



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 07:54 pm BST

PDB ID : 9FS6 / pdb_00009fs6
EMDB ID : EMD-50724
Title : Cryo-EM structure of *Saccharolobus solfataricus* 30S initiation complex bound to Ss-aIF2beta leaderless mRNA with h44 in up position
Authors : Bourgeois, G.; Coureux, P.D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2024-06-20
Resolution : 2.90 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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

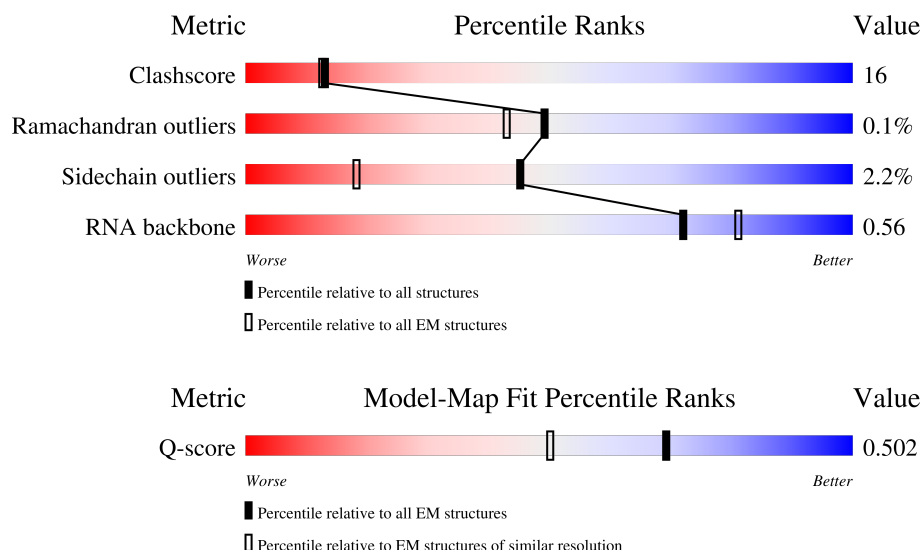
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



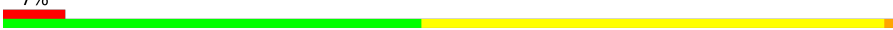
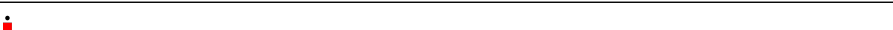
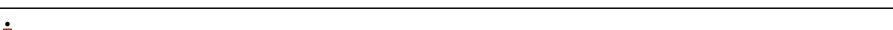
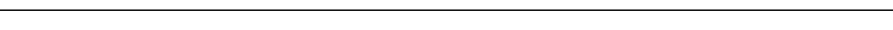
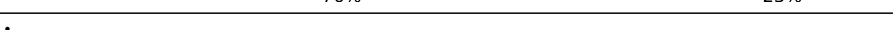
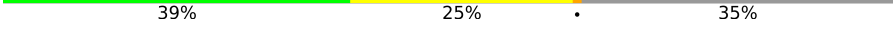
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	2	1497	
2	A	208	
3	B	231	

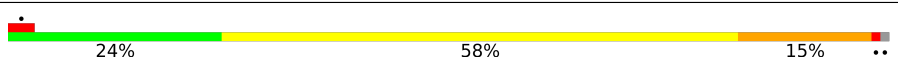
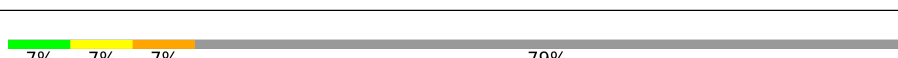
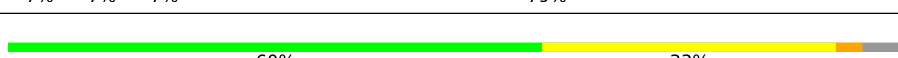
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Mol	Chain	Length	Quality of chain
4	C	65	
5	D	181	
6	E	239	
7	F	214	
8	G	214	
9	H	193	
10	I	133	
11	J	133	
12	K	137	
13	L	102	
14	N	147	
15	O	165	
16	Q	152	
17	R	114	
18	S	79	
19	T	140	
20	U	158	
21	V	120	
22	W	66	
23	X	83	
24	Y	75	
25	Z	229	
26	3	127	
27	c	110	
28	d	72	

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Mol	Chain	Length	Quality of chain
29	e	52	
30	4	77	
31	a	72	
32	P	54	
33	b	95	
34	5	14	
35	M	132	

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
36	SPM	2	1532	-	-	X	-

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 65629 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 rRNA 16S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1440	Total	C	N	O	P	0	0
			30982	13818	5732	9992	1440		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	843	4AC	C	modified residue	GB AE006641.1
2	930	C4J	U	modified residue	GB AE006641.1
2	1466	4AC	C	modified residue	GB AE006641.1
2	1467	4AC	C	modified residue	GB AE006641.1
2	1477	4AC	C	modified residue	GB AE006641.1
2	1478	4AC	C	modified residue	GB AE006641.1
2	1496	C	A	conflict	GB AE006641.1

- Molecule 2 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	186	Total	C	N	O	S	0	0
			1515	974	261	278	2		

- Molecule 3 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	215	Total	C	N	O	S	0	0
			1698	1092	291	312	3		

- Molecule 4 is a protein called Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	58	Total	C	N	O	S	0	0
			455	282	84	81	8		

- Molecule 5 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	166	Total	C	N	O	S	0	0
			1354	864	249	240	1		

- Molecule 6 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	238	Total	C	N	O	S	0	0
			1930	1238	342	344	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	210	Total	C	N	O	S	0	0
			1625	1041	275	303	6		

- Molecule 8 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	213	Total	C	N	O	S	0	0
			1661	1052	292	315	2		

- Molecule 9 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	192	Total	C	N	O	S	0	0
			1543	983	283	274	3		

- Molecule 10 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	132	Total	C	N	O	S	0	0
			1050	675	187	182	6		

- Molecule 11 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	127	Total	C	N	O		0	0
			982	617	186	179			

- Molecule 12 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	133	Total	C	N	O	S	0	0
			1068	675	201	185	7		

- Molecule 13 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	101	Total	C	N	O	S	0	0
			840	536	157	142	5		

- Molecule 14 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	146	Total	C	N	O	S	0	0
			1140	723	220	193	4		

- Molecule 15 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	140	Total	C	N	O	S	0	0
			1124	708	210	202	4		

- Molecule 16 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	145	Total	C	N	O	S	0	0
			1185	753	224	205	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	113	Total	C	N	O	S	0	0
			901	570	166	161	4		

- Molecule 18 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	66	Total	C	N	O	S	0	0
			571	364	101	105	1		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	128	Total	C	N	O	S	0	0
			1064	684	192	184	4		

- Molecule 20 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	154	Total	C	N	O	S	0	0
			1247	805	223	217	2		

- Molecule 21 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	107	Total	C	N	O	S	0	0
			836	524	154	156	2		

- Molecule 22 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	65	Total	C	N	O	S	0	0
			503	319	93	84	7		

- Molecule 23 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	67	Total	C	N	O	0	0
			535	335	103	97		

- Molecule 24 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	49	Total	C	N	O	S	0	0
			395	252	73	65	5		

- Molecule 25 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	196	Total	C	N	O	S	0	0
			1561	1009	274	272	6		

- Molecule 26 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	117	Total	C	N	O	S	0	0
			893	567	149	175	2		

- Molecule 27 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	109	Total	C	N	O	S	0	0
			856	539	152	164	1		

- Molecule 28 is a protein called VapB-type antitoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	68	Total	C	N	O	S	0	0
			557	362	90	103	2		

- Molecule 29 is a protein called LSU ribosomal protein S30E (Rps30E).

Mol	Chain	Residues	Atoms				AltConf	Trace
29	e	43	Total	C	N	O	0	0
			354	220	74	60		

- Molecule 30 is a RNA chain called tRNA met initiator.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	4	77	Total	C	N	O	P S	0	0
			1645	734	296	537	77 1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	A	C	engineered mutation	GB 1334604293
4	72	U	A	engineered mutation	GB 1334604293

- Molecule 31 is a protein called aS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	71	Total	C	N	O	S	0	0
			562	361	98	96	7		

- Molecule 32 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	P	53	Total	C	N	O	S	0	0
			440	282	80	74	4		

- Molecule 33 is a protein called LSU ribosomal protein S26E (Rps26E).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	93	Total	C	N	O	S	0	0
			723	449	139	128	7		

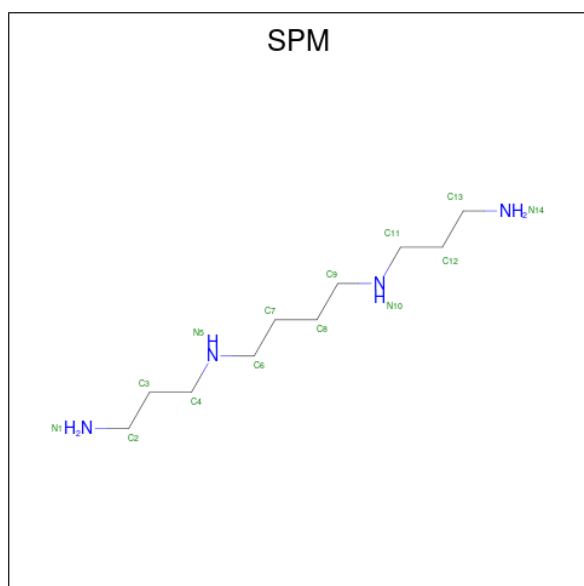
- Molecule 34 is a RNA chain called mRNA Ss-aIF2beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	5	3	Total	C	N	O	P	0	0
			47	19	7	18	3		

- Molecule 35 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	M	127	Total	C	N	O	S	0	0
			944	587	184	170	3		

- Molecule 36 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
36	2	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	
36	2	1	Total	C	N	0
			14	10	4	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	2	54	Total	Mg	0
			54	54	
37	F	1	Total	Mg	0
			1	1	

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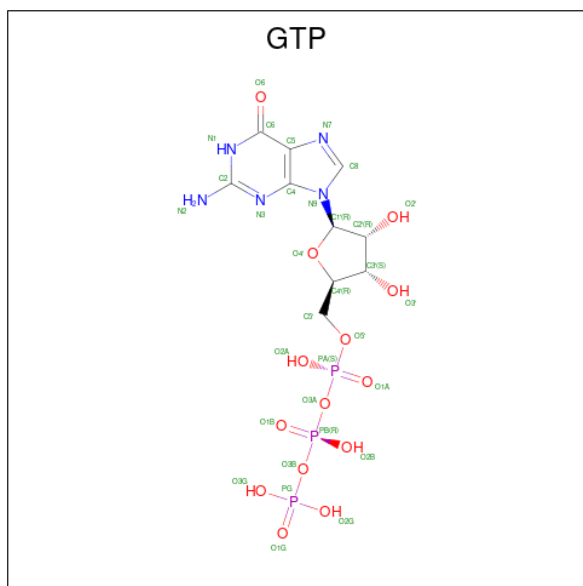
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Mol	Chain	Residues	Atoms		AltConf
37	R	1	Total	Mg	0
			1	1	
37	5	1	Total	Mg	0
			1	1	

- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	C	2	Total	Zn	0
			2	2	
38	F	1	Total	Zn	0
			1	1	
38	R	1	Total	Zn	0
			1	1	
38	W	1	Total	Zn	0
			1	1	
38	a	2	Total	Zn	0
			2	2	
38	P	1	Total	Zn	0
			1	1	
38	b	1	Total	Zn	0
			1	1	

- Molecule 39 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
39	5	1	Total	C	N	O	P	0
			32	10	5	14	3	

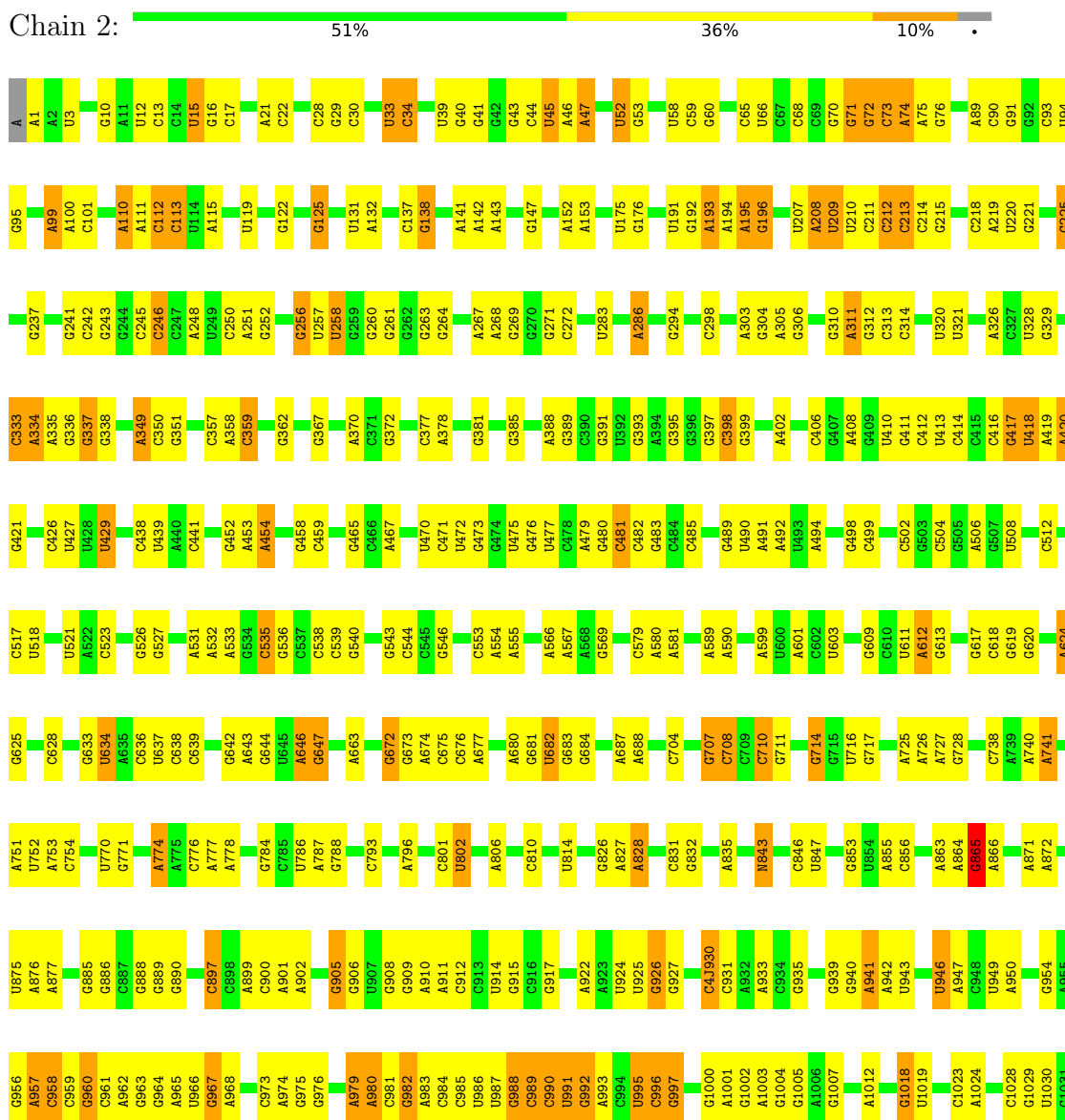
- Molecule 40 is water.

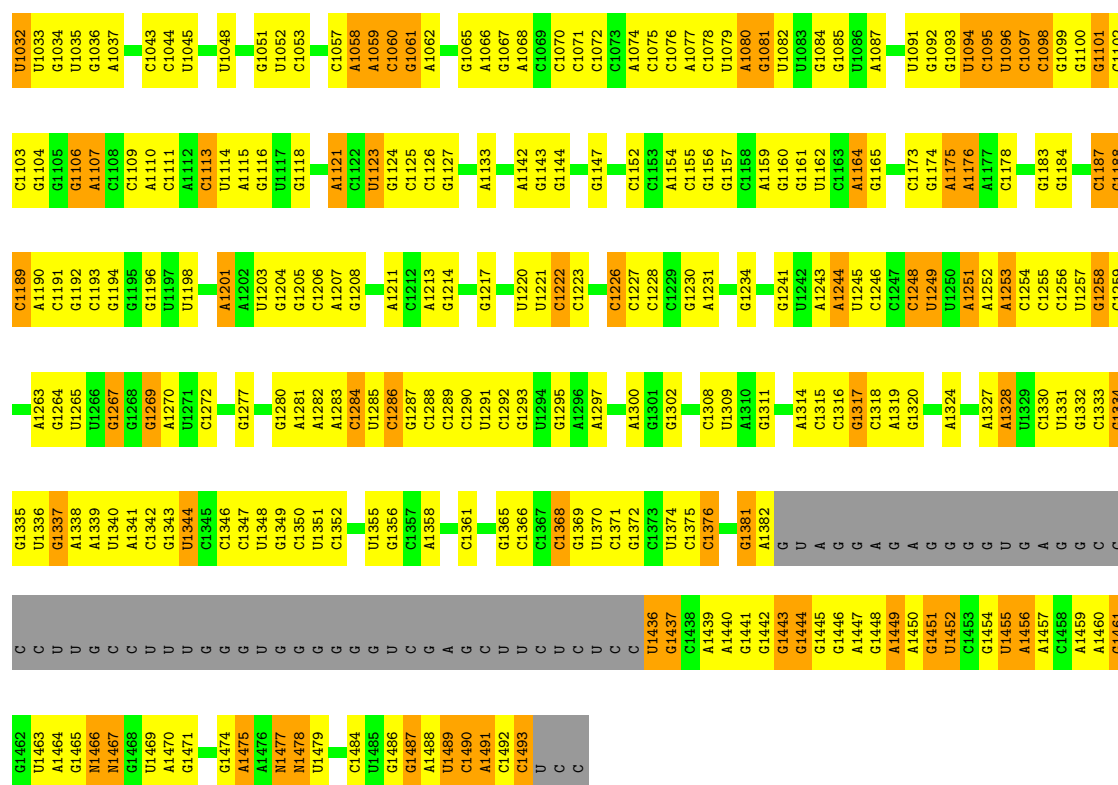
Mol	Chain	Residues	Atoms		AltConf
40	2	181	Total	O	0
			181	181	
40	D	1	Total	O	0
			1	1	
40	E	1	Total	O	0
			1	1	
40	H	1	Total	O	0
			1	1	
40	I	2	Total	O	0
			2	2	
40	J	2	Total	O	0
			2	2	
40	Q	1	Total	O	0
			1	1	
40	R	3	Total	O	0
			3	3	
40	U	1	Total	O	0
			1	1	
40	4	1	Total	O	0
			1	1	
40	b	2	Total	O	0
			2	2	
40	5	3	Total	O	0
			3	3	

3 Residue-property plots

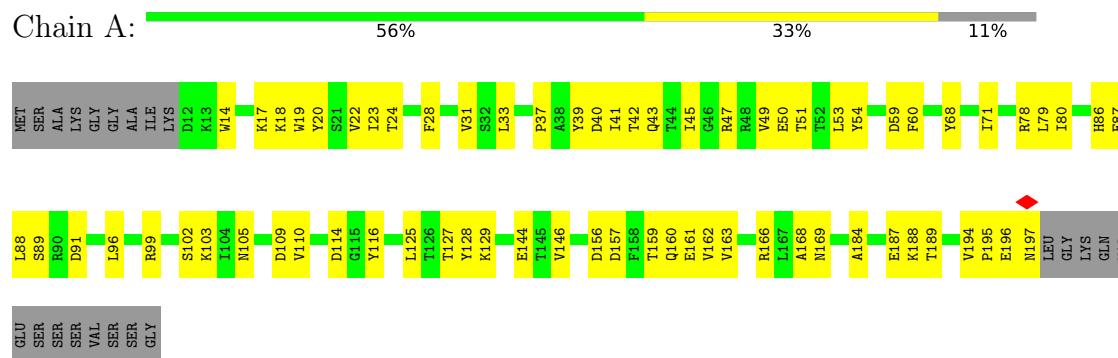
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: rRNA 16S

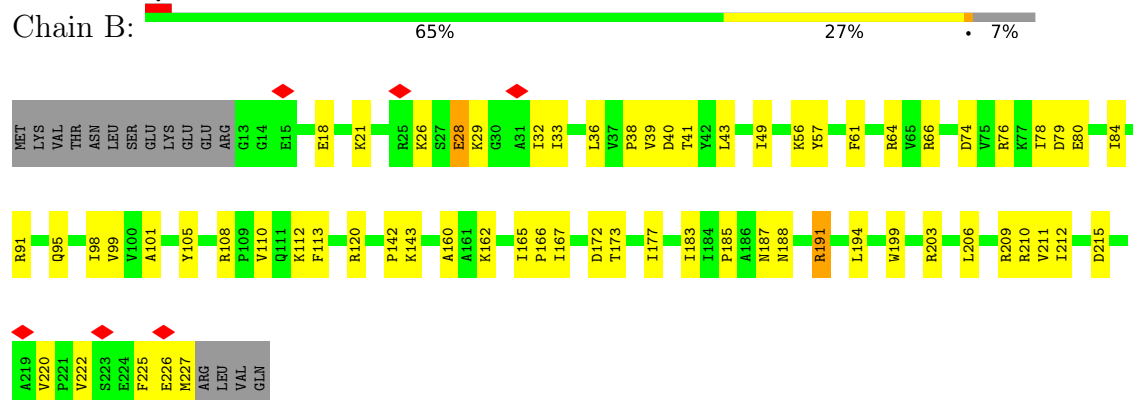




• Molecule 2: Small ribosomal subunit protein eS1

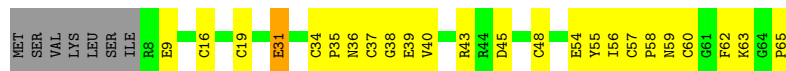


• Molecule 3: Small ribosomal subunit protein uS2



- Molecule 4: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein

Chain C: 



- Molecule 5: Small ribosomal subunit protein uS4

Chain D: 



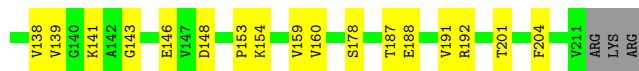
- Molecule 6: Small ribosomal subunit protein eS4

Chain E: 



- Molecule 7: Small ribosomal subunit protein uS5

Chain F: 



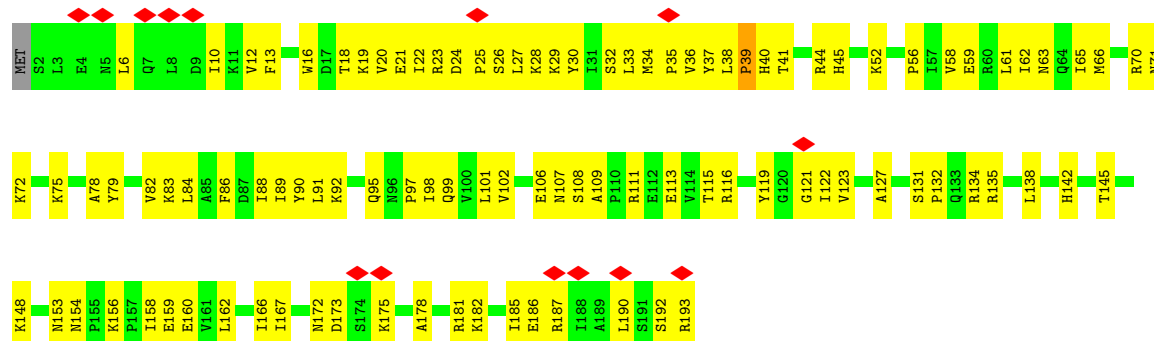
- Molecule 8: Small ribosomal subunit protein eS6

Chain G: 

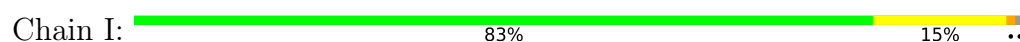




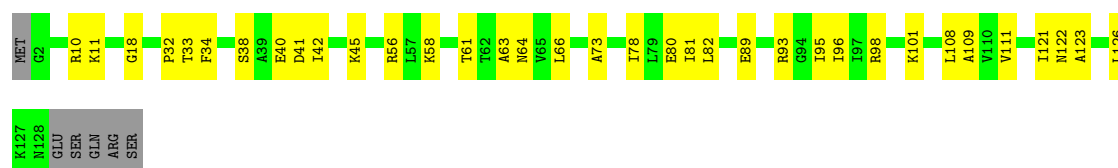
• Molecule 9: Small ribosomal subunit protein uS7



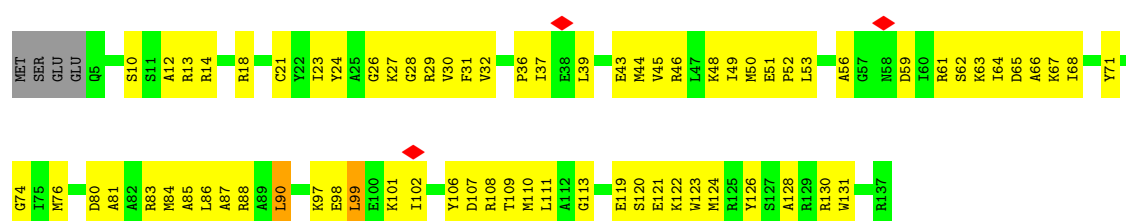
• Molecule 10: Small ribosomal subunit protein uS8



• Molecule 11: Small ribosomal subunit protein eS8

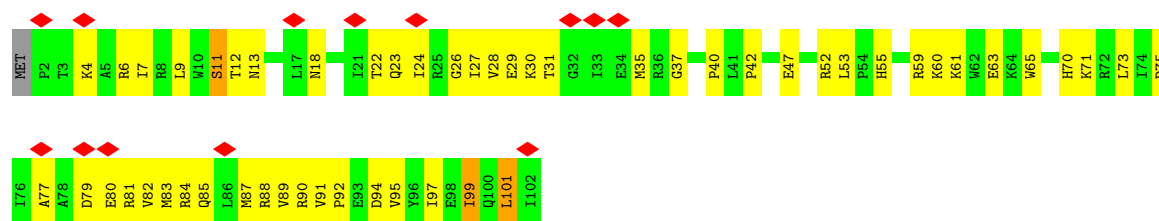


• Molecule 12: Small ribosomal subunit protein uS9

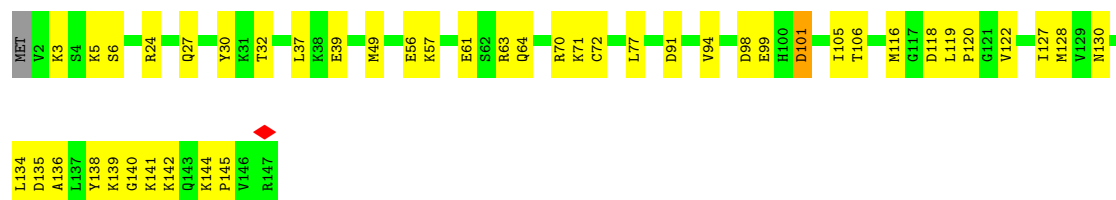


• Molecule 13: Small ribosomal subunit protein uS10

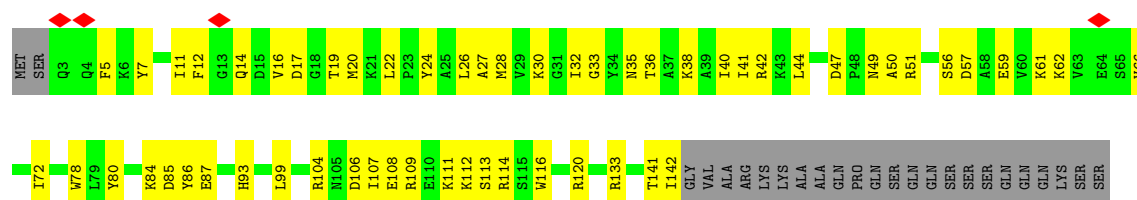




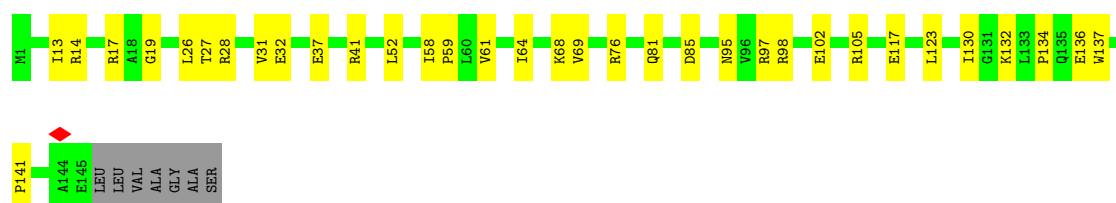
- Molecule 14: Small ribosomal subunit protein uS12



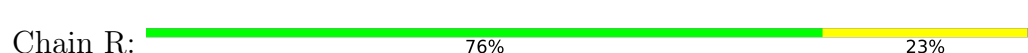
- Molecule 15: Small ribosomal subunit protein uS13



- Molecule 16: Small ribosomal subunit protein uS15



- Molecule 17: Small ribosomal subunit protein uS17



- Molecule 18: Small ribosomal subunit protein eS17

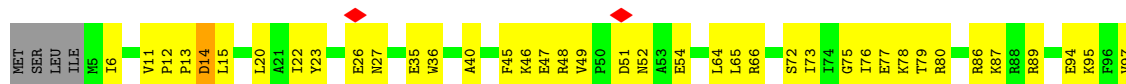




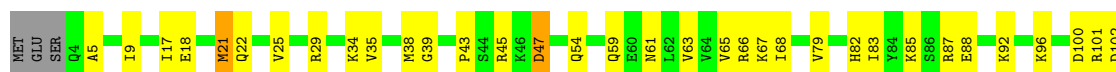
- Molecule 19: Small ribosomal subunit protein uS19



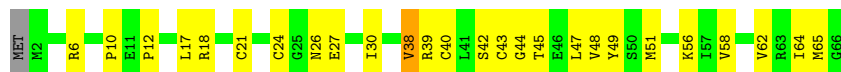
- Molecule 20: Small ribosomal subunit protein eS19



- Molecule 21: Small ribosomal subunit protein eS24



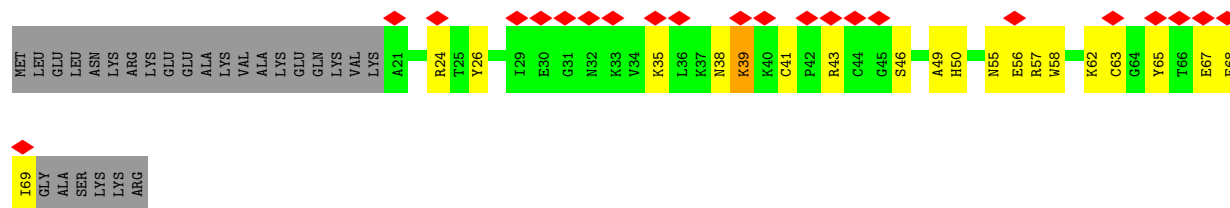
- Molecule 22: Small ribosomal subunit protein eS27



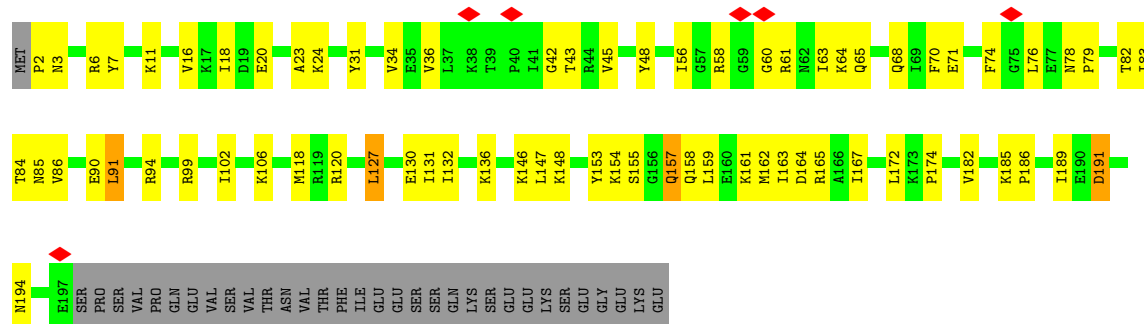
- Molecule 23: Small ribosomal subunit protein eS28



- Molecule 24: Small ribosomal subunit protein eS31



- Molecule 25: Small ribosomal subunit protein uS3

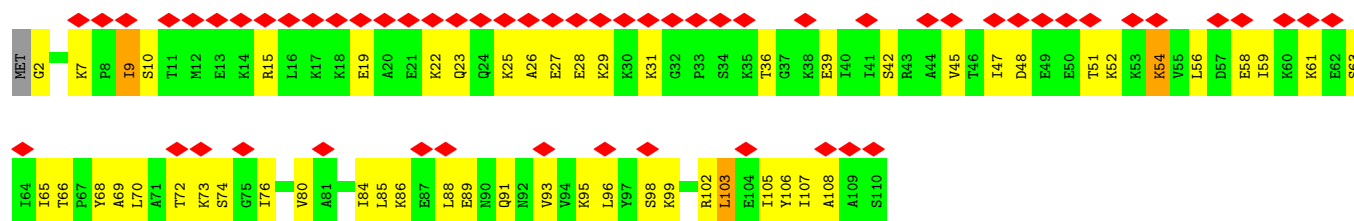


- Molecule 26: Large ribosomal subunit protein eL8



- Molecule 27: Small ribosomal subunit protein eS25

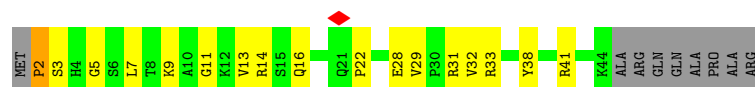




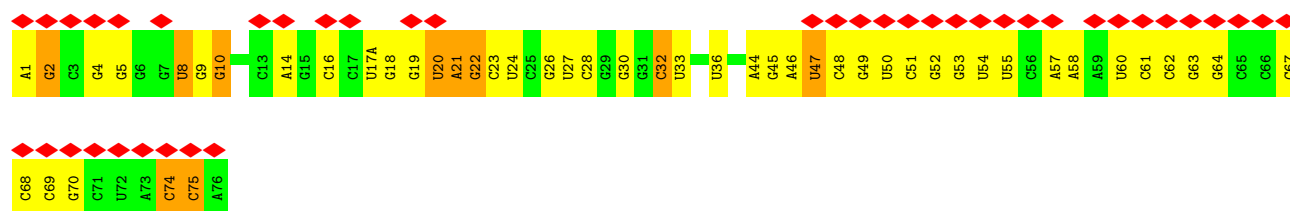
• Molecule 28: VapB-type antitoxin



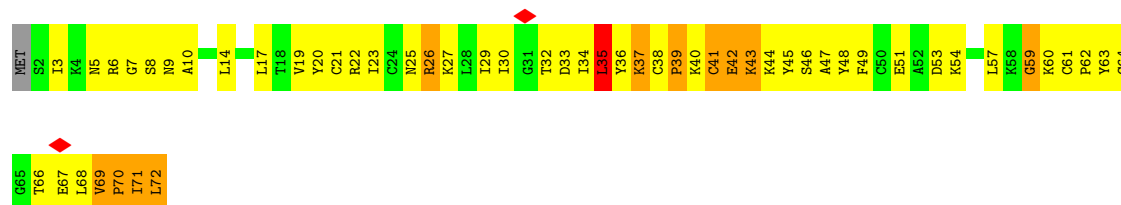
• Molecule 29: LSU ribosomal protein S30E (Rps30E)



• Molecule 30: tRNA met initiator



• Molecule 31: aS34



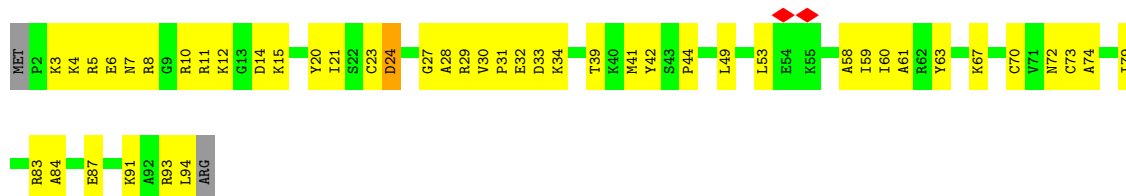
• Molecule 32: Small ribosomal subunit protein uS14

Chain P:  52% 46%



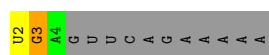
- Molecule 33: LSU ribosomal protein S26E (Rps26E)

Chain b:  49% 47%



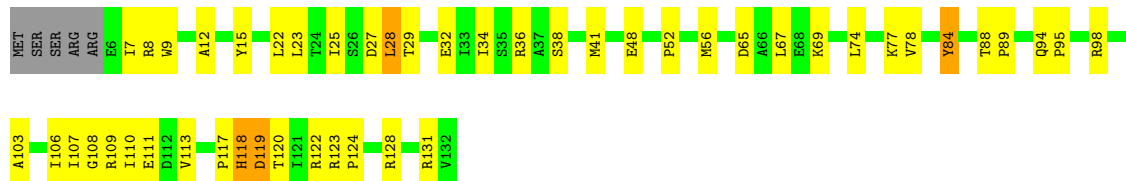
- Molecule 34: mRNA Ss-aIF2beta

Chain 5:  7% 7% 7% 79%



- Molecule 35: Small ribosomal subunit protein uS11

Chain M:  60% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49401	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.048	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0045	Depositor
Map size (Å)	361.19998, 361.19998, 361.19998	wwPDB
Map dimensions	516, 516, 516	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7, 0.7, 0.7	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, 4SU, ZN, H2U, OMC, GTP, C4J, MG, MA6, OMG, 4AC, SPM, 6MZ, 5MU, 5MC, A2M, OMU

