIS:HD2	1.76	0.50
1:A:291:C:H2'	1:A:292:G:H8	1.75	0.50
1:A:587:G:H21	8:H:1:MET:HE1	1.77	0.50
1:A:600:C:H2'	1:A:601:C:C6	2.47	0.50
1:A:917:G:H2'	1:A:918:A:H8	1.76	0.50
1:A:1099:G:C2	1:A:1100:C:O2	2.65	0.50
1:A:681:C:H42	1:A:709:G:H1	1.59	0.50
1:A:877:C:H2'	1:A:878:G:H8	1.76	0.50
1:A:1348:U:H2'	1:A:1349:A:C8	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1365:G:C2	1:A:1366:C:C2	2.99	0.50
1:A:743:U:H2'	1:A:744:C:C6	2.46	0.50
1:A:1361:G:C2	1:A:1362:C:O2	2.64	0.50
3:C:14:ILE:CD1	3:C:178:LEU:HD12	2.42	0.50
14:N:7:ILE:O	14:N:7:ILE:HG22	2.12	0.50
20:T:42:GLN:O	20:T:45:GLN:HB2	2.11	0.50
1:A:329:A:H4'	1:A:330:C:OP1	2.12	0.50
1:A:769:G:N1	1:A:770:C:C4	2.79	0.50
1:A:952:U:H2'	1:A:953:G:H8	1.76	0.50
1:A:99:U:H2'	1:A:100:C:C6	2.46	0.50
1:A:985:C:C2	1:A:1221:G:C2	3.00	0.50
1:A:1106:G:C2	1:A:1107:C:C4	3.00	0.50
1:A:1192:C:H2'	1:A:1193:G:O4'	2.12	0.50
1:A:1462:G:N2	1:A:1463:C:C2	2.79	0.50
4:D:109:GLY:HA3	4:D:165:MET:HG3	1.93	0.50
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.94	0.50
25:Z:64:G:C2	25:Z:65:C:C2	3.00	0.50
1:A:61:G:H2'	1:A:62:U:O4'	2.11	0.50
1:A:113:G:H2'	1:A:114:U:C6	2.46	0.50
1:A:189:G:C2	1:A:189(A):C:C2	3.00	0.50
1:A:433:C:H2'	1:A:434:U:C6	2.47	0.50
1:A:1384:C:H2'	1:A:1385:G:C8	2.46	0.50
11:K:110:ASP:HB3	18:R:85:LEU:HB3	1.93	0.50
15:O:39:LEU:HD22	15:O:56:LEU:HB2	1.94	0.50
1:A:623:C:H2'	1:A:624:C:O4'	2.12	0.50
1:A:1412:C:H4'	12:L:95:GLY:HA3	1.94	0.50
14:N:41:ARG:HE	14:N:42:ILE:HG13	1.77	0.50
17:Q:57:VAL:HG12	17:Q:76:LEU:HA	1.94	0.50
24:Y:24:A:H2'	24:Y:25:A:C8	2.47	0.50
1:A:17:U:H2'	1:A:18:C:H6	1.77	0.49
1:A:874:G:N1	1:A:875:C:C4	2.79	0.49
1:A:555:C:H2'	1:A:556:C:C6	2.47	0.49
1:A:590:C:H42	1:A:649:G:H1	1.59	0.49
1:A:814:A:H2'	1:A:816:A:H5''	1.95	0.49
1:A:880:C:H2'	1:A:881:G:C8	2.43	0.49
3:C:9:GLY:HA3	14:N:49:HIS:HA	1.94	0.49
1:A:401:C:H2'	1:A:402:G:H8	1.77	0.49
1:A:501:C:H2'	1:A:502:G:C8	2.47	0.49
1:A:583:A:H2'	1:A:584:G:O4'	2.11	0.49
1:A:674:G:H2'	1:A:675:A:C8	2.46	0.49
1:A:946:A:H2'	1:A:947:G:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:A:H2'	1:A:56:U:H6	1.72	0.49
1:A:504:C:N3	1:A:542:G:C2	2.80	0.49
4:D:177:ASP:HB3	4:D:182:LYS:HB2	1.94	0.49
25:Z:52:G:H2'	25:Z:53:G:C8	2.47	0.49
1:A:1001:A:H2'	1:A:1001(A):G:C8	2.48	0.49
1:A:1365:G:C6	1:A:1366:C:C4	3.00	0.49
1:A:1511:G:H2'	1:A:1512:U:O4'	2.13	0.49
25:Z:41:C:H2'	25:Z:42:G:C8	2.47	0.49
1:A:108:G:H5'	1:A:109:A:H5''	1.94	0.49
1:A:289:G:N2	1:A:290:C:C2	2.80	0.49
1:A:991:U:C4	1:A:1212:U:H1'	2.47	0.49
1:A:1074:G:C2	1:A:1075:C:C2	3.01	0.49
1:A:1133:G:H1	1:A:1141:C:H42	1.61	0.49
1:A:1399:C:C2	1:A:1502:A:N6	2.81	0.49
5:E:27:ARG:HH21	5:E:47:LYS:HB3	1.76	0.49
6:F:99:ALA:HB3	18:R:29:PHE:CE1	2.47	0.49
22:W:17:LEU:HD22	22:W:18:PRO:HD2	1.95	0.49
1:A:883:C:H2'	1:A:884:U:C6	2.47	0.49
1:A:1124:G:P	10:J:35:SER:O	2.69	0.49
1:A:1456:G:N2	1:A:1457:G:C8	2.81	0.49
5:E:33:VAL:HG21	5:E:109:ILE:HG12	1.95	0.49
1:A:998:G:N1	1:A:999:C:C4	2.80	0.49
23:X:3:LYS:CA	23:X:66:ARG:CZ	2.91	0.49
1:A:333:G:N2	1:A:334:C:C2	2.80	0.49
1:A:424:G:H2'	1:A:425:G:H8	1.77	0.49
1:A:734:G:C2	1:A:735:C:C2	3.00	0.49
1:A:931:C:O2	1:A:1387:G:C2	2.66	0.49
1:A:170:U:H2'	1:A:171:A:H8	1.78	0.49
1:A:216:G:C2	1:A:217:C:N3	2.81	0.49
1:A:1023:G:H2'	1:A:1023:G:N3	2.28	0.49
1:A:1532:U:H3'	1:A:1533:C:H5''	1.95	0.49
18:R:59:SER:HB3	18:R:62:GLU:HB2	1.95	0.49
22:W:17:LEU:CB	22:W:18:PRO:CD	2.91	0.49
1:A:171:A:H2'	1:A:172:A:C8	2.47	0.48
1:A:590:C:C2	1:A:650:G:N2	2.81	0.48
1:A:617:G:N1	1:A:618:C:C4	2.81	0.48
1:A:1390:U:H2'	1:A:1391:U:C6	2.48	0.48
1:A:1439:C:O2	1:A:1463:C:O2	2.31	0.48
19:S:37:ARG:HB3	19:S:37:ARG:NH1	2.28	0.48
25:Z:69:C:H2'	25:Z:70:G:H8	1.75	0.48
1:A:354:G:C6	1:A:355:C:N4	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:G:H3'	1:A:577:G:C5'	2.41	0.48
1:A:1353:G:N1	1:A:1354:C:C4	2.81	0.48
1:A:1416:G:H2'	1:A:1417:G:O4'	2.13	0.48
3:C:177:THR:HG23	3:C:180:ALA:HB2	1.95	0.48
10:J:92:THR:H	10:J:94:VAL:HG23	1.78	0.48
1:A:564:C:O2	1:A:564:C:H2'	2.14	0.48
1:A:601:C:H42	1:A:637:G:H1	1.61	0.48
10:J:61:GLU:OE2	14:N:58:LYS:CE	2.61	0.48
11:K:22:HIS:HB3	11:K:29:ILE:HG23	1.95	0.48
23:X:157:LEU:HB2	23:X:160:ASP:HB2	1.96	0.48
1:A:286:G:H2'	1:A:287:U:O4'	2.13	0.48
1:A:579:G:H5'	1:A:728:A:H1'	1.94	0.48
1:A:1086:U:O5'	1:A:1086:U:H6	1.96	0.48
1:A:1266:G:N2	1:A:1270:C:C2	2.82	0.48
4:D:62:GLN:O	4:D:66:ARG:HD3	2.13	0.48
1:A:148:G:C2	1:A:175:C:C2	3.02	0.48
1:A:407:G:C2	1:A:436:C:C2	3.01	0.48
1:A:877:C:H2'	1:A:878:G:C8	2.48	0.48
1:A:1230:C:H5'	25:Z:30:G:H5''	1.95	0.48
1:A:392:G:H2'	1:A:393:A:C8	2.48	0.48
1:A:999:C:O2	1:A:1043:C:O2	2.31	0.48
4:D:64:LEU:HD12	4:D:203:VAL:HG21	1.95	0.48
5:E:11:ILE:HD13	5:E:33:VAL:HB	1.94	0.48
17:Q:48:GLU:HB2	17:Q:50:LYS:HB2	1.96	0.48
1:A:259:G:H2'	1:A:260:G:C8	2.49	0.48
1:A:301:G:H2'	1:A:302:G:H8	1.77	0.48
1:A:671:G:C2	1:A:736:C:N3	2.81	0.48
1:A:1464:G:N2	1:A:1465:C:C2	2.82	0.48
1:A:30:U:H3'	1:A:31:G:C5'	2.42	0.48
1:A:225:C:H2'	1:A:226:G:H8	1.79	0.48
1:A:407:G:H5''	4:D:115:ARG:HD3	1.96	0.48
1:A:1074:G:C6	1:A:1075:C:C4	3.01	0.48
1:A:1420:C:H2'	1:A:1421:G:H8	1.78	0.48
3:C:91:LEU:HD23	3:C:99:VAL:HG21	1.95	0.48
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.94	0.48
5:E:135:THR:O	5:E:139:LEU:HD12	2.13	0.48
23:X:3:LYS:CB	23:X:66:ARG:HH22	1.87	0.48
23:X:11:ILE:HD13	23:X:45:LEU:HD23	1.94	0.48
23:X:45:LEU:HG	23:X:57:ALA:HB1	1.96	0.48
1:A:585:G:C2	1:A:586:C:C2	3.02	0.48
1:A:1105:A:H2'	1:A:1106:G:H8	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1301:U:H1'	1:A:1302:U:OP1	2.14	0.48
1:A:1410:G:H2'	1:A:1411:C:C6	2.49	0.48
1:A:22:G:C2	1:A:23:C:C2	3.01	0.48
1:A:253:U:H2'	1:A:254:G:C8	2.48	0.48
1:A:259:G:C2	1:A:268:C:C2	3.01	0.48
1:A:312:C:H2'	1:A:313:A:C8	2.49	0.48
1:A:504:C:C2	1:A:542:G:N2	2.82	0.48
1:A:1119:C:OP2	9:I:9:ARG:NH2	2.47	0.48
3:C:11:ARG:HG2	3:C:14:ILE:HD12	1.96	0.48
22:W:13:VAL:HB	22:W:50:GLY:H	1.78	0.48
22:W:40:MET:HA	22:W:45:ILE:HD12	1.95	0.48
1:A:21:G:H21	1:A:914:A:H62	1.62	0.47
1:A:616:G:H2'	1:A:617:G:H8	1.79	0.47
1:A:741:G:C5'	15:O:39:LEU:HD21	2.44	0.47
1:A:1127:G:H21	1:A:1147:C:N4	2.11	0.47
1:A:1127:G:N2	1:A:1145:C:C2	2.81	0.47
1:A:1132:C:H2'	1:A:1133:G:C8	2.49	0.47
1:A:1241:G:N2	1:A:1242:C:C2	2.82	0.47
1:A:1384:C:H2'	1:A:1385:G:H8	1.79	0.47
4:D:61:LYS:HD3	4:D:206:PHE:CE1	2.49	0.47
20:T:54:LYS:HA	20:T:57:ARG:HD3	1.95	0.47
1:A:1392:G:H21	1:A:1502:A:H8	1.62	0.47
1:A:19:C:H2'	1:A:20:U:H6	1.77	0.47
1:A:41:G:H2'	1:A:42:G:H8	1.78	0.47
1:A:98:G:H2'	1:A:99:U:O4'	2.13	0.47
1:A:189:G:C6	1:A:189(A):C:C4	3.02	0.47
1:A:824:C:H2'	1:A:825:G:C8	2.48	0.47
1:A:1347:G:O6	9:I:10:ARG:NH2	2.48	0.47
1:A:379:C:H2'	1:A:380:G:O4'	2.14	0.47
1:A:502:G:H2'	1:A:503:C:O4'	2.14	0.47
1:A:504:C:H42	1:A:541:G:H1	1.62	0.47
1:A:567:G:H2'	1:A:568:G:O4'	2.15	0.47
1:A:928:G:H1	1:A:1389:C:N4	2.12	0.47
1:A:1065:U:H4'	1:A:1066:C:O5'	2.15	0.47
11:K:110:ASP:HB2	18:R:88:LYS:HD2	1.95	0.47
15:O:38:ARG:HG3	15:O:38:ARG:HH11	1.78	0.47
1:A:1082:G:H2'	1:A:1083:U:O4'	2.14	0.47
1:A:1478:C:H2'	1:A:1479:C:C6	2.48	0.47
5:E:139:LEU:HA	5:E:142:LEU:HD12	1.95	0.47
1:A:102:G:N2	1:A:103:C:C2	2.83	0.47
1:A:178:C:H2'	1:A:179:A:H8	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:G:N2	1:A:395:C:C2	2.83	0.47
1:A:500:G:C6	1:A:501:C:N4	2.82	0.47
1:A:738:C:H2'	1:A:739:C:C6	2.50	0.47
1:A:1096:C:H2'	1:A:1097:C:C6	2.49	0.47
1:A:1228:C:H5'	13:M:108:ARG:NH2	2.30	0.47
1:A:1488:G:H2'	1:A:1489:G:H8	1.79	0.47
1:A:84:U:H2'	1:A:88:A:O4'	2.15	0.47
1:A:377:G:H1	1:A:386:C:H42	1.62	0.47
1:A:409:G:OP2	4:D:22:LYS:HB3	2.15	0.47
1:A:552:U:H2'	1:A:553:A:C8	2.48	0.47
1:A:953:G:H2'	1:A:954:G:O4'	2.14	0.47
1:A:1060:C:O2	1:A:1198:G:C2	2.67	0.47
1:A:1308:U:H2'	1:A:1309:G:C8	2.50	0.47
1:A:1430:C:C2	1:A:1471:G:N2	2.83	0.47
1:A:1534:A:H61	24:Y:31:U:H3	1.63	0.47
2:B:209:ARG:HA	2:B:239:VAL:HG11	1.96	0.47
3:C:63:ASN:HA	3:C:98:ASN:HB3	1.95	0.47
10:J:16:LEU:HD23	10:J:70:ARG:HG2	1.97	0.47
13:M:99:ARG:HB2	13:M:101:GLN:HE22	1.79	0.47
17:Q:81:ARG:HH21	17:Q:84:LEU:HD22	1.80	0.47
23:X:61:ASP:HB3	23:X:64:LYS:HB3	1.97	0.47
23:X:88:ILE:HG22	23:X:118:VAL:HG13	1.96	0.47
1:A:60:A:H4'	1:A:61:G:O5'	2.14	0.47
1:A:585:G:C6	1:A:586:C:C4	3.03	0.47
1:A:717:C:H2'	1:A:734:G:H5'	1.97	0.47
1:A:725:G:N1	1:A:726:C:C4	2.83	0.47
1:A:957:U:H4'	19:S:79:THR:HG23	1.96	0.47
1:A:1148:U:H2'	1:A:1149:C:O4'	2.14	0.47
18:R:53:ARG:HB3	18:R:53:ARG:HH11	1.78	0.47
20:T:53:LEU:HD23	20:T:100:ILE:HG22	1.96	0.47
1:A:867:G:N2	1:A:868:C:C2	2.83	0.47
1:A:1349:A:H3'	1:A:1350:A:C8	2.46	0.47
12:L:33:ARG:HB3	12:L:60:LEU:HD12	1.96	0.47
23:X:3:LYS:HB2	23:X:66:ARG:HH21	1.73	0.47
1:A:186:C:H5'	20:T:78:ALA:HB1	1.97	0.47
1:A:236:G:C2	1:A:237:C:C2	3.03	0.47
1:A:427:U:O2'	1:A:541:G:OP1	2.25	0.47
1:A:539:A:H2'	1:A:540:G:C8	2.50	0.47
1:A:891:U:H2'	1:A:892:A:H8	1.80	0.47
1:A:1431:C:H42	1:A:1469:G:H1	1.63	0.47
1:A:122:G:C6	1:A:123:C:N3	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:C:H42	1:A:166:G:H1	1.63	0.46
1:A:351:G:H4'	1:A:352:C:OP1	2.15	0.46
1:A:774:G:C2	1:A:806:C:C2	3.03	0.46
1:A:784:C:N3	1:A:799:G:C2	2.84	0.46
1:A:998:G:H1	1:A:1043:C:H42	1.63	0.46
1:A:1116:C:C2	1:A:1185:G:C2	3.03	0.46
1:A:1412:C:H2'	1:A:1413:A:O4'	2.15	0.46
4:D:13:ARG:HH21	4:D:36:ARG:CZ	2.27	0.46
4:D:157:LEU:HD23	4:D:157:LEU:H	1.80	0.46
18:R:26:LEU:HD21	18:R:39:VAL:HG22	1.96	0.46
1:A:509:A:H4'	1:A:510:A:OP1	2.15	0.46
1:A:1076:C:N3	1:A:1082:G:C2	2.83	0.46
3:C:26:LYS:HD3	14:N:36:PHE:HE1	1.78	0.46
1:A:56:U:H2'	1:A:57:G:H8	1.80	0.46
12:L:46:LYS:HG3	12:L:47:LYS:H	1.80	0.46
16:P:62:VAL:CG2	16:P:63:GLY:N	2.78	0.46
25:Z:73:A:C5'	25:Z:73:A:C8	2.98	0.46
1:A:18:C:H2'	1:A:19:C:O4'	2.14	0.46
1:A:93:G:H2'	1:A:96:U:O4'	2.15	0.46
1:A:333:G:C6	1:A:334:C:N4	2.83	0.46
1:A:616:G:H1	1:A:624:C:H42	1.63	0.46
1:A:693:G:H1'	7:G:81:GLY:O	2.16	0.46
1:A:1017:G:C6	1:A:1018:C:C4	3.04	0.46
1:A:1041:A:H2'	1:A:1042:G:H8	1.80	0.46
5:E:107:ARG:HH11	5:E:107:ARG:CB	2.27	0.46
23:X:122:PHE:CE2	23:X:161:MET:HB2	2.51	0.46
1:A:76:C:H2'	1:A:77:G:H5'	1.98	0.46
1:A:1287:A:H2'	1:A:1288:A:C8	2.51	0.46
1:A:1512:U:H2'	1:A:1513:A:H8	1.81	0.46
17:Q:54:GLY:HA2	17:Q:85:VAL:HG21	1.97	0.46
1:A:29:G:C2	1:A:555:C:N3	2.84	0.46
1:A:441:A:H3'	1:A:442:C:C6	2.50	0.46
1:A:546:G:H4'	1:A:548:G:H4'	1.98	0.46
1:A:734:G:C6	1:A:735:C:C4	3.04	0.46
1:A:881:G:C2	1:A:882:C:C2	3.04	0.46
1:A:1164:G:N1	1:A:1165:C:C4	2.84	0.46
2:B:109:SER:O	2:B:112:VAL:HG12	2.16	0.46
12:L:10:LEU:O	12:L:14:GLY:N	2.49	0.46
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	1.98	0.46
19:S:47:HIS:O	19:S:62:ILE:HG22	2.16	0.46
1:A:173:U:H5'	1:A:197:A:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1186:G:H2'	1:A:1187:G:O4'	2.16	0.46
12:L:8:ASN:O	12:L:12:ARG:HG3	2.16	0.46
12:L:27:LEU:HD23	12:L:33:ARG:HH21	1.81	0.46
1:A:1456:G:H2'	1:A:1457:G:O4'	2.15	0.46
3:C:77:ILE:HA	3:C:84:ILE:HB	1.98	0.46
13:M:87:TYR:O	13:M:91:ARG:HG2	2.15	0.46
1:A:200:G:N2	1:A:218:C:C2	2.84	0.46
1:A:714:G:H21	1:A:777:A:H1'	1.81	0.46
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.98	0.46
20:T:84:LEU:HD23	20:T:85:MET:HG3	1.97	0.46
1:A:446:G:N2	1:A:489:C:C2	2.84	0.46
1:A:690:G:OP2	11:K:27:ASN:HB3	2.15	0.46
1:A:1218:C:H2'	1:A:1219:U:C5	2.51	0.46
1:A:1520:G:H2'	1:A:1521:G:H8	1.80	0.46
9:I:48:GLU:H	9:I:49:PRO:HD2	1.81	0.46
1:A:13:U:H3	1:A:915:A:N6	2.14	0.45
1:A:28:G:H2'	1:A:29:G:O4'	2.16	0.45
1:A:72:C:N4	1:A:97:G:H1	2.14	0.45
1:A:661:G:C2	1:A:745:C:N3	2.84	0.45
1:A:885:G:H1	1:A:912:C:N4	2.14	0.45
1:A:1237:C:H5''	1:A:1238:A:O4'	2.15	0.45
2:B:71:VAL:HB	2:B:164:VAL:HA	1.97	0.45
25:Z:64:G:C6	25:Z:65:C:C4	3.04	0.45
1:A:409:G:OP1	4:D:24:GLU:HB3	2.15	0.45
1:A:1281:U:H3	10:J:5:ARG:HH22	1.63	0.45
1:A:1419:G:C6	1:A:1420:C:C4	3.04	0.45
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.97	0.45
6:F:41:GLU:HB2	6:F:62:TRP:CE3	2.50	0.45
8:H:53:VAL:HB	8:H:58:TYR:CD2	2.51	0.45
11:K:121:PRO:HD2	11:K:126:ARG:HD2	1.97	0.45
18:R:39:VAL:HG12	18:R:40:LEU:HD12	1.97	0.45
23:X:87:SER:HA	23:X:117:LYS:O	2.16	0.45
23:X:120:ILE:HD12	23:X:133:GLY:HA2	1.98	0.45
1:A:916:G:H2'	1:A:917:G:C8	2.52	0.45
1:A:1101:A:H4'	1:A:1102:A:O5'	2.16	0.45
1:A:1135:U:H4'	1:A:1136:U:C5	2.51	0.45
1:A:1172:C:H2'	1:A:1173:G:C8	2.51	0.45
1:A:1233:G:C2	1:A:1234:C:C2	3.04	0.45
1:A:1352:C:H2'	1:A:1353:G:C8	2.51	0.45
1:A:1456:G:C2	1:A:1457:G:C8	3.04	0.45
5:E:127:ASN:HD21	5:E:129:ILE:HD12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:84:ASN:HA	6:F:86:ARG:HH21	1.80	0.45
6:F:99:ALA:HB2	18:R:31:LEU:HD11	1.98	0.45
7:G:29:LYS:HB3	7:G:105:VAL:HG21	1.98	0.45
22:W:17:LEU:O	22:W:21:THR:O	2.34	0.45
1:A:13:U:H5'	1:A:14:U:C5	2.52	0.45
1:A:270:A:H2'	1:A:271:C:C6	2.51	0.45
1:A:301:G:H2'	1:A:302:G:C8	2.51	0.45
1:A:504:C:N4	1:A:541:G:H1	2.14	0.45
1:A:537:G:O5'	1:A:537:G:H8	1.99	0.45
1:A:1144:G:C2	1:A:1145:C:N3	2.85	0.45
1:A:1283:G:C6	1:A:1284:C:N4	2.85	0.45
1:A:1489:G:C2	1:A:1490:C:C2	3.04	0.45
2:B:187:LEU:HD12	2:B:205:ASP:HA	1.98	0.45
3:C:113:ALA:N	3:C:114:PRO:CD	2.80	0.45
3:C:187:ALA:HB3	3:C:198:VAL:HB	1.97	0.45
1:A:105:G:C2	1:A:106:C:C2	3.04	0.45
1:A:457:C:H2'	1:A:458:C:H6	1.80	0.45
1:A:632:A:H2'	1:A:633:G:O4'	2.16	0.45
1:A:786:G:C2	1:A:797:C:C2	3.04	0.45
1:A:947:G:C2	1:A:948:C:C2	3.04	0.45
15:O:17:ARG:HH11	15:O:17:ARG:HB3	1.82	0.45
1:A:42:G:C6	1:A:43:C:N3	2.85	0.45
1:A:254:G:H21	17:Q:16:GLN:HE22	1.65	0.45
1:A:542:G:C2	1:A:543:C:C2	3.05	0.45
1:A:577:G:C2	1:A:578:C:C2	3.04	0.45
1:A:729:A:H2'	1:A:730:G:H8	1.82	0.45
1:A:855:G:C6	1:A:856:C:C4	3.05	0.45
1:A:864:A:C2	1:A:865:A:C2	3.05	0.45
1:A:1233:G:N2	1:A:1234:C:C2	2.85	0.45
1:A:1462:G:N1	1:A:1463:C:C4	2.85	0.45
4:D:12:CYS:SG	4:D:19:LEU:HB2	2.57	0.45
4:D:101:LEU:HB2	4:D:138:TYR:HB3	1.98	0.45
23:X:46:VAL:HG11	23:X:65:TRP:CZ3	2.52	0.45
25:Z:73:A:C8	25:Z:73:A:O5'	2.69	0.45
1:A:198:G:H1	1:A:219:C:N4	2.15	0.45
1:A:590:C:C2	1:A:650:G:C2	3.04	0.45
1:A:616:G:H2'	1:A:617:G:C8	2.52	0.45
1:A:1124:G:H1	1:A:1149:C:H42	1.63	0.45
1:A:1265:G:H2'	1:A:1266:G:O4'	2.16	0.45
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.81	0.45
14:N:59:ALA:HB1	14:N:61:TRP:HZ3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:43:A:H2'	25:Z:44:A:C8	2.52	0.45
1:A:568:G:C6	1:A:569:C:N4	2.85	0.45
1:A:984:C:H2'	1:A:985:C:C6	2.52	0.45
1:A:1106:G:C6	1:A:1107:C:N4	2.85	0.45
1:A:1308:U:OP1	13:M:97:PRO:HA	2.16	0.45
1:A:1508:G:C2	1:A:1509:C:C2	3.05	0.45
12:L:93:LEU:HA	12:L:94:PRO:HD3	1.79	0.45
19:S:39:THR:HA	19:S:70:LYS:HA	1.97	0.45
25:Z:51:C:N4	25:Z:63:G:H1	2.15	0.45
1:A:128:G:C2	1:A:234:C:N3	2.84	0.45
1:A:137:C:H2'	1:A:138:G:H8	1.82	0.45
1:A:416:G:C6	1:A:417:C:C4	3.05	0.45
1:A:651:C:H2'	1:A:652:U:C6	2.52	0.45
1:A:881:G:P	12:L:12:ARG:HH22	2.40	0.45
1:A:1114:C:C2	1:A:1187:G:N2	2.85	0.45
1:A:1358:U:C2	1:A:1363(A):A:N6	2.75	0.45
2:B:130:ARG:HH22	3:C:207:VAL:HG21	1.81	0.45
13:M:52:GLU:HA	13:M:55:ARG:HE	1.82	0.45
23:X:64:LYS:O	23:X:68:GLU:HG2	2.16	0.45
23:X:103:LEU:HD12	23:X:140:VAL:HG13	1.99	0.45
1:A:1015:A:H2'	1:A:1016:A:C8	2.52	0.45
1:A:1207:G:C2	1:A:1208:C:C2	3.05	0.45
1:A:1369:C:H2'	1:A:1370:G:C8	2.52	0.45
2:B:208:ILE:HA	2:B:211:ILE:HD12	1.99	0.45
16:P:19:ILE:O	16:P:36:ILE:HG13	2.16	0.45
17:Q:92:ARG:O	17:Q:95:TYR:HB2	2.16	0.45
1:A:372:C:H1'	1:A:373:A:OP2	2.18	0.44
1:A:384:G:C6	1:A:385:C:N4	2.84	0.44
1:A:505:G:H2'	1:A:506:G:H8	1.82	0.44
1:A:577:G:C6	1:A:578:C:C4	3.05	0.44
1:A:1356:G:C2	1:A:1367:C:C2	3.05	0.44
1:A:1363(A):A:H1'	1:A:1365:G:C5	2.52	0.44
5:E:72:GLN:HG2	5:E:73:ASN:HD22	1.82	0.44
18:R:87:ARG:O	18:R:87:ARG:HD3	2.17	0.44
22:W:18:PRO:O	22:W:21:THR:CB	2.65	0.44
1:A:407:G:H2'	1:A:408:A:C8	2.53	0.44
1:A:504:C:C2	1:A:542:G:C2	3.06	0.44
1:A:712:A:H2'	1:A:713:G:O4'	2.17	0.44
3:C:44:GLU:HG2	3:C:52:LEU:HD11	1.99	0.44
10:J:38:ILE:HA	10:J:39:PRO:HD3	1.56	0.44
16:P:53:VAL:O	16:P:57:ARG:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:81:ARG:NH1	17:Q:81:ARG:HB2	2.32	0.44
1:A:201:C:H42	1:A:216:G:H1	1.65	0.44
1:A:501:C:OP1	12:L:117:ARG:NH2	2.50	0.44
1:A:548:G:C2	1:A:549:C:C2	3.05	0.44
1:A:827:U:N3	1:A:872:A:C6	2.77	0.44
1:A:881:G:C6	1:A:882:C:C4	3.05	0.44
1:A:1128:C:H2'	1:A:1139:G:N7	2.31	0.44
2:B:177:ALA:HA	2:B:182:ILE:HD12	1.99	0.44
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.99	0.44
1:A:57:G:C6	1:A:58:C:N3	2.86	0.44
1:A:63:C:H42	1:A:104:G:H1	1.65	0.44
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.99	0.44
13:M:3:ARG:HB3	13:M:7:VAL:HA	1.99	0.44
14:N:24:CYS:HB3	14:N:29:ARG:N	2.32	0.44
15:O:87:ILE:HG22	15:O:88:ARG:H	1.82	0.44
20:T:22:ARG:HA	20:T:25:ARG:HG2	2.00	0.44
23:X:18:VAL:HB	23:X:26:LEU:HB2	2.00	0.44
25:Z:48:C:H5''	25:Z:50:U:OP2	2.18	0.44
1:A:445:G:H1	1:A:489:C:H42	1.64	0.44
1:A:590:C:N4	1:A:649:G:H1	2.15	0.44
1:A:688:G:C6	1:A:689:C:N4	2.85	0.44
1:A:1001(A):G:N1	1:A:1002:G:C6	2.86	0.44
3:C:180:ALA:HA	3:C:206:GLU:HG2	2.00	0.44
4:D:25:ARG:HG3	4:D:30:LYS:HB3	1.98	0.44
10:J:6:ILE:HG22	10:J:98:ILE:HA	1.99	0.44
1:A:42:G:C6	1:A:43:C:C4	3.06	0.44
1:A:42:G:N1	1:A:43:C:C2	2.86	0.44
1:A:392:G:H2'	1:A:393:A:H8	1.81	0.44
1:A:447:G:H2'	1:A:485:G:N2	2.33	0.44
5:E:94:ALA:HB3	5:E:117:ASP:HB3	2.00	0.44
16:P:14:ASN:HA	16:P:42:ARG:HE	1.82	0.44
1:A:763:G:C2	1:A:764:C:C2	3.06	0.44
1:A:1050:G:C2	1:A:1209:C:O2	2.70	0.44
1:A:1126:U:O2	1:A:1126:U:C2'	2.65	0.44
1:A:1419:G:C2	1:A:1420:C:C2	3.06	0.44
