



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 02:10 am BST

PDB ID : 9FHL / pdb_00009fhl
EMDB ID : EMD-50445
Title : High-resolution cryo-EM structure of *Saccharolobus solfataricus* 30S ribosomal subunit bound to mRNA and initiator tRNA
Authors : Bourgeois, G.; Coureux, P.D.; Mechulam, Y.; Schmitt, E.
Deposited on : 2024-05-27
Resolution : 2.50 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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

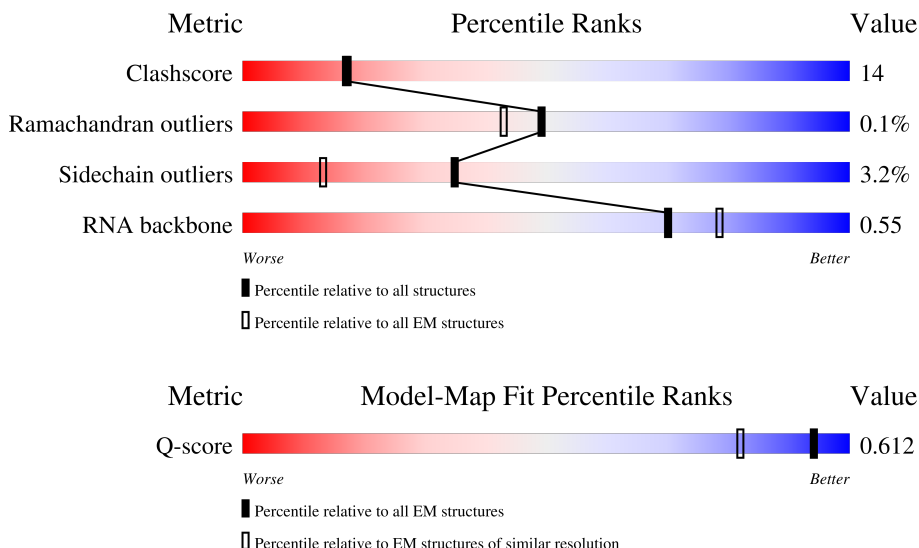
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 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	7115 (2.00 - 3.00)

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

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

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Mol	Chain	Length	Quality of chain
4	C	65	
5	D	181	
6	E	239	
7	F	214	
8	G	214	
9	H	193	
10	I	133	
11	J	133	
12	K	137	
13	L	102	
14	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	5	15	
34	s	15	
35	4	77	

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
37	SPM	2	1570	-	-	X	-
37	SPM	2	1581	-	-	X	-
37	SPM	2	1584	-	-	X	-
37	SPM	2	1589	-	-	X	-
37	SPM	2	1594	-	-	X	-
37	SPM	F	303	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 64047 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 Sso.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1430	Total	C	N	O	P	0	0
			30761	13720	5686	9925	1430		

There are 7 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is a protein called Small ribosomal subunit protein 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 VapB-type antitoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	70	Total	C	N	O	S	0	0
			570	370	92	105	3		

- 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 mRNA_Map.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5	3	Total	C	N	O	P	1	0
			105	39	17	41	8		

- Molecule 34 is a RNA chain called mRNA_Map.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	s	10	Total	C	N	O	P	0	0
			220	98	44	68	10		

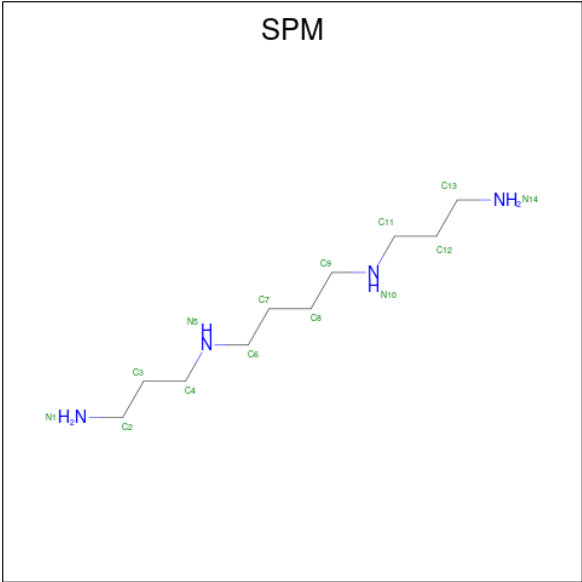
- Molecule 35 is a RNA chain called Initiator tRNA Met.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	4	17	Total	C	N	O	P	0	0
			361	162	64	118	17		

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	2	56	Total	Mg	0
			56	56	
36	F	1	Total	Mg	0
			1	1	
36	R	1	Total	Mg	0
			1	1	
36	5	1	Total	Mg	0
			1	1	

- Molecule 37 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			AltConf
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	

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Mol	Chain	Residues	Atoms			AltConf
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	2	1	Total	C	N	0
			14	10	4	
37	F	1	Total	C	N	0
			14	10	4	

- 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	

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		AltConf
39	2	434	Total	O	0
			434	434	
39	B	1	Total	O	0
			1	1	

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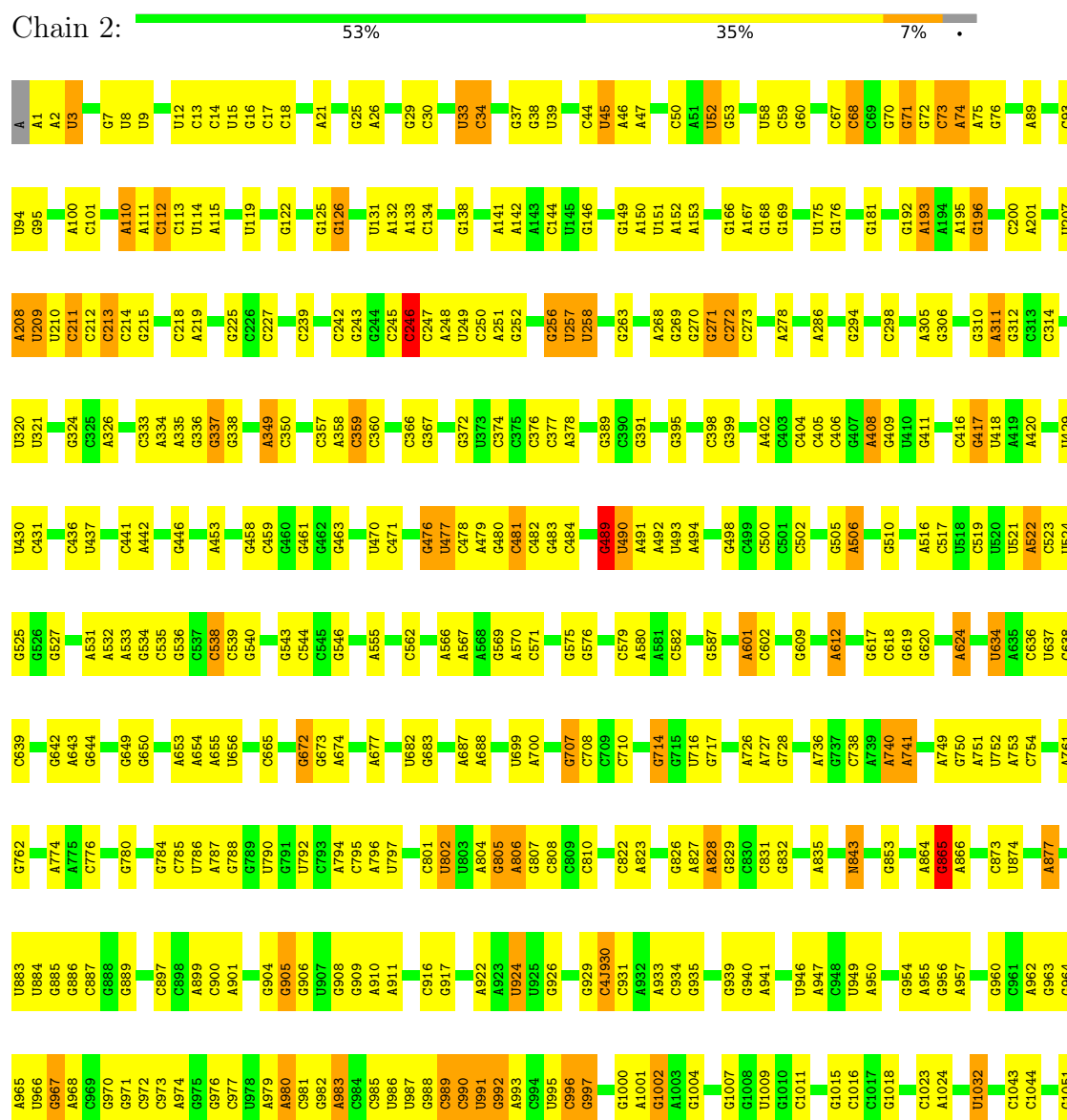
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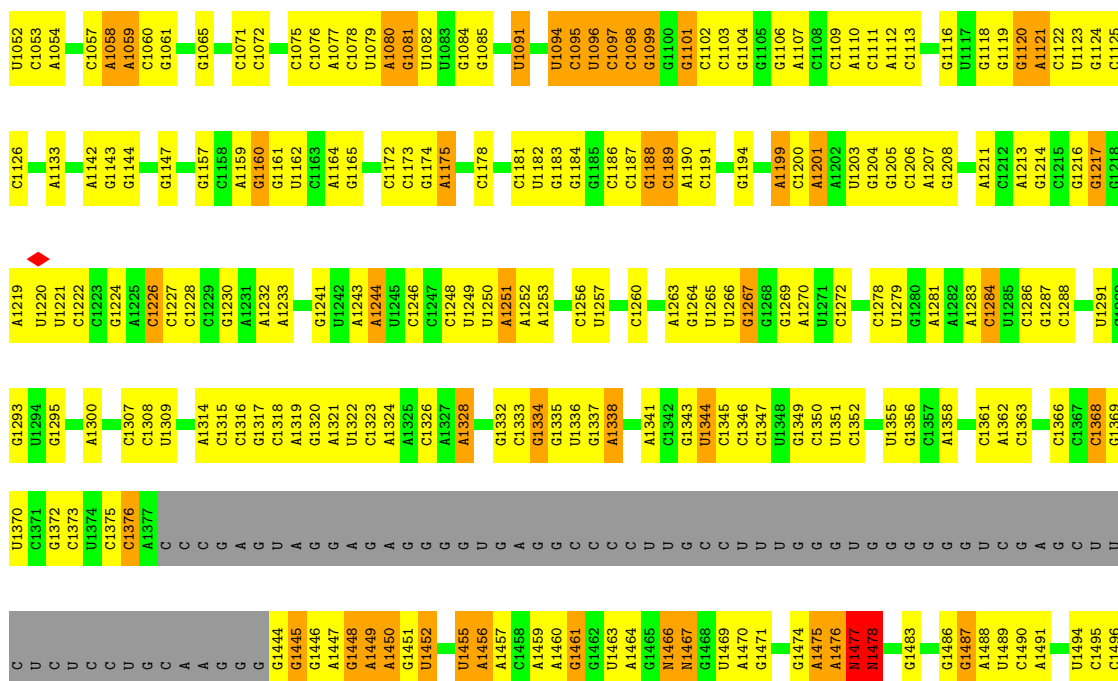
Mol	Chain	Residues	Atoms		AltConf
39	C	4	Total 4	O 4	0
39	D	8	Total 8	O 8	0
39	E	7	Total 7	O 7	0
39	F	15	Total 15	O 15	0
39	H	2	Total 2	O 2	0
39	I	5	Total 5	O 5	0
39	J	2	Total 2	O 2	0
39	K	3	Total 3	O 3	0
39	L	2	Total 2	O 2	0
39	Q	7	Total 7	O 7	0
39	R	4	Total 4	O 4	0
39	U	1	Total 1	O 1	0
39	V	1	Total 1	O 1	0
39	W	3	Total 3	O 3	0
39	5	12	Total 12	O 12	0
39	4	4	Total 4	O 4	0

3 Residue-property plots

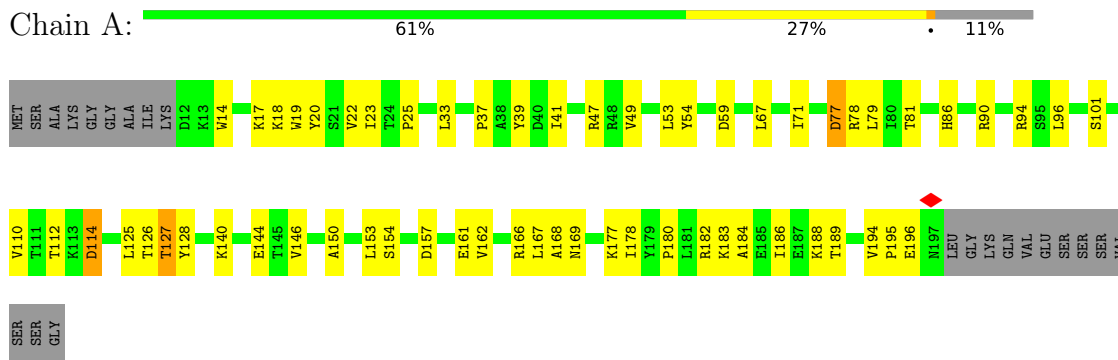
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: rRNA 16S Sso

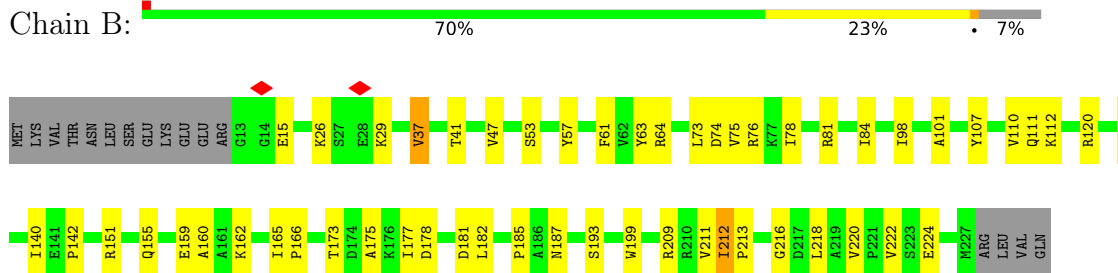




• Molecule 2: Small ribosomal subunit protein eS1

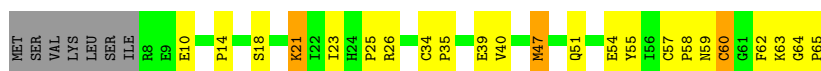


• Molecule 3: Small ribosomal subunit protein uS2



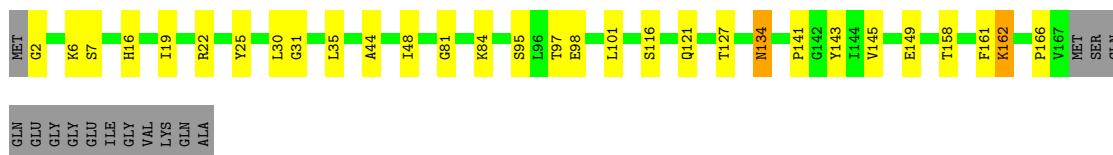
• Molecule 4: Small zinc finger protein HVO-2753-like zinc-binding pocket domain-containing protein





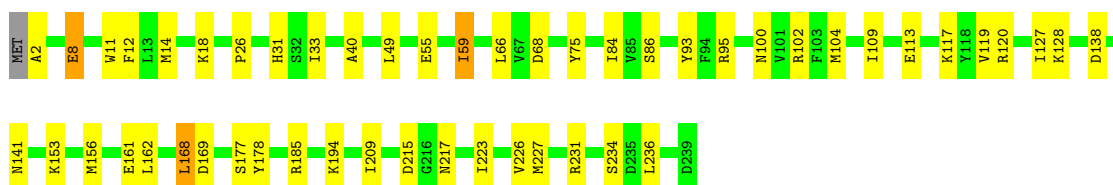
- Molecule 5: Small ribosomal subunit protein uS4