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	2	0.35	0/33843	0.31	0/52798
2	A	0.28	0/1543	0.48	0/2077
3	B	0.24	0/1731	0.45	1/2349 (0.0%)
4	C	0.28	0/466	0.43	0/625
5	D	0.32	0/1380	0.34	0/1859
6	E	0.32	0/1965	0.38	0/2644
7	F	0.33	0/1654	0.41	0/2240
8	G	0.27	1/1684 (0.1%)	0.53	3/2265 (0.1%)
9	H	0.62	4/1571 (0.3%)	0.72	4/2116 (0.2%)
10	I	0.35	0/1070	0.36	0/1444
11	J	0.31	0/994	0.43	0/1337
12	K	0.27	0/1084	0.62	0/1450
13	L	0.26	0/856	0.58	0/1154
14	N	0.33	0/1155	0.38	0/1540
15	O	0.21	0/1142	0.48	0/1532
16	Q	0.29	0/1206	0.39	0/1618
17	R	0.35	0/918	0.38	0/1236
18	S	0.25	0/578	0.51	0/770
19	T	0.18	0/1087	0.41	0/1456
20	U	0.22	0/1270	0.52	0/1710
21	V	0.30	0/843	0.45	0/1124
22	W	0.29	0/511	0.45	0/684
23	X	0.21	0/538	0.52	0/722
24	Y	0.20	0/404	0.50	0/540
25	Z	0.27	0/1584	0.48	0/2124
26	3	0.72	2/902 (0.2%)	1.20	5/1216 (0.4%)
27	c	0.17	0/861	0.47	0/1143
28	d	0.27	0/568	0.71	1/769 (0.1%)
29	e	0.33	0/360	0.81	2/477 (0.4%)
30	4	0.18	1/1725 (0.1%)	0.23	0/2687
31	a	0.76	1/574 (0.2%)	1.36	9/770 (1.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	P	0.33	0/451	0.73	0/600
33	b	0.32	0/732	0.76	1/976 (0.1%)
34	5	0.32	0/51	0.45	0/78
35	M	0.29	0/960	0.67	2/1294 (0.2%)
All	All	0.34	9/68261 (0.0%)	0.44	28/99424 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	3	12	PRO	CB-CG	17.20	2.35	1.49
9	H	39	PRO	CB-CG	14.77	2.23	1.49
9	H	39	PRO	CG-CD	-14.68	1.00	1.50
26	3	12	PRO	CG-CD	-10.07	1.16	1.50
31	a	70	PRO	CG-CD	-9.82	1.17	1.50
9	H	39	PRO	N-CD	6.96	1.57	1.47
9	H	39	PRO	CA-CB	-5.82	1.45	1.53
8	G	88	PRO	CG-CD	-5.18	1.33	1.50
30	4	8	4SU	O3'-P	5.00	1.61	1.56

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	12	PRO	CA-N-CD	-23.86	78.60	112.00
26	3	12	PRO	CB-CG-CD	-23.66	30.37	106.10
9	H	39	PRO	N-CD-CG	-16.07	79.09	103.20
29	e	2	PRO	CA-N-CD	-13.05	93.72	112.00
26	3	12	PRO	N-CD-CG	12.98	122.67	103.20
31	a	70	PRO	CA-N-CD	-12.20	94.92	112.00
9	H	39	PRO	CB-CG-CD	-10.50	72.50	106.10
8	G	88	PRO	CA-N-CD	-9.84	98.23	112.00
9	H	39	PRO	CA-CB-CG	-8.67	88.02	104.50
8	G	88	PRO	N-CD-CG	-8.11	91.04	103.20
9	H	39	PRO	N-CA-CB	-8.04	94.81	103.25
26	3	12	PRO	N-CA-CB	-6.95	94.18	103.15
31	a	35	LEU	CA-CB-CG	6.93	140.57	116.30
31	a	39	PRO	CA-N-CD	-6.62	102.73	112.00
35	M	118	HIS	CA-C-N	6.61	134.16	121.54
35	M	118	HIS	C-N-CA	6.61	134.16	121.54
29	e	2	PRO	N-CD-CG	-6.42	93.56	103.20
31	a	70	PRO	N-CD-CG	-6.39	93.61	103.20
8	G	2	PRO	CA-N-CD	-6.17	103.36	112.00
28	d	51	GLU	CA-CB-CG	6.00	126.09	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	42	GLU	N-CA-C	5.53	117.31	111.28
33	b	14	ASP	N-CA-C	5.43	117.20	111.28
31	a	41	CYS	N-CA-C	5.37	119.44	111.87
31	a	69	VAL	C-N-CD	5.23	146.44	125.00
26	3	24	ARG	CA-CB-CG	5.23	124.56	114.10
31	a	7	GLY	N-CA-C	-5.22	108.42	115.36
3	B	28	GLU	CB-CG-CD	5.08	121.23	112.60
31	a	59	GLY	N-CA-C	5.06	122.33	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2	30982	0	15677	628	0
2	A	1515	0	1565	67	0
3	B	1698	0	1753	50	0
4	C	455	0	437	22	0
5	D	1354	0	1419	37	0
6	E	1930	0	2013	38	0
7	F	1625	0	1689	35	0
8	G	1661	0	1737	67	0
9	H	1543	0	1611	115	0
10	I	1050	0	1100	14	0
11	J	982	0	1046	30	0
12	K	1068	0	1125	82	0
13	L	840	0	893	52	0
14	N	1140	0	1244	35	0
15	O	1124	0	1162	58	0
16	Q	1185	0	1260	28	0
17	R	901	0	935	19	0
18	S	571	0	598	25	0
19	T	1064	0	1107	41	0
20	U	1247	0	1329	65	0
21	V	836	0	894	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	W	503	0	532	20	0
23	X	535	0	572	44	0
24	Y	395	0	405	21	0
25	Z	1561	0	1667	62	0
26	3	893	0	940	70	0
27	c	856	0	941	53	0
28	d	557	0	576	73	0
29	e	354	0	386	19	0
30	4	1645	0	840	33	0
31	a	562	0	574	78	0
32	P	440	0	435	38	0
33	b	723	0	756	120	0
34	5	47	0	21	2	0
35	M	944	0	978	71	0
36	2	546	0	1014	81	0
37	2	54	0	0	0	0
37	5	1	0	0	0	0
37	F	1	0	0	0	0
37	R	1	0	0	0	0
38	C	2	0	0	0	0
38	F	1	0	0	0	0
38	P	1	0	0	0	0
38	R	1	0	0	0	0
38	W	1	0	0	0	0
38	a	2	0	0	0	0
38	b	1	0	0	0	0
39	5	32	0	11	1	0
40	2	181	0	0	16	0
40	4	1	0	0	0	0
40	5	3	0	0	0	0
40	D	1	0	0	0	0
40	E	1	0	0	0	0
40	H	1	0	0	0	0
40	I	2	0	0	0	0
40	J	2	0	0	0	0
40	Q	1	0	0	0	0
40	R	3	0	0	0	0
40	U	1	0	0	0	0
40	b	2	0	0	0	0
All	All	65629	0	51242	1900	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 16.