1:A:280:C:O2	17:Q:38:ARG:HG3	2.17	0.44
1:A:363:A:OP1	12:L:33:ARG:HA	2.18	0.44
1:A:505:G:H2'	1:A:506:G:C8	2.53	0.44
1:A:518:C:H2'	1:A:530:G:H8	1.74	0.44
1:A:941:G:H2'	1:A:942:G:O4'	2.17	0.44
24:Y:34:A:H3'	24:Y:35:A:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:G:C2	1:A:100:C:O2	2.71	0.44
1:A:184:G:H2'	1:A:185:A:C8	2.52	0.44
1:A:380:G:N2	1:A:383:A:OP2	2.51	0.44
1:A:402:G:N2	1:A:403:C:C2	2.85	0.44
1:A:501:C:H2'	1:A:502:G:H8	1.82	0.44
1:A:679:C:H2'	1:A:680:C:C6	2.53	0.44
1:A:903:G:C2	1:A:904:C:C2	3.06	0.44
1:A:947:G:H2'	1:A:948:C:O4'	2.17	0.44
1:A:948:C:H2'	1:A:949:A:H8	1.82	0.44
1:A:985:C:H2'	1:A:986:A:C8	2.52	0.44
1:A:1062:U:H2'	1:A:1063:C:C6	2.53	0.44
14:N:19:ARG:O	14:N:21:TYR:HD1	2.00	0.44
1:A:1484:C:H2'	1:A:1485:U:O4'	2.18	0.43
3:C:174:PRO:HB2	3:C:177:THR:HG22	2.00	0.43
16:P:27:LYS:C	16:P:29:ASP:H	2.20	0.43
1:A:21:G:H2'	1:A:22:G:H8	1.81	0.43
1:A:256:U:H2'	1:A:257:G:C8	2.53	0.43
1:A:522:C:OP2	12:L:69:TYR:OH	2.34	0.43
1:A:986:A:H1'	19:S:54:GLY:O	2.18	0.43
2:B:132:LYS:C	2:B:134:GLU:H	2.22	0.43
9:I:48:GLU:N	9:I:49:PRO:CD	2.81	0.43
25:Z:64:G:C5	25:Z:65:C:C4	3.06	0.43
1:A:502:G:C2	1:A:503:C:C2	3.06	0.43
1:A:562:C:H41	1:A:884:U:H2'	1.83	0.43
1:A:1050:G:N2	1:A:1051:C:C2	2.86	0.43
1:A:1221:G:OP1	19:S:36:ARG:HD2	2.18	0.43
4:D:26:CYS:HA	4:D:31:CYS:CB	2.41	0.43
4:D:61:LYS:HG3	4:D:203:VAL:HG13	1.99	0.43
6:F:26:ILE:O	6:F:30:LEU:HG	2.18	0.43
1:A:147:G:C2	1:A:176:C:C2	3.06	0.43
1:A:174:C:H2'	1:A:175:C:C6	2.53	0.43
1:A:299:G:C6	1:A:300:A:C6	3.06	0.43
1:A:663:A:H2'	1:A:664:G:O4'	2.18	0.43
1:A:767:A:H2'	1:A:768:A:O4'	2.19	0.43
1:A:810:C:H2'	1:A:811:C:O4'	2.17	0.43
1:A:992:U:H4'	1:A:993:G:O5'	2.18	0.43
1:A:1002:G:H2'	1:A:1003:G:O4'	2.19	0.43
1:A:1097:C:H5''	2:B:140:HIS:CE1	2.53	0.43
1:A:1108:G:H4'	1:A:1191:A:O4'	2.19	0.43
1:A:1125:U:H5'	1:A:1126:U:H5	1.83	0.43
1:A:1182:G:H4'	1:A:1183:A:O5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1253:G:C2	1:A:1254:C:C2	3.07	0.43
2:B:47:THR:HG23	2:B:202:PRO:HD2	1.99	0.43
4:D:22:LYS:HB2	4:D:26:CYS:HB2	1.99	0.43
18:R:52:PRO:HB2	18:R:54:ARG:HG3	1.99	0.43
1:A:67:C:H2'	1:A:68:G:H8	1.83	0.43
1:A:544:G:OP1	4:D:62:GLN:HG3	2.17	0.43
1:A:988:G:C6	1:A:989:C:C4	3.06	0.43
1:A:1283:G:N1	1:A:1284:C:C4	2.87	0.43
1:A:123:C:H2'	1:A:124:G:C8	2.53	0.43
1:A:299:G:H2'	1:A:300:A:C8	2.54	0.43
1:A:369:C:H2'	1:A:370:C:C6	2.54	0.43
1:A:384:G:C2	1:A:385:C:C2	3.06	0.43
1:A:568:G:C2	1:A:883:C:C2	3.06	0.43
1:A:977:A:H2'	1:A:978:A:H5''	2.00	0.43
1:A:1047:G:H1	1:A:1210:C:H42	1.66	0.43
1:A:1144:G:C6	1:A:1145:C:N4	2.86	0.43
1:A:1207:G:C6	1:A:1208:C:C4	3.07	0.43
17:Q:81:ARG:HB2	17:Q:81:ARG:HH11	1.83	0.43
1:A:33:A:H2'	1:A:34:C:C6	2.54	0.43
1:A:236:G:C6	1:A:237:C:C4	3.07	0.43
1:A:328:C:H4'	1:A:329:A:H5'	2.00	0.43
1:A:407:G:C2	1:A:436:C:O2	2.72	0.43
1:A:911:U:H2'	1:A:912:C:C6	2.54	0.43
1:A:952:U:H2'	1:A:953:G:C8	2.54	0.43
1:A:960:U:H4'	1:A:961:U:H5''	2.00	0.43
1:A:1119:C:H2'	1:A:1120:G:C8	2.54	0.43
1:A:1258:G:C6	1:A:1259:C:N4	2.87	0.43
3:C:6:HIS:HA	3:C:7:PRO:HD3	1.82	0.43
5:E:148:VAL:HG22	5:E:152:ARG:HE	1.83	0.43
6:F:3:ARG:HG3	6:F:93:SER:HB3	1.99	0.43
7:G:146:GLU:HA	7:G:149:ARG:CG	2.48	0.43
11:K:31:THR:HG23	11:K:42:TRP:HB3	2.01	0.43
15:O:9:GLN:HA	15:O:12:ILE:HD12	2.01	0.43
20:T:26:ASN:ND2	20:T:71:THR:HA	2.32	0.43
1:A:123:C:H2'	1:A:124:G:H8	1.83	0.43
1:A:381:C:H2'	1:A:382:A:O4'	2.19	0.43
1:A:489:C:H2'	1:A:490:G:H8	1.84	0.43
1:A:500:G:H2'	1:A:501:C:C6	2.54	0.43
1:A:582:U:H2'	1:A:583:A:H8	1.84	0.43
1:A:773:G:H1	1:A:806:C:H42	1.64	0.43
1:A:895:G:C2	1:A:896:C:C2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:C:H2'	1:A:986:A:H8	1.84	0.43
1:A:1021:G:H2'	1:A:1022:G:O4'	2.18	0.43
1:A:1144:G:N2	1:A:1146:A:H62	2.17	0.43
1:A:1253:G:C6	1:A:1254:C:C4	3.07	0.43
2:B:87:ARG:HE	2:B:219:VAL:HG11	1.83	0.43
17:Q:94:ASN:O	17:Q:97:SER:HB3	2.19	0.43
20:T:70:SER:HA	20:T:73:HIS:CD2	2.54	0.43
1:A:1001(A):G:N2	1:A:1040:U:C2	2.86	0.43
1:A:1050:G:C6	1:A:1051:C:N4	2.87	0.43
1:A:1346:A:H2'	7:G:10:ARG:HH22	1.84	0.43
1:A:1505:G:C2'	24:Y:35:A:OP2	2.55	0.43
2:B:15:VAL:HG21	2:B:209:ARG:HG2	2.01	0.43
19:S:53:ASN:HD22	19:S:53:ASN:HA	1.69	0.43
25:Z:36:U:H2'	25:Z:37:A:C8	2.54	0.43
1:A:109:A:C6	1:A:326:G:C6	3.07	0.43
1:A:582:U:H2'	1:A:583:A:C8	2.53	0.43
1:A:688:G:H2'	1:A:689:C:C6	2.54	0.43
1:A:777:A:H2'	1:A:778:G:C8	2.53	0.43
1:A:985:C:N3	1:A:1221:G:C2	2.87	0.43
1:A:1007:C:H42	1:A:1022:G:H1	1.66	0.43
1:A:1324:A:H2'	1:A:1325:C:O4'	2.19	0.43
11:K:14:VAL:HG21	11:K:34:ASP:HB2	2.01	0.43
1:A:276:G:C2	1:A:277:C:C2	3.07	0.42
1:A:416:G:C2	1:A:417:C:C2	3.06	0.42
1:A:418:C:C2	1:A:426:G:C2	3.07	0.42
1:A:683:G:C2	1:A:708:C:N3	2.87	0.42
1:A:1121:U:H2'	1:A:1122:U:C6	2.54	0.42
1:A:1235:U:H5''	21:V:3:LYS:CB	2.49	0.42
1:A:1235:U:H5''	21:V:3:LYS:HB2	2.01	0.42
1:A:1432:G:O2'	1:A:1468:A:N6	2.52	0.42
1:A:1459:C:OP1	20:T:28:ALA:HA	2.19	0.42
11:K:126:ARG:O	11:K:128:ALA:N	2.50	0.42
13:M:108:ARG:HE	13:M:114:ARG:HG2	1.82	0.42
17:Q:68:ARG:HG2	17:Q:68:ARG:HH11	1.84	0.42
1:A:67:C:H42	1:A:102:G:H1	1.66	0.42
1:A:778:G:C6	1:A:779:C:C4	3.06	0.42
1:A:778:G:C2	1:A:779:C:C2	3.08	0.42
1:A:1235:U:H2'	1:A:1236:A:O4'	2.19	0.42
1:A:1491:G:N2	22:W:18:PRO:HB3	2.34	0.42
5:E:87:SER:HA	5:E:125:SER:HB3	2.00	0.42
10:J:49:VAL:HG22	10:J:61:GLU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:72:A:O3'	25:Z:73:A:C8	2.72	0.42
25:Z:76:A:C8	25:Z:76:A:OP2	2.72	0.42
1:A:287:U:H2'	1:A:288:A:H8	1.82	0.42
1:A:538:G:H2'	1:A:539:A:H8	1.84	0.42
1:A:658:G:C6	1:A:749:C:N4	2.87	0.42
1:A:1218:C:H2'	1:A:1219:U:H6	1.82	0.42
1:A:1244:C:H2'	1:A:1245:A:H8	1.85	0.42
1:A:1263:C:H2'	1:A:1264:C:C6	2.54	0.42
1:A:1353:G:C6	1:A:1354:C:N4	2.88	0.42
1:A:1424:C:H42	1:A:1476:G:H1	1.67	0.42
6:F:60:PHE:CZ	18:R:78:LEU:HG	2.54	0.42
1:A:399:G:C6	1:A:400:C:N4	2.87	0.42
1:A:1074:G:C5	1:A:1075:C:C4	3.07	0.42
1:A:1217:C:N4	1:A:1218:C:N4	2.68	0.42
1:A:1225:A:H2'	1:A:1226:C:C6	2.54	0.42
25:Z:8:4SU:O2	25:Z:21:A:H2	2.02	0.42
1:A:166:G:H2'	1:A:167:G:C8	2.55	0.42
1:A:457:C:H2'	1:A:458:C:C6	2.54	0.42
1:A:947:G:C6	1:A:948:C:C4	3.07	0.42
1:A:1491:G:N2	22:W:18:PRO:CB	2.81	0.42
6:F:2:ARG:HD2	6:F:69:GLU:HB3	2.02	0.42
1:A:502:G:C6	1:A:503:C:C4	3.07	0.42
1:A:757:U:H2'	1:A:758:G:O4'	2.18	0.42
1:A:1076:C:C2	1:A:1082:G:C2	3.07	0.42
5:E:15:ARG:HG2	5:E:15:ARG:HH11	1.84	0.42
20:T:67:ALA:HA	20:T:73:HIS:H	1.85	0.42
22:W:37:SER:HB3	22:W:40:MET:HG3	2.02	0.42
23:X:14:LYS:H	23:X:14:LYS:HG3	1.60	0.42
25:Z:8:4SU:O5'	25:Z:8:4SU:H6	2.19	0.42
1:A:262:A:H2'	1:A:263:A:C8	2.54	0.42
1:A:669:U:H2'	1:A:670:G:C8	2.55	0.42
1:A:1004:A:H8	1:A:1038:C:O2	2.02	0.42
1:A:1038:C:H2'	1:A:1039:C:C6	2.54	0.42
1:A:1041:A:H2'	1:A:1042:G:C8	2.55	0.42
1:A:1353:G:C2	1:A:1354:C:C4	3.07	0.42
1:A:1464:G:N1	1:A:1465:C:C4	2.88	0.42
2:B:69:LEU:HB3	2:B:162:ILE:HG12	2.01	0.42
25:Z:39:C:H2'	25:Z:40:C:C6	2.55	0.42
25:Z:40:C:H2'	25:Z:41:C:C6	2.55	0.42
1:A:234:C:H2'	1:A:235:C:C6	2.55	0.42
1:A:309:G:H2'	1:A:310:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:G:C2	1:A:395:C:C2	3.07	0.42
1:A:492:G:H3'	1:A:493:G:C8	2.54	0.42
1:A:500:G:C2	1:A:501:C:C2	3.08	0.42
1:A:600:C:C2	1:A:639:G:C2	3.07	0.42
1:A:1368:G:N1	1:A:1369:C:C4	2.88	0.42
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.20	0.42
1:A:1526:G:C2	1:A:1527:C:C2	3.07	0.42
2:B:32:ILE:H	2:B:32:ILE:HG13	1.74	0.42
23:X:118:VAL:HG21	23:X:165:LEU:HD12	2.01	0.42
25:Z:72:A:H2'	25:Z:73:A:N7	2.35	0.42
1:A:21:G:C2	1:A:22:G:C5	3.07	0.42
1:A:35:G:C2	1:A:36:C:N3	2.88	0.42
1:A:70:G:N1	1:A:100:C:N3	2.68	0.42
1:A:250:A:H4'	1:A:251:G:O5'	2.20	0.42
1:A:289:G:C2	1:A:290:C:C2	3.08	0.42
1:A:333:G:C2	1:A:334:C:C2	3.08	0.42
1:A:372:C:H4'	1:A:373:A:O5'	2.20	0.42
1:A:916:G:H2'	1:A:917:G:H8	1.85	0.42
1:A:1356:G:N2	1:A:1367:C:C2	2.88	0.42
1:A:1479:C:H2'	1:A:1480:G:H8	1.85	0.42
1:A:1492:A:H2'	1:A:1493:A:H5'	2.02	0.42
11:K:114:VAL:HA	11:K:115:PRO:HD3	1.92	0.42
17:Q:56:VAL:HG12	17:Q:78:GLU:O	2.20	0.42
25:Z:7:G:H1	25:Z:66:C:N4	2.15	0.42
1:A:102:G:C2	1:A:103:C:C2	3.07	0.42
1:A:319:G:C2	1:A:320:C:C2	3.08	0.42
1:A:966:G:C2	1:A:967:C:C2	3.08	0.42
1:A:1241:G:C2	1:A:1242:C:C2	3.07	0.42
1:A:1423:G:C6	1:A:1424:C:C4	3.08	0.42
1:A:15:G:H2'	1:A:16:A:C8	2.55	0.41
1:A:43:C:H2'	1:A:44:G:C8	2.55	0.41
1:A:314:C:H2'	1:A:315:A:O4'	2.19	0.41
1:A:617:G:N2	1:A:618:C:C2	2.88	0.41
1:A:772:U:H2'	1:A:773:G:C8	2.55	0.41
1:A:926:G:H3'	1:A:1505:G:H21	1.84	0.41
1:A:1022:G:H2'	1:A:1023:G:C8	2.55	0.41
1:A:1190:G:H5'	3:C:176:HIS:CE1	2.55	0.41
1:A:1266:G:C2	1:A:1270:C:N3	2.88	0.41
1:A:1310:G:N2	1:A:1328:C:C2	2.88	0.41
1:A:1456:G:H5'	1:A:1457:G:OP2	2.20	0.41
1:A:1531:A:H2'	1:A:1532:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:TYR:HB2	4:D:70:ILE:HD11	2.01	0.41
4:D:76:ARG:HG3	4:D:207:TYR:HE1	1.84	0.41
10:J:8:LEU:HB2	10:J:70:ARG:HB2	2.00	0.41
11:K:109:VAL:HG13	18:R:84:LYS:HB2	2.01	0.41
17:Q:68:ARG:HG2	17:Q:68:ARG:NH1	2.35	0.41
1:A:245:C:C2	1:A:284:G:C2	3.08	0.41
1:A:318:G:N2	1:A:336:C:C2	2.89	0.41
1:A:520:A:N1	1:A:536:C:H1'	2.35	0.41
1:A:522:C:H5''	12:L:120:TYR:OH	2.20	0.41
1:A:643:C:H2'	1:A:644:G:C8	2.55	0.41
1:A:1008:C:C2	1:A:1022:G:N2	2.88	0.41
1:A:1119:C:C2	1:A:1155:G:N2	2.88	0.41
2:B:189:ASP:OD1	2:B:189:ASP:N	2.53	0.41
2:B:220:ASP:HA	2:B:230:VAL:HG11	2.02	0.41
3:C:113:ALA:HA	3:C:202:ILE:HD12	2.02	0.41
22:W:9:THR:HG23	22:W:26:LEU:HD22	2.01	0.41
25:Z:36:U:H2'	25:Z:37:A:H8	1.85	0.41
1:A:41:G:H2'	1:A:42:G:C8	2.55	0.41
1:A:436:C:H2'	1:A:437:U:H6	1.83	0.41
1:A:643:C:H2'	1:A:644:G:H8	1.85	0.41
1:A:742:G:H2'	1:A:743:U:O4'	2.19	0.41
1:A:1095:U:H2'	1:A:1096:C:C6	2.55	0.41
1:A:1476:G:C2	1:A:1477:C:C2	3.08	0.41
4:D:39:PRO:O	4:D:44:GLY:HA3	2.20	0.41
12:L:51:ALA:HB3	12:L:53:ARG:HH21	1.84	0.41
17:Q:26:GLN:HG2	17:Q:37:LYS:HA	2.01	0.41
1:A:42:G:C2	1:A:43:C:C2	3.09	0.41
1:A:51:A:N7	1:A:114:U:O2'	2.53	0.41
1:A:613:C:H2'	1:A:614:A:H8	1.85	0.41
1:A:1244:C:H2'	1:A:1245:A:C8	2.55	0.41
1:A:1407:C:H5''	23:X:123:ARG:HG3	2.03	0.41
1:A:1507:A:H2'	1:A:1508:G:H8	1.83	0.41
5:E:106:PRO:HA	5:E:109:ILE:HD12	2.03	0.41
7:G:81:GLY:N	24:Y:32:A:OP1	2.54	0.41
9:I:89:ASN:HD21	9:I:91:ASP:HB2	1.85	0.41
13:M:84:ILE:HD12	19:S:74:PHE:CE1	2.54	0.41
1:A:187:C:C2	20:T:105:SER:HB2	2.56	0.41
1:A:310:G:C2	1:A:311:C:C2	3.09	0.41
1:A:370:C:N3	1:A:392:G:C2	2.88	0.41
1:A:688:G:C2	1:A:689:C:C2	3.08	0.41
1:A:855:G:C2	1:A:856:C:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:G:H21	2:B:107:THR:HG21	1.85	0.41
1:A:1111:A:N1	3:C:177:THR:HB	2.35	0.41
1:A:1346:A:H4'	1:A:1347:G:O5'	2.21	0.41
1:A:1404:C:H2'	1:A:1405:G:C8	2.56	0.41
1:A:1489:G:H2'	1:A:1490:C:O4'	2.20	0.41
2:B:12:GLU:HG3	2:B:16:HIS:HB2	2.02	0.41
3:C:13:GLY:HA3	14:N:57:ARG:HE	1.85	0.41
16:P:2:VAL:HG13	16:P:64:ALA:HA	2.03	0.41
18:R:32:ARG:HA	18:R:69:THR:HG21	2.02	0.41
23:X:135:ARG:O	23:X:139:ARG:HB2	2.20	0.41
1:A:198:G:H1	1:A:219:C:H42	1.67	0.41
1:A:542:G:N2	1:A:543:C:C2	2.89	0.41
1:A:1306:A:H2'	1:A:1307:U:O4'	2.21	0.41
1:A:1423:G:C2	1:A:1424:C:C2	3.08	0.41
1:A:1489:G:C6	1:A:1490:C:C4	3.08	0.41
5:E:110:LEU:HD13	5:E:118:ILE:HG13	2.03	0.41
6:F:94:GLN:HB3	18:R:32:ARG:HD3	2.03	0.41
10:J:38:ILE:HG13	10:J:39:PRO:N	2.36	0.41
17:Q:98:LEU:HD23	17:Q:98:LEU:H	1.85	0.41
19:S:32:LYS:HA	19:S:50:ALA:HB3	2.02	0.41
22:W:13:VAL:HG22	22:W:24:VAL:HG22	2.03	0.41
1:A:11:G:H2'	1:A:12:U:O4'	2.21	0.41
1:A:354:G:N1	1:A:355:C:C4	2.89	0.41
1:A:434:U:H2'	1:A:435:C:C6	2.56	0.41
1:A:779:C:H2'	1:A:780:A:O4'	2.21	0.41
1:A:988:G:C2	1:A:989:C:C2	3.09	0.41
1:A:1074:G:C6	1:A:1075:C:N3	2.88	0.41
1:A:1076:C:C2	1:A:1082:G:N2	2.88	0.41
1:A:1169:A:H2'	1:A:1170:A:O4'	2.21	0.41
1:A:1387:G:C2	1:A:1388:C:C2	3.09	0.41
3:C:14:ILE:HD11	3:C:178:LEU:HD12	2.02	0.41
4:D:148:VAL:HB	4:D:181:MET:HB3	2.01	0.41
16:P:20:VAL:HG23	16:P:35:LYS:HA	2.02	0.41
1:A:98:G:C2	1:A:99:U:C2	3.08	0.41
1:A:105:G:C6	1:A:106:C:C4	3.08	0.41
1:A:110:C:H4'	16:P:25:ARG:HB3	2.03	0.41
1:A:285:G:H2'	1:A:286:G:O4'	2.20	0.41
1:A:399:G:C2	1:A:400:C:C2	3.08	0.41
1:A:681:C:N4	1:A:709:G:H1	2.18	0.41
1:A:774:G:N2	1:A:806:C:C2	2.89	0.41
1:A:948:C:OP1	13:M:109:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:A:H2'	1:A:1131:G:C8	2.55	0.41
4:D:162:LEU:HD12	4:D:178:VAL:HG23	2.02	0.41
5:E:80:ILE:HD12	5:E:91:LEU:HB3	2.03	0.41
5:E:107:ARG:HG2	5:E:108:ALA:N	2.35	0.41
8:H:7:ALA:HA	8:H:10:LEU:HD12	2.03	0.41
12:L:24:VAL:HA	12:L:25:PRO:HD3	1.92	0.41
13:M:3:ARG:HH21	13:M:9:ILE:HD11	1.86	0.41
23:X:46:VAL:HG22	23:X:62:TYR:HB2	2.03	0.41
25:Z:31:G:H2'	25:Z:32:OMC:C6	2.56	0.41
1:A:276:G:C6	1:A:277:C:C4	3.09	0.41
1:A:524:G:N2	1:A:525:C:C2	2.89	0.41
1:A:711:G:H2'	1:A:712:A:C8	2.56	0.41
1:A:825:G:C6	1:A:826:C:C4	3.09	0.41
1:A:861:G:C2	1:A:862:C:C2	3.09	0.41
1:A:876:G:C6	1:A:877:C:N4	2.89	0.41
1:A:881:G:OP2	12:L:12:ARG:NH2	2.53	0.41
1:A:1315:U:O2'	1:A:1360:A:N3	2.48	0.41
2:B:188:ALA:HB3	2:B:200:ILE:HG23	2.03	0.41
4:D:64:LEU:HD22	4:D:75:PHE:HE1	1.86	0.41
5:E:91:LEU:HD11	5:E:110:LEU:HD11	2.03	0.41
8:H:111:ILE:HG22	8:H:134:ILE:HD12	2.02	0.41
10:J:8:LEU:CB	10:J:70:ARG:HB2	2.51	0.41
10:J:30:SER:HB3	10:J:84:GLN:NE2	2.36	0.41
11:K:84:VAL:HG23	11:K:110:ASP:HA	2.01	0.41
19:S:6:LYS:HG3	19:S:7:LYS:H	1.85	0.41
20:T:43:LEU:HD23	20:T:48:LYS:HD2	2.02	0.41
25:Z:6:G:C2	25:Z:68:C:C2	3.09	0.41
1:A:229:U:H2'	1:A:230:G:H8	1.86	0.41
1:A:356:A:H2'	1:A:357:G:O4'	2.21	0.41
1:A:725:G:C6	1:A:726:C:N4	2.89	0.41
1:A:817:C:C2	1:A:819:A:O4'	2.74	0.41
1:A:838:G:N2	1:A:849:C:C2	2.88	0.41
1:A:983:A:H5''	1:A:984:C:H5	1.86	0.41
1:A:1333:A:H2'	1:A:1334:G:O4'	2.21	0.41
1:A:1422:G:H1	1:A:1478:C:N4	2.19	0.41
1:A:1535:C:C2	1:A:1536:C:C5	3.09	0.41
15:O:54:ARG:HG3	15:O:55:GLY:N	2.36	0.41
23:X:103:LEU:HD11	23:X:143:ASP:HB2	2.02	0.41
1:A:166:G:H2'	1:A:167:G:H8	1.86	0.40
1:A:403:C:H5''	4:D:136:PRO:HD2	2.02	0.40
1:A:584:G:H2'	1:A:585:G:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:G:C6	1:A:764:C:C4	3.09	0.40
1:A:895:G:C6	1:A:896:C:C4	3.08	0.40
4:D:3:ARG:HE	4:D:118:ARG:NE	2.19	0.40
10:J:54:PHE:H	14:N:41:ARG:NH2	2.19	0.40
12:L:90:VAL:HG11	12:L:93:LEU:HD12	2.03	0.40
1:A:98:G:H2'	1:A:99:U:C6	2.56	0.40
1:A:216:G:C2	1:A:217:C:C2	3.09	0.40
1:A:377:G:H2'	1:A:378:G:C8	2.57	0.40
1:A:445:G:H2'	1:A:446:G:O4'	2.20	0.40
1:A:550:G:H2'	1:A:551:U:C6	2.56	0.40
1:A:601:C:C2	1:A:638:G:N2	2.90	0.40
4:D:50:ARG:HA	4:D:51:PRO:HD3	1.85	0.40
9:I:112:LYS:HA	9:I:119:ALA:HA	2.03	0.40
1:A:129(A):G:O2'	1:A:130:A:OP2	2.31	0.40
1:A:131:C:C2	1:A:232:G:C2	3.09	0.40
1:A:284:G:H2'	1:A:285:G:C8	2.57	0.40
1:A:542:G:C6	1:A:543:C:N4	2.89	0.40
1:A:568:G:N2	1:A:569:C:C2	2.90	0.40
1:A:887:G:H3'	1:A:888:G:H8	1.87	0.40
1:A:903:G:C6	1:A:904:C:C4	3.10	0.40
1:A:1052:U:H2'	1:A:1200:C:H41	1.86	0.40
1:A:1115:C:C2	1:A:1186:G:N2	2.90	0.40
1:A:1493:A:N9	22:W:18:PRO:HA	2.35	0.40
9:I:93:ARG:HA	9:I:96:LEU:HB2	2.03	0.40
10:J:38:ILE:HG23	10:J:71:LEU:H	1.86	0.40
1:A:187:C:N3	20:T:105:SER:HB2	2.37	0.40
1:A:310:G:C6	1:A:311:C:C4	3.09	0.40
1:A:824:C:H42	1:A:876:G:H1	1.70	0.40
1:A:825:G:C2	1:A:826:C:C2	3.08	0.40
1:A:1030(B):C:H2'	1:A:1030(C):G:O4'	2.22	0.40
1:A:1157:A:H8	1:A:1157:A:OP1	2.05	0.40
1:A:1216:G:N1	1:A:1217:C:C4	2.90	0.40
1:A:1459:C:H2'	1:A:1460:A:O4'	2.21	0.40
4:D:67:ILE:O	4:D:114:ARG:HD2	2.22	0.40
6:F:44:GLY:HA2	6:F:59:TYR:CZ	2.57	0.40
23:X:3:LYS:HA	23:X:66:ARG:CZ	2.52	0.40
23:X:43:LEU:HB3	23:X:60:MET:HA	2.03	0.40
1:A:13:U:N3	1:A:915:A:N6	2.70	0.40
1:A:222:U:O3'	20:T:68:LYS:NZ	2.55	0.40
1:A:319:G:C6	1:A:320:C:C4	3.09	0.40
1:A:373:A:H2'	1:A:374:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:G:C2	1:A:403:C:C2	3.10	0.40
1:A:407:G:H2'	1:A:408:A:H8	1.86	0.40
1:A:661:G:N2	1:A:745:C:C2	2.90	0.40
1:A:662:G:H2'	1:A:663:A:H8	1.81	0.40
1:A:885:G:H1'	1:A:914:A:N1	2.37	0.40
1:A:1488:G:H2'	1:A:1489:G:C8	2.56	0.40
3:C:14:ILE:HD12	3:C:178:LEU:HD12	2.02	0.40
3:C:27:LYS:O	3:C:31:HIS:CD2	2.74	0.40
3:C:137:ALA:O	3:C:141:VAL:HG23	2.22	0.40
8:H:134:ILE:H	8:H:134:ILE:HG13	1.60	0.40
10:J:64:GLU:HG2	14:N:59:ALA:HA	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	189 (82%)	32 (14%)	11 (5%)	2	23
3	C	204/239 (85%)	179 (88%)	19 (9%)	6 (3%)	4	31
4	D	206/209 (99%)	185 (90%)	18 (9%)	3 (2%)	10	46
5	E	148/162 (91%)	132 (89%)	13 (9%)	3 (2%)	7	39
6	F	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	4	31
7	G	153/156 (98%)	139 (91%)	11 (7%)	3 (2%)	7	39
8	H	136/138 (99%)	124 (91%)	10 (7%)	2 (2%)	10	46
9	I	125/128 (98%)	106 (85%)	17 (14%)	2 (2%)	9	44
10	J	96/105 (91%)	81 (84%)	10 (10%)	5 (5%)	2	21
11	K	117/129 (91%)	101 (86%)	12 (10%)	4 (3%)	3	29
12	L	122/132 (92%)	104 (85%)	14 (12%)	4 (3%)	4	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	116/126 (92%)	106 (91%)	10 (9%)	0	100	100
14	N	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	2	21
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	P	81/88 (92%)	74 (91%)	7 (9%)	0	100	100
17	Q	97/105 (92%)	88 (91%)	9 (9%)	0	100	100
18	R	71/88 (81%)	66 (93%)	3 (4%)	2 (3%)	5	32
19	S	80/93 (86%)	70 (88%)	6 (8%)	4 (5%)	2	22
20	T	97/106 (92%)	84 (87%)	9 (9%)	4 (4%)	3	25
21	V	22/27 (82%)	22 (100%)	0	0	100	100
22	W	69/72 (96%)	58 (84%)	9 (13%)	2 (3%)	4	31
23	X	160/171 (94%)	138 (86%)	20 (12%)	2 (1%)	12	48
26	a	496/571 (87%)	434 (88%)	48 (10%)	14 (3%)	5	32
All	All	3071/3352 (92%)	2698 (88%)	296 (10%)	77 (2%)	9	34