Chain D: 75% 15% 8%



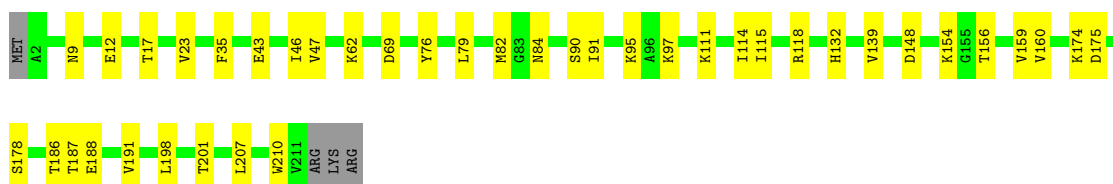
- Molecule 6: Small ribosomal subunit protein eS4

Chain E: 78% 20%



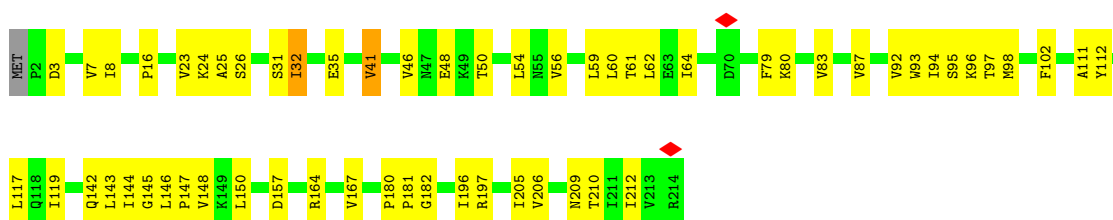
- Molecule 7: Small ribosomal subunit protein uS5

Chain F: 79% 19%



- Molecule 8: Small ribosomal subunit protein eS6

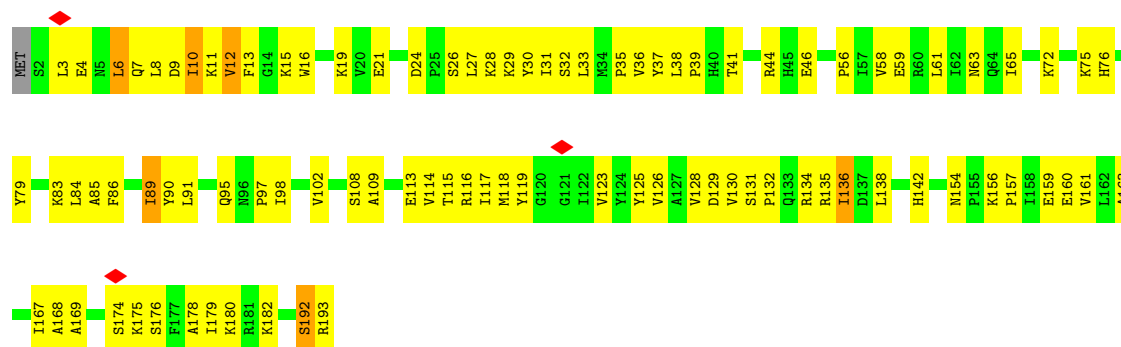
Chain G: 72% 27%



- Molecule 9: Small ribosomal subunit protein uS7

Chain H: 51% 45%





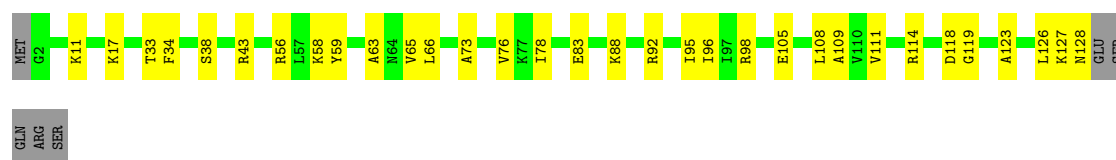
- Molecule 10: Small ribosomal subunit protein uS8

Chain I: 83% 16% .



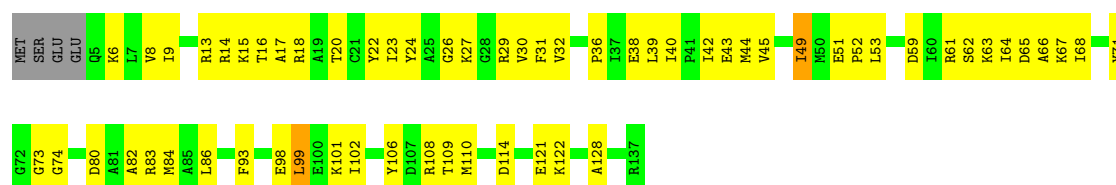
- Molecule 11: Small ribosomal subunit protein eS8

Chain J: 71% 24% 5%



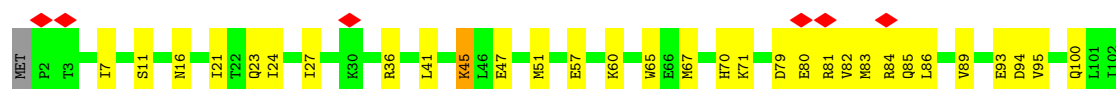
- Molecule 12: Small ribosomal subunit protein uS9

Chain K: 53% 43% ..



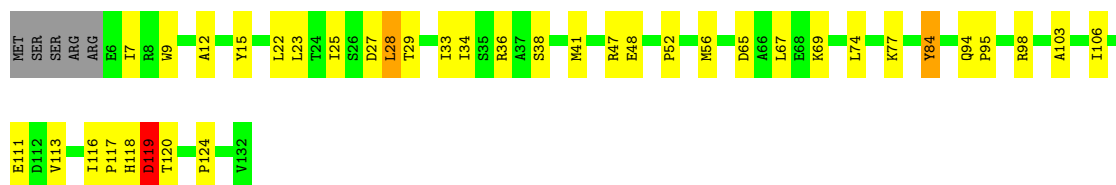
- Molecule 13: Small ribosomal subunit protein uS10

Chain L: 6% 69% 29% ..



- Molecule 14: Small ribosomal subunit protein uS11

Chain M: 67% 27% ...



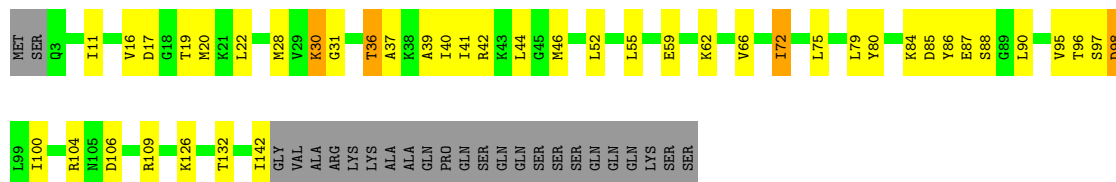
- Molecule 15: Small ribosomal subunit protein uS12

Chain N: 79% 20% ..



- Molecule 16: Small ribosomal subunit protein uS13

Chain O: 59% 24% 15%



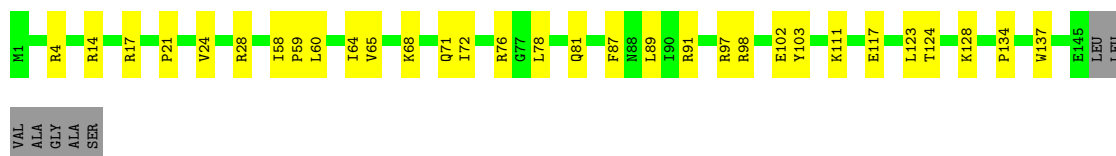
- Molecule 17: Small ribosomal subunit protein uS14

Chain P: 59% 37% ..



- Molecule 18: Small ribosomal subunit protein uS15

Chain Q: 75% 20% 5%

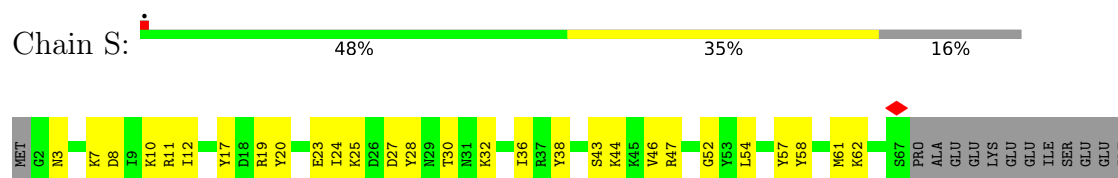


- Molecule 19: Small ribosomal subunit protein uS17

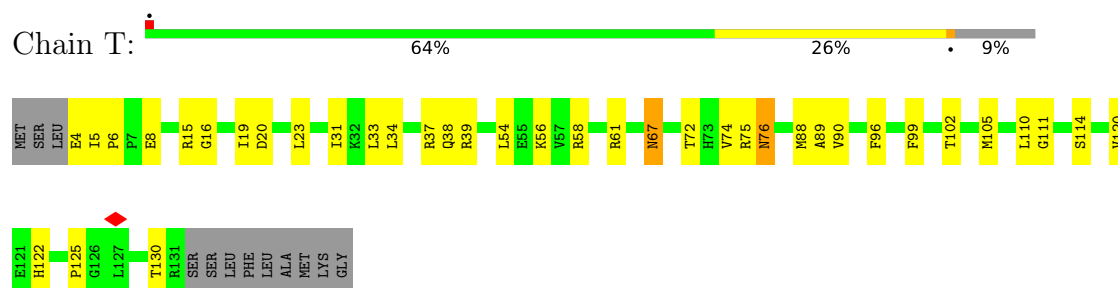
Chain R: 83% 16%



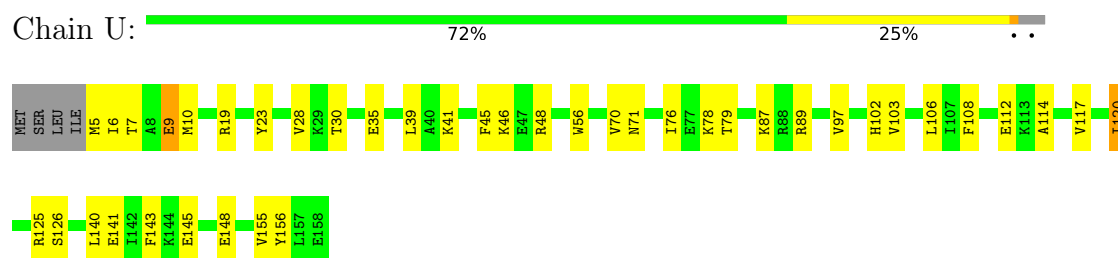
- Molecule 20: Small ribosomal subunit protein eS17



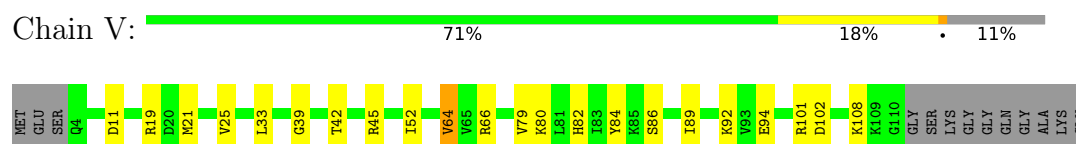
- Molecule 21: Small ribosomal subunit protein uS19



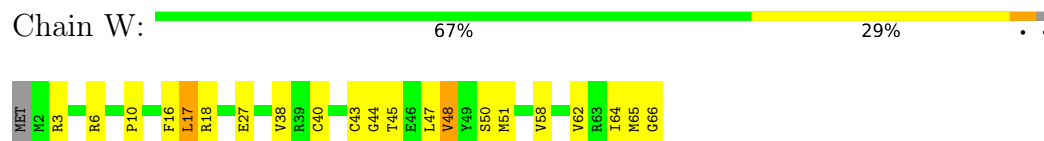
- Molecule 22: Small ribosomal subunit protein eS19



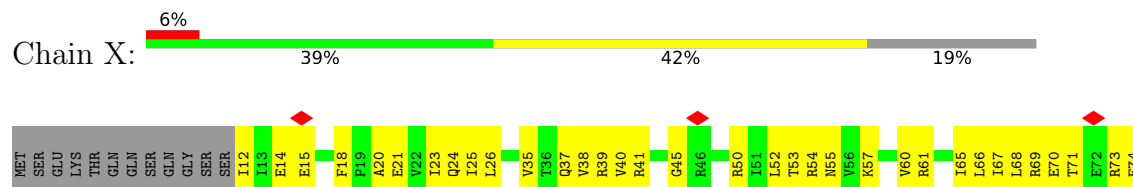
- Molecule 23: Small ribosomal subunit protein eS24



- Molecule 24: Small ribosomal subunit protein eS27



- Molecule 25: Small ribosomal subunit protein eS28







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	766000	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	0.177	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	365.292, 365.292, 365.292	wwPDB
Map dimensions	438, 438, 438	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 4AC, OMU, 5MC, OMC, MA6, OMG, SPM, ZN, 6MZ, C4J, A2M, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	2	0.36	2/33594 (0.0%)	0.38	4/52408 (0.0%)
2	A	0.25	0/1543	0.42	0/2077
3	B	0.22	0/1731	0.47	1/2349 (0.0%)
4	C	0.27	0/466	0.63	2/625 (0.3%)
5	D	0.28	0/1380	0.39	0/1859
6	E	0.31	0/1965	0.48	0/2644
7	F	0.36	0/1654	0.55	3/2240 (0.1%)
8	G	0.20	0/1684	0.42	0/2265
9	H	0.21	0/1571	0.50	2/2116 (0.1%)
10	I	0.32	0/1070	0.41	0/1444
11	J	0.29	0/994	0.45	0/1337
12	K	0.24	0/1084	0.47	0/1450
13	L	0.22	0/856	0.43	1/1154 (0.1%)
14	M	0.29	0/960	0.67	2/1294 (0.2%)
15	N	0.32	0/1155	0.50	1/1540 (0.1%)
16	O	0.21	0/1142	0.42	0/1532
17	P	0.26	0/451	0.59	2/600 (0.3%)
18	Q	0.29	0/1206	0.38	0/1618
19	R	0.32	0/918	0.44	0/1236
20	S	0.22	0/578	0.40	0/770
21	T	0.20	0/1087	0.37	0/1456
22	U	0.22	0/1270	0.40	0/1710
23	V	0.23	0/843	0.44	0/1124
24	W	0.27	0/511	0.42	0/684
25	X	0.20	0/538	0.52	0/722
26	Y	0.24	0/404	0.67	0/540
27	Z	0.24	0/1584	0.42	0/2124
28	3	0.24	0/902	0.57	0/1216
29	a	0.79	0/574	0.97	2/770 (0.3%)
30	c	0.36	1/861 (0.1%)	0.64	3/1143 (0.3%)
31	d	0.24	0/581	0.59	0/786
32	e	0.28	0/360	0.62	1/477 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	5	0.34	0/47	0.51	0/71
34	s	0.38	0/247	0.84	2/384 (0.5%)
35	4	0.24	0/379	0.30	0/588
All	All	0.33	3/66190 (0.0%)	0.44	26/96353 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	c	9	ILE	CA-C	-6.91	1.44	1.52
1	2	1450	A	O3'-P	-6.47	1.51	1.61
1	2	1373	C	O3'-P	5.16	1.68	1.61