All (1900) 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)
28:d:5:LYS:HG3	28:d:16:ILE:CG2	1.35	1.52
28:d:5:LYS:CG	28:d:16:ILE:CG2	1.89	1.49
33:b:59:ILE:CD1	35:M:109:ARG:HG2	1.48	1.41
28:d:5:LYS:HG2	28:d:16:ILE:CB	1.54	1.36
1:2:810:C:OP1	36:2:1535:SPM:H132	1.31	1.28
1:2:125:G:OP2	36:2:1521:SPM:H71	1.28	1.25
33:b:67:LYS:HE2	35:M:88:THR:CG2	1.65	1.25
33:b:21:ILE:CD1	33:b:32:GLU:HG2	1.66	1.24
33:b:20:TYR:CE2	33:b:29:ARG:HD2	1.73	1.22
1:2:125:G:OP2	36:2:1521:SPM:C7	1.89	1.20
28:d:5:LYS:CG	28:d:16:ILE:HG21	1.62	1.16
28:d:5:LYS:HD3	28:d:16:ILE:HG22	1.28	1.16
28:d:5:LYS:CD	28:d:16:ILE:HG22	1.75	1.15
33:b:59:ILE:HD13	35:M:109:ARG:HG2	1.26	1.14
33:b:53:LEU:HD11	35:M:107:ILE:HG21	1.25	1.13
28:d:5:LYS:CG	28:d:16:ILE:HB	1.78	1.11
1:2:810:C:OP1	36:2:1535:SPM:C13	1.98	1.11
1:2:683:G:O6	33:b:15:LYS:HE2	1.50	1.10
9:H:39:PRO:CB	9:H:39:PRO:CG	2.23	1.10
33:b:21:ILE:HD11	33:b:32:GLU:CG	1.83	1.08
28:d:5:LYS:CG	28:d:16:ILE:CB	2.20	1.07
33:b:67:LYS:CE	35:M:88:THR:HG23	1.84	1.07
33:b:21:ILE:HD11	33:b:32:GLU:HG2	1.32	1.06
33:b:59:ILE:CD1	35:M:109:ARG:CG	2.32	1.06
33:b:67:LYS:CE	35:M:88:THR:CG2	2.33	1.06
33:b:59:ILE:HD11	35:M:109:ARG:HG2	1.37	1.01
33:b:59:ILE:HD11	35:M:109:ARG:CG	1.87	1.01
33:b:67:LYS:HE2	35:M:88:THR:HG23	1.04	1.00
33:b:20:TYR:CE2	33:b:29:ARG:CD	2.44	0.99
28:d:5:LYS:CG	28:d:16:ILE:HG22	1.87	0.99
1:2:683:G:O6	33:b:15:LYS:CE	2.12	0.98
1:2:683:G:C6	33:b:15:LYS:CE	2.47	0.98
1:2:793:C:OP2	36:2:1535:SPM:H82	1.64	0.98
1:2:683:G:N7	33:b:15:LYS:NZ	2.13	0.97
1:2:393:G:OP1	36:2:1532:SPM:C4	2.12	0.96
33:b:21:ILE:CD1	33:b:32:GLU:CG	2.43	0.95
1:2:1091:U:H3	1:2:1104:G:H1	1.01	0.95
1:2:949:U:H3	1:2:1183:G:H1	0.98	0.94
12:K:39:LEU:HD22	20:U:12:PRO:HD3	1.49	0.93
33:b:29:ARG:NH1	35:M:122:ARG:HD2	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:53:LEU:CD1	35:M:107:ILE:HG21	2.00	0.92
33:b:20:TYR:CD2	33:b:29:ARG:HD2	2.03	0.92
1:2:1201:A:OP2	40:2:1601:HOH:O	1.88	0.91
1:2:125:G:P	36:2:1521:SPM:H71	2.10	0.91
28:d:5:LYS:HD2	28:d:5:LYS:H	1.34	0.91
1:2:683:G:C6	33:b:15:LYS:HE3	2.05	0.90
1:2:21:A:OP1	36:2:1529:SPM:H112	1.72	0.90
1:2:683:G:C6	33:b:15:LYS:HE2	2.05	0.90
4:C:57:CYS:SG	4:C:60:CYS:HB3	2.08	0.90
31:a:49:PHE:CD2	31:a:53:ASP:HB3	2.07	0.90
31:a:49:PHE:HB3	31:a:53:ASP:HB2	1.54	0.89
25:Z:16:VAL:HG21	32:P:48:LEU:HD23	1.52	0.88
1:2:310:G:HO2'	5:D:2:GLY:N	1.71	0.88
1:2:684:G:O6	33:b:15:LYS:HG2	1.74	0.88
31:a:51:GLU:HA	31:a:54:LYS:HE2	1.57	0.87
9:H:111:ARG:HG2	9:H:135:ARG:HH12	1.40	0.87
2:A:14:TRP:HH2	35:M:69:LYS:O	1.57	0.86
33:b:21:ILE:HD11	33:b:32:GLU:CD	1.99	0.86
31:a:41:CYS:HB2	31:a:44:LYS:HD3	1.56	0.86
2:A:17:LYS:HE3	35:M:32:GLU:OE2	1.75	0.86
31:a:57:LEU:HD21	32:P:4:TYR:CE2	2.11	0.86
15:O:104:ARG:HH21	27:c:10:SER:HB3	1.40	0.85
31:a:49:PHE:HD2	31:a:53:ASP:HB3	1.39	0.85
32:P:45:ALA:O	32:P:50:PHE:HB2	1.75	0.85
28:d:5:LYS:HG2	28:d:16:ILE:HB	0.85	0.85
31:a:5:ASN:ND2	32:P:42:ARG:HG2	1.90	0.84
35:M:117:PRO:HG3	35:M:120:THR:HB	1.58	0.83
1:2:943:U:H4'	36:2:1514:SPM:H112	1.58	0.83
2:A:19:TRP:CD1	35:M:8:ARG:HH21	1.97	0.83
1:2:683:G:C5	33:b:15:LYS:CE	2.62	0.83
1:2:941:A:N6	1:2:1187:C:OP1	2.12	0.83
31:a:36:TYR:CE2	31:a:70:PRO:HB3	2.13	0.83
31:a:5:ASN:HD21	32:P:42:ARG:HG2	1.42	0.83
1:2:1371:C:O2	1:2:1451:G:N2	2.12	0.82
28:d:5:LYS:CD	28:d:16:ILE:CG2	2.44	0.82
33:b:60:ILE:HG13	35:M:110:ILE:HB	1.58	0.82
3:B:172:ASP:OD1	3:B:173:THR:N	2.12	0.82
31:a:49:PHE:HB3	31:a:53:ASP:CB	2.10	0.81
1:2:681:G:OP1	2:A:99:ARG:HD3	1.79	0.81
8:G:17:LYS:HA	8:G:17:LYS:HE3	1.62	0.81
9:H:25:PRO:HA	9:H:28:LYS:HE2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:141:ASN:OD1	8:G:147:PRO:HA	1.80	0.80
31:a:57:LEU:HD21	32:P:4:TYR:HE2	1.44	0.80
9:H:90:TYR:HB2	9:H:97:PRO:HG3	1.63	0.80
1:2:786:U:OP2	22:W:6:ARG:NH2	2.15	0.80
30:4:9:G:O2'	30:4:10:G:N7	2.15	0.80
22:W:30:ILE:HD11	22:W:38:VAL:HG21	1.64	0.80
33:b:23:CYS:O	33:b:27:GLY:N	2.15	0.80
1:2:71:G:N2	1:2:213:C:O2	2.11	0.80
31:a:45:TYR:CE2	32:P:6:PRO:HB2	2.17	0.79
21:V:63:VAL:HG22	21:V:83:ILE:HG12	1.63	0.79
9:H:6:LEU:HB3	28:d:70:LYS:HD2	1.64	0.79
33:b:28:ALA:HB2	35:M:128:ARG:O	1.83	0.78
12:K:32:VAL:HA	12:K:68:ILE:HB	1.66	0.78
33:b:21:ILE:HD13	33:b:32:GLU:HG2	1.64	0.78
2:A:33:LEU:HD22	2:A:51:THR:HG21	1.65	0.78
33:b:67:LYS:CE	35:M:88:THR:HG21	2.12	0.78
5:D:116:SER:HB2	5:D:121:GLN:HG2	1.66	0.77
9:H:101:LEU:HA	9:H:166:ILE:HD11	1.65	0.77
1:2:579:C:H5''	36:2:1534:SPM:H132	1.66	0.77
33:b:42:TYR:OH	35:M:89:PRO:HG2	1.85	0.77
33:b:59:ILE:HD11	35:M:109:ARG:HG3	1.67	0.77
28:d:5:LYS:NZ	28:d:5:LYS:HB3	2.00	0.77
33:b:24:ASP:HA	35:M:123:ARG:NH2	1.99	0.77
33:b:70:CYS:SG	33:b:72:ASN:N	2.58	0.77
3:B:191:ARG:HH21	3:B:226:GLU:HB3	1.50	0.76
12:K:23:ILE:HD11	12:K:64:ILE:HG13	1.65	0.76
1:2:393:G:P	36:2:1532:SPM:H41	2.26	0.76
14:N:70:ARG:HG3	14:N:119:LEU:HD13	1.66	0.76
14:N:61:GLU:OE2	14:N:61:GLU:N	2.15	0.76
15:O:42:ARG:NH2	20:U:54:GLU:OE2	2.18	0.76
1:2:711:G:OP1	16:Q:132:LYS:NZ	2.18	0.76
1:2:1336:U:H3'	12:K:76:MET:HE2	1.66	0.76
28:d:48:GLU:HA	28:d:51:GLU:HB3	1.66	0.75
2:A:14:TRP:CH2	35:M:69:LYS:O	2.39	0.75
1:2:1456:A:OP1	40:2:1602:HOH:O	2.04	0.75
1:2:967:G:N1	26:3:38:GLU:OE2	2.20	0.74
12:K:29:ARG:N	12:K:65:ASP:OD2	2.20	0.74
28:d:5:LYS:HD2	28:d:5:LYS:N	2.01	0.74
28:d:21:ILE:HA	28:d:24:LEU:HB2	1.69	0.74
5:D:98:GLU:OE1	5:D:98:GLU:N	2.19	0.74
9:H:29:LYS:NZ	28:d:27:TYR:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:156:LYS:HZ2	9:H:160:GLU:HB3	1.52	0.74
1:2:1034:G:N2	1:2:1037:A:OP2	2.20	0.74
1:2:71:G:N1	1:2:213:C:N3	2.29	0.74
9:H:187:ARG:HA	9:H:190:LEU:HG	1.67	0.74
11:J:34:PHE:HB3	11:J:95:ILE:HG12	1.68	0.74
16:Q:136:GLU:N	16:Q:136:GLU:OE2	2.20	0.74
33:b:21:ILE:HD13	33:b:32:GLU:CA	2.18	0.74
20:U:47:GLU:N	20:U:47:GLU:OE1	2.21	0.73
31:a:34:ILE:HD12	31:a:34:ILE:O	1.87	0.73
1:2:1095:C:O2'	1:2:1096:U:O5'	2.07	0.73
1:2:1292:C:OP1	15:O:35:ASN:ND2	2.21	0.73
35:M:117:PRO:CG	35:M:120:THR:HB	2.19	0.73
3:B:18:GLU:OE1	3:B:18:GLU:N	2.20	0.73
9:H:132:PRO:HA	9:H:135:ARG:HD3	1.71	0.73
15:O:84:LYS:O	19:T:15:ARG:NH1	2.22	0.73
26:3:92:LEU:HD21	26:3:94:VAL:HG12	1.70	0.73
23:X:45:GLU:HA	23:X:49:LYS:HD2	1.71	0.72
23:X:35:GLU:N	23:X:35:GLU:OE1	2.22	0.72
3:B:49:ILE:O	3:B:187:ASN:ND2	2.22	0.72
30:4:50:U:H3	30:4:64:G:H1	0.78	0.72
33:b:7:ASN:C	33:b:8:ARG:HG2	2.14	0.72
1:2:796:A:OP1	40:2:1603:HOH:O	2.08	0.72
1:2:1097:C:H42	20:U:6:ILE:HB	1.54	0.72
28:d:5:LYS:HB3	28:d:5:LYS:HZ2	1.54	0.72
31:a:44:LYS:HG2	31:a:45:TYR:CD1	2.24	0.72
26:3:40:THR:HG22	26:3:66:LEU:HD11	1.70	0.72
1:2:125:G:OP2	36:2:1521:SPM:H72	1.90	0.71
3:B:101:ALA:HB2	3:B:110:VAL:HG21	1.72	0.71
4:C:16:CYS:HB3	4:C:19:CYS:SG	2.29	0.71
1:2:191:U:O3'	11:J:45:LYS:NZ	2.24	0.71
1:2:965:A:H2'	26:3:94:VAL:HG11	1.72	0.71
9:H:111:ARG:NH2	23:X:68:ILE:O	2.17	0.71
1:2:483:G:H5''	14:N:116:MET:HG3	1.73	0.71
1:2:683:G:N7	33:b:15:LYS:CE	2.53	0.71
1:2:967:G:N7	26:3:37:ASN:ND2	2.39	0.71
22:W:38:VAL:HG22	22:W:48:VAL:HG12	1.72	0.71
26:3:11:VAL:HG12	26:3:79:TYR:HD2	1.56	0.71
1:2:684:G:O6	33:b:15:LYS:CG	2.39	0.70
1:2:1074:A:OP1	12:K:13:ARG:NH2	2.24	0.70
1:2:393:G:OP1	36:2:1532:SPM:H42	1.88	0.70
1:2:1035:U:O3'	7:F:192:ARG:NH2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:134:PRO:HG2	16:Q:137:TRP:HB2	1.72	0.70
33:b:23:CYS:O	33:b:27:GLY:HA2	1.91	0.70
14:N:49:MET:HB3	14:N:106:THR:HG22	1.73	0.70
33:b:7:ASN:O	33:b:8:ARG:HG2	1.92	0.70
15:O:106:ASP:OD1	15:O:109:ARG:NH2	2.22	0.70
20:U:158:GLU:OE1	20:U:158:GLU:N	2.25	0.70
19:T:108:HIS:HD1	19:T:113:TYR:HH	1.38	0.70
1:2:1217:G:OP1	32:P:32:TYR:OH	2.05	0.70
7:F:121:CYS:SG	7:F:126:CYS:HB3	2.31	0.70
27:c:58:GLU:HG2	27:c:65:ILE:HG22	1.72	0.70
1:2:393:G:OP1	36:2:1532:SPM:H41	1.92	0.70
1:2:517:C:N3	40:2:1629:HOH:O	2.25	0.70
24:Y:26:TYR:OH	24:Y:38:ASN:OD1	2.08	0.70
1:2:192:G:P	11:J:45:LYS:HZ1	2.15	0.70
9:H:111:ARG:NH2	23:X:70:ARG:HB3	2.06	0.70
32:P:47:GLU:OE1	32:P:47:GLU:N	2.24	0.70
24:Y:41:CYS:HB3	24:Y:46:SER:H	1.57	0.69
1:2:644:G:OP1	2:A:39:TYR:OH	2.09	0.69
5:D:143:TYR:OH	5:D:149:GLU:OE2	2.08	0.69
33:b:67:LYS:HE2	35:M:88:THR:HG21	1.65	0.69
1:2:1446:G:H2'	1:2:1447:A:H8	1.57	0.69
23:X:22:GLU:OE2	28:d:33:THR:OG1	2.10	0.69
28:d:27:TYR:HB2	28:d:37:LEU:HD13	1.73	0.69
20:U:45:PHE:HB2	20:U:87:LYS:HB2	1.74	0.69
33:b:21:ILE:HD13	33:b:32:GLU:HA	1.74	0.69
1:2:1451:G:O2'	1:2:1452:U:H5'	1.93	0.69
9:H:111:ARG:HH22	23:X:18:GLY:HA3	1.56	0.69
10:I:101:GLU:N	10:I:101:GLU:OE2	2.26	0.69
25:Z:90:GLU:OE2	25:Z:120:ARG:NH2	2.26	0.69
1:2:962:A:H2'	1:2:963:G:H8	1.57	0.69
25:Z:16:VAL:CG2	32:P:48:LEU:HD23	2.23	0.69
33:b:23:CYS:O	33:b:27:GLY:CA	2.41	0.69
3:B:188:ASN:HA	3:B:194:LEU:HD13	1.75	0.68
16:Q:97:ARG:NH2	16:Q:117:GLU:OE2	2.21	0.68
1:2:1162:U:O4	36:2:1515:SPM:N1	2.25	0.68
13:L:101:LEU:N	13:L:101:LEU:HD22	2.07	0.68
1:2:962:A:H2'	1:2:963:G:C8	2.28	0.68
1:2:644:G:N3	35:M:36:ARG:NH2	2.39	0.68
1:2:910:A:H2'	1:2:911:A:C8	2.28	0.68
1:2:1198:U:OP1	40:2:1604:HOH:O	2.12	0.68
15:O:51:ARG:NH1	27:c:42:SER:OG	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:76:ILE:O	20:U:79:THR:OG1	2.08	0.68
12:K:28:GLY:O	12:K:61:ARG:NH2	2.27	0.68
28:d:5:LYS:HG3	28:d:16:ILE:HG21	0.70	0.68
8:G:26:SER:C	8:G:96:LYS:HZ1	2.02	0.68
1:2:1057:C:N4	1:2:1060:OMC:OP2	2.27	0.68
1:2:349:A:H5''	1:2:350:C:H5	1.59	0.67
1:2:964:G:N2	1:2:965:A:N1	2.42	0.67
10:I:114:MET:HE1	10:I:122:LEU:HD12	1.75	0.67
16:Q:98:ARG:NH1	16:Q:102:GLU:OE2	2.27	0.67
26:3:120:GLU:OE1	26:3:120:GLU:N	2.27	0.67
40:2:1601:HOH:O	9:H:153:ASN:OD1	2.12	0.67
11:J:89:GLU:OE2	11:J:89:GLU:N	2.25	0.67
1:2:777:A:H5''	33:b:8:ARG:NH2	2.09	0.67
26:3:112:ASP:HA	26:3:115:ILE:HD12	1.75	0.67
1:2:417:G:H21	1:2:419:A:H1'	1.59	0.67
7:F:160:VAL:HG12	7:F:178:SER:HB3	1.76	0.67
27:c:65:ILE:HD11	27:c:106:TYR:HB2	1.77	0.67
21:V:88:GLU:N	21:V:88:GLU:OE2	2.25	0.67
25:Z:70:PHE:HB3	25:Z:76:LEU:HD12	1.76	0.67
31:a:64:CYS:SG	31:a:66:THR:OG1	2.48	0.67
1:2:502:C:OP1	29:e:41:ARG:NH1	2.27	0.67
5:D:86:GLU:OE1	5:D:86:GLU:N	2.20	0.67
1:2:634:U:OP1	2:A:188:LYS:NZ	2.27	0.67
1:2:754:C:O2'	35:M:131:ARG:O	2.06	0.67
15:O:112:LYS:NZ	19:T:104:GLU:OE2	2.28	0.67
28:d:64:PRO:HG2	28:d:67:ILE:HG12	1.77	0.67
1:2:418:U:H1'	1:2:419:A:C5	2.30	0.66
1:2:619:G:H2'	1:2:620:G:C8	2.31	0.66
19:T:27:MET:HE2	19:T:27:MET:HA	1.75	0.66
26:3:93:GLN:NE2	26:3:93:GLN:O	2.27	0.66
1:2:613:G:OP2	40:2:1605:HOH:O	2.13	0.66
7:F:141:LYS:HG3	7:F:146:GLU:HG3	1.78	0.66
25:Z:36:VAL:HG12	25:Z:45:VAL:HG22	1.76	0.66
31:a:6:ARG:NE	32:P:46:TYR:CE2	2.64	0.66
1:2:337:OMG:HM22	1:2:338:G:H5'	1.77	0.66
1:2:680:A:OP1	2:A:129:LYS:HE3	1.95	0.66
1:2:1491:A:H2	33:b:94:LEU:HD21	1.58	0.66
19:T:15:ARG:HB2	19:T:33:LEU:HD23	1.75	0.66
21:V:107:GLN:HE21	21:V:109:LYS:HB2	1.60	0.66
9:H:10:ILE:HA	9:H:37:TYR:CE1	2.30	0.66
1:2:256:G:H4'	1:2:257:U:H5'	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:7:SER:HB2	7:F:53:LYS:HE3	1.78	0.66
5:D:30:LEU:HD23	5:D:35:LEU:HB2	1.77	0.66
12:K:98:GLU:OE1	12:K:98:GLU:N	2.28	0.66
1:2:714:G:H21	10:I:3:PHE:HZ	1.42	0.66
1:2:1114:U:H4'	13:L:42:PRO:HG3	1.77	0.66
1:2:1203:U:O2'	9:H:71:ASN:ND2	2.29	0.66
1:2:681:G:N7	2:A:129:LYS:NZ	2.44	0.66
1:2:393:G:OP1	36:2:1532:SPM:C3	2.44	0.65
5:D:21:GLU:OE1	5:D:21:GLU:N	2.22	0.65
15:O:104:ARG:O	15:O:108:GLU:HG2	1.96	0.65
1:2:917:G:OP1	36:2:1525:SPM:N10	2.27	0.65
9:H:18:THR:HG21	9:H:35:PRO:HA	1.78	0.65
13:L:99:ILE:HD12	13:L:99:ILE:O	1.95	0.65
25:Z:6:ARG:HB3	25:Z:6:ARG:NH1	2.11	0.65
31:a:43:LYS:HE3	31:a:43:LYS:HA	1.78	0.65
22:W:51:MET:HA	22:W:51:MET:HE3	1.79	0.65
26:3:27:LYS:HZ1	26:3:89:ALA:HB3	1.62	0.65
1:2:1443:G:H3'	1:2:1444:G:H8	1.59	0.65
3:B:112:LYS:HA	3:B:112:LYS:HE3	1.78	0.65
26:3:83:LYS:HZ2	26:3:95:ALA:HB1	1.61	0.65
1:2:1374:U:C2	1:2:1448:G:C2	2.84	0.65
14:N:119:LEU:HD12	14:N:120:PRO:HD2	1.79	0.65
16:Q:32:GLU:OE2	16:Q:76:ARG:NH1	2.26	0.65
33:b:67:LYS:HE3	35:M:88:THR:CG2	2.25	0.65
1:2:1161:G:O6	36:2:1515:SPM:N1	2.29	0.65
1:2:1443:G:H3'	1:2:1444:G:C8	2.32	0.65
3:B:98:ILE:HG12	3:B:142:PRO:HB3	1.77	0.65
33:b:70:CYS:SG	33:b:72:ASN:HB2	2.37	0.65
35:M:48:GLU:N	35:M:48:GLU:OE1	2.30	0.65
1:2:362:G:OP2	40:2:1606:HOH:O	2.14	0.64
1:2:628:C:OP1	16:Q:105:ARG:NH1	2.27	0.64
1:2:1318:C:H2'	1:2:1319:A:H8	1.62	0.64
20:U:35:GLU:OE1	20:U:35:GLU:N	2.22	0.64
31:a:41:CYS:CB	31:a:44:LYS:HD3	2.25	0.64
35:M:25:ILE:HG22	35:M:34:ILE:HB	1.80	0.64
1:2:1374:U:C2	1:2:1448:G:N2	2.64	0.64
21:V:38:MET:HA	21:V:38:MET:HE3	1.79	0.64
27:c:22:LYS:HA	27:c:25:LYS:HB3	1.79	0.64
31:a:38:CYS:HB2	31:a:61:CYS:HB2	1.77	0.64
1:2:672:OMG:H2'	1:2:673:G:C8	2.32	0.64
33:b:53:LEU:CD1	35:M:107:ILE:CG2	2.73	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:599:A:HO2'	10:I:110:SER:HG	1.46	0.64
1:2:1465:G:OP1	36:2:1523:SPM:N14	2.30	0.64
36:2:1516:SPM:N14	12:K:122:LYS:O	2.30	0.64
9:H:113:GLU:OE1	9:H:115:THR:HG23	1.98	0.64
1:2:141:A:OP1	40:2:1607:HOH:O	2.14	0.64
11:J:40:GLU:N	11:J:40:GLU:OE2	2.30	0.64
25:Z:65:GLN:OE1	25:Z:68:GLN:NE2	2.29	0.64
26:3:24:ARG:HG3	26:3:89:ALA:HB1	1.80	0.64
26:3:26:ALA:HB1	26:3:101:ILE:HD13	1.79	0.64
28:d:41:LEU:HD22	28:d:43:LEU:HB2	1.79	0.64
28:d:7:LYS:HB2	28:d:14:VAL:HB	1.78	0.64
9:H:26:SER:HA	23:X:66:ILE:HB	1.78	0.64
33:b:4:LYS:HB3	33:b:5:ARG:HD2	1.77	0.64
12:K:32:VAL:HG13	12:K:37:ILE:HD11	1.78	0.63
13:L:12:THR:OG1	13:L:13:ASN:OD1	2.15	0.63
12:K:10:SER:HB3	12:K:21:CYS:HB3	1.78	0.63
14:N:91:ASP:N	14:N:138:TYR:OH	2.31	0.63
20:U:20:LEU:HD21	20:U:65:LEU:HD23	1.79	0.63
1:2:481:OMC:HM22	1:2:482:C:H5'	1.79	0.63
9:H:91:LEU:O	27:c:63:SER:OG	2.14	0.63
11:J:33:THR:HG21	11:J:56:ARG:HD3	1.79	0.63
1:2:1251:A:H2'	1:2:1252:A:C8	2.34	0.63
8:G:128:ASN:HD21	8:G:143:LEU:HD21	1.63	0.63
25:Z:130:GLU:HB3	25:Z:182:VAL:HB	1.80	0.63
31:a:34:ILE:HD12	31:a:34:ILE:C	2.23	0.63
1:2:926:OMG:N7	36:2:1525:SPM:H82	2.13	0.63
27:c:80:VAL:O	27:c:84:ILE:HD12	1.98	0.63
5:D:19:ILE:HG22	5:D:22:ARG:H	1.64	0.63
12:K:30:VAL:HG23	12:K:37:ILE:HD13	1.81	0.63
20:U:77:GLU:OE2	20:U:77:GLU:N	2.30	0.63
11:J:63:ALA:HB2	11:J:78:ILE:HG13	1.81	0.63
12:K:37:ILE:HG21	12:K:50:MET:HE3	1.79	0.63
14:N:98:ASP:OD1	14:N:144:LYS:NZ	2.31	0.63
20:U:94:GLU:OE1	20:U:94:GLU:N	2.24	0.63
25:Z:118:MET:HE3	25:Z:147:LEU:HG	1.81	0.63
26:3:51:VAL:HG13	26:3:77:TYR:HB2	1.79	0.63
26:3:55:GLU:HB2	26:3:80:VAL:HG21	1.80	0.63
27:c:68:TYR:O	27:c:72:THR:HG23	1.98	0.63
36:2:1524:SPM:N14	36:2:1535:SPM:N1	2.46	0.63
13:L:81:ARG:HD2	13:L:84:ARG:HH12	1.63	0.63
22:W:40:CYS:CB	22:W:43:CYS:SG	2.86	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:81:ILE:HD11	11:J:96:ILE:HB	1.81	0.62
15:O:14:GLN:HE22	15:O:30:LYS:H	1.46	0.62
17:R:91:ASP:OD1	17:R:91:ASP:N	2.32	0.62
1:2:1324:A:C8	32:P:12:TYR:HB3	2.34	0.62
1:2:74:A:N1	1:2:213:C:O2'	2.33	0.62
1:2:636:C:H2'	1:2:637:U:C6	2.35	0.62
23:X:48:ASP:OD2	23:X:51:ARG:NE	2.30	0.62
33:b:53:LEU:HD11	35:M:107:ILE:CG2	2.14	0.62
1:2:683:G:C5	33:b:15:LYS:HE3	2.30	0.62
2:A:116:TYR:CD1	2:A:195:PRO:HD2	2.35	0.62
8:G:26:SER:HG	8:G:93:TRP:CG	2.18	0.62
25:Z:58:ARG:O	25:Z:58:ARG:NH1	2.28	0.62
33:b:7:ASN:O	33:b:8:ARG:CG	2.47	0.62
31:a:45:TYR:HE1	32:P:9:GLU:HB2	1.64	0.62
2:A:19:TRP:CG	35:M:8:ARG:HH21	2.16	0.62
26:3:19:VAL:HB	26:3:114:ILE:HG21	1.82	0.62
1:2:1076:C:H2'	1:2:1077:A:H8	1.64	0.62
9:H:89:ILE:HA	9:H:92:LYS:HB2	1.82	0.62
31:a:37:LYS:HE3	31:a:71:ILE:HB	1.81	0.62
1:2:1369:G:O2'	1:2:1475:MA6:O2'	2.17	0.61
30:4:36:U:H3	39:5:102:GTP:HN1	1.47	0.61
8:G:32:ILE:N	8:G:35:GLU:OE2	2.34	0.61
1:2:947:A:O2'	1:2:1007:G:OP2	2.15	0.61
16:Q:58:ILE:HG23	16:Q:64:ILE:HD12	1.83	0.61
1:2:1188:G:O2'	1:2:1189:C:OP1	2.18	0.61
1:2:1479:U:P	35:M:128:ARG:HH12	2.24	0.61
9:H:41:THR:O	9:H:44:ARG:NH1	2.33	0.61
1:2:119:U:O2	6:E:141:ASN:ND2	2.30	0.61
2:A:86:HIS:CE1	2:A:189:THR:HG23	2.36	0.61
8:G:202:SER:OG	8:G:203:GLN:N	2.31	0.61
15:O:7:TYR:OH	27:c:39:GLU:OE2	2.18	0.61
26:3:31:LYS:HB2	26:3:102:LEU:HB2	1.81	0.61
31:a:34:ILE:HD11	31:a:51:GLU:HB2	1.82	0.61
6:E:34:GLU:OE1	6:E:34:GLU:N	2.33	0.61
8:G:42:PRO:HB2	8:G:79:PHE:HD1	1.65	0.61
12:K:80:ASP:OD1	12:K:83:ARG:NH1	2.28	0.61
31:a:37:LYS:HA	31:a:47:ALA:O	1.99	0.61
1:2:438:C:N3	36:2:1518:SPM:N14	2.49	0.61
20:U:130:LYS:H	20:U:130:LYS:HD2	1.65	0.61
1:2:1189:C:HO2'	27:c:2:GLY:N	1.98	0.61
1:2:1436:U:H2'	1:2:1437:G:C8	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:987:U:H2'	1:2:988:G:C8	2.36	0.61
1:2:351:G:O2'	8:G:172:LYS:NZ	2.33	0.60
1:2:1272:C:O2'	27:c:7:LYS:NZ	2.33	0.60
7:F:90:SER:HB2	7:F:114:ILE:HA	1.83	0.60
12:K:29:ARG:NH2	20:U:158:GLU:OE1	2.34	0.60
21:V:22:GLN:HE22	21:V:85:LYS:NZ	1.99	0.60
2:A:19:TRP:CD1	35:M:8:ARG:NH2	2.69	0.60
2:A:47:ARG:HB3	35:M:29:THR:HG21	1.83	0.60
5:D:106:LEU:O	5:D:110:VAL:HG12	2.01	0.60
16:Q:97:ARG:CZ	16:Q:141:PRO:HB3	2.31	0.60
17:R:2:VAL:O	17:R:6:LYS:NZ	2.21	0.60
23:X:55:ARG:NH1	23:X:74:ARG:HB2	2.15	0.60
31:a:49:PHE:HD2	31:a:53:ASP:CB	2.11	0.60
1:2:1253:A:N1	1:2:1335:G:O2'	2.26	0.60
11:J:38:SER:O	11:J:61:THR:OG1	2.17	0.60
1:2:1343:G:H2'	1:2:1344:OMU:H6	1.83	0.60
5:D:99:GLN:O	5:D:103:GLU:HG2	2.01	0.60
1:2:1048:U:HO2'	18:S:2:GLY:N	1.99	0.60
1:2:1267:G:OP1	20:U:48:ARG:NH2	2.35	0.60
1:2:1449:A:H8	1:2:1449:A:OP2	1.84	0.60
4:C:34:CYS:HB3	4:C:38:GLY:H	1.65	0.60
8:G:30:LYS:H	8:G:30:LYS:HD3	1.67	0.60
9:H:18:THR:HA	9:H:98:ILE:HD11	1.83	0.60
10:I:55:ASP:OD2	10:I:60:LYS:NZ	2.34	0.60
16:Q:61:VAL:HG11	16:Q:69:VAL:HG23	1.84	0.60
28:d:22:ALA:HB2	28:d:65:LEU:HD23	1.82	0.60
33:b:33:ASP:OD1	33:b:33:ASP:N	2.34	0.60
5:D:31:GLY:HA3	29:e:38:TYR:CG	2.37	0.60
27:c:96:LEU:HB2	27:c:106:TYR:CE1	2.37	0.60
3:B:108:ARG:NH1	3:B:227:MET:O	2.35	0.60
22:W:24:CYS:HB2	22:W:43:CYS:HB3	1.82	0.60
26:3:44:GLU:HA	26:3:73:LYS:HE3	1.84	0.60
1:2:1469:U:H5''	36:2:1538:SPM:H22	1.84	0.60
15:O:85:ASP:OD1	15:O:86:TYR:N	2.34	0.60
1:2:1337:G:H5'	9:H:75:LYS:HB2	1.84	0.60
27:c:74:SER:HB2	27:c:76:ILE:HG12	1.83	0.59
1:2:617:G:H2'	1:2:618:C:C6	2.37	0.59
1:2:1066:A:OP2	25:Z:155:SER:OG	2.20	0.59
1:2:1070:C:H2'	1:2:1071:C:C6	2.37	0.59
1:2:1203:U:H5'	27:c:102:ARG:HD3	1.83	0.59
5:D:158:THR:HG21	21:V:39:GLY:HA3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:100:LYS:HG3	10:I:101:GLU:OE2	2.02	0.59
12:K:28:GLY:N	12:K:64:ILE:O	2.33	0.59
25:Z:18:ILE:HG22	25:Z:34:VAL:HG11	1.82	0.59
1:2:1282:A:HO2'	19:T:76:ASN:HD22	1.45	0.59
9:H:111:ARG:HG2	9:H:135:ARG:NH1	2.15	0.59
1:2:885:G:H2'	1:2:886:G:C8	2.37	0.59
25:Z:154:LYS:HA	31:a:3:ILE:HD11	1.84	0.59
1:2:788:G:H5''	3:B:56:LYS:HG3	1.84	0.59
6:E:113:GLU:OE2	6:E:237:ARG:NH2	2.34	0.59
7:F:79:LEU:HD11	7:F:188:GLU:HA	1.84	0.59
9:H:19:LYS:HD2	28:d:59:TRP:CZ2	2.38	0.59
12:K:23:ILE:HD13	12:K:66:ALA:HB2	1.83	0.59
30:4:50:U:O2	30:4:64:G:N2	2.20	0.59
1:2:483:G:O4'	36:2:1502:SPM:H131	2.03	0.59
1:2:988:G:O2'	1:2:989:C:O5'	2.19	0.59
24:Y:24:ARG:HD3	26:3:37:ASN:HB3	1.82	0.59
26:3:6:TYR:OH	26:3:77:TYR:OH	2.19	0.59
12:K:101:LYS:HZ3	28:d:65:LEU:HD12	1.67	0.59
1:2:475:U:H4'	29:e:16:GLN:HE21	1.67	0.59
1:2:1444:G:N2	1:2:1445:G:O6	2.35	0.59
28:d:4:LEU:N	28:d:4:LEU:HD23	2.18	0.59
30:4:58:A:O2'	30:4:60:U:OP2	2.13	0.59
1:2:922:A:N3	1:2:949:U:O2'	2.34	0.59
1:2:1097:C:N4	20:U:140:LEU:HB2	2.17	0.59
1:2:1451:G:C2'	1:2:1452:U:H5'	2.32	0.59
12:K:119:GLU:HG2	12:K:128:ALA:HB1	1.84	0.59
13:L:7:ILE:HG13	13:L:99:ILE:HG23	1.85	0.59
25:Z:42:GLY:HA3	25:Z:78:ASN:HB3	1.85	0.59
27:c:39:GLU:HB2	27:c:76:ILE:HA	1.84	0.59
25:Z:158:GLN:NE2	25:Z:191:ASP:OD2	2.35	0.59
5:D:110:VAL:HG13	5:D:122:ALA:HB1	1.85	0.58
12:K:99:LEU:HA	12:K:102:ILE:HG12	1.84	0.58
1:2:243:G:OP1	17:R:73:ARG:NH1	2.36	0.58
6:E:122:ILE:O	6:E:204:ARG:NH2	2.29	0.58
9:H:16:TRP:CZ3	9:H:86:PHE:HB3	2.39	0.58
23:X:30:THR:OG1	23:X:31:GLY:N	2.34	0.58
33:b:29:ARG:HH12	35:M:122:ARG:HD2	1.64	0.58
1:2:1318:C:H2'	1:2:1319:A:C8	2.38	0.58
17:R:20:GLU:OE2	17:R:20:GLU:N	2.25	0.58
1:2:465:G:O6	36:2:1502:SPM:N1	2.32	0.58
3:B:99:VAL:HG23	3:B:110:VAL:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:47:LEU:HA	22:W:58:VAL:HG22	1.84	0.58
36:2:1524:SPM:HN41	36:2:1535:SPM:HN12	1.50	0.58
9:H:39:PRO:HB3	9:H:58:VAL:HG23	1.83	0.58
33:b:67:LYS:HE3	35:M:88:THR:HG21	1.83	0.58
13:L:11:SER:OG	13:L:95:VAL:HG12	2.03	0.58
15:O:7:TYR:CZ	27:c:29:LYS:HD2	2.38	0.58
1:2:1282:A:O2'	19:T:76:ASN:ND2	2.24	0.58
2:A:156:ASP:O	2:A:160:GLN:HG2	2.03	0.58
19:T:83:LEU:HD23	19:T:88:MET:HE3	1.86	0.58
1:2:991:U:H2'	1:2:992:G:C4	2.39	0.58
1:2:1024:A:OP1	36:2:1537:SPM:N14	2.37	0.58
1:2:1152:C:OP1	32:P:52:LYS:NZ	2.36	0.58
8:G:80:LYS:NZ	8:G:145:GLY:O	2.35	0.58
9:H:158:ILE:HG23	9:H:159:GLU:OE1	2.03	0.58
14:N:127:ILE:HG13	14:N:128:MET:HG2	1.84	0.58
16:Q:26:LEU:HD12	16:Q:58:ILE:HD11	1.84	0.58
5:D:31:GLY:HA3	29:e:38:TYR:CD1	2.38	0.58
6:E:40:ALA:HB2	6:E:75:TYR:HB2	1.86	0.58
8:G:174:LYS:HG2	8:G:193:ARG:HG2	1.86	0.58
9:H:156:LYS:NZ	9:H:160:GLU:HB3	2.19	0.58
15:O:22:LEU:HD23	15:O:26:LEU:HD23	1.86	0.58
1:2:218:C:H2'	1:2:219:A:H8	1.67	0.57
7:F:141:LYS:NZ	7:F:143:GLY:O	2.37	0.57
9:H:111:ARG:NH2	23:X:18:GLY:HA3	2.19	0.57
12:K:97:LYS:O	12:K:97:LYS:NZ	2.29	0.57
31:a:59:GLY:O	31:a:68:LEU:HG	2.04	0.57
12:K:23:ILE:HD11	12:K:64:ILE:CG1	2.32	0.57
4:C:34:CYS:CB	4:C:37:CYS:SG	2.92	0.57
5:D:89:THR:OG1	5:D:90:VAL:N	2.36	0.57
7:F:69:ASP:N	7:F:69:ASP:OD1	2.36	0.57
18:S:64:LYS:O	18:S:67:SER:OG	2.22	0.57
20:U:51:ASP:OD1	20:U:52:ASN:N	2.36	0.57
26:3:35:GLY:O	26:3:39:THR:OG1	2.22	0.57
9:H:111:ARG:NH1	23:X:17:PHE:O	2.38	0.57
1:2:1004:G:HO2'	1:2:1178:C:HO2'	1.50	0.57
8:G:64:ILE:HG12	8:G:102:PHE:HD2	1.69	0.57
8:G:148:VAL:HB	8:G:212:ILE:HG23	1.86	0.57
13:L:4:LYS:HG3	13:L:77:ALA:HA	1.86	0.57
1:2:429:U:H1'	5:D:127:THR:HG22	1.87	0.57
1:2:1341:A:OP2	9:H:52:LYS:NZ	2.30	0.57
7:F:32:LYS:NZ	7:F:36:ASP:OD1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:34:CYS:HB3	4:C:37:CYS:SG	2.45	0.57
35:M:15:TYR:HB3	35:M:22:LEU:HB2	1.86	0.57
1:2:39:U:O4	6:E:18:LYS:NZ	2.38	0.57
6:E:109:ILE:HB	6:E:113:GLU:HG3	1.86	0.57
18:S:32:LYS:O	18:S:35:VAL:HG12	2.03	0.57
3:B:57:TYR:OH	4:C:65:PRO:O	2.21	0.57
15:O:78:TRP:HH2	20:U:40:ALA:HB2	1.70	0.57
18:S:19:ARG:NH1	18:S:20:TYR:OH	2.38	0.57
18:S:30:THR:O	18:S:34:ILE:HD12	2.04	0.57
1:2:682:U:O2	1:2:682:U:H2'	2.05	0.56
1:2:1311:G:O6	12:K:14:ARG:NH2	2.34	0.56
7:F:12:GLU:OE1	7:F:12:GLU:N	2.35	0.56
1:2:1019:U:OP1	13:L:59:ARG:HD3	2.04	0.56
4:C:59:ASN:OD1	4:C:60:CYS:N	2.38	0.56
11:J:96:ILE:HD13	11:J:121:ILE:HD13	1.88	0.56
12:K:84:MET:SD	12:K:113:GLY:HA2	2.45	0.56
1:2:93:C:H1'	1:2:359:C:H5'	1.88	0.56
1:2:518:U:OP2	36:2:1501:SPM:N5	2.38	0.56
1:2:1470:A:OP1	36:2:1538:SPM:N1	2.38	0.56
1:2:1492:C:H5	33:b:39:THR:HG1	1.53	0.56
3:B:199:TRP:NE1	3:B:220:VAL:O	2.30	0.56
12:K:120:SER:O	12:K:122:LYS:NZ	2.37	0.56
15:O:107:ILE:HG22	15:O:111:LYS:NZ	2.20	0.56
21:V:59:GLN:OE1	21:V:59:GLN:N	2.38	0.56
26:3:73:LYS:HB2	26:3:75:ILE:HG13	1.88	0.56
33:b:20:TYR:CD2	33:b:29:ARG:HB3	2.40	0.56
1:2:12:U:H2'	1:2:13:C:C6	2.40	0.56
1:2:458:G:H2'	1:2:459:C:C6	2.41	0.56
1:2:1032:OMU:HM22	1:2:1033:U:H5'	1.86	0.56
13:L:80:GLU:HA	13:L:83:MET:HE2	1.88	0.56
25:Z:11:LYS:HZ2	25:Z:11:LYS:HB3	1.69	0.56
23:X:19:PHE:HD1	23:X:70:ARG:HA	1.71	0.56
35:M:84:TYR:HD1	35:M:84:TYR:C	2.14	0.56
1:2:926:OMG:HM22	1:2:927:G:H5'	1.86	0.56
1:2:1070:C:H2'	1:2:1071:C:H6	1.71	0.56
1:2:1191:C:OP2	27:c:2:GLY:N	2.38	0.56
1:2:1213:A:H2'	1:2:1214:G:C8	2.41	0.56
1:2:1339:A:OP2	9:H:45:HIS:NE2	2.30	0.56
1:2:1368:5MC:H2'	1:2:1369:G:C8	2.41	0.56
8:G:35:GLU:OE1	8:G:97:THR:OG1	2.24	0.56
1:2:1253:A:H5'	20:U:86:ARG:HH12	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:101:LYS:NZ	28:d:65:LEU:HD12	2.20	0.56
23:X:38:GLN:NE2	23:X:78:LYS:HD3	2.21	0.56
26:3:114:ILE:O	26:3:118:VAL:HG13	2.06	0.56
1:2:237:G:OP2	36:2:1531:SPM:N1	2.37	0.56
1:2:1206:C:H5''	20:U:47:GLU:OE2	2.06	0.56
1:2:1335:G:O3'	12:K:74:GLY:HA3	2.05	0.56
21:V:96:LYS:NZ	21:V:100:ASP:OD1	2.33	0.56
8:G:60:LEU:HD11	8:G:111:ALA:HB1	1.87	0.56
20:U:12:PRO:HB2	20:U:15:LEU:HD23	1.87	0.56
1:2:989:C:O4'	24:Y:49:ALA:HB2	2.06	0.56
8:G:29:VAL:HA	8:G:45:LYS:HZ3	1.71	0.56
1:2:22:C:OP1	36:2:1529:SPM:H132	2.06	0.55
1:2:535:C:OP2	40:2:1609:HOH:O	2.18	0.55
6:E:26:PRO:HG2	6:E:33:ILE:HG12	1.87	0.55
8:G:140:ALA:HB1	8:G:144:ILE:HD12	1.88	0.55
9:H:21:GLU:OE1	28:d:58:ALA:N	2.37	0.55
25:Z:58:ARG:HH11	25:Z:58:ARG:C	2.14	0.55
1:2:1349:G:H2'	1:2:1350:C:H6	1.71	0.55
1:2:902:A:N3	1:2:1340:U:O2'	2.27	0.55
1:2:927:G:N7	36:2:1525:SPM:H91	2.21	0.55
28:d:29:ARG:HH21	28:d:62:TRP:HE3	1.54	0.55
28:d:43:LEU:HD21	28:d:48:GLU:HG2	1.89	0.55
31:a:17:LEU:HB3	31:a:30:ILE:HB	1.87	0.55
31:a:34:ILE:HD13	31:a:54:LYS:HE2	1.88	0.55
33:b:70:CYS:SG	33:b:73:CYS:N	2.77	0.55
1:2:334:A:OP2	36:2:1509:SPM:N5	2.35	0.55
1:2:1032:OMU:H5'	3:B:162:LYS:HE2	1.88	0.55
1:2:1241:G:H1'	1:2:1246:C:O2	2.06	0.55
1:2:1252:A:H2'	1:2:1253:A:C8	2.41	0.55
6:E:173:ILE:HG12	6:E:228:SER:HB2	1.88	0.55
22:W:40:CYS:HB3	22:W:44:GLY:H	1.71	0.55
6:E:10:PRO:HG3	6:E:34:GLU:HA	1.88	0.55
6:E:127:ILE:HG13	6:E:128:LYS:H	1.72	0.55
9:H:12:VAL:N	9:H:16:TRP:O	2.40	0.55
15:O:47:ASP:OD1	15:O:49:ASN:N	2.40	0.55
32:P:3:LYS:HD3	32:P:4:TYR:H	1.72	0.55
1:2:95:G:OP2	36:2:1507:SPM:N5	2.38	0.55
3:B:108:ARG:HH21	3:B:112:LYS:NZ	2.04	0.55
8:G:105:GLU:N	8:G:105:GLU:OE1	2.38	0.55
13:L:91:VAL:HG11	13:L:97:ILE:HG13	1.88	0.55
1:2:1097:C:C4	20:U:140:LEU:HB2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:23:ARG:HH22	9:H:99:GLN:HE22	1.55	0.55
9:H:78:ALA:O	9:H:82:VAL:HG13	2.06	0.55
27:c:47:ILE:HG22	27:c:84:ILE:HG23	1.89	0.55
33:b:70:CYS:SG	33:b:72:ASN:CB	2.94	0.55
1:2:385:G:N2	1:2:388:A:OP2	2.35	0.55
1:2:475:U:H4'	29:e:16:GLN:NE2	2.21	0.55
1:2:1191:C:H4'	15:O:141:THR:HA	1.89	0.55
6:E:127:ILE:HG13	6:E:128:LYS:N	2.21	0.55
9:H:142:HIS:CG	9:H:181:ARG:HD3	2.41	0.55
28:d:39:LYS:HE2	28:d:39:LYS:N	2.22	0.55
1:2:900:C:H2'	1:2:901:A:H8	1.71	0.55
4:C:54:GLU:OE1	4:C:63:LYS:HD2	2.07	0.55
23:X:22:GLU:HG3	23:X:66:ILE:HD13	1.89	0.55
1:2:636:C:H2'	1:2:637:U:H6	1.72	0.54
9:H:24:ASP:OD1	9:H:26:SER:N	2.37	0.54
9:H:30:TYR:HE1	23:X:62:ARG:HH12	1.54	0.54
9:H:172:ASN:HD22	9:H:172:ASN:N	2.04	0.54
12:K:10:SER:OG	12:K:85:ALA:O	2.20	0.54
13:L:9:LEU:O	13:L:71:LYS:HA	2.07	0.54
13:L:90:ARG:NH2	13:L:91:VAL:O	2.40	0.54
18:S:36:ILE:HG22	18:S:47:ARG:HD2	1.88	0.54
1:2:975:G:H2'	1:2:976:G:H8	1.72	0.54
1:2:1043:C:H2'	1:2:1044:C:H6	1.73	0.54
2:A:22:VAL:O	2:A:33:LEU:N	2.37	0.54
21:V:5:ALA:HB3	21:V:17:ILE:HB	1.89	0.54
29:e:29:VAL:HB	29:e:32:VAL:HB	1.89	0.54
1:2:1277:G:OP2	19:T:36:SER:OG	2.20	0.54
2:A:39:TYR:N	2:A:43:GLN:OE1	2.40	0.54
8:G:94:ILE:HD12	8:G:98:MET:HB2	1.90	0.54
31:a:37:LYS:CE	31:a:71:ILE:HB	2.38	0.54
1:2:682:U:C6	33:b:11:ARG:HD2	2.43	0.54
12:K:66:ALA:C	12:K:67:LYS:HD2	2.32	0.54
13:L:23:GLN:NE2	13:L:89:VAL:O	2.39	0.54
25:Z:6:ARG:HB3	25:Z:6:ARG:HH11	1.70	0.54
1:2:412:C:OP1	29:e:31:ARG:NH2	2.40	0.54
5:D:145:VAL:HG11	5:D:153:ILE:HD11	1.89	0.54
14:N:130:ASN:HB3	14:N:145:PRO:HG2	1.89	0.54
31:a:49:PHE:HB3	31:a:53:ASP:HB3	1.88	0.54
34:5:2:U:O2'	34:5:3:G:H5'	2.08	0.54
2:A:59:ASP:N	2:A:59:ASP:OD1	2.39	0.54
1:2:479:A:OP1	14:N:71:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1352:C:H4'	36:2:1537:SPM:H42	1.89	0.54
15:O:44:LEU:HD11	15:O:66:VAL:HG21	1.89	0.54
31:a:21:CYS:HB3	31:a:26:ARG:H	1.72	0.54
1:2:682:U:H1'	33:b:11:ARG:HH11	1.71	0.54
1:2:683:G:C5	33:b:15:LYS:HE2	2.36	0.54
1:2:1071:C:H2'	1:2:1072:C:H6	1.73	0.54
2:A:20:TYR:CE2	2:A:41:ILE:HD12	2.43	0.54
12:K:31:PHE:HE1	20:U:156:TYR:HE1	1.56	0.54
12:K:83:ARG:HB3	12:K:83:ARG:HH11	1.72	0.54
13:L:4:LYS:H	13:L:4:LYS:HE2	1.72	0.54
1:2:110:A:H1'	17:R:35:ARG:HG2	1.90	0.54
1:2:426:C:H2'	1:2:427:U:C6	2.42	0.54
1:2:1081:G:N2	1:2:1082:U:O4	2.36	0.54
2:A:110:VAL:HG11	2:A:146:VAL:HG12	1.89	0.54
8:G:8:ILE:HB	8:G:117:LEU:HD23	1.88	0.54
9:H:193:ARG:OXT	23:X:74:ARG:NH2	2.41	0.54
28:d:33:THR:HG23	28:d:35:GLU:H	1.73	0.54
2:A:19:TRP:CH2	2:A:37:PRO:HG3	2.43	0.53
3:B:61:PHE:CD1	3:B:185:PRO:HG3	2.43	0.53
14:N:91:ASP:OD2	29:e:11:GLY:HA2	2.08	0.53
33:b:20:TYR:CE2	33:b:29:ARG:HD3	2.38	0.53
1:2:981:C:H5'	19:T:52:HIS:HE1	1.73	0.53
15:O:57:ASP:O	15:O:61:LYS:HG2	2.09	0.53
26:3:79:TYR:HE1	26:3:118:VAL:HG12	1.74	0.53
1:2:45:U:O2'	1:2:46:A:H2'	2.07	0.53
2:A:23:ILE:HD11	2:A:80:ILE:HG22	1.91	0.53
21:V:9:ILE:H	21:V:9:ILE:HD12	1.73	0.53
32:P:45:ALA:C	32:P:50:PHE:HB2	2.33	0.53
1:2:708:C:OP1	16:Q:14:ARG:NH2	2.38	0.53
2:A:50:GLU:HG3	2:A:68:TYR:HE2	1.74	0.53
13:L:18:ASN:O	13:L:22:THR:HG23	2.09	0.53
19:T:50:GLN:HG2	19:T:77:LEU:HB2	1.90	0.53
19:T:124:GLU:OE2	19:T:125:PRO:HD2	2.08	0.53
22:W:17:LEU:H	22:W:17:LEU:HD12	1.74	0.53
33:b:30:VAL:HG23	33:b:31:PRO:HD2	1.89	0.53
1:2:625:G:OP1	36:2:1511:SPM:N5	2.42	0.53
1:2:1077:A:H2'	1:2:1078:C:C6	2.44	0.53
16:Q:37:GLU:OE2	16:Q:41:ARG:NH2	2.42	0.53
19:T:67:ASN:OD1	19:T:67:ASN:N	2.41	0.53
25:Z:56:ILE:HG13	25:Z:83:ILE:HD12	1.90	0.53
30:4:69:C:H2'	30:4:70:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:218:C:OP1	36:2:1521:SPM:N14	2.39	0.53
24:Y:56:GLU:HB3	24:Y:69:ILE:HB	1.91	0.53
30:4:50:U:O4	30:4:64:G:O6	2.26	0.53
30:4:67:C:H2'	30:4:68:C:C6	2.44	0.53
31:a:34:ILE:HD13	31:a:54:LYS:CE	2.39	0.53
35:M:84:TYR:C	35:M:84:TYR:CD1	2.86	0.53
1:2:681:G:H3'	1:2:681:G:N3	2.24	0.53
1:2:1487:G:O2'	33:b:5:ARG:NH1	2.32	0.53
20:U:143:PHE:HZ	20:U:156:TYR:HB3	1.73	0.53
35:M:12:ALA:HB2	35:M:74:LEU:HD13	1.90	0.53
1:2:673:G:H2'	1:2:674:A:C8	2.43	0.53
5:D:107:GLN:HE21	5:D:119:ILE:HG13	1.74	0.53
8:G:43:GLN:HE22	8:G:82:ASP:HB2	1.73	0.53
28:d:34:LEU:H	28:d:34:LEU:HD12	1.74	0.53
28:d:64:PRO:HB2	28:d:66:PRO:HD2	1.89	0.53
35:M:94:GLN:O	35:M:98:ARG:HG2	2.09	0.53
1:2:72:G:N1	1:2:209:U:O2'	2.40	0.53
1:2:257:U:H2'	1:2:258:U:C6	2.43	0.53
6:E:169:ASP:OD1	6:E:231:ARG:NH2	2.42	0.53
16:Q:27:THR:O	16:Q:31:VAL:HG12	2.09	0.53
26:3:66:LEU:O	26:3:70:CYS:N	2.41	0.53
30:4:74:C:H4'	30:4:75:C:O5'	2.08	0.53
12:K:36:PRO:HB3	20:U:156:TYR:CZ	2.43	0.52
15:O:22:LEU:HD22	15:O:41:ILE:HD11	1.90	0.52
25:Z:64:LYS:HD2	25:Z:64:LYS:C	2.34	0.52
1:2:958:C:H2'	1:2:959:C:H6	1.74	0.52
14:N:71:LYS:HG3	29:e:7:LEU:HD22	1.91	0.52
25:Z:130:GLU:OE1	25:Z:148:LYS:HB2	2.09	0.52
27:c:96:LEU:HD11	27:c:99:LYS:HB2	1.91	0.52
33:b:20:TYR:CD2	33:b:29:ARG:CD	2.83	0.52
33:b:58:ALA:HB2	35:M:107:ILE:O	2.09	0.52
1:2:611:U:O4	1:2:711:G:O2'	2.22	0.52
1:2:728:G:H4'	1:2:1470:A:H4'	1.91	0.52
5:D:104:ARG:NH2	5:D:145:VAL:O	2.38	0.52
6:E:120:ARG:NH2	6:E:137:GLU:OE2	2.37	0.52
14:N:57:LYS:HD2	14:N:94:VAL:HG22	1.90	0.52
18:S:34:ILE:HD12	18:S:34:ILE:H	1.75	0.52
1:2:900:C:C2	1:2:901:A:C8	2.97	0.52
1:2:1293:G:H5''	15:O:33:GLY:N	2.25	0.52
6:E:234:SER:OG	6:E:236:LEU:O	2.26	0.52
18:S:27:ASP:O	18:S:30:THR:OG1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:21:ILE:N	33:b:21:ILE:HD12	2.24	0.52
1:2:827:A:H2'	1:2:828:A:C8	2.45	0.52
1:2:1077:A:H2'	1:2:1078:C:H6	1.73	0.52
31:a:45:TYR:CE1	32:P:9:GLU:HB2	2.45	0.52
31:a:62:PRO:HG2	31:a:63:TYR:CZ	2.43	0.52
1:2:338:G:O2'	8:G:191:ARG:O	2.26	0.52
1:2:612:A:N6	22:W:10:PRO:HG3	2.24	0.52
1:2:1243:A:H4'	1:2:1245:U:C5	2.45	0.52
7:F:11:GLU:OE1	7:F:11:GLU:N	2.31	0.52
8:G:180:PRO:O	8:G:182:GLY:N	2.43	0.52
26:3:49:LYS:NZ	26:3:103:GLU:H	2.08	0.52
1:2:264:G:O2'	11:J:32:PRO:HB3	2.10	0.52
1:2:1243:A:O2'	1:2:1245:U:OP2	2.23	0.52
9:H:19:LYS:HG2	28:d:59:TRP:CD2	2.45	0.52
11:J:82:LEU:HD12	11:J:108:LEU:HD11	1.92	0.52
1:2:979:A:H2'	1:2:980:A:H8	1.75	0.52
13:L:101:LEU:N	13:L:101:LEU:CD2	2.73	0.52
19:T:28:ASP:O	19:T:31:ILE:HG22	2.10	0.52
20:U:109:GLN:O	20:U:113:LYS:HD3	2.10	0.52
31:a:59:GLY:C	31:a:68:LEU:HG	2.34	0.52
1:2:687:A:H2'	1:2:688:A:C8	2.45	0.52
1:2:704:C:OP1	1:2:814:U:O2'	2.26	0.52
1:2:1208:G:OP2	20:U:46:LYS:NZ	2.35	0.52
1:2:1280:G:N1	1:2:1283:A:OP2	2.42	0.52
9:H:182:LYS:O	9:H:186:GLU:HG2	2.10	0.52
12:K:107:ASP:OD2	12:K:109:THR:OG1	2.21	0.52
13:L:27:ILE:HG12	13:L:85:GLN:NE2	2.24	0.52
26:3:78:VAL:HG11	26:3:114:ILE:HD12	1.92	0.52
27:c:80:VAL:HG12	27:c:84:ILE:HD11	1.91	0.52
30:4:62:C:H2'	30:4:63:G:H8	1.74	0.52
31:a:45:TYR:HE2	32:P:6:PRO:HB2	1.67	0.52
1:2:406:C:O2'	1:2:580:A:N3	2.39	0.52
5:D:86:GLU:H	5:D:86:GLU:CD	2.16	0.52
6:E:117:LYS:HB2	6:E:162:LEU:HD11	1.91	0.52
12:K:130:ARG:NH1	12:K:131:TRP:O	2.43	0.52
23:X:62:ARG:HB2	28:d:31:GLN:HE22	1.75	0.52
26:3:66:LEU:HD22	26:3:66:LEU:H	1.74	0.52
27:c:95:LYS:HG2	27:c:107:ILE:HG22	1.92	0.52
35:M:65:ASP:O	35:M:69:LYS:HG2	2.10	0.52
1:2:793:C:OP2	36:2:1535:SPM:C8	2.46	0.51
1:2:914:U:H2'	1:2:915:G:H8	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:974:A:N3	24:Y:57:ARG:NH2	2.58	0.51
1:2:1095:C:H2'	1:2:1095:C:OP2	2.10	0.51
1:2:1196:G:OP1	12:K:126:TYR:OH	2.27	0.51
1:2:1484:C:P	33:b:10:ARG:HH12	2.33	0.51
7:F:17:THR:OG1	7:F:43:GLU:OE2	2.20	0.51
25:Z:23:ALA:HA	25:Z:31:TYR:HD1	1.75	0.51
28:d:5:LYS:HD3	28:d:16:ILE:O	2.11	0.51
31:a:39:PRO:HB3	31:a:69:VAL:HG11	1.92	0.51
9:H:22:ILE:HD13	9:H:102:VAL:CG1	2.41	0.51
9:H:22:ILE:HD11	9:H:106:GLU:HB3	1.92	0.51
9:H:193:ARG:NH2	23:X:71:GLU:OE1	2.42	0.51
12:K:59:ASP:HB2	12:K:63:LYS:NZ	2.25	0.51
15:O:24:TYR:O	15:O:28:MET:HG2	2.11	0.51
28:d:21:ILE:O	28:d:25:ASN:N	2.42	0.51
6:E:30:PRO:HD2	6:E:78:PRO:HG2	1.91	0.51
8:G:79:PHE:HE1	8:G:98:MET:HG3	1.75	0.51
19:T:31:ILE:HG13	19:T:39:ARG:HG2	1.92	0.51
22:W:43:CYS:SG	22:W:45:THR:HG23	2.51	0.51
31:a:67:GLU:OE1	31:a:68:LEU:N	2.41	0.51
35:M:22:LEU:HD13	35:M:38:SER:HB3	1.93	0.51
1:2:979:A:H2'	1:2:980:A:C8	2.44	0.51
1:2:1243:A:H1'	1:2:1246:C:N4	2.24	0.51
1:2:1253:A:H5'	20:U:86:ARG:HH22	1.74	0.51
8:G:95:SER:OG	8:G:97:THR:OG1	2.26	0.51
13:L:81:ARG:HA	13:L:84:ARG:HH11	1.75	0.51
30:4:4:G:H2'	30:4:5:G:H8	1.76	0.51
1:2:946:U:H4'	1:2:947:A:O4'	2.11	0.51
9:H:27:LEU:HD21	9:H:135:ARG:HE	1.74	0.51
13:L:81:ARG:HA	13:L:84:ARG:NH1	2.26	0.51
15:O:116:TRP:CD1	15:O:120:ARG:HG2	2.45	0.51
23:X:62:ARG:HB2	28:d:31:GLN:NE2	2.26	0.51
1:2:418:U:O2	1:2:419:A:N6	2.43	0.51
1:2:958:C:H2'	1:2:959:C:C6	2.46	0.51
3:B:211:VAL:HG23	3:B:212:ILE:HG12	1.92	0.51
9:H:91:LEU:HD13	27:c:107:ILE:HD13	1.93	0.51
12:K:52:PRO:HG2	12:K:86:LEU:HD12	1.92	0.51
26:3:108:LYS:HA	26:3:108:LYS:HE3	1.92	0.51
31:a:37:LYS:HG2	31:a:69:VAL:HG13	1.91	0.51
1:2:467:A:OP2	40:2:1611:HOH:O	2.19	0.51
1:2:476:G:H2'	1:2:490:U:C5	2.46	0.51
1:2:581:A:OP1	36:2:1534:SPM:H22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:843:4AC:HM72	14:N:3:LYS:HZ2	1.76	0.51
1:2:1272:C:H4'	27:c:7:LYS:HZ3	1.76	0.51
2:A:196:GLU:OE1	2:A:196:GLU:N	2.44	0.51
5:D:123:ARG:HD3	29:e:31:ARG:HD2	1.93	0.51
25:Z:61:ARG:O	25:Z:64:LYS:HE3	2.11	0.51
31:a:51:GLU:HG3	31:a:54:LYS:HE3	1.93	0.51
33:b:41:MET:HA	33:b:41:MET:HE3	1.91	0.51
2:A:116:TYR:CE1	2:A:194:VAL:HG12	2.46	0.51
8:G:197:ARG:HG2	8:G:205:ILE:HD11	1.91	0.51
15:O:11:ILE:HG22	15:O:12:PHE:CD1	2.47	0.51
19:T:15:ARG:HG3	19:T:33:LEU:HB3	1.92	0.51
27:c:22:LYS:O	27:c:26:ALA:N	2.39	0.51
1:2:349:A:H5''	1:2:350:C:C5	2.45	0.50
1:2:611:U:O2'	1:2:612:A:OP2	2.25	0.50
15:O:78:TRP:CH2	20:U:40:ALA:HB2	2.47	0.50
15:O:116:TRP:O	15:O:116:TRP:HD1	1.94	0.50
22:W:21:CYS:CB	22:W:40:CYS:SG	2.99	0.50
22:W:39:ARG:HD2	22:W:44:GLY:O	2.10	0.50
30:4:62:C:H2'	30:4:63:G:C8	2.46	0.50
1:2:100:A:H5''	11:J:11:LYS:HD3	1.93	0.50
1:2:1243:A:H4'	1:2:1245:U:H5	1.76	0.50
3:B:79:ASP:OD1	3:B:80:GLU:N	2.45	0.50
5:D:44:ALA:HA	5:D:101:LEU:HD23	1.93	0.50
8:G:3:ASP:OD1	8:G:3:ASP:N	2.44	0.50
8:G:164:ARG:NH1	8:G:181:PRO:O	2.44	0.50
8:G:168:ILE:H	8:G:168:ILE:HD12	1.76	0.50
26:3:15:LEU:HD21	26:3:114:ILE:HG22	1.93	0.50
1:2:1126:C:H2'	1:2:1127:G:H8	1.75	0.50
2:A:102:SER:HB2	2:A:129:LYS:HA	1.93	0.50
12:K:83:ARG:NH1	12:K:83:ARG:HB3	2.26	0.50
13:L:65:TRP:HB3	32:P:50:PHE:HB3	1.92	0.50
17:R:36:VAL:HG21	17:R:110:LEU:HD21	1.93	0.50
18:S:9:ILE:HD11	18:S:46:VAL:HG23	1.92	0.50
1:2:16:G:N7	36:2:1501:SPM:N14	2.60	0.50
1:2:220:U:H2'	1:2:221:G:H8	1.77	0.50
1:2:1184:G:OP2	36:2:1514:SPM:N14	2.38	0.50
26:3:11:VAL:HG12	26:3:79:TYR:CD2	2.42	0.50
1:2:826:G:O6	36:2:1513:SPM:H81	2.12	0.50
1:2:1204:G:H2'	1:2:1205:G:H8	1.75	0.50
9:H:111:ARG:HH22	23:X:70:ARG:HB3	1.77	0.50
9:H:192:SER:O	9:H:192:SER:OG	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:61:ARG:NH1	19:T:61:ARG:O	2.44	0.50
19:T:64:GLY:HA2	19:T:66:PHE:CE1	2.47	0.50
19:T:77:LEU:HD23	19:T:110:LEU:HD21	1.94	0.50
25:Z:161:LYS:O	25:Z:185:LYS:HG3	2.12	0.50
33:b:44:PRO:HG2	35:M:110:ILE:HG22	1.92	0.50
1:2:207:U:H2'	1:2:208:A:C8	2.46	0.50
1:2:539:C:H2'	1:2:540:G:O4'	2.11	0.50
1:2:968:A:H62	1:2:992:G:H21	1.60	0.50
1:2:673:G:H2'	1:2:674:A:H8	1.76	0.50
9:H:159:GLU:HB2	27:c:103:LEU:HD21	1.94	0.50
14:N:140:GLY:O	14:N:141:LYS:HG2	2.11	0.50
23:X:23:VAL:HG23	23:X:63:VAL:HA	1.94	0.50
32:P:5:LYS:HD2	32:P:5:LYS:N	2.27	0.50
32:P:48:LEU:HB2	32:P:50:PHE:CD1	2.46	0.50
1:2:603:U:OP1	36:2:1533:SPM:H61	2.12	0.50
1:2:1070:C:C2	1:2:1071:C:C5	3.00	0.50
6:E:161:GLU:HB2	6:E:168:LEU:HD21	1.93	0.50
12:K:43:GLU:HG3	12:K:44:MET:N	2.27	0.50
12:K:46:ARG:NH1	12:K:46:ARG:HB3	2.27	0.50
19:T:48:ASP:O	19:T:52:HIS:HD2	1.94	0.50
26:3:27:LYS:HZ2	26:3:90:CYS:H	1.58	0.50
31:a:34:ILE:CD1	31:a:54:LYS:HE2	2.41	0.50
1:2:1071:C:H4'	32:P:53:TYR:CD2	2.47	0.50
1:2:1084:G:H5'	1:2:1244:A:O2'	2.12	0.50
1:2:1336:U:H3'	12:K:76:MET:CE	2.39	0.50
2:A:24:THR:OG1	2:A:31:VAL:N	2.45	0.50
8:G:142:GLN:HG2	8:G:143:LEU:HD22	1.94	0.50
12:K:102:ILE:HD12	28:d:66:PRO:HB2	1.92	0.50
12:K:123:TRP:HE3	12:K:124:MET:HG3	1.77	0.50
13:L:83:MET:O	13:L:87:MET:HG3	2.12	0.50
15:O:56:SER:N	15:O:59:GLU:OE2	2.44	0.50
24:Y:57:ARG:HA	24:Y:68:PHE:HA	1.93	0.50
25:Z:60:GLY:O	25:Z:63:ILE:HG22	2.12	0.50
28:d:46:TRP:HA	28:d:49:ALA:HB3	1.93	0.50
33:b:30:VAL:CG2	33:b:31:PRO:HD2	2.42	0.50
6:E:169:ASP:CG	6:E:231:ARG:HH22	2.20	0.49
18:S:43:SER:HB3	18:S:46:VAL:HG12	1.93	0.49
27:c:19:GLU:O	27:c:23:GLN:N	2.41	0.49
1:2:908:G:N1	1:2:1302:G:OP2	2.45	0.49
1:2:1085:G:H21	1:2:1110:A:H62	1.60	0.49
1:2:1252:A:O2'	20:U:86:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:116:TYR:HD1	2:A:195:PRO:HD2	1.76	0.49
3:B:29:LYS:HA	3:B:29:LYS:HE2	1.92	0.49
13:L:53:LEU:HD11	13:L:60:LYS:HA	1.94	0.49
13:L:79:ASP:OD1	13:L:82:VAL:HG22	2.12	0.49
19:T:39:ARG:O	19:T:43:LYS:HB3	2.12	0.49
33:b:44:PRO:HD2	33:b:61:ALA:O	2.12	0.49
1:2:965:A:O4'	1:2:993:A:N6	2.46	0.49
1:2:1053:C:O2'	18:S:10:LYS:NZ	2.31	0.49
9:H:20:VAL:HB	9:H:99:GLN:OE1	2.11	0.49
13:L:24:ILE:HA	13:L:27:ILE:HD12	1.93	0.49
15:O:107:ILE:HG22	15:O:111:LYS:HZ3	1.77	0.49
31:a:39:PRO:HD2	31:a:40:LYS:N	2.27	0.49
1:2:914:U:H2'	1:2:915:G:C8	2.48	0.49
1:2:1004:G:H5''	31:a:27:LYS:HG2	1.93	0.49
1:2:1192:G:O2'	30:4:30:G:OP1	2.29	0.49
16:Q:17:ARG:NH1	16:Q:19:GLY:O	2.45	0.49
28:d:5:LYS:NZ	28:d:5:LYS:CB	2.73	0.49
32:P:28:VAL:HA	32:P:37:CYS:HA	1.93	0.49
35:M:77:LYS:HD3	35:M:111:GLU:OE1	2.12	0.49
1:2:707:G:N7	16:Q:17:ARG:NH2	2.61	0.49
1:2:1043:C:H2'	1:2:1044:C:C6	2.48	0.49
1:2:1081:G:H1'	1:2:1082:U:H5	1.78	0.49
15:O:30:LYS:NZ	27:c:9:ILE:O	2.35	0.49
25:Z:16:VAL:HG21	32:P:48:LEU:CD2	2.35	0.49
1:2:716:U:H2'	1:2:717:G:O4'	2.13	0.49
1:2:1081:G:N7	1:2:1109:C:O2'	2.45	0.49
1:2:1193:C:C5	36:2:1526:SPM:H22	2.47	0.49
1:2:1314:A:H1'	9:H:72:LYS:HG2	1.95	0.49
9:H:109:ALA:HB1	9:H:135:ARG:HB3	1.94	0.49
12:K:87:ALA:HA	12:K:90:LEU:HD12	1.94	0.49
30:4:69:C:H2'	30:4:70:G:H8	1.78	0.49
32:P:4:TYR:N	32:P:4:TYR:CD1	2.80	0.49
33:b:59:ILE:HD12	35:M:109:ARG:HA	1.93	0.49
1:2:1343:G:H2'	1:2:1344:OMU:C6	2.42	0.49
3:B:142:PRO:HG2	3:B:165:ILE:HD13	1.95	0.49
5:D:16:HIS:HB3	5:D:19:ILE:HD13	1.94	0.49
5:D:157:VAL:HG13	5:D:158:THR:HG23	1.95	0.49
13:L:65:TRP:HA	32:P:51:ARG:O	2.12	0.49
26:3:20:LEU:O	26:3:24:ARG:HD2	2.12	0.49
27:c:59:ILE:HG13	27:c:65:ILE:HG23	1.94	0.49
28:d:17:ASN:N	28:d:17:ASN:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:21:ILE:HD13	33:b:32:GLU:CB	2.43	0.49
1:2:29:G:H2'	1:2:30:C:C6	2.48	0.49
1:2:71:G:H2'	1:2:72:G:C8	2.48	0.49
1:2:1355:U:H5'	33:b:84:ALA:HA	1.93	0.49
11:J:66:LEU:HA	11:J:73:ALA:HA	1.93	0.49
26:3:70:CYS:SG	26:3:77:TYR:HB3	2.53	0.49
29:e:28:GLU:HB3	29:e:32:VAL:HG12	1.94	0.49
35:M:52:PRO:HB3	35:M:95:PRO:HG2	1.94	0.49
1:2:855:A:H2'	1:2:856:C:C6	2.47	0.49
1:2:1048:U:O3'	18:S:2:GLY:N	2.46	0.49
1:2:1096:U:O2	1:2:1100:G:C6	2.66	0.49
1:2:1337:G:OP2	12:K:76:MET:SD	2.71	0.49
12:K:67:LYS:C	12:K:68:ILE:HD13	2.37	0.49
1:2:207:U:H2'	1:2:208:A:H8	1.78	0.49
1:2:684:G:O6	33:b:15:LYS:CD	2.61	0.49
1:2:909:G:C2	1:2:910:A:C8	3.00	0.49
1:2:949:U:H2'	1:2:950:A:C8	2.48	0.49
2:A:116:TYR:CE1	2:A:195:PRO:HD2	2.47	0.49
5:D:36:ARG:HA	29:e:31:ARG:HG3	1.94	0.49
10:I:81:LEU:HB2	10:I:86:MET:HE2	1.95	0.49
22:W:18:ARG:HG3	22:W:27:GLU:OE2	2.13	0.49
28:d:49:ALA:O	28:d:52:LEU:HG	2.12	0.49
1:2:897:C:O2'	1:2:1308:C:OP2	2.27	0.48
1:2:1003:A:O2'	31:a:26:ARG:NH2	2.46	0.48
1:2:1058:A:H4'	1:2:1059:A:H5'	1.95	0.48
1:2:1204:G:H2'	1:2:1205:G:C8	2.48	0.48
1:2:1254:C:H2'	1:2:1255:C:H6	1.78	0.48
13:L:91:VAL:HG22	13:L:95:VAL:CG2	2.43	0.48
31:a:14:LEU:C	31:a:14:LEU:HD12	2.38	0.48
31:a:60:LYS:HA	31:a:66:THR:O	2.13	0.48
1:2:810:C:P	36:2:1535:SPM:H132	2.46	0.48
4:C:9:GLU:OE1	4:C:9:GLU:HA	2.13	0.48
5:D:164:ARG:HG3	5:D:164:ARG:O	2.13	0.48
9:H:121:GLY:C	9:H:122:ILE:HD13	2.39	0.48
11:J:93:ARG:HB2	11:J:95:ILE:HD12	1.95	0.48
16:Q:85:ASP:OD1	16:Q:85:ASP:N	2.47	0.48
23:X:27:LEU:HD12	23:X:38:GLN:HG2	1.95	0.48
24:Y:65:TYR:O	24:Y:65:TYR:CD2	2.66	0.48
25:Z:127:LEU:HD13	25:Z:186:PRO:HA	1.95	0.48
1:2:642:G:H2'	1:2:643:A:C8	2.48	0.48
1:2:1094:U:O3'	20:U:129:PRO:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1328:A:P	20:U:89:ARG:HH22	2.37	0.48
1:2:1493:C:OP1	33:b:93:ARG:HG2	2.13	0.48
2:A:103:LYS:HE3	2:A:105:ASN:ND2	2.28	0.48
4:C:40:VAL:HG11	4:C:58:PRO:HD2	1.95	0.48
9:H:33:LEU:HD12	28:d:62:TRP:CD1	2.48	0.48
13:L:101:LEU:HD22	13:L:101:LEU:H	1.75	0.48
15:O:38:LYS:HD3	20:U:49:VAL:HG23	1.94	0.48
15:O:44:LEU:HD22	15:O:62:LYS:HD2	1.96	0.48
20:U:13:PRO:HG3	20:U:66:ARG:NH2	2.29	0.48
1:2:828:A:OP2	1:2:828:A:H8	1.96	0.48
1:2:843:4AC:H5	14:N:6:SER:OG	2.13	0.48
3:B:26:LYS:HE2	3:B:39:VAL:HG21	1.94	0.48
7:F:121:CYS:SG	7:F:126:CYS:CB	2.92	0.48
9:H:63:ASN:O	9:H:66:MET:HB2	2.14	0.48
17:R:14:PRO:HB2	17:R:15:ASN:OD1	2.13	0.48
21:V:29:ARG:HG3	21:V:85:LYS:HE3	1.95	0.48
32:P:45:ALA:O	32:P:50:PHE:CB	2.57	0.48
1:2:580:A:OP1	36:2:1534:SPM:H91	2.13	0.48
1:2:1174:G:H5'	1:2:1176:A:H1'	1.95	0.48
13:L:26:GLY:HA2	13:L:29:GLU:CD	2.38	0.48
28:d:21:ILE:HD12	28:d:22:ALA:N	2.28	0.48
33:b:24:ASP:CA	35:M:123:ARG:NH2	2.75	0.48
1:2:476:G:H2'	1:2:490:U:C6	2.49	0.48
1:2:963:G:H2'	1:2:964:G:C8	2.49	0.48
1:2:964:G:O2'	1:2:993:A:N1	2.43	0.48
9:H:18:THR:HA	9:H:98:ILE:CD1	2.43	0.48
12:K:31:PHE:HE1	20:U:156:TYR:CE1	2.31	0.48
12:K:102:ILE:CD1	28:d:66:PRO:HB2	2.43	0.48
14:N:24:ARG:HD3	14:N:30:TYR:CZ	2.48	0.48
20:U:15:LEU:HD22	20:U:15:LEU:H	1.79	0.48
25:Z:106:LYS:HB2	25:Z:106:LYS:HE3	1.56	0.48
27:c:28:GLU:HA	27:c:31:LYS:HD2	1.95	0.48
1:2:141:A:H2'	1:2:142:A:O4'	2.14	0.48
1:2:1285:U:H4'	15:O:116:TRP:CZ3	2.49	0.48
18:S:57:TYR:O	18:S:60:ILE:HD12	2.14	0.48
25:Z:24:LYS:HG2	31:a:14:LEU:HB3	1.96	0.48
25:Z:165:ARG:HD2	31:a:3:ILE:HG23	1.96	0.48
27:c:48:ASP:OD1	27:c:51:THR:HG23	2.14	0.48
27:c:86:LYS:O	27:c:89:GLU:HG3	2.14	0.48
1:2:391:G:OP2	36:2:1517:SPM:H42	2.13	0.48
