



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 03:36 pm BST

PDB ID : 9FY0 / pdb_00009fy0
EMDB ID : EMD-50854
Title : Cryo-EM structure of *Saccharolobus solfataricus* 30S initiation complex bound to Ss-aIF2beta leaderless mRNA
Authors : Bourgeois, G.; Coureux, P.D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2024-07-02
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

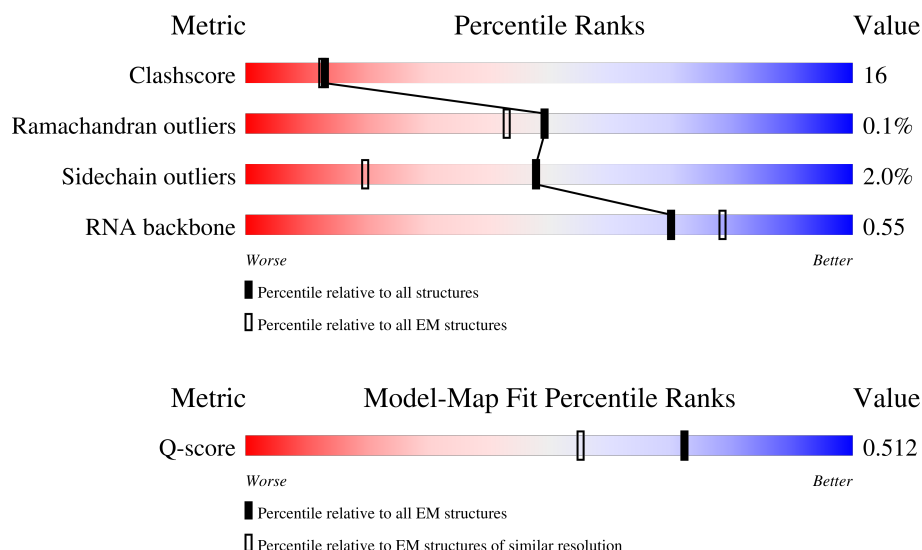
1 Overall quality at a glance i

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	46% 44% 10%
2	A	208	61% 28% 11%
3	B	231	61% 30% 7%

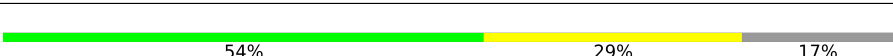
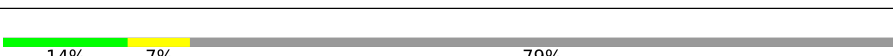
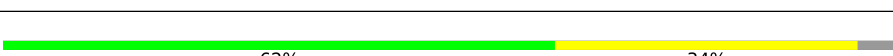
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Mol	Chain	Length	Quality of chain
4	C	65	
5	D	181	
6	E	239	
7	F	214	
8	G	214	
9	H	193	
10	I	133	
11	J	133	
12	K	137	
13	L	102	
14	M	132	
15	N	147	
16	O	165	
17	P	54	
18	Q	152	
19	R	114	
20	S	79	
21	T	140	
22	U	158	
23	V	120	
24	W	66	
25	X	83	
26	Y	75	
27	Z	229	
28	3	127	

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Mol	Chain	Length	Quality of chain
29	a	72	
30	c	110	
31	d	72	
32	e	52	
33	4	77	
34	5	14	
35	b	95	

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	1533	-	-	X	-
36	SPM	2	1540	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 66880 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	1494	Total	C	N	O	P	0	0
			32141	14332	5936	10379	1494		

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	191	Total	C	N	O	S	0	0
			1534	977	281	273	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 uS11.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 20 is a protein called Small ribosomal subunit protein eS17.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 22 is a protein called Small ribosomal subunit protein eS19.

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

- Molecule 23 is a protein called Small ribosomal subunit protein eS24.

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

- Molecule 24 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 25 is a protein called Small ribosomal subunit protein eS28.

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

- Molecule 26 is a protein called Small ribosomal subunit protein eS31.

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

- Molecule 27 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 28 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	117	Total	C	N	O	S	0	0
			893	567	149	175	2		

- Molecule 29 is a protein called aS34.

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

- Molecule 30 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 31 is a protein called aS33.

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

- Molecule 32 is a protein called LSU ribosomal protein S30E (Rps30E).

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

- Molecule 33 is a RNA chain called tRNA met initiator.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	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

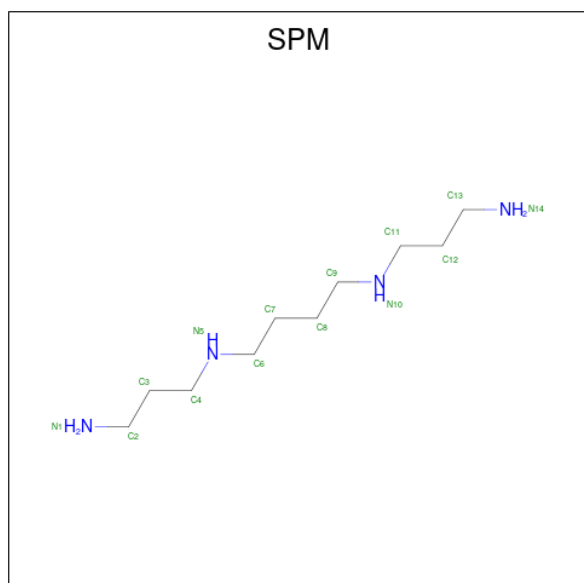
- Molecule 34 is a RNA chain called Ss_aIF2beta mRNA.

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 LSU ribosomal protein S26E (Rps26E).

Mol	Chain	Residues	Atoms						AltConf	Trace
35	b	91	Total	C	N	O	S		0	0
			704	437	134	126	7			

- Molecule 36 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



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	
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	

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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	
36	2	1	Total	C	N	0
			14	10	4	
36	E	1	Total	C	N	0
			14	10	4	

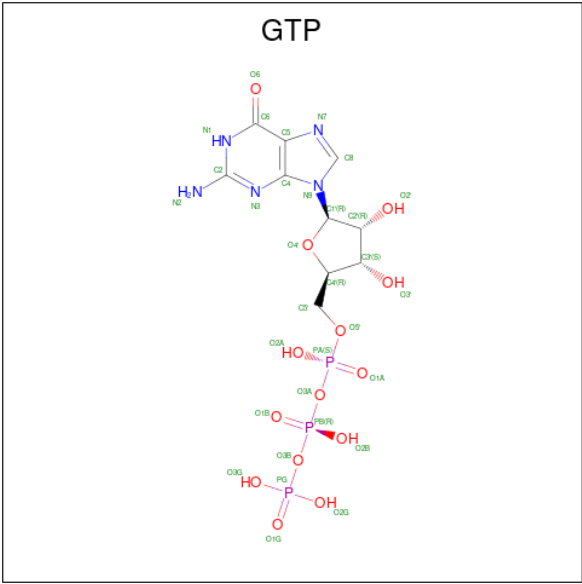
- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	2	46	Total	Mg	0
			46	46	
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	P	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	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	

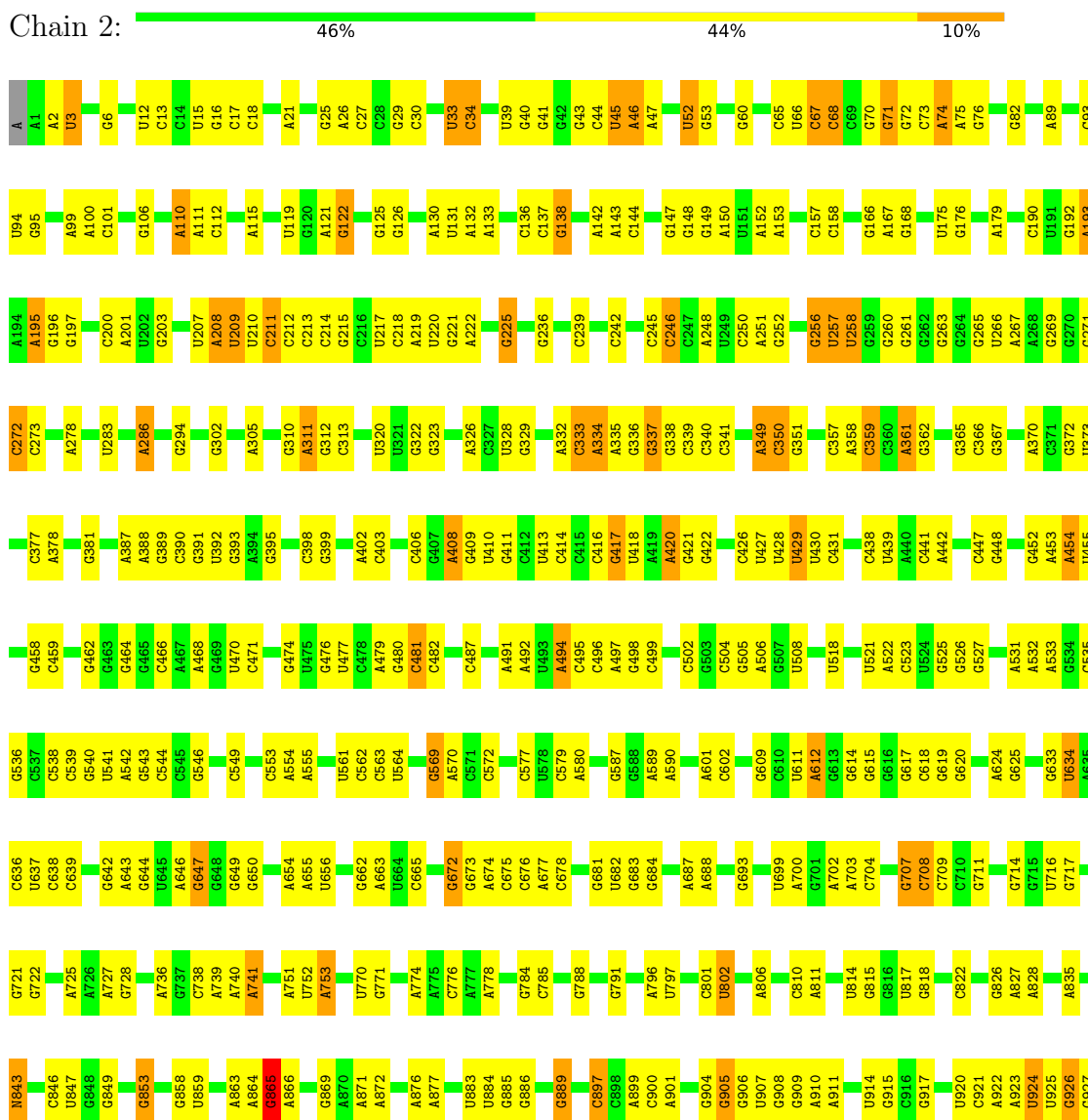
- Molecule 40 is water.

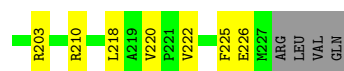
Mol	Chain	Residues	Atoms		AltConf
40	2	240	Total	O	0
			240	240	
40	E	3	Total	O	0
			3	3	
40	F	6	Total	O	0
			6	6	
40	H	1	Total	O	0
			1	1	
40	I	2	Total	O	0
			2	2	
40	J	1	Total	O	0
			1	1	
40	K	5	Total	O	0
			5	5	
40	L	2	Total	O	0
			2	2	
40	O	1	Total	O	0
			1	1	
40	Q	1	Total	O	0
			1	1	
40	R	1	Total	O	0
			1	1	
40	V	1	Total	O	0
			1	1	
40	W	1	Total	O	0
			1	1	
40	4	2	Total	O	0
			2	2	
40	5	3	Total	O	0
			3	3	
40	b	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

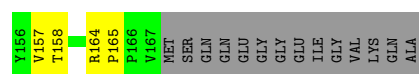




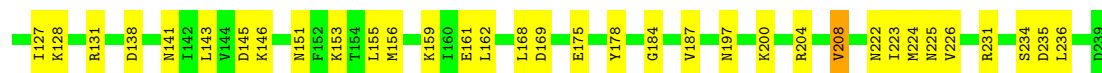
- Molecule 4: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein



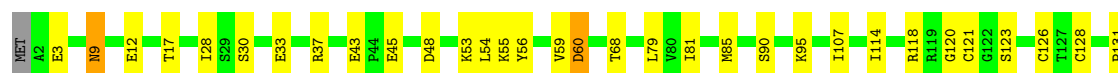
- Molecule 5: Small ribosomal subunit protein uS4



- Molecule 6: Small ribosomal subunit protein eS4

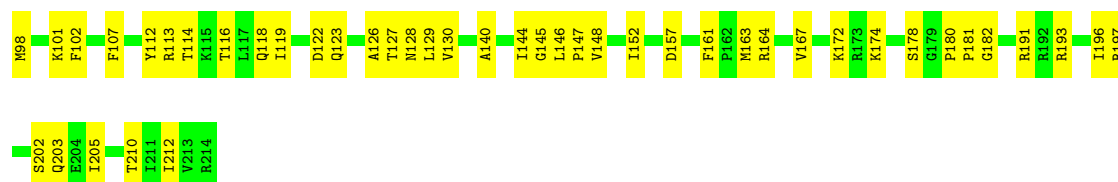


- Molecule 7: Small ribosomal subunit protein uS5



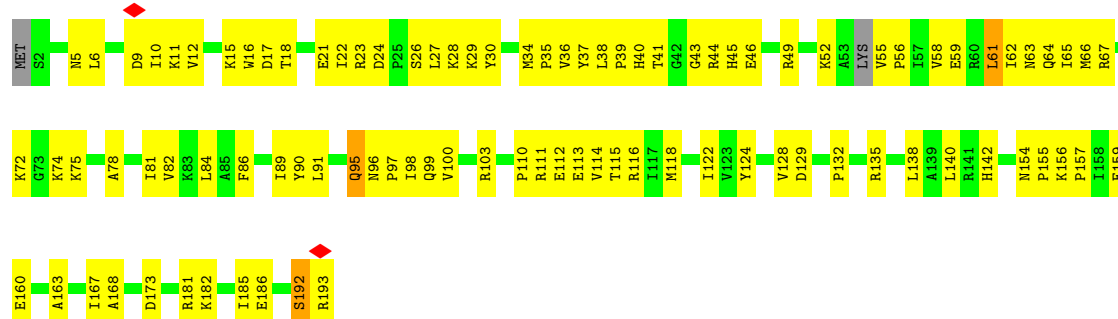
- Molecule 8: Small ribosomal subunit protein eS6





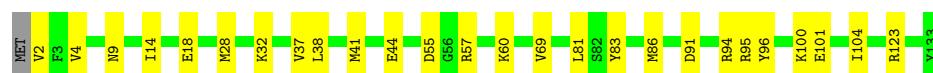
- Molecule 9: Small ribosomal subunit protein uS7

Chain H: 50% 48% ..



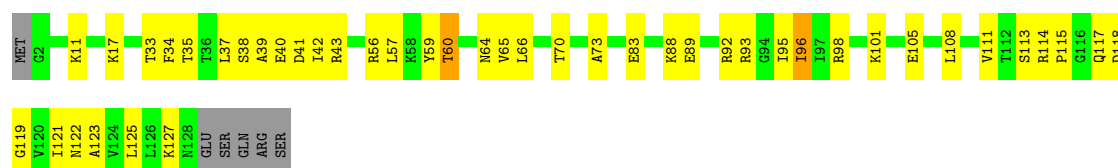
- Molecule 10: Small ribosomal subunit protein uS8

Chain I: 80% 20% .



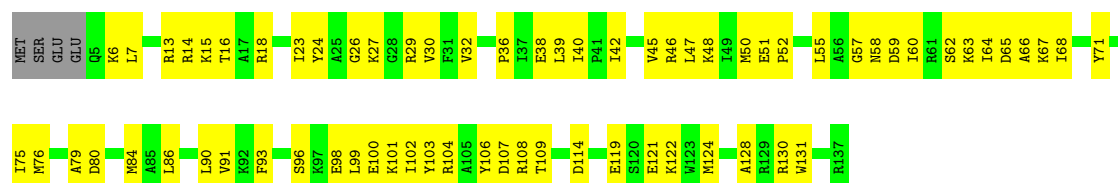
- Molecule 11: Small ribosomal subunit protein eS8

Chain J: 62% 32% 5%

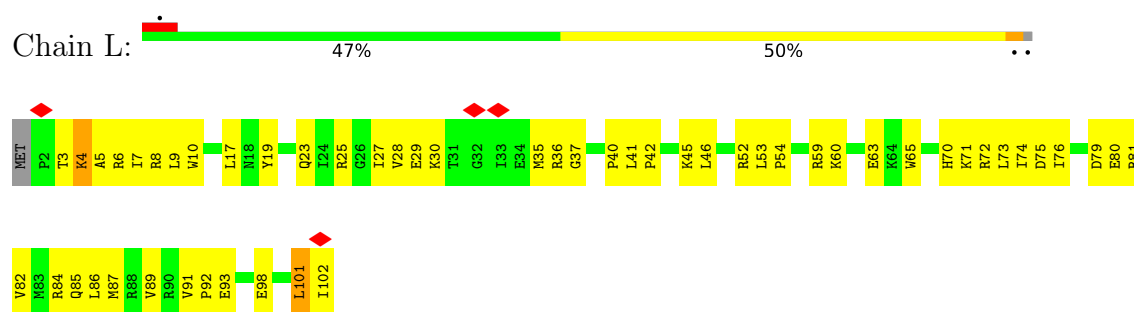


- Molecule 12: Small ribosomal subunit protein uS9

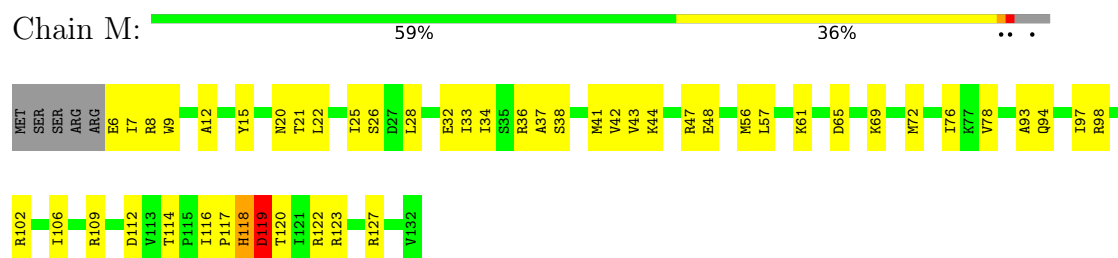
Chain K: 47% 50% .



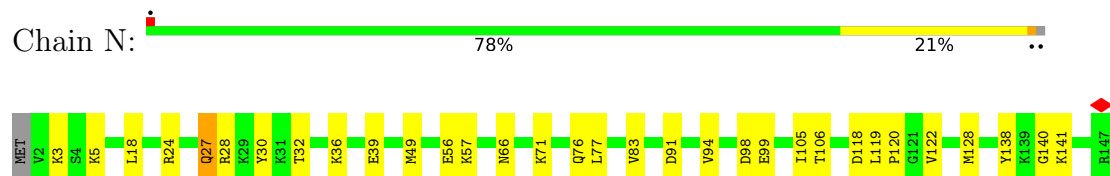
- Molecule 13: Small ribosomal subunit protein uS10



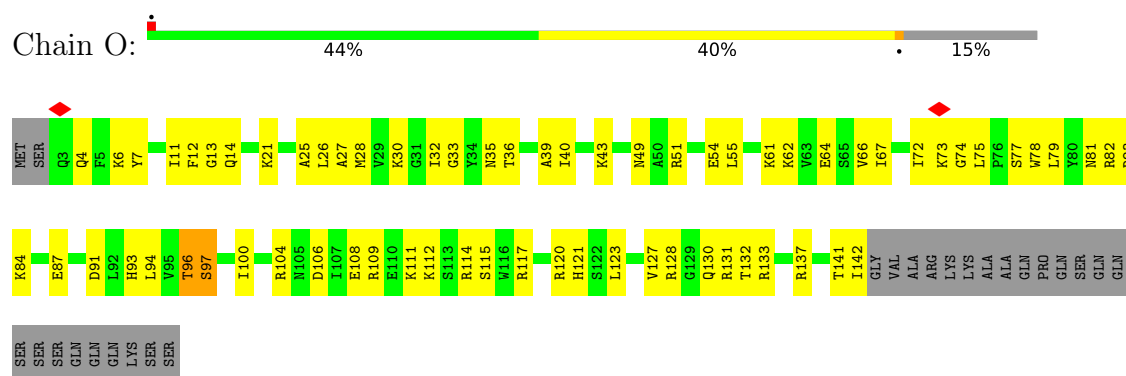
- Molecule 14: Small ribosomal subunit protein uS11



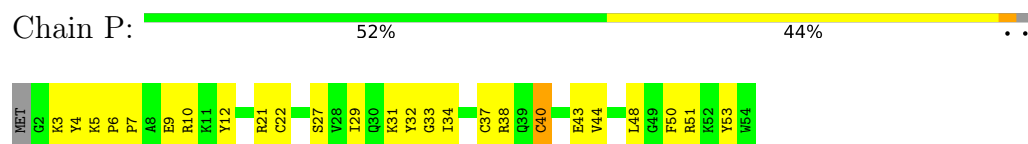
- Molecule 15: Small ribosomal subunit protein uS12



- Molecule 16: Small ribosomal subunit protein uS13

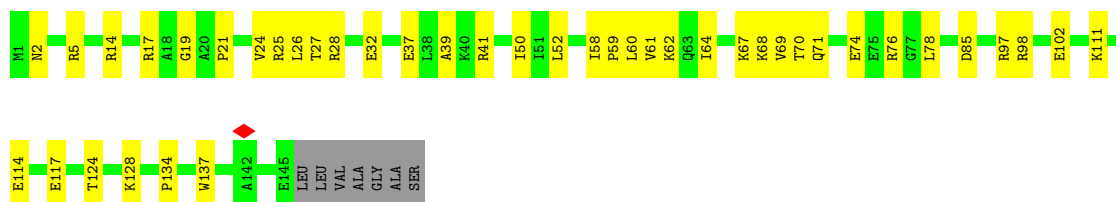


- Molecule 17: Small ribosomal subunit protein uS14

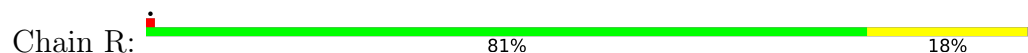


- Molecule 18: Small ribosomal subunit protein uS15





- Molecule 19: Small ribosomal subunit protein uS17



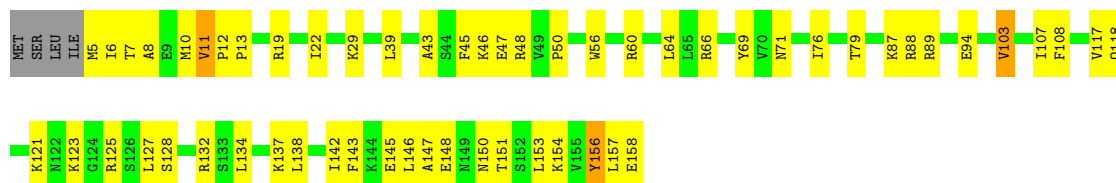
- Molecule 20: Small ribosomal subunit protein eS17



- Molecule 21: Small ribosomal subunit protein uS19

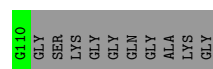


- Molecule 22: Small ribosomal subunit protein eS19



- Molecule 23: Small ribosomal subunit protein eS24





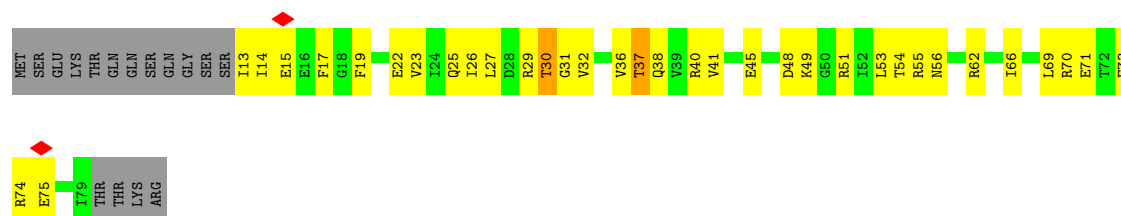
- Molecule 24: Small ribosomal subunit protein eS27

Chain W:  80% 17% ..

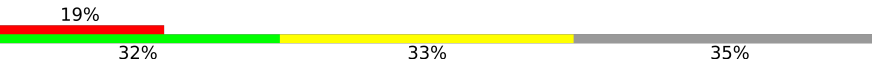


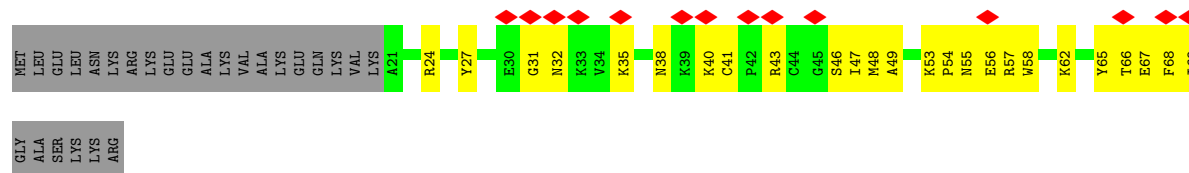
- Molecule 25: Small ribosomal subunit protein eS28

Chain X:  39% 40% 19%



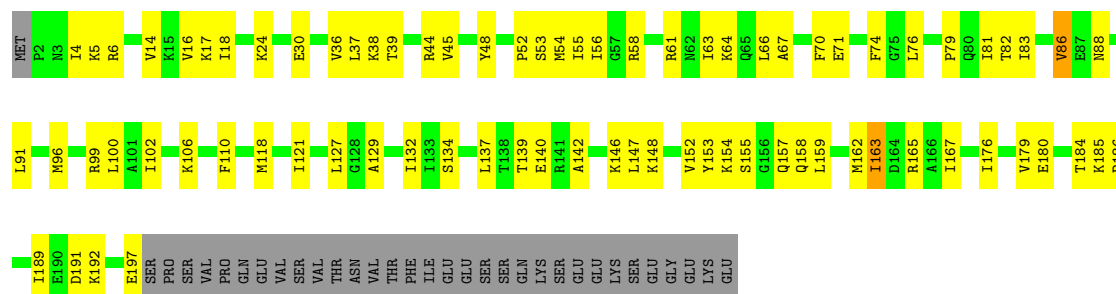
- Molecule 26: Small ribosomal subunit protein eS31

Chain Y:  19% 32% 33% 35%



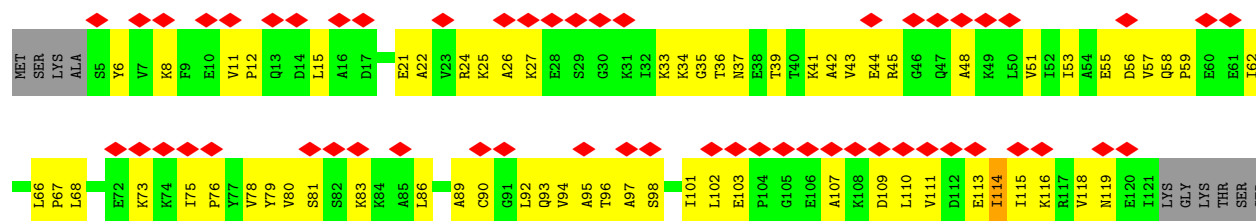
- Molecule 27: Small ribosomal subunit protein uS3

Chain Z:  52% 33% 14%



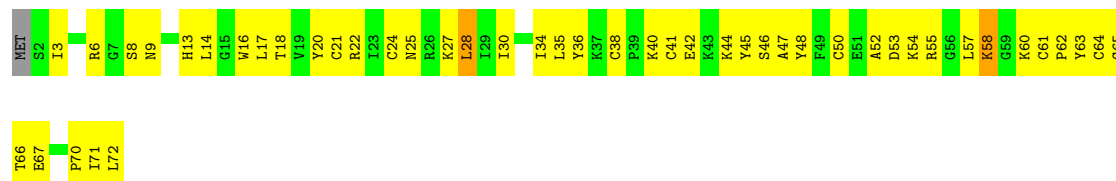
- Molecule 28: Large ribosomal subunit protein eL8

Chain 3:  43% 41% 50% 8%



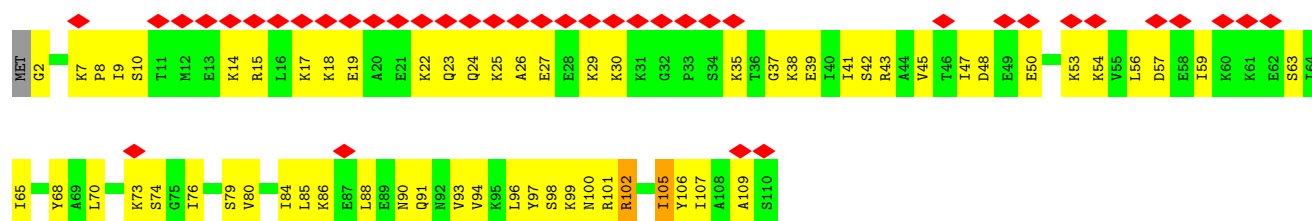
• Molecule 29: aS34

Chain a: 33% 62% ..



• Molecule 30: Small ribosomal subunit protein eS25

Chain c: 36% 43% 55% ..



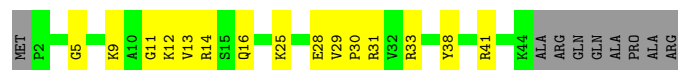
• Molecule 31: aS33

Chain d: 7% 50% 43% 6%



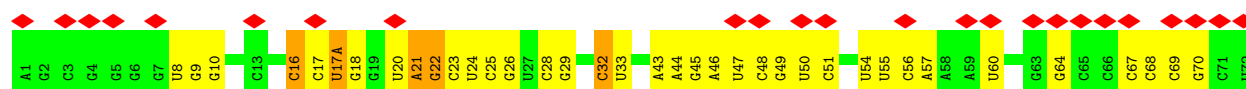
• Molecule 32: LSU ribosomal protein S30E (Rps30E)

Chain e: 54% 29% 17%



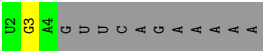
• Molecule 33: tRNA met initiator

Chain 4: 36% 49% 42% 9%





● Molecule 34: Ss_aIF2beta mRNA



● Molecule 35: LSU ribosomal protein S26E (Rps26E)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43812	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	0.045	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.004	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, H2U, 4AC, 5MU, ZN, A2M, 6MZ, MA6, OMC, GTP, 4SU, OMG, SPM, OMU, MG, C4J, 5MC

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	0.28	1/35139 (0.0%)	0.30	1/54824 (0.0%)
2	A	0.22	0/1543	0.35	0/2077
3	B	0.18	0/1731	0.35	0/2349
4	C	0.25	0/466	0.47	0/625
5	D	0.26	0/1380	0.34	0/1859
6	E	0.25	0/1965	0.32	0/2644
7	F	0.26	0/1654	0.36	0/2240
8	G	0.17	0/1684	0.32	0/2265
9	H	0.19	0/1561	0.46	0/2102
10	I	0.27	0/1070	0.34	0/1444
11	J	0.25	0/994	0.40	0/1337
12	K	0.20	0/1084	0.44	0/1450
13	L	0.21	0/856	0.49	0/1154
14	M	0.30	0/960	0.75	5/1294 (0.4%)
15	N	0.26	0/1155	0.40	0/1540
16	O	0.20	0/1142	0.50	1/1532 (0.1%)
17	P	0.23	0/451	0.39	0/600
18	Q	0.22	0/1206	0.34	0/1618
19	R	0.26	0/918	0.33	0/1236
20	S	0.20	0/578	0.44	0/770
21	T	0.18	0/1087	0.40	0/1456
22	U	0.18	0/1270	0.41	0/1710
23	V	0.21	0/843	0.34	0/1124
24	W	0.26	0/511	0.50	0/684
25	X	0.17	0/538	0.41	0/722
26	Y	0.22	0/404	0.57	0/540
27	Z	0.20	0/1584	0.41	0/2124
28	3	0.17	0/902	0.40	0/1216
29	a	0.20	0/574	0.52	0/770
30	c	0.19	0/861	0.49	0/1143
31	d	0.17	0/568	0.47	0/769

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	e	0.19	0/360	0.49	0/477
33	4	0.18	0/1725	0.25	0/2687
34	5	0.32	0/51	0.48	0/78
35	b	0.28	0/713	0.67	1/951 (0.1%)
All	All	0.25	1/69528 (0.0%)	0.36	8/101411 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1337	G	O3'-P	5.70	1.69	1.61

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1109	C	C5'-C4'-O4'	-15.04	86.53	109.10
14	M	116	ILE	O-C-N	-13.77	109.59	121.57
14	M	118	HIS	CA-C-N	6.62	134.18	121.54
14	M	118	HIS	C-N-CA	6.62	134.18	121.54
35	b	22	SER	CA-CB-OG	-6.28	98.55	111.10
16	O	96	THR	CB-CA-C	-6.05	109.58	116.54
14	M	116	ILE	CA-C-N	5.69	125.66	120.03
14	M	116	ILE	C-N-CA	5.69	125.66	120.03