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	24	TRP
6	F	69	GLU
9	I	119	ALA
10	J	34	VAL
10	J	39	PRO
11	K	89	ALA
12	L	27	LEU
12	L	45	PRO
23	X	8	ASN
23	X	54	PRO
26	a	550	ASP
2	B	21	ARG
3	C	81	GLY
3	C	175	LEU
4	D	5	ILE
4	D	42	GLN
7	G	55	GLY
8	H	92	ARG
9	I	56	LEU
11	K	127	LYS
2	B	9	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	16	HIS
2	B	99	GLY
2	B	130	ARG
2	B	229	VAL
2	B	233	SER
3	C	4	LYS
3	C	127	ARG
5	E	74	GLY
6	F	96	PRO
10	J	54	PHE
10	J	55	LYS
11	K	126	ARG
14	N	22	THR
14	N	23	ARG
19	S	30	LEU
20	T	95	ALA
26	a	73	PRO
26	a	138	GLN
26	a	260	ALA
26	a	354	ARG
26	a	468	GLY
5	E	39	GLY
7	G	7	ALA
7	G	114	ARG
12	L	25	PRO
12	L	105	TYR
18	R	17	SER
19	S	81	ARG
22	W	2	LYS
22	W	50	GLY
26	a	494	LYS
26	a	541	GLN
26	a	556	ARG
2	B	23	ARG
2	B	133	LYS
2	B	228	GLY
3	C	10	PHE
6	F	93	SER
8	H	5	PRO
14	N	15	LYS
19	S	6	LYS
19	S	13	ASP