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1450	A	O3'-P-O5'	9.53	118.29	104.00
29	a	24	CYS	N-CA-C	7.89	119.96	111.36
1	2	489	G	C2'-C3'-O3'	7.50	120.75	109.50
30	c	9	ILE	N-CA-C	7.02	117.16	110.42
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
3	B	212	ILE	N-CA-C	-6.49	103.87	109.19
32	e	10	ALA	O-C-N	-6.31	115.01	122.96
17	P	6	PRO	CA-C-N	6.26	126.23	119.78
17	P	6	PRO	C-N-CA	6.26	126.23	119.78
1	2	490	U	C1'-C2'-O2'	-6.16	102.56	111.80
30	c	103	LEU	N-CA-C	6.09	118.10	108.79
1	2	490	U	C3'-C2'-O2'	5.82	123.33	114.60
9	H	109	ALA	CA-C-N	5.82	126.70	120.13
9	H	109	ALA	C-N-CA	5.82	126.70	120.13
34	s	809	G	C4'-C3'-O3'	-5.72	104.42	113.00
30	c	9	ILE	O-C-N	5.54	127.34	121.91
34	s	813	G	C2'-C3'-O3'	5.46	117.68	109.50
15	N	64	GLN	N-CA-C	5.23	121.37	109.81
29	a	47	ALA	N-CA-C	5.20	117.79	108.17
7	F	156	THR	CA-C-N	-5.19	115.86	122.19
7	F	156	THR	C-N-CA	-5.19	115.86	122.19
7	F	84	ASN	N-CA-C	-5.18	101.71	109.95
13	L	45	LYS	N-CA-C	5.08	116.67	108.34
4	C	57	CYS	CA-C-N	5.06	124.84	119.28
4	C	57	CYS	C-N-CA	5.06	124.84	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	30761	0	15566	542	0
2	A	1515	0	1565	54	0
3	B	1698	0	1753	37	0
4	C	455	0	438	19	0
5	D	1354	0	1419	24	0
6	E	1930	0	2013	37	0
7	F	1625	0	1689	33	0
8	G	1661	0	1737	41	0
9	H	1543	0	1611	156	0
10	I	1050	0	1100	15	0
11	J	982	0	1046	21	0
12	K	1068	0	1125	65	0
13	L	840	0	893	32	0
14	M	944	0	978	31	0
15	N	1140	0	1244	26	0
16	O	1124	0	1162	42	0
17	P	440	0	436	29	0
18	Q	1185	0	1260	22	0
19	R	901	0	935	15	0
20	S	571	0	598	26	0
21	T	1064	0	1107	34	0
22	U	1247	0	1329	47	0
23	V	836	0	894	18	0
24	W	503	0	531	16	0
25	X	535	0	572	33	0
26	Y	395	0	405	37	0
27	Z	1561	0	1667	53	0
28	3	893	0	940	66	0
29	a	562	0	574	49	0
30	c	856	0	941	69	0
31	d	570	0	590	86	0
32	e	354	0	386	11	0
33	5	105	0	44	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	s	220	0	109	8	0
35	4	361	0	187	3	0
36	2	56	0	0	1	0
36	5	1	0	0	0	0
36	F	1	0	0	0	0
36	R	1	0	0	0	0
37	2	602	0	1117	152	0
37	F	14	0	26	11	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
39	2	434	0	0	21	0
39	4	4	0	0	0	0
39	5	12	0	0	0	0
39	B	1	0	0	0	0
39	C	4	0	0	1	0
39	D	8	0	0	1	0
39	E	7	0	0	1	0
39	F	15	0	0	0	0
39	H	2	0	0	0	0
39	I	5	0	0	0	0
39	J	2	0	0	0	0
39	K	3	0	0	0	0
39	L	2	0	0	1	0
39	Q	7	0	0	0	0
39	R	4	0	0	0	0
39	U	1	0	0	0	0
39	V	1	0	0	0	0
39	W	3	0	0	1	0
All	All	64047	0	49987	1553	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1553) 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)
9:H:19:LYS:NZ	31:d:71:LEU:CD1	1.87	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:7:G:OP1	37:2:1586:SPM:H131	1.40	1.20
31:d:56:VAL:HG22	31:d:57:PRO:CD	1.69	1.20
9:H:10:ILE:HG23	9:H:37:TYR:CD1	1.79	1.18
1:2:904:G:OP2	37:2:1583:SPM:N1	1.79	1.15
9:H:10:ILE:HA	9:H:37:TYR:CE2	1.82	1.15
9:H:19:LYS:NZ	31:d:71:LEU:HD12	1.60	1.14
9:H:113:GLU:O	9:H:128:VAL:HG12	1.48	1.14
9:H:168:ALA:HB2	9:H:175:LYS:NZ	1.61	1.14
10:I:28:MET:HE2	10:I:60:LYS:HE3	1.25	1.12
1:2:1184:G:OP2	37:2:1570:SPM:H122	1.49	1.11
26:Y:39:LYS:HZ3	26:Y:48:MET:HE3	1.13	1.11
26:Y:39:LYS:NZ	26:Y:48:MET:HE3	1.65	1.10
31:d:56:VAL:HG22	31:d:57:PRO:HD2	1.32	1.10
9:H:19:LYS:HZ3	31:d:71:LEU:CD1	1.52	1.08
9:H:19:LYS:HZ3	31:d:71:LEU:HD11	0.98	1.08
9:H:91:LEU:HD13	30:c:97:TYR:OH	1.51	1.07
1:2:21:A:OP1	37:2:1587:SPM:H71	1.54	1.06
29:a:20:TYR:HD1	29:a:25:ASN:ND2	1.54	1.05
9:H:3:LEU:HD12	12:K:98:GLU:HG2	1.08	1.04
22:U:5:MET:O	22:U:6:ILE:HD13	1.58	1.04
9:H:10:ILE:HG23	9:H:37:TYR:CG	1.93	1.03
9:H:19:LYS:HZ1	31:d:71:LEU:CD1	1.56	1.03
29:a:20:TYR:HD1	29:a:25:ASN:HD21	1.03	1.02
9:H:168:ALA:HB2	9:H:175:LYS:HZ1	1.09	1.01
31:d:7:LYS:HA	31:d:7:LYS:HE3	1.43	1.01
1:2:983:A:OP2	17:P:2:GLY:HA3	1.61	0.99
1:2:1189:C:HO2'	30:c:2:GLY:N	1.60	0.99
15:N:57:LYS:HD2	15:N:94:VAL:HG22	1.45	0.99
37:2:1581:SPM:H81	37:2:1581:SPM:H122	1.45	0.98
7:F:139:VAL:HG22	7:F:148:ASP:OD1	1.64	0.98
1:2:579:C:OP1	37:2:1594:SPM:H131	1.64	0.97
28:3:24:ARG:HG2	28:3:89:ALA:HB1	1.44	0.97
9:H:159:GLU:OE1	30:c:100:ASN:ND2	1.97	0.97
9:H:113:GLU:O	9:H:128:VAL:CG1	2.13	0.96
31:d:56:VAL:HG22	31:d:57:PRO:HD3	1.45	0.96
28:3:55:GLU:O	28:3:60:GLU:OE2	1.83	0.94
1:2:917:G:OP1	37:2:1581:SPM:H121	1.68	0.94
1:2:644:G:N3	14:M:36:ARG:NH2	2.15	0.94
4:C:40:VAL:HG21	4:C:58:PRO:HD2	1.49	0.94
1:2:949:U:H3	1:2:1183:G:H1	0.97	0.94
29:a:39:PRO:HD3	29:a:69:VAL:HG12	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:32:ILE:O	28:3:33:LYS:HG3	1.70	0.92
9:H:3:LEU:O	31:d:70:LYS:NZ	2.01	0.92
31:d:12:ARG:HG2	31:d:12:ARG:HH11	1.35	0.91
1:2:149:G:OP2	37:2:1589:SPM:H92	1.68	0.91
9:H:19:LYS:HZ1	31:d:71:LEU:HD12	1.21	0.91
1:2:243:G:OP2	37:2:1575:SPM:H32	1.71	0.91
2:A:23:ILE:HD13	2:A:78:ARG:CD	2.01	0.91
37:2:1594:SPM:H122	37:2:1594:SPM:H71	1.49	0.91
37:2:1586:SPM:H122	39:2:1928:HOH:O	1.71	0.90
31:d:4:LEU:HD21	31:d:16:ILE:O	1.72	0.89
2:A:23:ILE:HD13	2:A:78:ARG:HD2	1.52	0.89
9:H:10:ILE:HG12	9:H:37:TYR:CE1	2.08	0.89
9:H:108:SER:O	9:H:182:LYS:HD2	1.73	0.88
1:2:21:A:P	37:2:1587:SPM:H71	2.14	0.88
2:A:23:ILE:CG2	2:A:78:ARG:HD2	2.04	0.87
5:D:116:SER:HB2	5:D:121:GLN:HG2	1.55	0.87
9:H:3:LEU:HD12	12:K:98:GLU:CG	1.99	0.87
1:2:500:C:OP2	32:e:25:LYS:NZ	2.08	0.87
9:H:159:GLU:OE2	30:c:102:ARG:NE	2.07	0.87
1:2:983:A:P	17:P:2:GLY:HA3	2.16	0.86
3:B:98:ILE:HD13	3:B:142:PRO:HB3	1.58	0.86
9:H:19:LYS:NZ	31:d:71:LEU:HD11	1.68	0.85
30:c:7:LYS:HB2	30:c:9:ILE:HG22	1.58	0.85
1:2:463:G:H5'	1:2:493:U:O2	1.77	0.85
9:H:168:ALA:CB	9:H:175:LYS:NZ	2.39	0.85
26:Y:48:MET:SD	26:Y:58:TRP:HB3	2.16	0.85
37:2:1558:SPM:H122	37:2:1587:SPM:H22	1.59	0.84
1:2:1189:C:OP2	16:O:132:THR:OG1	1.94	0.84
1:2:477:U:H2'	1:2:489:G:C8	2.11	0.84
1:2:908:G:O6	37:2:1583:SPM:C13	2.25	0.84
2:A:23:ILE:HG21	2:A:78:ARG:HD2	1.60	0.84
9:H:128:VAL:HG23	25:X:55:ASN:O	1.77	0.84
1:2:1120:G:N7	20:S:44:LYS:NZ	2.26	0.83
8:G:56:VAL:HG23	8:G:59:LEU:O	1.76	0.83
14:M:117:PRO:HG3	14:M:120:THR:HB	1.58	0.83
15:N:28:ARG:O	15:N:32:THR:HG23	1.78	0.83
31:d:56:VAL:CG2	31:d:57:PRO:CD	2.56	0.83
18:Q:97:ARG:NH2	18:Q:117:GLU:OE2	2.12	0.83
1:2:21:A:OP1	37:2:1587:SPM:C7	2.26	0.82
1:2:1476:A:H8	1:2:1476:A:H5''	1.43	0.82
13:L:81:ARG:HG2	13:L:84:ARG:HH21	1.45	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:49:LYS:HG2	28:3:75:ILE:HG21	1.59	0.82
37:2:1594:SPM:H122	37:2:1594:SPM:C7	2.09	0.82
12:K:8:VAL:HG22	12:K:23:ILE:HG22	1.62	0.82
31:d:25:ASN:ND2	31:d:64:PRO:HA	1.93	0.82
12:K:14:ARG:HG2	12:K:80:ASP:HB3	1.61	0.82
26:Y:39:LYS:NZ	26:Y:48:MET:CE	2.43	0.82
1:2:1162:U:O4	37:2:1571:SPM:N1	2.13	0.82
2:A:23:ILE:HD13	2:A:78:ARG:NE	1.95	0.82
12:K:102:ILE:HD12	31:d:67:ILE:HD13	1.60	0.82
37:2:1594:SPM:H71	37:2:1594:SPM:C12	2.10	0.81
37:2:1570:SPM:HN11	37:2:1570:SPM:H62	1.43	0.81
1:2:983:A:P	17:P:2:GLY:CA	2.68	0.81
12:K:102:ILE:CD1	31:d:67:ILE:HD13	2.10	0.81
18:Q:98:ARG:NH1	18:Q:102:GLU:OE2	2.14	0.80
26:Y:32:ASN:O	26:Y:32:ASN:ND2	2.14	0.80
8:G:167:VAL:HG21	8:G:196:ILE:HD11	1.62	0.80
26:Y:56:GLU:HB3	26:Y:69:ILE:HB	1.63	0.80
28:3:57:VAL:O	28:3:60:GLU:CG	2.29	0.80
1:2:1216:G:OP1	13:L:45:LYS:NZ	2.15	0.80
1:2:1295:G:H4'	30:c:8:PRO:HG2	1.63	0.80
22:U:5:MET:HE3	22:U:7:THR:HG22	1.61	0.80
8:G:80:LYS:NZ	8:G:145:GLY:O	2.15	0.80
1:2:980:A:OP1	21:T:56:LYS:HE3	1.82	0.79
1:2:1160:G:OP1	39:2:1701:HOH:O	1.98	0.79
9:H:10:ILE:HG23	9:H:37:TYR:CE1	2.16	0.79
28:3:57:VAL:O	28:3:60:GLU:HG3	1.81	0.79
1:2:1091:U:H3	1:2:1104:G:H1	1.27	0.79
37:2:1570:SPM:HN11	37:2:1570:SPM:C6	1.95	0.79
1:2:522:A:H2'	1:2:522:A:N3	1.98	0.78
37:2:1589:SPM:H61	37:2:1589:SPM:HN0	1.46	0.78
22:U:30:THR:HG21	22:U:114:ALA:HB2	1.66	0.78
1:2:71:G:N1	1:2:213:C:N3	2.29	0.78
1:2:1101:G:O4'	22:U:5:MET:HE2	1.83	0.78
37:2:1576:SPM:H112	37:2:1588:SPM:H31	1.63	0.78
1:2:1143:G:OP1	12:K:108:ARG:NH2	2.15	0.78
1:2:337:OMG:HM22	1:2:338:G:H5'	1.65	0.78
9:H:108:SER:C	9:H:182:LYS:HD2	2.08	0.78
9:H:89:ILE:HD11	9:H:97:PRO:HA	1.65	0.77
1:2:95:G:OP2	37:2:1563:SPM:N5	2.16	0.77
1:2:481:OMC:HM22	1:2:482:C:H5'	1.67	0.77
31:d:56:VAL:CG2	31:d:57:PRO:HD3	2.12	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:310:G:HO2'	5:D:2:GLY:N	1.82	0.77
9:H:159:GLU:CD	30:c:102:ARG:HE	1.92	0.77
37:2:1558:SPM:H122	37:2:1587:SPM:C2	2.15	0.76
1:2:877:A:O5'	37:2:1586:SPM:H22	1.85	0.76
9:H:28:LYS:HE2	31:d:53:ILE:CG2	2.15	0.76
9:H:90:TYR:HB2	9:H:97:PRO:HG3	1.66	0.76
16:O:126:LYS:HG2	30:c:5:SER:HB3	1.66	0.76
12:K:27:LYS:NZ	22:U:155:VAL:O	2.19	0.76