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	32141	0	16256	766	0
2	A	1515	0	1565	52	0
3	B	1698	0	1753	54	0
4	C	455	0	437	29	0
5	D	1354	0	1419	32	0
6	E	1930	0	2013	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	1625	0	1689	42	0
8	G	1661	0	1737	55	0
9	H	1534	0	1597	110	0
10	I	1050	0	1100	19	0
11	J	982	0	1046	40	0
12	K	1068	0	1125	65	0
13	L	840	0	893	54	0
14	M	944	0	978	54	0
15	N	1140	0	1244	26	0
16	O	1124	0	1162	92	0
17	P	440	0	435	28	0
18	Q	1185	0	1260	29	0
19	R	901	0	935	18	0
20	S	571	0	598	26	0
21	T	1064	0	1107	52	0
22	U	1247	0	1329	51	0
23	V	836	0	894	24	0
24	W	503	0	532	9	0
25	X	535	0	572	31	0
26	Y	395	0	405	32	0
27	Z	1561	0	1667	81	0
28	3	893	0	940	58	0
29	a	562	0	575	52	0
30	c	856	0	939	82	0
31	d	557	0	576	48	0
32	e	354	0	386	20	0
33	4	1645	0	840	31	0
34	5	47	0	21	0	0
35	b	704	0	732	50	0
36	2	588	0	1092	93	0
36	E	14	0	26	1	0
37	2	46	0	0	0	0
37	5	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	2	0
40	2	240	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	4	2	0	0	0	0
40	5	3	0	0	0	0
40	E	3	0	0	0	0
40	F	6	0	0	3	0
40	H	1	0	0	0	0
40	I	2	0	0	0	0
40	J	1	0	0	0	0
40	K	5	0	0	0	0
40	L	2	0	0	0	0
40	O	1	0	0	1	0
40	Q	1	0	0	0	0
40	R	1	0	0	0	0
40	V	1	0	0	1	0
40	W	1	0	0	0	0
40	b	3	0	0	0	0
All	All	66880	0	51886	1926	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 (1926) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1189:C:N3	16:O:133:ARG:HA	1.06	1.37
1:2:1189:C:N3	16:O:133:ARG:CA	1.88	1.36
1:2:1337:G:N7	12:K:15:LYS:NZ	1.75	1.33
1:2:1189:C:C2	16:O:133:ARG:HA	1.65	1.32
1:2:1337:G:P	12:K:76:MET:HG3	1.68	1.31
1:2:924:U:C2	1:2:1188:G:O6	1.86	1.28
1:2:466:C:O2'	36:2:1502:SPM:N1	1.71	1.23
1:2:1189:C:H42	16:O:133:ARG:CG	1.53	1.21
1:2:1189:C:HO2'	30:c:2:GLY:N	1.40	1.17
1:2:468:A:H62	36:2:1502:SPM:H21	1.11	1.15
1:2:924:U:C2	1:2:1188:G:C6	2.36	1.14
31:d:67:ILE:HG22	31:d:71:LEU:HD11	1.30	1.13
1:2:1337:G:OP1	12:K:76:MET:HE3	1.46	1.12
1:2:126:G:OP2	36:2:1520:SPM:H62	1.48	1.12
1:2:1189:C:H42	16:O:133:ARG:CB	1.63	1.11
27:Z:63:ILE:HD11	27:Z:81:ILE:HB	1.18	1.10
1:2:1337:G:OP1	12:K:76:MET:HG3	1.47	1.09
1:2:924:U:O2	1:2:1188:G:O6	1.66	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:6:G:OP1	36:2:1528:SPM:H32	1.53	1.08
1:2:1189:C:N4	16:O:133:ARG:HB2	1.66	1.08
36:2:1540:SPM:H32	30:c:101:ARG:HH22	1.15	1.07
1:2:683:G:O6	35:b:15:LYS:NZ	1.85	1.07
4:C:16:CYS:HB3	4:C:19:CYS:SG	1.94	1.07
1:2:1189:C:OP2	16:O:132:THR:OG1	1.72	1.05
1:2:924:U:C5	1:2:1188:G:N7	2.25	1.05
1:2:468:A:N6	36:2:1502:SPM:H21	1.71	1.04
29:a:41:CYS:HB2	29:a:64:CYS:SG	1.95	1.04
35:b:12:LYS:HD2	35:b:18:VAL:HG23	1.38	1.01
1:2:924:U:H6	1:2:1185:G:HO2'	1.07	1.01
36:2:1540:SPM:H32	30:c:101:ARG:NH2	1.75	1.00
1:2:1337:G:OP1	12:K:76:MET:CE	2.09	1.00
4:C:57:CYS:SG	4:C:60:CYS:HB3	2.02	0.99
31:d:67:ILE:HG22	31:d:71:LEU:CD1	1.93	0.99
1:2:1091:U:H3	1:2:1104:G:H1	1.11	0.98
1:2:924:U:N3	1:2:1188:G:C6	2.30	0.98
1:2:1189:C:O2'	30:c:2:GLY:N	1.96	0.98
1:2:920:U:O2	1:2:1188:G:N1	1.97	0.98
27:Z:63:ILE:CD1	27:Z:81:ILE:HB	1.93	0.96
1:2:924:U:C4	1:2:1188:G:C5	2.52	0.96
1:2:1189:C:N4	16:O:133:ARG:CG	2.26	0.96
1:2:1189:C:N4	16:O:133:ARG:CB	2.25	0.95
1:2:1337:G:OP1	12:K:76:MET:CG	2.13	0.95
1:2:1482:G:OP1	14:M:122:ARG:NH2	1.99	0.95
1:2:949:U:H3	1:2:1183:G:H1	1.14	0.95
4:C:16:CYS:CB	4:C:19:CYS:SG	2.52	0.94
1:2:924:U:N3	1:2:1188:G:C5	2.36	0.93
1:2:1373:C:N3	1:2:1448:G:N1	2.16	0.93
1:2:924:U:C4	1:2:1188:G:N7	2.37	0.92
9:H:16:TRP:CH2	9:H:86:PHE:HB3	2.05	0.92
31:d:67:ILE:O	31:d:71:LEU:HG	1.70	0.91
31:d:7:LYS:HG3	31:d:16:ILE:HD11	1.52	0.90
1:2:1189:C:N3	16:O:133:ARG:CB	2.34	0.90
27:Z:63:ILE:HD11	27:Z:81:ILE:CB	2.02	0.89
26:Y:48:MET:HG3	26:Y:58:TRP:HB3	1.53	0.89
1:2:1189:C:H42	16:O:133:ARG:HB2	1.27	0.88
29:a:21:CYS:SG	29:a:24:CYS:N	2.43	0.88
1:2:1373:C:O2	1:2:1448:G:N2	2.08	0.87
9:H:29:LYS:HE2	31:d:28:VAL:HA	1.57	0.87
31:d:67:ILE:CG2	31:d:71:LEU:HD11	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:91:LEU:O	27:Z:185:LYS:NZ	2.08	0.86
1:2:1337:G:P	12:K:76:MET:CG	2.60	0.86
1:2:6:G:OP1	36:2:1528:SPM:C3	2.25	0.85
33:4:50:U:H3	33:4:64:G:H1	0.88	0.84
1:2:644:G:N3	14:M:36:ARG:NH2	2.24	0.84
14:M:117:PRO:HG3	14:M:120:THR:HB	1.58	0.83
31:d:7:LYS:HG3	31:d:16:ILE:CD1	2.08	0.83
29:a:60:LYS:HD2	29:a:65:GLY:HA2	1.59	0.83
1:2:1189:C:N4	16:O:133:ARG:HG3	1.92	0.83
1:2:1189:C:H42	16:O:133:ARG:CD	1.92	0.82
1:2:149:G:OP2	36:2:1531:SPM:H91	1.79	0.82
1:2:602:C:OP1	36:2:1534:SPM:H62	1.79	0.82
9:H:159:GLU:OE2	30:c:100:ASN:ND2	2.12	0.82
1:2:1189:C:C4	16:O:133:ARG:CB	2.64	0.81
1:2:6:G:OP1	36:2:1528:SPM:H41	1.81	0.81
9:H:16:TRP:HH2	9:H:86:PHE:HB3	1.41	0.81
1:2:683:G:C6	35:b:15:LYS:NZ	2.49	0.81
35:b:12:LYS:HD2	35:b:18:VAL:CG2	2.10	0.80
1:2:190:C:H4'	11:J:43:ARG:HH22	1.44	0.80
1:2:924:U:C5	1:2:1188:G:C8	2.69	0.80
1:2:1337:G:OP1	12:K:76:MET:SD	2.40	0.80
7:F:128:CYS:SG	7:F:132:HIS:HD2	2.00	0.80
1:2:126:G:OP2	36:2:1520:SPM:C6	2.30	0.78
35:b:12:LYS:CD	35:b:18:VAL:HG23	2.13	0.78
16:O:111:LYS:O	16:O:114:ARG:NH1	2.16	0.78
27:Z:185:LYS:HA	27:Z:185:LYS:HE3	1.64	0.78
9:H:26:SER:HA	25:X:66:ILE:HB	1.65	0.77
30:c:100:ASN:ND2	30:c:102:ARG:NH2	2.32	0.77
30:c:100:ASN:HD21	30:c:102:ARG:NH2	1.82	0.77
17:P:5:LYS:H	17:P:5:LYS:HD3	1.48	0.77
11:J:34:PHE:HB3	11:J:95:ILE:HG12	1.64	0.77
1:2:924:U:C6	1:2:1188:G:N7	2.52	0.76
30:c:100:ASN:ND2	30:c:102:ARG:HH21	1.81	0.76
29:a:67:GLU:OE2	29:a:67:GLU:N	2.17	0.76
13:L:7:ILE:HG22	13:L:74:ILE:HB	1.66	0.76
1:2:1189:C:C4	16:O:133:ARG:HB2	2.19	0.76
1:2:1311:G:O2'	1:2:1337:G:N1	2.15	0.76
9:H:84:LEU:HG	30:c:100:ASN:HB2	1.68	0.75
1:2:1337:G:OP2	12:K:76:MET:HG3	1.84	0.75
31:d:7:LYS:CG	31:d:16:ILE:CD1	2.65	0.75
18:Q:61:VAL:HG11	18:Q:69:VAL:HG23	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:45:PHE:HB2	22:U:87:LYS:HB2	1.67	0.75
36:2:1533:SPM:C3	36:2:1533:SPM:H71	2.17	0.74
6:E:204:ARG:HD3	6:E:224:MET:HE2	1.68	0.74
31:d:32:MET:HE1	31:d:36:GLU:HB2	1.70	0.74
1:2:1292:C:OP1	16:O:35:ASN:ND2	2.21	0.74
3:B:176:LYS:NZ	3:B:178:ASP:OD2	2.21	0.74
1:2:27:C:OP1	40:2:1601:HOH:O	2.06	0.74
1:2:1203:U:H5'	30:c:102:ARG:HD3	1.70	0.74
30:c:99:LYS:HD2	30:c:99:LYS:O	1.88	0.73
9:H:10:ILE:CG2	31:d:71:LEU:HD22	2.19	0.73
30:c:100:ASN:HD21	30:c:102:ARG:HH21	1.35	0.73
16:O:100:ILE:HG23	16:O:104:ARG:HH22	1.53	0.73
22:U:47:GLU:N	22:U:47:GLU:OE2	2.20	0.73
1:2:481:OMC:HM22	1:2:482:C:H5'	1.70	0.73
14:M:117:PRO:CG	14:M:120:THR:HB	2.19	0.73
2:A:33:LEU:HD22	2:A:51:THR:HG21	1.71	0.73
36:2:1540:SPM:HN11	30:c:101:ARG:NH1	1.85	0.72
29:a:21:CYS:CB	29:a:24:CYS:HB3	1.96	0.72
1:2:1245:U:O4	13:L:8:ARG:NH2	2.21	0.72
3:B:62:VAL:HG21	3:B:71:TYR:HD2	1.52	0.72
1:2:1188:G:N3	21:T:120:VAL:HG21	2.04	0.72
1:2:1335:G:OP1	12:K:16:THR:HG22	1.89	0.72
1:2:71:G:N2	1:2:213:C:O2	2.14	0.72
1:2:256:G:H4'	1:2:257:U:H5'	1.70	0.72
1:2:1189:C:C4	16:O:133:ARG:HG3	2.25	0.72
15:N:99:GLU:N	15:N:99:GLU:OE2	2.21	0.72
1:2:822:C:O2'	4:C:51:GLN:OE1	2.08	0.72
1:2:1311:G:N2	1:2:1337:G:H2'	2.05	0.72
1:2:1406:G:H1	1:2:1415:U:H3	1.37	0.72
14:M:61:LYS:C	14:M:61:LYS:HD3	2.14	0.72
31:d:7:LYS:HB2	31:d:14:VAL:HB	1.70	0.72
1:2:6:G:OP1	36:2:1528:SPM:C4	2.38	0.71
1:2:1034:G:N2	1:2:1037:A:OP2	2.22	0.71
1:2:1373:C:N4	1:2:1448:G:O6	2.22	0.71
22:U:138:LEU:O	22:U:142:ILE:HG13	1.91	0.71
31:d:25:ASN:ND2	31:d:61:MET:O	2.21	0.71
1:2:1187:C:OP2	36:2:1524:SPM:H21	1.90	0.71
12:K:52:PRO:HG2	12:K:86:LEU:HD11	1.72	0.71
1:2:910:A:H2'	1:2:911:A:C8	2.26	0.71
1:2:1393:G:H22	1:2:1428:U:H3	1.37	0.71
12:K:29:ARG:NH2	22:U:156:TYR:O	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:101:ARG:O	30:c:102:ARG:HG3	1.91	0.71
1:2:619:G:N7	40:2:1625:HOH:O	2.24	0.71
14:M:61:LYS:HD3	14:M:61:LYS:O	1.91	0.70
17:P:21:ARG:HH21	29:a:13:HIS:CD2	2.10	0.70
36:2:1540:SPM:H32	30:c:101:ARG:CZ	2.21	0.70
13:L:27:ILE:HG12	13:L:85:GLN:HE21	1.56	0.70
1:2:885:G:H2'	1:2:886:G:C8	2.26	0.70
8:G:57:ASP:OD2	8:G:113:ARG:NH2	2.25	0.70
1:2:71:G:N1	1:2:213:C:N3	2.34	0.70
1:2:1447:A:N6	1:2:1448:G:O6	2.25	0.70
28:3:73:LYS:HB2	28:3:75:ILE:HG13	1.72	0.70
31:d:7:LYS:CE	31:d:16:ILE:HD12	2.22	0.70
35:b:7:ASN:HD22	35:b:11:ARG:NH1	1.89	0.70
1:2:924:U:C4	1:2:1188:G:C8	2.80	0.70
11:J:93:ARG:HB2	11:J:95:ILE:HD12	1.72	0.69
7:F:28:ILE:HG23	7:F:33:GLU:HG3	1.74	0.69
1:2:218:C:H2'	1:2:219:A:H8	1.57	0.69
8:G:164:ARG:NH1	8:G:181:PRO:O	2.25	0.69
9:H:41:THR:O	9:H:44:ARG:NH1	2.26	0.69
31:d:7:LYS:CG	31:d:16:ILE:HD12	2.22	0.69
1:2:310:G:HO2'	5:D:2:GLY:N	1.89	0.69
1:2:337:OMG:HM22	1:2:338:G:H5'	1.73	0.69
3:B:181:ASP:OD2	4:C:49:ARG:NH1	2.25	0.69
18:Q:134:PRO:HG2	18:Q:137:TRP:HB2	1.73	0.69
36:2:1540:SPM:N1	30:c:101:ARG:NH1	2.40	0.69
12:K:26:GLY:HA3	12:K:65:ASP:HB2	1.75	0.69
1:2:410:U:OP2	32:e:31:ARG:NH2	2.25	0.68
1:2:502:C:OP1	32:e:41:ARG:NH1	2.26	0.68
1:2:634:U:OP1	2:A:188:LYS:NZ	2.26	0.68
5:D:158:THR:HG21	23:V:39:GLY:HA3	1.74	0.68
3:B:98:ILE:HG12	3:B:142:PRO:HB3	1.74	0.68
9:H:90:TYR:HB2	9:H:97:PRO:HG3	1.75	0.68
10:I:91:ASP:OD1	10:I:94:ARG:NH2	2.27	0.68
14:M:25:ILE:HG22	14:M:34:ILE:HB	1.74	0.68
1:2:1391:G:H2'	1:2:1392:G:C8	2.29	0.68
18:Q:98:ARG:NH1	18:Q:102:GLU:OE2	2.27	0.68
13:L:23:GLN:NE2	13:L:89:VAL:O	2.27	0.68
14:M:48:GLU:N	14:M:48:GLU:OE2	2.23	0.68
12:K:47:LEU:HA	12:K:50:MET:HG2	1.74	0.68
27:Z:58:ARG:NH1	27:Z:58:ARG:O	2.26	0.68
28:3:35:GLY:O	28:3:39:THR:OG1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:84:ARG:NH2	13:L:87:MET:SD	2.66	0.68
12:K:39:LEU:HD22	22:U:12:PRO:HD3	1.75	0.67
12:K:102:ILE:HD13	31:d:66:PRO:HB2	1.75	0.67
1:2:1391:G:H2'	1:2:1392:G:H8	1.57	0.67
6:E:153:LYS:H	6:E:156:MET:HE2	1.60	0.67
1:2:672:OMG:H2'	1:2:673:G:C8	2.29	0.67
24:W:18:ARG:HG2	24:W:65:MET:HE2	1.75	0.67
2:A:50:GLU:OE1	14:M:109:ARG:NH2	2.28	0.67
1:2:393:G:OP1	36:2:1533:SPM:H41	1.95	0.67
29:a:36:TYR:CE1	29:a:70:PRO:HB3	2.30	0.67
1:2:644:G:OP1	2:A:39:TYR:OH	2.13	0.67
2:A:156:ASP:OD1	2:A:157:ASP:N	2.27	0.67
5:D:30:LEU:HD23	5:D:35:LEU:HB2	1.77	0.67
1:2:322:G:OP2	40:2:1602:HOH:O	2.13	0.66
9:H:156:LYS:NZ	9:H:160:GLU:OE1	2.27	0.66
31:d:67:ILE:HG22	31:d:71:LEU:CG	2.25	0.66
1:2:468:A:H61	36:2:1502:SPM:H42	1.61	0.66
1:2:1188:G:N3	1:2:1188:G:H2'	2.10	0.66
33:4:16:C:H4'	33:4:60:U:O2	1.95	0.66
6:E:234:SER:OG	6:E:236:LEU:O	2.13	0.66
1:2:1335:G:H2'	1:2:1336:U:H6	1.60	0.66
1:2:190:C:O2'	11:J:43:ARG:NH2	2.29	0.66
1:2:1097:C:O2'	1:2:1099:G:N1	2.27	0.66
1:2:1316:C:OP2	36:2:1515:SPM:N1	2.28	0.66
30:c:9:ILE:HD12	30:c:9:ILE:H	1.61	0.66
1:2:920:U:C2	1:2:1188:G:N1	2.62	0.66
27:Z:96:MET:HA	27:Z:96:MET:HE3	1.78	0.66
24:W:47:LEU:HA	24:W:58:VAL:HG22	1.78	0.66
7:F:141:LYS:NZ	7:F:143:GLY:O	2.28	0.66
9:H:89:ILE:HG22	9:H:167:ILE:HD11	1.78	0.66
21:T:61:ARG:NH2	21:T:82:GLU:O	2.25	0.66
25:X:25:GLN:OE1	25:X:40:ARG:NH1	2.29	0.66
27:Z:17:LYS:HG3	29:a:16:TRP:CD2	2.30	0.66
1:2:636:C:H2'	1:2:637:U:C6	2.30	0.66
21:T:88:MET:HA	21:T:88:MET:HE3	1.78	0.66
1:2:1491:A:H4'	35:b:91:LYS:NZ	2.11	0.66
25:X:14:ILE:HG13	31:d:54:LYS:NZ	2.11	0.65
31:d:7:LYS:HE2	31:d:16:ILE:HD12	1.78	0.65
29:a:40:LYS:HE3	29:a:66:THR:HG21	1.78	0.65
1:2:971:G:H21	26:Y:62:LYS:HZ1	1.45	0.65
13:L:4:LYS:HE3	13:L:75:ASP:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:392:U:OP1	36:2:1533:SPM:N1	2.29	0.65
1:2:1189:C:C2	16:O:133:ARG:CA	2.60	0.65
1:2:1189:C:O2	16:O:132:THR:O	2.13	0.65
15:N:91:ASP:N	15:N:138:TYR:OH	2.29	0.65
1:2:421:G:H2'	1:2:422:G:H8	1.61	0.65
28:3:15:LEU:HD21	28:3:114:ILE:HG22	1.77	0.65
1:2:1161:G:O6	36:2:1514:SPM:N1	2.30	0.65
10:I:100:LYS:HG3	10:I:101:GLU:OE1	1.97	0.65
20:S:36:ILE:HG12	20:S:47:ARG:HD2	1.77	0.65
1:2:1076:C:H2'	1:2:1077:A:H8	1.62	0.65
16:O:100:ILE:CG2	16:O:104:ARG:HH22	2.09	0.65
1:2:655:A:H2'	1:2:656:U:H6	1.62	0.65
17:P:48:LEU:HD22	27:Z:16:VAL:HG21	1.78	0.65
28:3:34:LYS:NZ	28:3:86:LEU:O	2.29	0.65
16:O:14:GLN:HE22	16:O:30:LYS:H	1.44	0.65
16:O:104:ARG:O	16:O:108:GLU:HG2	1.97	0.65
22:U:19:ARG:HB2	22:U:19:ARG:HH11	1.62	0.65
31:d:7:LYS:HE3	31:d:56:VAL:HG12	1.79	0.65
1:2:392:U:OP1	36:2:1533:SPM:C2	2.45	0.64
14:M:42:VAL:HG23	14:M:43:VAL:HG13	1.79	0.64
22:U:29:LYS:HA	22:U:29:LYS:HE2	1.78	0.64
1:2:924:U:C2	1:2:1188:G:C5	2.84	0.64
1:2:940:G:OP1	40:2:1603:HOH:O	2.14	0.64
6:E:197:ASN:HB3	6:E:208:VAL:HG12	1.79	0.64
14:M:26:SER:HB3	14:M:33:ILE:HG22	1.78	0.64
16:O:13:GLY:O	30:c:15:ARG:NH2	2.31	0.64
18:Q:26:LEU:HD12	18:Q:58:ILE:HD11	1.80	0.64
27:Z:165:ARG:NH1	29:a:6:ARG:O	2.30	0.64
7:F:123:SER:O	10:I:100:LYS:NZ	2.25	0.64
18:Q:58:ILE:HG23	18:Q:64:ILE:HD12	1.79	0.64
1:2:497:A:OP1	32:e:14:ARG:NH1	2.31	0.64
1:2:1147:G:OP1	20:S:45:LYS:NZ	2.26	0.64
16:O:14:GLN:HG3	30:c:15:ARG:HH21	1.63	0.64
17:P:33:GLY:HA3	27:Z:6:ARG:HH12	1.62	0.64
30:c:22:LYS:HD3	30:c:25:LYS:HD2	1.78	0.64
1:2:1094:U:H3	1:2:1101:G:H1	1.45	0.64
26:Y:32:ASN:HA	28:3:68:LEU:HB2	1.78	0.64
9:H:10:ILE:HG21	31:d:71:LEU:HD22	1.79	0.64
1:2:132:A:OP2	36:2:1531:SPM:N14	2.31	0.64
3:B:21:LYS:HD3	3:B:22:GLU:HG3	1.79	0.64
15:N:49:MET:HB3	15:N:106:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:21:ARG:HH21	29:a:13:HIS:HD2	1.45	0.64
18:Q:70:THR:O	18:Q:74:GLU:HG2	1.98	0.64
26:Y:53:LYS:HG3	26:Y:54:PRO:HD3	1.80	0.64
1:2:442:A:OP1	23:V:108:LYS:NZ	2.30	0.64
1:2:962:A:H2'	1:2:963:G:H8	1.63	0.64
1:2:1057:C:N4	1:2:1060:OMC:OP2	2.31	0.64
8:G:68:GLU:O	8:G:71:LYS:NZ	2.27	0.64
18:Q:97:ARG:NH2	18:Q:117:GLU:OE2	2.30	0.64
1:2:683:G:N7	35:b:15:LYS:NZ	2.44	0.64
1:2:1318:C:H2'	1:2:1319:A:H8	1.63	0.64
9:H:16:TRP:CH2	9:H:97:PRO:HG2	2.32	0.64
9:H:193:ARG:NH2	25:X:73:GLU:OE2	2.31	0.64
12:K:80:ASP:O	12:K:84:MET:HG2	1.98	0.64
26:Y:41:CYS:HB3	26:Y:46:SER:H	1.62	0.64
9:H:91:LEU:O	30:c:63:SER:OG	2.16	0.63
28:3:79:TYR:HE1	28:3:118:VAL:HG23	1.62	0.63
1:2:897:C:O2'	1:2:1308:C:OP2	2.16	0.63
27:Z:36:VAL:HG12	27:Z:45:VAL:HG22	1.80	0.63
27:Z:88:ASN:HB3	27:Z:91:LEU:HB2	1.79	0.63
16:O:108:GLU:HB3	16:O:112:LYS:HE2	1.80	0.63
18:Q:32:GLU:OE1	18:Q:76:ARG:NH1	2.30	0.63
30:c:84:ILE:O	30:c:88:LEU:HG	1.98	0.63
1:2:349:A:H5''	1:2:350:C:H5	1.64	0.63
9:H:30:TYR:OH	25:X:62:ARG:NH1	2.30	0.63
15:N:56:GLU:N	15:N:56:GLU:OE2	2.31	0.63
17:P:50:PHE:O	17:P:51:ARG:NH1	2.29	0.63
27:Z:45:VAL:HG11	27:Z:70:PHE:HE2	1.63	0.63
1:2:119:U:O2	6:E:141:ASN:ND2	2.32	0.63
1:2:962:A:H2'	1:2:963:G:C8	2.33	0.63
7:F:3:GLU:OE1	7:F:3:GLU:N	2.31	0.63
5:D:110:VAL:HG13	5:D:122:ALA:HB1	1.79	0.63
12:K:107:ASP:OD2	12:K:109:THR:OG1	2.15	0.63
1:2:147:G:H2'	1:2:148:G:H8	1.64	0.63
1:2:1465:G:OP1	36:2:1522:SPM:N14	2.32	0.62
8:G:18:ARG:NH1	8:G:63:GLU:OE1	2.31	0.62
16:O:49:ASN:O	30:c:43:ARG:NH1	2.32	0.62
32:e:28:GLU:OE1	32:e:28:GLU:N	2.30	0.62
1:2:21:A:OP2	36:2:1530:SPM:N1	2.32	0.62
4:C:26:ARG:HH11	4:C:26:ARG:HG3	1.64	0.62
1:2:167:A:H2'	1:2:168:G:H8	1.63	0.62
25:X:30:THR:OG1	25:X:31:GLY:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:44:LYS:HG3	29:a:45:TYR:HD1	1.64	0.62
16:O:123:LEU:HD11	21:T:119:LYS:HD2	1.82	0.62
20:S:23:GLU:O	20:S:25:LYS:NZ	2.32	0.62
33:4:32:OMC:HM22	33:4:33:U:H5'	1.80	0.62
1:2:1189:C:H42	16:O:133:ARG:HD2	1.64	0.62
3:B:101:ALA:HB2	3:B:110:VAL:HG21	1.81	0.62
9:H:89:ILE:HG13	9:H:97:PRO:HB3	1.80	0.62
1:2:106:G:OP1	1:2:564:U:O2'	2.12	0.62
1:2:1191:C:H4'	16:O:141:THR:HA	1.81	0.62
12:K:36:PRO:HD2	12:K:39:LEU:HD11	1.82	0.62
1:2:1122:C:OP2	20:S:45:LYS:HG3	2.00	0.62
36:2:1533:SPM:H71	36:2:1533:SPM:H32	1.82	0.62
26:Y:57:ARG:HA	26:Y:68:PHE:HA	1.82	0.62
27:Z:14:VAL:O	27:Z:18:ILE:HG13	1.99	0.62
28:3:35:GLY:O	28:3:98:SER:OG	2.16	0.62
29:a:38:CYS:HB2	29:a:41:CYS:HB3	1.82	0.62
1:2:16:G:N7	36:2:1501:SPM:N14	2.48	0.61
2:A:50:GLU:OE2	2:A:66:HIS:ND1	2.33	0.61
5:D:78:LEU:HD22	5:D:83:LEU:HB2	1.82	0.61
1:2:1341:A:N6	9:H:46:GLU:OE2	2.30	0.61
17:P:37:CYS:SG	17:P:40:CYS:N	2.68	0.61
3:B:57:TYR:OH	4:C:65:PRO:O	2.18	0.61
7:F:160:VAL:HG12	7:F:178:SER:HB3	1.82	0.61
9:H:41:THR:HG21	9:H:55:VAL:HG12	1.81	0.61
2:A:19:TRP:CD1	14:M:8:ARG:HH21	2.19	0.61
3:B:40:ASP:OD1	3:B:41:THR:N	2.33	0.61
2:A:126:THR:OG1	2:A:128:TYR:O	2.15	0.61
9:H:16:TRP:CZ3	9:H:86:PHE:HB3	2.35	0.61
19:R:91:ASP:OD1	19:R:91:ASP:N	2.33	0.61
30:c:22:LYS:O	30:c:26:ALA:N	2.32	0.61
30:c:76:ILE:HD12	30:c:80:VAL:HG12	1.81	0.61
4:C:37:CYS:SG	4:C:60:CYS:HB2	2.40	0.61
1:2:619:G:H2'	1:2:620:G:C8	2.35	0.61
32:e:5:GLY:HA2	32:e:9:LYS:HD2	1.82	0.61
1:2:482:C:N3	15:N:118:ASP:HB3	2.15	0.61
3:B:181:ASP:OD1	4:C:44:ARG:NH1	2.34	0.61
9:H:154:ASN:HD21	9:H:156:LYS:HB3	1.65	0.61
23:V:11:ASP:N	23:V:11:ASP:OD1	2.32	0.61
1:2:971:G:H21	26:Y:62:LYS:NZ	1.99	0.60
16:O:137:ARG:NH1	40:O:201:HOH:O	2.33	0.60
22:U:76:ILE:O	22:U:79:THR:OG1	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1217:G:OP1	17:P:32:TYR:OH	2.12	0.60
9:H:142:HIS:CG	9:H:181:ARG:HD3	2.36	0.60
11:J:57:LEU:HD22	11:J:60:THR:HB	1.83	0.60
1:2:920:U:O2	1:2:1188:G:C2	2.54	0.60
36:2:1540:SPM:C3	30:c:101:ARG:HH22	2.04	0.60
8:G:63:GLU:OE2	8:G:74:LYS:NZ	2.30	0.60
31:d:7:LYS:CE	31:d:56:VAL:HG12	2.30	0.60
1:2:683:G:O6	35:b:15:LYS:CE	2.48	0.60
1:2:1189:C:N3	16:O:133:ARG:HG3	2.16	0.60
18:Q:37:GLU:OE2	18:Q:41:ARG:NH2	2.34	0.60
21:T:28:ASP:N	21:T:28:ASP:OD1	2.32	0.60
27:Z:54:MET:HA	27:Z:54:MET:HE3	1.83	0.60
29:a:42:GLU:OE1	29:a:47:ALA:N	2.34	0.60
1:2:413:U:O3'	5:D:117:ASN:ND2	2.34	0.60
1:2:1078:C:H2'	1:2:1079:U:H6	1.66	0.60
1:2:1133:A:O3'	20:S:10:LYS:NZ	2.30	0.60
36:2:1540:SPM:H32	30:c:101:ARG:NH1	2.16	0.60
16:O:100:ILE:HG22	16:O:104:ARG:HH12	1.66	0.60
21:T:22:LEU:HA	21:T:25:MET:HE2	1.82	0.60
1:2:684:G:O6	35:b:15:LYS:HG2	2.01	0.60
1:2:1101:G:H2'	1:2:1102:C:C6	2.37	0.60
1:2:1228:C:OP1	22:U:125:ARG:NH2	2.32	0.60
5:D:19:ILE:HG22	5:D:22:ARG:H	1.67	0.60
1:2:1261:G:OP1	16:O:51:ARG:NH2	2.35	0.60
2:A:86:HIS:ND1	2:A:189:THR:HG22	2.16	0.60
9:H:138:LEU:HB3	9:H:142:HIS:CE1	2.37	0.60
24:W:16:PHE:O	24:W:65:MET:HE3	2.00	0.60
35:b:12:LYS:HB2	35:b:33:ASP:OD2	2.02	0.60
1:2:340:C:O2'	1:2:1397:A:N3	2.34	0.60
1:2:886:G:O2'	1:2:1363:C:OP2	2.19	0.60
1:2:1393:G:H2'	1:2:1394:G:H8	1.66	0.60
1:2:1452:U:H2'	1:2:1453:C:C6	2.37	0.60
5:D:31:GLY:HA3	32:e:38:TYR:CG	2.37	0.60
15:N:91:ASP:HB3	32:e:14:ARG:HD3	1.82	0.60
16:O:43:LYS:HZ2	16:O:74:GLY:H	1.50	0.60
16:O:79:LEU:HD11	22:U:39:LEU:HD21	1.84	0.60
1:2:1189:C:N3	16:O:133:ARG:CG	2.64	0.59
1:2:579:C:OP1	36:2:1536:SPM:N14	2.35	0.59
1:2:817:U:H5''	35:b:14:ASP:OD2	2.02	0.59
1:2:1343:G:H2'	1:2:1344:OMU:H6	1.84	0.59
29:a:14:LEU:O	29:a:18:THR:OG1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b:46:ASP:OD1	35:b:47:ALA:N	2.34	0.59
30:c:42:SER:OG	30:c:43:ARG:NH2	2.35	0.59
11:J:88:LYS:HE2	11:J:88:LYS:H	1.67	0.59
30:c:94:VAL:HA	30:c:109:ALA:H	1.66	0.59
33:4:9:G:O2'	33:4:10:G:N7	2.34	0.59
1:2:549:C:O3'	10:I:32:LYS:NZ	2.34	0.59
1:2:683:G:C5	35:b:15:LYS:NZ	2.70	0.59
1:2:1311:G:O6	12:K:14:ARG:NH2	2.35	0.59
9:H:6:LEU:HB3	31:d:70:LYS:HD2	1.84	0.59
6:E:118:TYR:OH	6:E:235:ASP:OD1	2.16	0.59
12:K:90:LEU:HD11	12:K:103:TYR:CE2	2.38	0.59
25:X:36:VAL:HG21	25:X:56:ASN:HB3	1.85	0.59
30:c:98:SER:HB2	30:c:105:ILE:HD11	1.85	0.59
1:2:1415:U:H2'	1:2:1416:G:H8	1.66	0.59
11:J:33:THR:HG21	11:J:56:ARG:HD3	1.84	0.59
9:H:22:ILE:O	9:H:28:LYS:NZ	2.35	0.59
27:Z:118:MET:HE3	27:Z:147:LEU:HG	1.85	0.59
1:2:1130:G:N2	1:2:1133:A:OP2	2.35	0.59
8:G:45:LYS:HB2	8:G:93:TRP:HB2	1.85	0.59
9:H:10:ILE:HG22	31:d:71:LEU:HD22	1.85	0.59
8:G:42:PRO:HB2	8:G:79:PHE:HD1	1.68	0.58
8:G:52:GLN:OE1	8:G:52:GLN:N	2.35	0.58
8:G:80:LYS:NZ	8:G:145:GLY:O	2.36	0.58
30:c:47:ILE:HG13	30:c:47:ILE:O	2.02	0.58
1:2:922:A:N3	1:2:949:U:O2'	2.36	0.58
1:2:929:G:OP1	40:2:1606:HOH:O	2.17	0.58
36:2:1514:SPM:H131	27:Z:132:ILE:HG21	1.85	0.58
10:I:18:GLU:HG2	10:I:69:VAL:HB	1.85	0.58
11:J:89:GLU:HG3	11:J:92:ARG:HH21	1.68	0.58
22:U:43:ALA:HB3	22:U:46:LYS:HG3	1.86	0.58
31:d:48:GLU:HA	31:d:51:GLU:HB2	1.84	0.58
1:2:1285:U:OP2	40:2:1605:HOH:O	2.17	0.58
20:S:11:ARG:HH22	20:S:12:ILE:HD12	1.68	0.58
1:2:16:G:H2'	1:2:17:C:C6	2.38	0.58
1:2:1048:U:O3'	20:S:2:GLY:N	2.36	0.58
1:2:1483:G:OP2	14:M:127:ARG:NH2	2.36	0.58
36:2:1515:SPM:N14	12:K:122:LYS:O	2.37	0.58
3:B:36:LEU:O	3:B:203:ARG:NH2	2.34	0.58
1:2:1311:G:O2'	1:2:1337:G:C6	2.49	0.58
8:G:30:LYS:HE2	8:G:43:GLN:HG3	1.84	0.58
20:S:19:ARG:NH1	20:S:20:TYR:OH	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:e:28:GLU:HB2	32:e:33:ARG:HB2	1.85	0.58
3:B:111:GLN:O	3:B:115:GLU:HG3	2.03	0.58
23:V:44:SER:OG	23:V:47:ASP:OD1	2.20	0.58
1:2:71:G:H2'	1:2:72:G:C8	2.39	0.58
1:2:642:G:H2'	1:2:643:A:C8	2.39	0.58
1:2:770:U:O2'	1:2:864:A:N1	2.37	0.58
28:3:55:GLU:HB2	28:3:80:VAL:HG11	1.86	0.58
19:R:48:TYR:N	19:R:89:GLU:OE2	2.32	0.58
21:T:28:ASP:O	21:T:31:ILE:HG22	2.03	0.58
1:2:991:U:H2'	1:2:992:G:C4	2.39	0.58
1:2:1162:U:O4	36:2:1514:SPM:N1	2.36	0.58
1:2:1352:C:H4'	36:2:1539:SPM:H42	1.86	0.58
6:E:59:ILE:HD12	23:V:25:VAL:HG11	1.86	0.58
28:3:22:ALA:HB1	28:3:111:VAL:HG23	1.86	0.58
35:b:8:ARG:HG2	35:b:8:ARG:O	2.04	0.58
1:2:409:G:P	32:e:31:ARG:HH12	2.27	0.57
1:2:1284:C:OP2	40:2:1605:HOH:O	2.18	0.57
16:O:61:LYS:HA	16:O:64:GLU:OE1	2.03	0.57
36:2:1528:SPM:H131	40:F:405:HOH:O	2.04	0.57
9:H:34:MET:HE3	9:H:35:PRO:N	2.20	0.57
13:L:80:GLU:OE2	13:L:84:ARG:HD3	2.04	0.57
21:T:84:ILE:HD12	21:T:101:VAL:HG12	1.86	0.57
1:2:673:G:H2'	1:2:674:A:H8	1.69	0.57
3:B:168:VAL:HG13	3:B:182:LEU:HB3	1.86	0.57
10:I:28:MET:HE2	10:I:60:LYS:HE3	1.86	0.57
1:2:207:U:H2'	1:2:208:A:H8	1.70	0.57
9:H:38:LEU:HD13	12:K:47:LEU:HD12	1.85	0.57
16:O:112:LYS:HD3	16:O:112:LYS:N	2.20	0.57
26:Y:57:ARG:HB3	26:Y:68:PHE:HD1	1.69	0.57
1:2:1015:G:H5''	27:Z:167:ILE:HD13	1.86	0.57
1:2:1334:G:C2	1:2:1335:G:C8	2.93	0.57
7:F:121:CYS:SG	7:F:126:CYS:HB3	2.44	0.57
12:K:130:ARG:NH1	12:K:131:TRP:O	2.37	0.57
31:d:7:LYS:HG2	31:d:16:ILE:HD12	1.85	0.57
1:2:438:C:N3	36:2:1517:SPM:N14	2.52	0.57
20:S:20:TYR:OH	27:Z:197:GLU:OE1	2.23	0.57
30:c:96:LEU:HB2	30:c:106:TYR:CE1	2.40	0.57
9:H:16:TRP:CZ3	9:H:97:PRO:HG2	2.39	0.57
12:K:36:PRO:HB2	12:K:39:LEU:HG	1.86	0.57
28:3:51:VAL:HG21	28:3:66:LEU:HD11	1.87	0.57
28:3:56:ASP:HB2	28:3:83:LYS:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1066:A:OP2	27:Z:155:SER:OG	2.22	0.57
9:H:18:THR:HG21	9:H:35:PRO:HA	1.86	0.57
1:2:39:U:O4	6:E:18:LYS:NZ	2.37	0.57
1:2:1122:C:H6	20:S:28:TYR:CZ	2.23	0.57
7:F:79:LEU:HD11	7:F:188:GLU:HA	1.87	0.57
11:J:83:GLU:HG3	11:J:101:LYS:HB2	1.87	0.57
20:S:37:ARG:HH11	20:S:37:ARG:HG3	1.70	0.57
31:d:7:LYS:CE	31:d:16:ILE:CD1	2.83	0.57
4:C:56:ILE:HD12	4:C:56:ILE:O	2.05	0.57
12:K:47:LEU:O	12:K:51:GLU:HG2	2.04	0.57
33:4:74:C:H4'	33:4:75:C:O5'	2.04	0.57
1:2:1096:U:H1'	22:U:5:MET:HE2	1.87	0.56
1:2:1267:G:OP1	22:U:48:ARG:NH2	2.38	0.56
9:H:36:VAL:HG11	9:H:56:PRO:HG3	1.87	0.56
16:O:67:ILE:HG13	16:O:72:ILE:HG13	1.87	0.56
23:V:66:ARG:NH1	23:V:94:GLU:OE1	2.38	0.56
33:4:17:C:OP1	33:4:60:U:O2'	2.22	0.56
1:2:476:G:N2	1:2:492:A:OP2	2.38	0.56
9:H:15:LYS:C	9:H:16:TRP:CD1	2.83	0.56
15:N:66:ASN:ND2	15:N:118:ASP:OD1	2.36	0.56
1:2:12:U:H2'	1:2:13:C:C6	2.40	0.56
1:2:1318:C:H2'	1:2:1319:A:C8	2.39	0.56
9:H:157:PRO:HD3	30:c:68:TYR:CE2	2.40	0.56
16:O:104:ARG:CZ	16:O:104:ARG:HB2	2.36	0.56
21:T:90:VAL:HG23	21:T:114:SER:HB2	1.86	0.56
27:Z:48:TYR:HB3	27:Z:86:VAL:HG12	1.87	0.56
5:D:31:GLY:HA3	32:e:38:TYR:CD1	2.40	0.56
5:D:157:VAL:HG13	5:D:158:THR:HG23	1.87	0.56
9:H:132:PRO:HA	9:H:135:ARG:HD3	1.86	0.56
14:M:15:TYR:HB3	14:M:22:LEU:HB2	1.85	0.56
1:2:392:U:OP1	36:2:1533:SPM:H22	2.05	0.56
1:2:1061:OMG:HM22	1:2:1062:A:H5'	1.87	0.56
14:M:65:ASP:O	14:M:69:LYS:HG2	2.06	0.56
16:O:120:ARG:HB2	16:O:127:VAL:HG12	1.86	0.56
1:2:1334:G:N3	1:2:1335:G:C8	2.73	0.56
1:2:1100:G:C2	22:U:5:MET:HE1	2.41	0.56
1:2:1251:A:H2'	1:2:1252:A:C8	2.40	0.56
1:2:1436:U:H2'	1:2:1437:G:C8	2.41	0.56
7:F:53:LYS:N	40:F:401:HOH:O	2.39	0.56
7:F:85:MET:N	7:F:85:MET:SD	2.78	0.56
12:K:23:ILE:HG13	12:K:66:ALA:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:40:LYS:HD2	26:Y:47:ILE:HG22	1.86	0.56
1:2:709:C:OP2	18:Q:14:ARG:NH2	2.39	0.56
1:2:924:U:H6	1:2:1185:G:O2'	1.80	0.56
36:2:1540:SPM:C3	30:c:101:ARG:HH12	2.18	0.56
29:a:50:CYS:HB3	29:a:53:ASP:HB2	1.87	0.56
1:2:1189:C:N4	16:O:133:ARG:HD2	2.20	0.56
36:2:1540:SPM:H32	30:c:101:ARG:HH12	1.71	0.56
9:H:38:LEU:HD22	12:K:47:LEU:HB2	1.88	0.56
9:H:41:THR:OG1	9:H:59:GLU:OE2	2.21	0.56
24:W:64:ILE:HG22	24:W:66:GLY:H	1.71	0.56
1:2:95:G:OP2	36:2:1507:SPM:N5	2.34	0.56
1:2:617:G:H2'	1:2:618:C:C6	2.41	0.56
1:2:1024:A:N1	1:2:1065:G:O2'	2.32	0.56
7:F:30:SER:HB3	7:F:33:GLU:HB3	1.88	0.56
8:G:167:VAL:HG11	8:G:196:ILE:HD11	1.88	0.56
1:2:665:C:N3	14:M:36:ARG:NH1	2.54	0.55
1:2:1078:C:H2'	1:2:1079:U:C6	2.41	0.55
1:2:1189:C:O2'	1:2:1189:C:O2	2.24	0.55
13:L:7:ILE:CG2	13:L:74:ILE:HB	2.36	0.55
31:d:7:LYS:HE3	31:d:16:ILE:CD1	2.36	0.55
1:2:920:U:H1'	1:2:1188:G:N2	2.22	0.55
1:2:1204:G:H2'	1:2:1205:G:H8	1.71	0.55
35:b:12:LYS:CE	35:b:16:GLY:C	2.79	0.55
1:2:479:A:OP1	15:N:71:LYS:NZ	2.38	0.55
1:2:920:U:O2	1:2:1188:G:C6	2.58	0.55
1:2:1287:G:H2'	1:2:1288:C:C6	2.40	0.55
1:2:1433:U:O2	1:2:1433:U:H2'	2.07	0.55
25:X:29:ARG:HD3	25:X:37:THR:HB	1.88	0.55
33:4:69:C:H2'	33:4:70:G:H8	1.70	0.55
1:2:908:G:N1	1:2:1302:G:OP2	2.34	0.55
1:2:1334:G:C2	1:2:1335:G:C5	2.94	0.55
1:2:1334:G:C2	1:2:1335:G:N7	2.75	0.55
3:B:99:VAL:HG12	3:B:146:LEU:HB3	1.89	0.55
16:O:25:ALA:HA	16:O:28:MET:CE	2.36	0.55
1:2:266:U:OP1	11:J:56:ARG:NH2	2.39	0.55
2:A:90:ARG:NH2	14:M:114:THR:O	2.34	0.55
15:N:28:ARG:O	15:N:32:THR:HG23	2.06	0.55
1:2:167:A:H2'	1:2:168:G:C8	2.41	0.55
9:H:23:ARG:HH21	25:X:13:ILE:CG1	2.20	0.55
9:H:63:ASN:OD1	9:H:75:LYS:HE3	2.07	0.55
1:2:207:U:H2'	1:2:208:A:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:251:A:N1	1:2:283:U:O2'	2.36	0.55
1:2:611:U:O4	1:2:711:G:O2'	2.17	0.55
1:2:637:U:H2'	1:2:638:C:H6	1.71	0.55
2:A:19:TRP:CG	14:M:8:ARG:HH21	2.25	0.55
30:c:80:VAL:O	30:c:84:ILE:HG13	2.06	0.55
1:2:458:G:H2'	1:2:459:C:C6	2.42	0.55
1:2:788:G:H5''	3:B:56:LYS:HG3	1.88	0.55
1:2:1324:A:C8	17:P:12:TYR:HB3	2.42	0.55
2:A:14:TRP:CD1	2:A:17:LYS:HD2	2.42	0.55
19:R:20:GLU:H	19:R:20:GLU:CD	2.14	0.55
31:d:50:TYR:HA	31:d:53:ILE:HG22	1.89	0.55
1:2:1435:C:H2'	1:2:1436:U:C6	2.42	0.55
1:2:943:U:H4'	36:2:1513:SPM:H112	1.89	0.54
36:2:1533:SPM:C3	36:2:1533:SPM:C7	2.86	0.54
2:A:157:ASP:N	2:A:157:ASP:OD1	2.34	0.54
21:T:101:VAL:HA	21:T:105:MET:HE2	1.88	0.54
25:X:53:LEU:HD23	25:X:55:ARG:HD3	1.88	0.54
15:N:76:GLN:HG3	15:N:83:VAL:HG22	1.88	0.54
16:O:77:SER:OG	16:O:91:ASP:OD2	2.26	0.54
33:4:50:U:O2	33:4:64:G:N2	2.24	0.54
1:2:900:C:C2	1:2:901:A:C8	2.95	0.54
1:2:971:G:N2	26:Y:62:LYS:HZ1	2.05	0.54
1:2:1189:C:O2	16:O:133:ARG:HA	2.01	0.54
2:A:196:GLU:OE1	2:A:196:GLU:N	2.40	0.54
8:G:77:GLY:HA3	8:G:102:PHE:HZ	1.72	0.54
9:H:186:GLU:CD	25:X:70:ARG:HH22	2.16	0.54
1:2:93:C:H1'	1:2:359:C:H5'	1.90	0.54
1:2:1038:A:OP2	7:F:95:LYS:NZ	2.41	0.54
8:G:29:VAL:HG22	8:G:45:LYS:HD3	1.89	0.54
9:H:111:ARG:HE	9:H:135:ARG:HH22	1.55	0.54
9:H:163:ALA:O	9:H:167:ILE:HG12	2.08	0.54
27:Z:139:THR:OG1	27:Z:140:GLU:N	2.41	0.54
1:2:428:U:O2'	1:2:430:U:O4	2.20	0.54
1:2:974:A:H1'	26:Y:57:ARG:CZ	2.37	0.54
4:C:39:GLU:HG3	4:C:59:ASN:HD21	1.72	0.54
28:3:44:GLU:HA	28:3:73:LYS:HE3	1.89	0.54
1:2:987:U:H2'	1:2:988:G:C8	2.43	0.54
1:2:1204:G:H2'	1:2:1205:G:C8	2.42	0.54
5:D:164:ARG:O	5:D:164:ARG:NE	2.39	0.54
16:O:106:ASP:OD1	16:O:109:ARG:NH2	2.41	0.54
28:3:34:LYS:HZ2	28:3:92:LEU:HD13	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:45:U:O2'	1:2:46:A:H2'	2.06	0.54
1:2:683:G:C6	35:b:15:LYS:CE	2.91	0.54
1:2:1450:A:OP1	1:2:1450:A:H3'	2.07	0.54
4:C:23:ILE:HD13	4:C:43:ARG:HG2	1.88	0.54
9:H:90:TYR:HB2	9:H:97:PRO:CG	2.38	0.54
26:Y:56:GLU:HB2	26:Y:69:ILE:HB	1.90	0.54
29:a:38:CYS:CB	29:a:41:CYS:HB3	2.37	0.54
1:2:462:G:OP1	40:2:1608:HOH:O	2.18	0.54
1:2:904:G:H5''	9:H:67:ARG:HH21	1.72	0.54
1:2:1328:A:P	22:U:89:ARG:HH22	2.30	0.54
5:D:16:HIS:HB3	5:D:19:ILE:HD13	1.89	0.54
12:K:90:LEU:HD11	12:K:103:TYR:HE2	1.72	0.54
1:2:74:A:N1	1:2:213:C:O2'	2.38	0.54
1:2:272:C:H2'	1:2:273:C:C6	2.43	0.54
1:2:1077:A:H2'	1:2:1078:C:H6	1.73	0.54
1:2:152:A:H2'	1:2:153:A:C8	2.43	0.54
1:2:1287:G:H2'	1:2:1288:C:H6	1.72	0.54
36:2:1528:SPM:C13	40:F:405:HOH:O	2.55	0.54
2:A:127:THR:HG23	2:A:128:TYR:CD1	2.43	0.54
6:E:161:GLU:HB2	6:E:168:LEU:HD21	1.89	0.54
25:X:48:ASP:CG	25:X:51:ARG:HE	2.16	0.54
36:2:1540:SPM:HN11	30:c:101:ARG:HH12	1.53	0.53
8:G:157:ASP:OD1	8:G:161:PHE:N	2.39	0.53
21:T:28:ASP:O	21:T:32:LYS:HG2	2.07	0.53
35:b:24:ASP:OD1	35:b:24:ASP:N	2.37	0.53
14:M:109:ARG:HG2	35:b:59:ILE:HD11	1.90	0.53
30:c:14:LYS:HG3	30:c:17:LYS:HB3	1.90	0.53
30:c:19:GLU:O	30:c:23:GLN:N	2.41	0.53
1:2:323:G:OP2	36:2:1509:SPM:N14	2.41	0.53
1:2:1311:G:O2'	1:2:1337:G:O6	2.25	0.53
2:A:22:VAL:O	2:A:33:LEU:N	2.41	0.53
3:B:91:ARG:NH2	4:C:35:PRO:O	2.42	0.53
27:Z:17:LYS:HD2	27:Z:74:PHE:CE1	2.43	0.53
28:3:83:LYS:HZ2	28:3:95:ALA:HB1	1.73	0.53
28:3:93:GLN:OE1	28:3:93:GLN:N	2.42	0.53
1:2:996:C:O2'	1:2:997:G:H8	1.91	0.53
6:E:49:LEU:HD13	23:V:25:VAL:HG21	1.89	0.53
6:E:117:LYS:NZ	6:E:138:ASP:OD2	2.25	0.53
6:E:120:ARG:NH1	6:E:226:VAL:O	2.41	0.53
9:H:182:LYS:O	9:H:186:GLU:HG2	2.08	0.53
9:H:192:SER:O	9:H:192:SER:OG	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:50:GLN:O	21:T:54:LEU:HD22	2.08	0.53
1:2:971:G:H2'	1:2:972:C:O4'	2.08	0.53
1:2:1081:G:H5''	13:L:36:ARG:HB3	1.90	0.53
1:2:1431:U:H2'	1:2:1432:C:C6	2.43	0.53
13:L:81:ARG:NH2	13:L:85:GLN:OE1	2.40	0.53
14:M:34:ILE:HG23	14:M:69:LYS:HE2	1.91	0.53
33:4:69:C:H2'	33:4:70:G:C8	2.44	0.53
1:2:988:G:O2'	1:2:989:C:O5'	2.17	0.53
1:2:1491:A:H4'	35:b:91:LYS:HZ1	1.73	0.53
26:Y:58:TRP:N	26:Y:67:GLU:O	2.34	0.53
1:2:1077:A:H2'	1:2:1078:C:C6	2.44	0.53
2:A:19:TRP:CH2	2:A:37:PRO:HG3	2.44	0.53
6:E:169:ASP:OD1	6:E:231:ARG:NH2	2.41	0.53
8:G:119:ILE:HG21	8:G:144:ILE:HG23	1.91	0.53
9:H:18:THR:HA	9:H:98:ILE:HD11	1.91	0.53
5:D:154:ASP:OD2	5:D:155:TYR:N	2.37	0.53
6:E:40:ALA:HB2	6:E:75:TYR:HB2	1.91	0.53
18:Q:17:ARG:HG2	18:Q:19:GLY:H	1.74	0.53
1:2:406:C:O2'	1:2:580:A:N3	2.34	0.53
3:B:210:ARG:NH1	3:B:210:ARG:HA	2.23	0.53
16:O:84:LYS:O	21:T:15:ARG:NH1	2.42	0.53
1:2:190:C:H4'	11:J:43:ARG:NH2	2.21	0.53
5:D:106:LEU:O	5:D:110:VAL:HG12	2.08	0.53
8:G:36:LYS:HG2	8:G:101:LYS:HE2	1.91	0.53
21:T:31:ILE:HD12	21:T:34:LEU:HD12	1.90	0.53
22:U:134:LEU:HA	22:U:137:LYS:HD3	1.91	0.53
28:3:113:GLU:O	28:3:116:LYS:HG3	2.09	0.53
33:4:24:U:H2'	33:4:25:C:H6	1.73	0.53
1:2:707:G:C8	18:Q:59:PRO:HB2	2.44	0.52
23:V:45:ARG:NH1	23:V:65:VAL:O	2.35	0.52
29:a:57:LEU:HD21	29:a:62:PRO:HD3	1.92	0.52
1:2:218:C:H2'	1:2:219:A:C8	2.42	0.52
1:2:979:A:H2'	1:2:980:A:C8	2.45	0.52
11:J:105:GLU:CD	11:J:105:GLU:H	2.18	0.52
33:4:21:A:O4'	33:4:48:C:N4	2.42	0.52
4:C:31:GLU:OE2	4:C:43:ARG:HD3	2.09	0.52
8:G:122:ASP:OD1	8:G:123:GLN:N	2.42	0.52
27:Z:189:ILE:HG22	27:Z:192:LYS:H	1.74	0.52
32:e:12:LYS:O	32:e:12:LYS:HD2	2.08	0.52
1:2:1067:G:N2	27:Z:191:ASP:OD2	2.39	0.52
1:2:1241:G:H1'	1:2:1246:C:O2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1291:U:O2	16:O:83:ARG:NH2	2.32	0.52
1:2:1313:A:H1'	1:2:1338:A:N6	2.24	0.52
1:2:1431:U:H2'	1:2:1432:C:H6	1.72	0.52
8:G:21:VAL:HG21	8:G:92:VAL:HG23	1.90	0.52
8:G:26:SER:HG	8:G:93:TRP:CG	2.28	0.52
9:H:99:GLN:NE2	9:H:103:ARG:CG	2.72	0.52
12:K:59:ASP:OD1	12:K:60:ILE:N	2.42	0.52
22:U:11:VAL:HG21	22:U:142:ILE:HD12	1.90	0.52
28:3:42:ALA:HA	28:3:45:ARG:HG2	1.92	0.52
1:2:589:A:H2'	1:2:590:A:H8	1.73	0.52
1:2:637:U:H2'	1:2:638:C:C6	2.45	0.52
3:B:177:ILE:HD13	4:C:52:GLY:HA3	1.91	0.52
9:H:6:LEU:HD11	12:K:57:GLY:HA3	1.90	0.52
22:U:19:ARG:HB2	22:U:19:ARG:NH1	2.24	0.52
1:2:338:G:O2'	8:G:191:ARG:O	2.24	0.52
1:2:439:U:OP1	23:V:67:LYS:NZ	2.42	0.52
1:2:962:A:H2	1:2:996:C:N4	2.08	0.52
1:2:1112:A:O2'	12:K:71:TYR:OH	2.26	0.52
1:2:1188:G:N3	1:2:1188:G:C2'	2.73	0.52
1:2:1201:A:H2	1:2:1204:G:N3	2.06	0.52
1:2:1314:A:H1'	9:H:72:LYS:HG2	1.92	0.52
1:2:1402:C:H2'	1:2:1403:C:C6	2.45	0.52
1:2:1432:C:O2	1:2:1432:C:H2'	2.09	0.52
16:O:39:ALA:HB1	16:O:75:LEU:HD11	1.91	0.52
28:3:36:THR:HB	28:3:97:ALA:HB3	1.92	0.52
35:b:7:ASN:HB2	35:b:11:ARG:HH22	1.75	0.52
1:2:17:C:H2'	1:2:18:C:C6	2.45	0.52
1:2:126:G:OP2	36:2:1520:SPM:H42	2.09	0.52
1:2:801:C:H2'	1:2:802:U:O4'	2.10	0.52
1:2:949:U:H2'	1:2:950:A:C8	2.44	0.52
1:2:1017:C:H2'	1:2:1018:OMG:H8	1.75	0.52
7:F:132:HIS:ND1	7:F:175:ASP:OD2	2.41	0.52
9:H:110:PRO:O	9:H:135:ARG:NH1	2.42	0.52
21:T:21:GLU:O	21:T:25:MET:HG3	2.10	0.52
21:T:42:LEU:HD21	21:T:78:VAL:HB	1.91	0.52
28:3:21:GLU:O	28:3:24:ARG:HG3	2.10	0.52
33:4:23:C:H2'	33:4:24:U:C6	2.44	0.52
1:2:429:U:H1'	5:D:127:THR:HG22	1.91	0.52
2:A:36:THR:OG1	2:A:47:ARG:NH1	2.43	0.52
1:2:527:G:O2'	1:2:533:A:N1	2.35	0.52
1:2:625:G:OP1	36:2:1510:SPM:N5	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:885:G:H2'	1:2:886:G:H8	1.74	0.52
1:2:1179:C:H2'	1:2:1180:C:H6	1.74	0.52
1:2:1252:A:H2'	1:2:1253:A:C8	2.45	0.52
1:2:1343:G:H2'	1:2:1344:OMU:C6	2.40	0.52
1:2:1436:U:O2'	1:2:1437:G:OP1	2.27	0.52
8:G:35:GLU:HB3	8:G:98:MET:HE1	1.91	0.52
10:I:37:VAL:O	10:I:41:MET:HG3	2.10	0.52
11:J:37:LEU:HD12	11:J:60:THR:O	2.10	0.52
18:Q:52:LEU:HB3	18:Q:58:ILE:HB	1.92	0.52
35:b:7:ASN:HB2	35:b:11:ARG:NH2	2.25	0.52
1:2:728:G:H4'	1:2:1470:A:H4'	1.92	0.51
1:2:1053:C:O2'	20:S:10:LYS:NZ	2.30	0.51
1:2:1096:U:O2'	1:2:1099:G:O6	2.26	0.51
1:2:1313:A:N3	1:2:1338:A:C6	2.78	0.51
2:A:24:THR:HB	2:A:28:PHE:HB2	1.92	0.51
3:B:29:LYS:HB2	3:B:76:ARG:HH11	1.73	0.51
6:E:54:ARG:NH1	40:V:201:HOH:O	2.39	0.51
6:E:127:ILE:HG13	6:E:128:LYS:H	1.75	0.51
10:I:83:TYR:CZ	10:I:123:ARG:HG3	2.44	0.51
10:I:95:ARG:NH2	10:I:96:TYR:OH	2.43	0.51
22:U:145:GLU:HA	22:U:148:GLU:HG2	1.91	0.51
26:Y:35:LYS:HD2	26:Y:35:LYS:C	2.35	0.51
31:d:17:ASN:CG	31:d:18:ASP:H	2.18	0.51
1:2:1216:G:OP1	13:L:45:LYS:NZ	2.36	0.51
6:E:109:ILE:HB	6:E:113:GLU:HG3	1.92	0.51
16:O:87:GLU:OE1	16:O:87:GLU:N	2.44	0.51
22:U:143:PHE:CE1	22:U:153:LEU:HD12	2.45	0.51
8:G:3:ASP:OD1	8:G:3:ASP:N	2.40	0.51
14:M:94:GLN:HE22	35:b:46:ASP:HB2	1.74	0.51
28:3:115:ILE:O	28:3:118:VAL:HG12	2.10	0.51
1:2:965:A:N6	1:2:993:A:O2'	2.42	0.51
1:2:1334:G:N1	1:2:1335:G:C5	2.79	0.51
1:2:1450:A:H3'	1:2:1450:A:P	2.51	0.51
12:K:102:ILE:CD1	31:d:66:PRO:HB2	2.40	0.51
21:T:31:ILE:HG13	21:T:39:ARG:HG2	1.93	0.51
27:Z:70:PHE:HB3	27:Z:76:LEU:HD12	1.92	0.51
30:c:86:LYS:O	30:c:90:ASN:ND2	2.40	0.51
1:2:65:C:H2'	1:2:66:U:C6	2.46	0.51
1:2:272:C:H2'	1:2:273:C:H6	1.75	0.51
7:F:121:CYS:SG	7:F:126:CYS:CB	2.98	0.51
9:H:62:ILE:HG12	9:H:82:VAL:HG11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:22:CYS:HB3	17:P:40:CYS:SG	2.49	0.51
21:T:23:LEU:HD21	21:T:84:ILE:HG21	1.91	0.51
22:U:29:LYS:O	22:U:29:LYS:HD3	2.09	0.51
27:Z:71:GLU:HG3	27:Z:79:PRO:HD3	1.93	0.51
1:2:1019:U:OP1	13:L:59:ARG:NH1	2.31	0.51
5:D:21:GLU:OE1	5:D:21:GLU:N	2.41	0.51
6:E:43:ILE:HG21	6:E:59:ILE:HD11	1.93	0.51
9:H:115:THR:OG1	9:H:116:ARG:N	2.39	0.51
1:2:1446:G:H2'	1:2:1447:A:O4'	2.10	0.51
36:2:1533:SPM:H71	36:2:1533:SPM:H31	1.92	0.51
9:H:91:LEU:HD12	30:c:97:TYR:CZ	2.45	0.51
23:V:61:ASN:O	23:V:87:ARG:NH1	2.40	0.51
28:3:33:LYS:HZ1	28:3:42:ALA:HB3	1.75	0.51
28:3:76:PRO:HG2	28:3:115:ILE:HD12	1.93	0.51
31:d:7:LYS:O	31:d:14:VAL:N	2.31	0.51
1:2:362:G:OP2	40:2:1610:HOH:O	2.19	0.51
1:2:817:U:C5'	35:b:14:ASP:OD2	2.57	0.51
15:N:57:LYS:HD2	15:N:94:VAL:HG22	1.93	0.51
28:3:12:PRO:HG2	28:3:15:LEU:HB3	1.92	0.51
31:d:38:SER:HB2	31:d:43:LEU:HD23	1.93	0.51
33:4:16:C:O2'	33:4:17:C:O4'	2.29	0.51
35:b:7:ASN:HD22	35:b:11:ARG:CZ	2.23	0.51
1:2:176:G:N1	1:2:179:A:OP2	2.42	0.51
1:2:699:U:H2'	1:2:700:A:H8	1.76	0.51
1:2:1181:C:H5'	17:P:7:PRO:HA	1.92	0.51
1:2:1188:G:H2'	21:T:120:VAL:HG21	1.93	0.51
2:A:161:GLU:OE2	2:A:166:ARG:NH1	2.43	0.51
8:G:79:PHE:HE1	8:G:98:MET:HG2	1.75	0.51
14:M:37:ALA:HA	14:M:41:MET:HG2	1.93	0.51
16:O:78:TRP:O	16:O:83:ARG:NH1	2.43	0.51
16:O:82:ARG:NH1	16:O:106:ASP:OD2	2.42	0.51
28:3:11:VAL:HG23	28:3:79:TYR:HB3	1.93	0.51
30:c:50:GLU:HA	30:c:53:LYS:HE3	1.93	0.51
1:2:504:C:O2'	1:2:508:U:OP1	2.29	0.51
1:2:865:OMG:HM22	1:2:866:A:O4'	2.11	0.51
1:2:1336:U:C2'	1:2:1337:G:H5'	2.41	0.51
29:a:62:PRO:HG2	29:a:63:TYR:CE1	2.46	0.51
1:2:257:U:H2'	1:2:258:U:C6	2.46	0.50
1:2:269:G:O2'	19:R:100:PRO:O	2.26	0.50
1:2:871:A:H2'	1:2:872:A:C8	2.46	0.50
1:2:917:G:N7	16:O:133:ARG:NH2	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1190:A:H2'	16:O:142:ILE:HD11	1.93	0.50
14:M:44:LYS:H	14:M:44:LYS:CD	2.24	0.50
20:S:44:LYS:HD3	20:S:47:ARG:HH21	1.76	0.50
1:2:468:A:N6	36:2:1502:SPM:H42	2.26	0.50
1:2:589:A:H2'	1:2:590:A:C8	2.46	0.50
1:2:1392:G:H2'	1:2:1393:G:O4'	2.11	0.50
25:X:14:ILE:HA	25:X:17:PHE:HB2	1.92	0.50
26:Y:65:TYR:CG	26:Y:65:TYR:O	2.65	0.50
27:Z:58:ARG:H	27:Z:58:ARG:HD3	1.76	0.50
27:Z:110:PHE:CG	27:Z:137:LEU:HD12	2.46	0.50
29:a:24:CYS:N	29:a:53:ASP:OD2	2.44	0.50
29:a:71:ILE:HD12	29:a:72:LEU:H	1.74	0.50
30:c:8:PRO:HD2	30:c:9:ILE:HD12	1.93	0.50
1:2:260:G:H2'	1:2:261:G:H8	1.76	0.50
1:2:673:G:H2'	1:2:674:A:C8	2.46	0.50
1:2:972:C:H3'	1:2:982:G:C8	2.46	0.50
1:2:973:C:O2	26:Y:57:ARG:NH1	2.44	0.50
2:A:53:LEU:HD23	2:A:62:GLN:CD	2.37	0.50
2:A:101:SER:O	2:A:126:THR:OG1	2.28	0.50
8:G:157:ASP:HA	8:G:205:ILE:HA	1.93	0.50
9:H:61:LEU:HD23	9:H:140:LEU:HD22	1.93	0.50
13:L:79:ASP:O	13:L:82:VAL:HG22	2.11	0.50
16:O:104:ARG:HB2	16:O:104:ARG:NH1	2.26	0.50
16:O:4:GLN:O	16:O:6:LYS:NZ	2.41	0.50
16:O:62:LYS:O	16:O:66:VAL:HG23	2.10	0.50
28:3:59:PRO:HG2	28:3:62:ILE:HB	1.94	0.50
1:2:636:C:H2'	1:2:637:U:H6	1.73	0.50
1:2:1269:G:N2	1:2:1295:G:H1'	2.27	0.50
1:2:1355:U:H5'	35:b:84:ALA:HA	1.94	0.50
7:F:17:THR:OG1	7:F:43:GLU:OE2	2.23	0.50
8:G:202:SER:OG	8:G:203:GLN:N	2.45	0.50
13:L:28:VAL:HG21	13:L:35:MET:SD	2.52	0.50
30:c:70:LEU:O	30:c:74:SER:OG	2.16	0.50
1:2:17:C:H2'	1:2:18:C:H6	1.77	0.50
1:2:917:G:OP1	36:2:1524:SPM:N10	2.28	0.50
12:K:32:VAL:HA	12:K:68:ILE:HB	1.94	0.50
27:Z:99:ARG:O	27:Z:102:ILE:HD12	2.11	0.50
1:2:71:G:H2'	1:2:72:G:H8	1.76	0.50
1:2:190:C:C4'	11:J:43:ARG:HH22	2.21	0.50
1:2:612:A:N6	24:W:10:PRO:HG3	2.27	0.50
1:2:1453:C:H2'	1:2:1454:G:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:49:LYS:HA	8:G:52:GLN:HE22	1.76	0.50
9:H:37:TYR:HB2	12:K:51:GLU:OE2	2.11	0.50
13:L:93:GLU:OE1	27:Z:37:LEU:HA	2.12	0.50
1:2:142:A:H2'	1:2:143:A:C8	2.47	0.50
1:2:217:U:H2'	1:2:218:C:C6	2.47	0.50
1:2:1043:C:H2'	1:2:1044:C:H6	1.76	0.50
1:2:1081:G:O2'	1:2:1109:C:C4	2.65	0.50
3:B:188:ASN:HA	3:B:194:LEU:HD13	1.93	0.50
22:U:6:ILE:HG21	22:U:143:PHE:HB2	1.93	0.50
24:W:18:ARG:HG2	24:W:65:MET:CE	2.42	0.50
1:2:967:G:N7	28:3:37:ASN:ND2	2.60	0.50
5:D:110:VAL:HG23	5:D:115:LEU:HB2	1.93	0.50
9:H:10:ILE:HA	9:H:37:TYR:CZ	2.47	0.50
9:H:11:LYS:HD3	9:H:15:LYS:N	2.26	0.50
16:O:30:LYS:NZ	30:c:9:ILE:O	2.36	0.50
29:a:22:ARG:N	29:a:48:TYR:O	2.45	0.50
1:2:1019:U:OP1	13:L:59:ARG:HD3	2.12	0.49
1:2:1189:C:C2	16:O:132:THR:O	2.65	0.49
1:2:1288:C:H2'	1:2:1289:C:H6	1.76	0.49
2:A:14:TRP:HH2	14:M:69:LYS:O	1.95	0.49
3:B:112:LYS:HG2	3:B:225:PHE:HA	1.93	0.49
9:H:40:HIS:HD2	12:K:48:LYS:NZ	2.09	0.49
13:L:81:ARG:HH11	13:L:82:VAL:HA	1.77	0.49
33:4:22:G:H2'	33:4:23:C:H6	1.76	0.49
1:2:1050:A:OP1	36:2:1539:SPM:N14	2.31	0.49
1:2:1493:C:O2	1:2:1493:C:H2'	2.12	0.49
3:B:16:LEU:HB2	3:B:49:ILE:HG12	1.95	0.49
13:L:19:TYR:HE2	13:L:92:PRO:HD3	1.77	0.49
29:a:57:LEU:HD11	29:a:62:PRO:HG3	1.94	0.49
1:2:487:C:H41	15:N:66:ASN:ND2	2.10	0.49
1:2:699:U:H2'	1:2:700:A:C8	2.48	0.49
1:2:1101:G:H2'	1:2:1102:C:H6	1.77	0.49
1:2:1213:A:H2'	1:2:1214:G:C8	2.48	0.49
1:2:1293:G:H5''	16:O:33:GLY:H	1.77	0.49
1:2:1450:A:OP1	1:2:1450:A:H2'	2.13	0.49
5:D:44:ALA:HA	5:D:101:LEU:HD23	1.93	0.49
11:J:66:LEU:HA	11:J:73:ALA:HA	1.93	0.49
14:M:22:LEU:HD13	14:M:38:SER:HB3	1.92	0.49
18:Q:21:PRO:HG2	18:Q:24:VAL:HG23	1.92	0.49
27:Z:38:LYS:HD3	27:Z:38:LYS:H	1.78	0.49
29:a:20:TYR:CE1	29:a:27:LYS:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:60:LYS:NZ	29:a:61:CYS:O	2.41	0.49
30:c:100:ASN:O	30:c:102:ARG:N	2.44	0.49
1:2:979:A:O2'	1:2:980:A:OP1	2.26	0.49
1:2:1188:G:H21	21:T:120:VAL:HG11	1.77	0.49
1:2:1395:U:H2'	1:2:1396:G:O4'	2.12	0.49
13:L:76:ILE:CD1	13:L:86:LEU:HD11	2.43	0.49
1:2:421:G:H2'	1:2:422:G:C8	2.44	0.49
1:2:1099:G:H3'	1:2:1100:G:H8	1.77	0.49
6:E:82:MET:HE3	6:E:82:MET:HA	1.94	0.49
7:F:118:ARG:HB3	7:F:135:PRO:HG3	1.94	0.49
8:G:174:LYS:HG2	8:G:193:ARG:HG2	1.95	0.49
17:P:9:GLU:OE1	17:P:9:GLU:HA	2.12	0.49
21:T:15:ARG:HG3	21:T:33:LEU:HB3	1.93	0.49
22:U:19:ARG:O	22:U:22:ILE:HG13	2.12	0.49
1:2:971:G:OP1	17:P:3:LYS:N	2.22	0.49
1:2:1228:C:P	22:U:125:ARG:HH22	2.35	0.49
14:M:61:LYS:C	14:M:61:LYS:CD	2.85	0.49
1:2:65:C:H2'	1:2:66:U:H6	1.77	0.49
1:2:1328:A:OP2	22:U:89:ARG:NH2	2.45	0.49
1:2:1401:C:H2'	1:2:1402:C:C6	2.48	0.49
13:L:65:TRP:HB3	17:P:50:PHE:HB3	1.95	0.49
14:M:6:GLU:HG3	14:M:7:ILE:HG23	1.94	0.49
15:N:91:ASP:OD1	32:e:11:GLY:HA2	2.12	0.49
29:a:36:TYR:CD2	29:a:54:LYS:HD3	2.48	0.49
1:2:826:G:N7	36:2:1512:SPM:H111	2.28	0.49
1:2:1114:U:H4'	13:L:42:PRO:HG3	1.94	0.49
1:2:1313:A:H1'	1:2:1338:A:H61	1.78	0.49
4:C:31:GLU:OE2	4:C:43:ARG:NH1	2.45	0.49
6:E:55:GLU:O	6:E:59:ILE:HG23	2.12	0.49
1:2:828:A:OP2	1:2:828:A:H8	1.95	0.49
1:2:989:C:H2'	1:2:990:C:C6	2.48	0.49
1:2:1487:G:O2'	35:b:5:ARG:NH1	2.32	0.49
3:B:112:LYS:HD2	3:B:115:GLU:OE1	2.13	0.49
7:F:118:ARG:NH2	7:F:209:ASP:OD2	2.43	0.49
13:L:41:LEU:HD13	13:L:71:LYS:HE2	1.95	0.49
35:b:45:VAL:HG22	35:b:49:LEU:HB2	1.94	0.49
1:2:843:4AC:HM72	15:N:3:LYS:HE2	1.94	0.49
1:2:1350:C:H2'	1:2:1351:U:H6	1.77	0.49
1:2:1492:C:O2	1:2:1492:C:H2'	2.12	0.49
3:B:25:ARG:HH11	3:B:25:ARG:HG3	1.78	0.49
3:B:218:LEU:HG	3:B:220:VAL:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:66:LEU:HB2	6:E:86:SER:HB2	1.95	0.49
9:H:21:GLU:OE1	31:d:58:ALA:N	2.42	0.49
11:J:114:ARG:O	11:J:118:ASP:HB2	2.13	0.49
16:O:7:TYR:HE2	30:c:30:LYS:HE3	1.78	0.49
33:4:17:C:OP2	33:4:17(A):U:O2'	2.26	0.49
33:4:56:C:H2'	33:4:57:A:O4'	2.12	0.49
1:2:221:G:H2'	1:2:222:A:H8	1.77	0.48
1:2:426:C:H2'	1:2:427:U:C6	2.47	0.48
1:2:526:G:OP2	15:N:5:LYS:NZ	2.29	0.48
1:2:678:C:H1'	2:A:94:ARG:HH22	1.77	0.48
1:2:885:G:H4'	7:F:68:THR:HA	1.93	0.48
1:2:899:A:H2'	1:2:900:C:H6	1.78	0.48
1:2:926:OMG:HM22	1:2:927:G:H5'	1.95	0.48
1:2:975:G:H2'	1:2:976:G:H8	1.78	0.48
1:2:1081:G:N2	1:2:1082:U:O4	2.32	0.48
1:2:1404:U:H2'	1:2:1405:U:C6	2.49	0.48
1:2:1461:G:OP1	1:2:1464:A:H4'	2.13	0.48
8:G:152:ILE:HA	8:G:210:THR:HG22	1.94	0.48
10:I:18:GLU:HA	10:I:18:GLU:OE2	2.13	0.48
19:R:20:GLU:OE2	19:R:20:GLU:N	2.23	0.48
22:U:127:LEU:HD12	22:U:132:ARG:HB2	1.95	0.48
1:2:518:U:OP2	36:2:1501:SPM:N5	2.46	0.48
1:2:681:G:N7	2:A:129:LYS:NZ	2.60	0.48
1:2:964:G:O2'	1:2:967:G:O2'	2.26	0.48
1:2:1084:G:H2'	1:2:1085:G:C8	2.48	0.48
3:B:199:TRP:CD2	3:B:222:VAL:HG22	2.47	0.48
8:G:178:SER:HB3	8:G:191:ARG:HG2	1.94	0.48
16:O:81:ASN:OD1	16:O:94:LEU:N	2.45	0.48
22:U:7:THR:OG1	22:U:10:MET:HE2	2.13	0.48
1:2:521:U:C4	15:N:27:GLN:HG2	2.48	0.48
1:2:941:A:H3'	1:2:941:A:N3	2.28	0.48
9:H:27:LEU:HD21	9:H:135:ARG:HE	1.78	0.48
15:N:24:ARG:HG2	15:N:30:TYR:CD2	2.48	0.48
1:2:441:C:P	23:V:101:ARG:HH21	2.37	0.48
1:2:1001:A:H2'	1:2:1002:G:O4'	2.13	0.48
1:2:1058:A:H4'	1:2:1059:A:H5'	1.95	0.48
9:H:96:ASN:O	9:H:99:GLN:HB3	2.14	0.48
10:I:14:ILE:HD11	10:I:38:LEU:HD21	1.94	0.48
12:K:98:GLU:O	12:K:101:LYS:HG2	2.13	0.48
23:V:88:GLU:OE1	23:V:89:ILE:N	2.45	0.48
28:3:27:LYS:HE3	28:3:90:CYS:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:b:21:ILE:HD11	35:b:35:ALA:CB	2.43	0.48
1:2:853:G:O2'	1:2:869:G:O6	2.24	0.48
1:2:910:A:H2'	1:2:911:A:H8	1.74	0.48
1:2:941:A:N3	1:2:941:A:C2'	2.76	0.48
3:B:73:LEU:HD21	3:B:173:THR:HG22	1.94	0.48