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Mol	Chain	Res	Type
20	T	97	ALA
20	T	98	PRO
26	a	99	ALA
3	C	14	ILE
18	R	87	ARG
20	T	49	ALA
26	a	557	GLU
10	J	49	VAL
4	D	142	PRO
5	E	96	PRO
26	a	140	GLY
26	a	493	GLY
11	K	14	VAL
26	a	127	THR

### 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%)	166 (82%)	36 (18%)	2 11
3	C	160/188 (85%)	143 (89%)	17 (11%)	6 26
4	D	180/181 (99%)	148 (82%)	32 (18%)	2 11
5	E	115/123 (94%)	80 (70%)	35 (30%)	0 2
6	F	90/90 (100%)	76 (84%)	14 (16%)	2 15
7	G	126/127 (99%)	112 (89%)	14 (11%)	6 24
8	H	119/119 (100%)	96 (81%)	23 (19%)	1 9
9	I	98/99 (99%)	85 (87%)	13 (13%)	4 19
10	J	87/92 (95%)	75 (86%)	12 (14%)	3 19
11	K	90/99 (91%)	72 (80%)	18 (20%)	1 8
12	L	104/109 (95%)	89 (86%)	15 (14%)	3 17
13	M	94/101 (93%)	80 (85%)	14 (15%)	3 16
14	N	49/50 (98%)	42 (86%)	7 (14%)	3 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	79/80 (99%)	59 (75%)	20 (25%)	0	4
16	P	72/74 (97%)	64 (89%)	8 (11%)	6	24
17	Q	94/97 (97%)	85 (90%)	9 (10%)	8	29
18	R	64/77 (83%)	46 (72%)	18 (28%)	0	3
19	S	71/80 (89%)	60 (84%)	11 (16%)	2	15
20	T	76/82 (93%)	64 (84%)	12 (16%)	2	15
21	V	19/22 (86%)	16 (84%)	3 (16%)	2	15
22	W	62/63 (98%)	55 (89%)	7 (11%)	6	24
23	X	145/150 (97%)	125 (86%)	20 (14%)	3	19
26	a	374/460 (81%)	355 (95%)	19 (5%)	24	50
All	All	2570/2783 (92%)	2193 (85%)	377 (15%)	6	16