27:Z:36:VAL:HG12	27:Z:45:VAL:HG22	1.68	0.76
1:2:1187:C:OP2	37:2:1581:SPM:H31	1.87	0.75
11:J:33:THR:HG21	11:J:56:ARG:HD3	1.69	0.75
31:d:64:PRO:HG2	31:d:67:ILE:HB	1.69	0.75
1:2:904:G:P	37:2:1583:SPM:HN12	2.10	0.74
2:A:23:ILE:CD1	2:A:78:ARG:HD2	2.17	0.74
1:2:908:G:O6	37:2:1583:SPM:H131	1.87	0.74
17:P:19:CYS:SG	17:P:36:LEU:HA	2.28	0.74
31:d:52:LEU:C	31:d:52:LEU:HD12	2.13	0.74
14:M:117:PRO:CG	14:M:120:THR:HB	2.19	0.73
27:Z:63:ILE:H	27:Z:63:ILE:HD12	1.53	0.73
7:F:187:THR:H	37:F:303:SPM:H122	1.53	0.73
9:H:41:THR:O	9:H:44:ARG:NH1	2.22	0.73
22:U:45:PHE:HB2	22:U:87:LYS:HB2	1.71	0.72
29:a:57:LEU:HD23	29:a:62:PRO:HD3	1.70	0.72
16:O:126:LYS:CG	30:c:5:SER:HB3	2.19	0.72
1:2:1189:C:O2'	30:c:2:GLY:N	2.21	0.72
21:T:20:ASP:HA	21:T:23:LEU:HD12	1.71	0.72
31:d:4:LEU:CD2	31:d:16:ILE:O	2.38	0.72
37:2:1576:SPM:C11	37:2:1588:SPM:H31	2.19	0.72
18:Q:134:PRO:HG2	18:Q:137:TRP:HB2	1.72	0.72
12:K:38:GLU:OE1	12:K:61:ARG:NH2	2.23	0.72
1:2:484:C:H5''	37:2:1584:SPM:H132	1.72	0.72
1:2:1122:C:N3	1:2:1124:G:C8	2.58	0.72
9:H:3:LEU:CD1	12:K:98:GLU:HG2	2.04	0.72
1:2:483:G:H1'	37:2:1558:SPM:H121	1.70	0.71
18:Q:17:ARG:HH21	18:Q:21:PRO:HD3	1.54	0.71
27:Z:70:PHE:HB3	27:Z:76:LEU:HD12	1.70	0.71
1:2:1054:A:OP2	20:S:7:LYS:NZ	2.23	0.71
22:U:5:MET:HE3	22:U:7:THR:CG2	2.20	0.71
1:2:1011:C:OP1	39:2:1701:HOH:O	2.08	0.71
1:2:489:G:N3	1:2:489:G:H2'	2.05	0.71
9:H:8:LEU:HD12	9:H:8:LEU:C	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:10:ILE:HG12	9:H:37:TYR:CZ	2.26	0.71
12:K:24:TYR:HE1	12:K:65:ASP:HB3	1.56	0.71
18:Q:28:ARG:HG3	18:Q:65:VAL:HA	1.73	0.71
5:D:143:TYR:OH	5:D:149:GLU:OE2	2.06	0.71
17:P:4:TYR:O	29:a:63:TYR:HE1	1.74	0.71
1:2:39:U:O4	6:E:18:LYS:NZ	2.24	0.70
21:T:90:VAL:HG23	21:T:114:SER:HB2	1.73	0.70
1:2:1476:A:H5''	1:2:1476:A:C8	2.25	0.70
9:H:8:LEU:HD12	9:H:8:LEU:O	1.91	0.70
12:K:29:ARG:NH2	22:U:156:TYR:O	2.25	0.70
26:Y:25:THR:HG23	28:3:65:HIS:CE1	2.27	0.70
29:a:20:TYR:CD1	29:a:25:ASN:ND2	2.47	0.70
9:H:13:PHE:HE2	9:H:79:TYR:CE2	2.09	0.70
30:c:96:LEU:HD13	30:c:96:LEU:C	2.17	0.70
37:2:1585:SPM:H81	37:F:303:SPM:H92	1.71	0.70
29:a:36:TYR:CZ	29:a:54:LYS:NZ	2.60	0.70
31:d:12:ARG:HG2	31:d:12:ARG:NH1	2.07	0.70
31:d:24:LEU:HD21	31:d:53:ILE:HD11	1.71	0.70
1:2:910:A:H2'	1:2:911:A:C8	2.26	0.70
9:H:26:SER:HB3	25:X:67:ILE:HD11	1.72	0.70
25:X:26:LEU:HB2	25:X:37:GLN:HB3	1.73	0.69
9:H:168:ALA:CB	9:H:175:LYS:HZ3	2.05	0.69
27:Z:163:ILE:C	27:Z:163:ILE:HD12	2.17	0.69
34:s:812:U:OP1	34:s:812:U:C5	2.45	0.69
8:G:41:VAL:HG11	8:G:146:LEU:HD21	1.74	0.69
9:H:91:LEU:CD1	30:c:97:TYR:OH	2.36	0.69
27:Z:24:LYS:CG	29:a:14:LEU:HD22	2.23	0.69
31:d:7:LYS:HE2	31:d:55:GLN:HG3	1.73	0.69
1:2:71:G:O6	1:2:213:C:N4	2.24	0.69
1:2:940:G:OP1	39:2:1702:HOH:O	2.10	0.69
28:3:55:GLU:O	28:3:60:GLU:CD	2.34	0.69
1:2:1328:A:OP2	22:U:89:ARG:NH2	2.24	0.68
9:H:30:TYR:OH	25:X:61:ARG:NH1	2.26	0.68
1:2:908:G:O6	37:2:1583:SPM:H132	1.91	0.68
12:K:53:LEU:HD11	12:K:61:ARG:HD2	1.73	0.68
28:3:55:GLU:HB2	28:3:80:VAL:HG11	1.75	0.68
1:2:7:G:H2'	37:2:1584:SPM:H31	1.75	0.68
10:I:92:TYR:CE2	19:R:68:LYS:HD3	2.29	0.68
1:2:786:U:OP2	24:W:6:ARG:NH2	2.26	0.68
1:2:886:G:OP1	7:F:69:ASP:OD1	2.11	0.68
9:H:115:THR:HG21	25:X:35:VAL:HG21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:905:OMG:N7	37:2:1583:SPM:H42	2.09	0.68
28:3:11:VAL:HG22	28:3:12:PRO:HD2	1.75	0.68
31:d:7:LYS:HE3	31:d:7:LYS:CA	2.15	0.68
1:2:796:A:OP1	39:2:1703:HOH:O	2.11	0.68
9:H:13:PHE:CE2	9:H:79:TYR:CE2	2.82	0.68
9:H:119:TYR:HB3	25:X:76:ARG:NH2	2.10	0.67
9:H:3:LEU:HD11	12:K:99:LEU:HB2	1.77	0.67
9:H:28:LYS:HE2	31:d:53:ILE:HG22	1.76	0.67
37:2:1560:SPM:H121	6:E:8:GLU:OE2	1.95	0.67
30:c:96:LEU:HB2	30:c:106:TYR:CE1	2.30	0.67
34:s:812:U:OP1	34:s:812:U:C6	2.48	0.67
1:2:243:G:OP2	37:2:1575:SPM:C3	2.42	0.67
1:2:576:G:N7	37:2:1594:SPM:H72	2.08	0.67
16:O:42:ARG:NH2	22:U:35:GLU:OE1	2.26	0.67
1:2:1095:C:O2'	1:2:1096:U:O5'	2.10	0.67
28:3:34:LYS:HE3	28:3:92:LEU:CD2	2.24	0.67
29:a:36:TYR:CE1	29:a:54:LYS:NZ	2.63	0.67
1:2:71:G:N2	1:2:213:C:O2	2.20	0.67
1:2:964:G:N2	1:2:965:A:N1	2.42	0.67
9:H:10:ILE:CG2	9:H:37:TYR:CD1	2.70	0.67
25:X:37:GLN:OE1	25:X:37:GLN:HA	1.95	0.67
25:X:73:ARG:HH11	25:X:73:ARG:HG2	1.60	0.67
1:2:1272:C:H4'	30:c:7:LYS:HD3	1.74	0.67
9:H:83:LYS:NZ	12:K:43:GLU:OE1	2.28	0.67
27:Z:21:TYR:CD1	29:a:17:LEU:HD11	2.30	0.67
1:2:970:G:OP1	17:P:3:LYS:NZ	2.27	0.66
1:2:826:G:N7	37:2:1569:SPM:H111	2.10	0.66
12:K:13:ARG:HG2	12:K:18:ARG:HD3	1.76	0.66
1:2:983:A:OP1	17:P:2:GLY:HA2	1.95	0.66
2:A:54:TYR:HD2	2:A:59:ASP:O	1.78	0.66
2:A:126:THR:OG1	2:A:128:TYR:O	2.14	0.66
28:3:32:ILE:O	28:3:33:LYS:CG	2.42	0.66
1:2:1122:C:C5	1:2:1124:G:H1'	2.31	0.66
11:J:63:ALA:HB2	11:J:78:ILE:HG12	1.77	0.66
1:2:916:C:H5''	37:2:1581:SPM:H132	1.76	0.66
12:K:24:TYR:CE1	12:K:65:ASP:HB3	2.30	0.66
26:Y:39:LYS:HZ1	26:Y:48:MET:CE	2.07	0.66
1:2:1217:G:OP1	17:P:32:TYR:OH	2.11	0.66
26:Y:32:ASN:HD22	26:Y:32:ASN:C	2.03	0.66
1:2:917:G:OP1	37:2:1581:SPM:C12	2.43	0.66
1:2:983:A:P	17:P:2:GLY:HA2	2.36	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:57:LYS:CD	15:N:94:VAL:HG22	2.25	0.66
28:3:34:LYS:CE	28:3:92:LEU:HD22	2.27	0.66
2:A:23:ILE:CD1	2:A:78:ARG:CD	2.73	0.65
34:s:813:G:H8	34:s:813:G:OP2	1.78	0.65
1:2:965:A:H2'	28:3:94:VAL:HG11	1.78	0.65
4:C:40:VAL:CG2	4:C:58:PRO:HD2	2.26	0.65
6:E:153:LYS:H	6:E:156:MET:HE2	1.60	0.65
22:U:108:PHE:CD2	22:U:125:ARG:HD3	2.32	0.65
35:4:32:OMC:HM22	35:4:33:U:H5'	1.78	0.65
27:Z:56:ILE:HG23	27:Z:63:ILE:HD11	1.77	0.65
28:3:50:LEU:HD11	28:3:115:ILE:HD11	1.77	0.65
28:3:67:PRO:HB3	28:3:77:TYR:CZ	2.31	0.65
31:d:7:LYS:HE2	31:d:55:GLN:CG	2.27	0.65
9:H:91:LEU:HD13	30:c:97:TYR:CZ	2.31	0.65
29:a:55:ARG:CB	29:a:55:ARG:HH11	2.07	0.65
7:F:132:HIS:ND1	7:F:175:ASP:OD1	2.24	0.65
9:H:19:LYS:HZ1	31:d:71:LEU:HD13	1.57	0.65
11:J:34:PHE:HB3	11:J:95:ILE:HG12	1.76	0.65
12:K:23:ILE:HG13	12:K:66:ALA:HB2	1.77	0.65
26:Y:33:LYS:HG3	26:Y:35:LYS:HE3	1.79	0.65
28:3:20:LEU:O	28:3:24:ARG:HG3	1.95	0.65
28:3:78:VAL:HG21	28:3:114:ILE:HD12	1.79	0.65
1:2:873:C:OP2	15:N:114:ARG:NH2	2.28	0.65
3:B:57:TYR:OH	4:C:65:PRO:O	2.11	0.65
1:2:1076:C:H2'	1:2:1077:A:H8	1.62	0.65
29:a:38:CYS:HB2	29:a:61:CYS:HB2	1.79	0.65
31:d:12:ARG:C	31:d:12:ARG:HD3	2.21	0.65
1:2:1451:G:H2'	1:2:1452:U:H6	1.62	0.64
2:A:23:ILE:CG1	2:A:78:ARG:HD2	2.27	0.64
23:V:86:SER:HB3	23:V:89:ILE:HD12	1.79	0.64
16:O:11:ILE:HD11	16:O:52:LEU:HD21	1.79	0.64
31:d:21:ILE:HD11	31:d:60:VAL:HB	1.79	0.64
14:M:48:GLU:OE1	14:M:48:GLU:N	2.30	0.64
31:d:65:LEU:HD22	31:d:65:LEU:O	1.97	0.64
28:3:57:VAL:O	28:3:60:GLU:HG2	1.98	0.64
8:G:56:VAL:CG2	8:G:59:LEU:O	2.44	0.64
28:3:15:LEU:HD22	28:3:117:ARG:HE	1.62	0.64
14:M:25:ILE:HG22	14:M:34:ILE:HB	1.79	0.64
1:2:1355:U:H2'	1:2:1356:G:C8	2.33	0.64
37:2:1581:SPM:H122	37:2:1581:SPM:C8	2.23	0.64
9:H:10:ILE:HA	9:H:37:TYR:CD2	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:28:MET:CE	10:I:60:LYS:HE3	2.17	0.64
31:d:7:LYS:HE2	31:d:55:GLN:CD	2.23	0.64
3:B:151:ARG:HD3	3:B:175:ALA:HA	1.79	0.63
27:Z:69:ILE:HG12	29:a:72:LEU:HD21	1.79	0.63
4:C:18:SER:O	10:I:23:LYS:NZ	2.31	0.63
20:S:20:TYR:O	20:S:24:ILE:HD13	1.99	0.63
31:d:29:ARG:HH12	31:d:62:TRP:HA	1.62	0.63
8:G:54:LEU:HD21	8:G:111:ALA:HB1	1.81	0.63
1:2:636:C:H2'	1:2:637:U:C6	2.34	0.63
18:Q:87:PHE:CE2	18:Q:91:ARG:HD3	2.33	0.63
1:2:567:A:OP1	37:2:1566:SPM:H21	1.98	0.63
1:2:575:G:O6	37:2:1594:SPM:H32	1.99	0.63
5:D:19:ILE:HG22	5:D:22:ARG:H	1.63	0.63
9:H:7:GLN:OE1	9:H:7:GLN:HA	1.98	0.63
9:H:28:LYS:NZ	31:d:61:MET:HE1	2.12	0.63
1:2:929:G:H4'	1:2:930:C4J:O5'	1.98	0.63
21:T:15:ARG:HG3	21:T:33:LEU:HB3	1.81	0.63
1:2:461:G:H5'	37:2:1558:SPM:H21	1.79	0.63
30:c:22:LYS:HD3	30:c:25:LYS:HD2	1.81	0.63
1:2:617:G:H2'	1:2:618:C:C6	2.34	0.63
1:2:74:A:N1	1:2:213:C:O2'	2.31	0.62
36:2:1515:MG:MG	39:2:1838:HOH:O	1.42	0.62
16:O:72:ILE:O	16:O:80:TYR:OH	2.17	0.62
1:2:374:C:OP1	37:2:1591:SPM:N14	2.32	0.62
31:d:12:ARG:HD3	31:d:13:GLU:N	2.15	0.62
1:2:169:G:O6	39:2:1705:HOH:O	2.15	0.62
1:2:1324:A:C8	17:P:12:TYR:HB3	2.35	0.62
9:H:118:MET:HE1	9:H:123:VAL:HG22	1.80	0.62
20:S:23:GLU:O	20:S:25:LYS:CD	2.48	0.62
1:2:1318:C:H2'	1:2:1319:A:C8	2.35	0.62
16:O:37:ALA:O	16:O:41:ILE:HG12	1.99	0.62
1:2:7:G:H21	37:2:1584:SPM:H72	1.64	0.62
9:H:26:SER:HA	25:X:65:ILE:HB	1.80	0.62
15:N:57:LYS:HD2	15:N:94:VAL:CG2	2.27	0.62
18:Q:68:LYS:HB2	18:Q:71:GLN:HG3	1.80	0.62
26:Y:34:VAL:C	26:Y:35:LYS:HE2	2.24	0.62