11:J:66:LEU:HB2	11:J:73:ALA:HB2	1.95	0.48
27:Z:52:PRO:HA	27:Z:55:ILE:HG22	1.96	0.48
29:a:36:TYR:HD1	29:a:70:PRO:CA	2.26	0.48
1:2:452:G:O2'	1:2:454:A:H1'	2.14	0.48
1:2:914:U:H2'	1:2:915:G:H8	1.79	0.48
1:2:1173:C:H2'	1:2:1174:G:O4'	2.12	0.48
1:2:1477:4AC:O7	1:2:1477:4AC:H5	2.13	0.48
7:F:208:GLN:H	7:F:208:GLN:CD	2.20	0.48
9:H:111:ARG:NH1	25:X:17:PHE:O	2.47	0.48
12:K:119:GLU:HG2	12:K:128:ALA:HB1	1.95	0.48
31:d:49:ALA:HA	31:d:52:LEU:HD23	1.96	0.48
1:2:611:U:O2'	1:2:612:A:OP2	2.27	0.48
1:2:1475:MA6:H2'	1:2:1476:A:C8	2.49	0.48
7:F:9:ASN:HB2	7:F:12:GLU:CD	2.39	0.48
7:F:33:GLU:O	7:F:37:ARG:HD3	2.14	0.48
9:H:11:LYS:HB3	9:H:17:ASP:OD1	2.14	0.48
14:M:98:ARG:O	14:M:102:ARG:HG2	2.13	0.48
1:2:1208:G:OP2	22:U:46:LYS:NZ	2.34	0.48
6:E:30:PRO:HB2	6:E:31:HIS:CD2	2.49	0.48
8:G:41:VAL:HG21	8:G:146:LEU:HD21	1.95	0.48
16:O:123:LEU:HD11	21:T:119:LYS:NZ	2.28	0.48
19:R:23:CYS:HB2	19:R:83:PRO:HG2	1.96	0.48
21:T:54:LEU:HA	21:T:57:VAL:HG12	1.94	0.48
1:2:93:C:H2'	1:2:94:U:C6	2.48	0.48
1:2:367:G:N1	1:2:370:A:OP2	2.46	0.48
1:2:614:G:OP2	40:2:1611:HOH:O	2.20	0.48
1:2:1355:U:H2'	1:2:1356:G:C8	2.48	0.48
6:E:110:SER:OG	6:E:112:ASP:OD1	2.32	0.48
8:G:148:VAL:HB	8:G:212:ILE:HG23	1.96	0.48
27:Z:37:LEU:HD12	27:Z:44:ARG:HD3	1.96	0.48
1:2:381:G:O6	36:2:1516:SPM:N14	2.47	0.48
1:2:965:A:H5'	28:3:94:VAL:HG21	1.94	0.48
5:D:143:TYR:OH	5:D:149:GLU:OE2	2.23	0.48
1:2:579:C:H1'	5:D:143:TYR:HD1	1.77	0.47
1:2:644:G:H1'	14:M:36:ARG:NH2	2.29	0.47
1:2:704:C:OP1	1:2:814:U:O2'	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1189:C:OP1	16:O:120:ARG:NH1	2.45	0.47
12:K:40:ILE:HD12	12:K:46:ARG:HA	1.96	0.47
21:T:75:ARG:HB3	21:T:111:GLY:HA3	1.96	0.47
21:T:108:HIS:ND1	21:T:113:TYR:OH	2.36	0.47
22:U:45:PHE:HA	22:U:87:LYS:HD2	1.95	0.47
27:Z:30:GLU:CD	27:Z:99:ARG:HE	2.21	0.47
28:3:27:LYS:HZ1	28:3:89:ALA:HB3	1.79	0.47
30:c:41:ILE:O	30:c:80:VAL:HG22	2.14	0.47
35:b:33:ASP:OD1	35:b:33:ASP:N	2.46	0.47
1:2:633:G:H2'	1:2:634:U:C6	2.48	0.47
1:2:1070:C:H1'	27:Z:157:GLN:HG3	1.95	0.47
1:2:1143:G:OP1	12:K:108:ARG:NH2	2.35	0.47
7:F:128:CYS:SG	7:F:154:LYS:HD2	2.53	0.47
8:G:43:GLN:OE1	8:G:80:LYS:HB3	2.14	0.47
9:H:23:ARG:HH21	25:X:13:ILE:HG13	1.78	0.47
9:H:113:GLU:OE1	9:H:114:VAL:N	2.47	0.47
12:K:124:MET:HE1	13:L:59:ARG:HG2	1.96	0.47
35:b:90:GLN:HA	35:b:90:GLN:OE1	2.15	0.47
1:2:200:C:H2'	1:2:201:A:H8	1.80	0.47
1:2:995:U:H2'	1:2:996:C:C5	2.50	0.47
1:2:1349:G:H2'	1:2:1350:C:H6	1.79	0.47
7:F:59:VAL:HG11	7:F:81:ILE:HD12	1.94	0.47
8:G:80:LYS:HZ2	8:G:146:LEU:HA	1.80	0.47
1:2:82:G:O2'	1:2:132:A:N3	2.46	0.47
1:2:260:G:H2'	1:2:261:G:C8	2.50	0.47
1:2:1005:G:OP1	29:a:20:TYR:OH	2.25	0.47
1:2:1294:U:O2'	30:c:9:ILE:HG13	2.14	0.47
4:C:40:VAL:HG11	4:C:58:PRO:HD2	1.95	0.47
7:F:126:CYS:O	10:I:100:LYS:NZ	2.29	0.47
9:H:43:GLY:HA2	9:H:45:HIS:CE1	2.50	0.47
13:L:86:LEU:O	13:L:89:VAL:HG23	2.15	0.47
1:2:157:C:H2'	1:2:158:C:H6	1.78	0.47
1:2:1124:G:C2	1:2:1125:C:C6	3.02	0.47
1:2:1392:G:C4	1:2:1393:G:C8	3.03	0.47
13:L:10:TRP:CE2	27:Z:4:ILE:HG13	2.49	0.47
1:2:646:A:C2	1:2:663:A:C5	3.02	0.47
1:2:646:A:H4'	14:M:41:MET:HE2	1.96	0.47
1:2:1396:G:O2'	1:2:1425:A:N6	2.40	0.47
7:F:90:SER:HB3	7:F:114:ILE:HA	1.97	0.47
14:M:20:ASN:OD1	14:M:21:THR:N	2.43	0.47
30:c:25:LYS:O	30:c:29:LYS:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:328:U:H2'	1:2:329:G:O4'	2.15	0.47
1:2:716:U:H2'	1:2:717:G:O4'	2.15	0.47
1:2:827:A:H2'	1:2:828:A:C8	2.50	0.47
1:2:914:U:H2'	1:2:915:G:C8	2.50	0.47
1:2:953:G:O2'	17:P:5:LYS:NZ	2.37	0.47
1:2:1032:OMU:HM22	1:2:1033:U:H5'	1.96	0.47
1:2:1092:G:H2'	1:2:1093:G:C8	2.49	0.47
1:2:1179:C:H2'	1:2:1180:C:C6	2.50	0.47
1:2:1183:G:N7	36:2:1513:SPM:H71	2.29	0.47
1:2:1313:A:C4	1:2:1338:A:C6	3.02	0.47
3:B:48:HIS:CD2	3:B:49:ILE:HG13	2.50	0.47
4:C:59:ASN:OD1	4:C:60:CYS:N	2.48	0.47
9:H:12:VAL:HG13	9:H:39:PRO:HD3	1.97	0.47
21:T:38:GLN:OE1	21:T:38:GLN:N	2.47	0.47
21:T:90:VAL:HG11	21:T:110:LEU:HD12	1.97	0.47
21:T:105:MET:HB3	21:T:113:TYR:CZ	2.50	0.47
27:Z:37:LEU:HD22	27:Z:38:LYS:H	1.79	0.47
27:Z:66:LEU:HD12	27:Z:70:PHE:CZ	2.50	0.47
29:a:36:TYR:CE2	29:a:54:LYS:HD3	2.49	0.47
30:c:91:GLN:OE1	30:c:93:VAL:HG12	2.14	0.47
31:d:7:LYS:CD	31:d:56:VAL:HG12	2.43	0.47
1:2:633:G:O2'	14:M:118:HIS:ND1	2.32	0.47
1:2:1095:C:O2'	1:2:1096:U:O5'	2.28	0.47
1:2:1319:A:H2'	1:2:1320:G:C8	2.49	0.47
2:A:20:TYR:CD2	2:A:41:ILE:HD13	2.49	0.47
10:I:2:VAL:O	10:I:4:VAL:N	2.48	0.47
16:O:104:ARG:HH21	30:c:10:SER:HB3	1.79	0.47
23:V:19:ARG:NH1	23:V:21:MET:HG3	2.30	0.47
26:Y:24:ARG:HH11	28:3:37:ASN:HB3	1.79	0.47
27:Z:58:ARG:HH12	27:Z:61:ARG:HB2	1.80	0.47
1:2:649:G:H2'	1:2:650:G:C8	2.49	0.47
1:2:683:G:C6	35:b:15:LYS:HE2	2.49	0.47
1:2:1085:G:C2'	1:2:1086:U:H5'	2.45	0.47
36:2:1531:SPM:H122	36:2:1531:SPM:H92	1.68	0.47
9:H:10:ILE:HG21	31:d:71:LEU:CD2	2.43	0.47
13:L:27:ILE:HG23	13:L:85:GLN:NE2	2.29	0.47
20:S:19:ARG:HG2	20:S:20:TYR:CZ	2.50	0.47
22:U:118:GLN:HE22	22:U:128:SER:HA	1.79	0.47
27:Z:53:SER:O	27:Z:56:ILE:HG22	2.15	0.47
27:Z:88:ASN:ND2	27:Z:91:LEU:HD12	2.29	0.47
28:3:48:ALA:HA	28:3:102:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1035:U:O3'	7:F:192:ARG:NH1	2.48	0.47
3:B:150:PRO:HG2	3:B:175:ALA:HB1	1.95	0.47
11:J:40:GLU:N	11:J:40:GLU:OE2	2.48	0.47
12:K:16:THR:HA	12:K:18:ARG:HH12	1.79	0.47
18:Q:39:ALA:HB3	18:Q:78:LEU:HD23	1.97	0.47
21:T:67:ASN:OD1	21:T:68:LYS:N	2.48	0.47
22:U:147:ALA:HB1	22:U:154:LYS:HE3	1.97	0.47
26:Y:57:ARG:HB2	26:Y:66:THR:HG22	1.96	0.47
30:c:35:LYS:HA	30:c:38:LYS:HD2	1.96	0.47
1:2:687:A:H2'	1:2:688:A:C8	2.50	0.46
1:2:909:G:C2	1:2:910:A:C8	3.03	0.46
1:2:1185:G:H5''	21:T:117:THR:CG2	2.44	0.46
1:2:1232:A:N3	1:2:1290:C:O2'	2.40	0.46
1:2:1481:C:H2'	1:2:1482:G:C8	2.50	0.46
11:J:35:THR:HG22	11:J:60:THR:HG22	1.97	0.46
16:O:26:LEU:HD13	16:O:40:ILE:HD11	1.97	0.46
22:U:118:GLN:OE1	22:U:118:GLN:N	2.48	0.46
1:2:871:A:H2'	1:2:872:A:H8	1.80	0.46
1:2:940:G:H21	1:2:1327:A:H5'	1.79	0.46
1:2:989:C:O3'	26:Y:47:ILE:HD11	2.15	0.46
1:2:989:C:OP1	26:Y:49:ALA:HA	2.15	0.46
1:2:1273:G:O6	40:2:1609:HOH:O	2.19	0.46
1:2:1373:C:N3	1:2:1448:G:C6	2.83	0.46
36:2:1523:SPM:H61	36:2:1523:SPM:H31	1.65	0.46
2:A:168:ALA:HB1	2:A:184:ALA:O	2.15	0.46
7:F:55:LYS:HE3	7:F:55:LYS:HB2	1.76	0.46
8:G:102:PHE:HD2	8:G:107:PHE:CZ	2.33	0.46
8:G:128:ASN:N	8:G:128:ASN:OD1	2.47	0.46
12:K:90:LEU:HD13	12:K:99:LEU:HD21	1.96	0.46
14:M:12:ALA:HB3	14:M:76:ILE:HD13	1.97	0.46
16:O:36:THR:O	16:O:40:ILE:HG23	2.16	0.46
18:Q:25:ARG:H	18:Q:25:ARG:HD2	1.80	0.46
20:S:19:ARG:NH1	27:Z:197:GLU:OE1	2.44	0.46
25:X:23:VAL:HA	25:X:41:VAL:HA	1.97	0.46
30:c:37:GLY:O	30:c:41:ILE:HG12	2.15	0.46
30:c:106:TYR:O	30:c:107:ILE:HD13	2.15	0.46
1:2:538:OMC:HM21	18:Q:111:LYS:HE2	1.97	0.46
1:2:1243:A:O2'	1:2:1245:U:OP2	2.19	0.46
9:H:44:ARG:NE	12:K:114:ASP:OD2	2.41	0.46
9:H:78:ALA:O	9:H:82:VAL:HG12	2.15	0.46
12:K:96:SER:HB3	12:K:99:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:64:ILE:C	24:W:66:GLY:H	2.24	0.46
27:Z:56:ILE:HD12	27:Z:56:ILE:HA	1.86	0.46
30:c:24:GLN:HA	30:c:27:GLU:HG2	1.97	0.46
33:4:23:C:H2'	33:4:24:U:H6	1.79	0.46
1:2:539:C:H2'	1:2:540:G:O4'	2.15	0.46
1:2:721:G:H2'	1:2:722:G:C8	2.51	0.46
1:2:1368:5MC:H2'	1:2:1369:G:C8	2.51	0.46
2:A:12:ASP:N	2:A:12:ASP:OD1	2.48	0.46
3:B:26:LYS:HE3	3:B:63:TYR:CD1	2.51	0.46
6:E:26:PRO:HG2	6:E:33:ILE:HG12	1.98	0.46
9:H:86:PHE:HA	9:H:89:ILE:HG12	1.98	0.46
11:J:60:THR:HG21	11:J:121:ILE:HD11	1.97	0.46
15:N:140:GLY:O	15:N:141:LYS:HG2	2.15	0.46
21:T:69:THR:HA	21:T:87:LYS:HB2	1.98	0.46
25:X:70:ARG:HG3	25:X:71:GLU:OE2	2.16	0.46
27:Z:148:LYS:HZ3	27:Z:152:VAL:HB	1.80	0.46
29:a:42:GLU:O	29:a:46:SER:N	2.49	0.46
30:c:39:GLU:HB2	30:c:76:ILE:HA	1.97	0.46
31:d:24:LEU:HD13	31:d:61:MET:HB3	1.97	0.46
1:2:615:G:OP1	18:Q:2:ASN:ND2	2.48	0.46
1:2:638:C:H2'	1:2:639:C:H6	1.80	0.46
1:2:947:A:H5'	1:2:948:C:OP2	2.15	0.46
1:2:974:A:N3	26:Y:57:ARG:NH2	2.63	0.46
1:2:1226:C:H2'	1:2:1227:C:C6	2.51	0.46
1:2:1316:C:N3	1:2:1335:G:N1	2.64	0.46
1:2:1331:U:C5	36:2:1515:SPM:H111	2.50	0.46
2:A:183:LYS:HG3	2:A:185:GLU:OE1	2.14	0.46
9:H:128:VAL:HG23	25:X:56:ASN:O	2.16	0.46
19:R:56:ILE:HD13	19:R:79:ALA:HB3	1.96	0.46
29:a:17:LEU:HB3	29:a:30:ILE:HB	1.98	0.46
31:d:40:ARG:NH1	31:d:40:ARG:HB2	2.31	0.46
1:2:138:G:N7	36:2:1521:SPM:H32	2.30	0.46
9:H:118:MET:HA	9:H:118:MET:HE3	1.98	0.46
9:H:193:ARG:HA	25:X:74:ARG:NH2	2.31	0.46
27:Z:127:LEU:HG	27:Z:186:PRO:HA	1.98	0.46
30:c:97:TYR:CE1	30:c:105:ILE:HD13	2.50	0.46
1:2:136:C:O2'	8:G:116:THR:O	2.32	0.46
1:2:147:G:H2'	1:2:148:G:C8	2.47	0.46
1:2:655:A:H2'	1:2:656:U:C6	2.46	0.46
1:2:1262:C:C4	9:H:155:PRO:HA	2.50	0.46
1:2:1277:G:OP2	40:2:1612:HOH:O	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:65:VAL:HG11	11:J:125:LEU:HD13	1.98	0.46
23:V:47:ASP:OD1	23:V:47:ASP:N	2.48	0.46
1:2:221:G:H2'	1:2:222:A:C8	2.50	0.46
1:2:464:G:OP2	36:2:1502:SPM:H22	2.16	0.46
1:2:907:U:O4	36:2:1527:SPM:N10	2.40	0.46
1:2:1479:U:H2'	1:2:1480:G:H8	1.81	0.46
28:3:25:LYS:HE2	28:3:25:LYS:HB2	1.81	0.46
28:3:116:LYS:HD2	28:3:116:LYS:C	2.40	0.46
1:2:1057:C:OP2	3:B:125:ARG:HD2	2.16	0.46
16:O:115:SER:HB3	21:T:113:TYR:CE1	2.51	0.46
29:a:36:TYR:HE1	29:a:70:PRO:HB3	1.80	0.46
1:2:468:A:H61	36:2:1502:SPM:C4	2.27	0.46
1:2:1342:C:OP1	25:X:29:ARG:NH2	2.30	0.46
2:A:19:TRP:CD1	14:M:8:ARG:NH2	2.83	0.46
12:K:64:ILE:HD12	12:K:64:ILE:HA	1.83	0.46
23:V:35:VAL:HG11	23:V:43:PRO:HG2	1.97	0.46
29:a:46:SER:O	29:a:46:SER:OG	2.28	0.46
30:c:48:ASP:HB2	30:c:50:GLU:HG3	1.97	0.46
33:4:67:C:H2'	33:4:68:C:C6	2.51	0.46
1:2:504:C:H2'	1:2:505:G:O4'	2.16	0.45
1:2:778:A:OP2	35:b:8:ARG:NH1	2.39	0.45
1:2:926:OMG:N7	36:2:1524:SPM:H82	2.30	0.45
1:2:964:G:N2	1:2:965:A:N1	2.64	0.45
1:2:988:G:O2'	1:2:989:C:H6	1.98	0.45
1:2:1099:G:N2	22:U:158:GLU:O	2.48	0.45
1:2:1422:U:H2'	1:2:1423:C:C6	2.51	0.45
23:V:84:TYR:OH	23:V:94:GLU:OE2	2.19	0.45
27:Z:148:LYS:NZ	27:Z:152:VAL:HB	2.32	0.45
27:Z:154:LYS:HD2	29:a:3:ILE:HD13	1.98	0.45
1:2:351:G:O2'	8:G:172:LYS:NZ	2.49	0.45
1:2:949:U:H2'	1:2:950:A:H8	1.81	0.45
1:2:973:C:C2	1:2:974:A:C8	3.05	0.45
2:A:159:THR:HA	2:A:162:VAL:HG22	1.98	0.45
30:c:7:LYS:NZ	30:c:9:ILE:HD13	2.31	0.45
33:4:22:G:H2'	33:4:23:C:C6	2.51	0.45
1:2:195:A:N1	1:2:225:G:O2'	2.39	0.45
1:2:1070:C:C1'	27:Z:157:GLN:HG3	2.46	0.45
1:2:1207:A:H4'	22:U:50:PRO:HA	1.98	0.45
1:2:1283:A:O2'	1:2:1287:G:N7	2.39	0.45
1:2:1350:C:H2'	1:2:1351:U:C6	2.50	0.45
1:2:1481:C:OP1	35:b:29:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:60:ASP:HB3	7:F:79:LEU:HB2	1.97	0.45
9:H:36:VAL:HG23	12:K:106:TYR:OH	2.16	0.45
14:M:41:MET:HA	14:M:41:MET:HE3	1.98	0.45
21:T:76:ASN:OD1	21:T:76:ASN:N	2.42	0.45
25:X:27:LEU:HD12	25:X:38:GLN:HB3	1.98	0.45
30:c:65:ILE:HG23	30:c:106:TYR:HB2	1.98	0.45
1:2:3:U:H5'	7:F:159:VAL:HG12	1.98	0.45
1:2:67:C:C2'	1:2:68:C:H5'	2.46	0.45
1:2:751:A:O2'	1:2:753:A:N7	2.45	0.45
1:2:981:C:H5'	21:T:52:HIS:CE1	2.52	0.45
23:V:84:TYR:C	23:V:85:LYS:HE2	2.41	0.45
23:V:105:THR:O	23:V:105:THR:OG1	2.32	0.45
29:a:71:ILE:HD12	29:a:72:LEU:N	2.32	0.45
30:c:56:LEU:O	30:c:59:ILE:HG22	2.16	0.45
1:2:33:U:H2'	1:2:34:C:O4'	2.16	0.45
1:2:387:A:H2'	1:2:388:A:C8	2.51	0.45
1:2:905:OMG:H2'	1:2:906:G:O4'	2.16	0.45
1:2:1075:C:H1'	1:2:1142:A:C4	2.51	0.45
1:2:1099:G:H3'	1:2:1100:G:C8	2.51	0.45
1:2:1403:C:O2	1:2:1403:C:H2'	2.17	0.45
13:L:46:LEU:HD21	27:Z:5:LYS:HB3	1.99	0.45
18:Q:68:LYS:HB2	18:Q:71:GLN:OE1	2.17	0.45
31:d:17:ASN:ND2	31:d:18:ASP:OD1	2.50	0.45
33:4:24:U:H2'	33:4:25:C:C6	2.51	0.45
1:2:311:A:O2'	1:2:312:G:H5'	2.17	0.45
1:2:702:A:H2'	1:2:703:A:H8	1.82	0.45
1:2:899:A:H2'	1:2:900:C:C6	2.52	0.45
1:2:961:C:C2	1:2:962:A:C8	3.04	0.45
1:2:1016:C:OP1	29:a:8:SER:OG	2.33	0.45
1:2:1106:G:H2'	1:2:1107:A:O4'	2.16	0.45
3:B:103:ARG:NE	3:B:103:ARG:HA	2.31	0.45
6:E:200:LYS:HA	6:E:200:LYS:HD2	1.67	0.45
13:L:3:THR:HG23	13:L:3:THR:O	2.17	0.45
21:T:104:GLU:OE1	21:T:104:GLU:HA	2.16	0.45
26:Y:31:GLY:C	26:Y:32:ASN:OD1	2.59	0.45
27:Z:37:LEU:HD22	27:Z:38:LYS:N	2.32	0.45
27:Z:37:LEU:HB3	27:Z:44:ARG:HG3	1.98	0.45
28:3:76:PRO:CG	28:3:115:ILE:HD12	2.46	0.45
29:a:54:LYS:HZ2	29:a:54:LYS:C	2.24	0.45
31:d:7:LYS:HD2	31:d:56:VAL:HG12	1.98	0.45
1:2:946:U:H4'	1:2:947:A:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:968:A:H62	1:2:992:G:H21	1.64	0.45
1:2:985:C:C2	1:2:986:U:H5	2.34	0.45
2:A:110:VAL:HG11	2:A:146:VAL:HG12	1.97	0.45
3:B:100:VAL:HG12	3:B:122:LEU:HB2	1.98	0.45
6:E:96:VAL:HG11	6:E:104:MET:HE3	1.99	0.45
7:F:90:SER:HB3	7:F:114:ILE:HD13	1.99	0.45
15:N:77:LEU:HD21	15:N:105:ILE:HD11	1.99	0.45
21:T:5:ILE:HD12	21:T:5:ILE:O	2.17	0.45
28:3:107:ALA:HB1	28:3:110:LEU:HB3	1.97	0.45
1:2:121:A:H2'	1:2:122:G:O4'	2.16	0.45
1:2:149:G:H2'	1:2:150:A:H8	1.81	0.45
1:2:941:A:N3	1:2:941:A:H2'	2.31	0.45
1:2:1311:G:C2	1:2:1337:G:H2'	2.51	0.45
1:2:1313:A:C2	1:2:1338:A:C5	3.05	0.45
1:2:1344:OMU:HM23	1:2:1344:OMU:H1'	1.82	0.45
1:2:1489:U:O4	35:b:34:LYS:HE3	2.17	0.45
4:C:37:CYS:SG	4:C:38:GLY:N	2.90	0.45
5:D:21:GLU:H	5:D:21:GLU:CD	2.20	0.45
5:D:69:ARG:HE	5:D:69:ARG:HB3	1.56	0.45
6:E:169:ASP:CG	6:E:231:ARG:HH22	2.24	0.45
9:H:155:PRO:O	30:c:68:TYR:HE2	2.00	0.45
16:O:32:ILE:HD12	16:O:93:HIS:HE2	1.81	0.45
19:R:27:ASP:OD2	19:R:101:LEU:HD22	2.16	0.45
27:Z:55:ILE:HG23	27:Z:83:ILE:HD13	1.99	0.45
30:c:94:VAL:CG2	30:c:106:TYR:HB3	2.47	0.45
1:2:553:C:H2'	1:2:554:A:O4'	2.17	0.45
1:2:654:A:H2'	1:2:655:A:C8	2.52	0.45
1:2:1043:C:H2'	1:2:1044:C:C6	2.52	0.45
1:2:1319:A:H2'	1:2:1320:G:H8	1.80	0.45
1:2:1470:A:H2'	1:2:1471:G:C8	2.52	0.45
9:H:64:GLN:HG3	9:H:140:LEU:HB3	1.98	0.45
12:K:66:ALA:C	12:K:67:LYS:HE2	2.42	0.45
17:P:4:TYR:CE2	29:a:57:LEU:HD12	2.51	0.45
33:4:28:C:H2'	33:4:29:G:H8	1.82	0.45
35:b:37:CYS:HA	35:b:68:CYS:HA	1.98	0.45
1:2:166:G:H2'	1:2:167:A:H8	1.82	0.45
1:2:209:U:H2'	1:2:210:U:C6	2.52	0.45
1:2:940:G:N2	1:2:1327:A:H5'	2.32	0.45
1:2:981:C:H5'	21:T:52:HIS:HE1	1.82	0.45
1:2:1029:G:H2'	1:2:1030:U:C6	2.51	0.45
1:2:1199:A:H2'	1:2:1200:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1307:C:H2'	1:2:1308:C:C6	2.51	0.45
9:H:95:GLN:N	9:H:95:GLN:OE1	2.50	0.45
9:H:181:ARG:O	9:H:185:ILE:HG12	2.17	0.45
15:N:119:LEU:HD23	15:N:120:PRO:HD2	1.98	0.45
25:X:14:ILE:HG13	31:d:54:LYS:HZ1	1.79	0.45
26:Y:55:ASN:ND2	26:Y:57:ARG:HG2	2.32	0.45
1:2:784:G:O2'	10:I:9:ASN:OD1	2.34	0.44
1:2:941:A:C2	1:2:941:A:OP1	2.70	0.44
1:2:1092:G:H2'	1:2:1093:G:H8	1.82	0.44
1:2:1109:C:H6	1:2:1109:C:O5'	2.00	0.44
1:2:1122:C:O2	1:2:1122:C:H3'	2.17	0.44
1:2:1341:A:OP2	9:H:52:LYS:NZ	2.34	0.44
4:C:54:GLU:HG3	4:C:63:LYS:HE3	1.99	0.44
9:H:97:PRO:HA	9:H:100:VAL:HG23	1.99	0.44
11:J:64:ASN:ND2	11:J:122:ASN:OD1	2.48	0.44
20:S:12:ILE:O	20:S:16:ILE:HG12	2.17	0.44
25:X:54:THR:OG1	25:X:75:GLU:OE2	2.34	0.44
27:Z:37:LEU:HB3	27:Z:44:ARG:CG	2.47	0.44
28:3:57:VAL:HG21	28:3:97:ALA:HA	1.99	0.44
1:2:496:C:H4'	32:e:14:ARG:HG3	1.99	0.44
1:2:957:A:O5'	1:2:958:C:H5	1.99	0.44
1:2:1254:C:OP1	9:H:74:LYS:NZ	2.34	0.44
1:2:1281:A:H2'	1:2:1282:A:O4'	2.17	0.44
8:G:180:PRO:O	8:G:182:GLY:N	2.51	0.44
16:O:49:ASN:C	30:c:43:ARG:HD2	2.42	0.44
23:V:52:ILE:HG23	23:V:56:LEU:HD23	1.98	0.44
23:V:96:LYS:NZ	23:V:100:ASP:OD2	2.50	0.44
1:2:175:U:H2'	1:2:176:G:O4'	2.17	0.44
1:2:333:C:H4'	1:2:334:A:H5''	2.00	0.44
1:2:675:C:O2'	14:M:119:ASP:OD2	2.35	0.44
1:2:943:U:O2	17:P:10:ARG:HD3	2.17	0.44
1:2:1250:U:H3	22:U:71:ASN:HD21	1.65	0.44
7:F:9:ASN:OD1	7:F:9:ASN:N	2.45	0.44
9:H:30:TYR:CE2	9:H:132:PRO:HG2	2.52	0.44
16:O:51:ARG:O	16:O:55:LEU:HD13	2.17	0.44
16:O:78:TRP:HA	16:O:83:ARG:HD3	1.99	0.44
16:O:82:ARG:HH12	16:O:106:ASP:CG	2.25	0.44
17:P:44:VAL:O	17:P:48:LEU:HD23	2.17	0.44
18:Q:62:LYS:HD3	18:Q:68:LYS:HG3	1.98	0.44
30:c:97:TYR:CZ	30:c:105:ILE:HD13	2.52	0.44
33:4:25:C:C2	33:4:26:G:C8	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:361:A:N3	1:2:373:U:O2'	2.38	0.44
1:2:1447:A:C5	1:2:1448:G:N7	2.85	0.44
36:2:1531:SPM:HN11	36:2:1531:SPM:H41	1.60	0.44
2:A:17:LYS:NZ	14:M:32:GLU:OE2	2.46	0.44
3:B:29:LYS:HB3	3:B:33:ILE:HG12	2.00	0.44
11:J:127:LYS:HD2	11:J:127:LYS:C	2.42	0.44
13:L:7:ILE:HD12	13:L:98:GLU:O	2.18	0.44
13:L:52:ARG:NE	13:L:63:GLU:OE2	2.50	0.44
13:L:53:LEU:HD11	13:L:60:LYS:HA	1.99	0.44
22:U:8:ALA:HB3	22:U:69:TYR:CE1	2.52	0.44
25:X:22:GLU:C	25:X:41:VAL:HG23	2.42	0.44
26:Y:47:ILE:C	26:Y:47:ILE:HD12	2.43	0.44
28:3:53:ILE:HD13	28:3:67:PRO:HD3	2.00	0.44
1:2:986:U:H2'	1:2:987:U:C6	2.52	0.44
1:2:1293:G:H5''	16:O:33:GLY:N	2.32	0.44
36:2:1542:SPM:H71	36:2:1542:SPM:H42	1.73	0.44
3:B:191:ARG:HG2	3:B:226:GLU:CD	2.43	0.44
9:H:157:PRO:HD3	30:c:68:TYR:CD2	2.52	0.44
11:J:42:ILE:CG1	11:J:59:TYR:HB2	2.48	0.44
12:K:38:GLU:H	12:K:38:GLU:CD	2.25	0.44
22:U:8:ALA:HB3	22:U:69:TYR:CD1	2.52	0.44
27:Z:176:ILE:HD12	27:Z:176:ILE:N	2.32	0.44
30:c:94:VAL:HG22	30:c:106:TYR:HB3	2.00	0.44
32:e:13:VAL:O	32:e:16:GLN:HG3	2.17	0.44
1:2:1187:C:H4'	16:O:131:ARG:HD2	1.99	0.44
1:2:1313:A:C2	1:2:1338:A:C4	3.06	0.44
2:A:53:LEU:HB3	2:A:62:GLN:HG2	1.99	0.44
6:E:117:LYS:HB2	6:E:162:LEU:HD11	1.99	0.44
9:H:142:HIS:CD2	9:H:181:ARG:HD3	2.52	0.44
11:J:33:THR:O	11:J:33:THR:OG1	2.31	0.44
19:R:58:ARG:HB3	19:R:75:SER:OG	2.16	0.44
27:Z:159:LEU:HD22	27:Z:163:ILE:HG12	1.99	0.44
35:b:45:VAL:HG13	35:b:46:ASP:O	2.18	0.44
1:2:1232:A:H2'	1:2:1233:A:C8	2.53	0.44
1:2:1260:C:OP1	30:c:43:ARG:NH2	2.51	0.44
1:2:1261:G:H1'	1:2:1262:C:H5	1.83	0.44
1:2:1346:C:H2'	1:2:1347:C:H6	1.83	0.44
1:2:1449:A:OP2	1:2:1449:A:H2'	2.18	0.44
7:F:120:GLY:HA2	7:F:131:PRO:HA	1.98	0.44
8:G:12:GLN:HB2	8:G:113:ARG:NH2	2.33	0.44
8:G:49:LYS:HD3	8:G:89:ASP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:24:ASP:OD2	9:H:27:LEU:N	2.34	0.44
9:H:154:ASN:ND2	9:H:156:LYS:HB3	2.32	0.44
13:L:4:LYS:HG2	13:L:76:ILE:O	2.17	0.44
14:M:94:GLN:NE2	35:b:46:ASP:HB2	2.33	0.44
19:R:49:ARG:NH1	19:R:89:GLU:OE2	2.51	0.44
27:Z:24:LYS:HG2	29:a:14:LEU:HB2	1.99	0.44
28:3:55:GLU:HB2	28:3:80:VAL:HG21	2.00	0.44
31:d:67:ILE:HG22	31:d:71:LEU:HG	1.99	0.44
1:2:738:C:H2'	1:2:739:A:O4'	2.18	0.44
3:B:15:GLU:OE1	3:B:15:GLU:N	2.51	0.44
8:G:87:VAL:HG23	8:G:93:TRP:CE2	2.51	0.44
9:H:99:GLN:HE22	9:H:103:ARG:HD3	1.83	0.44
12:K:6:LYS:NZ	12:K:93:PHE:HA	2.33	0.44
16:O:121:HIS:CE1	16:O:127:VAL:HG11	2.52	0.44
28:3:33:LYS:HE3	28:3:102:LEU:HD21	2.00	0.44
1:2:474:G:O2'	32:e:16:GLN:OE1	2.35	0.44
1:2:924:U:H1'	1:2:1185:G:O2'	2.18	0.44
1:2:1075:C:H2'	1:2:1076:C:C6	2.53	0.44
1:2:1255:C:H2'	1:2:1256:C:H6	1.83	0.44
1:2:1494:U:O2	1:2:1494:U:O2'	2.28	0.44
2:A:14:TRP:CZ2	14:M:69:LYS:HE3	2.53	0.44
2:A:19:TRP:CZ2	2:A:37:PRO:HG3	2.53	0.44
8:G:80:LYS:NZ	8:G:147:PRO:HD3	2.33	0.44
11:J:38:SER:OG	11:J:39:ALA:N	2.42	0.44
12:K:100:GLU:O	12:K:104:ARG:HG2	2.18	0.44
27:Z:153:TYR:HE2	27:Z:184:THR:HG21	1.82	0.44
1:2:410:U:O4	32:e:30:PRO:HD2	2.18	0.43
1:2:980:A:O3'	21:T:52:HIS:ND1	2.50	0.43
1:2:1021:G:N2	1:2:1153:C:O2'	2.51	0.43
1:2:1113:C:OP1	12:K:18:ARG:NE	2.51	0.43
1:2:1136:C:H2'	1:2:1137:G:H8	1.82	0.43
1:2:1484:C:H2'	1:2:1485:U:C6	2.53	0.43
4:C:26:ARG:HG3	4:C:26:ARG:NH1	2.33	0.43
6:E:15:ILE:HG22	6:E:45:ASP:OD2	2.18	0.43
8:G:60:LEU:HD13	8:G:61:THR:N	2.33	0.43
10:I:44:GLU:HG3	10:I:104:ILE:HD13	2.00	0.43
12:K:45:VAL:HG22	12:K:79:ALA:HB2	1.99	0.43
19:R:101:LEU:HD12	19:R:105:ILE:HG22	1.98	0.43
22:U:145:GLU:HA	22:U:148:GLU:CG	2.48	0.43
26:Y:27:TYR:OH	28:3:44:GLU:HG3	2.18	0.43
27:Z:165:ARG:HH21	27:Z:180:GLU:CD	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1316:C:N3	1:2:1335:G:C6	2.86	0.43
2:A:20:TYR:CE2	2:A:41:ILE:HD13	2.53	0.43
2:A:102:SER:HB2	2:A:129:LYS:HA	2.00	0.43
3:B:81:ARG:HD3	3:B:81:ARG:HA	1.77	0.43
6:E:6:ARG:HG2	6:E:23:THR:HB	2.00	0.43
9:H:81:ILE:HA	9:H:159:GLU:HG2	2.00	0.43
10:I:101:GLU:OE1	10:I:101:GLU:N	2.51	0.43
13:L:5:ALA:HB3	13:L:76:ILE:HG13	2.00	0.43
26:Y:24:ARG:HD3	28:3:37:ASN:HB3	2.00	0.43
31:d:43:LEU:HD21	31:d:48:GLU:OE1	2.18	0.43
35:b:12:LYS:CE	35:b:16:GLY:O	2.66	0.43
1:2:334:A:OP2	36:2:1509:SPM:N5	2.46	0.43
1:2:858:G:H2'	1:2:859:U:C6	2.53	0.43
1:2:865:OMG:H4'	36:2:1541:SPM:H42	2.00	0.43
1:2:1216:G:N1	1:2:1249:U:O4	2.51	0.43
1:2:1342:C:P	9:H:49:ARG:HH21	2.42	0.43
3:B:97:ILE:HB	3:B:119:SER:OG	2.17	0.43
5:D:74:VAL:O	5:D:78:LEU:HD23	2.18	0.43
5:D:158:THR:O	5:D:158:THR:OG1	2.35	0.43
9:H:116:ARG:NH1	9:H:116:ARG:HB2	2.32	0.43
17:P:29:ILE:HD11	17:P:38:ARG:HA	1.99	0.43
35:b:21:ILE:HD11	35:b:35:ALA:HB2	2.00	0.43
1:2:2:A:H2'	7:F:177:TRP:CD1	2.53	0.43
1:2:137:C:O2'	8:G:118:GLN:HB2	2.18	0.43
1:2:725:A:OP2	1:2:771:G:N2	2.51	0.43
1:2:923:A:C2	1:2:1185:G:O4'	2.71	0.43
1:2:995:U:H2'	1:2:996:C:C6	2.54	0.43
1:2:1075:C:H2'	1:2:1076:C:H6	1.83	0.43
1:2:1111:C:H2'	1:2:1112:A:O4'	2.17	0.43
1:2:1161:G:H2'	1:2:1162:U:C6	2.53	0.43
1:2:1335:G:H2'	1:2:1336:U:C6	2.46	0.43
13:L:79:ASP:O	13:L:82:VAL:N	2.46	0.43
21:T:46:PHE:CE2	21:T:54:LEU:HD21	2.53	0.43
27:Z:185:LYS:HA	27:Z:185:LYS:CE	2.41	0.43
29:a:44:LYS:HG3	29:a:45:TYR:CD1	2.49	0.43
1:2:826:G:O6	36:2:1512:SPM:H81	2.19	0.43
1:2:849:G:OP2	40:2:1614:HOH:O	2.21	0.43
1:2:956:G:H22	1:2:1175:A:P	2.40	0.43
1:2:1165:G:N1	17:P:43:GLU:OE2	2.43	0.43
1:2:1375:C:O2'	1:2:1376:C:O5'	2.33	0.43
4:C:36:ASN:HB3	4:C:60:CYS:SG	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:57:ASP:OD1	8:G:58:THR:N	2.45	0.43
20:S:33:GLN:OE1	20:S:33:GLN:HA	2.18	0.43
21:T:99:PHE:CD2	21:T:105:MET:HE1	2.54	0.43
22:U:147:ALA:HB2	22:U:157:LEU:HD21	2.00	0.43
27:Z:64:LYS:HE3	27:Z:64:LYS:HB3	1.77	0.43
27:Z:118:MET:CE	27:Z:147:LEU:HG	2.47	0.43
28:3:90:CYS:O	28:3:92:LEU:HD12	2.19	0.43
29:a:36:TYR:HD1	29:a:70:PRO:HA	1.84	0.43
1:2:617:G:H2'	1:2:618:C:H6	1.83	0.43
1:2:938:U:OP2	17:P:27:SER:OG	2.19	0.43
1:2:979:A:HO2'	1:2:980:A:P	2.41	0.43
1:2:1399:G:H2'	1:2:1400:C:H6	1.84	0.43
3:B:22:GLU:O	3:B:26:LYS:HG2	2.19	0.43
9:H:122:ILE:HB	9:H:124:TYR:HE1	1.82	0.43
9:H:168:ALA:HB1	9:H:173:ASP:HB2	2.01	0.43
11:J:41:ASP:HA	11:J:59:TYR:O	2.19	0.43
17:P:43:GLU:O	29:a:9:ASN:ND2	2.51	0.43
27:Z:162:MET:HE3	27:Z:162:MET:HB3	1.87	0.43
1:2:29:G:H2'	1:2:30:C:C6	2.53	0.43
1:2:889:G:H22	39:5:102:GTP:PA	2.42	0.43
2:A:156:ASP:O	2:A:160:GLN:HG2	2.18	0.43
6:E:31:HIS:CG	6:E:80:GLY:HA3	2.54	0.43
6:E:116:TYR:CD1	6:E:159:LYS:HE3	2.53	0.43
6:E:131:ARG:HH21	6:E:143:LEU:HB3	1.83	0.43
9:H:112:GLU:HA	9:H:129:ASP:HA	2.01	0.43
13:L:54:PRO:O	17:P:38:ARG:NH2	2.50	0.43
16:O:72:ILE:CG2	16:O:75:LEU:HD23	2.49	0.43
16:O:96:THR:O	16:O:100:ILE:HG13	2.19	0.43
20:S:53:TYR:HA	20:S:56:ARG:HG2	2.01	0.43
31:d:27:TYR:HD1	31:d:32:MET:HB3	1.84	0.43
1:2:883:U:H2'	1:2:884:U:C6	2.54	0.43
1:2:1260:C:H5'	16:O:21:LYS:HE3	2.00	0.43
1:2:1388:A:HO2'	1:2:1389:G:H8	1.64	0.43
3:B:122:LEU:HD13	3:B:126:ILE:HD13	1.99	0.43
8:G:127:THR:O	8:G:130:VAL:HG12	2.19	0.43
14:M:33:ILE:O	14:M:33:ILE:HD12	2.19	0.43
20:S:9:ILE:HD12	20:S:9:ILE:H	1.84	0.43
23:V:19:ARG:HG2	23:V:32:SER:HB3	2.01	0.43
30:c:39:GLU:H	30:c:39:GLU:CD	2.27	0.43
30:c:53:LYS:HD2	30:c:54:LYS:N	2.33	0.43
1:2:132:A:H2'	1:2:133:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:391:G:OP2	36:2:1516:SPM:H42	2.19	0.43
1:2:906:G:O6	36:2:1527:SPM:H81	2.19	0.43
1:2:907:U:OP1	36:2:1526:SPM:N1	2.52	0.43
1:2:1312:U:OP2	40:2:1613:HOH:O	2.21	0.43
3:B:21:LYS:HD3	3:B:22:GLU:N	2.33	0.43
3:B:34:GLU:OE1	3:B:34:GLU:C	2.62	0.43
4:C:40:VAL:HG21	4:C:58:PRO:HG2	2.01	0.43
12:K:58:ASN:OD1	12:K:58:ASN:N	2.51	0.43
16:O:96:THR:OG1	16:O:97:SER:N	2.52	0.43
17:P:51:ARG:HB2	17:P:53:TYR:CE1	2.53	0.43
29:a:52:ALA:HA	29:a:55:ARG:HG2	2.00	0.43
35:b:89:LYS:HA	35:b:89:LYS:HD2	1.79	0.43
1:2:741:A:H4'	1:2:1471:G:O2'	2.18	0.43
1:2:1188:G:C2	21:T:120:VAL:HG21	2.53	0.43
1:2:1280:G:N2	1:2:1282:A:H3'	2.33	0.43
1:2:1316:C:C2	1:2:1335:G:C2	3.07	0.43
1:2:1336:U:H2'	1:2:1337:G:H5'	2.00	0.43
36:2:1533:SPM:C7	36:2:1533:SPM:H31	2.48	0.43
4:C:31:GLU:CD	4:C:43:ARG:HD3	2.43	0.43
4:C:45:ASP:OD1	4:C:48:CYS:HB2	2.19	0.43
7:F:148:ASP:OD1	7:F:148:ASP:N	2.51	0.43
11:J:35:THR:CG2	11:J:60:THR:HG22	2.49	0.43
14:M:123:ARG:NH1	35:b:24:ASP:HA	2.33	0.43
15:N:49:MET:HB3	15:N:49:MET:HE2	1.86	0.43
20:S:34:ILE:HA	20:S:37:ARG:HG2	2.00	0.43
29:a:21:CYS:HB3	29:a:25:ASN:N	2.34	0.43
1:2:25:G:H2'	1:2:26:A:C8	2.54	0.42
1:2:683:G:O6	35:b:15:LYS:HE2	2.19	0.42
1:2:927:G:OP2	36:2:1524:SPM:H112	2.19	0.42
1:2:1053:C:H2'	1:2:1054:A:H8	1.84	0.42
1:2:1316:C:H2'	1:2:1317:G:C8	2.54	0.42
1:2:1457:6MZ:OP1	40:2:1615:HOH:O	2.21	0.42
11:J:96:ILE:HD11	11:J:111:VAL:HG21	2.00	0.42
12:K:13:ARG:HE	12:K:13:ARG:HB3	1.61	0.42
13:L:4:LYS:CE	13:L:75:ASP:HB3	2.47	0.42
13:L:9:LEU:O	13:L:71:LYS:HA	2.19	0.42
13:L:17:LEU:HD21	13:L:72:ARG:HG2	2.00	0.42
13:L:76:ILE:CD1	13:L:86:LEU:CD1	2.97	0.42
16:O:27:ALA:HA	16:O:32:ILE:HG22	1.99	0.42
33:4:43:A:H2'	33:4:44:A:C8	2.54	0.42
1:2:365:G:H2'	1:2:366:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:413:U:H2'	1:2:414:C:C6	2.54	0.42
1:2:1013:U:OP1	27:Z:142:ALA:N	2.33	0.42
1:2:1445:G:H2'	1:2:1446:G:C8	2.55	0.42
3:B:183:ILE:HD13	3:B:183:ILE:HA	1.87	0.42
4:C:8:ARG:HH21	4:C:9:GLU:CD	2.27	0.42
7:F:198:LEU:O	7:F:201:THR:OG1	2.23	0.42
8:G:80:LYS:HZ1	8:G:147:PRO:HD3	1.84	0.42
8:G:140:ALA:HB1	8:G:144:ILE:HD13	2.01	0.42
9:H:5:ASN:OD1	9:H:5:ASN:N	2.52	0.42
9:H:30:TYR:HD2	9:H:132:PRO:HB2	1.83	0.42
10:I:55:ASP:OD2	10:I:60:LYS:NZ	2.52	0.42
14:M:26:SER:HA	14:M:33:ILE:HA	2.02	0.42
14:M:112:ASP:OD2	14:M:112:ASP:C	2.62	0.42
17:P:21:ARG:HG3	29:a:16:TRP:CZ2	2.54	0.42
22:U:64:LEU:HD22	22:U:108:PHE:CZ	2.54	0.42
22:U:143:PHE:CZ	22:U:153:LEU:HD12	2.54	0.42
28:3:116:LYS:HA	28:3:119:ASN:HB2	2.00	0.42
31:d:69:LYS:HE2	31:d:70:LYS:NZ	2.34	0.42
1:2:302:G:N2	1:2:305:A:OP2	2.41	0.42
1:2:504:C:OP1	5:D:38:LYS:NZ	2.37	0.42
1:2:642:G:H2'	1:2:643:A:H8	1.81	0.42
36:2:1509:SPM:H92	36:2:1509:SPM:H122	1.73	0.42
36:2:1540:SPM:C3	30:c:101:ARG:NH1	2.79	0.42
3:B:195:ALA:HB2	3:B:226:GLU:OE1	2.20	0.42
8:G:59:LEU:HD13	8:G:114:THR:HG21	2.01	0.42
9:H:15:LYS:O	9:H:16:TRP:HD1	2.02	0.42
13:L:9:LEU:HD12	13:L:9:LEU:HA	1.82	0.42
15:N:119:LEU:HD13	15:N:122:VAL:HB	2.01	0.42
22:U:5:MET:O	22:U:6:ILE:HD13	2.19	0.42
27:Z:132:ILE:HD11	27:Z:146:LYS:HE2	2.00	0.42
1:2:239:C:H4'	19:R:100:PRO:HG3	2.02	0.42
1:2:286:A:H8	1:2:286:A:OP2	2.02	0.42
1:2:1084:G:H2'	1:2:1085:G:H8	1.83	0.42
1:2:1399:G:H2'	1:2:1400:C:C6	2.55	0.42
3:B:64:ARG:HD3	3:B:64:ARG:HA	1.85	0.42
7:F:28:ILE:HG22	7:F:30:SER:H	1.83	0.42
26:Y:54:PRO:HG2	26:Y:57:ARG:HE	1.84	0.42
29:a:28:LEU:CB	29:a:35:LEU:HD23	2.49	0.42
29:a:57:LEU:HD23	29:a:58:LYS:N	2.34	0.42
1:2:211:C:O2	1:2:211:C:H3'	2.20	0.42
1:2:242:C:OP1	19:R:75:SER:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:408:A:O5'	5:D:141:PRO:HD2	2.20	0.42
1:2:420:A:H4'	1:2:421:G:O4'	2.20	0.42
1:2:846:C:O2'	1:2:847:U:H5'	2.19	0.42
1:2:968:A:C2	1:2:993:A:C4	3.08	0.42
1:2:1000:G:H2'	1:2:1001:A:O4'	2.19	0.42
1:2:1032:OMU:H5'	3:B:162:LYS:HE2	2.01	0.42
1:2:1136:C:H2'	1:2:1137:G:C8	2.54	0.42
1:2:1207:A:H2'	1:2:1208:G:H8	1.84	0.42
1:2:1327:A:O2'	1:2:1329:U:O4	2.29	0.42
8:G:144:ILE:HD12	8:G:144:ILE:N	2.35	0.42
13:L:30:LYS:HE3	13:L:30:LYS:HB2	1.82	0.42
16:O:123:LEU:HD11	21:T:119:LYS:CD	2.47	0.42
21:T:19:ILE:H	21:T:19:ILE:HD12	1.83	0.42
26:Y:43:ARG:HB3	26:Y:43:ARG:NH1	2.34	0.42
29:a:36:TYR:CD1	29:a:70:PRO:HB3	2.55	0.42
1:2:391:G:OP2	36:2:1516:SPM:H61	2.19	0.42
1:2:796:A:H2'	1:2:797:U:C6	2.54	0.42
1:2:810:C:H2'	1:2:811:A:H8	1.84	0.42
1:2:1243:A:OP2	27:Z:4:ILE:HG12	2.19	0.42
1:2:1299:G:N3	40:2:1663:HOH:O	2.37	0.42
1:2:1418:G:H2'	1:2:1419:G:H8	1.84	0.42
2:A:23:ILE:HG22	2:A:32:SER:HA	2.00	0.42
2:A:53:LEU:HD12	2:A:56:LEU:HD12	2.01	0.42
2:A:89:SER:OG	2:A:91:ASP:OD1	2.36	0.42
4:C:34:CYS:HB3	4:C:37:CYS:SG	2.59	0.42
9:H:9:ASP:OD1	9:H:11:LYS:HE3	2.18	0.42
9:H:10:ILE:HA	9:H:37:TYR:CE1	2.53	0.42
13:L:81:ARG:NH1	13:L:82:VAL:HA	2.33	0.42
23:V:20:ASP:OD2	23:V:20:ASP:C	2.62	0.42
28:3:58:GLN:OE1	28:3:58:GLN:N	2.51	0.42
28:3:109:ASP:OD1	28:3:109:ASP:N	2.52	0.42
35:b:10:ARG:HD2	35:b:34:LYS:HB2	2.01	0.42
1:2:150:A:OP2	36:2:1531:SPM:H71	2.20	0.42
1:2:192:G:O2'	1:2:193:A:H5''	2.19	0.42
1:2:1255:C:H2'	1:2:1256:C:C6	2.55	0.42
36:2:1528:SPM:H121	7:F:183:GLU:OE2	2.20	0.42
3:B:128:PRO:HA	3:B:159:GLU:OE2	2.20	0.42
8:G:16:PRO:HB2	8:G:112:TYR:HB2	2.00	0.42
9:H:91:LEU:HD12	30:c:97:TYR:OH	2.18	0.42
11:J:65:VAL:HG22	11:J:123:ALA:HB3	2.01	0.42
12:K:40:ILE:HG22	12:K:42:ILE:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:28:LEU:HD13	14:M:28:LEU:HA	1.89	0.42
22:U:60:ARG:HG3	22:U:107:ILE:HD12	2.00	0.42
23:V:37:HIS:HB2	23:V:40:SER:OG	2.20	0.42
28:3:78:VAL:HG12	28:3:79:TYR:N	2.35	0.42
1:2:810:C:H2'	1:2:811:A:C8	2.55	0.42
1:2:924:U:H4'	1:2:925:U:H5''	2.01	0.42
1:2:1125:C:H2'	1:2:1126:C:H6	1.85	0.42
1:2:1265:U:OP1	30:c:14:LYS:NZ	2.26	0.42
1:2:1366:OMC:HM22	1:2:1367:C:H5'	2.02	0.42
5:D:81:GLY:O	5:D:84:LYS:NZ	2.52	0.42
9:H:111:ARG:HE	9:H:135:ARG:HH12	1.68	0.42
12:K:27:LYS:HA	12:K:62:SER:O	2.19	0.42
25:X:53:LEU:HG	25:X:75:GLU:OE1	2.19	0.42
27:Z:106:LYS:HZ3	27:Z:106:LYS:HG3	1.72	0.42
1:2:612:A:H5''	10:I:57:ARG:HE	1.84	0.42
1:2:784:G:H2'	1:2:785:C:H6	1.84	0.42
1:2:943:U:N3	17:P:12:TYR:O	2.53	0.42
1:2:990:C:C4	1:2:991:U:C5	3.08	0.42
1:2:1466:4AC:O7	1:2:1466:4AC:H5	2.19	0.42
1:2:1469:U:O4	36:2:1522:SPM:H22	2.20	0.42
2:A:14:TRP:CH2	14:M:69:LYS:HE3	2.54	0.42
12:K:55:LEU:HD11	12:K:106:TYR:CG	2.55	0.42
16:O:11:ILE:HG22	16:O:12:PHE:CD2	2.54	0.42
16:O:54:GLU:OE1	30:c:41:ILE:HG23	2.19	0.42
17:P:31:LYS:O	17:P:34:ILE:HD12	2.20	0.42
27:Z:96:MET:HG3	27:Z:121:ILE:HG12	2.02	0.42
31:d:29:ARG:NH1	31:d:62:TRP:O	2.52	0.42
33:4:44:A:H2'	33:4:45:G:O4'	2.20	0.42
1:2:219:A:H2'	1:2:220:U:C6	2.55	0.42
1:2:236:G:O6	36:2:1532:SPM:H81	2.18	0.42
1:2:263:G:OP1	11:J:98:ARG:NE	2.52	0.42
1:2:326:A:H2	1:2:337:OMG:HN21	1.66	0.42
1:2:409:G:OP2	32:e:31:ARG:NH1	2.39	0.42
1:2:975:G:H1'	26:Y:53:LYS:NZ	2.35	0.42
1:2:989:C:H2'	1:2:990:C:H6	1.84	0.42
1:2:1012:A:O2'	27:Z:140:GLU:OE2	2.38	0.42
1:2:1340:U:H2'	1:2:1341:A:H8	1.84	0.42
12:K:7:LEU:HD12	12:K:24:TYR:HD2	1.84	0.42
12:K:46:ARG:O	12:K:50:MET:HG2	2.20	0.42
15:N:128:MET:HE3	15:N:128:MET:HB3	1.92	0.42
22:U:88:ARG:HA	22:U:94:GLU:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:410:U:C4	32:e:29:VAL:HB	2.55	0.41
1:2:522:A:O2'	1:2:525:G:O2'	2.35	0.41
1:2:563:C:OP1	6:E:184:GLY:HA3	2.20	0.41
1:2:708:C:H1'	18:Q:50:ILE:HG12	2.02	0.41
1:2:727:A:H4'	1:2:1480:G:N2	2.35	0.41
1:2:1028:C:H2'	1:2:1029:G:H8	1.85	0.41
1:2:1110:A:H5'	1:2:1111:C:OP2	2.20	0.41
1:2:1154:A:H4'	27:Z:154:LYS:HG3	2.01	0.41
1:2:1336:U:OP2	12:K:15:LYS:CD	2.67	0.41
1:2:1403:C:C6	1:2:1403:C:H5''	2.55	0.41
1:2:1435:C:H2'	1:2:1436:U:H6	1.85	0.41
36:2:1514:SPM:N14	27:Z:180:GLU:OE1	2.35	0.41
36:2:1520:SPM:HN11	36:2:1520:SPM:H41	1.54	0.41
36:2:1531:SPM:H42	36:2:1531:SPM:H72	1.82	0.41
3:B:98:ILE:HG13	3:B:140:ILE:HD12	2.02	0.41
6:E:146:LYS:CD	6:E:146:LYS:H	2.33	0.41
8:G:32:ILE:H	8:G:35:GLU:CD	2.28	0.41
9:H:132:PRO:O	9:H:135:ARG:HB2	2.20	0.41
11:J:113:SER:O	11:J:115:PRO:HD3	2.20	0.41
25:X:19:PHE:HB2	25:X:69:LEU:O	2.19	0.41
26:Y:54:PRO:CG	26:Y:57:ARG:HE	2.34	0.41
28:3:6:TYR:CZ	28:3:8:LYS:HD2	2.54	0.41
1:2:329:G:N1	1:2:332:A:OP2	2.51	0.41
1:2:494:A2M:HM'2	1:2:495:C:H6	1.86	0.41
1:2:572:C:OP1	5:D:54:GLN:NE2	2.47	0.41
1:2:612:A:C6	24:W:10:PRO:HG3	2.56	0.41
1:2:674:A:H2'	1:2:675:C:C6	2.55	0.41
1:2:990:C:H1'	26:Y:62:LYS:NZ	2.34	0.41
2:A:22:VAL:HG23	2:A:33:LEU:HB2	2.01	0.41
2:A:156:ASP:O	2:A:159:THR:OG1	2.30	0.41
3:B:45:ALA:HA	3:B:192:LYS:HD2	2.01	0.41
4:C:37:CYS:HB3	4:C:60:CYS:HB2	2.01	0.41
8:G:2:PRO:O	8:G:123:GLN:HB2	2.20	0.41
9:H:15:LYS:C	9:H:16:TRP:HD1	2.27	0.41
19:R:88:ARG:CZ	19:R:88:ARG:HB3	2.49	0.41
25:X:14:ILE:HA	25:X:17:PHE:CB	2.50	0.41
28:3:51:VAL:HB	28:3:66:LEU:HD21	2.03	0.41
28:3:73:LYS:C	28:3:75:ILE:H	2.28	0.41
35:b:12:LYS:CD	35:b:18:VAL:CG2	2.88	0.41
1:2:430:U:C4	1:2:431:C:C5	3.07	0.41
1:2:647:G:H4'	14:M:41:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:965:A:H2'	28:3:94:VAL:HG11	2.02	0.41
1:2:1222:C:H2'	1:2:1223:C:C6	2.55	0.41
1:2:1226:C:H2'	1:2:1227:C:H6	1.85	0.41
36:2:1515:SPM:H91	12:K:121:GLU:OE1	2.19	0.41
2:A:96:LEU:HB3	2:A:125:LEU:HD11	2.01	0.41
2:A:114:ASP:OD1	2:A:114:ASP:N	2.34	0.41
3:B:63:TYR:CD2	3:B:64:ARG:HG2	2.55	0.41
3:B:136:LEU:HD12	3:B:136:LEU:HA	1.85	0.41
6:E:43:ILE:CG2	6:E:59:ILE:HD11	2.50	0.41
18:Q:14:ARG:HD3	18:Q:60:LEU:HD11	2.02	0.41
18:Q:114:GLU:OE1	18:Q:114:GLU:HA	2.20	0.41
21:T:6:PRO:HG2	21:T:9:TRP:CZ2	2.55	0.41
27:Z:67:ALA:N	27:Z:81:ILE:HD11	2.35	0.41
27:Z:118:MET:SD	27:Z:129:ALA:HB3	2.60	0.41
28:3:25:LYS:HG3	28:3:26:ALA:N	2.35	0.41
28:3:39:THR:O	28:3:43:VAL:HG23	2.20	0.41
30:c:45:VAL:HG21	30:c:84:ILE:HG12	2.02	0.41
1:2:203:G:O6	1:2:219:A:N6	2.53	0.41
1:2:541:U:H2'	1:2:542:A:H8	1.85	0.41
1:2:924:U:C4	1:2:1188:G:C4	3.07	0.41
1:2:1170:C:H2'	1:2:1171:C:H6	1.85	0.41
1:2:1273:G:OP1	16:O:117:ARG:NH1	2.44	0.41
1:2:1481:C:H2'	1:2:1482:G:H8	1.86	0.41
6:E:175:GLU:N	6:E:175:GLU:OE2	2.54	0.41
6:E:178:TYR:CE1	6:E:234:SER:HB2	2.55	0.41
14:M:47:ARG:HB3	14:M:47:ARG:CZ	2.50	0.41
18:Q:17:ARG:CZ	18:Q:17:ARG:HB3	2.51	0.41
22:U:127:LEU:CD1	22:U:132:ARG:HB2	2.50	0.41
30:c:7:LYS:HA	30:c:7:LYS:HD2	1.70	0.41
30:c:14:LYS:HD2	30:c:18:LYS:HG2	2.02	0.41
30:c:17:LYS:HA	30:c:17:LYS:HD2	1.90	0.41
30:c:85:LEU:HD23	30:c:106:TYR:CE2	2.55	0.41
33:4:16:C:O2'	33:4:17:C:N1	2.53	0.41
1:2:339:C:H2'	1:2:340:C:H6	1.85	0.41
1:2:505:G:C4	32:e:30:PRO:HG3	2.56	0.41
1:2:1070:C:H2'	1:2:1071:C:H6	1.85	0.41
1:2:1091:U:O4	1:2:1104:G:O6	2.39	0.41
1:2:1237:G:H2'	1:2:1238:A:O4'	2.19	0.41
2:A:119:ARG:HD2	2:A:190:LYS:HE2	2.02	0.41
7:F:138:VAL:HG11	7:F:201:THR:HG22	2.02	0.41
11:J:108:LEU:HD13	11:J:108:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:90:LEU:HD12	12:K:91:VAL:N	2.36	0.41
12:K:124:MET:CE	13:L:60:LYS:H	2.33	0.41
13:L:6:ARG:HH11	13:L:73:LEU:HD21	1.86	0.41
13:L:84:ARG:HA	13:L:87:MET:HG2	2.02	0.41
21:T:60:TYR:CE2	21:T:68:LYS:HG2	2.55	0.41
22:U:13:PRO:HG3	22:U:66:ARG:NH2	2.36	0.41
29:a:27:LYS:HB3	29:a:27:LYS:HE2	1.78	0.41
1:2:263:G:H5''	11:J:98:ARG:HB3	2.02	0.41
1:2:683:G:OP2	1:2:791:G:N2	2.53	0.41
1:2:843:4AC:O7	1:2:843:4AC:H5	2.20	0.41
1:2:1004:G:O2'	1:2:1178:C:O2'	2.32	0.41
1:2:1200:C:H4'	1:2:1267:G:H21	1.85	0.41
36:2:1506:SPM:H62	36:2:1506:SPM:H31	1.78	0.41
2:A:15:LYS:HD3	2:A:15:LYS:N	2.35	0.41
6:E:155:LEU:HD13	6:E:223:ILE:HG12	2.03	0.41
6:E:222:ASN:OD1	6:E:225:ASN:ND2	2.51	0.41
9:H:10:ILE:HG12	9:H:35:PRO:O	2.20	0.41
14:M:72:MET:SD	14:M:72:MET:N	2.94	0.41
18:Q:85:ASP:OD1	18:Q:85:ASP:N	2.50	0.41
19:R:42:GLU:OE1	19:R:113:VAL:HG21	2.20	0.41
21:T:56:LYS:HE2	21:T:56:LYS:HB2	1.86	0.41
22:U:10:MET:N	22:U:10:MET:SD	2.93	0.41
1:2:100:A:H4'	11:J:17:LYS:HD2	2.02	0.41
1:2:131:U:OP1	36:2:1531:SPM:N10	2.53	0.41
1:2:439:U:N3	1:2:442:A:OP2	2.41	0.41
1:2:561:U:H2'	1:2:562:C:H6	1.86	0.41
1:2:1076:C:H2'	1:2:1077:A:C8	2.50	0.41
1:2:1188:G:H2'	21:T:120:VAL:CG2	2.49	0.41
1:2:1273:G:N7	16:O:128:ARG:NH2	2.69	0.41
1:2:1342:C:H5''	1:2:1343:G:O5'	2.20	0.41
1:2:1373:C:O2	1:2:1448:G:C2	2.71	0.41
1:2:1403:C:H3'	1:2:1404:U:C6	2.56	0.41
8:G:126:ALA:HB1	8:G:129:LEU:HD12	2.03	0.41
9:H:116:ARG:HH12	25:X:32:VAL:HG11	1.84	0.41
13:L:4:LYS:O	13:L:102:ILE:HG12	2.20	0.41
14:M:72:MET:O	14:M:106:ILE:HG13	2.21	0.41
15:N:98:ASP:N	15:N:98:ASP:OD1	2.54	0.41
19:R:88:ARG:HB3	19:R:88:ARG:NH1	2.36	0.41
20:S:43:SER:HB3	20:S:46:VAL:HG22	2.02	0.41
21:T:5:ILE:H	21:T:5:ILE:HG13	1.73	0.41
25:X:14:ILE:HG13	31:d:54:LYS:HZ3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:38:ASN:HB3	26:Y:48:MET:HE3	2.01	0.41
33:4:16:C:HO2'	33:4:17:C:CI'	2.34	0.41
1:2:569:G:C4	1:2:570:A:C8	3.08	0.41
1:2:727:A:N3	1:2:1469:U:O2'	2.54	0.41
2:A:24:THR:OG1	2:A:31:VAL:N	2.53	0.41
5:D:164:ARG:HD2	5:D:165:PRO:O	2.21	0.41
11:J:101:LYS:HE2	11:J:101:LYS:HB3	1.89	0.41
18:Q:67:LYS:HB2	18:Q:67:LYS:HE2	1.88	0.41
20:S:42:LYS:HE3	20:S:42:LYS:HB3	1.98	0.41
22:U:121:LYS:O	22:U:123:LYS:HG2	2.21	0.41
28:3:27:LYS:HA	28:3:101:ILE:HD11	2.03	0.41
30:c:73:LYS:O	30:c:73:LYS:HG3	2.21	0.41
31:d:65:LEU:HB3	31:d:66:PRO:HD3	2.02	0.41
33:4:50:U:O4	33:4:64:G:O6	2.38	0.41
1:2:110:A:N6	1:2:176:G:H1'	2.35	0.41
1:2:413:U:H2'	1:2:414:C:H6	1.86	0.41
1:2:439:U:OP2	23:V:101:ARG:NH1	2.44	0.41
1:2:543:G:H2'	1:2:544:C:C6	2.55	0.41
1:2:587:G:OP1	36:E:301:SPM:H122	2.21	0.41
1:2:676:C:O2'	1:2:693:G:O4'	2.37	0.41
1:2:900:C:H2'	1:2:901:A:H8	1.86	0.41
1:2:910:A:OP1	36:2:1525:SPM:H92	2.21	0.41
1:2:964:G:O2'	1:2:993:A:N1	2.38	0.41
1:2:1003:A:H2'	1:2:1004:G:O4'	2.21	0.41
1:2:1115:A:O4'	13:L:40:PRO:HB2	2.21	0.41
1:2:1116:G:OP1	13:L:70:HIS:ND1	2.54	0.41
1:2:1155:C:H2'	1:2:1156:G:O4'	2.21	0.41
1:2:1350:C:C2	1:2:1351:U:C5	3.09	0.41
1:2:1397:A:H3'	1:2:1398:G:H8	1.86	0.41
1:2:1455:U:OP2	39:5:102:GTP:O2'	2.36	0.41
1:2:1466:4AC:HM73	1:2:1467:4AC:HM72	2.02	0.41
2:A:47:ARG:HB2	2:A:71:ILE:HD12	2.02	0.41
3:B:29:LYS:HB2	3:B:76:ARG:HD2	2.02	0.41
3:B:95:GLN:HE21	3:B:95:GLN:HB2	1.59	0.41
4:C:39:GLU:HG3	4:C:59:ASN:ND2	2.35	0.41
5:D:145:VAL:HG13	5:D:149:GLU:HG3	2.02	0.41
9:H:61:LEU:O	9:H:65:ILE:HG12	2.21	0.41
13:L:79:ASP:O	13:L:81:ARG:N	2.54	0.41
15:N:36:LYS:HB3	15:N:39:GLU:HG3	2.03	0.41
20:S:27:ASP:OD2	20:S:27:ASP:C	2.63	0.41
21:T:89:ALA:HA	21:T:97:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:T:90:VAL:HG22	21:T:99:PHE:HE1	1.84	0.41
22:U:69:TYR:HE2	22:U:132:ARG:HG3	1.85	0.41
24:W:28:GLN:OE1	24:W:40:CYS:HA	2.20	0.41
25:X:15:GLU:N	25:X:15:GLU:OE1	2.53	0.41
27:Z:91:LEU:HD23	27:Z:91:LEU:HA	1.85	0.41
27:Z:100:LEU:HB3	27:Z:179:VAL:HG11	2.02	0.41
35:b:7:ASN:ND2	35:b:11:ARG:NH1	2.63	0.41
35:b:84:ALA:O	35:b:88:ARG:HG3	2.20	0.41
1:2:989:C:C2	1:2:990:C:C5	3.09	0.41
1:2:1126:C:H2'	1:2:1127:G:H8	1.86	0.41
1:2:1384:U:H3'	1:2:1385:A:H8	1.85	0.41
2:A:94:ARG:HB2	35:b:63:TYR:HB2	2.03	0.41
5:D:134:ASN:OD1	5:D:134:ASN:C	2.64	0.41
7:F:45:GLU:HA	7:F:48:ASP:OD1	2.21	0.41
10:I:81:LEU:HB2	10:I:86:MET:HE2	2.02	0.41
14:M:93:ALA:O	14:M:97:ILE:HG12	2.21	0.41
18:Q:27:THR:OG1	18:Q:28:ARG:N	2.54	0.41
19:R:21:LYS:H	19:R:21:LYS:HG2	1.61	0.41
20:S:24:ILE:HG13	20:S:58:TYR:CE2	2.57	0.41
20:S:58:TYR:HD1	20:S:58:TYR:O	2.04	0.41
1:2:147:G:N3	1:2:148:G:C8	2.89	0.40
1:2:340:C:H2'	1:2:341:C:H6	1.86	0.40
1:2:863:A:H2'	1:2:864:A:C8	2.56	0.40
1:2:926:OMG:C8	36:2:1524:SPM:H82	2.56	0.40
36:2:1517:SPM:H72	36:2:1517:SPM:H41	1.71	0.40
9:H:65:ILE:O	9:H:67:ARG:N	2.54	0.40
18:Q:2:ASN:HA	18:Q:5:ARG:HG3	2.03	0.40
20:S:24:ILE:O	20:S:58:TYR:HE2	2.03	0.40
27:Z:17:LYS:HG3	29:a:16:TRP:CG	2.56	0.40
28:3:81:SER:HB2	28:3:86:LEU:HG	2.04	0.40
33:4:23:C:C2	33:4:24:U:C5	3.09	0.40
33:4:67:C:H2'	33:4:68:C:H6	1.86	0.40
1:2:390:C:P	36:2:1516:SPM:H41	2.61	0.40
1:2:1080:A:H4'	13:L:37:GLY:HA3	2.02	0.40
1:2:1207:A:H2'	1:2:1208:G:C8	2.56	0.40
1:2:1311:G:H22	1:2:1337:G:H2'	1.83	0.40
1:2:1393:G:H2'	1:2:1394:G:C8	2.52	0.40
3:B:113:PHE:O	3:B:117:VAL:HG22	2.21	0.40
6:E:68:ASP:HA	6:E:162:LEU:HD13	2.03	0.40
6:E:145:ASP:N	6:E:145:ASP:OD1	2.51	0.40
7:F:54:LEU:HD23	7:F:54:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:163:MET:HA	8:G:197:ARG:HB3	2.03	0.40
11:J:57:LEU:HG	11:J:119:GLY:O	2.22	0.40
16:O:73:LYS:HA	16:O:73:LYS:HD3	1.89	0.40
33:4:25:C:C4	33:4:26:G:N7	2.90	0.40
33:4:50:U:H2'	33:4:51:C:C6	2.56	0.40
1:2:40:G:H2'	1:2:41:G:C8	2.57	0.40
1:2:52:OMU:HM22	1:2:53:G:O4'	2.22	0.40
1:2:100:A:H5''	11:J:11:LYS:HD3	2.02	0.40
1:2:644:G:O4'	14:M:33:ILE:HD11	2.20	0.40
1:2:1014:G:H5''	27:Z:134:SER:OG	2.21	0.40
1:2:1271:U:P	16:O:130:GLN:HE21	2.43	0.40
1:2:1342:C:OP1	9:H:49:ARG:NH2	2.54	0.40
1:2:1478:4AC:O7	1:2:1478:4AC:H5	2.21	0.40
1:2:1492:C:O2	1:2:1492:C:C2'	2.70	0.40
5:D:164:ARG:HE	5:D:164:ARG:C	2.28	0.40
7:F:56:TYR:CE1	7:F:107:ILE:HD11	2.56	0.40
11:J:42:ILE:HG12	11:J:59:TYR:HB2	2.04	0.40
13:L:25:ARG:O	13:L:29:GLU:HG2	2.21	0.40
13:L:101:LEU:HD23	13:L:101:LEU:HA	1.82	0.40
16:O:114:ARG:NH1	16:O:114:ARG:HA	2.36	0.40
22:U:56:TRP:CH2	22:U:103:VAL:HG21	2.56	0.40
22:U:146:LEU:O	22:U:150:ASN:HB3	2.22	0.40
27:Z:74:PHE:CE1	29:a:17:LEU:HD21	2.57	0.40
27:Z:158:GLN:OE1	27:Z:158:GLN:N	2.52	0.40
28:3:103:GLU:N	28:3:103:GLU:OE1	2.54	0.40
30:c:97:TYR:CE1	30:c:107:ILE:HG12	2.57	0.40
35:b:11:ARG:HA	35:b:11:ARG:NE	2.35	0.40
35:b:12:LYS:HE3	35:b:16:GLY:O	2.21	0.40
1:2:265:G:P	11:J:117:GLN:HE21	2.45	0.40
1:2:416:C:H2'	1:2:417:G:O4'	2.22	0.40
1:2:498:G:H2'	1:2:499:C:C6	2.57	0.40
1:2:872:A:OP1	15:N:28:ARG:NH2	2.32	0.40
1:2:1191:C:H2'	1:2:1192:G:C8	2.57	0.40
1:2:1242:U:H5''	1:2:1243:A:O4'	2.20	0.40
1:2:1470:A:H2'	1:2:1471:G:H8	1.87	0.40
6:E:30:PRO:HD2	6:E:78:PRO:HG2	2.03	0.40
9:H:115:THR:HG22	9:H:128:VAL:HG11	2.04	0.40
13:L:30:LYS:HG2	13:L:81:ARG:HH21	1.87	0.40
14:M:56:MET:SD	14:M:57:LEU:HD22	2.61	0.40
21:T:7:PRO:HA	21:T:10:LYS:HG2	2.03	0.40
28:3:41:LYS:HB3	28:3:41:LYS:HE3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:101:ILE:O	28:3:102:LEU:HD13	2.21	0.40
1:2:310:G:H5''	1:2:311:A:OP1	2.21	0.40
1:2:447:C:C4	1:2:448:G:N7	2.90	0.40
1:2:815:G:O6	36:2:1542:SPM:H41	2.21	0.40
1:2:920:U:H2'	1:2:921:C:O4'	2.22	0.40
1:2:967:G:O6	28:3:37:ASN:HB2	2.22	0.40
1:2:1373:C:C2	1:2:1448:G:N1	2.82	0.40
1:2:1390:A:OP2	1:2:1390:A:H8	2.05	0.40
3:B:25:ARG:HH12	3:B:76:ARG:HH22	1.70	0.40
7:F:118:ARG:HH22	7:F:209:ASP:CG	2.26	0.40
12:K:13:ARG:HG2	12:K:18:ARG:HD3	2.02	0.40
13:L:41:LEU:HB2	13:L:71:LYS:HB3	2.03	0.40
14:M:9:TRP:CB	14:M:28:LEU:HD21	2.51	0.40
14:M:57:LEU:HD13	14:M:57:LEU:HA	1.96	0.40
16:O:108:GLU:HB3	16:O:112:LYS:CE	2.48	0.40
17:P:6:PRO:HB2	29:a:45:TYR:OH	2.21	0.40
18:Q:124:THR:HG22	18:Q:128:LYS:HE3	2.04	0.40
19:R:49:ARG:HH12	19:R:89:GLU:CD	2.29	0.40
21:T:31:ILE:HD12	21:T:31:ILE:HA	1.91	0.40
25:X:45:GLU:HG3	25:X:49:LYS:HE2	2.02	0.40
27:Z:37:LEU:HD22	27:Z:38:LYS:HD3	2.03	0.40
32:e:25:LYS:HA	32:e:25:LYS:HD3	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	184/208 (88%)	178 (97%)	6 (3%)	0	100	100
3	B	213/231 (92%)	207 (97%)	6 (3%)	0	100	100
4	C	56/65 (86%)	54 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	D	164/181 (91%)	163 (99%)	1 (1%)	0	100	100
6	E	236/239 (99%)	228 (97%)	8 (3%)	0	100	100
7	F	208/214 (97%)	202 (97%)	6 (3%)	0	100	100
8	G	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
9	H	187/193 (97%)	176 (94%)	11 (6%)	0	100	100
10	I	130/133 (98%)	127 (98%)	3 (2%)	0	100	100
11	J	125/133 (94%)	124 (99%)	1 (1%)	0	100	100
12	K	131/137 (96%)	122 (93%)	9 (7%)	0	100	100
13	L	99/102 (97%)	95 (96%)	4 (4%)	0	100	100
14	M	125/132 (95%)	117 (94%)	7 (6%)	1 (1%)	16	44
15	N	144/147 (98%)	135 (94%)	9 (6%)	0	100	100
16	O	138/165 (84%)	131 (95%)	7 (5%)	0	100	100
17	P	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
18	Q	143/152 (94%)	143 (100%)	0	0	100	100
19	R	111/114 (97%)	110 (99%)	1 (1%)	0	100	100
20	S	64/79 (81%)	63 (98%)	1 (2%)	0	100	100
21	T	126/140 (90%)	123 (98%)	3 (2%)	0	100	100
22	U	152/158 (96%)	145 (95%)	7 (5%)	0	100	100
23	V	105/120 (88%)	102 (97%)	3 (3%)	0	100	100
24	W	63/66 (96%)	57 (90%)	6 (10%)	0	100	100
25	X	65/83 (78%)	54 (83%)	11 (17%)	0	100	100
26	Y	47/75 (63%)	39 (83%)	8 (17%)	0	100	100
27	Z	194/229 (85%)	189 (97%)	5 (3%)	0	100	100
28	3	115/127 (91%)	104 (90%)	11 (10%)	0	100	100
29	a	69/72 (96%)	63 (91%)	6 (9%)	0	100	100
30	c	107/110 (97%)	96 (90%)	10 (9%)	1 (1%)	14	41
31	d	66/72 (92%)	63 (96%)	3 (4%)	0	100	100
32	e	41/52 (79%)	40 (98%)	1 (2%)	0	100	100
35	b	89/95 (94%)	89 (100%)	0	0	100	100
All	All	3959/4292 (92%)	3792 (96%)	165 (4%)	2 (0%)	49	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	M	119	ASP
30	c	102	ARG