1:2:498:G:H2'	1:2:499:C:C6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:589:A:H2'	1:2:590:A:C8	2.49	0.48
7:F:3:GLU:OE1	7:F:3:GLU:N	2.46	0.48
8:G:18:ARG:NH1	8:G:63:GLU:OE1	2.41	0.48
28:d:50:TYR:HD1	28:d:53:ILE:HG22	1.79	0.48
31:a:19:VAL:HG21	31:a:48:TYR:CD1	2.49	0.48
35:M:38:SER:H	35:M:41:MET:HG3	1.78	0.48
1:2:498:G:H5''	29:e:22:PRO:HB3	1.96	0.48
1:2:527:G:O2'	1:2:533:A:N1	2.38	0.48
1:2:680:A:OP1	2:A:129:LYS:CE	2.61	0.48
1:2:865:OMG:HM22	1:2:866:A:O4'	2.11	0.48
1:2:949:U:H2'	1:2:950:A:H8	1.79	0.48
1:2:1012:A:O2'	25:Z:136:LYS:HD3	2.13	0.48
30:4:1:A:H3'	30:4:2:G:H8	1.79	0.48
30:4:47:U:H5''	30:4:48:C:H5'	1.96	0.48
33:b:44:PRO:HB3	35:M:78:VAL:HG21	1.95	0.48
1:2:131:U:H2'	1:2:132:A:C8	2.48	0.48
1:2:417:G:N2	1:2:419:A:H1'	2.26	0.48
1:2:633:G:H2'	1:2:634:U:C6	2.49	0.48
1:2:777:A:H5''	33:b:8:ARG:HH21	1.78	0.48
1:2:1070:C:H1'	25:Z:157:GLN:OE1	2.14	0.48
2:A:159:THR:HA	2:A:162:VAL:HG22	1.95	0.48
19:T:79:ILE:HD11	19:T:110:LEU:HD13	1.95	0.48
26:3:49:LYS:HZ3	26:3:103:GLU:H	1.61	0.48
28:d:55:GLN:CD	28:d:55:GLN:H	2.22	0.48
1:2:419:A:H2'	1:2:420:A:C8	2.49	0.47
1:2:777:A:H3'	33:b:8:ARG:NH2	2.29	0.47
11:J:58:LYS:HA	11:J:58:LYS:HD2	1.65	0.47
13:L:24:ILE:O	13:L:28:VAL:HG12	2.14	0.47
14:N:39:GLU:CD	14:N:39:GLU:H	2.22	0.47
1:2:439:U:OP1	21:V:67:LYS:NZ	2.48	0.47
1:2:589:A:H2'	1:2:590:A:H8	1.79	0.47
2:A:24:THR:HB	2:A:28:PHE:HB2	1.97	0.47
3:B:38:PRO:HB2	3:B:40:ASP:OD1	2.13	0.47
4:C:54:GLU:CD	4:C:63:LYS:HD2	2.39	0.47
5:D:110:VAL:HG23	5:D:115:LEU:HB2	1.96	0.47
8:G:16:PRO:HB2	8:G:112:TYR:HB2	1.96	0.47
9:H:38:LEU:O	9:H:40:HIS:N	2.48	0.47
21:V:18:GLU:OE2	21:V:34:LYS:HB2	2.14	0.47
21:V:61:ASN:O	21:V:87:ARG:NH1	2.43	0.47
30:4:32:OMC:HM22	30:4:33:U:H5'	1.96	0.47
1:2:52:OMU:HM22	1:2:53:G:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:778:A:OP1	33:b:3:LYS:NZ	2.34	0.47
1:2:810:C:OP1	36:2:1535:SPM:C12	2.58	0.47
1:2:910:A:H2'	1:2:911:A:H8	1.76	0.47
8:G:60:LEU:HD13	8:G:61:THR:N	2.30	0.47
9:H:132:PRO:HA	9:H:135:ARG:HB2	1.95	0.47
1:2:410:U:C2	29:e:29:VAL:HG22	2.50	0.47
1:2:1226:C:OP2	20:U:75:GLY:HA3	2.15	0.47
1:2:1477:4AC:HM73	1:2:1478:4AC:HM72	1.97	0.47
1:2:1489:U:OP2	33:b:5:ARG:NH2	2.47	0.47
2:A:23:ILE:HD13	2:A:78:ARG:CZ	2.44	0.47
13:L:30:LYS:NZ	13:L:31:THR:HG22	2.29	0.47
15:O:30:LYS:HG2	15:O:99:LEU:HD23	1.95	0.47
1:2:974:A:N6	1:2:975:G:O6	2.48	0.47
1:2:1466:4AC:HM73	1:2:1467:4AC:HM72	1.97	0.47
2:A:18:LYS:HB2	2:A:20:TYR:CE1	2.49	0.47
6:E:222:ASN:OD1	6:E:225:ASN:ND2	2.47	0.47
7:F:128:CYS:SG	7:F:154:LYS:HD2	2.55	0.47
15:O:62:LYS:O	15:O:66:VAL:HG23	2.14	0.47
15:O:116:TRP:HD1	15:O:120:ARG:HG2	1.80	0.47
20:U:72:SER:O	20:U:73:ILE:HG12	2.15	0.47
25:Z:58:ARG:CZ	25:Z:61:ARG:HE	2.28	0.47
26:3:6:TYR:HB2	26:3:55:GLU:OE2	2.15	0.47
33:b:7:ASN:C	33:b:8:ARG:CG	2.85	0.47
33:b:79:ILE:HG22	33:b:94:LEU:HD13	1.97	0.47
1:2:942:A:C2	1:2:1283:A:C4	3.03	0.47
1:2:1490:C:H5'	1:2:1491:A:C8	2.50	0.47
2:A:157:ASP:OD1	2:A:157:ASP:N	2.46	0.47
9:H:36:VAL:HG23	12:K:106:TYR:OH	2.14	0.47
9:H:40:HIS:HD2	12:K:48:LYS:NZ	2.12	0.47
9:H:79:TYR:CD1	9:H:79:TYR:C	2.93	0.47
13:L:94:ASP:OD1	13:L:94:ASP:N	2.41	0.47
15:O:116:TRP:HE1	15:O:120:ARG:HD3	1.79	0.47
17:R:48:TYR:N	17:R:89:GLU:OE2	2.47	0.47
25:Z:48:TYR:HB3	25:Z:86:VAL:HG12	1.96	0.47
29:e:28:GLU:HB2	29:e:33:ARG:HB2	1.95	0.47
1:2:99:A:OP1	11:J:18:GLY:N	2.41	0.47
1:2:131:U:H2'	1:2:132:A:H8	1.80	0.47
1:2:147:G:N7	36:2:1522:SPM:H131	2.29	0.47
1:2:1024:A:N1	1:2:1065:G:O2'	2.36	0.47
1:2:1113:C:OP1	12:K:13:ARG:NH1	2.48	0.47
1:2:1143:G:P	12:K:108:ARG:HH21	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1382:A:P	1:2:1382:A:H8	2.36	0.47
1:2:1477:4AC:O7	1:2:1477:4AC:H5	2.14	0.47
2:A:60:PHE:HE1	33:b:59:ILE:CG2	2.28	0.47
2:A:109:ASP:N	2:A:109:ASP:OD1	2.48	0.47
7:F:138:VAL:HG11	7:F:201:THR:HG22	1.96	0.47
8:G:18:ARG:HB3	8:G:110:PHE:CD1	2.49	0.47
8:G:157:ASP:HA	8:G:205:ILE:HA	1.97	0.47
9:H:131:SER:HB2	23:X:61:VAL:HG22	1.96	0.47
9:H:162:LEU:O	9:H:166:ILE:HG22	2.14	0.47
12:K:30:VAL:O	20:U:156:TYR:OH	2.33	0.47
23:X:22:GLU:OE2	23:X:64:GLY:HA2	2.15	0.47
27:c:52:LYS:HE3	27:c:91:GLN:NE2	2.29	0.47
31:a:51:GLU:HA	31:a:54:LYS:CE	2.37	0.47
32:P:34:ILE:CG2	32:P:36:LEU:HD12	2.45	0.47
35:M:52:PRO:O	35:M:56:MET:HG3	2.15	0.47
1:2:242:C:OP1	17:R:75:SER:HB2	2.14	0.47
1:2:981:C:H5'	19:T:52:HIS:CE1	2.50	0.47
1:2:1188:G:H2'	1:2:1188:G:N3	2.30	0.47
8:G:155:GLY:H	8:G:163:MET:HG2	1.79	0.47
16:Q:136:GLU:H	16:Q:136:GLU:CD	2.21	0.47
19:T:97:VAL:HG11	19:T:114:SER:HA	1.95	0.47
23:X:30:THR:HG23	23:X:36:VAL:HG13	1.97	0.47
33:b:6:GLU:OE1	33:b:6:GLU:HA	2.15	0.47
1:2:112:C:H2'	1:2:113:OMC:C6	2.50	0.47
1:2:1071:C:H2'	1:2:1072:C:C6	2.48	0.47
1:2:1075:C:H1'	1:2:1142:A:C4	2.50	0.47
1:2:1253:A:C5'	20:U:86:ARG:HH22	2.28	0.47
3:B:105:TYR:HB2	3:B:191:ARG:HD2	1.96	0.47
12:K:121:GLU:HA	12:K:128:ALA:HA	1.97	0.47
23:X:45:GLU:HA	23:X:49:LYS:HA	1.96	0.47
25:Z:7:TYR:C	25:Z:7:TYR:CD1	2.92	0.47
27:c:58:GLU:HG2	27:c:65:ILE:CG2	2.42	0.47
28:d:61:MET:SD	28:d:61:MET:N	2.86	0.47
1:2:28:C:O4'	14:N:49:MET:HE1	2.14	0.47
1:2:263:G:H5''	11:J:98:ARG:HD2	1.97	0.47
1:2:393:G:OP1	36:2:1532:SPM:H32	2.15	0.47
1:2:801:C:H2'	1:2:802:U:O4'	2.15	0.47
5:D:154:ASP:OD1	5:D:155:TYR:N	2.42	0.47
6:E:102:ARG:HD3	6:E:102:ARG:HA	1.74	0.47
10:I:108:SER:HB2	10:I:129:LEU:HD11	1.97	0.47
20:U:108:PHE:CD2	20:U:125:ARG:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:57:ARG:HB3	24:Y:68:PHE:HD1	1.79	0.47
28:d:4:LEU:N	28:d:4:LEU:CD2	2.78	0.47
31:a:37:LYS:HD3	31:a:42:GLU:OE2	2.15	0.47
1:2:137:C:O2'	8:G:118:GLN:HB2	2.15	0.46
1:2:452:G:O2'	1:2:454:A:H1'	2.15	0.46
1:2:973:C:O2	24:Y:57:ARG:NH1	2.48	0.46
1:2:974:A:H1'	24:Y:57:ARG:CZ	2.45	0.46
1:2:1349:G:H2'	1:2:1350:C:C6	2.49	0.46
36:2:1532:SPM:HN41	36:2:1532:SPM:H111	1.55	0.46
11:J:41:ASP:OD1	11:J:61:THR:N	2.39	0.46
12:K:37:ILE:HG12	12:K:50:MET:HE3	1.97	0.46
14:N:136:ALA:HB1	14:N:142:LYS:HB2	1.97	0.46
17:R:20:GLU:H	17:R:20:GLU:CD	2.20	0.46
19:T:12:PHE:HB3	19:T:19:ILE:HD11	1.97	0.46
25:Z:20:GLU:OE2	31:a:9:ASN:ND2	2.48	0.46
26:3:50:LEU:HD12	26:3:50:LEU:O	2.15	0.46
1:2:393:G:P	36:2:1532:SPM:C4	2.95	0.46
1:2:408:A:O5'	5:D:141:PRO:HD2	2.15	0.46
1:2:543:G:H2'	1:2:544:C:C6	2.50	0.46
1:2:784:G:O2'	10:I:9:ASN:OD1	2.33	0.46
1:2:1285:U:H3'	1:2:1286:C:H2'	1.97	0.46
14:N:56:GLU:HA	14:N:99:GLU:OE2	2.16	0.46
16:Q:130:ILE:HD11	16:Q:132:LYS:HD2	1.97	0.46
18:S:9:ILE:HD11	18:S:46:VAL:CG2	2.45	0.46
19:T:80:LEU:H	19:T:83:LEU:HD13	1.79	0.46
22:W:21:CYS:HB2	22:W:40:CYS:SG	2.55	0.46
25:Z:159:LEU:HD22	25:Z:163:ILE:HG12	1.98	0.46
26:3:36:THR:HB	26:3:97:ALA:HB3	1.96	0.46
1:2:152:A:H2'	1:2:153:A:C8	2.51	0.46
1:2:617:G:H2'	1:2:618:C:H6	1.79	0.46
1:2:1116:G:OP1	13:L:70:HIS:ND1	2.48	0.46
1:2:1123:U:OP1	18:S:49:ARG:NH1	2.47	0.46
11:J:109:ALA:HB1	11:J:123:ALA:HB1	1.96	0.46
23:X:24:ILE:HD11	23:X:42:ARG:HB3	1.97	0.46
26:3:41:LYS:HE3	26:3:45:ARG:HH22	1.80	0.46
30:4:20:H2U:O2'	30:4:22:G:OP1	2.30	0.46
1:2:418:U:H4'	1:2:419:A:H5'	1.96	0.46
1:2:521:U:C4	14:N:27:GLN:HG2	2.50	0.46
1:2:964:G:O2'	1:2:967:G:O2'	2.34	0.46
1:2:1028:C:H2'	1:2:1029:G:H8	1.80	0.46
1:2:1110:A:H5'	1:2:1111:C:OP2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1125:C:H2'	1:2:1126:C:H6	1.80	0.46
1:2:1315:C:OP1	36:2:1527:SPM:H61	2.15	0.46
36:2:1526:SPM:H31	36:2:1526:SPM:H61	1.80	0.46
2:A:88:LEU:HG	2:A:187:GLU:HA	1.97	0.46
9:H:30:TYR:CE2	9:H:132:PRO:HG2	2.50	0.46
23:X:47:ARG:NH1	23:X:48:ASP:OD1	2.46	0.46
26:3:59:PRO:HG2	26:3:62:ILE:HB	1.97	0.46
1:2:826:G:N7	36:2:1513:SPM:H111	2.30	0.46
1:2:990:C:H1'	24:Y:62:LYS:HD3	1.97	0.46
1:2:1100:G:N2	1:2:1101:G:C8	2.83	0.46
1:2:1446:G:H2'	1:2:1447:A:C8	2.45	0.46
5:D:80:MET:HE3	5:D:80:MET:HB2	1.78	0.46
7:F:188:GLU:OE2	7:F:192:ARG:NH1	2.48	0.46
11:J:96:ILE:HD11	11:J:111:VAL:HG21	1.97	0.46
18:S:18:ASP:OD2	18:S:19:ARG:N	2.48	0.46
20:U:22:ILE:O	20:U:26:GLU:HG3	2.16	0.46
25:Z:84:THR:OG1	25:Z:85:ASN:N	2.47	0.46
27:c:45:VAL:HG21	27:c:84:ILE:HG13	1.96	0.46
1:2:1018:OMG:H5''	13:L:61:LYS:HE3	1.98	0.46
3:B:36:LEU:O	3:B:203:ARG:NH2	2.43	0.46
8:G:2:PRO:O	8:G:123:GLN:HB2	2.16	0.46
8:G:7:VAL:C	8:G:8:ILE:HD13	2.40	0.46
12:K:18:ARG:HB2	12:K:71:TYR:CZ	2.50	0.46
14:N:32:THR:HG22	14:N:37:LEU:HD12	1.98	0.46
19:T:31:ILE:HD11	19:T:42:LEU:HB2	1.97	0.46
19:T:101:VAL:HA	19:T:105:MET:HE2	1.96	0.46
26:3:80:VAL:HG22	26:3:81:SER:O	2.16	0.46
1:2:675:C:H2'	1:2:676:C:C6	2.50	0.46
1:2:875:U:OP1	14:N:63:ARG:NH2	2.35	0.46
3:B:91:ARG:NH2	4:C:35:PRO:O	2.48	0.46
3:B:95:GLN:OE1	3:B:120:ARG:NH1	2.49	0.46
15:O:22:LEU:HB2	15:O:50:ALA:O	2.15	0.46
23:X:24:ILE:N	23:X:24:ILE:HD12	2.31	0.46
27:c:65:ILE:C	27:c:65:ILE:HD12	2.40	0.46
33:b:91:LYS:HD3	33:b:91:LYS:HA	1.68	0.46
1:2:305:A:O2'	17:R:68:LYS:NZ	2.49	0.46
1:2:1087:A:N6	1:2:1107:A:H61	2.14	0.46
1:2:1173:C:H2'	1:2:1174:G:O4'	2.16	0.46
3:B:199:TRP:HD1	3:B:225:PHE:CD1	2.34	0.46
5:D:146:ASN:HB2	5:D:148:ASP:OD1	2.16	0.46
8:G:36:LYS:HD3	8:G:36:LYS:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:56:ASP:HB3	26:3:83:LYS:HD2	1.97	0.46
27:c:39:GLU:HA	27:c:76:ILE:HG22	1.97	0.46
33:b:83:ARG:HB3	33:b:87:GLU:HG3	1.98	0.46
35:M:41:MET:HE3	35:M:41:MET:HB3	1.83	0.46
1:2:391:G:OP2	36:2:1517:SPM:H61	2.15	0.46
1:2:871:A:H2'	1:2:872:A:C8	2.51	0.46
1:2:1078:C:H2'	1:2:1079:U:H6	1.80	0.46
1:2:1284:C:OP2	40:2:1614:HOH:O	2.20	0.46
1:2:1350:C:H2'	1:2:1351:U:H6	1.80	0.46
1:2:1465:G:H2'	1:2:1466:4AC:H6	1.98	0.46
4:C:55:TYR:C	4:C:56:ILE:HD13	2.40	0.46
7:F:108:ARG:O	7:F:112:MET:HG2	2.16	0.46
26:3:32:ILE:HD12	26:3:32:ILE:HA	1.82	0.46
31:a:29:ILE:HG22	31:a:32:THR:HG22	1.97	0.46
35:M:67:LEU:HD11	35:M:103:ALA:O	2.15	0.46
1:2:741:A:H4'	1:2:1471:G:O2'	2.16	0.46
2:A:40:ASP:C	2:A:40:ASP:OD1	2.59	0.46
2:A:96:LEU:HB3	2:A:125:LEU:HD11	1.98	0.46
2:A:197:ASN:OD1	2:A:197:ASN:N	2.48	0.46
10:I:43:LYS:HB2	10:I:43:LYS:NZ	2.31	0.46
13:L:6:ARG:NH1	13:L:73:LEU:HD21	2.31	0.46
28:d:5:LYS:CD	28:d:5:LYS:N	2.73	0.46
1:2:33:U:H2'	1:2:34:C:O4'	2.16	0.45
1:2:73:C:OP2	1:2:209:U:N3	2.45	0.45
1:2:1287:G:OP2	40:2:1613:HOH:O	2.20	0.45
3:B:177:ILE:O	3:B:177:ILE:HG22	2.16	0.45
7:F:13:TRP:O	7:F:24:LYS:HE3	2.16	0.45
15:O:72:ILE:O	15:O:80:TYR:OH	2.32	0.45
35:M:9:TRP:HB2	35:M:28:LEU:HD21	1.98	0.45
1:2:93:C:H2'	1:2:94:U:C6	2.51	0.45
1:2:175:U:H2'	1:2:176:G:O4'	2.16	0.45
1:2:303:A:H2'	1:2:304:G:O4'	2.16	0.45
1:2:985:C:C2	1:2:986:U:H5	2.35	0.45
1:2:1207:A:H2'	1:2:1208:G:C8	2.51	0.45
1:2:1248:C:H3'	1:2:1249:U:H6	1.81	0.45
1:2:1328:A:OP2	20:U:89:ARG:NH2	2.47	0.45
9:H:13:PHE:CE1	9:H:83:LYS:HB2	2.51	0.45
13:L:101:LEU:CD2	13:L:101:LEU:H	2.28	0.45
30:4:27:U:H2'	30:4:28:C:C6	2.52	0.45
33:b:49:LEU:HD11	35:M:98:ARG:CG	2.37	0.45
1:2:142:A:H2'	1:2:143:A:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:393:G:OP2	36:2:1532:SPM:H41	2.16	0.45
1:2:553:C:H2'	1:2:554:A:O4'	2.17	0.45
1:2:956:G:H22	1:2:1175:A:P	2.39	0.45
1:2:1164:A:H4'	1:2:1165:G:H5''	1.97	0.45
1:2:1258:G:H2'	1:2:1259:C:C6	2.51	0.45
6:E:208:VAL:C	6:E:209:ILE:HD12	2.40	0.45
8:G:12:GLN:HG3	8:G:214:ARG:HD2	1.98	0.45
17:R:15:ASN:O	17:R:16:ILE:HD13	2.16	0.45
20:U:142:ILE:HA	20:U:145:GLU:OE1	2.15	0.45
26:3:101:ILE:C	26:3:102:LEU:HD23	2.41	0.45
27:c:15:ARG:O	27:c:19:GLU:HB2	2.17	0.45
1:2:218:C:H2'	1:2:219:A:C8	2.50	0.45
1:2:646:A:C2	1:2:663:A:C5	3.05	0.45
3:B:206:LEU:HD22	3:B:211:VAL:HG21	1.98	0.45
5:D:29:LEU:HD21	5:D:99:GLN:NE2	2.32	0.45
9:H:107:ASN:ND2	9:H:172:ASN:HD21	2.15	0.45
27:c:54:LYS:HE2	27:c:70:LEU:HD12	1.98	0.45
28:d:20:THR:O	28:d:23:VAL:HG12	2.17	0.45
31:a:63:TYR:CD1	32:P:6:PRO:HB3	2.51	0.45
32:P:19:CYS:CB	32:P:22:CYS:SG	3.03	0.45
1:2:1096:U:O2	1:2:1100:G:O6	2.35	0.45
1:2:1369:G:H2'	1:2:1370:U:H6	1.81	0.45
2:A:14:TRP:HE1	2:A:17:LYS:HD2	1.82	0.45
3:B:21:LYS:HD2	3:B:21:LYS:O	2.16	0.45
20:U:77:GLU:HA	20:U:80:ARG:HG3	1.98	0.45
25:Z:68:GLN:HE22	31:a:72:LEU:CD1	2.30	0.45
26:3:27:LYS:NZ	26:3:89:ALA:HB3	2.31	0.45
31:a:51:GLU:HA	31:a:54:LYS:HG2	1.99	0.45
33:b:30:VAL:HG22	33:b:34:LYS:HB3	1.98	0.45
1:2:899:A:H2'	1:2:900:C:C6	2.51	0.45
4:C:31:GLU:OE1	4:C:43:ARG:NE	2.49	0.45
6:E:49:LEU:HD13	21:V:25:VAL:HG21	1.97	0.45
9:H:10:ILE:HA	9:H:37:TYR:CZ	2.51	0.45
13:L:85:GLN:O	13:L:88:ARG:NE	2.47	0.45
22:W:64:ILE:O	22:W:65:MET:HG3	2.17	0.45
26:3:42:ALA:HA	26:3:45:ARG:HG2	1.99	0.45
28:d:51:GLU:OE2	28:d:51:GLU:O	2.35	0.45
30:4:4:G:H2'	30:4:5:G:C8	2.51	0.45
30:4:68:C:H2'	30:4:69:C:C6	2.51	0.45
32:P:3:LYS:HG3	32:P:4:TYR:CE1	2.50	0.45
33:b:42:TYR:CE1	35:M:89:PRO:HD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:634:U:H1'	35:M:118:HIS:ND1	2.31	0.45
1:2:707:G:O2'	16:Q:59:PRO:O	2.32	0.45
1:2:1061:OMG:HM22	1:2:1062:A:H5'	1.98	0.45
1:2:1124:G:C2	1:2:1125:C:C6	3.05	0.45
6:E:16:SER:HB2	6:E:19:GLN:HB2	1.98	0.45
8:G:20:LYS:HE3	8:G:108:GLU:OE1	2.17	0.45
8:G:128:ASN:OD1	8:G:128:ASN:N	2.50	0.45
9:H:25:PRO:O	9:H:28:LYS:HG2	2.16	0.45
9:H:193:ARG:HD2	23:X:74:ARG:NH2	2.32	0.45
22:W:49:TYR:HB2	22:W:56:LYS:HG2	1.98	0.45
25:Z:71:GLU:HG3	25:Z:79:PRO:HD3	1.99	0.45
26:3:104:PRO:O	26:3:108:LYS:NZ	2.50	0.45
31:a:59:GLY:O	31:a:68:LEU:N	2.47	0.45
33:b:24:ASP:HA	35:M:123:ARG:HH21	1.79	0.45
1:2:193:A:H2'	1:2:194:A:C8	2.52	0.45
1:2:257:U:H4'	11:J:10:ARG:HD3	1.98	0.45
1:2:975:G:H2'	1:2:976:G:C8	2.52	0.45
1:2:1029:G:H2'	1:2:1030:U:C6	2.52	0.45
1:2:1355:U:H2'	1:2:1356:G:C8	2.52	0.45
3:B:199:TRP:CZ3	3:B:203:ARG:HD3	2.52	0.45
10:I:118:GLU:OE1	10:I:121:ARG:NE	2.35	0.45
14:N:134:LEU:HD23	14:N:134:LEU:HA	1.85	0.45
22:W:40:CYS:C	22:W:42:SER:H	2.23	0.45
30:4:67:C:H2'	30:4:68:C:H6	1.80	0.45
31:a:21:CYS:SG	31:a:49:PHE:HA	2.57	0.45
1:2:770:U:O2'	1:2:864:A:N1	2.47	0.45
1:2:1155:C:H2'	1:2:1156:G:O4'	2.17	0.45
36:2:1510:SPM:H61	6:E:11:TRP:CH2	2.51	0.45
6:E:182:VAL:HG11	6:E:227:MET:HE3	1.99	0.45
15:O:109:ARG:O	15:O:113:SER:OG	2.28	0.45
26:3:101:ILE:HD11	26:3:104:PRO:HG3	1.99	0.45
30:4:21:A:O4'	30:4:48:C:N4	2.50	0.45
33:b:21:ILE:CD1	33:b:32:GLU:CB	2.95	0.45
1:2:980:A:H2'	1:2:981:C:C6	2.51	0.45
4:C:57:CYS:HB3	4:C:62:PHE:H	1.82	0.45
6:E:209:ILE:HD11	6:E:223:ILE:HD13	1.98	0.45
8:G:41:VAL:HG11	8:G:146:LEU:HD21	1.99	0.45
10:I:83:TYR:CZ	10:I:123:ARG:HG3	2.52	0.45
12:K:59:ASP:HB2	12:K:63:LYS:HZ3	1.82	0.45
14:N:77:LEU:HD21	14:N:105:ILE:HD11	1.99	0.45
25:Z:99:ARG:O	25:Z:102:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:c:88:LEU:HB3	27:c:93:VAL:HB	1.99	0.45
1:2:397:G:OP1	36:2:1520:SPM:H92	2.16	0.44
1:2:567:A:OP2	40:2:1616:HOH:O	2.21	0.44
1:2:637:U:H2'	1:2:638:C:C6	2.52	0.44
1:2:1376:C:H42	1:2:1444:G:N2	2.15	0.44
6:E:209:ILE:HD12	6:E:209:ILE:N	2.32	0.44
8:G:168:ILE:HD12	8:G:168:ILE:N	2.33	0.44
9:H:39:PRO:HB3	9:H:39:PRO:HD3	1.74	0.44
9:H:108:SER:OG	9:H:178:ALA:HB1	2.17	0.44
11:J:101:LYS:HE2	11:J:101:LYS:HB3	1.90	0.44
14:N:91:ASP:HB3	29:e:14:ARG:HD3	1.99	0.44
27:c:98:SER:HB2	27:c:105:ILE:HD11	1.99	0.44
33:b:20:TYR:CD2	33:b:20:TYR:O	2.70	0.44
1:2:47:A:OP2	40:2:1612:HOH:O	2.20	0.44
1:2:441:C:P	21:V:101:ARG:HH21	2.40	0.44
1:2:1125:C:H2'	1:2:1126:C:C6	2.52	0.44
3:B:40:ASP:OD1	3:B:41:THR:N	2.50	0.44
14:N:98:ASP:O	14:N:101:ASP:HB2	2.18	0.44
19:T:63:GLU:N	19:T:63:GLU:OE1	2.50	0.44
20:U:27:ASN:OD1	20:U:27:ASN:C	2.60	0.44
20:U:64:LEU:HD22	20:U:108:PHE:CZ	2.53	0.44
33:b:11:ARG:HA	33:b:11:ARG:HD3	1.84	0.44
1:2:195:A:N1	1:2:225:G:O2'	2.45	0.44
1:2:381:G:O6	36:2:1517:SPM:N14	2.51	0.44
1:2:638:C:H2'	1:2:639:C:H6	1.81	0.44
1:2:682:U:O4'	33:b:11:ARG:HD2	2.17	0.44
3:B:160:ALA:HB3	3:B:167:ILE:HD11	1.99	0.44
3:B:177:ILE:CG2	3:B:183:ILE:HD11	2.47	0.44
5:D:134:ASN:OD1	5:D:152:LEU:HD13	2.17	0.44
9:H:37:TYR:HB2	12:K:51:GLU:OE2	2.18	0.44
9:H:95:GLN:NE2	9:H:99:GLN:HG3	2.31	0.44
9:H:134:ARG:O	9:H:138:LEU:HD12	2.17	0.44
13:L:97:ILE:O	13:L:97:ILE:HD12	2.16	0.44
15:O:85:ASP:OD1	15:O:87:GLU:HG3	2.18	0.44
16:Q:123:LEU:HD23	16:Q:123:LEU:HA	1.81	0.44
18:S:18:ASP:OD2	18:S:18:ASP:C	2.60	0.44
27:c:56:LEU:O	27:c:59:ILE:HG22	2.18	0.44
1:2:682:U:C2	33:b:11:ARG:NH1	2.85	0.44
1:2:871:A:H2'	1:2:872:A:H8	1.82	0.44
1:2:1075:C:H2'	1:2:1076:C:H6	1.82	0.44
2:A:91:ASP:HA	33:b:63:TYR:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:37:ILE:N	12:K:37:ILE:HD12	2.32	0.44
13:L:52:ARG:NE	13:L:63:GLU:OE2	2.51	0.44
28:d:15:GLU:OE1	28:d:17:ASN:ND2	2.50	0.44
30:4:10:G:N2	30:4:26:G:H1'	2.32	0.44
31:a:57:LEU:HD21	32:P:4:TYR:CD2	2.51	0.44
32:P:44:VAL:O	32:P:47:GLU:HB2	2.18	0.44
1:2:326:A:O2'	8:G:191:ARG:NH2	2.51	0.44
1:2:942:A:C8	1:2:943:U:C5	3.06	0.44
1:2:1287:G:H2'	1:2:1288:C:C6	2.52	0.44
36:2:1537:SPM:N10	40:2:1641:HOH:O	2.35	0.44
2:A:50:GLU:HG3	2:A:68:TYR:CE2	2.53	0.44
2:A:114:ASP:OD1	2:A:114:ASP:N	2.40	0.44
9:H:38:LEU:HA	9:H:39:PRO:HG2	1.98	0.44
12:K:81:ALA:HA	12:K:84:MET:HE3	2.00	0.44
14:N:128:MET:HE3	14:N:128:MET:HB3	1.84	0.44
20:U:23:TYR:HA	20:U:26:GLU:OE1	2.17	0.44
1:2:1226:C:H2'	1:2:1227:C:C6	2.53	0.44
1:2:1269:G:N2	1:2:1295:G:H1'	2.33	0.44
1:2:1319:A:H2'	1:2:1320:G:C8	2.52	0.44
3:B:64:ARG:HG2	3:B:66:ARG:NH1	2.33	0.44
13:L:11:SER:HG	13:L:95:VAL:HG12	1.80	0.44
14:N:135:ASP:O	14:N:139:LYS:HG2	2.18	0.44
19:T:20:ASP:OD1	19:T:20:ASP:N	2.49	0.44
20:U:143:PHE:CZ	20:U:156:TYR:HB3	2.52	0.44
28:d:41:LEU:CD2	28:d:43:LEU:HB2	2.48	0.44
1:2:314:C:O2'	1:2:566:A:N1	2.47	0.44
1:2:863:A:H2'	1:2:864:A:C8	2.52	0.44
1:2:1372:G:H22	1:2:1449:A:H2	1.64	0.44
2:A:22:VAL:HG12	2:A:79:LEU:HB2	1.99	0.44
6:E:118:TYR:OH	6:E:235:ASP:OD2	2.28	0.44
7:F:126:CYS:HB2	7:F:153:PRO:HA	1.99	0.44
8:G:152:ILE:HA	8:G:210:THR:HG22	1.99	0.44
12:K:23:ILE:HD12	12:K:24:TYR:H	1.83	0.44
12:K:45:VAL:O	12:K:49:ILE:HG12	2.17	0.44
22:W:26:ASN:OD1	22:W:27:GLU:N	2.51	0.44
26:3:14:ASP:OD1	26:3:15:LEU:N	2.51	0.44
26:3:33:LYS:HZ3	26:3:42:ALA:HB3	1.82	0.44
31:a:23:ILE:HD12	31:a:49:PHE:HE2	1.82	0.44
1:2:472:U:H2'	1:2:473:G:H8	1.81	0.44
1:2:885:G:H4'	7:F:68:THR:HA	1.99	0.44
1:2:996:C:H2'	1:2:996:C:OP2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1226:C:OP2	20:U:78:LYS:HD3	2.18	0.44
9:H:39:PRO:HB2	9:H:62:ILE:HD12	2.00	0.44
20:U:45:PHE:CE1	20:U:46:LYS:HE2	2.53	0.44
25:Z:7:TYR:CZ	25:Z:11:LYS:HE3	2.52	0.44
26:3:39:THR:O	26:3:43:VAL:HG23	2.18	0.44
31:a:51:GLU:HG3	31:a:54:LYS:CE	2.47	0.44
1:2:311:A:O2'	1:2:312:G:H5'	2.18	0.44
1:2:419:A:H2'	1:2:420:A:N9	2.33	0.44
1:2:1283:A:OP1	19:T:41:SER:OG	2.27	0.44
4:C:16:CYS:CB	4:C:19:CYS:SG	2.99	0.44
16:Q:95:ASN:OD1	16:Q:98:ARG:NH2	2.38	0.44
21:V:21:MET:HE3	21:V:21:MET:HB2	1.84	0.44
26:3:6:TYR:CZ	26:3:8:LYS:HD2	2.53	0.44
26:3:55:GLU:N	26:3:80:VAL:HG21	2.33	0.44
26:3:79:TYR:CE1	26:3:118:VAL:HG12	2.53	0.44
31:a:49:PHE:CD2	31:a:53:ASP:CB	2.89	0.44
1:2:310:G:H5''	1:2:311:A:OP1	2.18	0.43
1:2:710:OMC:OP1	16:Q:68:LYS:HB3	2.17	0.43
1:2:1293:G:H5''	15:O:33:GLY:H	1.83	0.43
36:2:1534:SPM:H91	36:2:1534:SPM:H122	1.67	0.43
8:G:28:GLN:OE1	8:G:45:LYS:HE2	2.18	0.43
9:H:193:ARG:HA	23:X:74:ARG:HH22	1.82	0.43
15:O:5:PHE:C	15:O:5:PHE:CD2	2.96	0.43
23:X:32:VAL:HG13	23:X:33:THR:HG23	1.99	0.43
28:d:65:LEU:HB3	28:d:66:PRO:HD3	1.99	0.43
30:4:14:A:C4	30:4:22:G:C2	3.06	0.43
35:M:111:GLU:OE2	35:M:113:VAL:HG13	2.18	0.43
1:2:777:A:H3'	33:b:8:ARG:HH22	1.82	0.43
1:2:831:C:H2'	1:2:832:G:O4'	2.18	0.43
1:2:855:A:H2'	1:2:856:C:H6	1.83	0.43
1:2:1003:A:H61	1:2:1174:G:H1'	1.83	0.43
1:2:1125:C:C2	1:2:1126:C:C5	3.06	0.43
1:2:1479:U:H5''	35:M:131:ARG:NH2	2.33	0.43
7:F:14:LYS:HD3	7:F:14:LYS:HA	1.81	0.43
13:L:27:ILE:HG12	13:L:85:GLN:CD	2.43	0.43
23:X:73:GLU:OE1	23:X:73:GLU:N	2.51	0.43
25:Z:167:ILE:HD12	31:a:8:SER:HA	2.00	0.43
30:4:23:C:H2'	30:4:24:U:C6	2.52	0.43
1:2:286:A:H8	1:2:286:A:OP2	2.00	0.43
1:2:381:G:P	6:E:44:ARG:HH22	2.41	0.43
1:2:504:C:O2'	1:2:508:U:OP1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1000:G:H2'	1:2:1001:A:O4'	2.18	0.43
1:2:1133:A:O3'	18:S:10:LYS:NZ	2.44	0.43
1:2:1155:C:OP1	25:Z:146:LYS:NZ	2.51	0.43
1:2:1201:A:H2	1:2:1204:G:N3	2.16	0.43
1:2:1461:G:OP1	1:2:1464:A:H4'	2.18	0.43
5:D:158:THR:O	5:D:158:THR:OG1	2.34	0.43
7:F:11:GLU:HA	7:F:24:LYS:NZ	2.33	0.43
9:H:30:TYR:HE2	9:H:132:PRO:HG2	1.81	0.43
9:H:127:ALA:HB3	23:X:74:ARG:NH2	2.33	0.43
14:N:98:ASP:OD1	14:N:98:ASP:N	2.51	0.43
16:Q:13:ILE:O	22:W:12:PRO:HB3	2.18	0.43
16:Q:52:LEU:HB3	16:Q:58:ILE:HB	2.00	0.43
1:2:991:U:H2'	1:2:992:G:C8	2.53	0.43
1:2:1314:A:H2'	1:2:1315:C:C6	2.53	0.43
2:A:54:TYR:CD1	2:A:54:TYR:C	2.97	0.43
3:B:199:TRP:CD1	3:B:222:VAL:HA	2.53	0.43
7:F:118:ARG:NH2	7:F:204:PHE:O	2.51	0.43
8:G:48:GLU:OE1	8:G:83:VAL:HG21	2.18	0.43
9:H:41:THR:HG23	9:H:59:GLU:CD	2.44	0.43
20:U:45:PHE:HB3	20:U:97:VAL:HB	1.99	0.43
20:U:113:LYS:HD3	20:U:113:LYS:H	1.83	0.43
20:U:133:SER:HA	20:U:136:ASP:OD1	2.18	0.43
21:V:22:GLN:HE22	21:V:85:LYS:HZ1	1.66	0.43
23:X:47:ARG:CZ	23:X:47:ARG:HB3	2.48	0.43
26:3:41:LYS:HE3	26:3:41:LYS:HB3	1.80	0.43
26:3:75:ILE:HG13	26:3:75:ILE:H	1.66	0.43
26:3:87:GLY:O	26:3:92:LEU:HD22	2.19	0.43
1:2:416:C:H2'	1:2:417:G:O4'	2.18	0.43
1:2:526:G:OP2	14:N:5:LYS:NZ	2.47	0.43
1:2:726:A:H2'	1:2:727:A:H8	1.84	0.43
1:2:1228:C:OP1	20:U:125:ARG:NH2	2.35	0.43
1:2:1332:G:O6	36:2:1516:SPM:H92	2.18	0.43
1:2:1337:G:C8	12:K:76:MET:HE1	2.53	0.43
3:B:18:GLU:OE2	3:B:43:LEU:HD22	2.17	0.43
6:E:14:MET:SD	6:E:102:ARG:NH1	2.91	0.43
6:E:50:ALA:HB1	6:E:55:GLU:HB2	1.99	0.43
6:E:58:HIS:CE1	21:V:92:LYS:HZ3	2.36	0.43
18:S:57:TYR:HA	18:S:60:ILE:HD11	2.01	0.43
20:U:12:PRO:HA	20:U:13:PRO:HD3	1.90	0.43
21:V:66:ARG:HD3	21:V:82:HIS:CE1	2.53	0.43
23:X:13:ILE:O	23:X:16:GLU:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:14:ILE:HD12	23:X:15:GLU:N	2.34	0.43
25:Z:164:ASP:OD2	25:Z:164:ASP:C	2.62	0.43
1:2:65:C:H2'	1:2:66:U:C6	2.54	0.43
1:2:1466:4AC:O7	1:2:1466:4AC:H5	2.18	0.43
4:C:39:GLU:OE1	4:C:39:GLU:N	2.52	0.43
12:K:31:PHE:CE1	12:K:36:PRO:HG3	2.54	0.43
17:R:51:THR:HG22	17:R:52:LYS:HG3	2.01	0.43
19:T:56:LYS:HE2	19:T:56:LYS:HB2	1.74	0.43
20:U:108:PHE:HD1	20:U:108:PHE:HA	1.72	0.43
1:2:482:C:O2'	1:2:485:C:N4	2.47	0.43
1:2:988:G:H4'	24:Y:50:HIS:CD2	2.54	0.43
1:2:1106:G:H2'	1:2:1107:A:O4'	2.18	0.43
7:F:77:LYS:NZ	7:F:188:GLU:OE1	2.40	0.43
9:H:111:ARG:NH2	23:X:68:ILE:HG22	2.33	0.43
9:H:138:LEU:HB3	9:H:142:HIS:NE2	2.32	0.43
15:O:104:ARG:HH11	15:O:104:ARG:HG2	1.83	0.43
16:Q:27:THR:OG1	16:Q:28:ARG:N	2.52	0.43
17:R:3:SER:OG	17:R:4:LYS:N	2.50	0.43
19:T:105:MET:HB3	19:T:113:TYR:CZ	2.54	0.43
21:V:45:ARG:NH1	21:V:65:VAL:O	2.41	0.43
28:d:55:GLN:CD	28:d:55:GLN:N	2.75	0.43
28:d:68:TYR:C	28:d:68:TYR:CD1	2.97	0.43
1:2:967:G:O6	26:3:37:ASN:HB2	2.19	0.43
1:2:992:G:N7	26:3:38:GLU:HG2	2.34	0.43
1:2:1067:G:H2'	1:2:1068:A:O4'	2.19	0.43
1:2:1316:C:H2'	1:2:1317:G:C8	2.54	0.43
1:2:1342:C:OP2	23:X:60:PRO:HB3	2.19	0.43
2:A:47:ARG:HD3	35:M:29:THR:HG21	2.00	0.43
3:B:209:ARG:O	3:B:210:ARG:HG2	2.19	0.43
8:G:51:LYS:HB3	8:G:51:LYS:HE2	1.76	0.43
9:H:116:ARG:HB3	9:H:123:VAL:CG2	2.49	0.43
9:H:142:HIS:CE1	9:H:181:ARG:HD3	2.54	0.43
9:H:173:ASP:OD2	9:H:175:LYS:HG2	2.18	0.43
12:K:24:TYR:OH	12:K:67:LYS:HD3	2.18	0.43
12:K:26:GLY:HA3	12:K:65:ASP:OD1	2.18	0.43
13:L:84:ARG:HA	13:L:87:MET:SD	2.59	0.43
24:Y:58:TRP:HB2	24:Y:67:GLU:HG2	2.01	0.43
27:c:36:THR:O	27:c:36:THR:OG1	2.36	0.43
33:b:70:CYS:SG	33:b:72:ASN:CA	3.06	0.43
1:2:682:U:C6	33:b:11:ARG:CZ	3.01	0.43
1:2:1096:U:C2	1:2:1098:C:N3	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1272:C:H4'	27:c:7:LYS:NZ	2.33	0.43
11:J:41:ASP:O	11:J:42:ILE:HD13	2.19	0.43
15:O:14:GLN:NE2	15:O:30:LYS:H	2.13	0.43
19:T:22:LEU:HD13	19:T:106:ILE:HD13	2.00	0.43
25:Z:56:ILE:CG1	25:Z:83:ILE:HD12	2.49	0.43
1:2:219:A:H2'	1:2:220:U:C6	2.54	0.43
1:2:961:C:H2'	1:2:962:A:H8	1.84	0.43
1:2:1226:C:H2'	1:2:1227:C:H6	1.83	0.43
1:2:1346:C:H2'	1:2:1347:C:H6	1.83	0.43
3:B:39:VAL:O	3:B:43:LEU:HG	2.19	0.43
12:K:37:ILE:HG12	12:K:50:MET:CE	2.49	0.43
21:V:107:GLN:HG3	21:V:109:LYS:HD3	2.01	0.43
27:c:27:GLU:O	27:c:31:LYS:N	2.51	0.43
30:4:50:U:H2'	30:4:51:C:C6	2.54	0.43
1:2:40:G:H2'	1:2:41:G:C8	2.54	0.42
1:2:910:A:O2'	1:2:1297:A:N3	2.41	0.42
1:2:965:A:H5'	26:3:94:VAL:HG21	2.00	0.42
1:2:1028:C:H2'	1:2:1029:G:C8	2.54	0.42
1:2:1319:A:H2'	1:2:1320:G:H8	1.83	0.42
1:2:1330:C:OP2	36:2:1527:SPM:N14	2.52	0.42
2:A:144:GLU:OE1	2:A:144:GLU:HA	2.18	0.42
9:H:142:HIS:CD2	9:H:181:ARG:HD3	2.54	0.42
9:H:182:LYS:O	9:H:185:ILE:HG22	2.18	0.42
13:L:28:VAL:HG21	13:L:35:MET:HB2	2.01	0.42
13:L:53:LEU:HD21	13:L:59:ARG:O	2.19	0.42
1:2:58:U:H2'	1:2:59:C:C6	2.54	0.42
1:2:682:U:C1'	33:b:11:ARG:HD2	2.48	0.42
2:A:86:HIS:HE1	2:A:189:THR:HG23	1.84	0.42
8:G:72:LYS:HA	8:G:72:LYS:HD2	1.78	0.42
8:G:157:ASP:OD1	8:G:161:PHE:N	2.51	0.42
9:H:160:GLU:OE1	9:H:160:GLU:HA	2.19	0.42
15:O:72:ILE:HD11	15:O:93:HIS:CD2	2.55	0.42
19:T:94:LYS:HB2	19:T:94:LYS:HE3	1.79	0.42
1:2:251:A:N1	1:2:283:U:O2'	2.43	0.42
1:2:268:A:H2'	1:2:269:G:C8	2.53	0.42
1:2:305:A:C5	1:2:306:G:H1'	2.54	0.42
1:2:917:G:N7	15:O:133:ARG:NH2	2.53	0.42
1:2:988:G:H4'	24:Y:50:HIS:HD2	1.85	0.42
1:2:990:C:C4	1:2:991:U:C5	3.07	0.42
1:2:1369:G:H2'	1:2:1370:U:C6	2.54	0.42
7:F:51:LEU:HB3	7:F:54:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:26:SER:HB2	8:G:29:VAL:HG23	2.01	0.42
12:K:53:LEU:HD13	12:K:86:LEU:HD11	2.01	0.42
15:O:11:ILE:HB	15:O:16:VAL:HG21	2.01	0.42
20:U:121:LYS:HD3	20:U:122:ASN:N	2.34	0.42
25:Z:43:THR:O	25:Z:79:PRO:HA	2.20	0.42
25:Z:64:LYS:HD2	25:Z:65:GLN:N	2.35	0.42
25:Z:74:PHE:N	25:Z:74:PHE:CD2	2.85	0.42
27:c:59:ILE:HG21	27:c:108:ALA:HB2	2.01	0.42
30:4:22:G:H2'	30:4:23:C:C6	2.54	0.42
1:2:333:C:H4'	1:2:334:A:H5''	2.01	0.42
1:2:942:A:C8	1:2:943:U:H5	2.37	0.42
1:2:957:A:O5'	1:2:958:C:H5	2.02	0.42
1:2:991:U:H2'	1:2:992:G:C5	2.54	0.42
1:2:996:C:O2'	1:2:997:G:H8	2.02	0.42
1:2:1005:G:P	31:a:27:LYS:HZ1	2.42	0.42
1:2:1091:U:O4	1:2:1104:G:O6	2.37	0.42
1:2:1092:G:H2'	1:2:1093:G:H8	1.84	0.42
1:2:1207:A:H2'	1:2:1208:G:H8	1.84	0.42
1:2:1333:C:H2'	1:2:1334:G:C8	2.54	0.42
36:2:1516:SPM:H91	12:K:121:GLU:OE1	2.19	0.42
2:A:40:ASP:OD1	2:A:42:THR:N	2.49	0.42
8:G:155:GLY:N	8:G:163:MET:HG2	2.34	0.42
9:H:70:ARG:HG3	9:H:71:ASN:N	2.35	0.42
11:J:126:LEU:HD23	11:J:126:LEU:HA	1.88	0.42
12:K:36:PRO:O	12:K:39:LEU:HD12	2.19	0.42
20:U:14:ASP:OD1	20:U:14:ASP:N	2.50	0.42
21:V:54:GLN:OE1	21:V:54:GLN:C	2.63	0.42
27:c:61:LYS:HD2	27:c:61:LYS:C	2.44	0.42
27:c:66:THR:HG23	27:c:69:ALA:H	1.83	0.42
27:c:69:ALA:O	27:c:73:LYS:HG2	2.20	0.42
31:a:57:LEU:CD1	31:a:62:PRO:HD3	2.50	0.42
33:b:21:ILE:HD13	33:b:32:GLU:CG	2.33	0.42
33:b:24:ASP:CA	35:M:123:ARG:HH22	2.31	0.42
35:M:27:ASP:OD1	35:M:27:ASP:N	2.41	0.42
1:2:1085:G:N2	1:2:1110:A:H62	2.17	0.42
36:2:1516:SPM:H122	12:K:121:GLU:OE1	2.20	0.42
36:2:1520:SPM:H121	36:2:1520:SPM:H91	1.64	0.42
7:F:139:VAL:HG22	7:F:148:ASP:OD2	2.20	0.42
12:K:64:ILE:HD12	12:K:64:ILE:HA	1.80	0.42
26:3:50:LEU:HD11	26:3:101:ILE:HG13	2.01	0.42
31:a:5:ASN:ND2	32:P:42:ARG:NH1	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:72:G:C2	1:2:209:U:H1'	2.55	0.42
1:2:885:G:H2'	1:2:886:G:H8	1.84	0.42
1:2:1371:C:C2	1:2:1451:G:N2	2.64	0.42
1:2:1442:G:N3	1:2:1443:G:C8	2.88	0.42
36:2:1528:SPM:H62	36:2:1528:SPM:H32	1.73	0.42
8:G:28:GLN:OE1	8:G:28:GLN:C	2.62	0.42
9:H:36:VAL:HG11	9:H:56:PRO:HG3	2.00	0.42
11:J:89:GLU:H	11:J:89:GLU:CD	2.24	0.42
12:K:56:ALA:HB2	12:K:90:LEU:HD22	2.01	0.42
13:L:47:GLU:OE1	13:L:47:GLU:HA	2.20	0.42
19:T:69:THR:HA	19:T:87:LYS:HB2	2.01	0.42
25:Z:154:LYS:HD2	31:a:3:ILE:CD1	2.49	0.42
30:4:27:U:H2'	30:4:28:C:H6	1.84	0.42
32:P:13:GLY:O	32:P:16:VAL:HG22	2.20	0.42
1:2:17:C:O2'	1:2:876:A:N1	2.50	0.42
1:2:209:U:H2'	1:2:210:U:C2	2.54	0.42
1:2:646:A:O2'	1:2:647:G:OP2	2.37	0.42
1:2:1101:G:C6	1:2:1102:C:C4	3.07	0.42
36:2:1518:SPM:H72	36:2:1518:SPM:H41	1.73	0.42
36:2:1520:SPM:HN0	36:2:1530:SPM:H31	1.85	0.42
3:B:113:PHE:CD1	3:B:113:PHE:C	2.96	0.42
11:J:33:THR:O	11:J:33:THR:OG1	2.29	0.42
16:Q:81:GLN:C	16:Q:81:GLN:OE1	2.62	0.42
18:S:28:TYR:CD1	18:S:28:TYR:C	2.98	0.42
1:2:138:G:N7	36:2:1522:SPM:H32	2.35	0.42
1:2:413:U:H2'	1:2:414:C:C6	2.55	0.42
1:2:579:C:H1'	5:D:143:TYR:HD1	1.83	0.42
1:2:613:G:O4'	10:I:2:VAL:HG12	2.19	0.42
1:2:963:G:H2'	1:2:964:G:H8	1.85	0.42
1:2:1213:A:N3	1:2:1334:G:O2'	2.38	0.42
3:B:74:ASP:O	3:B:78:ILE:HG13	2.20	0.42
8:G:122:ASP:OD1	8:G:123:GLN:N	2.50	0.42
9:H:21:GLU:O	9:H:23:ARG:NH1	2.51	0.42
9:H:182:LYS:HA	9:H:185:ILE:HG22	2.02	0.42
11:J:80:GLU:OE1	11:J:81:ILE:N	2.43	0.42
18:S:39:VAL:HG23	25:Z:194:ASN:O	2.19	0.42
26:3:74:LYS:HA	26:3:74:LYS:HD2	1.73	0.42
28:d:53:ILE:HD12	28:d:53:ILE:HA	1.80	0.42
1:2:940:G:H21	1:2:1327:A:H5'	1.85	0.42
1:2:1478:4AC:O7	1:2:1478:4AC:H5	2.19	0.42
2:A:14:TRP:NE1	2:A:17:LYS:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:127:THR:HG23	2:A:128:TYR:CD2	2.55	0.42
8:G:119:ILE:HD12	8:G:119:ILE:HA	1.86	0.42
9:H:63:ASN:OD1	9:H:75:LYS:HE3	2.19	0.42
9:H:181:ARG:HB2	9:H:181:ARG:CZ	2.50	0.42
12:K:53:LEU:HD12	12:K:90:LEU:HD21	2.02	0.42
15:O:114:ARG:CZ	15:O:114:ARG:HB2	2.50	0.42
25:Z:153:TYR:OH	25:Z:189:ILE:HG12	2.20	0.42
27:c:47:ILE:CG2	27:c:84:ILE:HG23	2.50	0.42
28:d:34:LEU:HD23	28:d:50:TYR:HB2	2.02	0.42
35:M:7:ILE:HD12	35:M:106:ILE:HD12	2.01	0.42
1:2:778:A:OP2	33:b:8:ARG:NH2	2.53	0.42
1:2:1252:A:N1	1:2:1335:G:H1'	2.35	0.42
9:H:34:MET:HA	9:H:35:PRO:HD3	1.93	0.42
9:H:41:THR:HG23	9:H:59:GLU:OE1	2.20	0.42
9:H:193:ARG:HD2	23:X:74:ARG:HH22	1.84	0.42
12:K:124:MET:CE	13:L:60:LYS:H	2.33	0.42
25:Z:91:LEU:O	25:Z:91:LEU:HD13	2.20	0.42
28:d:15:GLU:OE1	28:d:17:ASN:CG	2.63	0.42
30:4:44:A:H2'	30:4:45:G:O4'	2.20	0.42
1:2:959:C:C4	1:2:960:G:N7	2.88	0.41
1:2:1071:C:H4'	32:P:53:TYR:HD2	1.83	0.41
1:2:1228:C:P	20:U:125:ARG:HH22	2.41	0.41
2:A:20:TYR:CD2	2:A:41:ILE:HD12	2.55	0.41
9:H:111:ARG:CZ	23:X:68:ILE:HG22	2.50	0.41
14:N:63:ARG:HG3	14:N:118:ASP:O	2.20	0.41
25:Z:172:LEU:HB3	25:Z:174:PRO:HD2	2.01	0.41
28:d:18:ASP:HA	28:d:65:LEU:HD21	2.01	0.41
29:e:28:GLU:OE1	29:e:33:ARG:HD3	2.20	0.41
2:A:47:ARG:HB3	35:M:29:THR:CG2	2.48	0.41
7:F:43:GLU:H	7:F:46:ILE:HD12	1.85	0.41
9:H:88:ILE:HD13	9:H:160:GLU:OE1	2.20	0.41
12:K:12:ALA:HB2	12:K:88:ARG:HH12	1.85	0.41
12:K:27:LYS:HA	12:K:62:SER:O	2.20	0.41
15:O:17:ASP:OD1	15:O:17:ASP:C	2.63	0.41
15:O:36:THR:O	15:O:40:ILE:HG23	2.19	0.41
15:O:47:ASP:OD1	15:O:47:ASP:C	2.63	0.41
15:O:116:TRP:CD1	15:O:116:TRP:O	2.72	0.41
18:S:57:TYR:CZ	18:S:61:MET:HE2	2.55	0.41
21:V:47:ASP:OD2	21:V:47:ASP:N	2.51	0.41
21:V:102:ASP:OD2	21:V:102:ASP:N	2.53	0.41
21:V:106:LYS:O	21:V:108:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:165:ARG:HB2	25:Z:182:VAL:HG22	2.03	0.41
31:a:29:ILE:HG22	31:a:30:ILE:O	2.20	0.41
1:2:1:A:H1'	7:F:159:VAL:HG13	2.02	0.41
1:2:212:C:H2'	1:2:213:C:C6	2.55	0.41
1:2:682:U:N1	33:b:11:ARG:NH1	2.68	0.41
1:2:707:G:C8	16:Q:59:PRO:HB2	2.55	0.41
1:2:1115:A:O4'	13:L:40:PRO:HB2	2.20	0.41
1:2:1161:G:H2'	1:2:1162:U:C6	2.55	0.41
1:2:1256:C:H2'	1:2:1257:U:C6	2.55	0.41
1:2:1331:U:OP2	36:2:1516:SPM:H132	2.20	0.41
1:2:1436:U:O2'	1:2:1437:G:OP1	2.37	0.41
3:B:108:ARG:HH21	3:B:112:LYS:HZ1	1.68	0.41
3:B:172:ASP:OD1	3:B:173:THR:HG22	2.21	0.41
3:B:199:TRP:CD2	3:B:222:VAL:HG22	2.55	0.41
8:G:142:GLN:OE1	8:G:142:GLN:N	2.33	0.41
11:J:82:LEU:CD1	11:J:108:LEU:HD11	2.50	0.41
24:Y:38:ASN:ND2	24:Y:58:TRP:HZ3	2.18	0.41
26:3:22:ALA:HB1	26:3:111:VAL:HG23	2.01	0.41
31:a:22:ARG:HD2	31:a:46:SER:O	2.20	0.41
1:2:196:G:H3'	36:2:1521:SPM:H92	2.02	0.41
1:2:637:U:H2'	1:2:638:C:H6	1.86	0.41
1:2:905:OMG:H2'	1:2:906:G:O4'	2.20	0.41
1:2:980:A:O3'	19:T:52:HIS:ND1	2.52	0.41
1:2:986:U:H2'	1:2:987:U:C6	2.55	0.41
1:2:1057:C:C4	1:2:1059:A:H5''	2.55	0.41
1:2:1317:G:OP1	20:U:94:GLU:HB2	2.20	0.41
2:A:45:ILE:HA	2:A:71:ILE:HG22	2.02	0.41
4:C:37:CYS:SG	4:C:60:CYS:HB2	2.60	0.41
6:E:145:ASP:N	6:E:145:ASP:OD1	2.45	0.41
7:F:187:THR:O	7:F:191:VAL:HG23	2.20	0.41
8:G:26:SER:O	8:G:96:LYS:NZ	2.39	0.41
13:L:90:ARG:HH21	13:L:92:PRO:HA	1.85	0.41
15:O:104:ARG:HD3	15:O:108:GLU:OE2	2.19	0.41
32:P:48:LEU:HB2	32:P:50:PHE:HD1	1.85	0.41
33:b:74:ALA:HA	33:b:79:ILE:HD12	2.02	0.41
33:b:83:ARG:HD2	33:b:87:GLU:HG3	2.03	0.41
1:2:328:U:H2'	1:2:329:G:O4'	2.21	0.41
1:2:624:A:N6	33:b:15:LYS:HD3	2.36	0.41
36:2:1514:SPM:H61	36:2:1514:SPM:H32	1.79	0.41
7:F:100:ARG:O	7:F:104:GLN:HG2	2.20	0.41
8:G:87:VAL:HA	8:G:93:TRP:CZ2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:78:VAL:HA	19:T:108:HIS:O	2.21	0.41
26:3:86:LEU:HD11	26:3:99:ALA:CB	2.51	0.41
1:2:726:A:H2'	1:2:727:A:C8	2.56	0.41
1:2:843:4AC:H5	1:2:843:4AC:O7	2.20	0.41
1:2:1005:G:P	31:a:27:LYS:NZ	2.93	0.41
1:2:1036:G:P	7:F:192:ARG:HH22	2.43	0.41
1:2:1080:A:H4'	13:L:37:GLY:HA3	2.01	0.41
1:2:1096:U:H2'	1:2:1098:C:C4	2.56	0.41
1:2:1348:U:H2'	1:2:1349:G:C8	2.56	0.41
3:B:26:LYS:O	3:B:76:ARG:HD3	2.20	0.41
8:G:148:VAL:HB	8:G:212:ILE:CG2	2.51	0.41
8:G:177:LEU:HD23	8:G:177:LEU:HA	1.91	0.41
14:N:105:ILE:O	14:N:105:ILE:HG13	2.21	0.41
15:O:56:SER:OG	15:O:59:GLU:OE1	2.36	0.41
17:R:23:CYS:HB2	17:R:83:PRO:HG2	2.02	0.41
24:Y:35:LYS:HA	24:Y:35:LYS:HE3	2.02	0.41
24:Y:39:LYS:H	24:Y:39:LYS:HG3	1.72	0.41
26:3:101:ILE:O	26:3:102:LEU:HD23	2.20	0.41
31:a:20:TYR:HD2	31:a:25:ASN:ND2	2.18	0.41
31:a:30:ILE:CD1	31:a:35:LEU:HD11	2.51	0.41
1:2:125:G:OP2	36:2:1521:SPM:C6	2.61	0.41
1:2:218:C:P	36:2:1521:SPM:N14	2.93	0.41
1:2:725:A:OP2	1:2:771:G:N2	2.53	0.41
1:2:741:A:OP1	36:2:1512:SPM:H21	2.21	0.41
1:2:787:A:H2'	1:2:788:G:O4'	2.21	0.41
1:2:1093:G:C6	1:2:1094:U:C4	3.09	0.41
1:2:1154:A:H4'	25:Z:154:LYS:HG3	2.03	0.41
1:2:1230:G:C2	1:2:1234:G:C6	3.09	0.41
2:A:168:ALA:HB1	2:A:184:ALA:O	2.21	0.41
3:B:21:LYS:HD2	3:B:21:LYS:C	2.45	0.41
3:B:33:ILE:O	3:B:33:ILE:HD12	2.21	0.41
9:H:84:LEU:CB	9:H:159:GLU:HG2	2.51	0.41
9:H:145:THR:O	9:H:148:LYS:N	2.53	0.41
9:H:167:ILE:HD13	9:H:167:ILE:HA	1.91	0.41
13:L:7:ILE:HG13	13:L:99:ILE:CG2	2.50	0.41
20:U:130:LYS:HD2	20:U:130:LYS:N	2.33	0.41
28:d:5:LYS:N	28:d:5:LYS:HZ3	2.19	0.41
30:4:52:G:H2'	30:4:53:G:H8	1.85	0.41
1:2:398:C:OP1	36:2:1530:SPM:H32	2.21	0.41
1:2:771:G:OP1	1:2:865:OMG:N2	2.53	0.41
1:2:846:C:O2'	1:2:847:U:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:982:G:H4'	1:2:984:C:H41	1.86	0.41
1:2:1044:C:H2'	1:2:1045:U:C6	2.55	0.41
1:2:1203:U:OP2	9:H:158:ILE:HG22	2.21	0.41
1:2:1257:U:H5''	27:c:99:LYS:NZ	2.36	0.41
3:B:143:LYS:O	3:B:166:PRO:HD2	2.20	0.41
9:H:10:ILE:HG22	9:H:35:PRO:O	2.20	0.41
15:O:44:LEU:HD13	15:O:62:LYS:NZ	2.35	0.41
32:P:47:GLU:N	32:P:47:GLU:CD	2.78	0.41
33:b:30:VAL:CG2	33:b:31:PRO:CD	2.99	0.41
1:2:90:C:H2'	1:2:91:G:O4'	2.21	0.41
1:2:220:U:H2'	1:2:221:G:C8	2.55	0.41
1:2:241:G:H2'	1:2:242:C:O4'	2.21	0.41
1:2:298:C:O2'	5:D:3:ASP:O	2.36	0.41
1:2:381:G:OP1	6:E:44:ARG:NH2	2.43	0.41
1:2:476:G:N1	1:2:492:A:OP2	2.53	0.41
1:2:684:G:O6	33:b:15:LYS:HD3	2.21	0.41
1:2:925:U:OP1	36:2:1525:SPM:H41	2.21	0.41
1:2:1078:C:H2'	1:2:1079:U:C6	2.55	0.41
1:2:1288:C:H2'	1:2:1289:C:H6	1.85	0.41
1:2:1455:U:C4	34:5:2:U:H5''	2.56	0.41
2:A:161:GLU:OE1	2:A:166:ARG:HD2	2.21	0.41
5:D:161:PHE:HD2	5:D:166:PRO:HD3	1.86	0.41
8:G:137:VAL:HA	8:G:150:LEU:O	2.21	0.41
9:H:61:LEU:O	9:H:65:ILE:HG12	2.21	0.41
12:K:61:ARG:O	12:K:64:ILE:HG22	2.21	0.41
14:N:72:CYS:SG	14:N:122:VAL:HG21	2.60	0.41
15:O:28:MET:HE3	15:O:28:MET:HB3	1.79	0.41
17:R:82:PRO:HG2	17:R:85:ILE:HG12	2.02	0.41
18:S:5:TYR:O	18:S:10:LYS:HE3	2.20	0.41
23:X:55:ARG:CZ	23:X:74:ARG:HB2	2.51	0.41
24:Y:56:GLU:OE1	24:Y:56:GLU:HA	2.20	0.41
28:d:23:VAL:HG13	28:d:37:LEU:HD11	2.02	0.41
28:d:39:LYS:HE2	28:d:39:LYS:H	1.84	0.41
29:e:5:GLY:HA2	29:e:9:LYS:HD2	2.03	0.41
30:4:9:G:H1'	30:4:45:G:H2'	2.02	0.41
30:4:19:G:C2	30:4:57:A:H1'	2.56	0.41
1:2:367:G:N1	1:2:370:A:OP2	2.47	0.41
1:2:738:C:H5''	35:M:124:PRO:HB3	2.03	0.41
1:2:1036:G:H2'	1:2:1037:A:C8	2.56	0.41
1:2:1222:C:H2'	1:2:1223:C:C6	2.56	0.41
1:2:1336:U:OP1	12:K:76:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1382:A:N7	1:2:1439:A:H2	2.19	0.41
2:A:159:THR:O	2:A:163:VAL:HG22	2.21	0.41
3:B:84:ILE:CD1	4:C:36:ASN:HB2	2.51	0.41
4:C:45:ASP:OD1	4:C:48:CYS:HB2	2.21	0.41
6:E:175:GLU:HA	6:E:175:GLU:OE1	2.20	0.41
9:H:84:LEU:HB3	9:H:159:GLU:HG2	2.03	0.41
11:J:64:ASN:ND2	11:J:122:ASN:OD1	2.53	0.41
17:R:88:ARG:CZ	17:R:88:ARG:HB2	2.50	0.41
19:T:12:PHE:HD2	19:T:19:ILE:HD11	1.86	0.41
20:U:65:LEU:HD12	20:U:65:LEU:HA	1.84	0.41
25:Z:165:ARG:NH1	31:a:6:ARG:O	2.52	0.41
26:3:25:LYS:HB2	26:3:25:LYS:HE2	1.76	0.41
27:c:84:ILE:O	27:c:88:LEU:HG	2.21	0.41
1:2:638:C:H2'	1:2:639:C:C6	2.56	0.40
1:2:1280:G:N2	1:2:1282:A:H3'	2.36	0.40
2:A:60:PHE:HE1	33:b:59:ILE:HG21	1.85	0.40
2:A:166:ARG:HA	2:A:169:ASN:OD1	2.21	0.40
6:E:120:ARG:HG3	6:E:227:MET:HE2	2.02	0.40
7:F:59:VAL:HG11	7:F:81:ILE:HD12	2.02	0.40
8:G:119:ILE:HG12	8:G:144:ILE:HG23	2.02	0.40
12:K:110:MET:H	12:K:110:MET:HG3	1.64	0.40
13:L:90:ARG:HD2	13:L:90:ARG:HA	1.75	0.40
15:O:7:TYR:OH	27:c:29:LYS:HD2	2.21	0.40
18:S:30:THR:O	18:S:33:GLN:N	2.54	0.40
23:X:68:ILE:O	23:X:68:ILE:HG22	2.21	0.40
26:3:23:VAL:HG11	26:3:86:LEU:HD22	2.04	0.40
28:d:5:LYS:HE3	28:d:68:TYR:CE1	2.56	0.40
33:b:58:ALA:HB1	35:M:108:GLY:O	2.21	0.40
1:2:774:A:N7	1:2:1466:4AC:O2'	2.54	0.40
1:2:911:A:H2'	1:2:912:C:C6	2.56	0.40
1:2:1222:C:H2'	1:2:1223:C:H6	1.86	0.40
1:2:1231:A:H4'	20:U:36:TRP:CE3	2.55	0.40
1:2:1290:C:H2'	1:2:1291:U:H6	1.86	0.40
1:2:1365:G:H2'	1:2:1366:OMC:O4'	2.22	0.40
1:2:1451:G:N2	1:2:1452:U:C2	2.89	0.40
2:A:53:LEU:HA	2:A:53:LEU:HD12	1.87	0.40
2:A:80:ILE:HD12	2:A:80:ILE:O	2.21	0.40
3:B:76:ARG:HA	3:B:79:ASP:OD2	2.21	0.40
4:C:63:LYS:HA	4:C:63:LYS:HD3	1.93	0.40
8:G:22:LYS:HB3	8:G:91:GLU:HG2	2.04	0.40
12:K:29:ARG:HA	20:U:156:TYR:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:86:ARG:HA	20:U:95:LYS:O	2.22	0.40
25:Z:2:PRO:HB2	25:Z:3:ASN:H	1.60	0.40
27:c:85:LEU:HA	27:c:85:LEU:HD23	1.81	0.40
29:e:2:PRO:HB2	29:e:3:SER:H	1.63	0.40
31:a:34:ILE:HD13	31:a:54:LYS:NZ	2.37	0.40
33:b:10:ARG:NH2	33:b:12:LYS:HD3	2.35	0.40
1:2:10:G:O2'	7:F:72:GLU:HG2	2.21	0.40
1:2:15:OMU:HM22	1:2:16:G:H5'	2.02	0.40
1:2:260:G:H2'	1:2:261:G:H8	1.86	0.40
1:2:1082:U:C2	1:2:1084:G:C8	3.09	0.40
1:2:1443:G:H2'	1:2:1443:G:N3	2.36	0.40
36:2:1524:SPM:H31	36:2:1524:SPM:H61	1.67	0.40
9:H:20:VAL:HG11	9:H:99:GLN:HB2	2.04	0.40
9:H:32:SER:HA	28:d:62:TRP:CE2	2.56	0.40
9:H:79:TYR:CE1	9:H:83:LYS:HE2	2.56	0.40
9:H:79:TYR:O	9:H:82:VAL:HG22	2.21	0.40
12:K:98:GLU:O	12:K:102:ILE:HG12	2.21	0.40
17:R:92:LYS:NZ	17:R:92:LYS:HB3	2.36	0.40
19:T:10:LYS:HD3	19:T:10:LYS:HA	1.78	0.40
21:V:68:ILE:HG12	21:V:79:VAL:HG22	2.02	0.40
24:Y:43:ARG:NH2	24:Y:63:CYS:SG	2.95	0.40
25:Z:94:ARG:NE	31:a:10:ALA:HB1	2.37	0.40
25:Z:131:ILE:C	25:Z:132:ILE:HD12	2.47	0.40
26:3:66:LEU:HA	26:3:69:LEU:HG	2.03	0.40
26:3:79:TYR:OH	26:3:121:ILE:HG12	2.21	0.40
28:d:38:SER:HB2	28:d:43:LEU:CD2	2.51	0.40
1:2:413:U:H2'	1:2:414:C:H6	1.87	0.40
1:2:979:A:O2'	1:2:980:A:OP1	2.32	0.40
1:2:1121:A:N3	1:2:1144:G:C2	2.89	0.40
1:2:1165:G:OP2	13:L:55:HIS:ND1	2.50	0.40
1:2:1201:A:N3	1:2:1201:A:H2'	2.37	0.40
4:C:37:CYS:SG	4:C:38:GLY:N	2.95	0.40
6:E:152:PHE:HA	6:E:156:MET:HE1	2.03	0.40
8:G:24:LYS:HB2	8:G:93:TRP:CD1	2.56	0.40
15:O:27:ALA:HA	15:O:32:ILE:HG22	2.03	0.40
17:R:23:CYS:HB3	17:R:84:CYS:HB3	2.03	0.40
18:S:24:ILE:H	18:S:24:ILE:HG12	1.71	0.40
25:Z:158:GLN:O	25:Z:162:MET:HB2	2.21	0.40
31:a:59:GLY:O	31:a:67:GLU:OE1	2.39	0.40
1:2:634:U:H1'	35:M:118:HIS:CG	2.57	0.40
1:2:683:G:N7	33:b:15:LYS:HE2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:888:G:C2	1:2:890:G:C8	3.10	0.40
1:2:995:U:H6	1:2:995:U:H5''	1.86	0.40
1:2:1121:A:C2	1:2:1144:G:C4	3.10	0.40
1:2:1381:G:C2	1:2:1439:A:C4	3.10	0.40
2:A:80:ILE:HD12	2:A:80:ILE:C	2.47	0.40
2:A:89:SER:OG	2:A:91:ASP:OD2	2.27	0.40
9:H:29:LYS:HD2	9:H:29:LYS:HA	1.74	0.40
10:I:10:ALA:HA	10:I:27:ILE:HG12	2.02	0.40
19:T:89:ALA:HA	19:T:97:VAL:O	2.22	0.40
21:V:9:ILE:HD12	21:V:9:ILE:N	2.36	0.40
21:V:35:VAL:HG11	21:V:43:PRO:HG2	2.03	0.40
24:Y:55:ASN:ND2	24:Y:57:ARG:HG2	2.36	0.40
25:Z:165:ARG:CD	31:a:3:ILE:HG23	2.51	0.40
26:3:53:ILE:HD13	26:3:67:PRO:HD3	2.04	0.40
28:d:17:ASN:HB2	28:d:18:ASP:H	1.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	184/208 (88%)	179 (97%)	5 (3%)	0	100	100
3	B	213/231 (92%)	205 (96%)	8 (4%)	0	100	100
4	C	56/65 (86%)	55 (98%)	1 (2%)	0	100	100
5	D	164/181 (91%)	161 (98%)	3 (2%)	0	100	100
6	E	236/239 (99%)	230 (98%)	6 (2%)	0	100	100
7	F	208/214 (97%)	202 (97%)	6 (3%)	0	100	100
8	G	211/214 (99%)	200 (95%)	11 (5%)	0	100	100
9	H	190/193 (98%)	182 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	I	130/133 (98%)	126 (97%)	4 (3%)	0	100	100
11	J	125/133 (94%)	123 (98%)	2 (2%)	0	100	100
12	K	131/137 (96%)	123 (94%)	8 (6%)	0	100	100
13	L	99/102 (97%)	92 (93%)	7 (7%)	0	100	100
14	N	144/147 (98%)	138 (96%)	6 (4%)	0	100	100
15	O	138/165 (84%)	130 (94%)	8 (6%)	0	100	100
16	Q	143/152 (94%)	142 (99%)	1 (1%)	0	100	100
17	R	111/114 (97%)	108 (97%)	3 (3%)	0	100	100
18	S	64/79 (81%)	63 (98%)	1 (2%)	0	100	100
19	T	126/140 (90%)	123 (98%)	3 (2%)	0	100	100
20	U	152/158 (96%)	146 (96%)	6 (4%)	0	100	100
21	V	105/120 (88%)	102 (97%)	3 (3%)	0	100	100
22	W	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
23	X	65/83 (78%)	57 (88%)	8 (12%)	0	100	100
24	Y	47/75 (63%)	36 (77%)	11 (23%)	0	100	100
25	Z	194/229 (85%)	191 (98%)	3 (2%)	0	100	100
26	3	115/127 (91%)	103 (90%)	12 (10%)	0	100	100
27	c	107/110 (97%)	99 (92%)	8 (8%)	0	100	100
28	d	66/72 (92%)	60 (91%)	5 (8%)	1 (2%)	8	28
29	e	41/52 (79%)	41 (100%)	0	0	100	100
31	a	69/72 (96%)	64 (93%)	5 (7%)	0	100	100
32	P	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
33	b	91/95 (96%)	90 (99%)	1 (1%)	0	100	100
35	M	125/132 (95%)	118 (94%)	6 (5%)	1 (1%)	16	44
All	All	3964/4292 (92%)	3794 (96%)	168 (4%)	2 (0%)	49	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
35	M	119	ASP
28	d	17	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	168/184 (91%)	166 (99%)	2 (1%)	63	86
3	B	182/198 (92%)	178 (98%)	4 (2%)	45	77
4	C	51/58 (88%)	50 (98%)	1 (2%)	48	78
5	D	147/158 (93%)	147 (100%)	0	100	100
6	E	214/215 (100%)	213 (100%)	1 (0%)	81	93
7	F	180/184 (98%)	180 (100%)	0	100	100
8	G	186/187 (100%)	183 (98%)	3 (2%)	55	83
9	H	166/167 (99%)	164 (99%)	2 (1%)	63	86
10	I	113/114 (99%)	112 (99%)	1 (1%)	70	90
11	J	104/110 (94%)	104 (100%)	0	100	100
12	K	109/113 (96%)	106 (97%)	3 (3%)	38	72
13	L	93/94 (99%)	89 (96%)	4 (4%)	26	60
14	N	122/123 (99%)	120 (98%)	2 (2%)	55	83
15	O	121/142 (85%)	118 (98%)	3 (2%)	42	74
16	Q	125/129 (97%)	125 (100%)	0	100	100
17	R	101/102 (99%)	101 (100%)	0	100	100
18	S	63/75 (84%)	58 (92%)	5 (8%)	11	34
19	T	116/126 (92%)	112 (97%)	4 (3%)	32	66
20	U	134/138 (97%)	131 (98%)	3 (2%)	45	77
21	V	92/99 (93%)	90 (98%)	2 (2%)	45	77
22	W	57/58 (98%)	55 (96%)	2 (4%)	32	66
23	X	58/73 (80%)	55 (95%)	3 (5%)	21	52
24	Y	43/65 (66%)	42 (98%)	1 (2%)	44	76
25	Z	163/195 (84%)	158 (97%)	5 (3%)	35	69
26	3	97/105 (92%)	93 (96%)	4 (4%)	27	61
27	c	95/96 (99%)	92 (97%)	3 (3%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	d	62/65 (95%)	58 (94%)	4 (6%)	15	44
29	e	40/46 (87%)	39 (98%)	1 (2%)	42	74
31	a	61/62 (98%)	54 (88%)	7 (12%)	5	18
32	P	45/46 (98%)	45 (100%)	0	100	100
33	b	77/79 (98%)	76 (99%)	1 (1%)	61	86
35	M	93/98 (95%)	89 (96%)	4 (4%)	26	60
All	All	3478/3704 (94%)	3403 (98%)	75 (2%)	45	77