28:3:34:LYS:CE	28:3:92:LEU:CD2	2.78	0.62
30:c:35:LYS:O	30:c:38:LYS:HG2	2.00	0.62
37:2:1589:SPM:H61	37:2:1589:SPM:N10	2.14	0.62
28:3:34:LYS:HE2	28:3:92:LEU:HD22	1.82	0.62
16:O:142:ILE:HD12	21:T:125:PRO:HG3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:24:ILE:HG12	20:S:54:LEU:HD11	1.81	0.62
1:2:256:G:H4'	1:2:257:U:H5'	1.81	0.62
1:2:1250:U:H3	22:U:71:ASN:ND2	1.98	0.62
15:N:64:GLN:CB	15:N:65:PRO:CD	2.78	0.61
26:Y:32:ASN:ND2	26:Y:32:ASN:C	2.58	0.61
27:Z:17:LYS:HG3	29:a:16:TRP:CD2	2.35	0.61
1:2:458:G:H2'	1:2:459:C:C6	2.35	0.61
31:d:18:ASP:OD1	31:d:19:ASP:N	2.32	0.61
1:2:132:A:OP2	37:2:1589:SPM:C13	2.48	0.61
1:2:150:A:N7	37:2:1589:SPM:N14	2.48	0.61
1:2:483:G:N3	37:2:1558:SPM:H111	2.16	0.61
2:A:77:ASP:OD2	2:A:77:ASP:N	2.33	0.61
9:H:91:LEU:O	30:c:63:SER:OG	2.14	0.61
10:I:27:ILE:N	10:I:27:ILE:HD12	2.15	0.61
17:P:6:PRO:HB3	29:a:63:TYR:CD1	2.34	0.61
6:E:66:LEU:HB2	6:E:86:SER:HB2	1.81	0.61
9:H:16:TRP:CZ3	9:H:86:PHE:HB3	2.35	0.61
1:2:644:G:H1'	14:M:33:ILE:HD11	1.82	0.61
1:2:962:A:H2'	1:2:963:G:H8	1.65	0.61
21:T:31:ILE:HG23	21:T:39:ARG:HG2	1.81	0.61
25:X:26:LEU:HD12	25:X:37:GLN:HG3	1.83	0.61
1:2:741:A:OP1	37:2:1568:SPM:H21	2.01	0.61
1:2:1097:C:O2'	1:2:1099:G:N1	2.32	0.61
12:K:29:ARG:N	12:K:65:ASP:OD1	2.30	0.61
31:d:65:LEU:HD22	31:d:65:LEU:C	2.26	0.61
37:2:1594:SPM:H122	37:2:1594:SPM:C8	2.31	0.61
22:U:19:ARG:NH2	22:U:141:GLU:OE1	2.33	0.61
28:3:6:TYR:HB2	28:3:55:GLU:OE2	2.00	0.61
1:2:727:A:OP2	39:2:1706:HOH:O	2.16	0.61
27:Z:154:LYS:HD2	29:a:3:ILE:HD12	1.82	0.61
28:3:79:TYR:HE1	28:3:118:VAL:HG23	1.65	0.61
1:2:1203:U:H5'	30:c:102:ARG:HD3	1.83	0.60
6:E:109:ILE:HB	6:E:113:GLU:HG3	1.83	0.60
9:H:28:LYS:HE2	31:d:53:ILE:HG23	1.82	0.60
1:2:1183:G:N7	37:2:1570:SPM:C7	2.64	0.60
1:2:1321:A:H5''	17:P:31:LYS:HD3	1.82	0.60
29:a:55:ARG:NH1	29:a:55:ARG:HB2	2.15	0.60
7:F:90:SER:HB3	7:F:114:ILE:HA	1.82	0.60
12:K:80:ASP:O	12:K:84:MET:HG3	2.00	0.60
16:O:30:LYS:HE3	30:c:13:GLU:CD	2.26	0.60
7:F:62:LYS:HE3	37:F:303:SPM:H111	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1183:G:N7	37:2:1570:SPM:H71	2.16	0.60
37:2:1575:SPM:H131	19:R:73:ARG:HH22	1.66	0.60
5:D:44:ALA:HA	5:D:101:LEU:HD23	1.83	0.60
28:3:112:ASP:HA	28:3:115:ILE:HD12	1.83	0.60
1:2:534:G:O6	15:N:3:LYS:NZ	2.34	0.60
6:E:31:HIS:O	39:E:301:HOH:O	2.16	0.60
31:d:16:ILE:CG2	31:d:21:ILE:HD13	2.31	0.60
1:2:1032:OMU:H5'	3:B:162:LYS:HE2	1.84	0.60
1:2:1250:U:H3	22:U:71:ASN:HD21	1.48	0.60
1:2:1315:C:OP1	37:2:1582:SPM:H61	2.02	0.60
1:2:17:C:H2'	1:2:18:C:C6	2.37	0.60
27:Z:20:GLU:HG2	29:a:13:HIS:N	2.17	0.60
16:O:30:LYS:HE3	30:c:13:GLU:OE1	2.01	0.60
17:P:4:TYR:O	29:a:63:TYR:CE1	2.53	0.60
25:X:61:ARG:HD2	31:d:31:GLN:HG3	1.84	0.60
24:W:3:ARG:NH1	39:W:201:HOH:O	2.34	0.60
24:W:17:LEU:HD12	24:W:64:ILE:HD12	1.84	0.59
6:E:40:ALA:HB2	6:E:75:TYR:HB2	1.84	0.59
27:Z:127:LEU:HG	27:Z:186:PRO:HA	1.84	0.59
1:2:687:A:H2'	1:2:688:A:C8	2.38	0.59
15:N:49:MET:HB3	15:N:106:THR:HG22	1.84	0.59
26:Y:57:ARG:HA	26:Y:68:PHE:HA	1.84	0.59
31:d:65:LEU:N	31:d:66:PRO:HD2	2.17	0.59
1:2:12:U:H2'	1:2:13:C:C6	2.37	0.59
1:2:983:A:OP1	17:P:2:GLY:CA	2.49	0.59
2:A:18:LYS:HB2	2:A:20:TYR:CE1	2.38	0.59
11:J:38:SER:OG	11:J:59:TYR:HB3	2.02	0.59
16:O:30:LYS:HE3	30:c:13:GLU:OE2	2.01	0.59
21:T:6:PRO:HB2	21:T:8:GLU:OE1	2.03	0.59
1:2:1122:C:H6	20:S:28:TYR:CZ	2.21	0.59
9:H:29:LYS:NZ	31:d:27:TYR:O	2.34	0.59
12:K:52:PRO:HG2	12:K:86:LEU:HD23	1.83	0.59
1:2:1004:G:HO2'	1:2:1178:C:HO2'	1.50	0.59
1:2:1189:C:O2	21:T:122:HIS:HE1	1.86	0.59
13:L:93:GLU:OE1	27:Z:37:LEU:HA	2.03	0.59
31:d:24:LEU:CD2	31:d:53:ILE:HD11	2.32	0.59
9:H:113:GLU:HG2	9:H:130:VAL:HG22	1.85	0.58
30:c:56:LEU:O	30:c:59:ILE:HG22	2.03	0.58
1:2:962:A:H2'	1:2:963:G:C8	2.37	0.58
1:2:1477:4AC:H5	1:2:1477:4AC:O7	2.01	0.58
27:Z:159:LEU:HD13	29:a:3:ILE:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1188:G:H2'	1:2:1188:G:N3	2.18	0.58
6:E:161:GLU:HB2	6:E:168:LEU:HD21	1.85	0.58
11:J:96:ILE:HD11	11:J:111:VAL:HG21	1.85	0.58
31:d:7:LYS:CG	31:d:16:ILE:HD11	2.33	0.58
9:H:119:TYR:HB3	25:X:76:ARG:HH21	1.67	0.58
15:N:70:ARG:HG3	15:N:119:LEU:HD13	1.84	0.58
16:O:39:ALA:HB1	16:O:75:LEU:HD11	1.86	0.58
21:T:76:ASN:OD1	21:T:76:ASN:N	2.36	0.58
30:c:39:GLU:HB2	30:c:76:ILE:HA	1.84	0.58
1:2:906:G:N7	37:2:1583:SPM:H81	2.19	0.58
31:d:52:LEU:HD12	31:d:52:LEU:O	2.04	0.58
1:2:740:A:P	37:2:1568:SPM:H112	2.44	0.58
37:2:1571:SPM:H131	27:Z:132:ILE:HG21	1.85	0.58
1:2:1253:A:N1	1:2:1335:G:O2'	2.29	0.58
1:2:1451:G:O2'	1:2:1452:U:H5'	2.04	0.58
1:2:1318:C:H2'	1:2:1319:A:H8	1.66	0.58
9:H:157:PRO:HB3	30:c:102:ARG:HB3	1.84	0.58
1:2:17:C:H2'	1:2:18:C:H6	1.69	0.57
1:2:272:C:H2'	1:2:273:C:C6	2.38	0.57
1:2:1447:A:H2'	1:2:1448:G:H8	1.68	0.57
7:F:118:ARG:HD2	7:F:201:THR:O	2.04	0.57
30:c:100:ASN:ND2	30:c:102:ARG:HH21	2.01	0.57
1:2:1333:C:H2'	1:2:1334:G:C8	2.39	0.57
28:3:34:LYS:HE3	28:3:92:LEU:HD23	1.85	0.57
1:2:13:C:OP1	39:2:1707:HOH:O	2.17	0.57
1:2:714:G:H21	10:I:3:PHE:HZ	1.50	0.57
1:2:1328:A:P	22:U:89:ARG:HH22	2.27	0.57
1:2:1337:G:N7	12:K:15:LYS:NZ	2.52	0.57
6:E:120:ARG:HG3	6:E:227:MET:HE2	1.85	0.57
12:K:31:PHE:HB2	12:K:67:LYS:HD3	1.86	0.57
1:2:990:C:H4'	26:Y:62:LYS:HE2	1.84	0.57
1:2:1096:U:N3	1:2:1098:C:N3	2.52	0.57
2:A:20:TYR:HE2	2:A:41:ILE:HA	1.69	0.57
15:N:57:LYS:HG2	15:N:73:VAL:HG12	1.85	0.57
16:O:30:LYS:HD2	16:O:100:ILE:HD11	1.86	0.57
31:d:54:LYS:HG2	31:d:54:LYS:O	2.03	0.57
1:2:991:U:H2'	1:2:992:G:C4	2.40	0.57
1:2:1164:A:OP1	37:2:1596:SPM:N1	2.37	0.57
37:2:1572:SPM:H91	12:K:121:GLU:OE1	2.04	0.57
1:2:1015:G:H5''	27:Z:167:ILE:HD13	1.86	0.57
18:Q:58:ILE:HG23	18:Q:64:ILE:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:510:G:OP1	37:2:1558:SPM:H32	2.05	0.57
7:F:198:LEU:O	7:F:201:THR:OG1	2.18	0.57
14:M:15:TYR:HB3	14:M:22:LEU:HB2	1.86	0.57
1:2:93:C:H2'	1:2:94:U:C6	2.39	0.57
9:H:10:ILE:CG1	9:H:37:TYR:CZ	2.88	0.57
9:H:168:ALA:CB	9:H:175:LYS:HZ1	1.98	0.57
13:L:79:ASP:O	13:L:82:VAL:HG22	2.04	0.57
1:2:1375:C:O2'	1:2:1376:C:O5'	2.16	0.56
6:E:117:LYS:HB2	6:E:162:LEU:HD11	1.87	0.56
1:2:562:C:OP1	6:E:185:ARG:NH1	2.38	0.56
9:H:27:LEU:HD21	9:H:135:ARG:HE	1.70	0.56
9:H:176:SER:O	9:H:180:LYS:HB2	2.05	0.56
15:N:140:GLY:O	15:N:141:LYS:HG2	2.04	0.56
26:Y:57:ARG:HB3	26:Y:68:PHE:HD1	1.68	0.56
31:d:7:LYS:HG2	31:d:16:ILE:HD11	1.87	0.56
1:2:218:C:H2'	1:2:219:A:H8	1.71	0.56
1:2:1094:U:H3	1:2:1101:G:H1	1.53	0.56
4:C:40:VAL:HG21	4:C:58:PRO:CD	2.29	0.56
18:Q:14:ARG:HD3	18:Q:60:LEU:HD11	1.88	0.56
27:Z:20:GLU:HG2	29:a:13:HIS:H	1.68	0.56
1:2:973:C:O2	26:Y:57:ARG:NH1	2.38	0.56
1:2:505:G:C4	32:e:30:PRO:HG3	2.40	0.56
1:2:922:A:N3	1:2:949:U:O2'	2.37	0.56
25:X:23:ILE:HD11	25:X:41:ARG:HB2	1.88	0.56
28:3:15:LEU:HD21	28:3:114:ILE:HG22	1.88	0.56
1:2:790:U:O2'	1:2:1496:C:OP1	2.17	0.56
1:2:1116:G:OP1	13:L:70:HIS:ND1	2.38	0.56
37:2:1560:SPM:C12	6:E:8:GLU:OE2	2.54	0.56
7:F:79:LEU:HD11	7:F:188:GLU:HA	1.86	0.56
27:Z:69:ILE:HD11	29:a:31:GLY:HA3	1.88	0.56
1:2:7:G:OP1	37:2:1586:SPM:C13	2.33	0.56
1:2:8:U:OP1	37:2:1586:SPM:H91	2.05	0.56
9:H:10:ILE:HG23	9:H:37:TYR:CD2	2.41	0.56
1:2:1081:G:N2	1:2:1082:U:O4	2.39	0.56
2:A:47:ARG:HB3	14:M:29:THR:HG21	1.88	0.56
5:D:31:GLY:HA3	32:e:38:TYR:CG	2.41	0.56
14:M:84:TYR:C	14:M:84:TYR:HD1	2.14	0.56
1:2:877:A:OP1	37:2:1586:SPM:H32	2.06	0.56
1:2:1213:A:H2'	1:2:1214:G:C8	2.41	0.56
31:d:50:TYR:CZ	31:d:54:LYS:HE3	2.40	0.56
1:2:1122:C:C4	1:2:1124:G:N9	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:196:GLU:OE1	2:A:196:GLU:N	2.38	0.55
5:D:16:HIS:HB3	5:D:19:ILE:HD13	1.86	0.55
1:2:150:A:OP2	37:2:1589:SPM:H61	2.06	0.55
8:G:24:LYS:HB2	8:G:93:TRP:CD1	2.41	0.55
1:2:1122:C:C4	1:2:1124:G:C8	2.95	0.55
2:A:90:ARG:HD3	2:A:94:ARG:NH1	2.21	0.55
27:Z:185:LYS:HB3	27:Z:187:LEU:HD13	1.88	0.55
28:3:56:ASP:HA	28:3:60:GLU:OE2	2.06	0.55
31:d:51:GLU:OE1	31:d:51:GLU:HA	2.05	0.55
1:2:521:U:C4	15:N:27:GLN:HG2	2.41	0.55
1:2:538:OMC:HM21	18:Q:111:LYS:HE2	1.89	0.55
1:2:1099:G:C2	22:U:5:MET:N	2.75	0.55
1:2:1188:G:H2'	21:T:120:VAL:HG21	1.89	0.55
9:H:6:LEU:C	9:H:6:LEU:HD12	2.32	0.55
9:H:37:TYR:HB2	12:K:51:GLU:OE1	2.07	0.55
1:2:152:A:H2'	1:2:153:A:C8	2.42	0.55
9:H:10:ILE:CG2	9:H:37:TYR:CG	2.81	0.55
1:2:1081:G:N7	1:2:1109:C:O2'	2.38	0.55
2:A:140:LYS:HE3	2:A:144:GLU:OE2	2.06	0.55
8:G:3:ASP:OD1	8:G:3:ASP:N	2.39	0.55
17:P:4:TYR:CE1	29:a:57:LEU:HD11	2.41	0.55
1:2:965:A:O4'	1:2:993:A:N6	2.40	0.55
1:2:967:G:N7	28:3:37:ASN:ND2	2.54	0.55
37:2:1585:SPM:H111	37:F:303:SPM:H72	1.89	0.55