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%)	51 (100%)	0	100	100
5	D	147/158 (93%)	146 (99%)	1 (1%)	76	92
6	E	214/215 (100%)	209 (98%)	5 (2%)	44	76
7	F	180/184 (98%)	178 (99%)	2 (1%)	65	88
8	G	186/187 (100%)	185 (100%)	1 (0%)	81	93
9	H	165/167 (99%)	160 (97%)	5 (3%)	36	70
10	I	113/114 (99%)	113 (100%)	0	100	100
11	J	104/110 (94%)	101 (97%)	3 (3%)	37	71
12	K	109/113 (96%)	106 (97%)	3 (3%)	38	72
13	L	93/94 (99%)	90 (97%)	3 (3%)	34	68
14	M	93/98 (95%)	91 (98%)	2 (2%)	45	77
15	N	122/123 (99%)	120 (98%)	2 (2%)	55	83
16	O	121/142 (85%)	120 (99%)	1 (1%)	73	90
17	P	45/46 (98%)	44 (98%)	1 (2%)	45	77
18	Q	125/129 (97%)	125 (100%)	0	100	100
19	R	101/102 (99%)	99 (98%)	2 (2%)	48	78
20	S	63/75 (84%)	61 (97%)	2 (3%)	34	68
21	T	116/126 (92%)	113 (97%)	3 (3%)	40	73
22	U	134/138 (97%)	129 (96%)	5 (4%)	30	64
23	V	92/99 (93%)	90 (98%)	2 (2%)	45	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	W	57/58 (98%)	54 (95%)	3 (5%)	20	52
25	X	58/73 (80%)	55 (95%)	3 (5%)	21	52
26	Y	43/65 (66%)	43 (100%)	0	100	100
27	Z	163/195 (84%)	159 (98%)	4 (2%)	42	74
28	3	97/105 (92%)	95 (98%)	2 (2%)	47	77
29	a	61/62 (98%)	58 (95%)	3 (5%)	22	54
30	c	95/96 (99%)	92 (97%)	3 (3%)	34	68
31	d	62/65 (95%)	61 (98%)	1 (2%)	55	83
32	e	40/46 (87%)	40 (100%)	0	100	100
35	b	75/79 (95%)	73 (97%)	2 (3%)	39	73
All	All	3475/3704 (94%)	3405 (98%)	70 (2%)	48	78