All (377) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	11	LEU
2	B	16	HIS
2	B	21	ARG
2	B	23	ARG
2	B	44	LEU
2	B	45	GLN
2	B	49	GLU
2	B	51	LEU
2	B	52	GLU
2	B	61	LEU
2	B	64	ARG
2	B	83	MET
2	B	93	VAL
2	B	102	LEU
2	B	107	THR
2	B	108	ILE
2	B	112	VAL
2	B	130	ARG
2	B	136	VAL
2	B	142	LEU
2	B	144	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	157	ARG
2	B	168	THR
2	B	172	ILE
2	B	178	ARG
2	B	187	LEU
2	B	204	ASN
2	B	205	ASP
2	B	206	ASP
2	B	209	ARG
2	B	211	ILE
2	B	220	ASP
2	B	221	LEU
2	B	229	VAL
3	C	3	ASN
3	C	16	ARG
3	C	42	LEU
3	C	52	LEU
3	C	59	ARG
3	C	83	ARG
3	C	87	LEU
3	C	101	LEU
3	C	104	GLN
3	C	107	GLN
3	C	108	ASN
3	C	115	LEU
3	C	119	ARG
3	C	136	GLN
3	C	165	THR
3	C	175	LEU
3	C	191	THR
4	D	3	ARG
4	D	8	VAL
4	D	10	ARG
4	D	11	LEU
4	D	13	ARG
4	D	15	GLU
4	D	19	LEU
4	D	24	GLU
4	D	25	ARG
4	D	26	CYS
4	D	35	ARG
4	D	49	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	D	50	ARG
4	D	66	ARG
4	D	70	ILE
4	D	78	LEU
4	D	94	LEU
4	D	112	VAL
4	D	118	ARG
4	D	119	GLN
4	D	122	ARG
4	D	131	ARG
4	D	132	ARG
4	D	135	LEU
4	D	141	ARG
4	D	144	ASP
4	D	159	ARG
4	D	162	LEU
4	D	165	MET
4	D	176	LEU
4	D	192	GLU
4	D	196	LEU
5	E	5	ASP
5	E	7	GLU
5	E	14	ARG
5	E	15	ARG
5	E	19	MET
5	E	24	ARG
5	E	25	ARG
5	E	32	VAL
5	E	34	VAL
5	E	40	ARG
5	E	41	VAL
5	E	55	VAL
5	E	64	ARG
5	E	68	GLU
5	E	71	LEU
5	E	76	ILE
5	E	80	ILE
5	E	83	GLU
5	E	90	VAL
5	E	91	LEU
5	E	107	ARG
5	E	116	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	E	118	ILE
5	E	123	LEU
5	E	126	ARG
5	E	133	TYR
5	E	136	MET
5	E	139	LEU
5	E	142	LEU
5	E	143	ARG
5	E	144	THR
5	E	147	ASP
5	E	148	VAL
5	E	151	LEU
5	E	152	ARG
6	F	3	ARG
6	F	18	GLN
6	F	19	LEU
6	F	28	ARG
6	F	42	GLU
6	F	45	LEU
6	F	47	ARG
6	F	54	LYS
6	F	61	LEU
6	F	64	GLN
6	F	69	GLU
6	F	75	LEU
6	F	82	ARG
6	F	86	ARG
7	G	16	LEU
7	G	45	ASP
7	G	52	GLU
7	G	57	GLU
7	G	72	ARG
7	G	75	VAL
7	G	84	ASN
7	G	91	VAL
7	G	94	ARG
7	G	96	GLN
7	G	99	LEU
7	G	113	GLU
7	G	126	ASP
7	G	156	TRP
8	H	2	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	H	6	ILE
8	H	18	ARG
8	H	21	LYS
8	H	26	VAL
8	H	34	GLU
8	H	45	ILE
8	H	50	ARG
8	H	56	LYS
8	H	58	TYR
8	H	70	GLN
8	H	75	ARG
8	H	83	ILE
8	H	85	ARG
8	H	102	ARG
8	H	104	ARG
8	H	114	THR
8	H	121	ASP
8	H	122	ARG
8	H	127	LEU
8	H	129	VAL
8	H	133	LEU
8	H	134	ILE
9	I	38	GLN
9	I	40	LEU
9	I	44	VAL
9	I	54	ASP
9	I	78	LYS
9	I	85	LEU
9	I	87	GLN
9	I	104	ARG
9	I	112	LYS
9	I	118	LYS
9	I	120	ARG
9	I	121	ARG
9	I	128	ARG
10	J	16	LEU
10	J	17	ASP
10	J	19	SER
10	J	43	ARG
10	J	51	ARG
10	J	57	LYS
10	J	59	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	J	61	GLU
10	J	70	ARG
10	J	73	ASP
10	J	89	ASP
10	J	94	VAL
11	K	12	ARG
11	K	18	ARG
11	K	29	ILE
11	K	34	ASP
11	K	40	ILE
11	K	41	THR
11	K	48	ILE
11	K	54	ARG
11	K	57	THR
11	K	77	MET
11	K	84	VAL
11	K	85	ARG
11	K	87	THR
11	K	91	ARG
11	K	92	GLU
11	K	93	GLN
11	K	96	ARG
11	K	116	HIS
12	L	7	ILE
12	L	15	ARG
12	L	19	ARG
12	L	39	VAL
12	L	41	ARG
12	L	42	THR
12	L	52	LEU
12	L	55	VAL
12	L	59	ARG
12	L	60	LEU
12	L	83	VAL
12	L	97	ARG
12	L	102	ARG
12	L	113	ARG
12	L	127	GLU
13	M	3	ARG
13	M	9	ILE
13	M	32	GLU
13	M	37	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	M	43	THR
13	M	48	LEU
13	M	49	THR
13	M	66	LEU
13	M	70	LEU
13	M	83	ASP
13	M	86	CYS
13	M	102	ARG
13	M	110	ARG
13	M	115	LYS
14	N	8	GLU
14	N	12	ARG
14	N	17	LYS
14	N	26	ARG
14	N	31	ARG
14	N	32	SER
14	N	41	ARG
15	O	10	LYS
15	O	17	ARG
15	O	29	VAL
15	O	31	LEU
15	O	37	ASN
15	O	38	ARG
15	O	39	LEU
15	O	41	GLU
15	O	43	LEU
15	O	49	ASP
15	O	54	ARG
15	O	56	LEU
15	O	64	ARG
15	O	66	LEU
15	O	70	LEU
15	O	71	GLN
15	O	72	ARG
15	O	77	ARG
15	O	83	GLU
15	O	88	ARG
16	P	1	MET
16	P	5	ARG
16	P	20	VAL
16	P	27	LYS
16	P	28	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
16	P	44	THR
16	P	49	LEU
16	P	81	ARG
17	Q	25	ARG
17	Q	34	LYS
17	Q	62	SER
17	Q	63	ARG
17	Q	68	ARG
17	Q	76	LEU
17	Q	81	ARG
17	Q	83	ASP
17	Q	92	ARG
18	R	18	ARG
18	R	23	LYS
18	R	29	PHE
18	R	31	LEU
18	R	35	ARG
18	R	36	ASN
18	R	39	VAL
18	R	42	ARG
18	R	44	LEU
18	R	46	GLU
18	R	54	ARG
18	R	63	GLN
18	R	68	LYS
18	R	75	ILE
18	R	76	LEU
18	R	81	PHE
18	R	84	LYS
18	R	87	ARG
19	S	5	LEU
19	S	7	LYS
19	S	25	LYS
19	S	29	ARG
19	S	37	ARG
19	S	39	THR
19	S	41	VAL
19	S	53	ASN
19	S	63	THR
19	S	77	THR
19	S	80	TYR
20	T	15	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
20	T	22	ARG
20	T	23	ARG
20	T	24	LEU
20	T	25	ARG
20	T	36	LEU
20	T	43	LEU
20	T	53	LEU
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	84	LEU
21	V	9	ARG
21	V	12	LYS
21	V	25	LYS
22	W	14	THR
22	W	23	ARG
22	W	27	ASP
22	W	32	ILE
22	W	46	ARG
22	W	47	ILE
22	W	58	THR
23	X	3	LYS
23	X	4	GLU
23	X	12	ARG
23	X	18	VAL
23	X	24	LYS
23	X	28	ILE
23	X	30	ASP
23	X	32	ARG
23	X	59	ILE
23	X	67	TYR
23	X	73	GLU
23	X	74	LYS
23	X	77	ARG
23	X	88	ILE
23	X	92	VAL
23	X	105	HIS
23	X	119	THR
23	X	125	ARG
23	X	163	MET
23	X	164	LEU
26	a	72	ARG

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Mol	Chain	Res	Type
26	a	78	ILE
26	a	83	ASP
26	a	86	LYS
26	a	87	THR
26	a	89	LEU
26	a	126	ASP
26	a	135	THR
26	a	154	ASP
26	a	167	HIS
26	a	308	VAL
26	a	311	LEU
26	a	317	PRO
26	a	321	ASP
26	a	397	THR
26	a	419	LEU
26	a	490	LEU
26	a	520	VAL
26	a	552	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	212	GLN
3	C	3	ASN
3	C	28	GLN
3	C	31	HIS
3	C	104	GLN
3	C	108	ASN
3	C	123	GLN
4	D	123	HIS
4	D	129	ASN
4	D	161	ASN
4	D	201	GLN
5	E	73	ASN
6	F	13	ASN
6	F	73	ASN
7	G	122	HIS
8	H	15	ASN
9	I	89	ASN
10	J	56	HIS
10	J	68	HIS
10	J	84	GLN

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Mol	Chain	Res	Type
11	K	13	GLN
12	L	8	ASN
12	L	49	ASN
12	L	75	HIS
13	M	77	ASN
15	O	9	GLN
17	Q	16	GLN
18	R	36	ASN
18	R	63	GLN
19	S	47	HIS
19	S	53	ASN
20	T	26	ASN
23	X	111	GLN
23	X	138	ASN
23	X	162	ASN
26	a	108	GLN
26	a	382	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1509/1522 (99%)	407 (26%)	89 (5%)
24	Y	19/42 (45%)	7 (36%)	1 (5%)
25	Z	76/77 (98%)	27 (35%)	4 (5%)
All	All	1604/1641 (97%)	441 (27%)	94 (5%)