28:3:43:VAL:HG12	28:3:73:LYS:HG3	1.89	0.55
29:a:55:ARG:HH11	29:a:55:ARG:HB2	1.71	0.55
1:2:1494:U:H2'	1:2:1495:C:C6	2.42	0.55
9:H:113:GLU:HG3	25:X:57:LYS:HD3	1.88	0.55
1:2:905:OMG:O6	37:2:1583:SPM:H62	2.06	0.55
12:K:102:ILE:HD12	31:d:67:ILE:CD1	2.35	0.55
27:Z:154:LYS:HA	29:a:3:ILE:CD1	2.37	0.55
27:Z:154:LYS:HA	29:a:3:ILE:HD12	1.89	0.55
1:2:3:U:H5'	7:F:159:VAL:HG12	1.90	0.54
9:H:28:LYS:CE	31:d:53:ILE:CG2	2.86	0.54
28:3:27:LYS:HE3	28:3:90:CYS:HB2	1.89	0.54
1:2:619:G:H2'	1:2:620:G:C8	2.42	0.54
7:F:160:VAL:HG12	7:F:178:SER:HB3	1.88	0.54
22:U:6:ILE:HA	22:U:10:MET:SD	2.48	0.54
2:A:110:VAL:HG11	2:A:146:VAL:HG12	1.89	0.54
5:D:25:TYR:OH	5:D:98:GLU:OE2	2.25	0.54
16:O:36:THR:O	16:O:40:ILE:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1461:G:OP1	1:2:1464:A:H4'	2.08	0.54
14:M:84:TYR:C	14:M:84:TYR:CD1	2.85	0.54
16:O:22:LEU:HD12	16:O:52:LEU:HD12	1.88	0.54
1:2:72:G:N1	1:2:209:U:O2'	2.38	0.54
13:L:80:GLU:HA	13:L:83:MET:HG2	1.89	0.54
32:e:35:ARG:O	32:e:39:GLU:HG2	2.07	0.54
1:2:634:U:OP1	2:A:188:LYS:NZ	2.39	0.54
1:2:1189:C:H41	37:2:1581:SPM:HN12	1.55	0.54
28:3:49:LYS:HG2	28:3:75:ILE:CG2	2.33	0.54
1:2:479:A:H4'	32:e:12:LYS:HG2	1.90	0.54
1:2:1189:C:O2	21:T:122:HIS:CE1	2.61	0.54
3:B:29:LYS:HB2	3:B:76:ARG:HH11	1.73	0.54
3:B:98:ILE:HD11	3:B:120:ARG:HH21	1.73	0.54
8:G:62:LEU:HB2	8:G:79:PHE:HE1	1.72	0.54
14:M:12:ALA:HB2	14:M:74:LEU:HD13	1.90	0.54
26:Y:56:GLU:O	26:Y:58:TRP:NE1	2.40	0.54
1:2:481:OMC:N4	15:N:70:ARG:HH21	2.06	0.54
1:2:1251:A:H2'	1:2:1252:A:C8	2.43	0.54
1:2:1314:A:H1'	9:H:72:LYS:HG2	1.90	0.54
21:T:67:ASN:OD1	21:T:67:ASN:N	2.36	0.54
22:U:141:GLU:O	22:U:145:GLU:HG3	2.08	0.54
1:2:298:C:H5'	1:2:569:G:N3	2.23	0.54
5:D:81:GLY:O	5:D:84:LYS:NZ	2.40	0.54
1:2:112:C:H2'	1:2:113:OMC:C6	2.42	0.54
11:J:92:ARG:HA	11:J:92:ARG:NE	2.23	0.54
27:Z:21:TYR:CD1	29:a:17:LEU:CD1	2.91	0.54
30:c:64:ILE:HG23	30:c:105:ILE:HG23	1.90	0.54
2:A:22:VAL:HG23	2:A:33:LEU:HB2	1.91	0.53
3:B:84:ILE:HD13	4:C:62:PHE:CE1	2.43	0.53
5:D:161:PHE:HD2	5:D:166:PRO:HD3	1.72	0.53
16:O:22:LEU:HD21	16:O:46:MET:HE2	1.89	0.53
25:X:12:ILE:O	25:X:15:GLU:HG3	2.08	0.53
27:Z:165:ARG:HB2	27:Z:182:VAL:HG22	1.89	0.53
1:2:125:G:OP2	37:2:1577:SPM:N5	2.42	0.53
9:H:28:LYS:HZ1	31:d:61:MET:HE1	1.70	0.53
26:Y:41:CYS:HB3	26:Y:46:SER:H	1.72	0.53
1:2:349:A:H5''	1:2:350:C:H5	1.73	0.53
16:O:85:ASP:OD2	16:O:86:TYR:N	2.41	0.53
31:d:68:TYR:O	31:d:71:LEU:HB2	2.08	0.53
2:A:86:HIS:ND1	2:A:189:THR:OG1	2.20	0.53
12:K:15:LYS:O	12:K:16:THR:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:80:GLU:O	13:L:84:ARG:HG3	2.08	0.53
28:3:53:ILE:HD13	28:3:67:PRO:HD3	1.91	0.53
1:2:1188:G:N3	1:2:1188:G:C2'	2.72	0.53
2:A:86:HIS:HE1	2:A:186:ILE:HG22	1.74	0.53
8:G:157:ASP:HB3	8:G:197:ARG:HD3	1.90	0.53
12:K:26:GLY:HA3	12:K:65:ASP:HB2	1.90	0.53
14:M:94:GLN:O	14:M:98:ARG:HG2	2.09	0.53
24:W:3:ARG:HB2	24:W:6:ARG:HB2	1.91	0.53
1:2:479:A:H1'	32:e:13:VAL:HG23	1.90	0.53
1:2:707:G:C8	18:Q:59:PRO:HB2	2.44	0.53
1:2:930:C4J:C6	1:2:930:C4J:C4'	2.87	0.53
2:A:23:ILE:HG12	2:A:78:ARG:HG2	1.91	0.53
9:H:21:GLU:OE1	31:d:58:ALA:N	2.38	0.53
26:Y:65:TYR:O	26:Y:65:TYR:CG	2.62	0.53
1:2:522:A:H5''	1:2:524:U:O4	2.08	0.53
9:H:115:THR:HG21	25:X:35:VAL:CG2	2.38	0.53
11:J:33:THR:O	11:J:33:THR:OG1	2.27	0.53
18:Q:72:ILE:O	18:Q:76:ARG:HG2	2.08	0.53
30:c:35:LYS:O	30:c:38:LYS:CG	2.57	0.53
1:2:947:A:O2'	1:2:1007:G:OP2	2.24	0.53
1:2:1332:G:O6	37:2:1572:SPM:H92	2.09	0.53
5:D:31:GLY:HA3	32:e:38:TYR:CD1	2.43	0.53
1:2:483:G:H21	37:2:1558:SPM:H111	1.74	0.53
1:2:1122:C:N4	1:2:1124:G:C4	2.77	0.53
1:2:1287:G:H2'	1:2:1288:C:C6	2.44	0.53
9:H:10:ILE:CA	9:H:37:TYR:CE2	2.75	0.53
16:O:62:LYS:O	16:O:66:VAL:HG23	2.09	0.53
1:2:539:C:H2'	1:2:540:G:O4'	2.09	0.53
1:2:1075:C:H1'	1:2:1142:A:C4	2.44	0.53
1:2:1191:C:OP2	30:c:2:GLY:N	2.42	0.53
1:2:1320:G:O2'	1:2:1321:A:H5'	2.09	0.53
7:F:186:THR:OG1	37:F:303:SPM:H81	2.08	0.53
27:Z:24:LYS:HG2	29:a:14:LEU:HD22	1.90	0.53
1:2:741:A:H4'	1:2:1471:G:O2'	2.08	0.52
1:2:1143:G:P	12:K:108:ARG:HH22	2.32	0.52
1:2:1332:G:N7	37:2:1572:SPM:H111	2.23	0.52
9:H:9:ASP:O	9:H:37:TYR:HE2	1.92	0.52
9:H:12:VAL:N	9:H:16:TRP:O	2.42	0.52
10:I:49:GLU:OE1	10:I:49:GLU:HA	2.10	0.52
16:O:30:LYS:CE	30:c:13:GLU:OE2	2.57	0.52
19:R:25:ASP:OD2	19:R:28:CYS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:11:ASP:N	23:V:11:ASP:OD1	2.43	0.52
30:c:59:ILE:HG21	30:c:108:ALA:HB2	1.90	0.52
1:2:1466:4AC:HM73	1:2:1467:4AC:HM72	1.91	0.52
9:H:12:VAL:HG21	9:H:98:ILE:HD11	1.91	0.52
12:K:13:ARG:HH11	12:K:13:ARG:HB2	1.74	0.52
18:Q:21:PRO:HG2	18:Q:24:VAL:HG23	1.91	0.52
21:T:75:ARG:HB3	21:T:111:GLY:HA3	1.91	0.52
1:2:1186:C:OP2	1:2:1187:C:H6	1.93	0.52
8:G:95:SER:OG	8:G:97:THR:OG1	2.27	0.52
9:H:163:ALA:O	9:H:167:ILE:HG13	2.09	0.52
12:K:13:ARG:HH11	12:K:13:ARG:CB	2.22	0.52
13:L:81:ARG:CG	13:L:84:ARG:HH21	2.20	0.52
1:2:446:G:H21	23:V:42:THR:HG21	1.75	0.52
1:2:489:G:N3	1:2:489:G:C2'	2.72	0.52
1:2:677:A:H5'	14:M:119:ASP:OD1	2.09	0.52
28:3:116:LYS:HA	28:3:119:ASN:HB2	1.92	0.52
1:2:16:G:H2'	1:2:17:C:C6	2.45	0.52
1:2:305:A:C5	1:2:306:G:H1'	2.44	0.52
1:2:1284:C:OP2	39:2:1710:HOH:O	2.19	0.52
12:K:83:ARG:HD3	12:K:110:MET:HG2	1.92	0.52
15:N:119:LEU:HD12	15:N:120:PRO:HD2	1.92	0.52
18:Q:87:PHE:O	18:Q:91:ARG:HG3	2.10	0.52
1:2:9:U:OP2	39:2:1709:HOH:O	2.19	0.52
1:2:493:U:O2	1:2:493:U:H2'	2.09	0.52
1:2:1295:G:H4'	30:c:8:PRO:CG	2.36	0.52
7:F:69:ASP:OD1	7:F:69:ASP:N	2.41	0.52
9:H:192:SER:OG	9:H:192:SER:O	2.25	0.52
11:J:109:ALA:HB1	11:J:123:ALA:HB1	1.90	0.52
16:O:75:LEU:HD13	22:U:39:LEU:HD13	1.92	0.52
1:2:784:G:O2'	10:I:9:ASN:OD1	2.27	0.52
1:2:1226:C:H2'	1:2:1227:C:H6	1.75	0.52
2:A:161:GLU:OE2	2:A:166:ARG:NH1	2.33	0.52
6:E:234:SER:OG	6:E:236:LEU:O	2.28	0.52
27:Z:17:LYS:HD2	27:Z:74:PHE:CE1	2.44	0.52
30:c:103:LEU:HD12	30:c:103:LEU:O	2.09	0.52
12:K:32:VAL:HG21	12:K:40:ILE:HD11	1.90	0.52
13:L:82:VAL:O	13:L:86:LEU:HG	2.10	0.52
30:c:7:LYS:HB2	30:c:9:ILE:CG2	2.37	0.52
1:2:1183:G:OP2	37:2:1570:SPM:H111	2.10	0.52
7:F:23:VAL:HG21	7:F:46:ILE:HG23	1.91	0.52
17:P:50:PHE:O	17:P:51:ARG:NH1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:84:THR:OG1	27:Z:85:ASN:N	2.42	0.52
34:s:808:A:H2'	34:s:809:G:H5''	1.90	0.52
1:2:740:A:OP1	37:2:1568:SPM:H112	2.09	0.52
1:2:1475:MA6:H2'	1:2:1476:A:C8	2.44	0.52
10:I:81:LEU:HB2	10:I:86:MET:HE2	1.92	0.52
22:U:28:VAL:HG12	22:U:30:THR:HG22	1.91	0.52
1:2:644:G:C1'	14:M:33:ILE:HD11	2.39	0.51
37:2:1572:SPM:N14	12:K:122:LYS:O	2.43	0.51
7:F:187:THR:O	7:F:191:VAL:HG23	2.10	0.51
9:H:3:LEU:HD11	12:K:99:LEU:CB	2.40	0.51
9:H:159:GLU:OE2	30:c:102:ARG:CD	2.58	0.51
1:2:796:A:H2'	1:2:797:U:C6	2.45	0.51
1:2:1079:U:H2'	1:2:1080:A:O4'	2.11	0.51
2:A:20:TYR:CE2	2:A:41:ILE:HD12	2.45	0.51
8:G:148:VAL:HB	8:G:212:ILE:HG23	1.92	0.51
11:J:76:VAL:HB	11:J:105:GLU:HG2	1.92	0.51
12:K:13:ARG:CB	12:K:13:ARG:NH1	2.74	0.51
25:X:73:ARG:HG2	25:X:73:ARG:NH1	2.23	0.51
29:a:38:CYS:SG	29:a:61:CYS:CB	2.98	0.51
29:a:38:CYS:SG	29:a:61:CYS:HB2	2.49	0.51
34:s:807:G:H2'	34:s:808:A:C8	2.44	0.51
1:2:1469:U:H5''	37:2:1599:SPM:H22	1.92	0.51
8:G:24:LYS:HB2	8:G:93:TRP:HD1	1.76	0.51
23:V:66:ARG:NH1	23:V:94:GLU:OE1	2.40	0.51
25:X:24:GLN:OE1	25:X:39:ARG:NH1	2.42	0.51
26:Y:58:TRP:N	26:Y:67:GLU:O	2.43	0.51
1:2:481:OMC:N4	15:N:70:ARG:NH2	2.59	0.51
9:H:41:THR:HG23	9:H:59:GLU:OE2	2.10	0.51
9:H:160:GLU:HG2	30:c:103:LEU:CD2	2.40	0.51
14:M:22:LEU:HD13	14:M:38:SER:HB3	1.93	0.51
14:M:65:ASP:O	14:M:69:LYS:HG2	2.10	0.51
8:G:164:ARG:HB3	8:G:196:ILE:HD12	1.92	0.51
1:2:119:U:O2	6:E:141:ASN:ND2	2.39	0.51
1:2:954:G:H2'	1:2:955:A:C8	2.46	0.51
1:2:971:G:H2'	1:2:972:C:O4'	2.11	0.51
1:2:1101:G:O4'	22:U:5:MET:CE	2.56	0.51
1:2:1204:G:H2'	1:2:1205:G:C8	2.45	0.51
31:d:25:ASN:HD22	31:d:64:PRO:HA	1.76	0.51
1:2:1101:G:H1'	22:U:5:MET:HE1	1.92	0.51
1:2:1183:G:N7	37:2:1570:SPM:H72	2.25	0.51
9:H:117:ILE:HD13	9:H:126:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:23:GLN:NE2	13:L:89:VAL:O	2.43	0.51
1:2:200:C:H2'	1:2:201:A:H8	1.76	0.51
1:2:1076:C:H2'	1:2:1077:A:C8	2.44	0.51
12:K:13:ARG:NH1	12:K:13:ARG:HB3	2.25	0.51
26:Y:41:CYS:HA	26:Y:65:TYR:OH	2.11	0.51
1:2:200:C:H2'	1:2:201:A:C8	2.45	0.51
1:2:654:A:H2'	1:2:655:A:C8	2.45	0.51
1:2:916:C:OP1	37:2:1581:SPM:N14	2.44	0.51
16:O:132:THR:HB	30:c:3:GLY:HA3	1.93	0.51
34:s:810:G:H8	34:s:810:G:H5''	1.76	0.51
1:2:218:C:H2'	1:2:219:A:C8	2.45	0.51
1:2:567:A:OP1	37:2:1566:SPM:C2	2.59	0.51