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	49	VAL
2	A	77	ASP
3	B	16	LEU
3	B	37	VAL
3	B	126	ILE
3	B	182	LEU
5	D	97	THR
6	E	81	LEU
6	E	112	ASP
6	E	151	ASN
6	E	187	VAL
6	E	208	VAL
7	F	9	ASN
7	F	60	ASP
8	G	56	VAL
9	H	58	VAL
9	H	61	LEU
9	H	66	MET
9	H	95	GLN
9	H	192	SER
11	J	60	THR
11	J	70	THR
11	J	96	ILE

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Mol	Chain	Res	Type
12	K	30	VAL
12	K	63	LYS
12	K	75	ILE
13	L	4	LYS
13	L	91	VAL
13	L	101	LEU
14	M	78	VAL
14	M	119	ASP
15	N	18	LEU
15	N	27	GLN
16	O	97	SER
17	P	40	CYS
19	R	17	THR
19	R	97	GLU
20	S	42	LYS
20	S	46	VAL
21	T	20	ASP
21	T	28	ASP
21	T	127	LEU
22	U	11	VAL
22	U	103	VAL
22	U	117	VAL
22	U	151	THR
22	U	156	TYR
23	V	7	VAL
23	V	16	ILE
24	W	48	VAL
24	W	58	VAL
24	W	62	VAL
25	X	26	ILE
25	X	30	THR
25	X	37	THR
27	Z	39	THR
27	Z	82	THR
27	Z	86	VAL
27	Z	163	ILE
28	3	96	THR
28	3	114	ILE
29	a	28	LEU
29	a	34	ILE
29	a	58	LYS
30	c	57	ASP