All (441) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	13	U
1	A	19	C
1	A	22	G
1	A	26	A
1	A	30	U
1	A	31	G
1	A	32	A
1	A	39	G
1	A	40	C
1	A	44	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	63	C
1	A	68	G
1	A	73	G
1	A	76	C
1	A	77	G
1	A	78	G
1	A	79	G
1	A	81	U
1	A	82	U
1	A	91	C
1	A	97	G
1	A	98	G
1	A	100	C
1	A	108	G
1	A	110	C
1	A	116	A
1	A	120	A
1	A	121	C
1	A	122	G
1	A	123	C
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	163	C
1	A	181	G
1	A	182	U
1	A	189(E)	U
1	A	189(F)	U
1	A	189(G)	G
1	A	189(H)	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	195	A
1	A	197	A
1	A	198	G
1	A	199	G
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	222	U
1	A	244	U
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	253	U
1	A	262	A
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	289	G
1	A	291	C
1	A	298	A
1	A	299	G
1	A	300	A
1	A	301	G
1	A	306	G
1	A	315	A
1	A	316	G
1	A	321	A
1	A	325	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	342	C
1	A	344	A
1	A	345	C
1	A	347	G
1	A	350	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	351	G
1	A	352	C
1	A	353	A
1	A	367	U
1	A	368	U
1	A	372	C
1	A	373	A
1	A	375	U
1	A	378	G
1	A	384	G
1	A	390	C
1	A	392	G
1	A	397	A
1	A	398	C
1	A	399	G
1	A	406	G
1	A	412	A
1	A	413	G
1	A	419	C
1	A	421	U
1	A	422	C
1	A	423	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	446	G
1	A	451	A
1	A	452	A
1	A	453	A
1	A	454	C
1	A	455	C
1	A	470	C
1	A	480	U
1	A	484	G
1	A	485	G
1	A	492	G
1	A	495	A
1	A	496	A
1	A	498	U
1	A	510	A
1	A	511	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	529	G
1	A	531	U
1	A	532	A
1	A	534	U
1	A	535	A
1	A	545	C
1	A	547	A
1	A	548	G
1	A	550	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	588	G
1	A	593	G
1	A	596	C
1	A	607	A
1	A	641	U
1	A	653	A
1	A	665	A
1	A	672	U
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	715	A
1	A	716	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	717	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	728	A
1	A	731	G
1	A	748	C
1	A	749	C
1	A	752	G
1	A	753	A
1	A	755	G
1	A	760	G
1	A	785	G
1	A	787	A
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	804	U
1	A	805	C
1	A	810	C
1	A	812	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	818	G
1	A	820	U
1	A	821	G
1	A	828	A
1	A	835	U
1	A	839	U
1	A	841	U
1	A	851	G
1	A	853	G
1	A	855	G
1	A	864	A
1	A	873	A
1	A	876	G
1	A	885	G
1	A	887	G
1	A	889	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	891	U
1	A	900	A
1	A	902	G
1	A	914	A
1	A	919	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	956	U
1	A	958	A
1	A	960	U
1	A	961	U
1	A	965	A
1	A	966	G
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	998	G
1	A	1000	U
1	A	1002	G
1	A	1005	A
1	A	1007	C
1	A	1009	G
1	A	1023	G
1	A	1025	U
1	A	1026	G
1	A	1028	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1029	C
1	A	1030	C
1	A	1031	G
1	A	1045	C
1	A	1046	A
1	A	1049	U
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1054	C
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1074	G
1	A	1085	U
1	A	1086	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1104	G
1	A	1117	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1134	G
1	A	1135	U
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1145	C
1	A	1146	A
1	A	1150	U
1	A	1152	A
1	A	1154	G
1	A	1155	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1159	U
1	A	1160	G
1	A	1170	A
1	A	1175	G
1	A	1183	A
1	A	1184	G
1	A	1187	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	1214	C
1	A	1215	G
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1236	A
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1250	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1270	C
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1303	C
1	A	1305	G
1	A	1312	G
1	A	1317	C
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1321	C
1	A	1322	C
1	A	1323	G
1	A	1332	A
1	A	1336	C
1	A	1346	A
1	A	1347	G
1	A	1349	A
1	A	1353	G
1	A	1357	A
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	1378	C
1	A	1379	G
1	A	1381	U
1	A	1394	A
1	A	1397	C
1	A	1398	A
1	A	1399	C
1	A	1400	C
1	A	1402	C
1	A	1419	G
1	A	1423	G
1	A	1440	C
1	A	1442	G
1	A	1443	G
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1473	A
1	A	1488	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1492	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1519	A
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1534	A
1	A	1536	C
1	A	1539	C
1	A	1541	U
24	Y	21	G
24	Y	28	A
24	Y	32	A
24	Y	33	A
24	Y	37	U
24	Y	38	G
24	Y	39	U
25	Z	3	C
25	Z	9	G
25	Z	10	G
25	Z	17	C
25	Z	17(A)	U
25	Z	18	G
25	Z	20	U
25	Z	21	A
25	Z	22	G
25	Z	23	C
25	Z	34	C
25	Z	42	G
25	Z	43	A
25	Z	47	U
25	Z	48	C
25	Z	52	G
25	Z	55	PSU
25	Z	57	A

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Mol	Chain	Res	Type
25	Z	59	A
25	Z	67	C
25	Z	68	C
25	Z	69	C
25	Z	72	A
25	Z	73	A
25	Z	74	C
25	Z	75	C
25	Z	76	A

All (94) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	A
1	A	30	U
1	A	31	G
1	A	48	C
1	A	51	A
1	A	60	A
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	189(F)	U
1	A	197	A
1	A	202	U
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	279	A
1	A	281	G
1	A	305	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	428	G
1	A	429	U
1	A	484	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	495	A
1	A	496	A
1	A	509	A
1	A	518	C
1	A	524	G
1	A	535	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	572	A
1	A	641	U
1	A	687	A
1	A	701	C
1	A	703	G
1	A	748	C
1	A	792	A
1	A	840	C
1	A	872	A
1	A	873	A
1	A	884	U
1	A	913	A
1	A	934	C
1	A	960	U
1	A	965	A
1	A	975	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1065	U
1	A	1101	A
1	A	1128	C
1	A	1137	C
1	A	1145	C
1	A	1151	A
1	A	1182	G
1	A	1190	G
1	A	1196	U
1	A	1201	A
1	A	1212	U
1	A	1225	A
1	A	1226	C
1	A	1239	A

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Mol	Chain	Res	Type
1	A	1257	U
1	A	1279	A
1	A	1285	A
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1331	G
1	A	1335	C
1	A	1346	A
1	A	1364	U
1	A	1380	U
1	A	1442(B)	A
1	A	1447	A
1	A	1452	C
1	A	1498	U
1	A	1504	G
1	A	1529	G
1	A	1533	C
24	Y	32	A
25	Z	19	G
25	Z	47	U
25	Z	60	U
25	Z	73	A

## 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	OMC	Z	32	25	19,22,23	0.87	1 (5%)	26,31,34	1.15	3 (11%)
25	PSU	Z	55	25	18,21,22	1.39	2 (11%)	22,30,33	2.08	6 (27%)
25	G7M	Z	46	25	20,26,27	2.76	3 (15%)	17,39,42	1.07	1 (5%)
25	5MU	Z	54	25	19,22,23	1.56	4 (21%)	28,32,35	1.85	8 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
25	4SU	Z	8	25	18,21,22	1.72	4 (22%)	26,30,33	2.26	9 (34%)

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	OMC	Z	32	25	-	1/9/27/28	0/2/2/2
25	PSU	Z	55	25	-	4/7/25/26	0/2/2/2
25	G7M	Z	46	25	-	0/3/25/26	0/3/3/3
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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	46	G7M	C8-N9	7.95	1.47	1.33
25	Z	46	G7M	C8-N7	7.28	1.46	1.33
25	Z	46	G7M	C5-C4	4.67	1.48	1.39
25	Z	8	4SU	C4-S4	-4.38	1.60	1.68
25	Z	55	PSU	C6-C5	4.26	1.40	1.35
25	Z	54	5MU	C6-C5	3.87	1.40	1.34
25	Z	8	4SU	C2-N1	3.26	1.43	1.38
25	Z	54	5MU	C4-C5	2.84	1.49	1.44
25	Z	8	4SU	C4-N3	-2.81	1.34	1.37
25	Z	54	5MU	C2-N1	2.70	1.42	1.38
25	Z	54	5MU	C4-N3	-2.37	1.34	1.38
25	Z	55	PSU	C4-N3	-2.28	1.34	1.38
25	Z	8	4SU	C6-C5	2.28	1.40	1.35
25	Z	32	OMC	C6-C5	2.04	1.39	1.35

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	8	4SU	C4-N3-C2	-6.26	121.26	127.34
25	Z	55	PSU	N1-C2-N3	5.78	121.68	115.13
25	Z	8	4SU	C5-C4-N3	5.62	119.90	114.69
25	Z	54	5MU	N3-C2-N1	4.85	121.32	114.89
25	Z	8	4SU	N3-C2-N1	4.46	120.81	114.89
25	Z	55	PSU	C4-N3-C2	-3.87	120.76	126.34
25	Z	54	5MU	C4-N3-C2	-3.82	122.40	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	55	PSU	C3'-C2'-C1'	3.75	106.00	101.64
25	Z	54	5MU	C5-C4-N3	3.45	118.26	115.31
25	Z	55	PSU	O2-C2-N1	-3.31	119.15	122.79
25	Z	8	4SU	C5-C4-S4	-2.81	120.84	124.47
25	Z	32	OMC	O2-C2-N3	-2.72	117.90	122.33
25	Z	46	G7M	CN7-N7-C8	-2.67	112.58	125.43
25	Z	54	5MU	O4'-C1'-N1	2.59	114.29	108.36
25	Z	54	5MU	O4-C4-C5	-2.48	122.03	124.90
25	Z	55	PSU	C6-C5-C4	-2.44	116.49	118.20
25	Z	54	5MU	C5-C6-N1	-2.44	120.83	123.34
25	Z	8	4SU	C3'-C2'-C1'	2.43	106.04	101.43
25	Z	8	4SU	O2-C2-N3	-2.35	117.12	121.50
25	Z	8	4SU	C6-N1-C2	-2.34	118.00	120.99
25	Z	54	5MU	C3'-C2'-C1'	2.22	105.65	101.43
25	Z	32	OMC	C2'-C1'-N1	-2.21	109.93	114.22
25	Z	32	OMC	O4'-C1'-N1	2.20	113.39	108.36
25	Z	8	4SU	C1'-N1-C2	2.14	121.44	117.57
25	Z	54	5MU	C6-N1-C2	-2.09	119.18	121.30
25	Z	8	4SU	O4'-C1'-N1	2.07	113.11	108.36
25	Z	55	PSU	O3'-C3'-C4'	2.05	116.99	111.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	Z	55	PSU	C3'-C4'-C5'-O5'
25	Z	55	PSU	O4'-C4'-C5'-O5'
25	Z	32	OMC	C3'-C2'-O2'-CM2
25	Z	55	PSU	C4'-C5'-O5'-P
25	Z	55	PSU	O4'-C1'-C5-C6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	32	OMC	2	0
25	Z	8	4SU	2	0

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	FME	Z	101	-	8,8,10	0.51	0	7,8,11	0.83	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	FME	Z	101	-	-	1/7/7/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	Z	101	FME	C-CA-N-CN

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	Z	101	FME	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1442(A):G	O3'	1442(B):A	P	5.40
1	A	84:U	O3'	88:A	P	5.02
1	A	93:G	O3'	96:U	P	4.43
1	A	204:U	O3'	216:G	P	4.27
1	A	841:U	O3'	848:C	P	3.83

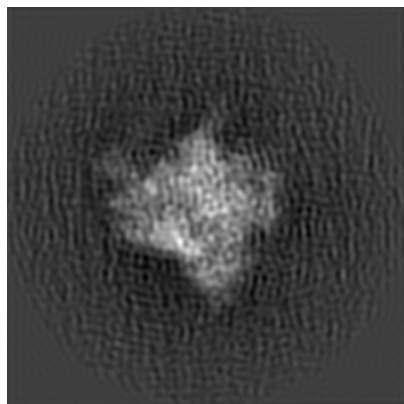
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4083. These allow visual inspection of the internal detail of the map and identification of artifacts.

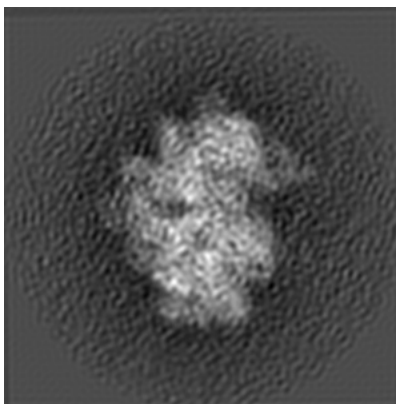
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

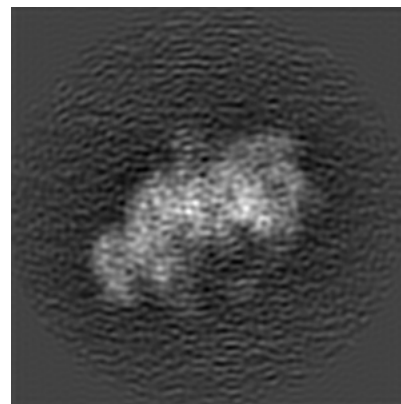
#### 6.1.1 Primary map



X

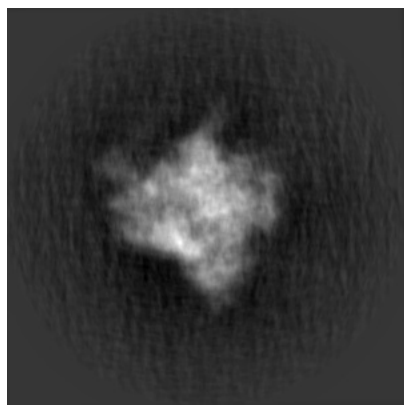


Y

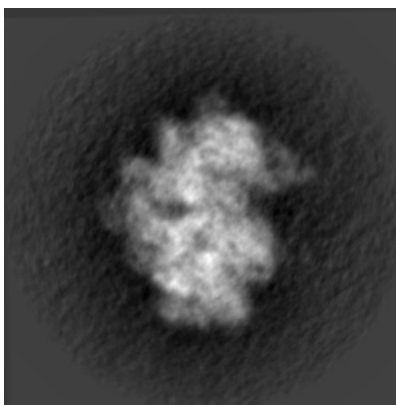


Z

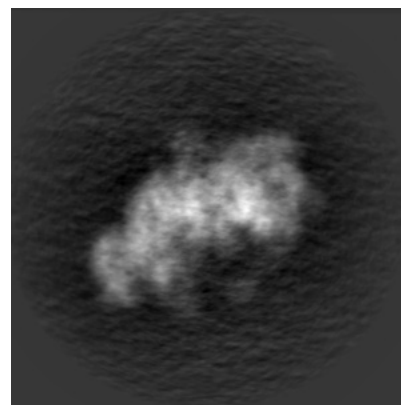
#### 6.1.2 Raw map



X



Y

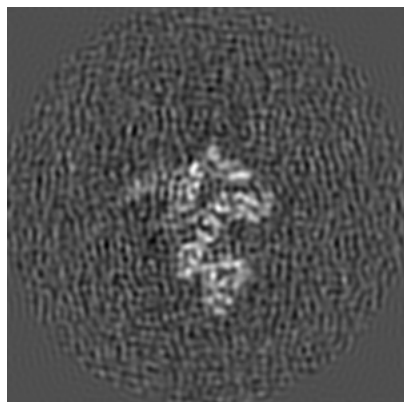


Z

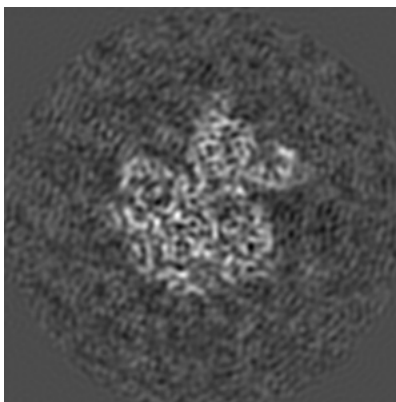
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