1:2:864:A:O2'	37:2:1599:SPM:H132	2.11	0.51
1:2:1455:U:H4'	1:2:1476:A:H2	1.76	0.51
37:2:1581:SPM:H81	37:2:1581:SPM:C12	2.25	0.51
20:S:23:GLU:O	20:S:25:LYS:HD2	2.11	0.51
20:S:24:ILE:C	20:S:25:LYS:HD2	2.36	0.51
21:T:54:LEU:O	21:T:58:ARG:HD2	2.10	0.51
27:Z:62:ASN:O	27:Z:66:LEU:HG	2.11	0.51
1:2:989:C:OP1	26:Y:49:ALA:HA	2.11	0.50
9:H:84:LEU:HG	30:c:100:ASN:HB2	1.92	0.50
16:O:106:ASP:OD1	16:O:109:ARG:NH2	2.44	0.50
21:T:99:PHE:CE2	21:T:105:MET:HE1	2.46	0.50
28:3:115:ILE:O	28:3:119:ASN:N	2.44	0.50
1:2:442:A:OP1	23:V:108:LYS:NZ	2.33	0.50
1:2:1291:U:OP1	22:U:41:LYS:NZ	2.24	0.50
8:G:48:GLU:OE1	8:G:83:VAL:HG21	2.12	0.50
8:G:197:ARG:HG2	8:G:205:ILE:HD11	1.93	0.50
20:S:43:SER:HB3	20:S:46:VAL:HG22	1.93	0.50
23:V:64:VAL:HG11	23:V:94:GLU:HG3	1.93	0.50
29:a:54:LYS:C	29:a:54:LYS:HD2	2.35	0.50
1:2:637:U:H2'	1:2:638:C:C6	2.46	0.50
1:2:1187:C:H3'	1:2:1188:G:H5''	1.93	0.50
12:K:102:ILE:HD13	31:d:67:ILE:HD13	1.89	0.50
16:O:19:THR:HG23	30:c:40:ILE:HD12	1.92	0.50
28:3:51:VAL:O	28:3:77:TYR:HB2	2.11	0.50
29:a:26:ARG:NH1	29:a:33:ASP:OD2	2.45	0.50
1:2:612:A:N6	24:W:10:PRO:HG3	2.26	0.50
1:2:1122:C:O2	1:2:1122:C:H3'	2.11	0.50
27:Z:153:TYR:O	29:a:3:ILE:HD11	2.12	0.50
1:2:1478:4AC:OP1	37:2:1579:SPM:N14	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:1566:SPM:H61	6:E:11:TRP:CZ3	2.46	0.50
14:M:27:ASP:OD1	14:M:27:ASP:N	2.41	0.50
30:c:103:LEU:HD12	30:c:103:LEU:C	2.36	0.50
31:d:7:LYS:HB3	31:d:55:GLN:NE2	2.26	0.50
31:d:12:ARG:NH1	31:d:12:ARG:CG	2.73	0.50
31:d:38:SER:HB2	31:d:43:LEU:HD23	1.94	0.50
1:2:7:G:O2'	37:2:1584:SPM:H61	2.11	0.50
1:2:7:G:N2	37:2:1584:SPM:H72	2.26	0.50
1:2:484:C:O3'	37:2:1584:SPM:H112	2.11	0.50
1:2:1343:G:H2'	1:2:1344:OMU:H6	1.93	0.50
8:G:62:LEU:HB2	8:G:79:PHE:CE1	2.46	0.50
16:O:55:LEU:HG	16:O:59:GLU:HG3	1.93	0.50
1:2:810:C:OP2	37:2:1595:SPM:H111	2.12	0.50
37:2:1575:SPM:H131	19:R:73:ARG:NH2	2.25	0.50
9:H:115:THR:HG23	9:H:117:ILE:CD1	2.41	0.50
14:M:52:PRO:HB3	14:M:95:PRO:HG2	1.94	0.50
1:2:527:G:O2'	1:2:533:A:N1	2.43	0.50
1:2:917:G:P	37:2:1581:SPM:C12	3.00	0.50
1:2:1122:C:C2	1:2:1124:G:C8	2.99	0.50
1:2:1372:G:C6	1:2:1451:G:C6	2.99	0.50
37:2:1566:SPM:H61	6:E:11:TRP:CH2	2.47	0.50
23:V:33:LEU:HB3	23:V:79:VAL:HB	1.94	0.50
1:2:38:G:N7	37:2:1588:SPM:H41	2.26	0.50
1:2:826:G:O6	37:2:1569:SPM:H81	2.12	0.50
1:2:1232:A:H2'	1:2:1233:A:C8	2.47	0.50
7:F:12:GLU:OE1	7:F:12:GLU:N	2.45	0.50
9:H:4:GLU:OE1	9:H:4:GLU:N	2.32	0.50
16:O:17:ASP:HB3	16:O:20:MET:HE2	1.94	0.50
24:W:38:VAL:HB	24:W:48:VAL:HG13	1.94	0.50
24:W:43:CYS:SG	24:W:45:THR:HG22	2.52	0.50
1:2:688:A:H5'	18:Q:4:ARG:HH21	1.76	0.49
3:B:101:ALA:HB2	3:B:110:VAL:HG21	1.93	0.49
8:G:54:LEU:HD21	8:G:111:ALA:CB	2.42	0.49
1:2:612:A:C6	24:W:10:PRO:HG3	2.47	0.49
1:2:985:C:C2	1:2:986:U:H5	2.30	0.49
9:H:30:TYR:O	9:H:136:ILE:HD13	2.12	0.49
12:K:6:LYS:HG3	12:K:93:PHE:CE2	2.47	0.49
20:S:44:LYS:HG3	20:S:47:ARG:NH2	2.27	0.49
1:2:463:G:C5'	1:2:493:U:O2	2.57	0.49
7:F:62:LYS:HE3	37:F:303:SPM:C11	2.42	0.49
9:H:36:VAL:HG11	9:H:56:PRO:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:134:ARG:O	9:H:138:LEU:HD12	2.12	0.49
14:M:77:LYS:HD3	14:M:111:GLU:OE1	2.12	0.49
30:c:29:LYS:NZ	30:c:40:ILE:HD11	2.27	0.49
1:2:502:C:OP1	32:e:41:ARG:NH1	2.45	0.49
37:2:1566:SPM:H111	6:E:100:ASN:O	2.13	0.49
37:2:1594:SPM:H122	37:2:1594:SPM:H81	1.94	0.49
3:B:112:LYS:NZ	3:B:224:GLU:OE2	2.37	0.49
1:2:7:G:C2	37:2:1584:SPM:H42	2.48	0.49
1:2:1119:G:H2'	1:2:1120:G:O4'	2.12	0.49
1:2:1352:C:H4'	37:2:1597:SPM:H42	1.94	0.49
3:B:15:GLU:OE1	3:B:15:GLU:N	2.44	0.49
9:H:157:PRO:CB	30:c:102:ARG:HB3	2.43	0.49
12:K:68:ILE:HD11	12:K:86:LEU:HD13	1.94	0.49
26:Y:38:ASN:HB3	26:Y:48:MET:HB3	1.93	0.49
1:2:1316:C:H2'	1:2:1317:G:C8	2.48	0.49
1:2:1489:U:H2'	1:2:1490:C:C6	2.48	0.49
6:E:215:ASP:OD2	6:E:217:ASN:ND2	2.45	0.49
8:G:157:ASP:HA	8:G:205:ILE:HA	1.93	0.49
15:N:64:GLN:HB2	15:N:65:PRO:CD	2.43	0.49
17:P:19:CYS:HA	17:P:35:TYR:O	2.13	0.49
1:2:1:A:H1'	7:F:159:VAL:HG13	1.95	0.49
1:2:479:A:H1'	32:e:13:VAL:CG2	2.43	0.49
2:A:114:ASP:OD1	2:A:114:ASP:N	2.30	0.49
2:A:154:SER:HB3	2:A:157:ASP:OD1	2.12	0.49
3:B:98:ILE:HG12	3:B:140:ILE:HD12	1.95	0.49
13:L:7:ILE:HD13	13:L:24:ILE:HD11	1.93	0.49
30:c:8:PRO:HA	30:c:11:THR:HB	1.93	0.49
4:C:54:GLU:OE1	4:C:63:LYS:HD2	2.12	0.49
21:T:90:VAL:HG22	21:T:99:PHE:HE1	1.78	0.49
22:U:76:ILE:O	22:U:79:THR:OG1	2.23	0.49
27:Z:24:LYS:HG3	29:a:14:LEU:HD22	1.94	0.49
30:c:29:LYS:HB3	30:c:39:GLU:OE2	2.12	0.49
1:2:543:G:H2'	1:2:544:C:C6	2.48	0.49
1:2:962:A:H2	1:2:996:C:N4	2.10	0.49
1:2:1477:4AC:H2'	1:2:1478:4AC:H6	1.95	0.49
3:B:47:VAL:HA	3:B:187:ASN:HB3	1.94	0.49
8:G:164:ARG:NH1	8:G:181:PRO:O	2.46	0.49
16:O:100:ILE:HG22	16:O:104:ARG:HH21	1.78	0.49
26:Y:32:ASN:HA	28:3:68:LEU:HB2	1.95	0.49
1:2:728:G:H4'	1:2:1470:A:H4'	1.93	0.49
1:2:909:G:C2	1:2:910:A:C8	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:27:ILE:HG21	13:L:86:LEU:HD21	1.95	0.49
14:M:38:SER:H	14:M:41:MET:HG3	1.78	0.49
22:U:143:PHE:HD2	22:U:143:PHE:O	1.96	0.49
27:Z:46:ILE:HA	27:Z:82:THR:O	2.13	0.49
1:2:430:U:C4	1:2:431:C:C5	3.00	0.48
1:2:996:C:O2'	1:2:997:G:H8	1.95	0.48
2:A:22:VAL:HG12	2:A:79:LEU:HB2	1.95	0.48
2:A:54:TYR:CD2	2:A:59:ASP:O	2.63	0.48
3:B:213:PRO:HD2	3:B:216:GLY:HA3	1.94	0.48
5:D:158:THR:HG21	23:V:39:GLY:HA3	1.95	0.48
12:K:17:ALA:HB2	12:K:73:GLY:HA3	1.95	0.48
26:Y:24:ARG:HH11	28:3:37:ASN:HB3	1.78	0.48
26:Y:35:LYS:HE2	26:Y:35:LYS:N	2.28	0.48
1:2:406:C:O2'	1:2:580:A:N3	2.42	0.48
1:2:1024:A:N1	1:2:1065:G:O2'	2.43	0.48
3:B:166:PRO:HA	3:B:181:ASP:OD2	2.13	0.48
4:C:59:ASN:OD1	4:C:60:CYS:N	2.46	0.48
8:G:180:PRO:O	8:G:182:GLY:N	2.46	0.48
28:3:27:LYS:HA	28:3:32:ILE:HG22	1.94	0.48
1:2:638:C:H2'	1:2:639:C:H6	1.79	0.48
1:2:1204:G:H2'	1:2:1205:G:H8	1.78	0.48
2:A:18:LYS:HB2	2:A:20:TYR:HE1	1.76	0.48
9:H:16:TRP:CE3	9:H:97:PRO:HG2	2.49	0.48
9:H:156:LYS:HD3	9:H:161:VAL:HG12	1.94	0.48
30:c:96:LEU:C	30:c:96:LEU:CD1	2.86	0.48
1:2:1113:C:OP1	12:K:18:ARG:NE	2.46	0.48
28:3:11:VAL:CG2	28:3:12:PRO:HD2	2.43	0.48
30:c:96:LEU:HB2	30:c:106:TYR:HE1	1.76	0.48
1:2:207:U:H2'	1:2:208:A:C8	2.49	0.48
1:2:874:U:OP2	15:N:114:ARG:NH1	2.47	0.48
1:2:1057:C:N4	1:2:1060:OMC:OP2	2.46	0.48
2:A:19:TRP:CZ2	2:A:37:PRO:HG3	2.48	0.48
4:C:25:PRO:HB3	7:F:35:PHE:CD1	2.48	0.48
9:H:30:TYR:CE2	9:H:132:PRO:HG2	2.48	0.48
2:A:14:TRP:HD1	2:A:17:LYS:HD2	1.79	0.48
1:2:522:A:N3	1:2:522:A:C2'	2.73	0.48
1:2:843:4AC:H5	15:N:6:SER:OG	2.13	0.48
1:2:1122:C:C5	1:2:1124:G:C1'	2.95	0.48
7:F:17:THR:OG1	7:F:43:GLU:OE2	2.27	0.48
8:G:87:VAL:HB	8:G:93:TRP:CZ3	2.49	0.48
31:d:25:ASN:HD21	31:d:64:PRO:HA	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:33:U:H2'	1:2:34:C:O4'	2.14	0.48
1:2:624:A:H4'	37:2:1567:SPM:H81	1.95	0.48
1:2:989:C:H2'	1:2:990:C:H6	1.79	0.48
9:H:108:SER:O	9:H:182:LYS:HB2	2.14	0.48
23:V:45:ARG:NH1	23:V:102:ASP:OD1	2.34	0.48
1:2:582:C:H41	37:2:1594:SPM:H31	1.79	0.48
37:2:1575:SPM:H62	37:2:1575:SPM:H31	1.60	0.48
30:c:86:LYS:O	30:c:89:GLU:HG3	2.14	0.48
1:2:1269:G:N2	1:2:1295:G:H1'	2.29	0.48
1:2:1455:U:H1'	1:2:1456:A:N7	2.29	0.48
19:R:23:CYS:HB2	19:R:83:PRO:HG2	1.94	0.48
28:3:93:GLN:OE1	28:3:93:GLN:N	2.47	0.48
29:a:55:ARG:CB	29:a:55:ARG:NH1	2.73	0.48
1:2:1165:G:N1	17:P:43:GLU:OE2	2.44	0.47
37:2:1571:SPM:N14	27:Z:180:GLU:OE1	2.27	0.47
2:A:101:SER:O	2:A:126:THR:OG1	2.32	0.47
1:2:672:OMG:H2'	1:2:673:G:C8	2.50	0.47
1:2:1101:G:H2'	1:2:1102:C:H6	1.79	0.47
1:2:1125:C:H2'	1:2:1126:C:H6	1.79	0.47
6:E:194:LYS:HD2	6:E:194:LYS:HA	1.70	0.47
22:U:9:GLU:OE1	22:U:70:VAL:HG22	2.14	0.47
1:2:29:G:H2'	1:2:30:C:C6	2.49	0.47
1:2:257:U:H2'	1:2:258:U:C6	2.48	0.47
6:E:14:MET:SD	6:E:102:ARG:HG3	2.54	0.47
9:H:169:ALA:HA	9:H:179:ILE:HG12	1.95	0.47
1:2:416:C:H2'	1:2:417:G:O4'	2.13	0.47
1:2:576:G:N7	37:2:1594:SPM:C7	2.75	0.47
1:2:877:A:H5''	37:2:1584:SPM:HN5	1.79	0.47
1:2:1241:G:H1'	1:2:1246:C:O2	2.14	0.47
1:2:1372:G:H22	1:2:1449:A:H2	1.62	0.47
3:B:155:GLN:NE2	3:B:159:GLU:OE2	2.36	0.47
4:C:39:GLU:HB2	4:C:59:ASN:HD21	1.79	0.47
8:G:32:ILE:HG23	8:G:35:GLU:HG3	1.96	0.47
26:Y:27:TYR:OH	28:3:44:GLU:HG3	2.14	0.47
27:Z:55:ILE:HG22	27:Z:83:ILE:HD13	1.95	0.47
30:c:92:ASN:CG	30:c:92:ASN:O	2.57	0.47
1:2:1081:G:H5''	13:L:36:ARG:HB3	1.96	0.47
20:S:36:ILE:HG12	20:S:47:ARG:HD2	1.97	0.47
11:J:114:ARG:O	11:J:118:ASP:HB2	2.13	0.47
13:L:57:GLU:O	39:L:201:HOH:O	2.20	0.47