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Mol	Chain	Res	Type
30	c	79	SER
30	c	105	ILE
31	d	14	VAL
35	b	20	TYR
35	b	60	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	62	GLN
8	G	123	GLN
8	G	186	ASN
8	G	188	ASN
9	H	40	HIS
9	H	71	ASN
9	H	99	GLN
11	J	30	ASN
11	J	52	ASN
14	M	13	HIS
14	M	60	ASN
20	S	29	ASN
20	S	31	ASN
21	T	122	HIS
22	U	104	ASN
23	V	59	GLN
26	Y	50	HIS
27	Z	62	ASN
30	c	100	ASN
31	d	17	ASN
31	d	55	GLN
32	e	26	HIS
35	b	7	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1493/1497 (99%)	266 (17%)	7 (0%)
33	4	76/77 (98%)	12 (15%)	1 (1%)
34	5	1/14 (7%)	1 (100%)	0
All	All	1570/1588 (98%)	279 (17%)	8 (0%)

All (279) 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	46	A
1	2	47	A
1	2	60	G
1	2	67	C
1	2	68	C
1	2	70	G
1	2	71	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	130	A
1	2	138	G
1	2	144	C
1	2	193	A
1	2	195	A
1	2	196	G
1	2	197	G
1	2	208	A
1	2	209	U
1	2	211	C
1	2	212	C
1	2	214	C
1	2	215	G
1	2	225	G
1	2	245	C
1	2	246	OMC

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Mol	Chain	Res	Type
1	2	248	A
1	2	250	C
1	2	252	G
1	2	256	G
1	2	257	U
1	2	258	U
1	2	267	A
1	2	271	G
1	2	272	C
1	2	278	A
1	2	286	A
1	2	294	G
1	2	311	A
1	2	320	U
1	2	333	C
1	2	334	A
1	2	335	A
1	2	336	G
1	2	349	A
1	2	350	C
1	2	357	C
1	2	358	A
1	2	359	C
1	2	361	A
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	403	C
1	2	408	A
1	2	411	G
1	2	417	G
1	2	418	U
1	2	420	A
1	2	429	U
1	2	453	A
1	2	454	A
1	2	455	U
1	2	470	U

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Mol	Chain	Res	Type
1	2	471	C
1	2	477	U
1	2	480	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	577	C
1	2	601	A
1	2	609	G
1	2	612	A
1	2	624	A
1	2	634	U
1	2	647	G
1	2	662	G
1	2	677	A
1	2	682	U
1	2	707	G
1	2	708	C
1	2	714	G
1	2	736	A
1	2	740	A
1	2	741	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	818	G
1	2	835	A
1	2	853	G
1	2	865	OMG
1	2	876	A
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	1085	G
1	2	1086	U
1	2	1091	U
1	2	1094	U
1	2	1095	C
1	2	1096	U
1	2	1097	C
1	2	1098	C

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Mol	Chain	Res	Type
1	2	1099	G
1	2	1101	G
1	2	1103	C
1	2	1106	G
1	2	1107	A
1	2	1110	A
1	2	1121	A
1	2	1123	U
1	2	1124	G
1	2	1139	A
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	1199	A
1	2	1201	A
1	2	1211	A
1	2	1219	A
1	2	1220	U
1	2	1221	U
1	2	1222	C
1	2	1244	A
1	2	1249	U
1	2	1251	A
1	2	1263	A
1	2	1264	G
1	2	1265	U
1	2	1267	G
1	2	1270	A
1	2	1281	A
1	2	1284	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	1335	G
1	2	1337	G
1	2	1338	A
1	2	1339	A
1	2	1358	A
1	2	1361	C
1	2	1362	A
1	2	1376	C
1	2	1383	G
1	2	1386	G
1	2	1387	G
1	2	1389	G
1	2	1391	G
1	2	1394	G
1	2	1402	C
1	2	1403	C
1	2	1404	U
1	2	1410	U
1	2	1411	U
1	2	1412	G
1	2	1413	G
1	2	1421	G
1	2	1424	G
1	2	1425	A
1	2	1428	U
1	2	1429	U
1	2	1432	C
1	2	1433	U
1	2	1437	G
1	2	1440	A
1	2	1441	G
1	2	1442	G
1	2	1443	G
1	2	1444	G
1	2	1445	G
1	2	1448	G
1	2	1449	A
1	2	1450	A
1	2	1451	G
1	2	1452	U
1	2	1454	G

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Mol	Chain	Res	Type
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	1492	C
1	2	1493	C
33	4	8	4SU
33	4	16	C
33	4	17(A)	U
33	4	18	G
33	4	20	H2U
33	4	21	A
33	4	22	G
33	4	46	A
33	4	47	U
33	4	49	G
33	4	74	C
33	4	75	C
34	5	3	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	402	A
1	2	979	A
1	2	1123	U
1	2	1187	C
1	2	1188	G
1	2	1436	U
1	2	1443	G
33	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	OMG	2	672	1	23,26,27	1.23	3 (13%)	33,38,41	1.92	6 (18%)
1	OMC	2	1060	1	19,22,23	0.84	0	26,31,34	0.78	0
1	OMC	2	113	1	19,22,23	0.84	0	26,31,34	0.84	0
1	OMC	2	481	1	19,22,23	0.87	0	26,31,34	1.16	4 (15%)
33	5MU	4	54	33	19,22,23	1.38	6 (31%)	28,32,35	2.04	7 (25%)
1	OMG	2	337	1	23,26,27	1.23	4 (17%)	33,38,41	1.98	7 (21%)
1	OMG	2	546	1	23,26,27	1.21	3 (13%)	33,38,41	1.93	6 (18%)
1	OMG	2	399	1	23,26,27	1.23	3 (13%)	33,38,41	1.92	6 (18%)
1	C4J	2	930	1	24,29,30	0.65	1 (4%)	29,42,45	0.53	0
1	OMG	2	865	1	23,26,27	1.24	3 (13%)	33,38,41	1.94	6 (18%)
1	4AC	2	1477	1	21,24,25	1.03	2 (9%)	29,34,37	1.69	5 (17%)
1	OMG	2	1194	1	23,26,27	1.23	3 (13%)	33,38,41	1.95	5 (15%)
1	4AC	2	1467	1	21,24,25	1.00	2 (9%)	29,34,37	1.29	4 (13%)
33	OMC	4	32	33	19,22,23	0.85	0	26,31,34	1.11	2 (7%)
1	OMC	2	538	1	19,22,23	0.85	0	26,31,34	0.82	0
1	OMG	2	926	1	23,26,27	1.22	3 (13%)	33,38,41	1.96	6 (18%)
33	H2U	4	20	33	18,21,22	0.32	0	21,30,33	0.44	0
1	4AC	2	1478	1	21,24,25	1.00	2 (9%)	29,34,37	1.31	4 (13%)
1	MA6	2	1475	1	23,26,27	1.45	5 (21%)	34,38,41	2.10	10 (29%)
1	OMG	2	1061	1	23,26,27	1.22	3 (13%)	33,38,41	1.94	6 (18%)
1	6MZ	2	1457	1	22,25,26	1.45	4 (18%)	30,36,39	2.21	10 (33%)
33	PSU	4	55	33	18,21,22	1.31	2 (11%)	22,30,33	1.89	3 (13%)
1	OMU	2	15	1	19,22,23	1.34	3 (15%)	26,31,34	1.77	4 (15%)
1	OMG	2	1018	1	23,26,27	1.24	3 (13%)	33,38,41	1.93	6 (18%)
33	4SU	4	8	33	18,21,22	0.28	0	26,30,33	0.34	0
1	OMC	2	710	1	19,22,23	0.84	0	26,31,34	0.82	0
1	OMU	2	1032	1	19,22,23	1.29	3 (15%)	26,31,34	1.75	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	2	1344	1	19,22,23	1.22	3 (15%)	26,31,34	1.71	5 (19%)
1	5MC	2	1368	1	18,22,23	0.89	2 (11%)	26,32,35	1.07	3 (11%)
1	4AC	2	843	1	21,24,25	1.07	2 (9%)	29,34,37	1.34	4 (13%)
1	OMC	2	512	1	19,22,23	0.83	0	26,31,34	0.79	0
1	OMU	2	52	1	19,22,23	1.25	3 (15%)	26,31,34	1.75	5 (19%)
1	OMC	2	1366	1	19,22,23	0.82	0	26,31,34	0.76	0
1	4AC	2	1466	1	21,24,25	1.02	2 (9%)	29,34,37	1.30	4 (13%)
1	OMC	2	313	1	19,22,23	0.86	1 (5%)	26,31,34	0.97	1 (3%)
1	OMC	2	246	1	19,22,23	0.87	0	26,31,34	1.03	1 (3%)
1	OMG	2	905	1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	A2M	2	494	1	22,25,26	1.43	5 (22%)	31,36,39	2.08	9 (29%)

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	OMG	2	672	1	-	0/9/27/28	0/3/3/3
1	OMC	2	1060	1	-	0/9/27/28	0/2/2/2
1	OMC	2	113	1	-	0/9/27/28	0/2/2/2
1	OMC	2	481	1	-	0/9/27/28	0/2/2/2
33	5MU	4	54	33	-	0/7/25/26	0/2/2/2
1	OMG	2	337	1	-	1/9/27/28	0/3/3/3
1	OMG	2	546	1	-	0/9/27/28	0/3/3/3
1	OMG	2	399	1	-	0/9/27/28	0/3/3/3
1	C4J	2	930	1	-	6/16/34/35	0/2/2/2
1	OMG	2	865	1	-	3/9/27/28	0/3/3/3
1	4AC	2	1477	1	-	2/11/29/30	0/2/2/2
1	OMG	2	1194	1	-	0/9/27/28	0/3/3/3
1	4AC	2	1467	1	-	0/11/29/30	0/2/2/2
33	OMC	4	32	33	-	2/9/27/28	0/2/2/2
1	OMC	2	538	1	-	0/9/27/28	0/2/2/2
1	OMG	2	926	1	-	1/9/27/28	0/3/3/3
33	H2U	4	20	33	-	3/7/38/39	0/2/2/2
1	4AC	2	1478	1	-	0/11/29/30	0/2/2/2
1	MA6	2	1475	1	-	0/11/29/30	0/3/3/3
1	OMG	2	1061	1	-	0/9/27/28	0/3/3/3
1	6MZ	2	1457	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PSU	4	55	33	-	0/7/25/26	0/2/2/2
1	OMU	2	15	1	-	0/9/27/28	0/2/2/2
1	OMG	2	1018	1	-	0/9/27/28	0/3/3/3
33	4SU	4	8	33	-	0/7/25/26	0/2/2/2
1	OMC	2	710	1	-	0/9/27/28	0/2/2/2
1	OMU	2	1032	1	-	0/9/27/28	0/2/2/2
1	OMU	2	1344	1	-	0/9/27/28	0/2/2/2
1	5MC	2	1368	1	-	0/7/25/26	0/2/2/2
1	4AC	2	843	1	-	0/11/29/30	0/2/2/2
1	OMC	2	512	1	-	0/9/27/28	0/2/2/2
1	OMU	2	52	1	-	0/9/27/28	0/2/2/2
1	OMC	2	1366	1	-	0/9/27/28	0/2/2/2
1	4AC	2	1466	1	-	0/11/29/30	0/2/2/2
1	OMC	2	313	1	-	1/9/27/28	0/2/2/2
1	OMC	2	246	1	-	3/9/27/28	0/2/2/2
1	OMG	2	905	1	-	0/9/27/28	0/3/3/3
1	A2M	2	494	1	-	0/9/27/28	0/3/3/3

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1475	MA6	C5-C4	4.40	1.47	1.39
1	2	1457	6MZ	C5-C4	4.38	1.47	1.39
1	2	494	A2M	C5-C4	4.13	1.46	1.39
33	4	55	PSU	C6-C5	3.10	1.38	1.35
1	2	15	OMU	C4-N3	-3.07	1.33	1.38
1	2	865	OMG	C5-C4	2.95	1.47	1.38
1	2	926	OMG	C5-C4	2.92	1.46	1.38
1	2	672	OMG	C5-C4	2.89	1.46	1.38
1	2	546	OMG	C5-C4	2.88	1.46	1.38
1	2	1061	OMG	C5-C4	2.85	1.46	1.38
1	2	1194	OMG	C5-C4	2.83	1.46	1.38
1	2	905	OMG	C5-C4	2.83	1.46	1.38
1	2	1194	OMG	C6-N1	-2.83	1.33	1.38
1	2	1018	OMG	C5-C4	2.82	1.46	1.38
1	2	399	OMG	C6-N1	-2.82	1.33	1.38
1	2	1032	OMU	C4-N3	-2.82	1.33	1.38
1	2	865	OMG	C6-N1	-2.82	1.33	1.38
1	2	399	OMG	C5-C4	2.81	1.46	1.38
1	2	1018	OMG	C6-N1	-2.80	1.33	1.38
1	2	15	OMU	C2-N3	-2.77	1.33	1.38
1	2	843	4AC	C4-N3	-2.76	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	672	OMG	C6-N1	-2.75	1.33	1.38
1	2	52	OMU	C4-N3	-2.73	1.33	1.38
1	2	337	OMG	C5-C4	2.72	1.46	1.38
1	2	1061	OMG	C6-N1	-2.72	1.33	1.38
1	2	843	4AC	C5-C4	2.72	1.46	1.40
1	2	1466	4AC	C5-C4	2.71	1.46	1.40
1	2	337	OMG	C6-N1	-2.70	1.33	1.38
1	2	1478	4AC	C5-C4	2.70	1.46	1.40
1	2	1475	MA6	C5-C6	2.66	1.48	1.41
33	4	54	5MU	C6-C5	2.62	1.38	1.34
1	2	1457	6MZ	C5-C6	2.61	1.48	1.41
1	2	905	OMG	C6-N1	-2.61	1.34	1.38
1	2	926	OMG	C6-N1	-2.61	1.34	1.38
1	2	1344	OMU	C4-N3	-2.60	1.33	1.38
1	2	1467	4AC	C5-C4	2.60	1.46	1.40
1	2	546	OMG	C6-N1	-2.59	1.34	1.38
1	2	930	C4J	O4'-C1'	-2.58	1.40	1.43
33	4	55	PSU	C4-N3	-2.51	1.34	1.38
33	4	54	5MU	C4-N3	-2.51	1.34	1.38
1	2	1467	4AC	C4-N3	-2.48	1.28	1.32
1	2	1477	4AC	C5-C4	2.47	1.46	1.40
1	2	1018	OMG	C5-N7	-2.45	1.34	1.39
1	2	1061	OMG	C5-N7	-2.44	1.34	1.39
1	2	52	OMU	C2-N3	-2.44	1.33	1.38
1	2	15	OMU	C5-C4	-2.44	1.38	1.43
1	2	865	OMG	C5-N7	-2.43	1.34	1.39
1	2	494	A2M	C5-N7	-2.43	1.34	1.39
1	2	672	OMG	C5-N7	-2.43	1.34	1.39
1	2	1466	4AC	C4-N3	-2.41	1.28	1.32
1	2	1032	OMU	C2-N3	-2.41	1.33	1.38
1	2	399	OMG	C5-N7	-2.40	1.34	1.39
1	2	494	A2M	C5-C6	2.39	1.47	1.41
33	4	54	5MU	C6-N1	-2.38	1.34	1.38
1	2	1194	OMG	C5-N7	-2.37	1.34	1.39
1	2	1368	5MC	C6-N1	-2.35	1.34	1.38
1	2	926	OMG	C5-N7	-2.34	1.34	1.39
1	2	337	OMG	C5-N7	-2.33	1.34	1.39
1	2	1368	5MC	C6-C5	2.33	1.38	1.34
1	2	1478	4AC	C4-N3	-2.32	1.28	1.32
1	2	1457	6MZ	C5-N7	-2.30	1.34	1.39
1	2	1032	OMU	C5-C4	-2.28	1.38	1.43
1	2	905	OMG	C5-N7	-2.25	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1475	MA6	C5-N7	-2.25	1.34	1.39
1	2	546	OMG	C5-N7	-2.25	1.34	1.39
33	4	54	5MU	C4-C5	2.23	1.48	1.44
1	2	1344	OMU	C2-N3	-2.21	1.34	1.38
1	2	1344	OMU	C5-C4	-2.20	1.38	1.43
1	2	52	OMU	C5-C4	-2.17	1.38	1.43
1	2	494	A2M	C8-N7	2.14	1.35	1.31
1	2	1475	MA6	C8-N7	2.14	1.35	1.31
1	2	1477	4AC	C4-N3	-2.13	1.29	1.32
33	4	54	5MU	C2-N1	2.07	1.41	1.38
1	2	337	OMG	C4-N9	-2.05	1.32	1.38
1	2	1475	MA6	C4-N9	-2.05	1.33	1.37
1	2	494	A2M	C4-N9	-2.04	1.33	1.37
33	4	54	5MU	C2-N3	-2.04	1.34	1.38
1	2	1457	6MZ	C8-N7	2.03	1.35	1.31
1	2	313	OMC	C6-N1	-2.01	1.33	1.38