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	49	VAL
2	A	87	GLU
3	B	28	GLU
3	B	32	ILE
3	B	191	ARG
3	B	215	ASP
4	C	31	GLU
6	E	187	VAL
8	G	41	VAL
8	G	56	VAL
8	G	71	LYS
9	H	119	TYR
9	H	154	ASN
10	I	110	SER
12	K	90	LEU
12	K	99	LEU
12	K	111	LEU
13	L	11	SER
13	L	75	ASP
13	L	99	ILE
13	L	101	LEU
14	N	64	GLN
14	N	101	ASP
15	O	19	THR
15	O	20	MET
15	O	142	ILE
18	S	3	ASN
18	S	8	ASP
18	S	35	VAL

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Mol	Chain	Res	Type
18	S	61	MET
18	S	63	GLU
19	T	31	ILE
19	T	43	LYS
19	T	76	ASN
19	T	102	THR
20	U	11	VAL
20	U	14	ASP
20	U	103	VAL
21	V	21	MET
21	V	47	ASP
22	W	38	VAL
22	W	62	VAL
23	X	30	THR
23	X	37	THR
23	X	72	THR
24	Y	39	LYS
25	Z	82	THR
25	Z	91	LEU
25	Z	127	LEU
25	Z	157	GLN
25	Z	191	ASP
26	3	19	VAL
26	3	72	GLU
26	3	77	TYR
26	3	88	GLU
27	c	9	ILE
27	c	54	LYS
27	c	103	LEU
28	d	5	LYS
28	d	17	ASN
28	d	26	GLU
28	d	44	SER
29	e	13	VAL
31	a	26	ARG
31	a	33	ASP
31	a	35	LEU
31	a	37	LYS
31	a	43	LYS
31	a	71	ILE
31	a	72	LEU
33	b	24	ASP