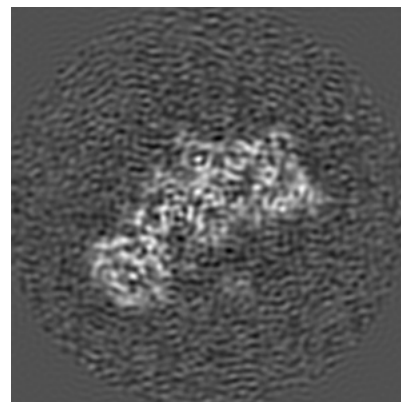
### 6.2.1 Primary map



X Index: 130

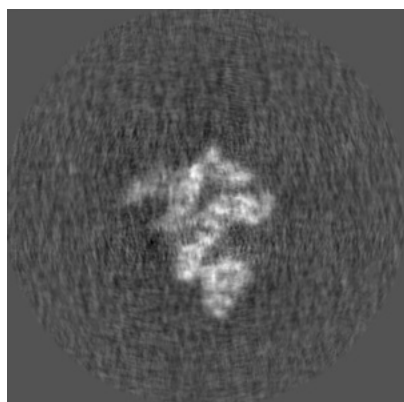


Y Index: 130

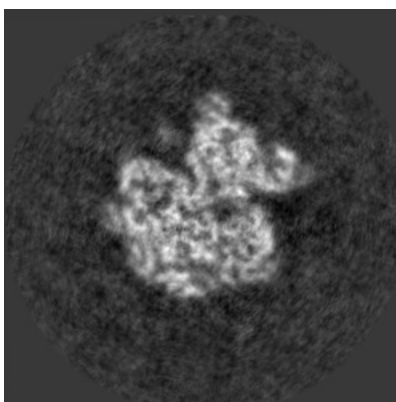


Z Index: 130

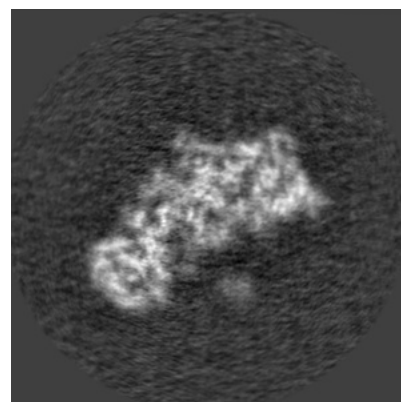
### 6.2.2 Raw map



X Index: 130



Y Index: 130



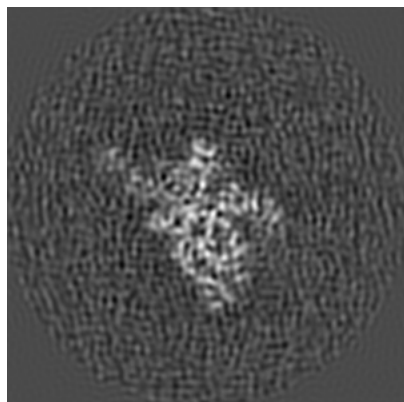
Z Index: 130

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

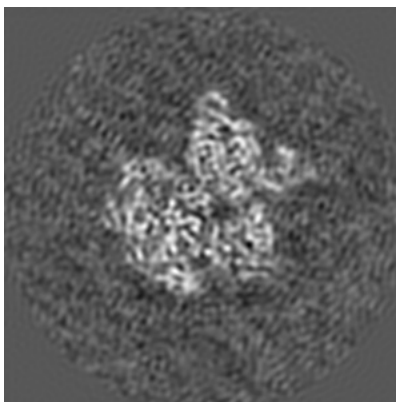


## 6.3 Largest variance slices [i](#)

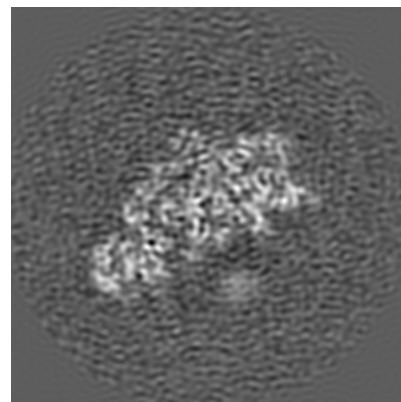
### 6.3.1 Primary map



X Index: 121

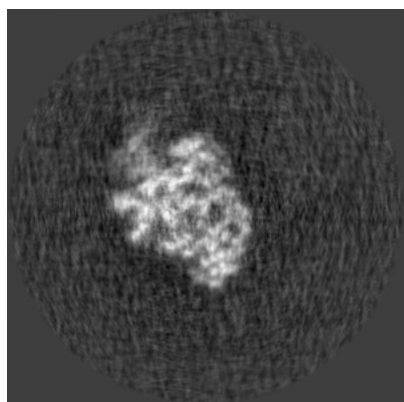


Y Index: 132

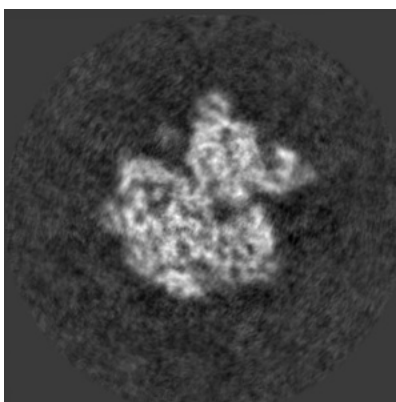


Z Index: 126

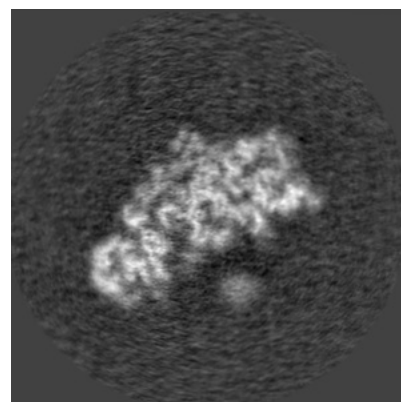
### 6.3.2 Raw map



X Index: 96



Y Index: 131



Z Index: 127

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



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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



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

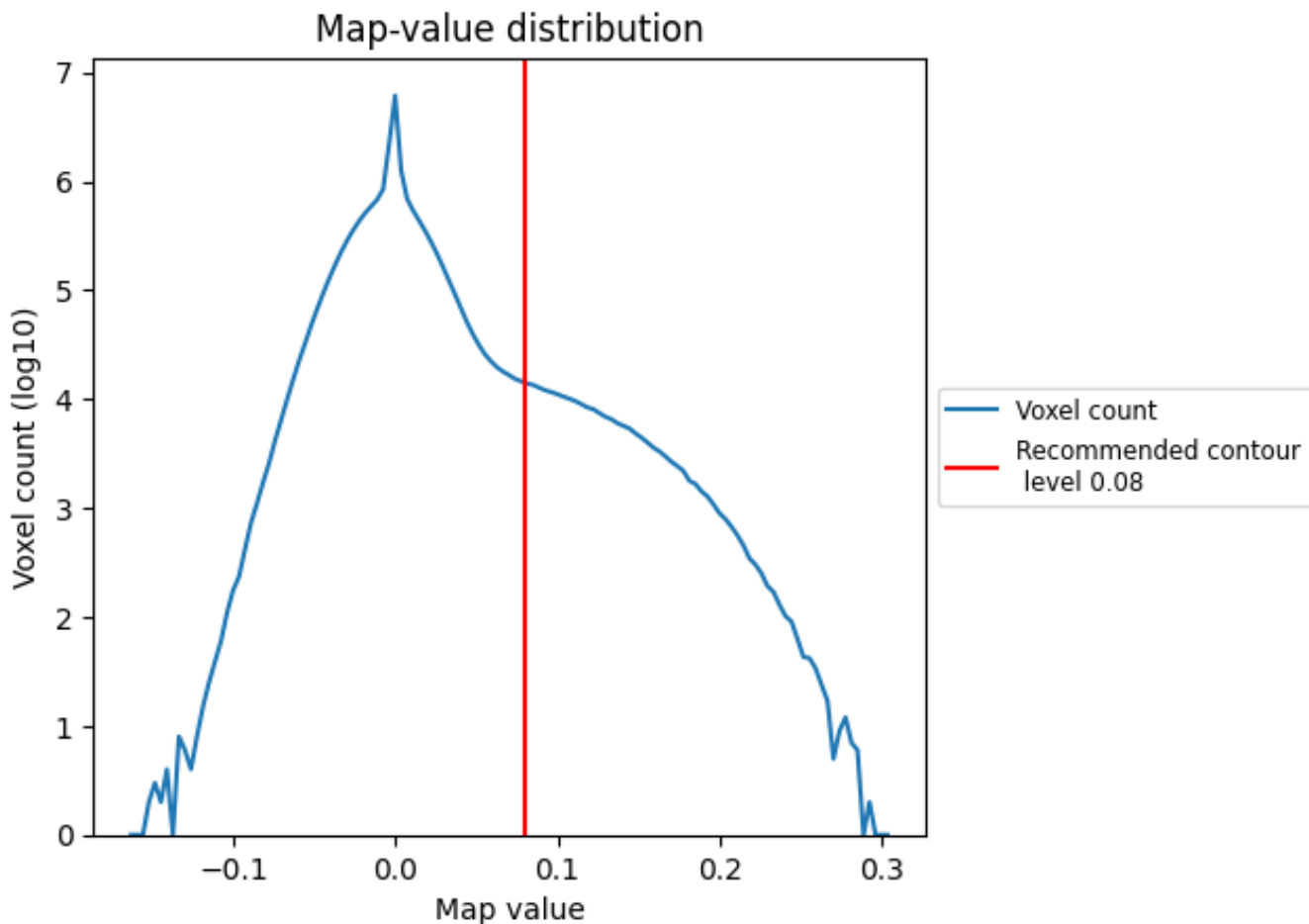
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

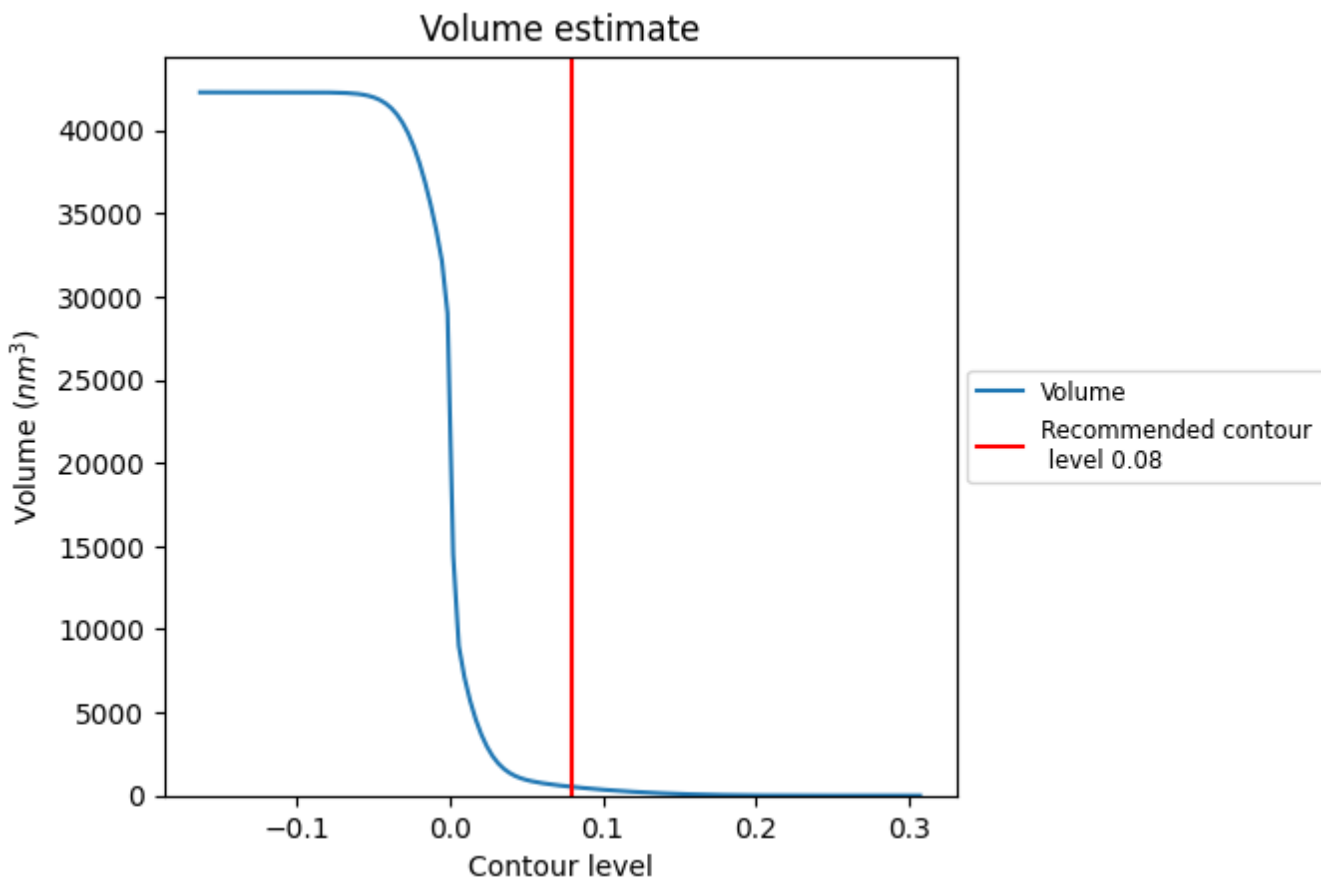
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

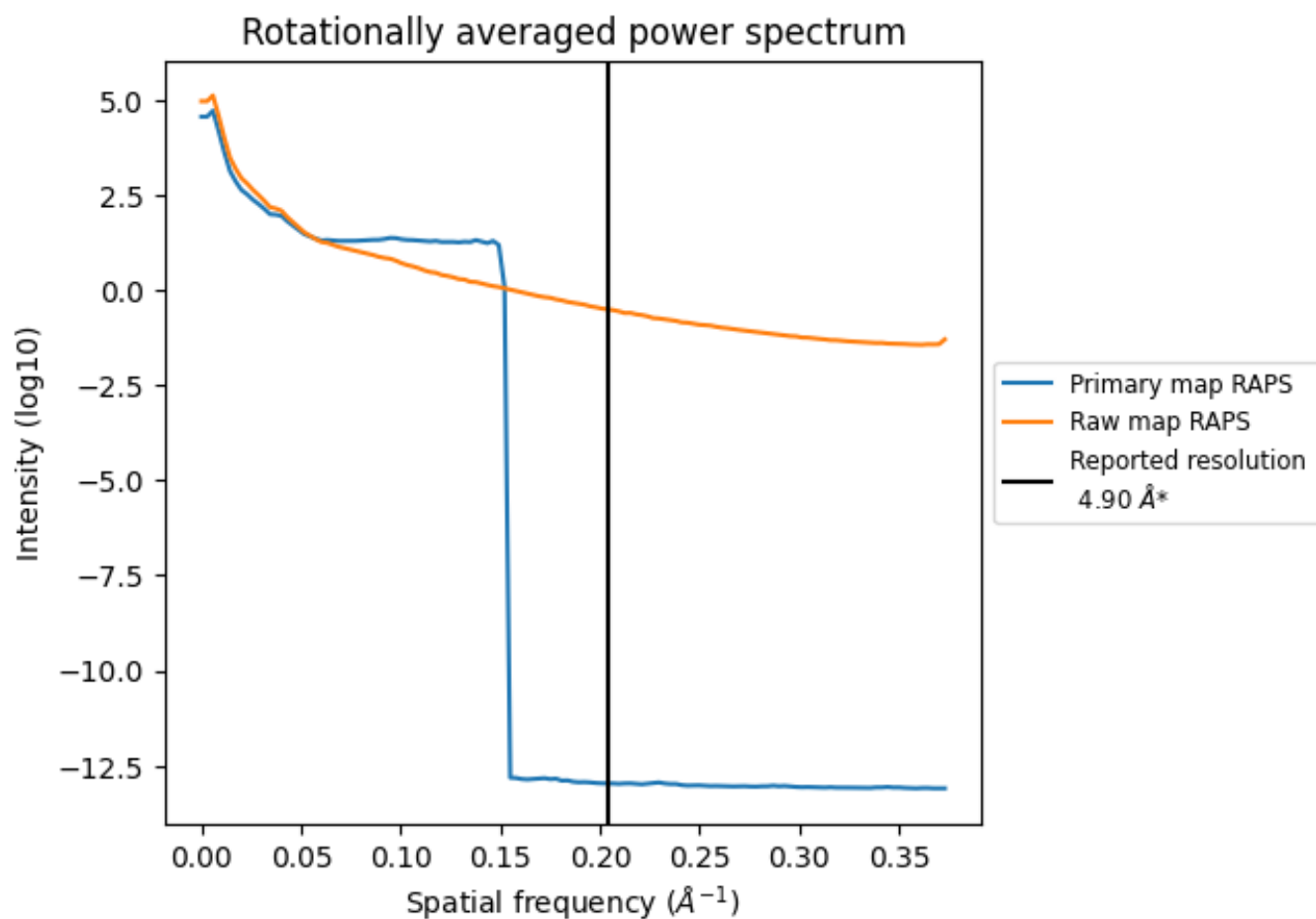
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 522  $\text{nm}^3$ ; this corresponds to an approximate mass of 471 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](#)