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	865	OMG	C5-C4-N3	-6.28	118.28	128.46
1	2	926	OMG	C5-C4-N3	-6.19	118.42	128.46
1	2	1194	OMG	C5-C4-N3	-6.19	118.42	128.46
1	2	1061	OMG	C5-C4-N3	-6.18	118.44	128.46
1	2	1018	OMG	C5-C4-N3	-6.14	118.49	128.46
1	2	672	OMG	C5-C4-N3	-6.13	118.51	128.46
1	2	1457	6MZ	C5-C4-N3	-6.09	118.80	126.75
1	2	494	A2M	C5-C4-N3	-6.04	118.86	126.75
1	2	1475	MA6	C5-C4-N3	-5.92	119.02	126.75
1	2	905	OMG	C5-C4-N3	-5.90	118.89	128.46
1	2	399	OMG	C5-C4-N3	-5.89	118.91	128.46
33	4	55	PSU	N1-C2-N3	5.84	121.75	115.13
1	2	337	OMG	C5-C4-N3	-5.76	119.11	128.46
1	2	546	OMG	C5-C4-N3	-5.76	119.11	128.46
1	2	1477	4AC	O7-C7-N4	5.06	130.01	121.82
33	4	54	5MU	C4-N3-C2	-5.04	120.83	127.35
1	2	905	OMG	C2-N3-C4	4.92	121.06	112.30
1	2	865	OMG	C2-N3-C4	4.90	121.03	112.30
1	2	1018	OMG	C2-N3-C4	4.90	121.03	112.30
1	2	1194	OMG	C2-N3-C4	4.88	120.99	112.30
1	2	926	OMG	C2-N3-C4	4.88	120.99	112.30
1	2	494	A2M	N3-C4-N9	4.87	135.10	127.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	672	OMG	C2-N3-C4	4.82	120.89	112.30
1	2	337	OMG	C2-N3-C4	4.81	120.87	112.30
1	2	1061	OMG	C2-N3-C4	4.80	120.85	112.30
33	4	54	5MU	N3-C2-N1	4.75	121.19	114.89
1	2	399	OMG	C2-N3-C4	4.75	120.76	112.30
1	2	546	OMG	C2-N3-C4	4.75	120.76	112.30
1	2	865	OMG	N9-C4-N3	4.70	135.37	125.94
1	2	15	OMU	C4-N3-C2	-4.69	120.40	126.58
1	2	1061	OMG	N9-C4-N3	4.68	135.34	125.94
1	2	926	OMG	N9-C4-N3	4.60	135.17	125.94
1	2	1018	OMG	N9-C4-N3	4.58	135.13	125.94
1	2	1457	6MZ	N3-C4-N9	4.57	134.61	127.08
1	2	52	OMU	C4-N3-C2	-4.56	120.56	126.58
1	2	672	OMG	N9-C4-N3	4.55	135.08	125.94
1	2	1032	OMU	C4-N3-C2	-4.54	120.60	126.58
1	2	1194	OMG	N9-C4-N3	4.48	134.93	125.94
1	2	399	OMG	N9-C4-N3	4.46	134.88	125.94
1	2	843	4AC	O7-C7-N4	4.43	128.99	121.82
1	2	1344	OMU	C4-N3-C2	-4.43	120.74	126.58
1	2	1478	4AC	O7-C7-N4	4.41	128.95	121.82
1	2	1475	MA6	N3-C4-N9	4.40	134.34	127.08
1	2	1475	MA6	C2-N1-C6	4.38	122.11	111.75
33	4	54	5MU	C5-C4-N3	4.32	119.00	115.31
1	2	1466	4AC	O7-C7-N4	4.32	128.81	121.82
1	2	1467	4AC	O7-C7-N4	4.31	128.80	121.82
1	2	905	OMG	N9-C4-N3	4.29	134.54	125.94
1	2	337	OMG	N9-C4-N3	4.28	134.53	125.94
1	2	15	OMU	C5-C4-N3	4.23	121.17	114.84
1	2	1457	6MZ	C6-C5-N7	4.15	136.88	132.39
1	2	546	OMG	N9-C4-N3	4.15	134.26	125.94
1	2	1032	OMU	N3-C2-N1	4.11	120.34	114.89
1	2	52	OMU	N3-C2-N1	4.08	120.31	114.89
1	2	1344	OMU	N3-C2-N1	3.98	120.18	114.89
33	4	54	5MU	O4-C4-C5	-3.96	120.31	124.90
1	2	1457	6MZ	C2-N3-C4	3.93	121.03	111.75
1	2	1477	4AC	N4-C4-N3	3.89	120.38	113.85
33	4	55	PSU	C4-N3-C2	-3.87	120.76	126.34
1	2	1475	MA6	C2-N3-C4	3.85	120.85	111.75
1	2	15	OMU	N3-C2-N1	3.83	119.98	114.89
1	2	1475	MA6	C4-C5-N7	-3.82	105.97	110.62
1	2	1457	6MZ	C4-C5-N7	-3.81	105.98	110.62
1	2	494	A2M	C2-N3-C4	3.80	120.73	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1477	4AC	C5-C4-N4	-3.76	116.38	122.92
1	2	52	OMU	C5-C4-N3	3.76	120.46	114.84
1	2	1032	OMU	C5-C4-N3	3.71	120.39	114.84
1	2	1344	OMU	C5-C4-N3	3.59	120.22	114.84
33	4	55	PSU	O2-C2-N1	-3.53	118.91	122.79
33	4	54	5MU	C5-C6-N1	-3.47	119.77	123.34
1	2	337	OMG	C6-C5-N7	3.44	136.64	130.25
1	2	905	OMG	C6-C5-N7	3.43	136.62	130.25
1	2	546	OMG	C6-C5-N7	3.38	136.53	130.25
1	2	1457	6MZ	N1-C2-N3	-3.36	123.35	128.60
1	2	1194	OMG	C6-C5-N7	3.25	136.30	130.25
1	2	1475	MA6	N1-C2-N3	-3.23	123.54	128.60
1	2	399	OMG	C6-C5-N7	3.22	136.24	130.25
1	2	15	OMU	O4-C4-C5	-3.21	119.52	125.16
1	2	1344	OMU	O4-C4-C5	-3.20	119.53	125.16
1	2	494	A2M	N3-C2-N1	-3.17	123.64	128.60
1	2	926	OMG	C6-C5-N7	3.09	135.99	130.25
1	2	1018	OMG	C6-C5-N7	3.09	135.99	130.25
1	2	672	OMG	C6-C5-N7	3.09	135.99	130.25
1	2	494	A2M	C4-C5-N7	-3.07	106.88	110.62
1	2	52	OMU	O4-C4-C5	-3.07	119.77	125.16
1	2	1032	OMU	O4-C4-C5	-3.06	119.78	125.16
1	2	1475	MA6	C5-N7-C8	3.05	107.85	103.51
1	2	865	OMG	C6-C5-N7	3.05	135.91	130.25
1	2	1457	6MZ	C5-N7-C8	3.04	107.83	103.51
1	2	1467	4AC	CM7-C7-N4	-2.99	110.11	115.29
1	2	246	OMC	O2-C2-N3	-2.95	117.53	122.33
1	2	1466	4AC	C5-C4-N4	-2.91	117.86	122.92
1	2	1061	OMG	C6-C5-N7	2.91	135.65	130.25
1	2	494	A2M	C4-N9-C8	2.86	108.82	105.73
1	2	1368	5MC	C5-C6-N1	-2.84	120.42	123.34
1	2	1466	4AC	N4-C4-N3	2.83	118.61	113.85
1	2	1478	4AC	CM7-C7-N4	-2.79	110.47	115.29
1	2	1194	OMG	C4-C5-N7	-2.78	106.31	110.72
33	4	32	OMC	O2-C2-N3	-2.78	117.81	122.33
1	2	1467	4AC	N4-C4-N3	2.75	118.47	113.85
1	2	1467	4AC	C5-C4-N4	-2.75	118.14	122.92
1	2	1478	4AC	N4-C4-N3	2.74	118.46	113.85
1	2	843	4AC	CM7-C7-N4	-2.70	110.62	115.29
1	2	1478	4AC	C5-C4-N4	-2.70	118.23	122.92
1	2	1466	4AC	CM7-C7-N4	-2.69	110.63	115.29
1	2	905	OMG	C4-C5-N7	-2.69	106.47	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1475	MA6	C4-N9-C8	2.64	108.59	105.73
1	2	926	OMG	C4-C5-N7	-2.64	106.54	110.72
1	2	494	A2M	C5-N7-C8	2.63	107.24	103.51
1	2	546	OMG	C4-C5-N7	-2.61	106.59	110.72
1	2	337	OMG	C4-C5-N7	-2.60	106.60	110.72
1	2	843	4AC	C5-C4-N4	-2.59	118.42	122.92
1	2	1477	4AC	C1'-N1-C2	2.58	124.18	118.42
1	2	672	OMG	C4-C5-N7	-2.57	106.65	110.72
1	2	1477	4AC	CM7-C7-N4	-2.56	110.87	115.29
1	2	1368	5MC	C5-C4-N3	-2.56	118.92	121.67
1	2	865	OMG	C4-C5-N7	-2.55	106.68	110.72
33	4	32	OMC	C1'-N1-C2	2.52	124.06	118.42
1	2	1018	OMG	C4-C5-N7	-2.50	106.76	110.72
1	2	1457	6MZ	C4-N9-C8	2.50	108.44	105.73
1	2	1061	OMG	C4-C5-N7	-2.48	106.80	110.72
33	4	54	5MU	O2-C2-N1	-2.48	119.49	122.79
1	2	481	OMC	O2-C2-N3	-2.47	118.32	122.33
1	2	399	OMG	C4-C5-N7	-2.46	106.82	110.72
1	2	313	OMC	O2-C2-N3	-2.40	118.43	122.33
1	2	481	OMC	C6-C5-C4	2.39	121.36	117.50
1	2	843	4AC	N4-C4-N3	2.33	117.76	113.85
1	2	399	OMG	O6-C6-C5	-2.26	120.61	126.60
1	2	1032	OMU	C1'-N1-C2	2.26	121.66	117.57
1	2	1475	MA6	C6-C5-N7	2.25	137.06	133.28
1	2	1061	OMG	O6-C6-C5	-2.24	120.64	126.60
1	2	546	OMG	O6-C6-C5	-2.18	120.81	126.60
1	2	337	OMG	C2'-C1'-N9	-2.18	109.99	114.22
1	2	1457	6MZ	C2-N1-C6	2.18	122.55	115.25
1	2	1475	MA6	N9-C8-N7	-2.17	110.95	113.91
1	2	481	OMC	C5-C4-N3	-2.16	117.65	121.33
1	2	1018	OMG	O6-C6-C5	-2.16	120.88	126.60
1	2	337	OMG	O6-C6-C5	-2.16	120.88	126.60
1	2	1344	OMU	C1'-N1-C2	2.13	121.43	117.57
1	2	481	OMC	N4-C4-N3	2.12	121.69	117.97
1	2	494	A2M	N9-C8-N7	-2.12	111.02	113.91
1	2	926	OMG	O6-C6-C5	-2.11	121.01	126.60
1	2	672	OMG	O6-C6-C5	-2.10	121.04	126.60
1	2	865	OMG	O6-C6-C5	-2.10	121.04	126.60
1	2	494	A2M	C6-C5-N7	2.09	135.91	132.02
1	2	1368	5MC	O2-C2-N3	-2.08	118.94	122.33
1	2	905	OMG	O6-C6-C5	-2.07	121.11	126.60
33	4	54	5MU	C5M-C5-C4	2.05	121.02	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1457	6MZ	N9-C8-N7	-2.01	111.16	113.91
1	2	52	OMU	C1'-N1-C2	2.00	121.20	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'
1	2	246	OMC	O4'-C4'-C5'-O5'
33	4	20	H2U	O4'-C1'-N1-C6
1	2	930	C4J	C4'-C5'-O5'-P
33	4	20	H2U	O4'-C1'-N1-C2
1	2	865	OMG	C3'-C4'-C5'-O5'
1	2	865	OMG	C4'-C5'-O5'-P
1	2	930	C4J	N3-C3-C31-C32
1	2	930	C4J	C31-C32-C34-O36
33	4	20	H2U	C4'-C5'-O5'-P
1	2	930	C4J	C31-C32-C34-O35
1	2	930	C4J	C3'-C4'-C5'-O5'
33	4	32	OMC	C2'-C1'-N1-C6
1	2	865	OMG	O4'-C4'-C5'-O5'
1	2	246	OMC	C2'-C1'-N1-C2
1	2	313	OMC	C2'-C1'-N1-C2
33	4	32	OMC	C2'-C1'-N1-C2
1	2	930	C4J	C3-C31-C32-N33
1	2	1477	4AC	C2'-C1'-N1-C2
1	2	926	OMG	C3'-C2'-O2'-CM2
1	2	337	OMG	C4'-C5'-O5'-P
1	2	1477	4AC	C4'-C5'-O5'-P

There are no ring outliers.

24 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	672	OMG	1	0
1	2	1060	OMC	1	0
1	2	481	OMC	1	0
1	2	337	OMG	2	0
1	2	865	OMG	2	0
1	2	1477	4AC	1	0
1	2	1467	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	4	32	OMC	1	0
1	2	538	OMC	1	0
1	2	926	OMG	3	0
1	2	1478	4AC	1	0
1	2	1475	MA6	1	0
1	2	1061	OMG	1	0
1	2	1457	6MZ	1	0
1	2	1018	OMG	1	0
1	2	1032	OMU	2	0
1	2	1344	OMU	3	0
1	2	1368	5MC	1	0
1	2	843	4AC	2	0
1	2	52	OMU	1	0
1	2	1366	OMC	1	0
1	2	1466	4AC	2	0
1	2	905	OMG	1	0
1	2	494	A2M	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 100 ligands modelled in this entry, 56 are monoatomic - leaving 44 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	1520	-	13,13,13	0.11	0	12,12,12	0.07	0
39	GTP	5	102	34	30,34,34	0.83	1 (3%)	46,54,54	1.73	11 (23%)
36	SPM	2	1506	-	13,13,13	0.09	0	12,12,12	0.07	0
36	SPM	2	1542	-	13,13,13	0.10	0	12,12,12	0.06	0
36	SPM	2	1505	-	13,13,13	0.06	0	12,12,12	0.14	0
36	SPM	2	1538	-	13,13,13	0.11	0	12,12,12	0.09	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	0.13	0	12,12,12	0.11	0
36	SPM	2	1540	-	13,13,13	0.11	0	12,12,12	0.10	0
36	SPM	2	1530	-	13,13,13	0.10	0	12,12,12	0.08	0
36	SPM	2	1528	-	13,13,13	0.12	0	12,12,12	0.06	0
36	SPM	2	1532	-	13,13,13	0.11	0	12,12,12	0.08	0
36	SPM	2	1513	-	13,13,13	0.10	0	12,12,12	0.07	0
36	SPM	2	1516	-	13,13,13	0.07	0	12,12,12	0.14	0
36	SPM	2	1514	-	13,13,13	0.09	0	12,12,12	0.09	0
36	SPM	2	1510	-	13,13,13	0.08	0	12,12,12	0.10	0
36	SPM	2	1515	-	13,13,13	0.07	0	12,12,12	0.14	0
36	SPM	2	1522	-	13,13,13	0.07	0	12,12,12	0.13	0
36	SPM	2	1507	-	13,13,13	0.10	0	12,12,12	0.08	0
36	SPM	2	1535	-	13,13,13	0.10	0	12,12,12	0.08	0
36	SPM	2	1541	-	13,13,13	0.10	0	12,12,12	0.16	0
36	SPM	2	1509	-	13,13,13	0.06	0	12,12,12	0.11	0
36	SPM	2	1521	-	13,13,13	0.11	0	12,12,12	0.08	0
36	SPM	2	1537	-	13,13,13	0.10	0	12,12,12	0.11	0
36	SPM	2	1526	-	13,13,13	0.09	0	12,12,12	0.09	0
36	SPM	E	301	-	13,13,13	0.08	0	12,12,12	0.09	0
36	SPM	2	1508	-	13,13,13	0.07	0	12,12,12	0.10	0
36	SPM	2	1518	-	13,13,13	0.11	0	12,12,12	0.08	0
36	SPM	2	1512	-	13,13,13	0.10	0	12,12,12	0.12	0
36	SPM	2	1536	-	13,13,13	0.11	0	12,12,12	0.09	0
36	SPM	2	1517	-	13,13,13	0.08	0	12,12,12	0.17	0
36	SPM	2	1529	-	13,13,13	0.11	0	12,12,12	0.07	0
36	SPM	2	1523	-	13,13,13	0.11	0	12,12,12	0.10	0
36	SPM	2	1524	-	13,13,13	0.10	0	12,12,12	0.10	0
36	SPM	2	1511	-	13,13,13	0.12	0	12,12,12	0.14	0
36	SPM	2	1534	-	13,13,13	0.12	0	12,12,12	0.06	0
36	SPM	2	1501	-	13,13,13	0.08	0	12,12,12	0.11	0
36	SPM	2	1519	-	13,13,13	0.11	0	12,12,12	0.10	0
36	SPM	2	1525	-	13,13,13	0.11	0	12,12,12	0.14	0
36	SPM	2	1533	-	13,13,13	0.11	0	12,12,12	0.07	0
36	SPM	2	1531	-	13,13,13	0.11	0	12,12,12	0.07	0
36	SPM	2	1527	-	13,13,13	0.12	0	12,12,12	0.10	0
36	SPM	2	1503	-	13,13,13	0.09	0	12,12,12	0.11	0
36	SPM	2	1504	-	13,13,13	0.09	0	12,12,12	0.08	0
36	SPM	2	1502	-	13,13,13	0.12	0	12,12,12	0.07	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	1520	-	-	8/11/11/11	-
39	GTP	5	102	34	-	6/22/38/38	0/3/3/3
36	SPM	2	1506	-	-	4/11/11/11	-
36	SPM	2	1542	-	-	3/11/11/11	-
36	SPM	2	1505	-	-	2/11/11/11	-
36	SPM	2	1538	-	-	1/11/11/11	-
36	SPM	2	1539	-	-	2/11/11/11	-
36	SPM	2	1540	-	-	5/11/11/11	-
36	SPM	2	1530	-	-	3/11/11/11	-
36	SPM	2	1528	-	-	6/11/11/11	-
36	SPM	2	1532	-	-	2/11/11/11	-
36	SPM	2	1513	-	-	3/11/11/11	-
36	SPM	2	1516	-	-	5/11/11/11	-
36	SPM	2	1514	-	-	2/11/11/11	-
36	SPM	2	1510	-	-	3/11/11/11	-
36	SPM	2	1515	-	-	2/11/11/11	-
36	SPM	2	1522	-	-	4/11/11/11	-
36	SPM	2	1507	-	-	2/11/11/11	-
36	SPM	2	1535	-	-	3/11/11/11	-
36	SPM	2	1541	-	-	4/11/11/11	-
36	SPM	2	1509	-	-	2/11/11/11	-
36	SPM	2	1521	-	-	2/11/11/11	-
36	SPM	2	1537	-	-	2/11/11/11	-
36	SPM	2	1526	-	-	4/11/11/11	-
36	SPM	E	301	-	-	2/11/11/11	-
36	SPM	2	1508	-	-	3/11/11/11	-
36	SPM	2	1518	-	-	1/11/11/11	-
36	SPM	2	1512	-	-	1/11/11/11	-
36	SPM	2	1536	-	-	1/11/11/11	-
36	SPM	2	1517	-	-	4/11/11/11	-
36	SPM	2	1529	-	-	4/11/11/11	-
36	SPM	2	1523	-	-	3/11/11/11	-
36	SPM	2	1524	-	-	2/11/11/11	-
36	SPM	2	1511	-	-	4/11/11/11	-
36	SPM	2	1534	-	-	7/11/11/11	-
36	SPM	2	1501	-	-	2/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SPM	2	1519	-	-	5/11/11/11	-
36	SPM	2	1525	-	-	1/11/11/11	-
36	SPM	2	1533	-	-	4/11/11/11	-
36	SPM	2	1531	-	-	9/11/11/11	-
36	SPM	2	1527	-	-	2/11/11/11	-
36	SPM	2	1503	-	-	4/11/11/11	-
36	SPM	2	1504	-	-	2/11/11/11	-
36	SPM	2	1502	-	-	9/11/11/11	-

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	4.44	120.21	112.30
39	5	102	GTP	PB-O3B-PG	-3.30	121.51	132.83
39	5	102	GTP	PA-O3A-PB	-3.25	121.68	132.83
39	5	102	GTP	N9-C4-N3	3.20	132.35	125.94
39	5	102	GTP	C2-N1-C6	-2.85	119.90	125.10
39	5	102	GTP	N9-C8-N7	-2.63	108.43	113.39
39	5	102	GTP	C2'-C1'-N9	-2.59	105.88	113.22
39	5	102	GTP	C5-C6-N1	2.52	119.59	113.19
39	5	102	GTP	C8-N7-C5	2.47	108.71	104.24
39	5	102	GTP	O6-C6-C5	-2.36	120.34	126.60

There are no chirality outliers.

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	2	1509	SPM	C12-C11-N10-C9
36	2	1517	SPM	C7-C6-N5-C4
36	2	1520	SPM	C11-C12-C13-N14
36	2	1523	SPM	C3-C4-N5-C6
36	2	1525	SPM	C3-C4-N5-C6
36	2	1531	SPM	C7-C6-N5-C4
36	2	1531	SPM	C12-C11-N10-C9

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Mol	Chain	Res	Type	Atoms
36	2	1531	SPM	C11-C12-C13-N14
36	2	1535	SPM	C12-C11-N10-C9
39	5	102	GTP	C5'-O5'-PA-O1A
36	2	1512	SPM	C8-C9-N10-C11
36	2	1519	SPM	C7-C8-C9-N10
36	2	1531	SPM	N5-C6-C7-C8
39	5	102	GTP	C3'-C4'-C5'-O5'
36	2	1516	SPM	N10-C11-C12-C13
36	2	1529	SPM	N5-C6-C7-C8
36	2	1531	SPM	C7-C8-C9-N10
36	2	1533	SPM	N5-C6-C7-C8
36	2	1541	SPM	N5-C6-C7-C8
36	2	1520	SPM	C2-C3-C4-N5
36	2	1506	SPM	C12-C11-N10-C9
36	2	1511	SPM	C12-C11-N10-C9
36	2	1515	SPM	C3-C4-N5-C6
36	2	1516	SPM	C8-C9-N10-C11
36	2	1520	SPM	C7-C6-N5-C4
36	2	1529	SPM	C7-C6-N5-C4
36	2	1529	SPM	C12-C11-N10-C9
36	2	1532	SPM	C8-C9-N10-C11
36	2	1540	SPM	C3-C4-N5-C6
39	5	102	GTP	O4'-C4'-C5'-O5'
36	2	1528	SPM	C2-C3-C4-N5
36	2	1502	SPM	C12-C11-N10-C9
36	2	1503	SPM	C8-C9-N10-C11
36	2	1510	SPM	C12-C11-N10-C9
36	2	1516	SPM	C3-C4-N5-C6
36	2	1519	SPM	C12-C11-N10-C9
36	2	1521	SPM	C8-C9-N10-C11
36	2	1523	SPM	C8-C9-N10-C11
36	2	1527	SPM	C8-C9-N10-C11
36	2	1528	SPM	C8-C9-N10-C11
36	2	1540	SPM	C7-C6-N5-C4
36	2	1540	SPM	C8-C9-N10-C11
36	2	1541	SPM	C12-C11-N10-C9
36	2	1542	SPM	C3-C4-N5-C6
36	2	1533	SPM	C2-C3-C4-N5
36	2	1507	SPM	C8-C9-N10-C11
36	2	1528	SPM	C3-C4-N5-C6
36	2	1531	SPM	C8-C9-N10-C11
36	2	1533	SPM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
36	2	1517	SPM	C3-C4-N5-C6
36	2	1519	SPM	C8-C9-N10-C11
36	2	1523	SPM	C7-C6-N5-C4
36	2	1526	SPM	C3-C4-N5-C6
36	2	1532	SPM	C7-C6-N5-C4
36	2	1534	SPM	C3-C4-N5-C6
36	2	1539	SPM	C7-C6-N5-C4
36	2	1502	SPM	C11-C12-C13-N14
36	2	1522	SPM	C11-C12-C13-N14
36	2	1502	SPM	N10-C11-C12-C13
36	2	1513	SPM	C3-C4-N5-C6
36	2	1537	SPM	C3-C4-N5-C6
36	2	1522	SPM	C6-C7-C8-C9
36	2	1528	SPM	C6-C7-C8-C9
36	2	1531	SPM	C6-C7-C8-C9
36	2	1526	SPM	C7-C6-N5-C4
36	2	1526	SPM	C12-C11-N10-C9
36	2	1530	SPM	C12-C11-N10-C9
36	2	1541	SPM	C8-C9-N10-C11
36	2	1542	SPM	C7-C6-N5-C4
36	2	1520	SPM	N10-C11-C12-C13
36	2	1502	SPM	N5-C6-C7-C8
36	2	1502	SPM	C7-C8-C9-N10
36	2	1505	SPM	C12-C11-N10-C9
36	2	1506	SPM	C7-C6-N5-C4
36	2	1518	SPM	C8-C9-N10-C11
36	2	1522	SPM	C8-C9-N10-C11
36	2	1531	SPM	C2-C3-C4-N5
36	2	1511	SPM	C3-C4-N5-C6
36	2	1524	SPM	C7-C6-N5-C4
36	2	1530	SPM	C7-C6-N5-C4
36	2	1538	SPM	C3-C4-N5-C6
36	2	1502	SPM	N1-C2-C3-C4
36	2	1531	SPM	N1-C2-C3-C4
36	2	1534	SPM	C11-C12-C13-N14
39	5	102	GTP	C5'-O5'-PA-O3A
36	2	1503	SPM	C12-C11-N10-C9
36	2	1511	SPM	C7-C6-N5-C4
36	2	1542	SPM	C12-C11-N10-C9
39	5	102	GTP	C5'-O5'-PA-O2A
36	2	1507	SPM	C3-C4-N5-C6
36	2	1519	SPM	C3-C4-N5-C6

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Mol	Chain	Res	Type	Atoms
36	2	1521	SPM	C3-C4-N5-C6
36	2	1526	SPM	C8-C9-N10-C11
36	2	1536	SPM	C7-C6-N5-C4
36	2	1534	SPM	C7-C8-C9-N10
36	2	1508	SPM	C3-C4-N5-C6
36	2	1528	SPM	C12-C11-N10-C9
36	2	1534	SPM	C2-C3-C4-N5
36	2	1540	SPM	C6-C7-C8-C9
36	2	1535	SPM	C6-C7-C8-C9
36	2	1533	SPM	N10-C11-C12-C13
36	2	1503	SPM	C3-C4-N5-C6
36	2	1516	SPM	C7-C6-N5-C4
36	2	1520	SPM	C8-C9-N10-C11
36	2	1522	SPM	C7-C6-N5-C4
36	2	1528	SPM	C7-C6-N5-C4
36	2	1539	SPM	C12-C11-N10-C9
36	2	1502	SPM	C2-C3-C4-N5
36	2	1537	SPM	C6-C7-C8-C9
36	2	1508	SPM	N5-C6-C7-C8
36	2	1534	SPM	N5-C6-C7-C8
36	2	1541	SPM	C6-C7-C8-C9
36	2	1502	SPM	C6-C7-C8-C9
36	2	1506	SPM	C3-C4-N5-C6
36	2	1516	SPM	C12-C11-N10-C9
36	2	1534	SPM	C7-C6-N5-C4
36	2	1520	SPM	N1-C2-C3-C4
36	2	1517	SPM	C6-C7-C8-C9
36	2	1520	SPM	C6-C7-C8-C9
36	2	1502	SPM	C8-C9-N10-C11
36	2	1515	SPM	C12-C11-N10-C9
36	2	1511	SPM	C8-C9-N10-C11
36	2	1508	SPM	C12-C11-N10-C9
36	2	1509	SPM	C8-C9-N10-C11
36	2	1524	SPM	C12-C11-N10-C9
36	2	1534	SPM	C8-C9-N10-C11
36	2	1503	SPM	C7-C6-N5-C4
36	2	1510	SPM	C3-C4-N5-C6
36	2	1540	SPM	C12-C11-N10-C9
36	2	1519	SPM	C6-C7-C8-C9
36	2	1501	SPM	C8-C9-N10-C11
36	2	1505	SPM	C7-C6-N5-C4
36	2	1520	SPM	C12-C11-N10-C9

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Mol	Chain	Res	Type	Atoms
36	2	1530	SPM	C8-C9-N10-C11
36	E	301	SPM	C3-C4-N5-C6
36	2	1510	SPM	C8-C9-N10-C11
36	2	1513	SPM	C12-C11-N10-C9
36	2	1514	SPM	C7-C6-N5-C4
36	2	1514	SPM	C12-C11-N10-C9
36	2	1517	SPM	C8-C9-N10-C11
36	2	1527	SPM	C12-C11-N10-C9
36	2	1529	SPM	C8-C9-N10-C11
39	5	102	GTP	PG-O3B-PB-O2B
36	2	1506	SPM	C6-C7-C8-C9
36	2	1504	SPM	C8-C9-N10-C11
36	2	1513	SPM	C8-C9-N10-C11
36	2	1535	SPM	C8-C9-N10-C11
36	E	301	SPM	C12-C11-N10-C9
36	2	1504	SPM	C6-C7-C8-C9
36	2	1501	SPM	C7-C8-C9-N10

There are no ring outliers.

33 monomers are involved in 96 short contacts:

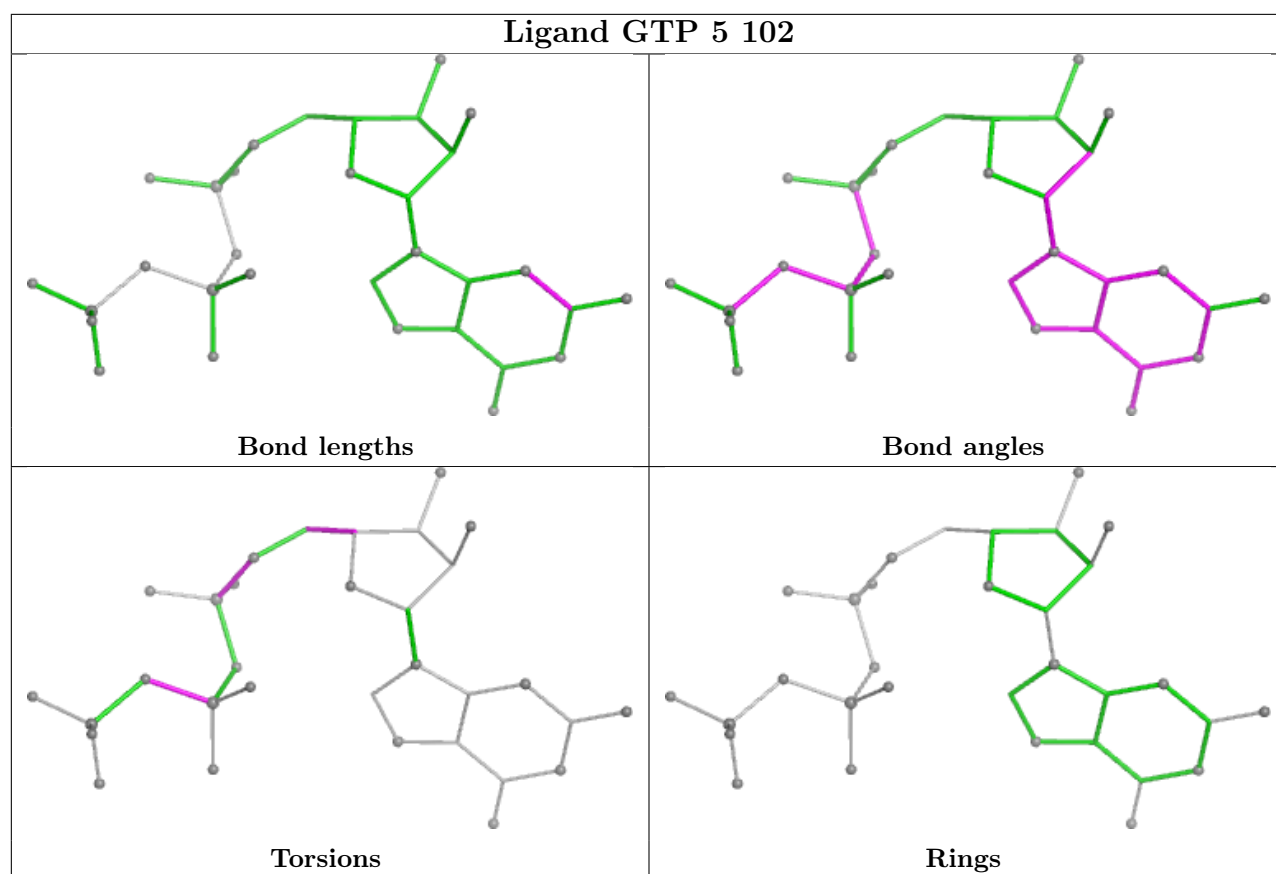
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	2	1520	SPM	4	0
39	5	102	GTP	2	0
36	2	1506	SPM	1	0
36	2	1542	SPM	2	0
36	2	1539	SPM	2	0
36	2	1540	SPM	11	0
36	2	1530	SPM	1	0
36	2	1528	SPM	7	0
36	2	1532	SPM	1	0
36	2	1513	SPM	2	0
36	2	1516	SPM	4	0
36	2	1514	SPM	4	0
36	2	1510	SPM	1	0
36	2	1515	SPM	4	0
36	2	1522	SPM	2	0
36	2	1507	SPM	1	0
36	2	1541	SPM	1	0
36	2	1509	SPM	3	0
36	2	1521	SPM	1	0
36	2	1526	SPM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	E	301	SPM	1	0
36	2	1512	SPM	2	0
36	2	1536	SPM	1	0
36	2	1517	SPM	2	0
36	2	1523	SPM	1	0
36	2	1524	SPM	5	0
36	2	1534	SPM	1	0
36	2	1501	SPM	2	0
36	2	1525	SPM	1	0
36	2	1533	SPM	9	0
36	2	1531	SPM	7	0
36	2	1527	SPM	2	0
36	2	1502	SPM	7	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.

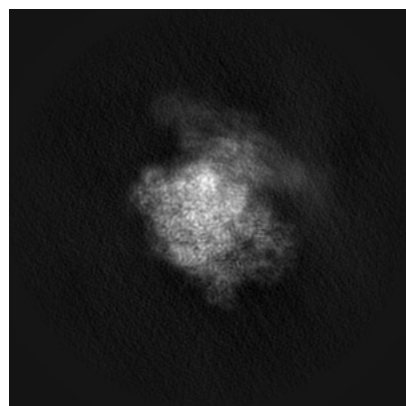
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50854. These allow visual inspection of the internal detail of the map and identification of artifacts.

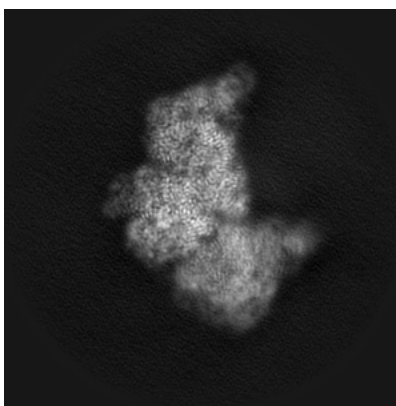
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

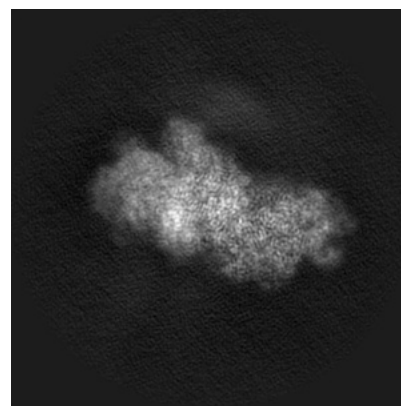
6.1.1 Primary map



X

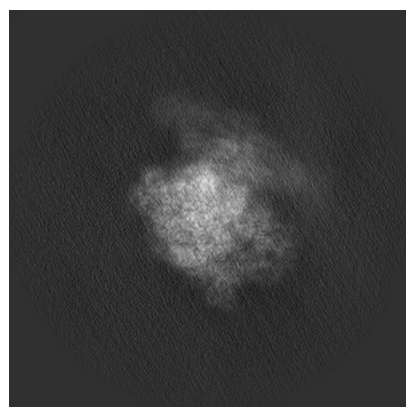


Y

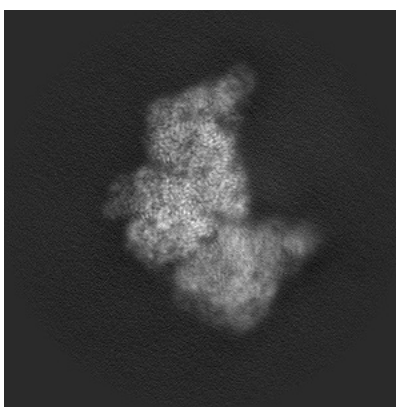


Z

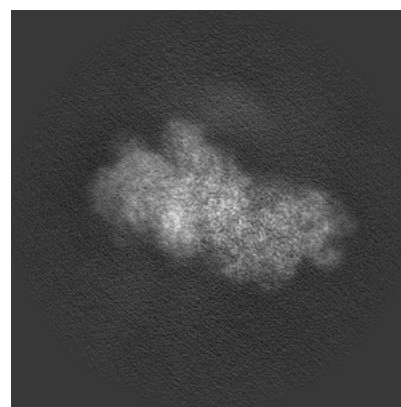
6.1.2 Raw map



X



Y

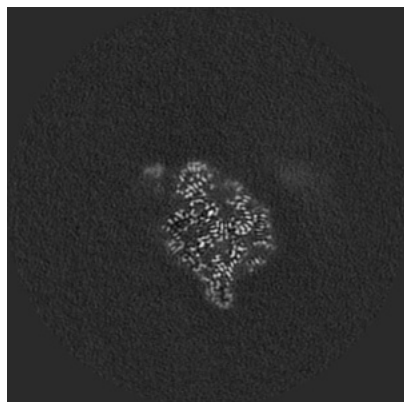


Z

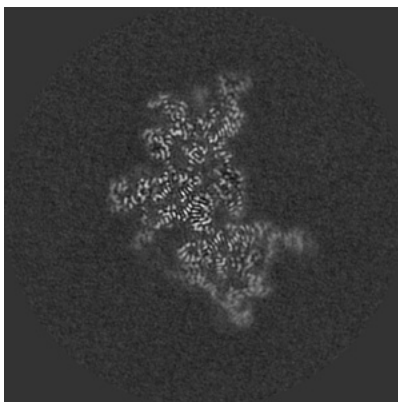
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

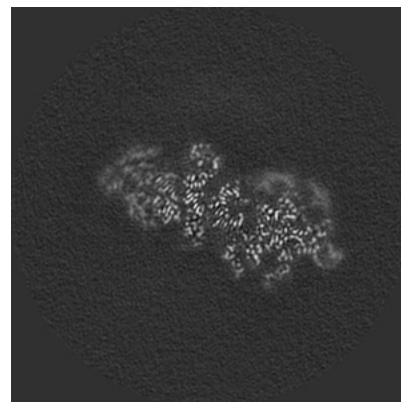
6.2.1 Primary map



X Index: 258

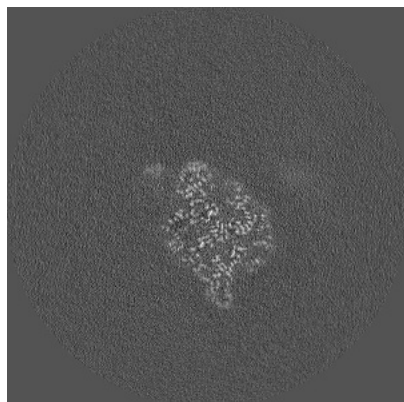


Y Index: 258

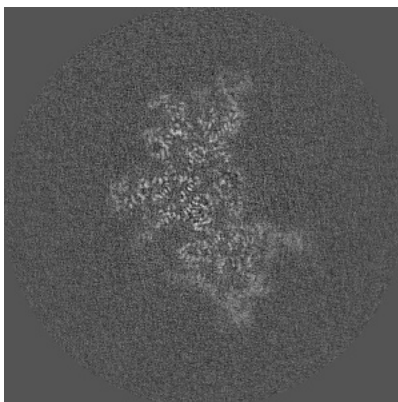


Z Index: 258

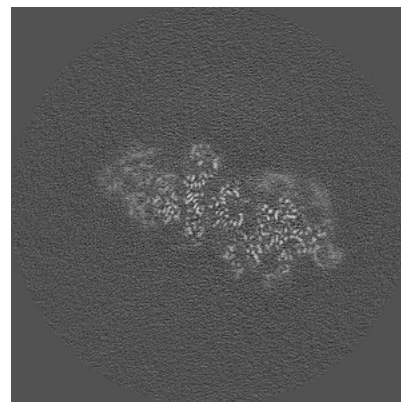
6.2.2 Raw map



X Index: 258



Y Index: 258

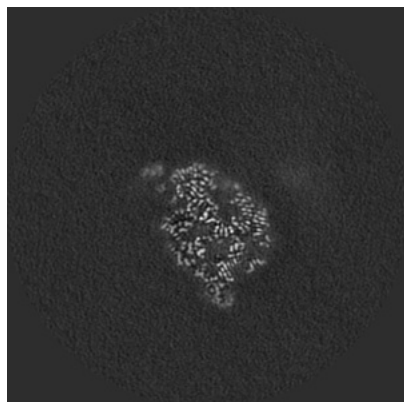


Z Index: 258

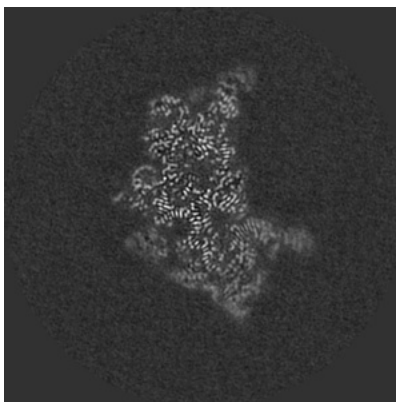
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

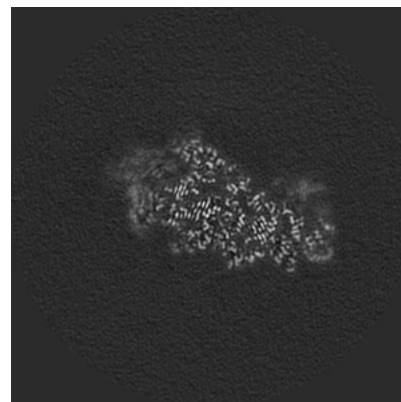
6.3.1 Primary map



X Index: 261

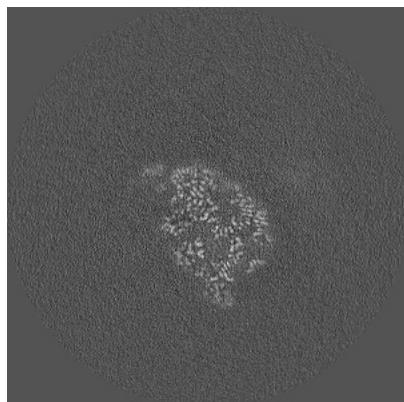


Y Index: 251

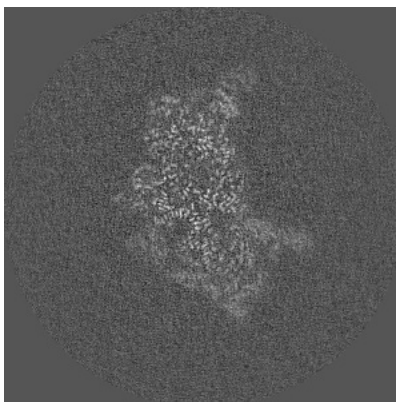


Z Index: 244

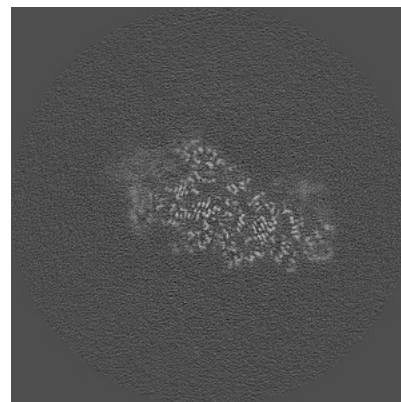
6.3.2 Raw map



X Index: 262



Y Index: 251

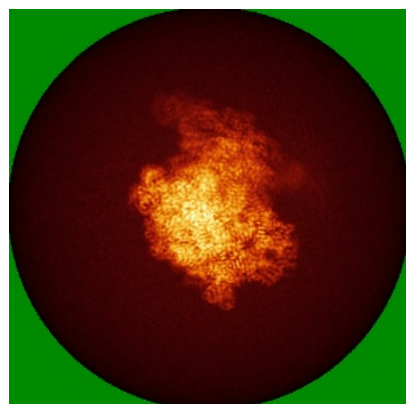


Z Index: 244

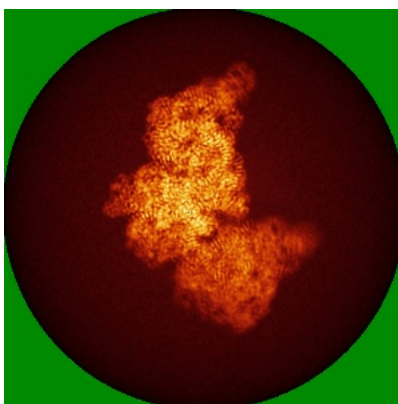
The images above show the largest variance slices of the map in three orthogonal directions.