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Mol	Chain	Res	Type
35	M	23	LEU
35	M	28	LEU
35	M	84	TYR
35	M	119	ASP

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

Mol	Chain	Res	Type
2	A	86	HIS
2	A	105	ASN
3	B	187	ASN
5	D	99	GLN
5	D	121	GLN
6	E	19	GLN
6	E	58	HIS
8	G	188	ASN
9	H	5	ASN
9	H	47	HIS
9	H	71	ASN
9	H	95	GLN
9	H	172	ASN
11	J	52	ASN
12	K	78	GLN
13	L	100	GLN
14	N	130	ASN
15	O	14	GLN
15	O	121	HIS
16	Q	2	ASN
16	Q	55	GLN
18	S	31	ASN
21	V	22	GLN
22	W	23	ASN
24	Y	50	HIS
24	Y	51	HIS
25	Z	3	ASN
27	c	91	GLN
27	c	100	ASN
31	a	5	ASN
31	a	25	ASN
35	M	13	HIS
35	M	18	GLN
35	M	60	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1439/1497 (96%)	233 (16%)	4 (0%)
30	4	76/77 (98%)	15 (19%)	1 (1%)
34	5	1/14 (7%)	1 (100%)	0
All	All	1516/1588 (95%)	249 (16%)	5 (0%)

All (249) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	33	U
1	2	34	C
1	2	43	G
1	2	44	C
1	2	45	U
1	2	47	A
1	2	60	G
1	2	68	C
1	2	70	G
1	2	71	G
1	2	72	G
1	2	73	C
1	2	74	A
1	2	75	A
1	2	76	G
1	2	89	A
1	2	99	A
1	2	101	C
1	2	110	A
1	2	111	A
1	2	112	C
1	2	115	A
1	2	122	G
1	2	125	G
1	2	138	G
1	2	193	A
1	2	195	A
1	2	196	G
1	2	208	A
1	2	209	U
1	2	211	C
1	2	212	C

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Mol	Chain	Res	Type
1	2	213	C
1	2	214	C
1	2	215	G
1	2	225	G
1	2	245	C
1	2	246	OMC
1	2	248	A
1	2	250	C
1	2	252	G
1	2	256	G
1	2	258	U
1	2	267	A
1	2	271	G
1	2	272	C
1	2	286	A
1	2	294	G
1	2	311	A
1	2	320	U
1	2	321	U
1	2	333	C
1	2	334	A
1	2	335	A
1	2	336	G
1	2	349	A
1	2	357	C
1	2	358	A
1	2	359	C
1	2	372	G
1	2	377	C
1	2	378	A
1	2	389	G
1	2	395	G
1	2	398	C
1	2	402	A
1	2	411	G
1	2	417	G
1	2	418	U
1	2	420	A
1	2	421	G
1	2	429	U
1	2	453	A
1	2	454	A

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Mol	Chain	Res	Type
1	2	470	U
1	2	471	C
1	2	477	U
1	2	480	G
1	2	489	G
1	2	491	A
1	2	506	A
1	2	523	C
1	2	531	A
1	2	532	A
1	2	535	C
1	2	536	G
1	2	555	A
1	2	569	G
1	2	601	A
1	2	609	G
1	2	612	A
1	2	624	A
1	2	634	U
1	2	646	A
1	2	647	G
1	2	677	A
1	2	682	U
1	2	707	G
1	2	708	C
1	2	714	G
1	2	740	A
1	2	741	A
1	2	751	A
1	2	752	U
1	2	753	A
1	2	774	A
1	2	776	C
1	2	802	U
1	2	806	A
1	2	828	A
1	2	835	A
1	2	853	G
1	2	865	OMG
1	2	877	A
1	2	889	G
1	2	897	C

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Mol	Chain	Res	Type
1	2	924	U
1	2	930	C4J
1	2	931	C
1	2	933	A
1	2	935	G
1	2	939	G
1	2	941	A
1	2	946	U
1	2	954	G
1	2	957	A
1	2	958	C
1	2	960	G
1	2	966	U
1	2	967	G
1	2	979	A
1	2	980	A
1	2	982	G
1	2	983	A
1	2	988	G
1	2	989	C
1	2	990	C
1	2	991	U
1	2	992	G
1	2	995	U
1	2	996	C
1	2	997	G
1	2	1002	G
1	2	1023	C
1	2	1051	G
1	2	1052	U
1	2	1058	A
1	2	1059	A
1	2	1080	A
1	2	1081	G
1	2	1094	U
1	2	1095	C
1	2	1096	U
1	2	1097	C
1	2	1098	C
1	2	1099	G
1	2	1101	G
1	2	1103	C

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Mol	Chain	Res	Type
1	2	1106	G
1	2	1107	A
1	2	1113	C
1	2	1118	G
1	2	1121	A
1	2	1123	U
1	2	1147	G
1	2	1157	G
1	2	1159	A
1	2	1160	G
1	2	1164	A
1	2	1175	A
1	2	1176	A
1	2	1187	C
1	2	1188	G
1	2	1189	C
1	2	1190	A
1	2	1201	A
1	2	1211	A
1	2	1220	U
1	2	1221	U
1	2	1222	C
1	2	1226	C
1	2	1244	A
1	2	1248	C
1	2	1249	U
1	2	1251	A
1	2	1253	A
1	2	1258	G
1	2	1263	A
1	2	1264	G
1	2	1265	U
1	2	1267	G
1	2	1269	G
1	2	1270	A
1	2	1281	A
1	2	1284	C
1	2	1286	C
1	2	1300	A
1	2	1309	U
1	2	1317	G
1	2	1328	A

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Mol	Chain	Res	Type
1	2	1334	G
1	2	1337	G
1	2	1338	A
1	2	1358	A
1	2	1361	C
1	2	1375	C
1	2	1376	C
1	2	1381	G
1	2	1437	G
1	2	1440	A
1	2	1441	G
1	2	1443	G
1	2	1444	G
1	2	1449	A
1	2	1450	A
1	2	1451	G
1	2	1452	U
1	2	1454	G
1	2	1455	U
1	2	1456	A
1	2	1459	A
1	2	1460	A
1	2	1461	G
1	2	1463	U
1	2	1474	G
1	2	1486	G
1	2	1487	G
1	2	1488	A
1	2	1489	U
1	2	1490	C
1	2	1491	A
1	2	1493	C
30	4	2	G
30	4	8	4SU
30	4	10	G
30	4	16	C
30	4	17(A)	U
30	4	18	G
30	4	20	H2U
30	4	21	A
30	4	22	G
30	4	46	A

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Mol	Chain	Res	Type
30	4	47	U
30	4	49	G
30	4	61	C
30	4	74	C
30	4	75	C
34	5	3	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	44	C
1	2	979	A
1	2	1188	G
1	2	1436	U
30	4	74	C

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

38 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	$\# Z > 2$
1	4AC	2	1466	1	21,24,25	1.03	2 (9%)	29,34,37	1.30	4 (13%)
1	MA6	2	1475	1	23,26,27	1.47	4 (17%)	34,38,41	2.08	10 (29%)
1	OMC	2	512	1	19,22,23	0.86	2 (10%)	26,31,34	0.86	0
1	OMG	2	672	1	23,26,27	1.25	3 (13%)	33,38,41	1.94	6 (18%)
1	OMG	2	546	1	23,26,27	1.24	3 (13%)	33,38,41	1.93	6 (18%)
1	OMG	2	1018	1	23,26,27	1.25	3 (13%)	33,38,41	1.93	6 (18%)
30	5MU	4	54	30	19,22,23	1.39	5 (26%)	28,32,35	2.10	8 (28%)
1	C4J	2	930	1	24,29,30	0.65	1 (4%)	29,42,45	0.55	0
1	OMU	2	52	1	19,22,23	1.28	3 (15%)	26,31,34	1.75	5 (19%)
1	OMG	2	865	1	23,26,27	1.23	4 (17%)	33,38,41	1.96	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	2	337	1	23,26,27	1.25	4 (17%)	33,38,41	1.95	7 (21%)
1	OMU	2	1344	1	19,22,23	1.22	3 (15%)	26,31,34	1.67	6 (23%)
1	OMC	2	1366	1	19,22,23	0.81	0	26,31,34	0.74	0
1	OMC	2	246	1	19,22,23	0.88	1 (5%)	26,31,34	1.03	1 (3%)
30	H2U	4	20	30	18,21,22	0.30	0	21,30,33	0.44	0
1	OMC	2	538	1	19,22,23	0.88	2 (10%)	26,31,34	0.87	1 (3%)
1	6MZ	2	1457	37,1	22,25,26	1.47	4 (18%)	30,36,39	2.25	10 (33%)
1	OMG	2	926	1	23,26,27	1.24	3 (13%)	33,38,41	1.98	6 (18%)
1	OMG	2	399	1	23,26,27	1.25	3 (13%)	33,38,41	1.97	7 (21%)
1	OMG	2	1061	1	23,26,27	1.23	3 (13%)	33,38,41	1.93	6 (18%)
1	OMC	2	1060	1	19,22,23	0.85	1 (5%)	26,31,34	0.73	0
30	OMC	4	32	30	19,22,23	0.84	0	26,31,34	1.04	2 (7%)
1	OMG	2	905	1	23,26,27	1.24	3 (13%)	33,38,41	1.96	6 (18%)
1	5MC	2	1368	1	18,22,23	0.92	2 (11%)	26,32,35	1.05	2 (7%)
1	4AC	2	1478	1	21,24,25	1.03	2 (9%)	29,34,37	1.35	4 (13%)
1	OMG	2	1194	1	23,26,27	1.22	3 (13%)	33,38,41	1.95	6 (18%)
1	OMU	2	15	1	19,22,23	1.35	4 (21%)	26,31,34	1.82	5 (19%)
1	4AC	2	1467	1	21,24,25	1.04	2 (9%)	29,34,37	1.27	4 (13%)
1	OMC	2	481	1	19,22,23	0.94	1 (5%)	26,31,34	1.05	3 (11%)
1	OMU	2	1032	1	19,22,23	1.29	3 (15%)	26,31,34	1.74	4 (15%)
1	4AC	2	843	1	21,24,25	1.11	3 (14%)	29,34,37	1.39	4 (13%)
30	PSU	4	55	30	18,21,22	1.31	2 (11%)	22,30,33	1.89	3 (13%)
1	OMC	2	113	1	19,22,23	0.86	1 (5%)	26,31,34	0.86	0
1	4AC	2	1477	1	21,24,25	1.03	2 (9%)	29,34,37	1.60	7 (24%)
30	4SU	4	8	30	18,21,22	0.28	0	26,30,33	0.35	0
1	OMC	2	710	1	19,22,23	0.88	2 (10%)	26,31,34	0.79	0
1	A2M	2	494	1	22,25,26	1.42	5 (22%)	31,36,39	2.05	7 (22%)
1	OMC	2	313	1	19,22,23	0.89	2 (10%)	26,31,34	0.95	1 (3%)

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
1	4AC	2	1466	1	-	0/11/29/30	0/2/2/2
1	MA6	2	1475	1	-	0/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	2	512	1	-	0/9/27/28	0/2/2/2
1	OMG	2	672	1	-	0/9/27/28	0/3/3/3
1	OMG	2	546	1	-	0/9/27/28	0/3/3/3
1	OMG	2	1018	1	-	0/9/27/28	0/3/3/3
30	5MU	4	54	30	-	0/7/25/26	0/2/2/2
1	C4J	2	930	1	-	3/16/34/35	0/2/2/2
1	OMU	2	52	1	-	0/9/27/28	0/2/2/2
1	OMG	2	865	1	-	3/9/27/28	0/3/3/3
1	OMG	2	337	1	-	1/9/27/28	0/3/3/3
1	OMU	2	1344	1	-	0/9/27/28	0/2/2/2
1	OMC	2	1366	1	-	0/9/27/28	0/2/2/2
1	OMC	2	246	1	-	3/9/27/28	0/2/2/2
30	H2U	4	20	30	-	3/7/38/39	0/2/2/2
1	OMC	2	538	1	-	0/9/27/28	0/2/2/2
1	6MZ	2	1457	37,1	-	0/9/27/28	0/3/3/3
1	OMG	2	926	1	-	1/9/27/28	0/3/3/3
1	OMG	2	399	1	-	0/9/27/28	0/3/3/3
1	OMG	2	1061	1	-	0/9/27/28	0/3/3/3
1	OMC	2	1060	1	-	0/9/27/28	0/2/2/2
30	OMC	4	32	30	-	4/9/27/28	0/2/2/2
1	OMG	2	905	1	-	0/9/27/28	0/3/3/3
1	5MC	2	1368	1	-	0/7/25/26	0/2/2/2
1	4AC	2	1478	1	-	0/11/29/30	0/2/2/2
1	OMG	2	1194	1	-	0/9/27/28	0/3/3/3
1	OMU	2	15	1	-	0/9/27/28	0/2/2/2
1	4AC	2	1467	1	-	0/11/29/30	0/2/2/2
1	OMC	2	481	1	-	0/9/27/28	0/2/2/2
1	OMU	2	1032	1	-	0/9/27/28	0/2/2/2
1	4AC	2	843	1	-	0/11/29/30	0/2/2/2
30	PSU	4	55	30	-	1/7/25/26	0/2/2/2
1	OMC	2	113	1	-	0/9/27/28	0/2/2/2
1	4AC	2	1477	1	-	2/11/29/30	0/2/2/2
30	4SU	4	8	30	-	0/7/25/26	0/2/2/2
1	OMC	2	710	1	-	0/9/27/28	0/2/2/2
1	A2M	2	494	1	-	0/9/27/28	0/3/3/3
1	OMC	2	313	1	-	1/9/27/28	0/2/2/2

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1475	MA6	C5-C4	4.38	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1457	6MZ	C5-C4	4.31	1.47	1.39
1	2	494	A2M	C5-C4	3.98	1.46	1.39
1	2	15	OMU	C4-N3	-3.15	1.32	1.38
30	4	55	PSU	C6-C5	3.12	1.39	1.35
1	2	399	OMG	C6-N1	-3.03	1.33	1.38
1	2	1032	OMU	C4-N3	-2.99	1.33	1.38
1	2	1018	OMG	C6-N1	-2.93	1.33	1.38
1	2	1061	OMG	C6-N1	-2.93	1.33	1.38
1	2	672	OMG	C6-N1	-2.92	1.33	1.38
1	2	843	4AC	C4-N3	-2.91	1.27	1.32
1	2	337	OMG	C6-N1	-2.90	1.33	1.38
1	2	546	OMG	C6-N1	-2.87	1.33	1.38
1	2	905	OMG	C5-C4	2.87	1.46	1.38
1	2	1194	OMG	C5-C4	2.86	1.46	1.38
1	2	672	OMG	C5-C4	2.86	1.46	1.38
1	2	52	OMU	C4-N3	-2.86	1.33	1.38
1	2	546	OMG	C5-C4	2.84	1.46	1.38
1	2	865	OMG	C6-N1	-2.84	1.33	1.38
1	2	15	OMU	C2-N3	-2.82	1.32	1.38
1	2	926	OMG	C5-C4	2.81	1.46	1.38
1	2	905	OMG	C6-N1	-2.80	1.33	1.38
1	2	1475	MA6	C5-C6	2.80	1.48	1.41
1	2	1061	OMG	C5-C4	2.78	1.46	1.38
1	2	1018	OMG	C5-C4	2.76	1.46	1.38
1	2	926	OMG	C6-N1	-2.75	1.33	1.38
1	2	1467	4AC	C4-N3	-2.71	1.28	1.32
1	2	1194	OMG	C6-N1	-2.69	1.33	1.38
1	2	865	OMG	C5-C4	2.67	1.46	1.38
30	4	54	5MU	C6-C5	2.63	1.38	1.34
1	2	399	OMG	C5-C4	2.62	1.46	1.38
30	4	55	PSU	C4-N3	-2.61	1.34	1.38
1	2	1457	6MZ	C5-C6	2.61	1.48	1.41
1	2	337	OMG	C5-C4	2.61	1.46	1.38
1	2	52	OMU	C2-N3	-2.60	1.33	1.38
1	2	399	OMG	C5-N7	-2.59	1.34	1.39
1	2	1478	4AC	C5-C4	2.58	1.46	1.40
1	2	1344	OMU	C4-N3	-2.58	1.33	1.38
1	2	843	4AC	C5-C4	2.58	1.46	1.40
1	2	494	A2M	C5-N7	-2.57	1.34	1.39
1	2	930	C4J	O4'-C1'	-2.57	1.40	1.43
1	2	1467	4AC	C5-C4	2.56	1.46	1.40
1	2	1032	OMU	C2-N3	-2.56	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1466	4AC	C4-N3	-2.55	1.28	1.32
1	2	1478	4AC	C4-N3	-2.55	1.28	1.32
30	4	54	5MU	C4-N3	-2.54	1.34	1.38
1	2	1466	4AC	C5-C4	2.54	1.46	1.40
1	2	1368	5MC	C6-N1	-2.52	1.33	1.38
1	2	1457	6MZ	C5-N7	-2.52	1.34	1.39
1	2	672	OMG	C5-N7	-2.51	1.34	1.39
1	2	15	OMU	C5-C4	-2.50	1.38	1.43
1	2	1018	OMG	C5-N7	-2.48	1.34	1.39
1	2	926	OMG	C5-N7	-2.46	1.34	1.39
1	2	1477	4AC	C5-C4	2.44	1.46	1.40
1	2	905	OMG	C5-N7	-2.40	1.34	1.39
1	2	1194	OMG	C5-N7	-2.39	1.34	1.39
1	2	1477	4AC	C4-N3	-2.38	1.28	1.32
30	4	54	5MU	C4-C5	2.38	1.48	1.44
1	2	337	OMG	C5-N7	-2.38	1.34	1.39
1	2	865	OMG	C5-N7	-2.34	1.34	1.39
1	2	546	OMG	C5-N7	-2.33	1.34	1.39
1	2	1061	OMG	C5-N7	-2.33	1.34	1.39
1	2	1344	OMU	C2-N3	-2.31	1.33	1.38
1	2	1032	OMU	C5-C4	-2.31	1.38	1.43
1	2	1368	5MC	C6-C5	2.31	1.38	1.34
1	2	1475	MA6	C5-N7	-2.30	1.34	1.39
1	2	494	A2M	C5-C6	2.29	1.47	1.41
30	4	54	5MU	C6-N1	-2.28	1.34	1.38
1	2	52	OMU	C5-C4	-2.27	1.38	1.43
30	4	54	5MU	C2-N1	2.25	1.42	1.38
1	2	1344	OMU	C5-C4	-2.24	1.38	1.43
1	2	337	OMG	C4-N9	-2.21	1.32	1.38
1	2	1457	6MZ	C8-N9	-2.13	1.33	1.37
1	2	494	A2M	C4-N9	-2.13	1.32	1.37
1	2	494	A2M	C8-N7	2.12	1.35	1.31
1	2	843	4AC	C4-N4	-2.11	1.36	1.39
1	2	538	OMC	C6-N1	-2.11	1.32	1.38
1	2	313	OMC	C6-N1	-2.10	1.32	1.38
1	2	246	OMC	C5-C4	-2.09	1.38	1.42
1	2	1475	MA6	C4-N9	-2.08	1.33	1.37
1	2	15	OMU	C6-N1	-2.07	1.33	1.38
1	2	481	OMC	C6-N1	-2.07	1.33	1.38
1	2	313	OMC	C5-C4	-2.07	1.38	1.42
1	2	512	OMC	C5-C4	-2.05	1.38	1.42
1	2	538	OMC	C5-C4	-2.05	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	865	OMG	C4-N9	-2.04	1.32	1.38
1	2	113	OMC	C6-N1	-2.03	1.33	1.38
1	2	710	OMC	C5-C4	-2.03	1.38	1.42
1	2	1060	OMC	C6-N1	-2.02	1.33	1.38
1	2	512	OMC	C6-N1	-2.02	1.33	1.38
1	2	710	OMC	C6-N1	-2.02	1.33	1.38