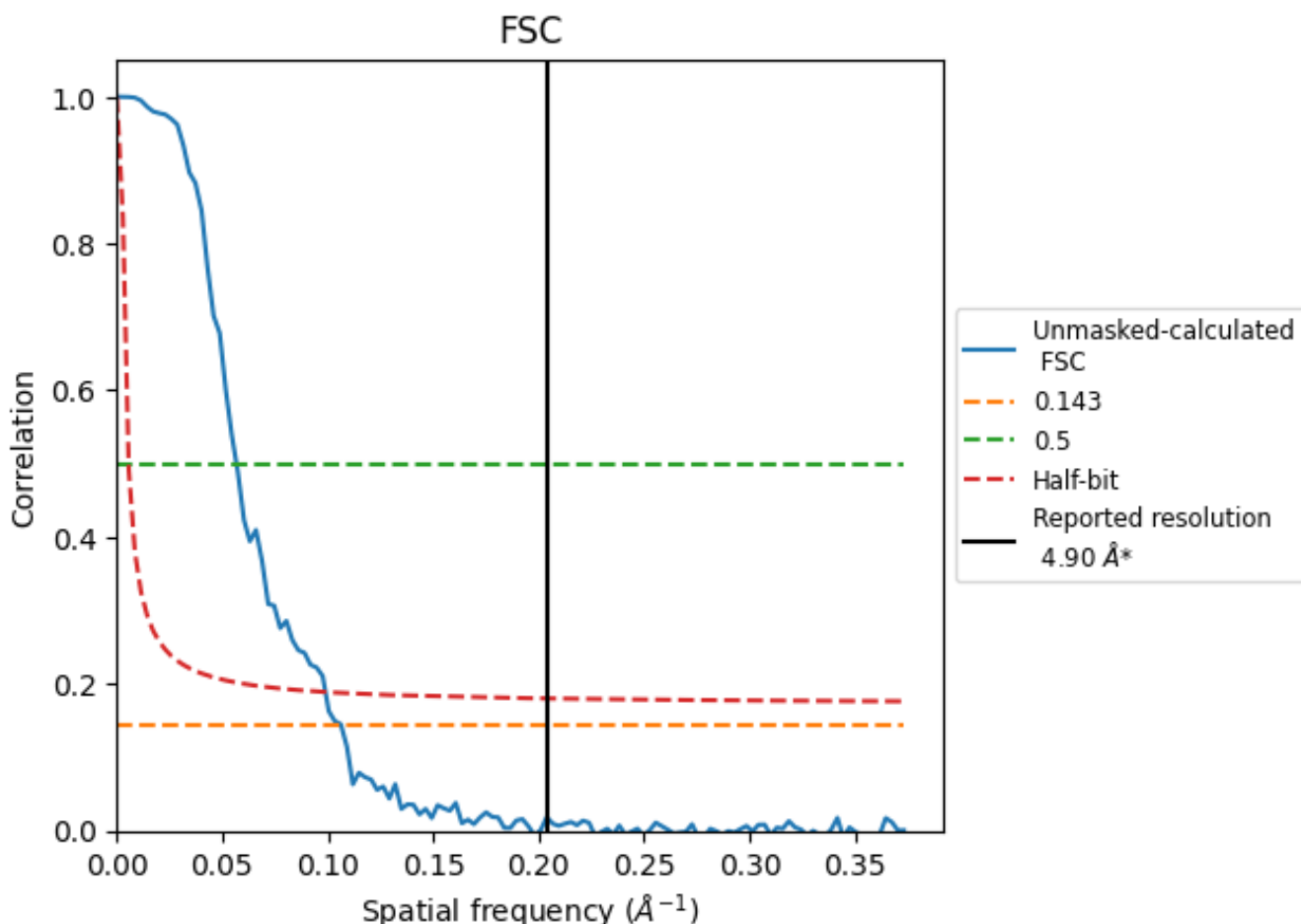


\*Reported resolution corresponds to spatial frequency of  $0.204 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.204 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

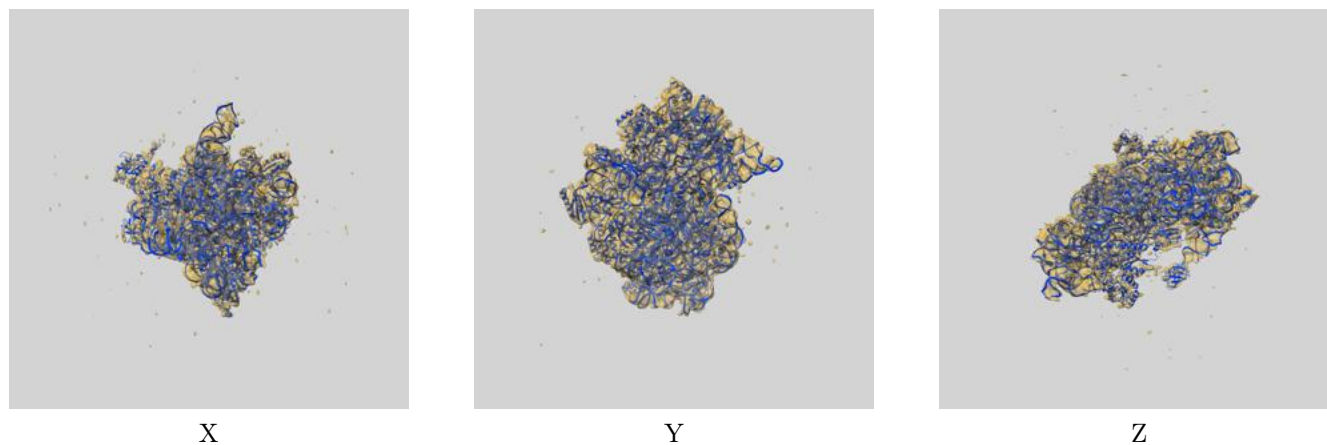
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.40	17.64	10.11

\*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 9.40 differs from the reported value 4.9 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-4083 and PDB model 5LMV. Per-residue inclusion information can be found in section [3](#) on page [9](#).

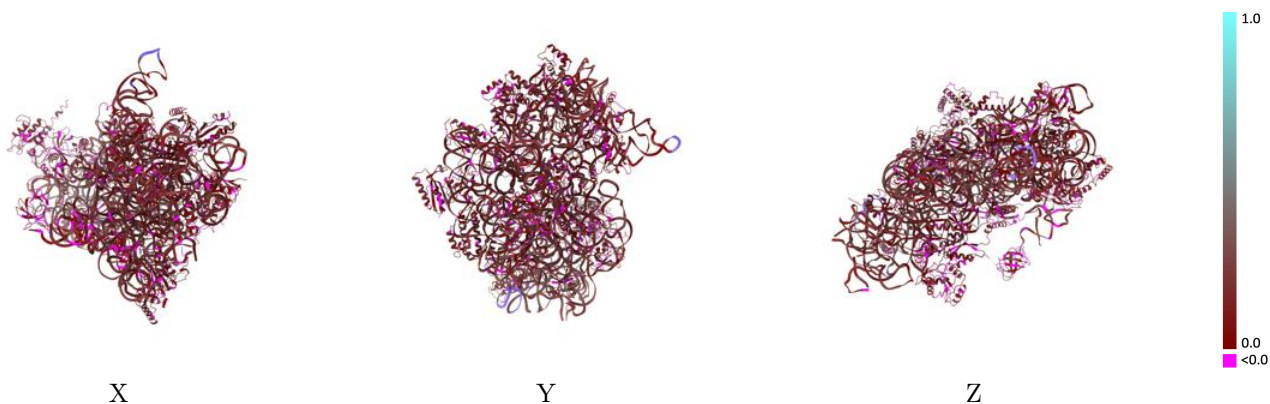
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

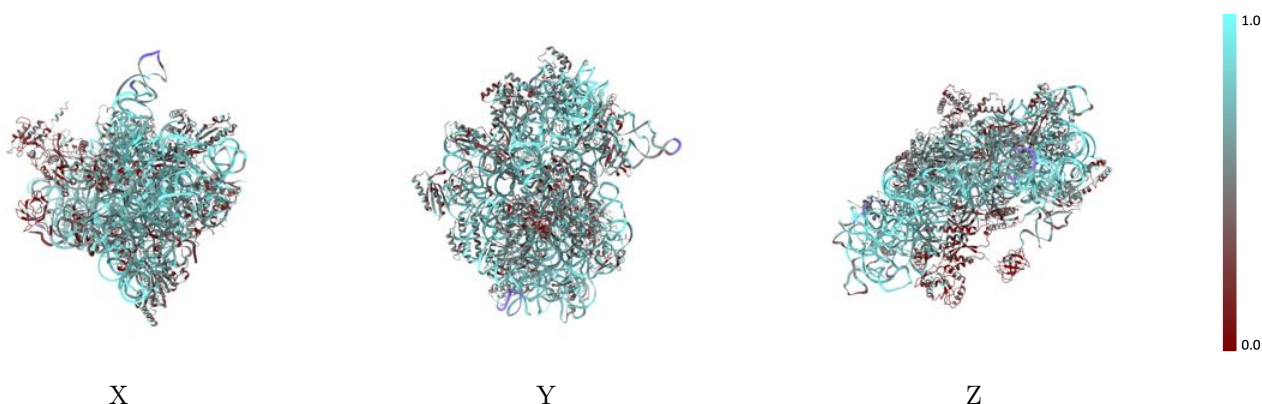


## 9.2 Q-score mapped to coordinate model [i](#)



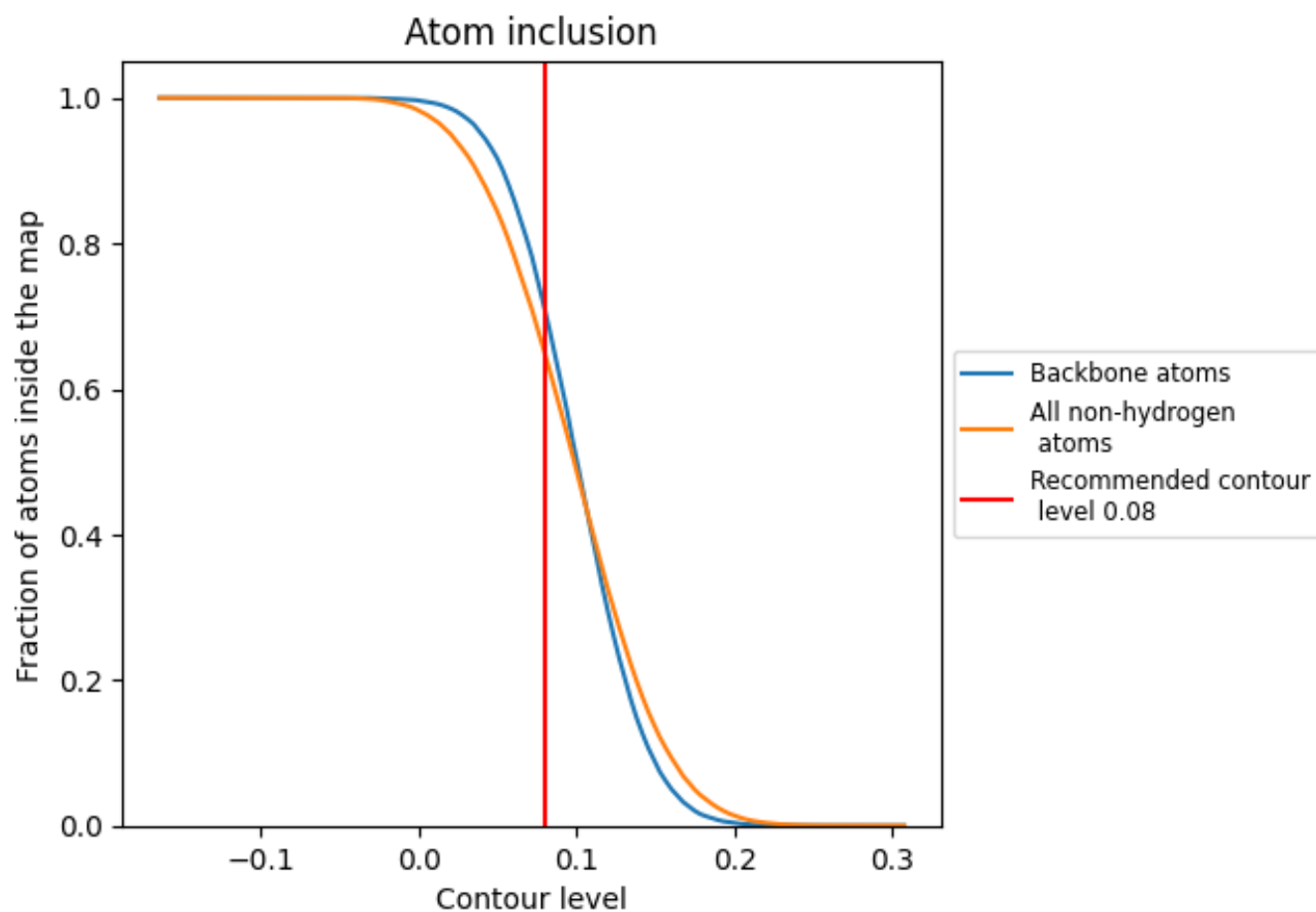
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 65% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6497	 0.1640
A	 0.8068	 0.1960
B	 0.3431	 0.1260
C	 0.5003	 0.1400
D	 0.4914	 0.1350
E	 0.5365	 0.1430
F	 0.4932	 0.1360
G	 0.5108	 0.1540
H	 0.5257	 0.1410
I	 0.4825	 0.1290
J	 0.4401	 0.1160
K	 0.5110	 0.1410
L	 0.4055	 0.1420
M	 0.4955	 0.1270
N	 0.4530	 0.1150
O	 0.5650	 0.1520
P	 0.5622	 0.1290
Q	 0.5363	 0.1330
R	 0.4504	 0.1120
S	 0.5117	 0.1430
T	 0.5318	 0.1420
V	 0.5550	 0.1130
W	 0.2196	 0.1060
X	 0.4189	 0.0740
Y	 0.4784	 0.1220
Z	 0.6473	 0.1360
a	 0.2534	 0.1010