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

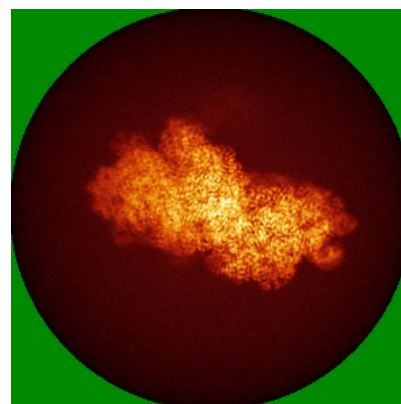
6.4.1 Primary map



X

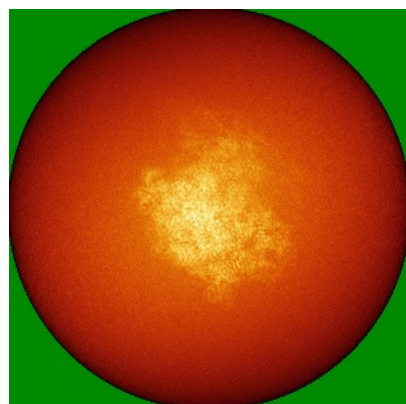


Y

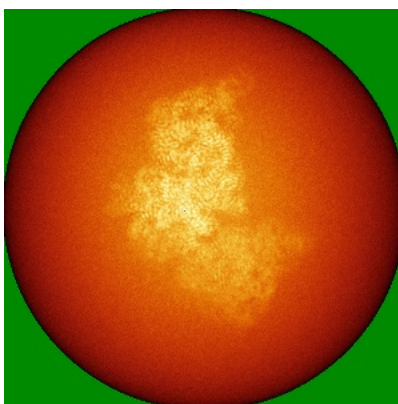


Z

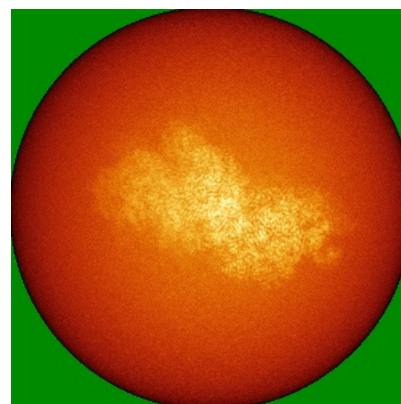
6.4.2 Raw map



X



Y

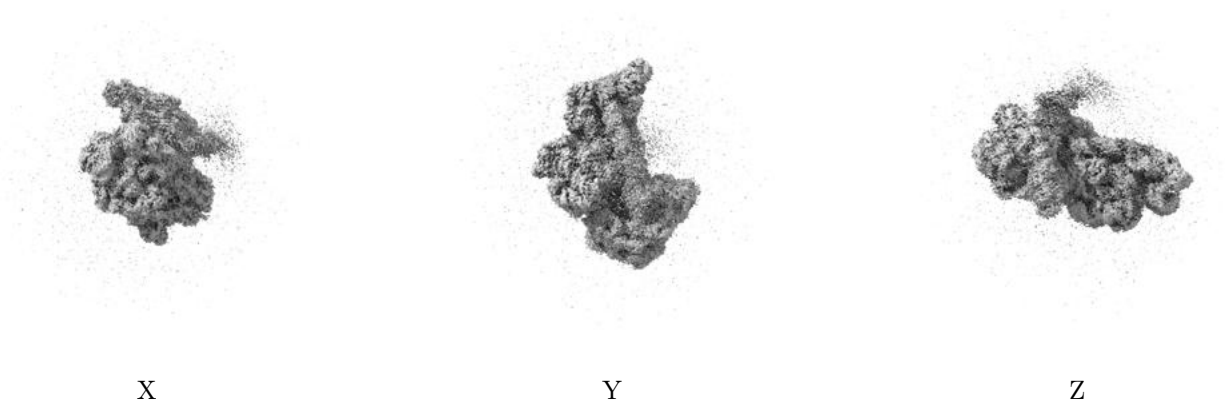


Z

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.

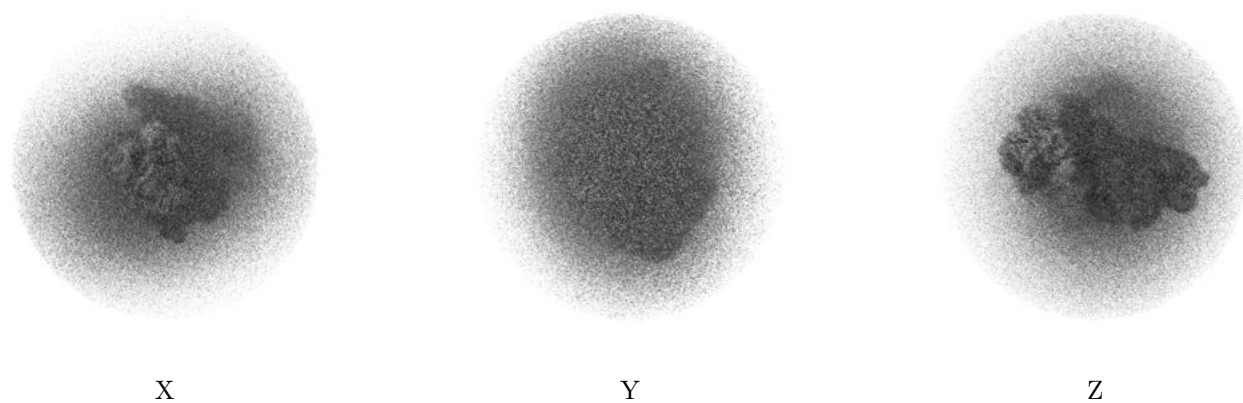
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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.

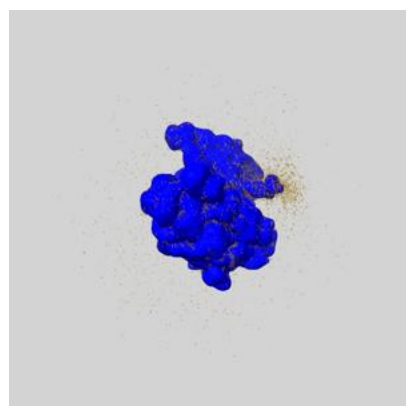
6.6 Mask visualisation [i](#)

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

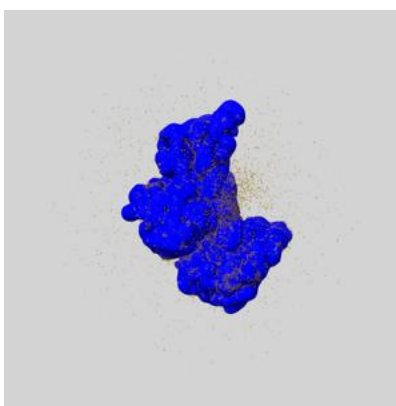
A mask typically either:

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

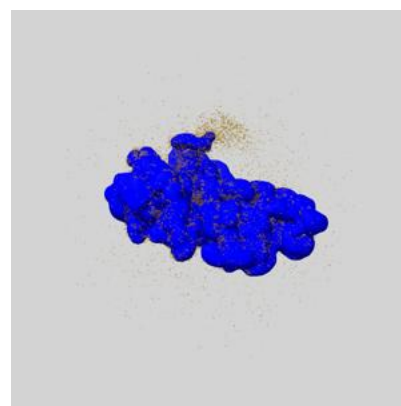
6.6.1 emd_50854_msk_1.map [i](#)



X



Y

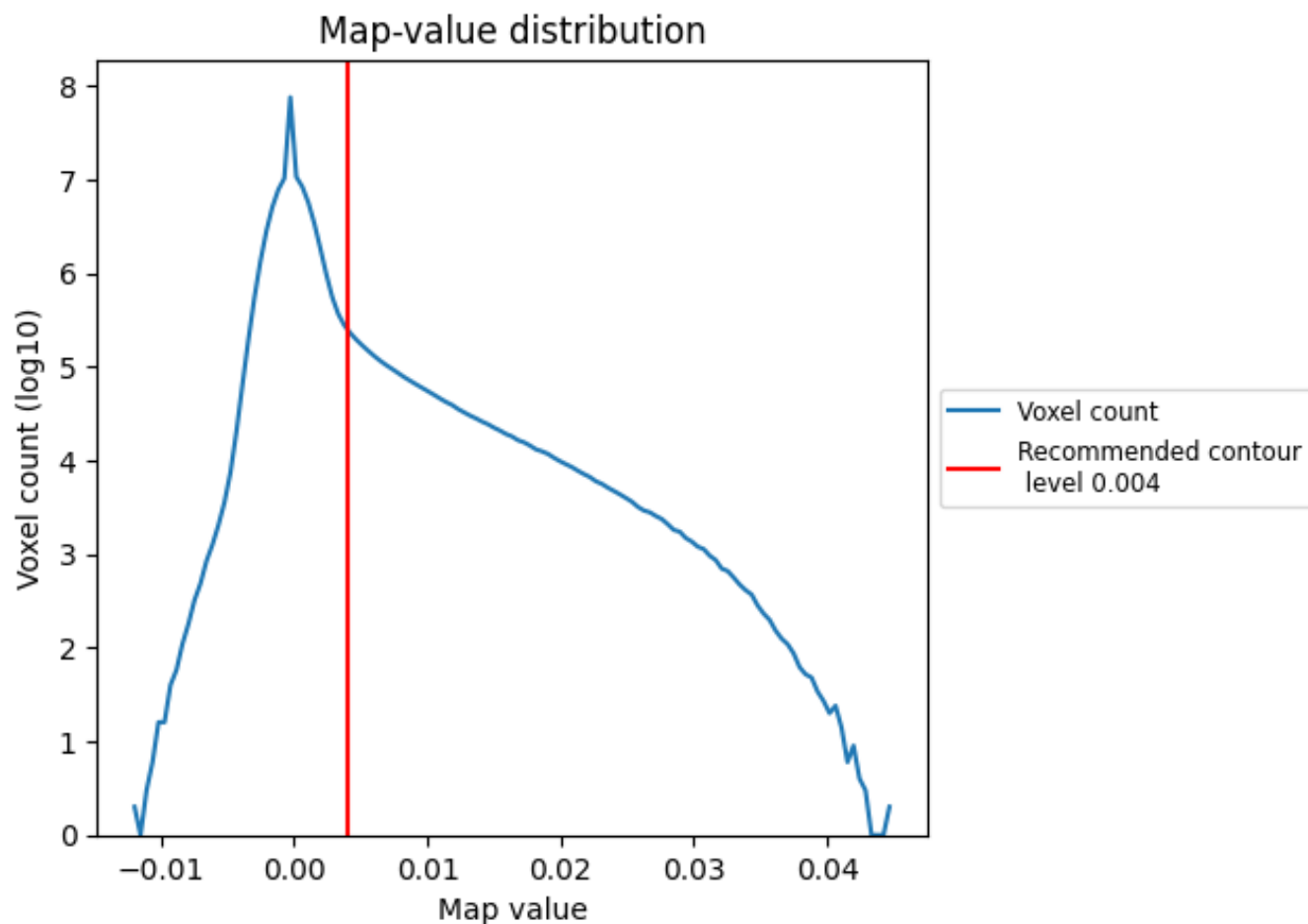


Z

7 Map analysis [i](#)

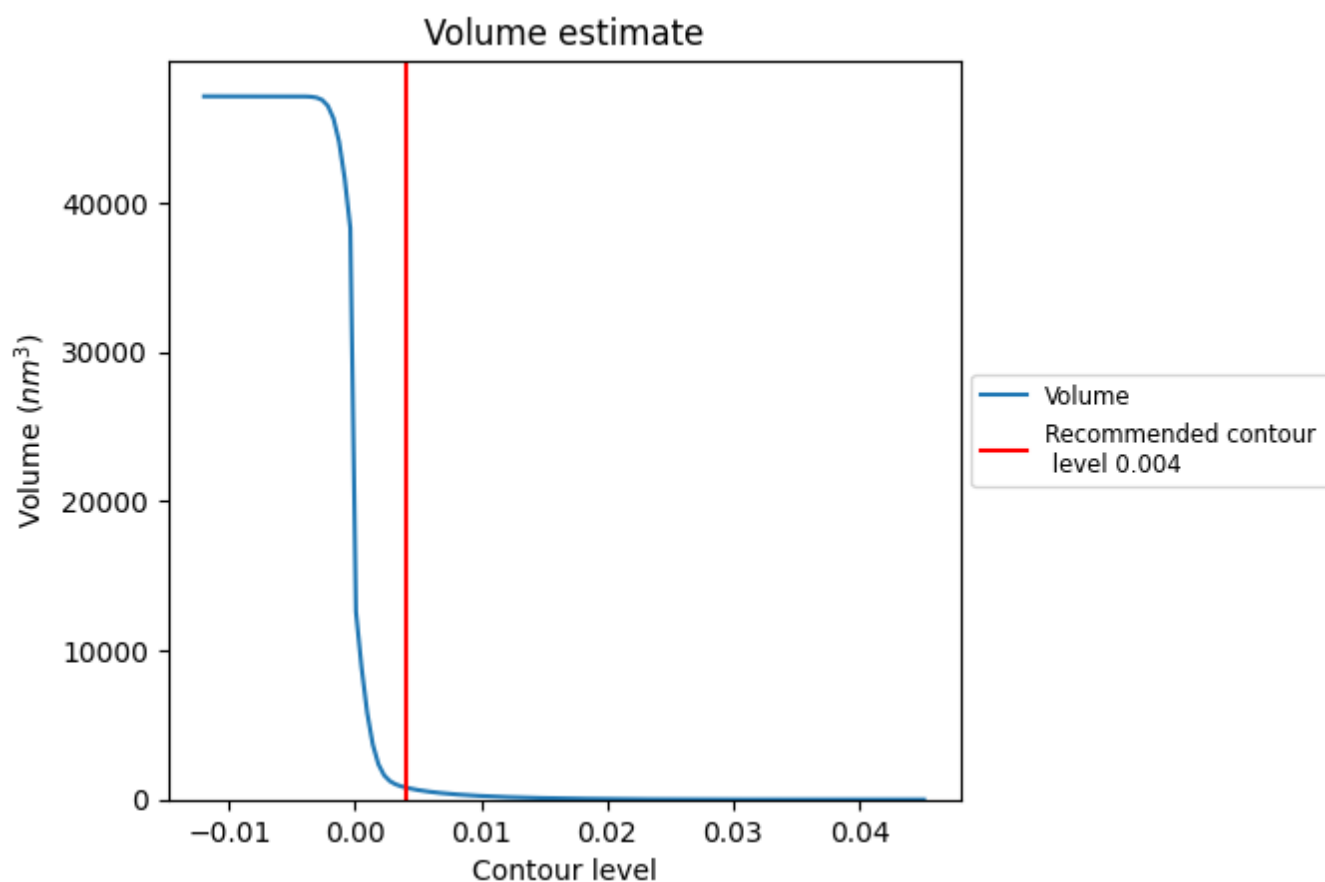
This section contains the results of statistical analysis of the map.

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.

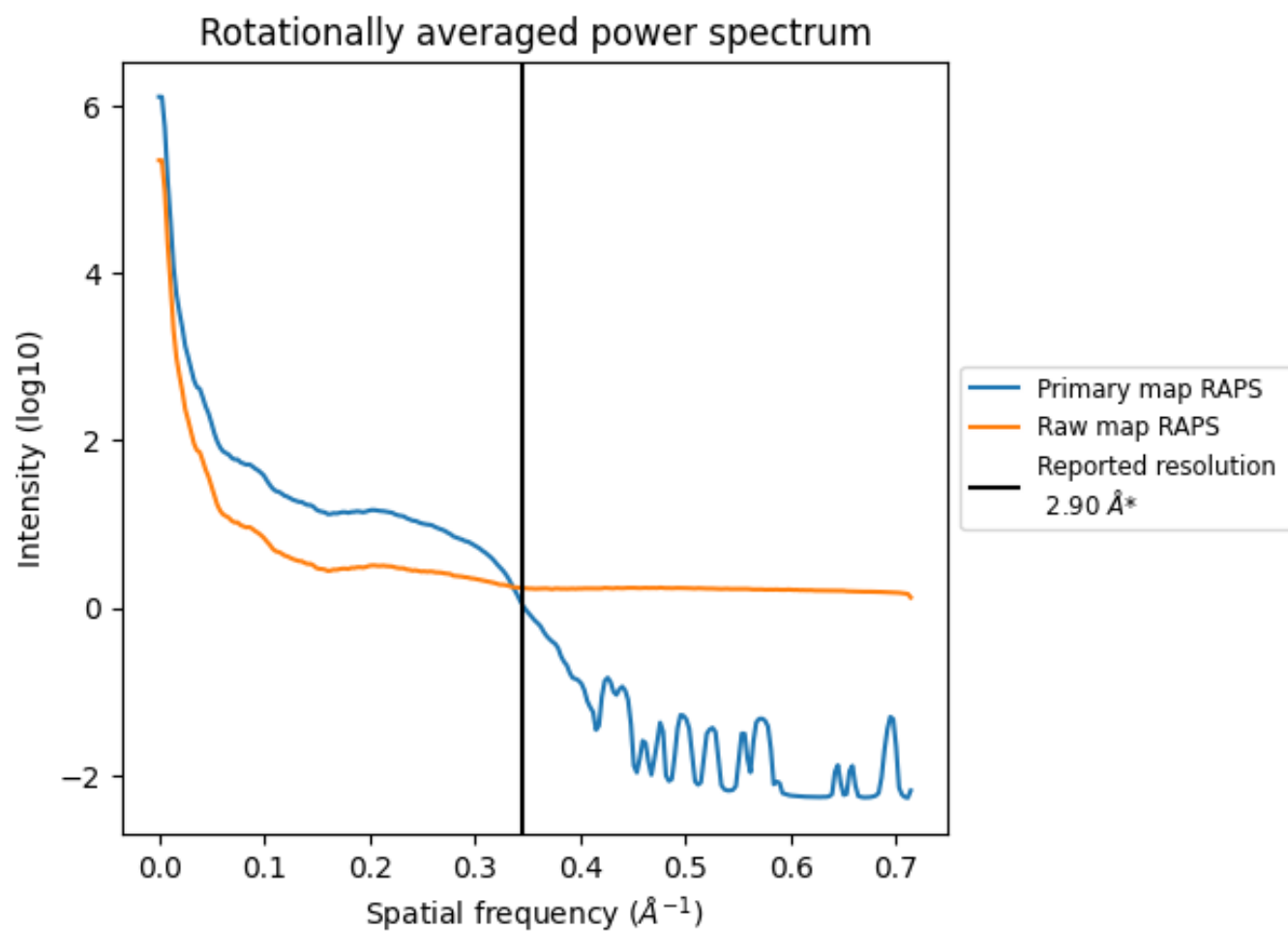
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 810 nm³; this corresponds to an approximate mass of 732 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 ⓘ

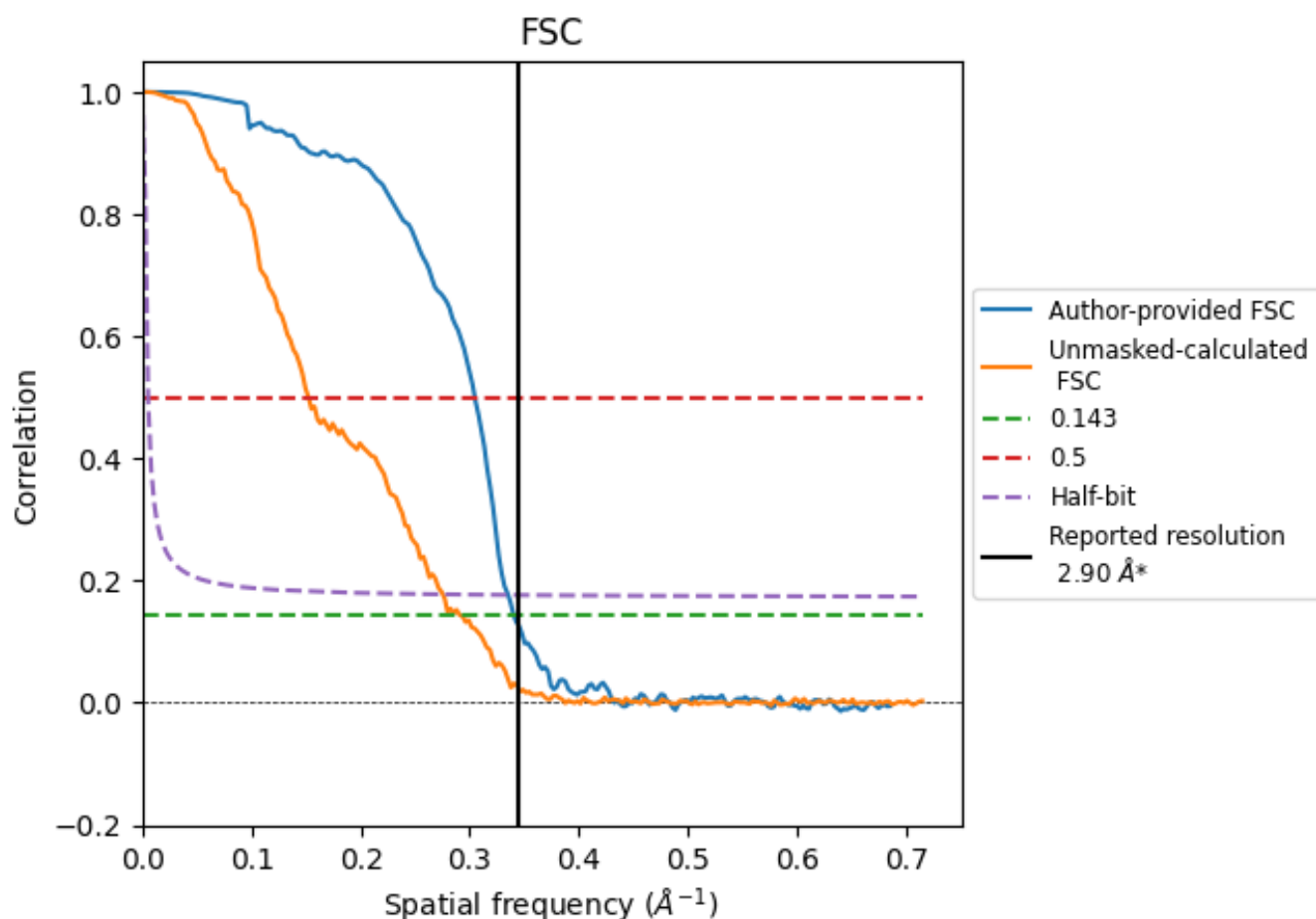


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

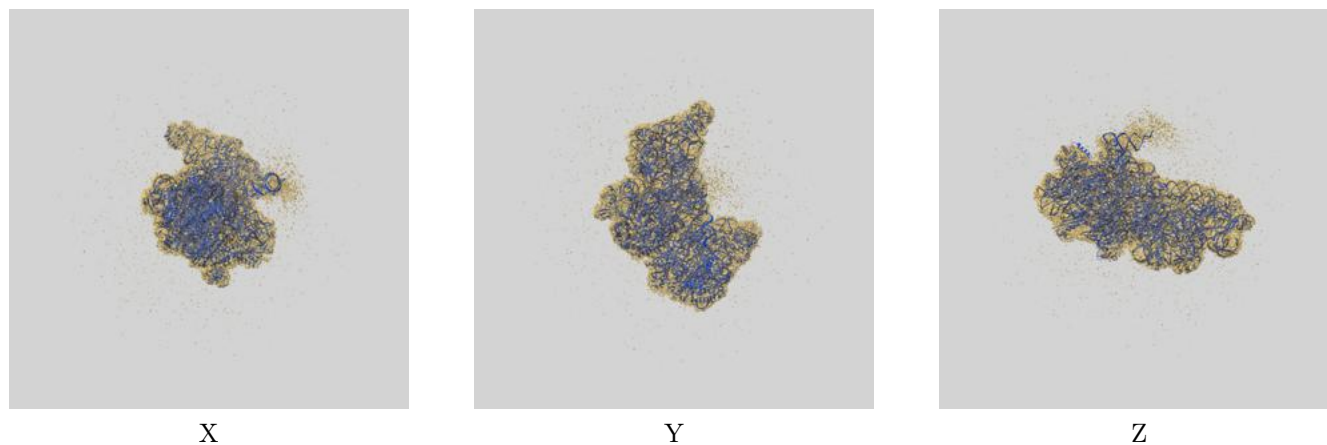
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.94	3.28	2.98
Unmasked-calculated*	3.43	6.57	3.63

*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 3.43 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

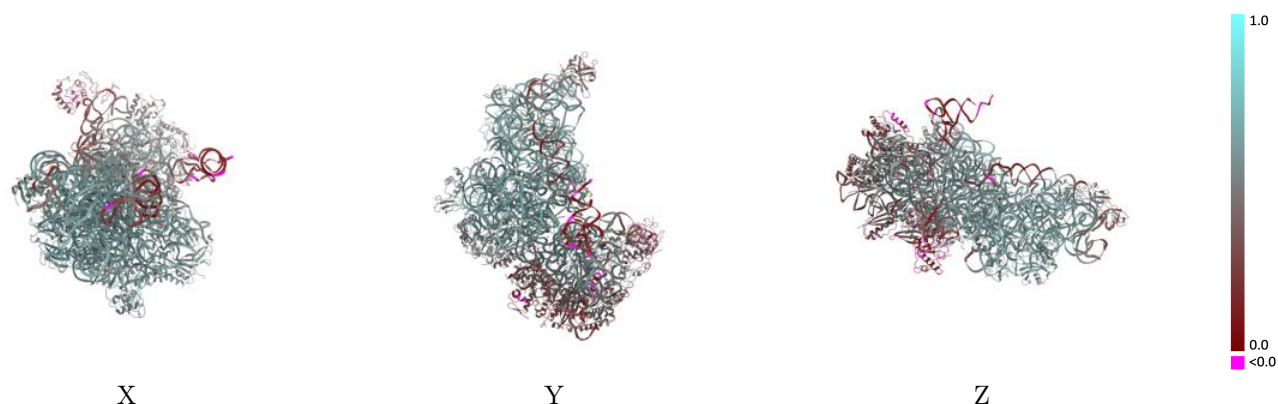
This section contains information regarding the fit between EMDB map EMD-50854 and PDB model 9FY0. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



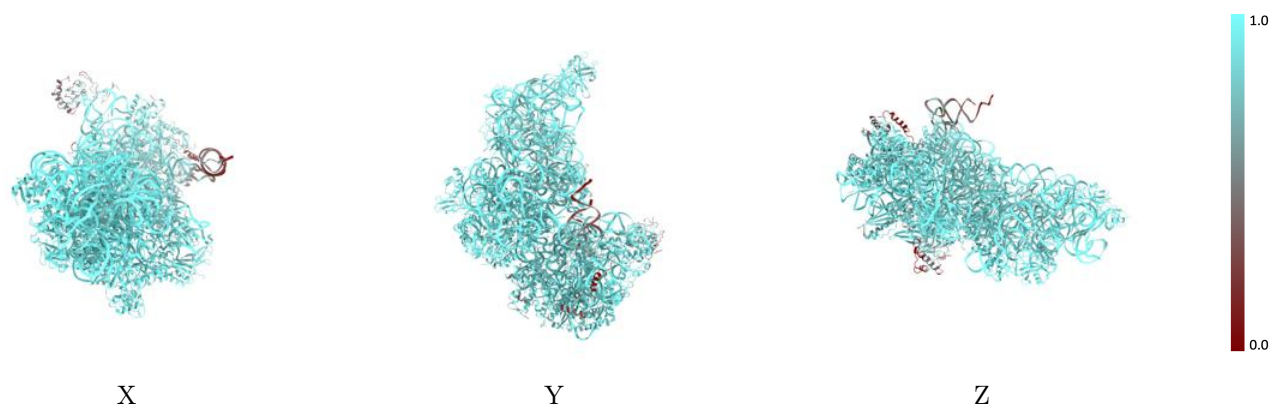
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



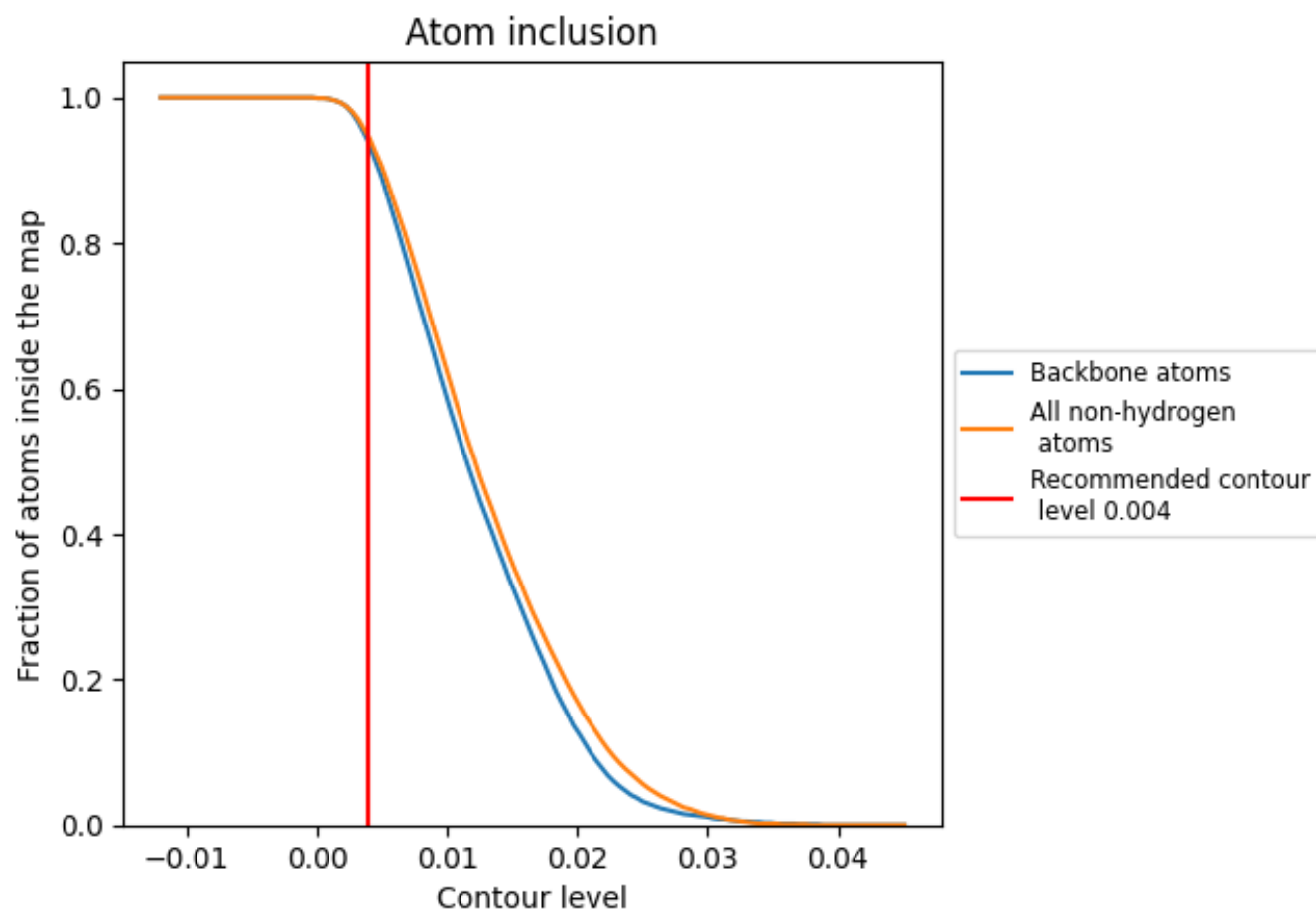
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.004).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9470	 0.5120
2	 0.9930	 0.5590
3	 0.4600	 0.1420
4	 0.5790	 0.2150
5	 0.9880	 0.5630
A	 0.9640	 0.5270
B	 0.9210	 0.4740
C	 0.9800	 0.5530
D	 0.9770	 0.5840
E	 0.9890	 0.5980
F	 0.9780	 0.5900
G	 0.9290	 0.4400
H	 0.8850	 0.3660
I	 0.9860	 0.6070
J	 0.9830	 0.5700
K	 0.9500	 0.4130
L	 0.8900	 0.3850
M	 0.9780	 0.5340
N	 0.9790	 0.5810
O	 0.9280	 0.4380
P	 0.9910	 0.5320
Q	 0.9680	 0.5640
R	 0.9870	 0.6080
S	 0.9440	 0.4120
T	 0.9090	 0.4180
U	 0.9440	 0.4360
V	 0.9560	 0.5580
W	 0.9760	 0.5510
X	 0.8720	 0.3290
Y	 0.5380	 0.1730
Z	 0.9490	 0.4610
a	 0.9510	 0.4220
b	 0.9450	 0.5400
c	 0.5280	 0.2520
d	 0.8440	 0.2650
e	 0.8830	 0.5270