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1457	6MZ	C5-C4-N3	-6.37	118.44	126.75
1	2	672	OMG	C5-C4-N3	-6.30	118.24	128.46
1	2	399	OMG	C5-C4-N3	-6.27	118.30	128.46
1	2	926	OMG	C5-C4-N3	-6.17	118.46	128.46
1	2	905	OMG	C5-C4-N3	-6.12	118.52	128.46
1	2	1018	OMG	C5-C4-N3	-6.11	118.54	128.46
1	2	1194	OMG	C5-C4-N3	-6.06	118.63	128.46
1	2	865	OMG	C5-C4-N3	-6.05	118.65	128.46
1	2	1061	OMG	C5-C4-N3	-6.01	118.70	128.46
1	2	494	A2M	C5-C4-N3	-5.93	119.02	126.75
1	2	546	OMG	C5-C4-N3	-5.92	118.86	128.46
30	4	55	PSU	N1-C2-N3	5.78	121.67	115.13
1	2	1475	MA6	C5-C4-N3	-5.75	119.25	126.75
1	2	337	OMG	C5-C4-N3	-5.60	119.38	128.46
30	4	54	5MU	C4-N3-C2	-5.17	120.66	127.35
1	2	865	OMG	C2-N3-C4	4.97	121.15	112.30
1	2	399	OMG	C2-N3-C4	4.93	121.08	112.30
1	2	1194	OMG	C2-N3-C4	4.92	121.06	112.30
1	2	905	OMG	C2-N3-C4	4.91	121.04	112.30
1	2	15	OMU	C4-N3-C2	-4.88	120.14	126.58
30	4	54	5MU	N3-C2-N1	4.85	121.33	114.89
1	2	1018	OMG	C2-N3-C4	4.84	120.92	112.30
1	2	1457	6MZ	N3-C4-N9	4.82	135.03	127.08
1	2	926	OMG	C2-N3-C4	4.81	120.88	112.30
1	2	672	OMG	C2-N3-C4	4.80	120.85	112.30
1	2	337	OMG	C2-N3-C4	4.77	120.80	112.30
1	2	546	OMG	C2-N3-C4	4.77	120.80	112.30
1	2	672	OMG	N9-C4-N3	4.77	135.52	125.94
1	2	494	A2M	N3-C4-N9	4.77	134.94	127.08
1	2	843	4AC	O7-C7-N4	4.71	129.44	121.82
1	2	926	OMG	N9-C4-N3	4.70	135.38	125.94
1	2	1061	OMG	C2-N3-C4	4.68	120.64	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	399	OMG	N9-C4-N3	4.68	135.34	125.94
1	2	1478	4AC	O7-C7-N4	4.64	129.32	121.82
1	2	1018	OMG	N9-C4-N3	4.57	135.12	125.94
1	2	52	OMU	C4-N3-C2	-4.56	120.56	126.58
1	2	1061	OMG	N9-C4-N3	4.55	135.07	125.94
1	2	1032	OMU	C4-N3-C2	-4.54	120.59	126.58
1	2	905	OMG	N9-C4-N3	4.52	135.01	125.94
1	2	1477	4AC	O7-C7-N4	4.49	129.08	121.82
1	2	1475	MA6	C2-N1-C6	4.46	122.28	111.75
1	2	865	OMG	N9-C4-N3	4.43	134.83	125.94
1	2	1194	OMG	N9-C4-N3	4.41	134.79	125.94
1	2	1466	4AC	O7-C7-N4	4.40	128.94	121.82
30	4	54	5MU	C5-C4-N3	4.39	119.06	115.31
1	2	1475	MA6	N3-C4-N9	4.33	134.22	127.08
1	2	1344	OMU	C4-N3-C2	-4.32	120.88	126.58
1	2	1467	4AC	O7-C7-N4	4.30	128.78	121.82
1	2	546	OMG	N9-C4-N3	4.28	134.54	125.94
1	2	337	OMG	N9-C4-N3	4.26	134.49	125.94
1	2	52	OMU	N3-C2-N1	4.16	120.42	114.89
1	2	15	OMU	N3-C2-N1	4.15	120.40	114.89
1	2	1032	OMU	N3-C2-N1	4.15	120.40	114.89
1	2	15	OMU	C5-C4-N3	4.10	120.98	114.84
30	4	55	PSU	C4-N3-C2	-4.01	120.56	126.34
1	2	1457	6MZ	C4-C5-N7	-3.97	105.78	110.62
1	2	1344	OMU	N3-C2-N1	3.84	119.99	114.89
1	2	494	A2M	C2-N3-C4	3.81	120.76	111.75
1	2	1032	OMU	C5-C4-N3	3.78	120.50	114.84
1	2	1475	MA6	C4-C5-N7	-3.78	106.01	110.62
1	2	1457	6MZ	C2-N3-C4	3.77	120.65	111.75
1	2	1475	MA6	C2-N3-C4	3.76	120.63	111.75
30	4	54	5MU	O4-C4-C5	-3.75	120.56	124.90
1	2	52	OMU	C5-C4-N3	3.71	120.40	114.84
1	2	1457	6MZ	C6-C5-N7	3.69	136.38	132.39
1	2	1344	OMU	C5-C4-N3	3.66	120.32	114.84
30	4	54	5MU	C5-C6-N1	-3.60	119.64	123.34
1	2	1477	4AC	N4-C4-N3	3.57	119.85	113.85
1	2	337	OMG	C6-C5-N7	3.46	136.69	130.25
1	2	1477	4AC	C5-C4-N4	-3.41	117.00	122.92
30	4	55	PSU	O2-C2-N1	-3.33	119.12	122.79
1	2	494	A2M	N3-C2-N1	-3.33	123.39	128.60
1	2	865	OMG	C6-C5-N7	3.29	136.36	130.25
1	2	1194	OMG	C6-C5-N7	3.28	136.35	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	546	OMG	C6-C5-N7	3.27	136.33	130.25
1	2	15	OMU	O4-C4-C5	-3.26	119.43	125.16
1	2	1467	4AC	CM7-C7-N4	-3.25	109.67	115.29
1	2	1457	6MZ	C5-N7-C8	3.24	108.11	103.51
1	2	1475	MA6	N1-C2-N3	-3.22	123.56	128.60
1	2	905	OMG	C6-C5-N7	3.17	136.15	130.25
1	2	1061	OMG	C6-C5-N7	3.09	135.99	130.25
1	2	1018	OMG	C6-C5-N7	3.08	135.98	130.25
1	2	1368	5MC	C5-C6-N1	-3.08	120.17	123.34
1	2	1344	OMU	O4-C4-C5	-3.07	119.76	125.16
1	2	926	OMG	C6-C5-N7	3.06	135.94	130.25
1	2	52	OMU	O4-C4-C5	-3.06	119.78	125.16
1	2	1475	MA6	C5-N7-C8	3.05	107.84	103.51
1	2	399	OMG	C6-C5-N7	2.95	135.73	130.25
1	2	1457	6MZ	N1-C2-N3	-2.92	124.03	128.60
1	2	672	OMG	C6-C5-N7	2.89	135.63	130.25
1	2	1466	4AC	C5-C4-N4	-2.88	117.91	122.92
1	2	843	4AC	CM7-C7-N4	-2.88	110.32	115.29
1	2	1478	4AC	C5-C4-N4	-2.87	117.93	122.92
1	2	1466	4AC	N4-C4-N3	2.85	118.63	113.85
1	2	1032	OMU	O4-C4-C5	-2.85	120.16	125.16
1	2	1466	4AC	CM7-C7-N4	-2.84	110.38	115.29
1	2	494	A2M	C4-C5-N7	-2.79	107.22	110.62
30	4	32	OMC	O2-C2-N3	-2.75	117.86	122.33
1	2	246	OMC	O2-C2-N3	-2.75	117.86	122.33
1	2	1478	4AC	CM7-C7-N4	-2.74	110.55	115.29
1	2	1477	4AC	C1'-N1-C2	2.74	124.53	118.42
1	2	1478	4AC	N4-C4-N3	2.70	118.39	113.85
1	2	1194	OMG	C4-C5-N7	-2.69	106.46	110.72
1	2	1475	MA6	C4-N9-C8	2.68	108.63	105.73
1	2	843	4AC	C5-C4-N4	-2.66	118.30	122.92
1	2	865	OMG	C4-C5-N7	-2.64	106.54	110.72
1	2	494	A2M	C4-N9-C8	2.63	108.58	105.73
1	2	926	OMG	C4-C5-N7	-2.63	106.56	110.72
1	2	905	OMG	C4-C5-N7	-2.59	106.62	110.72
1	2	546	OMG	C4-C5-N7	-2.55	106.69	110.72
1	2	1018	OMG	C4-C5-N7	-2.54	106.70	110.72
1	2	1467	4AC	C5-C4-N4	-2.54	118.51	122.92
1	2	1368	5MC	C5-C4-N3	-2.52	118.96	121.67
1	2	1477	4AC	CM7-C7-N4	-2.51	110.96	115.29
1	2	672	OMG	C4-C5-N7	-2.50	106.76	110.72
1	2	1457	6MZ	C4-N9-C8	2.50	108.44	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	4	54	5MU	O2-C2-N1	-2.48	119.48	122.79
1	2	1061	OMG	C4-C5-N7	-2.48	106.80	110.72
1	2	313	OMC	O2-C2-N3	-2.44	118.36	122.33
1	2	337	OMG	C4-C5-N7	-2.42	106.89	110.72
1	2	399	OMG	C4-C5-N7	-2.41	106.91	110.72
1	2	1467	4AC	N4-C4-N3	2.39	117.86	113.85
1	2	494	A2M	C5-N7-C8	2.38	106.89	103.51
1	2	481	OMC	C5-C4-N3	-2.37	117.29	121.33
1	2	481	OMC	C6-C5-C4	2.37	121.33	117.50
1	2	399	OMG	O6-C6-C5	-2.35	120.36	126.60
1	2	15	OMU	O2-C2-N1	-2.34	119.67	122.79
30	4	54	5MU	C5M-C5-C4	2.33	121.33	118.77
30	4	32	OMC	C1'-N1-C2	2.30	123.56	118.42
1	2	843	4AC	N4-C4-N3	2.27	117.67	113.85
1	2	337	OMG	O6-C6-C5	-2.25	120.63	126.60
1	2	481	OMC	N4-C4-N3	2.25	121.91	117.97
1	2	1475	MA6	C6-C5-N7	2.21	137.00	133.28
1	2	1477	4AC	O2-C2-N3	-2.19	118.78	122.33
1	2	52	OMU	C1'-N1-C2	2.18	121.52	117.57
1	2	926	OMG	O6-C6-C5	-2.17	120.84	126.60
1	2	865	OMG	O6-C6-C5	-2.16	120.86	126.60
1	2	1061	OMG	O6-C6-C5	-2.15	120.88	126.60
1	2	1018	OMG	O6-C6-C5	-2.15	120.89	126.60
1	2	1475	MA6	N9-C8-N7	-2.14	110.98	113.91
1	2	672	OMG	O6-C6-C5	-2.12	120.97	126.60
1	2	905	OMG	O6-C6-C5	-2.12	120.97	126.60
1	2	546	OMG	O6-C6-C5	-2.11	121.00	126.60
1	2	1457	6MZ	C2-N1-C6	2.10	122.31	115.25
1	2	538	OMC	O2-C2-N3	-2.10	118.91	122.33
30	4	54	5MU	C5M-C5-C6	-2.09	120.05	122.85
1	2	399	OMG	C5-C6-N1	2.09	118.50	113.19
1	2	1194	OMG	O6-C6-C5	-2.08	121.09	126.60
1	2	1344	OMU	O2-C2-N1	-2.06	120.04	122.79
1	2	337	OMG	C5-C6-N1	2.06	118.41	113.19
1	2	1477	4AC	C1'-N1-C6	-2.04	116.40	120.84
1	2	1457	6MZ	N9-C8-N7	-2.03	111.14	113.91
1	2	1344	OMU	C1'-N1-C2	2.02	121.23	117.57

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	246	OMC	C3'-C4'-C5'-O5'
30	4	20	H2U	O4'-C1'-N1-C6
1	2	930	C4J	C4'-C5'-O5'-P
1	2	246	OMC	O4'-C4'-C5'-O5'
1	2	930	C4J	C3'-C4'-C5'-O5'
30	4	20	H2U	O4'-C1'-N1-C2
30	4	32	OMC	C1'-C2'-O2'-CM2
1	2	865	OMG	C3'-C4'-C5'-O5'
1	2	926	OMG	C3'-C2'-O2'-CM2
1	2	865	OMG	C4'-C5'-O5'-P
1	2	930	C4J	N3-C3-C31-C32
30	4	20	H2U	C4'-C5'-O5'-P
30	4	32	OMC	C3'-C2'-O2'-CM2
1	2	337	OMG	C4'-C5'-O5'-P
30	4	32	OMC	C2'-C1'-N1-C6
30	4	55	PSU	O4'-C1'-C5-C4
1	2	246	OMC	C2'-C1'-N1-C2
1	2	313	OMC	C2'-C1'-N1-C2
30	4	32	OMC	C2'-C1'-N1-C2
1	2	1477	4AC	C2'-C1'-N1-C2
1	2	865	OMG	O4'-C4'-C5'-O5'
1	2	1477	4AC	C2'-C1'-N1-C6

There are no ring outliers.

25 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1466	4AC	4	0
1	2	1475	MA6	1	0
1	2	672	OMG	1	0
1	2	1018	OMG	1	0
1	2	52	OMU	1	0
1	2	865	OMG	2	0
1	2	337	OMG	1	0
1	2	1344	OMU	2	0
1	2	1366	OMC	1	0
30	4	20	H2U	1	0
1	2	926	OMG	2	0
1	2	1061	OMG	1	0
1	2	1060	OMC	1	0
30	4	32	OMC	1	0
1	2	905	OMG	1	0
1	2	1368	5MC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1478	4AC	2	0
1	2	15	OMU	1	0
1	2	1467	4AC	1	0
1	2	481	OMC	1	0
1	2	1032	OMU	2	0
1	2	843	4AC	3	0
1	2	113	OMC	1	0
1	2	1477	4AC	2	0
1	2	710	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 106 ligands modelled in this entry, 66 are monoatomic - leaving 40 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	$\# Z > 2$
36	SPM	2	1521	-	13,13,13	0.12	0	12,12,12	0.07	0
36	SPM	2	1522	-	13,13,13	0.09	0	12,12,12	0.09	0
36	SPM	2	1516	-	13,13,13	0.06	0	12,12,12	0.21	0
36	SPM	2	1519	-	13,13,13	0.10	0	12,12,12	0.08	0
36	SPM	2	1527	-	13,13,13	0.09	0	12,12,12	0.08	0
36	SPM	2	1502	-	13,13,13	0.11	0	12,12,12	0.06	0
36	SPM	2	1517	-	13,13,13	0.07	0	12,12,12	0.18	0
36	SPM	2	1534	-	13,13,13	0.12	0	12,12,12	0.07	0
36	SPM	2	1509	-	13,13,13	0.06	0	12,12,12	0.14	0
36	SPM	2	1518	-	13,13,13	0.07	0	12,12,12	0.14	0
36	SPM	2	1501	-	13,13,13	0.08	0	12,12,12	0.12	0
36	SPM	2	1532	-	13,13,13	0.11	0	12,12,12	0.06	0
36	SPM	2	1505	-	13,13,13	0.07	0	12,12,12	0.21	0
36	SPM	2	1536	-	13,13,13	0.12	0	12,12,12	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	SPM	2	1539	-	13,13,13	0.09	0	12,12,12	0.12	0
36	SPM	2	1503	-	13,13,13	0.08	0	12,12,12	0.17	0
36	SPM	2	1504	-	13,13,13	0.08	0	12,12,12	0.10	0
36	SPM	2	1524	-	13,13,13	0.11	0	12,12,12	0.13	0
36	SPM	2	1525	-	13,13,13	0.08	0	12,12,12	0.16	0
36	SPM	2	1535	-	13,13,13	0.12	0	12,12,12	0.07	0
36	SPM	2	1515	-	13,13,13	0.08	0	12,12,12	0.12	0
36	SPM	2	1508	-	13,13,13	0.06	0	12,12,12	0.12	0
36	SPM	2	1507	-	13,13,13	0.08	0	12,12,12	0.12	0
36	SPM	2	1514	-	13,13,13	0.10	0	12,12,12	0.09	0
36	SPM	2	1506	-	13,13,13	0.09	0	12,12,12	0.10	0
36	SPM	2	1530	-	13,13,13	0.09	0	12,12,12	0.12	0
36	SPM	2	1529	-	13,13,13	0.12	0	12,12,12	0.06	0
36	SPM	2	1510	-	13,13,13	0.08	0	12,12,12	0.17	0
36	SPM	2	1513	-	13,13,13	0.09	0	12,12,12	0.19	0
36	SPM	2	1526	-	13,13,13	0.11	0	12,12,12	0.11	0
36	SPM	2	1538	-	13,13,13	0.09	0	12,12,12	0.14	0
36	SPM	2	1512	-	13,13,13	0.11	0	12,12,12	0.09	0
36	SPM	2	1528	-	13,13,13	0.11	0	12,12,12	0.09	0
39	GTP	5	102	34	30,34,34	0.83	1 (3%)	46,54,54	1.72	11 (23%)
36	SPM	2	1520	-	13,13,13	0.11	0	12,12,12	0.14	0
36	SPM	2	1523	-	13,13,13	0.08	0	12,12,12	0.19	0
36	SPM	2	1511	-	13,13,13	0.07	0	12,12,12	0.11	0
36	SPM	2	1531	-	13,13,13	0.09	0	12,12,12	0.09	0
36	SPM	2	1533	-	13,13,13	0.11	0	12,12,12	0.08	0
36	SPM	2	1537	-	13,13,13	0.13	0	12,12,12	0.11	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
36	SPM	2	1521	-	-	7/11/11/11	-
36	SPM	2	1522	-	-	2/11/11/11	-
36	SPM	2	1516	-	-	0/11/11/11	-
36	SPM	2	1519	-	-	2/11/11/11	-
36	SPM	2	1527	-	-	3/11/11/11	-
36	SPM	2	1502	-	-	11/11/11/11	-
36	SPM	2	1517	-	-	4/11/11/11	-
36	SPM	2	1534	-	-	9/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SPM	2	1509	-	-	2/11/11/11	-
36	SPM	2	1518	-	-	4/11/11/11	-
36	SPM	2	1501	-	-	2/11/11/11	-
36	SPM	2	1532	-	-	9/11/11/11	-
36	SPM	2	1505	-	-	4/11/11/11	-
36	SPM	2	1536	-	-	1/11/11/11	-
36	SPM	2	1539	-	-	2/11/11/11	-
36	SPM	2	1503	-	-	3/11/11/11	-
36	SPM	2	1504	-	-	2/11/11/11	-
36	SPM	2	1524	-	-	3/11/11/11	-
36	SPM	2	1525	-	-	1/11/11/11	-
36	SPM	2	1535	-	-	5/11/11/11	-
36	SPM	2	1515	-	-	2/11/11/11	-
36	SPM	2	1508	-	-	2/11/11/11	-
36	SPM	2	1507	-	-	4/11/11/11	-
36	SPM	2	1514	-	-	3/11/11/11	-
36	SPM	2	1506	-	-	4/11/11/11	-
36	SPM	2	1530	-	-	4/11/11/11	-
36	SPM	2	1529	-	-	6/11/11/11	-
36	SPM	2	1510	-	-	1/11/11/11	-
36	SPM	2	1513	-	-	1/11/11/11	-
36	SPM	2	1526	-	-	4/11/11/11	-
36	SPM	2	1538	-	-	5/11/11/11	-
36	SPM	2	1512	-	-	3/11/11/11	-
36	SPM	2	1528	-	-	4/11/11/11	-
39	GTP	5	102	34	-	6/22/38/38	0/3/3/3
36	SPM	2	1520	-	-	4/11/11/11	-
36	SPM	2	1523	-	-	4/11/11/11	-
36	SPM	2	1511	-	-	2/11/11/11	-
36	SPM	2	1531	-	-	2/11/11/11	-
36	SPM	2	1533	-	-	1/11/11/11	-
36	SPM	2	1537	-	-	2/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	5	102	GTP	C2-N3	2.20	1.38	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	5	102	GTP	C5-C4-N3	-4.91	120.50	128.46
39	5	102	GTP	C2-N3-C4	4.41	120.16	112.30
39	5	102	GTP	PB-O3B-PG	-3.30	121.50	132.83
39	5	102	GTP	PA-O3A-PB	-3.25	121.67	132.83
39	5	102	GTP	N9-C4-N3	3.18	132.31	125.94
39	5	102	GTP	C2-N1-C6	-2.84	119.92	125.10
39	5	102	GTP	N9-C8-N7	-2.63	108.44	113.39
39	5	102	GTP	C2'-C1'-N9	-2.58	105.91	113.22
39	5	102	GTP	C5-C6-N1	2.50	119.55	113.19
39	5	102	GTP	C8-N7-C5	2.46	108.69	104.24
39	5	102	GTP	O6-C6-C5	-2.35	120.36	126.60

There are no chirality outliers.

All (140) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	2	1509	SPM	C12-C11-N10-C9
36	2	1520	SPM	C12-C11-N10-C9
36	2	1524	SPM	C3-C4-N5-C6
36	2	1525	SPM	C3-C4-N5-C6
36	2	1533	SPM	C7-C6-N5-C4
39	5	102	GTP	C5'-O5'-PA-O1A
36	2	1502	SPM	N5-C6-C7-C8
36	2	1507	SPM	C7-C8-C9-N10
36	2	1521	SPM	C7-C8-C9-N10
36	2	1528	SPM	C3-C4-N5-C6
36	2	1529	SPM	N5-C6-C7-C8
39	5	102	GTP	C3'-C4'-C5'-O5'
36	2	1517	SPM	N10-C11-C12-C13
36	2	1532	SPM	N5-C6-C7-C8
36	2	1532	SPM	C7-C8-C9-N10
36	2	1502	SPM	C7-C8-C9-N10
36	2	1502	SPM	N10-C11-C12-C13
36	2	1521	SPM	N5-C6-C7-C8
36	2	1532	SPM	N10-C11-C12-C13
36	2	1501	SPM	C8-C9-N10-C11
36	2	1503	SPM	C8-C9-N10-C11

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Mol	Chain	Res	Type	Atoms
36	2	1512	SPM	C7-C6-N5-C4
36	2	1517	SPM	C3-C4-N5-C6
36	2	1519	SPM	C8-C9-N10-C11
36	2	1520	SPM	C8-C9-N10-C11
36	2	1522	SPM	C8-C9-N10-C11
36	2	1523	SPM	C7-C6-N5-C4
36	2	1535	SPM	C3-C4-N5-C6
39	5	102	GTP	O4'-C4'-C5'-O5'
36	2	1529	SPM	C2-C3-C4-N5
36	2	1502	SPM	C3-C4-N5-C6
36	2	1506	SPM	C3-C4-N5-C6
36	2	1507	SPM	C12-C11-N10-C9
36	2	1514	SPM	C8-C9-N10-C11
36	2	1517	SPM	C8-C9-N10-C11
36	2	1518	SPM	C3-C4-N5-C6
36	2	1520	SPM	C3-C4-N5-C6
36	2	1521	SPM	C7-C6-N5-C4
36	2	1522	SPM	C7-C6-N5-C4
36	2	1524	SPM	C8-C9-N10-C11
36	2	1527	SPM	C8-C9-N10-C11
36	2	1538	SPM	C8-C9-N10-C11
36	2	1529	SPM	C6-C7-C8-C9
36	2	1518	SPM	C7-C6-N5-C4
36	2	1521	SPM	C3-C4-N5-C6
36	2	1536	SPM	C3-C4-N5-C6
36	2	1534	SPM	C6-C7-C8-C9
36	2	1532	SPM	C6-C7-C8-C9
36	2	1521	SPM	C6-C7-C8-C9
36	2	1502	SPM	C2-C3-C4-N5
36	2	1512	SPM	C12-C11-N10-C9
36	2	1515	SPM	C8-C9-N10-C11
36	2	1527	SPM	C12-C11-N10-C9
36	2	1528	SPM	C7-C6-N5-C4
36	2	1528	SPM	C8-C9-N10-C11
36	2	1530	SPM	C3-C4-N5-C6
36	2	1531	SPM	C7-C6-N5-C4
36	2	1539	SPM	C3-C4-N5-C6
36	2	1523	SPM	C6-C7-C8-C9
36	2	1502	SPM	C11-C12-C13-N14
36	2	1521	SPM	C11-C12-C13-N14
36	2	1523	SPM	C11-C12-C13-N14
36	2	1502	SPM	C8-C9-N10-C11

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Mol	Chain	Res	Type	Atoms
36	2	1506	SPM	C12-C11-N10-C9
36	2	1535	SPM	C6-C7-C8-C9
36	2	1514	SPM	C3-C4-N5-C6
36	2	1532	SPM	C7-C6-N5-C4
36	2	1508	SPM	C3-C4-N5-C6
36	2	1529	SPM	C7-C6-N5-C4
36	2	1534	SPM	C7-C8-C9-N10
36	2	1502	SPM	C7-C6-N5-C4
36	2	1505	SPM	C12-C11-N10-C9
36	2	1509	SPM	C8-C9-N10-C11
36	2	1511	SPM	C12-C11-N10-C9
36	2	1512	SPM	C3-C4-N5-C6
36	2	1518	SPM	C8-C9-N10-C11
36	2	1526	SPM	C8-C9-N10-C11
36	2	1534	SPM	C7-C6-N5-C4
36	2	1538	SPM	C3-C4-N5-C6
36	2	1521	SPM	N1-C2-C3-C4
36	2	1529	SPM	N1-C2-C3-C4
36	2	1532	SPM	N1-C2-C3-C4
36	2	1534	SPM	C11-C12-C13-N14
39	5	102	GTP	C5'-O5'-PA-O3A
36	2	1514	SPM	C12-C11-N10-C9
36	2	1534	SPM	C12-C11-N10-C9
39	5	102	GTP	C5'-O5'-PA-O2A
36	2	1503	SPM	C12-C11-N10-C9
36	2	1507	SPM	C8-C9-N10-C11
36	2	1528	SPM	C12-C11-N10-C9
36	2	1530	SPM	C7-C6-N5-C4
36	2	1531	SPM	C8-C9-N10-C11
36	2	1535	SPM	C12-C11-N10-C9
36	2	1532	SPM	C2-C3-C4-N5
36	2	1524	SPM	C7-C6-N5-C4
36	2	1505	SPM	C7-C6-N5-C4
36	2	1510	SPM	C3-C4-N5-C6
36	2	1513	SPM	C8-C9-N10-C11
36	2	1535	SPM	N10-C11-C12-C13
36	2	1508	SPM	C12-C11-N10-C9
36	2	1517	SPM	C7-C6-N5-C4
36	2	1527	SPM	C3-C4-N5-C6
36	2	1537	SPM	C7-C6-N5-C4
36	2	1538	SPM	C12-C11-N10-C9
36	2	1534	SPM	C2-C3-C4-N5

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Mol	Chain	Res	Type	Atoms
36	2	1526	SPM	C3-C4-N5-C6
36	2	1539	SPM	C7-C6-N5-C4
36	2	1502	SPM	N1-C2-C3-C4
36	2	1532	SPM	C11-C12-C13-N14
36	2	1534	SPM	N1-C2-C3-C4
36	2	1503	SPM	C3-C4-N5-C6
36	2	1506	SPM	C8-C9-N10-C11
36	2	1511	SPM	C3-C4-N5-C6
36	2	1530	SPM	C8-C9-N10-C11
36	2	1532	SPM	C3-C4-N5-C6
36	2	1534	SPM	C3-C4-N5-C6
36	2	1505	SPM	C8-C9-N10-C11
36	2	1515	SPM	C7-C6-N5-C4
36	2	1526	SPM	C12-C11-N10-C9
36	2	1535	SPM	C8-C9-N10-C11
36	2	1505	SPM	C7-C8-C9-N10
36	2	1506	SPM	C6-C7-C8-C9
36	2	1502	SPM	C6-C7-C8-C9
36	2	1501	SPM	C12-C11-N10-C9
36	2	1537	SPM	C12-C11-N10-C9
36	2	1538	SPM	C6-C7-C8-C9
36	2	1504	SPM	C8-C9-N10-C11
36	2	1507	SPM	C3-C4-N5-C6
36	2	1519	SPM	C3-C4-N5-C6
36	2	1526	SPM	C7-C6-N5-C4
36	2	1529	SPM	C8-C9-N10-C11
36	2	1530	SPM	C12-C11-N10-C9
36	2	1518	SPM	C6-C7-C8-C9
39	5	102	GTP	PG-O3B-PB-O2B
36	2	1520	SPM	C6-C7-C8-C9
36	2	1502	SPM	C12-C11-N10-C9
36	2	1523	SPM	C8-C9-N10-C11
36	2	1534	SPM	C8-C9-N10-C11
36	2	1504	SPM	C6-C7-C8-C9
36	2	1538	SPM	N5-C6-C7-C8

There are no ring outliers.

32 monomers are involved in 82 short contacts:

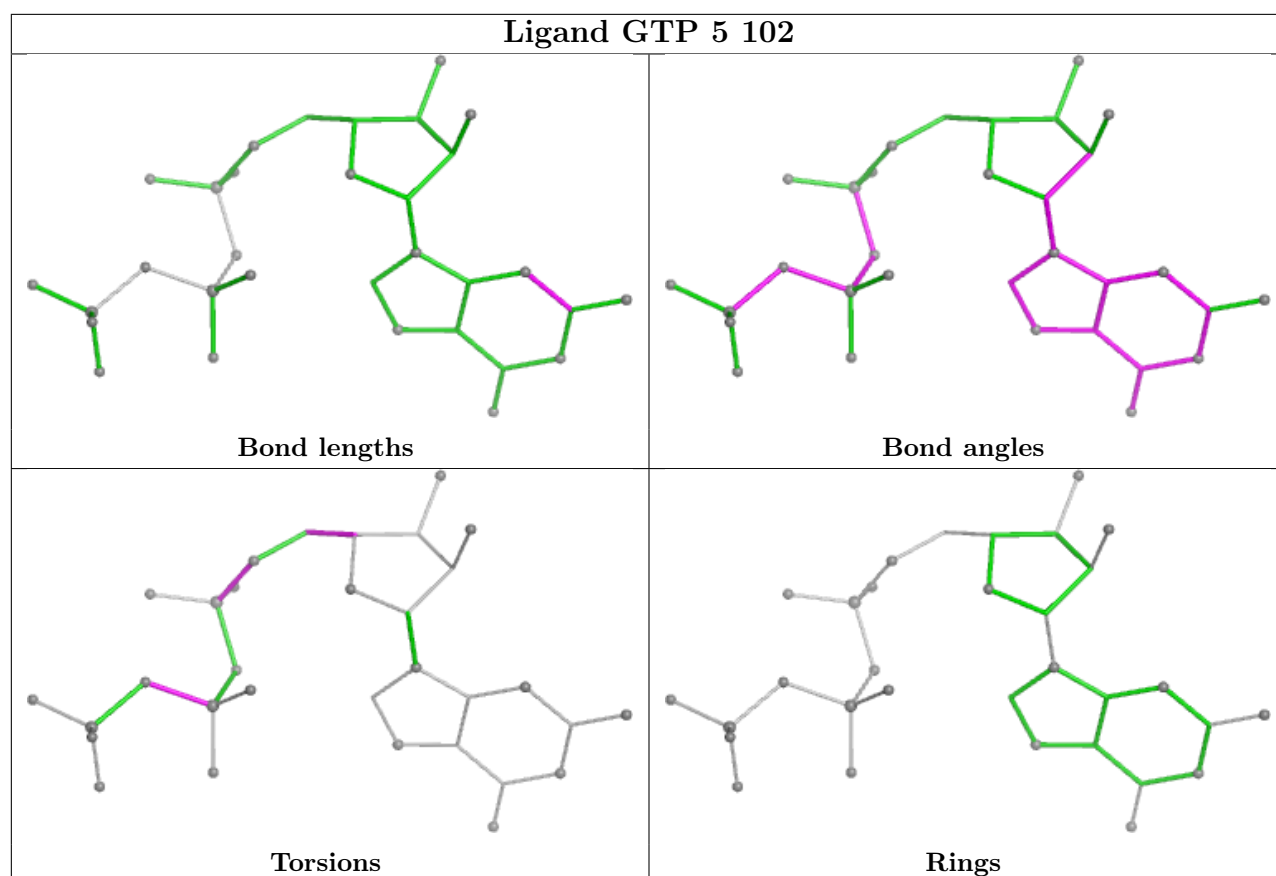
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	2	1521	SPM	8	0
36	2	1522	SPM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	2	1516	SPM	5	0
36	2	1527	SPM	2	0
36	2	1502	SPM	2	0
36	2	1517	SPM	3	0
36	2	1534	SPM	4	0
36	2	1509	SPM	1	0
36	2	1518	SPM	2	0
36	2	1501	SPM	2	0
36	2	1532	SPM	9	0
36	2	1524	SPM	3	0
36	2	1525	SPM	4	0
36	2	1535	SPM	8	0
36	2	1515	SPM	2	0
36	2	1507	SPM	1	0
36	2	1514	SPM	3	0
36	2	1530	SPM	2	0
36	2	1529	SPM	2	0
36	2	1510	SPM	1	0
36	2	1513	SPM	2	0
36	2	1526	SPM	2	0
36	2	1538	SPM	2	0
36	2	1512	SPM	1	0
36	2	1528	SPM	1	0
39	5	102	GTP	1	0
36	2	1520	SPM	3	0
36	2	1523	SPM	1	0
36	2	1511	SPM	1	0
36	2	1531	SPM	1	0
36	2	1533	SPM	1	0
36	2	1537	SPM	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

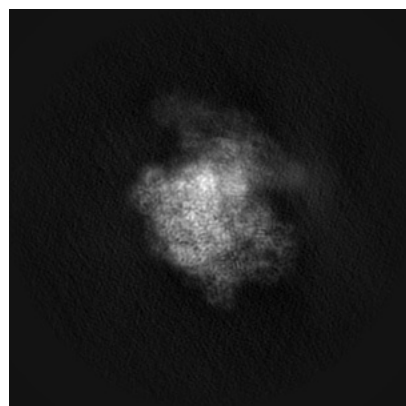
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50724. These allow visual inspection of the internal detail of the map and identification of artifacts.

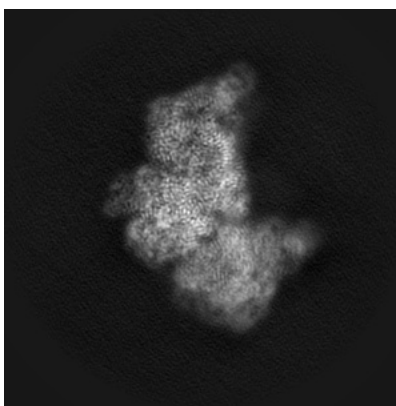
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

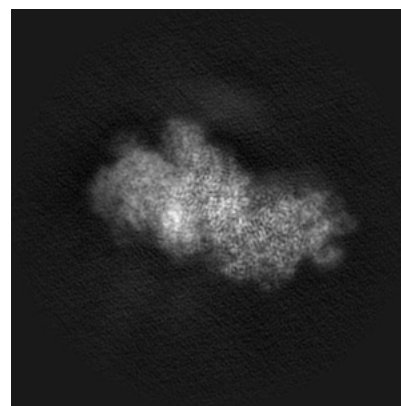
6.1.1 Primary map



X

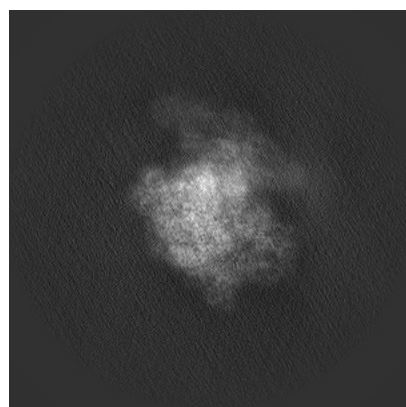


Y

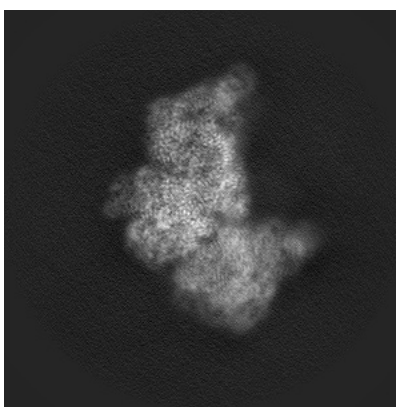


Z

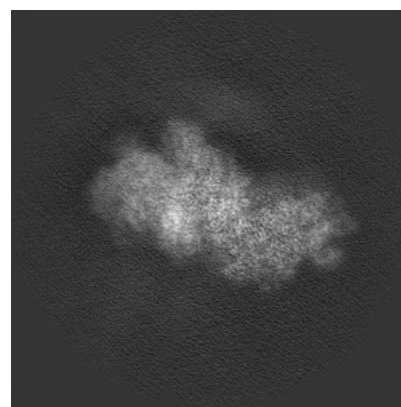
6.1.2 Raw map



X



Y

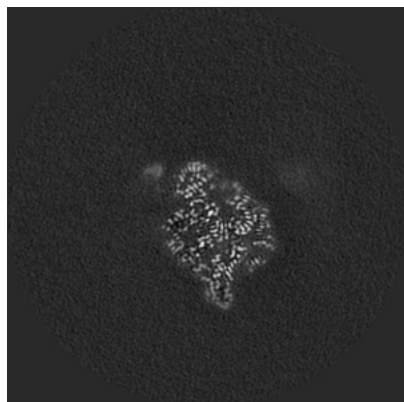


Z

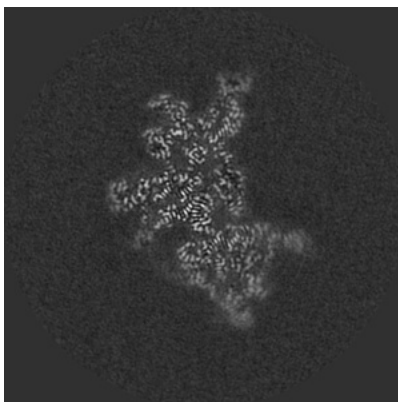
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

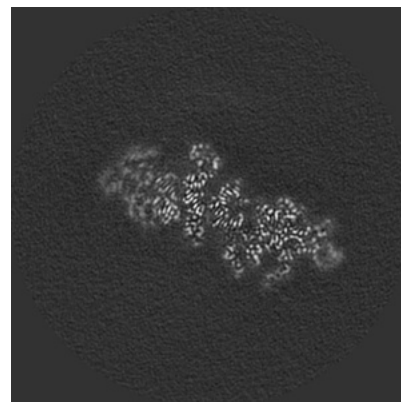
6.2.1 Primary map



X Index: 258

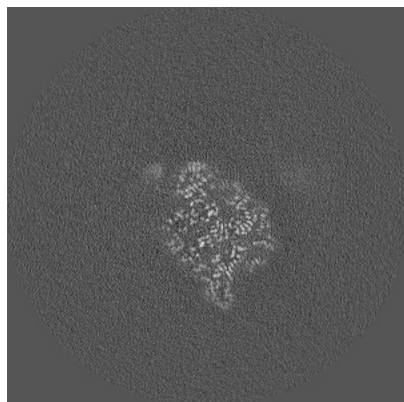


Y Index: 258

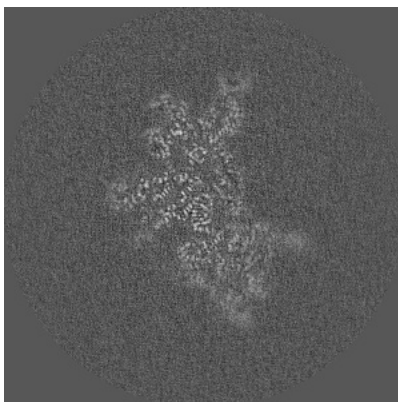


Z Index: 258

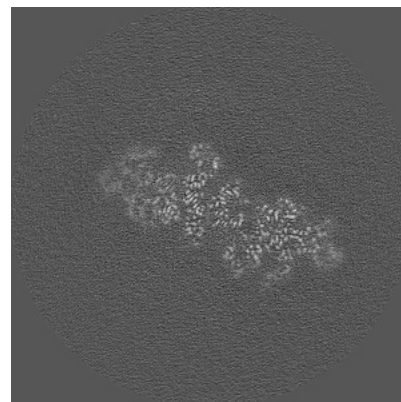
6.2.2 Raw map



X Index: 258



Y Index: 258

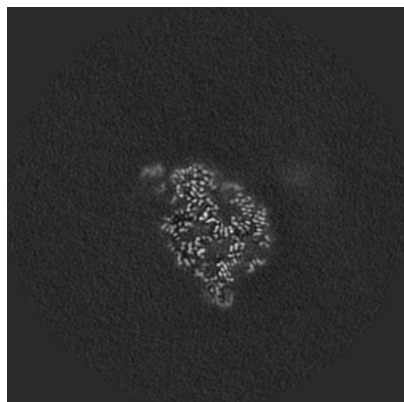


Z Index: 258

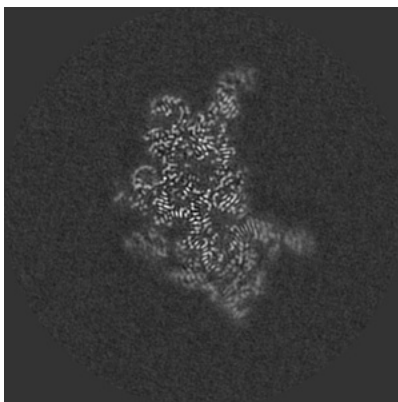
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

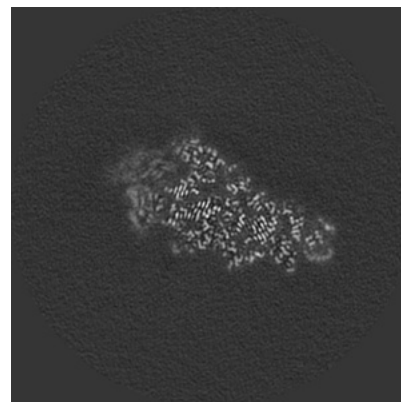
6.3.1 Primary map



X Index: 261

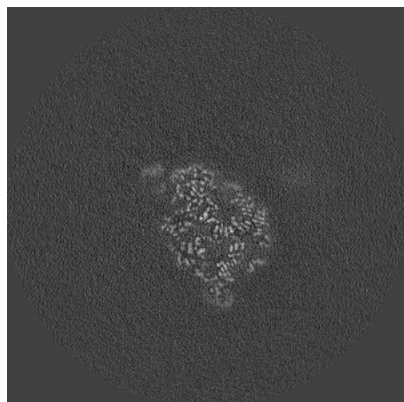


Y Index: 251

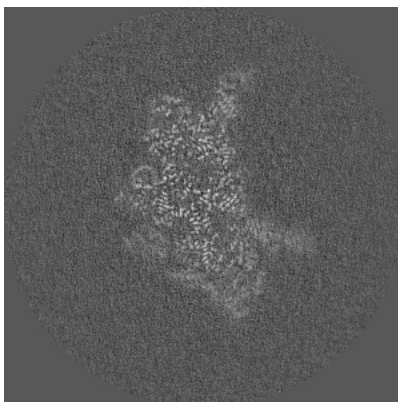


Z Index: 244

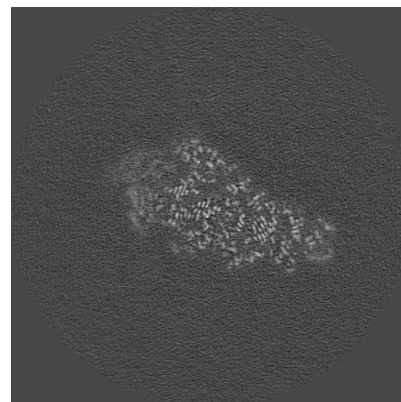
6.3.2 Raw map



X Index: 261



Y Index: 251

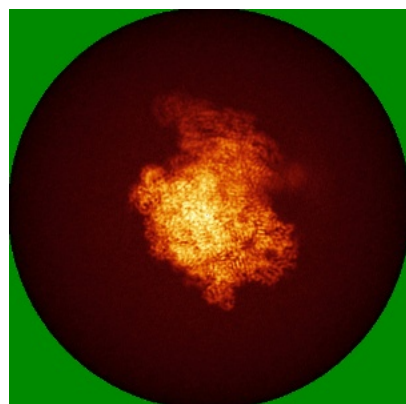


Z Index: 244

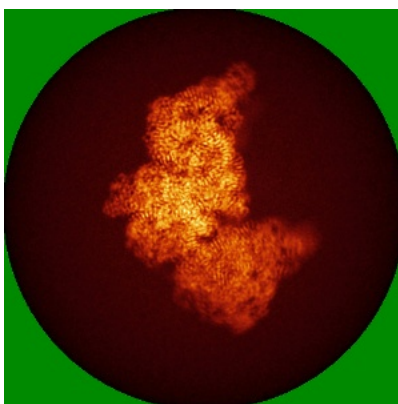
The images above show the largest variance slices of the map in three orthogonal directions.

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

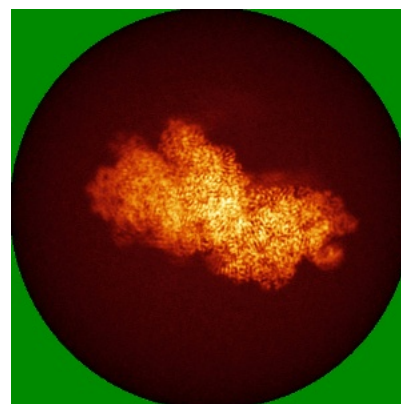
6.4.1 Primary map



X

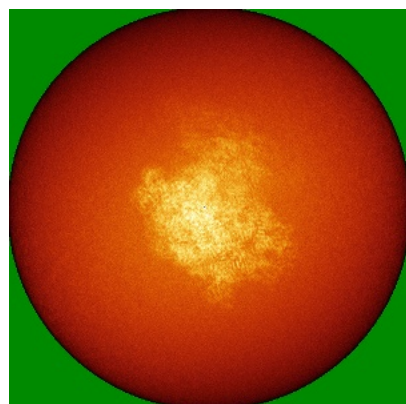


Y

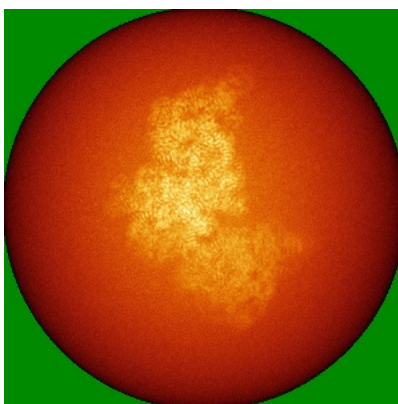


Z

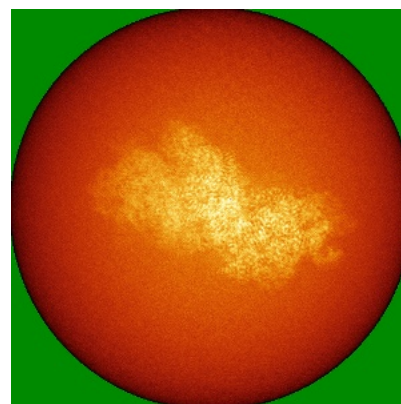
6.4.2 Raw map



X



Y

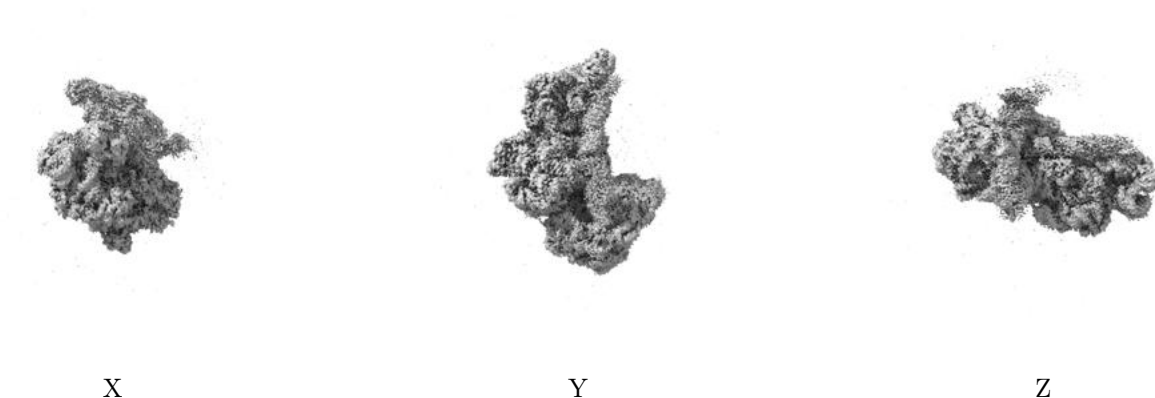


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

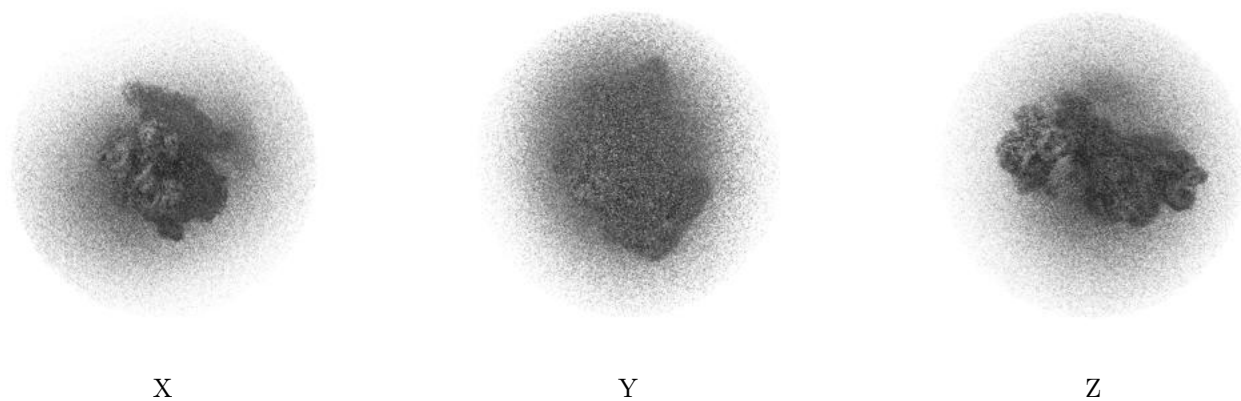
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

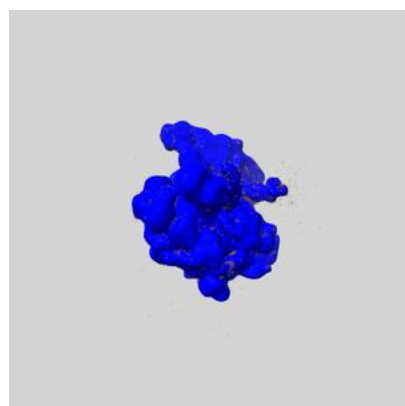
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

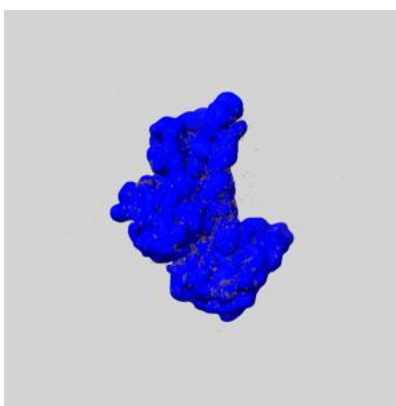
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

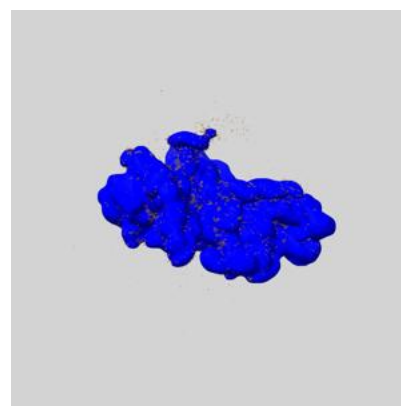
6.6.1 emd_50724_msk_1.map [i](#)



X



Y

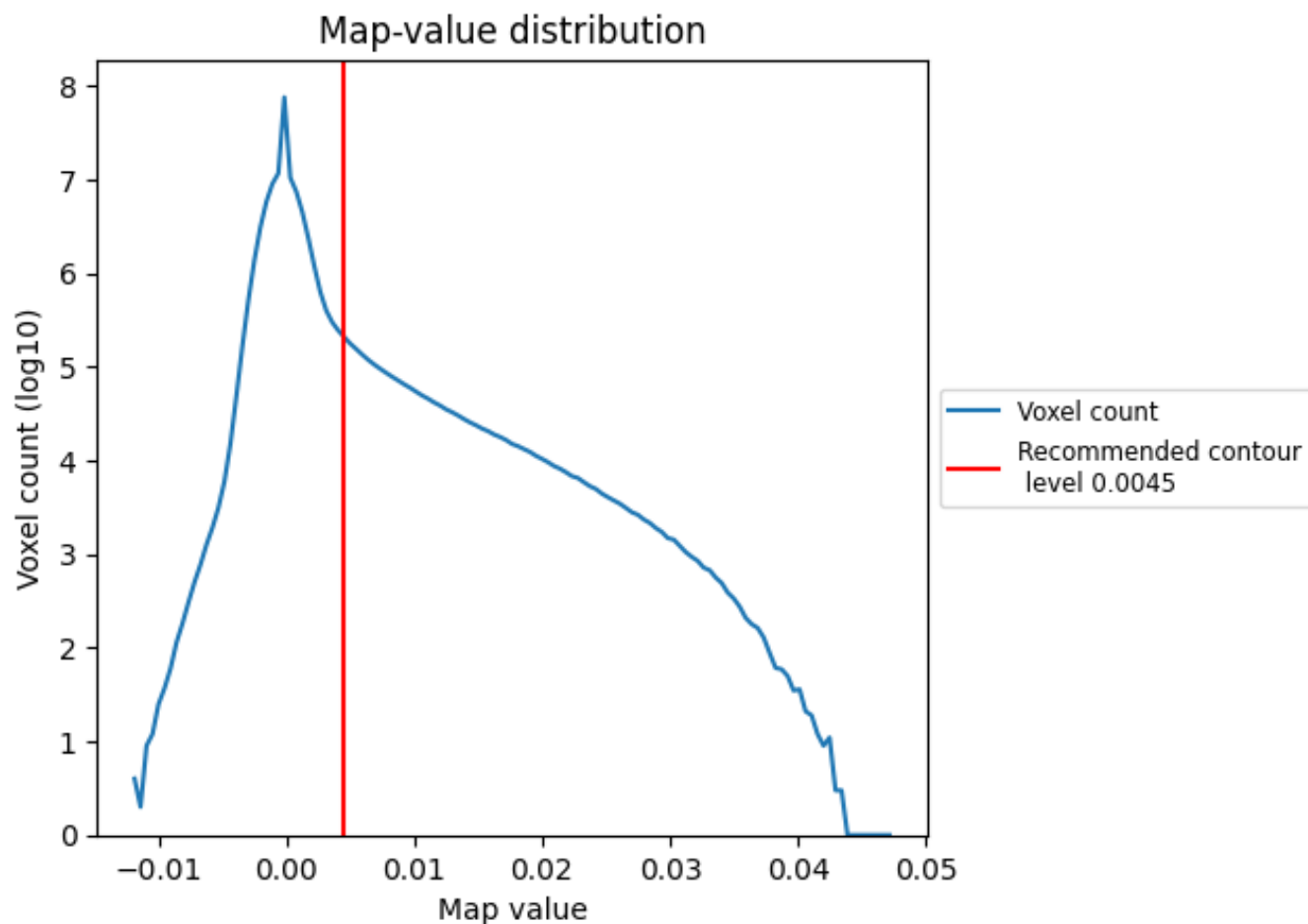


Z

7 Map analysis [i](#)

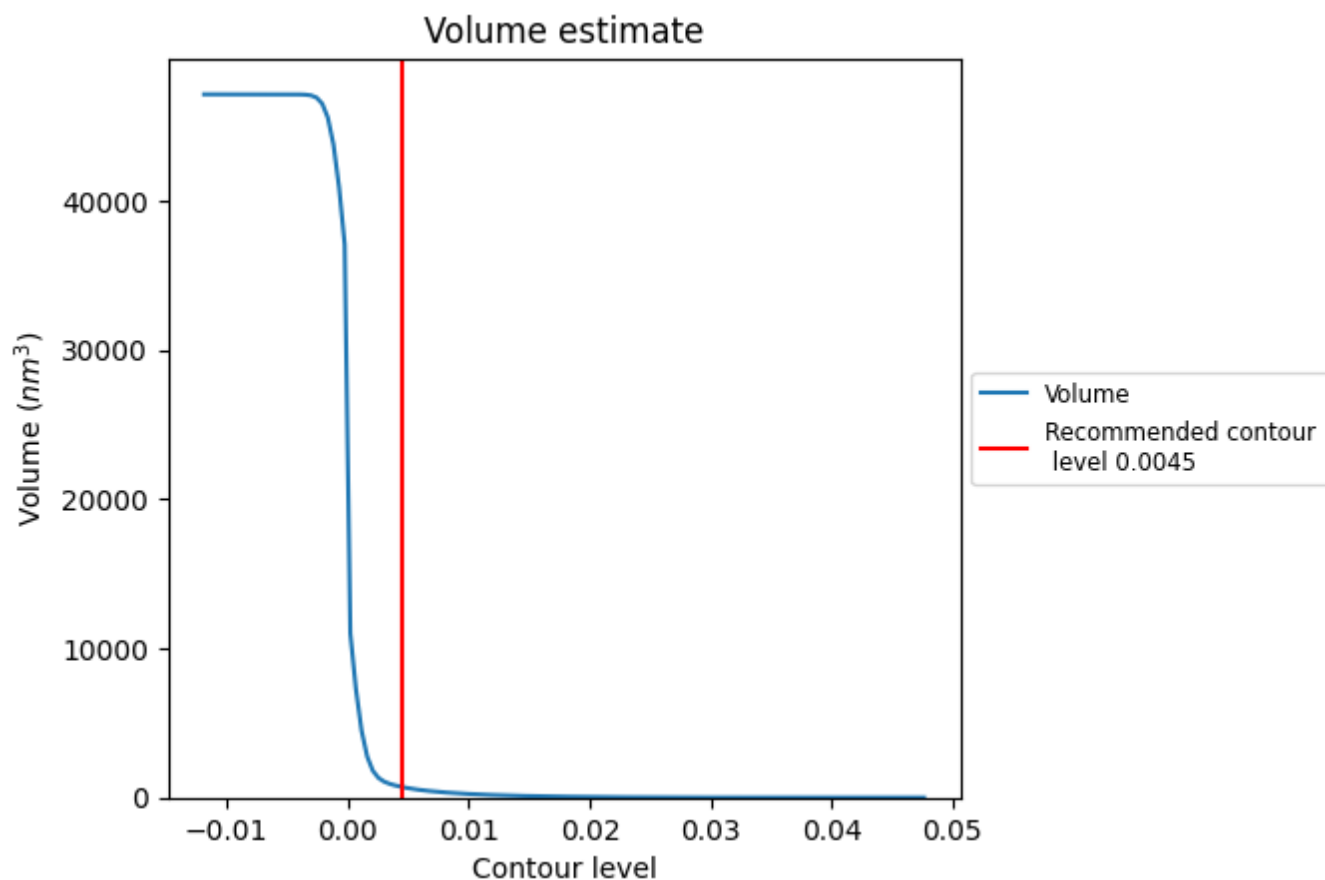
This section contains the results of statistical analysis of the map.

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.

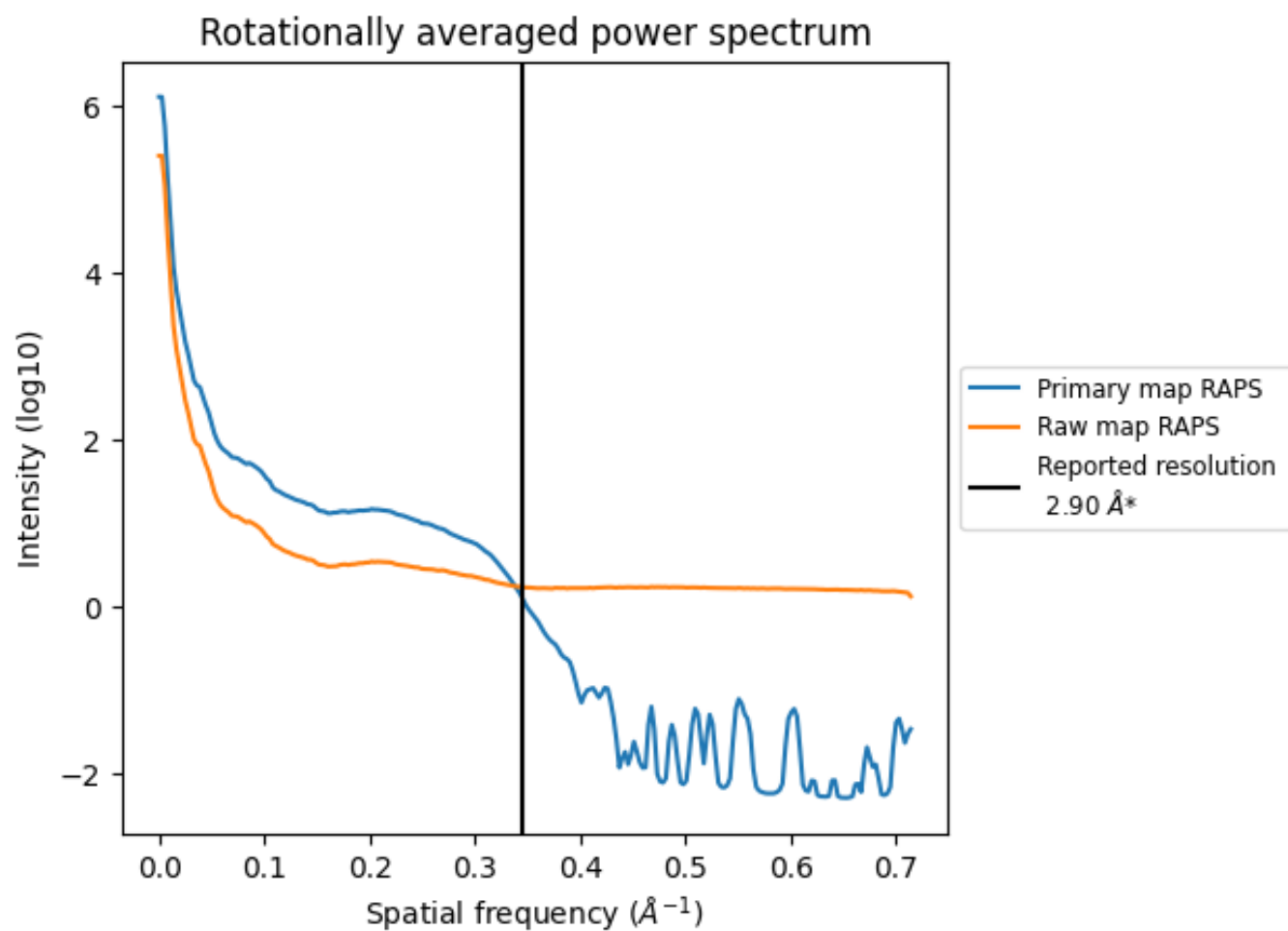
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 709 nm^3 ; this corresponds to an approximate mass of 640 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

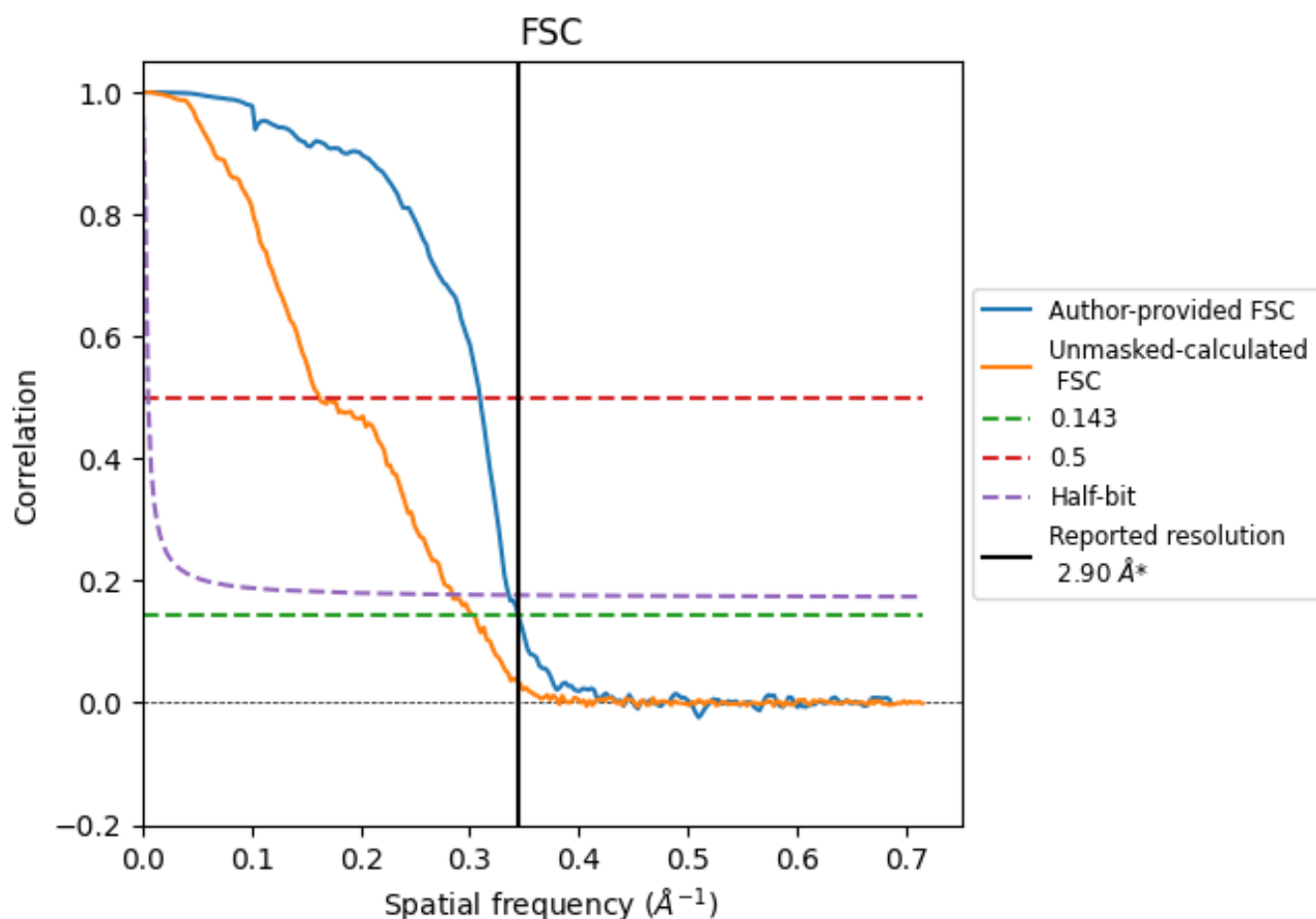


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

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 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

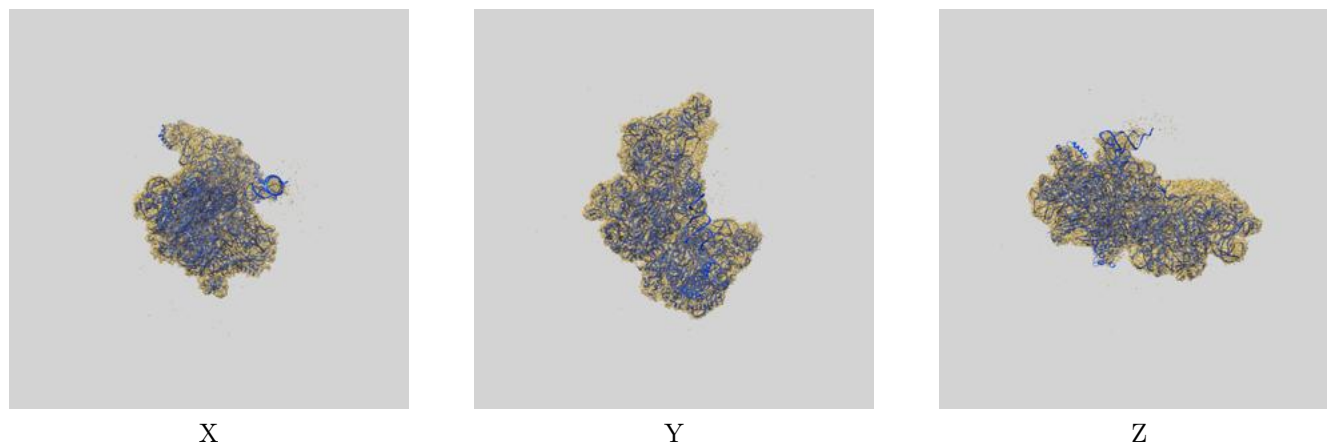
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.23	2.98
Unmasked-calculated*	3.29	6.17	3.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.29 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

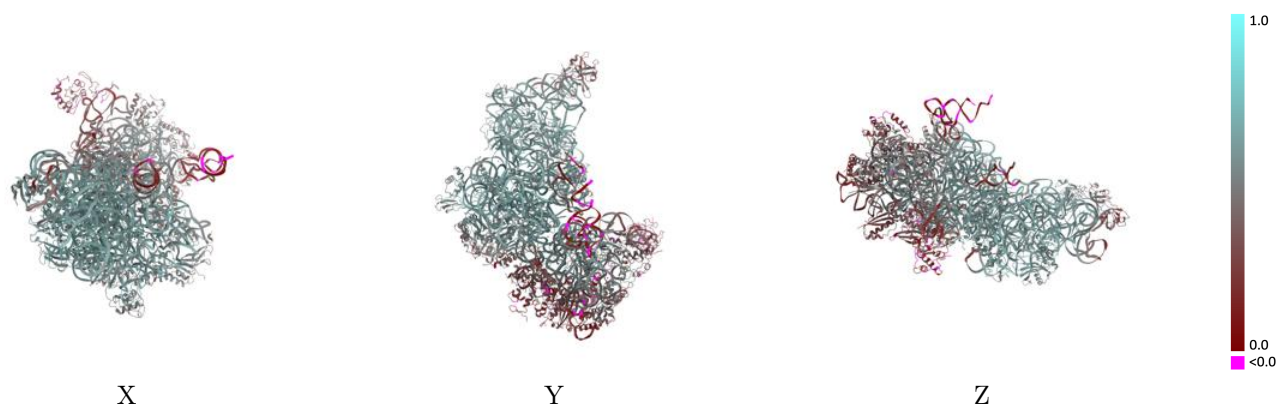
This section contains information regarding the fit between EMDB map EMD-50724 and PDB model 9FS6. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



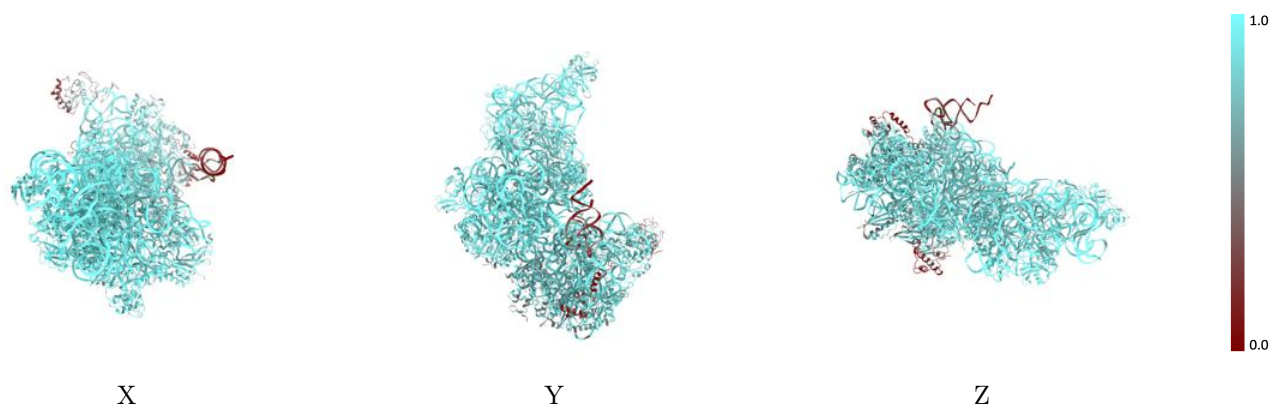
The images above show the 3D surface view of the map at the recommended contour level 0.0045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



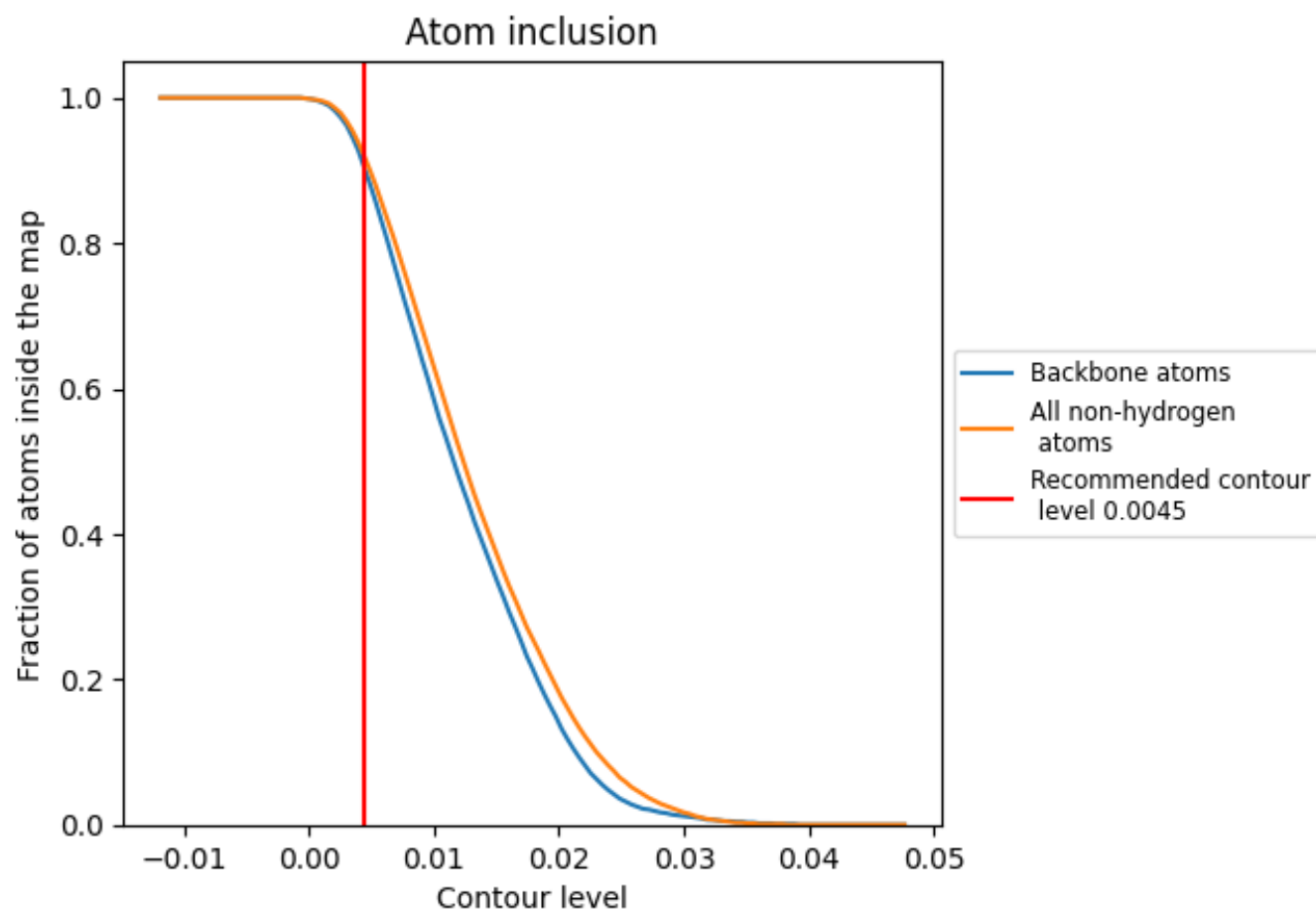
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0045).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 92% 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 (0.0045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.5020
2	 0.9890	 0.5630
3	 0.3250	 0.1480
4	 0.4510	 0.1940
5	 1.0000	 0.5780
A	 0.9260	 0.5060
B	 0.8830	 0.4540
C	 0.9510	 0.5540
D	 0.9700	 0.5900
E	 0.9760	 0.5940
F	 0.9640	 0.5880
G	 0.8990	 0.4210
H	 0.7870	 0.3100
I	 0.9840	 0.6110
J	 0.9660	 0.5680
K	 0.8760	 0.3820
L	 0.7920	 0.3470
M	 0.9120	 0.4910
N	 0.9770	 0.5820
O	 0.8730	 0.4350
P	 0.9810	 0.5110
Q	 0.9540	 0.5440
R	 0.9780	 0.6050
S	 0.8930	 0.3790
T	 0.8490	 0.3970
U	 0.8890	 0.3900
V	 0.9400	 0.5490
W	 0.9530	 0.5480
X	 0.7360	 0.2790
Y	 0.4130	 0.1340
Z	 0.8910	 0.4320
a	 0.8710	 0.3610
b	 0.9090	 0.5140
c	 0.3830	 0.2050
d	 0.7300	 0.2360
e	 0.8370	 0.5300