30:c:25:LYS:O	30:c:29:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:146:G:O6	37:2:1578:SPM:H91	2.14	0.47
1:2:209:U:H2'	1:2:210:U:C2	2.50	0.47
1:2:391:G:OP2	37:2:1573:SPM:H42	2.15	0.47
1:2:980:A:H2'	1:2:981:C:C6	2.50	0.47
1:2:1487:G:H2'	1:2:1488:A:C8	2.50	0.47
5:D:145:VAL:HG13	5:D:149:GLU:HG3	1.97	0.47
8:G:80:LYS:HZ1	8:G:147:PRO:HD3	1.80	0.47
9:H:10:ILE:HA	9:H:37:TYR:CZ	2.41	0.47
9:H:193:ARG:CZ	25:X:70:GLU:HG3	2.45	0.47
10:I:83:TYR:CD1	10:I:123:ARG:HA	2.49	0.47
13:L:93:GLU:O	27:Z:11:LYS:NZ	2.48	0.47
14:M:52:PRO:O	14:M:56:MET:HG3	2.15	0.47
15:N:64:GLN:CB	15:N:65:PRO:HD3	2.45	0.47
24:W:64:ILE:C	24:W:66:GLY:H	2.22	0.47
28:3:51:VAL:HB	28:3:66:LEU:HD21	1.96	0.47
29:a:38:CYS:CB	29:a:61:CYS:HB2	2.43	0.47
29:a:39:PRO:HD3	29:a:69:VAL:CG1	2.35	0.47
30:c:29:LYS:HE2	30:c:39:GLU:OE2	2.15	0.47
1:2:37:G:H3'	37:2:1588:SPM:H22	1.97	0.47
1:2:326:A:H2	1:2:337:OMG:HN21	1.63	0.47
1:2:885:G:H2'	1:2:886:G:C8	2.49	0.47
1:2:916:C:H5''	37:2:1581:SPM:C13	2.44	0.47
3:B:218:LEU:HG	3:B:220:VAL:H	1.80	0.47
9:H:8:LEU:C	9:H:8:LEU:CD1	2.87	0.47
12:K:49:ILE:HD13	12:K:82:ALA:HB3	1.96	0.47
15:N:51:ARG:HD2	15:N:102:GLU:OE2	2.15	0.47
16:O:126:LYS:HG3	30:c:5:SER:HB3	1.94	0.47
1:2:673:G:H2'	1:2:674:A:H8	1.80	0.47
1:2:792:U:OP2	37:2:1595:SPM:H121	2.15	0.47
1:2:1352:C:H1'	37:2:1597:SPM:H82	1.96	0.47
37:2:1593:SPM:H122	5:D:7:SER:OG	2.15	0.47
6:E:177:SER:HA	6:E:231:ARG:O	2.15	0.47
27:Z:24:LYS:HG2	29:a:14:LEU:HB2	1.97	0.47
28:3:11:VAL:HG23	28:3:79:TYR:HB3	1.97	0.47
31:d:4:LEU:HD22	31:d:5:LYS:H	1.80	0.47
1:2:196:G:H3'	37:2:1577:SPM:H81	1.96	0.47
1:2:827:A:H2'	1:2:828:A:C8	2.49	0.47
1:2:883:U:H2'	1:2:884:U:C6	2.50	0.47
1:2:1335:G:O3'	12:K:74:GLY:HA3	2.15	0.47
2:A:18:LYS:NZ	2:A:39:TYR:O	2.49	0.47
2:A:19:TRP:CH2	2:A:37:PRO:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:132:PRO:HA	9:H:135:ARG:HD3	1.96	0.47
19:R:21:LYS:HD2	19:R:84:CYS:HA	1.97	0.47
20:S:57:TYR:CE1	20:S:61:MET:HE2	2.50	0.47
21:T:90:VAL:HG11	21:T:110:LEU:HD12	1.95	0.47
22:U:145:GLU:HA	22:U:148:GLU:OE1	2.14	0.47
27:Z:90:GLU:OE2	27:Z:120:ARG:NH2	2.47	0.47
30:c:15:ARG:O	30:c:19:GLU:HB2	2.15	0.47
31:d:68:TYR:CD1	31:d:68:TYR:C	2.92	0.47
1:2:900:C:C2	1:2:901:A:C8	3.03	0.46
1:2:1199:A:H2'	1:2:1200:C:C6	2.50	0.46
4:C:55:TYR:CZ	4:C:64:GLY:HA3	2.50	0.46
7:F:187:THR:OG1	37:F:303:SPM:N14	2.46	0.46
22:U:56:TRP:CH2	22:U:103:VAL:HG21	2.51	0.46
1:2:37:G:H3'	37:2:1588:SPM:C2	2.45	0.46
1:2:482:C:N4	15:N:118:ASP:OD2	2.47	0.46
1:2:785:C:OP1	24:W:6:ARG:NH1	2.48	0.46
1:2:1122:C:O2'	20:S:52:GLY:HA3	2.16	0.46
3:B:53:SER:O	3:B:173:THR:OG1	2.21	0.46
9:H:76:HIS:HA	12:K:44:MET:HE3	1.98	0.46
25:X:23:ILE:HD11	25:X:41:ARG:CB	2.45	0.46
28:3:73:LYS:HB2	28:3:75:ILE:HG13	1.96	0.46
29:a:21:CYS:HB3	29:a:25:ASN:N	2.31	0.46
31:d:46:TRP:HA	31:d:49:ALA:HB3	1.98	0.46
1:2:132:A:OP2	37:2:1589:SPM:N14	2.48	0.46
1:2:175:U:H2'	1:2:176:G:O4'	2.16	0.46
1:2:314:C:O2'	1:2:566:A:N1	2.45	0.46
1:2:1110:A:H5'	1:2:1111:C:OP2	2.15	0.46
3:B:73:LEU:HD21	3:B:173:THR:HG22	1.97	0.46
5:D:30:LEU:HD23	5:D:35:LEU:HB2	1.97	0.46
13:L:82:VAL:HG23	13:L:83:MET:SD	2.55	0.46
21:T:56:LYS:HE2	21:T:56:LYS:HB2	1.76	0.46
24:W:40:CYS:HB3	24:W:44:GLY:H	1.80	0.46
25:X:54:ARG:NH1	25:X:73:ARG:HB2	2.29	0.46
28:3:72:GLU:OE1	28:3:72:GLU:N	2.49	0.46
1:2:801:C:H2'	1:2:802:U:O4'	2.15	0.46
1:2:877:A:OP2	37:2:1584:SPM:H62	2.15	0.46
1:2:1053:C:H5'	20:S:7:LYS:HG2	1.98	0.46
2:A:53:LEU:HD13	2:A:67:LEU:HD11	1.97	0.46
3:B:199:TRP:NE1	3:B:218:LEU:HD23	2.30	0.46
8:G:150:LEU:HB3	8:G:210:THR:HB	1.97	0.46
17:P:34:ILE:HG12	27:Z:9:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:69:ARG:HG3	25:X:70:GLU:OE2	2.15	0.46
28:3:56:ASP:OD2	28:3:83:LYS:HD2	2.16	0.46
30:c:95:LYS:HZ2	30:c:109:ALA:HA	1.79	0.46
1:2:193:A:N3	1:2:227:C:O2'	2.44	0.46
1:2:1201:A:H2	1:2:1204:G:N3	2.13	0.46
2:A:20:TYR:CD2	2:A:41:ILE:HD12	2.51	0.46
23:V:64:VAL:HG13	23:V:82:HIS:HB2	1.98	0.46
32:e:6:SER:OG	32:e:8:THR:HG23	2.16	0.46
1:2:441:C:P	23:V:101:ARG:HH21	2.38	0.46
1:2:617:G:H2'	1:2:618:C:H6	1.81	0.46
15:N:139:LYS:HE2	15:N:139:LYS:HB3	1.70	0.46
29:a:54:LYS:C	29:a:54:LYS:CD	2.88	0.46
1:2:93:C:H1'	1:2:359:C:H5'	1.97	0.46
1:2:1057:C:C4	1:2:1059:A:H5''	2.51	0.46
1:2:1341:A:N6	9:H:46:GLU:OE2	2.45	0.46
2:A:162:VAL:HG12	2:A:167:LEU:HD23	1.97	0.46
9:H:4:GLU:N	9:H:4:GLU:CD	2.73	0.46
12:K:36:PRO:HB2	12:K:39:LEU:HD23	1.98	0.46
14:M:67:LEU:HD11	14:M:103:ALA:O	2.15	0.46
18:Q:81:GLN:H	18:Q:81:GLN:CD	2.24	0.46
30:c:81:ALA:O	30:c:85:LEU:HD23	2.16	0.46
35:4:27:U:H2'	35:4:28:C:H6	1.80	0.46
1:2:210:U:H5''	1:2:211:C:H5'	1.98	0.46
3:B:29:LYS:HE2	3:B:29:LYS:HA	1.98	0.46
31:d:43:LEU:HD21	31:d:48:GLU:HG2	1.98	0.46
1:2:478:C:OP2	15:N:67:SER:OG	2.30	0.46
1:2:1344:OMU:HM22	1:2:1345:C:O4'	2.16	0.46
10:I:72:CYS:HB3	10:I:132:VAL:HG23	1.98	0.46
12:K:59:ASP:HB3	12:K:63:LYS:NZ	2.31	0.46
25:X:21:GLU:HG3	25:X:65:ILE:HD13	1.97	0.46
1:2:429:U:H1'	5:D:127:THR:HG22	1.97	0.46
39:2:1858:HOH:O	6:E:2:ALA:HB3	2.15	0.46
3:B:29:LYS:HB2	3:B:76:ARG:HD2	1.98	0.46
7:F:139:VAL:CG2	7:F:148:ASP:OD1	2.51	0.46
9:H:174:SER:O	9:H:180:LYS:HE2	2.16	0.46
19:R:92:LYS:HG2	19:R:113:VAL:CG1	2.46	0.46
20:S:27:ASP:OD2	20:S:30:THR:HG23	2.16	0.46
1:2:973:C:C2	1:2:974:A:C8	3.04	0.45
1:2:1445:G:H2'	1:2:1446:G:C8	2.51	0.45
5:D:95:SER:OG	7:F:154:LYS:NZ	2.35	0.45
1:2:133:A:C8	1:2:134:C:C5	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:498:G:H5''	32:e:22:PRO:HB3	1.98	0.45
1:2:543:G:H2'	1:2:544:C:H6	1.81	0.45
1:2:956:G:H22	1:2:1175:A:P	2.38	0.45
1:2:1101:G:H2'	1:2:1102:C:C6	2.51	0.45
1:2:1287:G:OP2	39:2:1711:HOH:O	2.21	0.45
9:H:180:LYS:HB2	9:H:180:LYS:HE3	1.73	0.45
14:M:9:TRP:HB2	14:M:28:LEU:HD21	1.98	0.45
19:R:92:LYS:HG2	19:R:113:VAL:HG13	1.98	0.45
1:2:7:G:H1'	37:2:1584:SPM:H81	1.98	0.45
3:B:212:ILE:HG13	3:B:213:PRO:CD	2.46	0.45
13:L:83:MET:SD	13:L:83:MET:N	2.90	0.45
27:Z:35:GLU:HG3	27:Z:48:TYR:HE1	1.81	0.45
1:2:239:C:H4'	19:R:100:PRO:HG3	1.98	0.45
1:2:761:A:H2'	1:2:762:G:O4'	2.16	0.45
1:2:805:G:H4'	2:A:177:LYS:O	2.17	0.45
1:2:967:G:O6	28:3:37:ASN:HB2	2.17	0.45
4:C:21:LYS:HE3	39:C:204:HOH:O	2.15	0.45
5:D:22:ARG:HD2	39:D:205:HOH:O	2.16	0.45
9:H:95:GLN:H	9:H:95:GLN:HG2	1.63	0.45
13:L:27:ILE:HG13	13:L:85:GLN:NE2	2.32	0.45
20:S:23:GLU:OE2	20:S:38:TYR:OH	2.31	0.45
31:d:32:MET:HE3	31:d:32:MET:HB3	1.79	0.45
31:d:57:PRO:O	31:d:60:VAL:HG22	2.15	0.45
1:2:16:G:H22	37:2:1584:SPM:H41	1.81	0.45
1:2:242:C:OP1	19:R:75:SER:HB2	2.17	0.45
1:2:409:G:H5'	5:D:127:THR:HG21	1.99	0.45
1:2:829:G:OP1	37:2:1569:SPM:H21	2.17	0.45
1:2:1111:C:H2'	1:2:1112:A:O4'	2.15	0.45
1:2:1112:A:HO2'	12:K:71:TYR:HH	1.51	0.45
9:H:4:GLU:CD	9:H:4:GLU:H	2.19	0.45
9:H:85:ALA:O	9:H:89:ILE:HG23	2.17	0.45
16:O:30:LYS:HB2	16:O:30:LYS:HE2	1.42	0.45
21:T:5:ILE:HD12	21:T:5:ILE:O	2.17	0.45
1:2:7:G:H5''	37:2:1586:SPM:H111	1.99	0.45
1:2:126:G:N7	37:2:1577:SPM:H21	2.32	0.45
1:2:962:A:H2	1:2:996:C:H41	1.65	0.45
1:2:1181:C:H2'	1:2:1182:U:C6	2.51	0.45
1:2:1226:C:H2'	1:2:1227:C:C6	2.51	0.45
3:B:74:ASP:O	3:B:78:ILE:HG13	2.17	0.45
7:F:207:LEU:HD22	7:F:210:TRP:CZ2	2.52	0.45
16:O:44:LEU:HD11	16:O:66:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:964:G:O2'	1:2:993:A:N1	2.38	0.45
2:A:23:ILE:HG12	2:A:78:ARG:CG	2.45	0.45
3:B:131:PHE:HB2	3:B:159:GLU:HB3	1.99	0.45
8:G:60:LEU:HD22	8:G:62:LEU:HD22	1.98	0.45
9:H:10:ILE:CG2	9:H:35:PRO:O	2.65	0.45
12:K:23:ILE:HD11	12:K:64:ILE:HG12	1.97	0.45
30:c:11:THR:O	30:c:12:MET:C	2.60	0.45
1:2:72:G:C2	1:2:209:U:H1'	2.52	0.45
1:2:1256:C:H2'	1:2:1257:U:C6	2.52	0.45
3:B:187:ASN:O	3:B:193:SER:OG	2.20	0.45
5:D:48:ILE:HG13	5:D:97:THR:O	2.17	0.45
9:H:39:PRO:HB3	9:H:58:VAL:HG23	1.98	0.45
9:H:108:SER:OG	9:H:178:ALA:HB1	2.16	0.45
21:T:34:LEU:HD13	21:T:38:GLN:HB3	1.98	0.45
30:c:35:LYS:HB2	30:c:36:THR:H	1.65	0.45
31:d:50:TYR:O	31:d:50:TYR:CG	2.70	0.45
1:2:754:C:OP1	37:2:1568:SPM:C6	2.65	0.45
1:2:908:G:OP1	39:2:1712:HOH:O	2.21	0.45
1:2:934:C:OP1	13:L:60:LYS:NZ	2.44	0.45
1:2:1133:A:O3'	20:S:10:LYS:NZ	2.43	0.45
15:N:136:ALA:HB1	15:N:142:LYS:HB2	1.98	0.45
24:W:47:LEU:HA	24:W:58:VAL:HG22	1.98	0.45
27:Z:29:ALA:HB2	27:Z:54:MET:HG3	1.98	0.45
20:S:25:LYS:HD2	20:S:25:LYS:N	2.32	0.45
30:c:103:LEU:C	30:c:103:LEU:CD1	2.90	0.45
37:2:1580:SPM:H31	37:2:1580:SPM:H61	1.66	0.44
8:G:26:SER:HG	8:G:93:TRP:CG	2.34	0.44
9:H:63:ASN:OD1	9:H:75:LYS:HE3	2.16	0.44
9:H:129:ASP:OD2	25:X:66:LEU:HD23	2.17	0.44
21:T:89:ALA:HB1	21:T:96:PHE:HB3	1.99	0.44
1:2:1184:G:N7	37:2:1570:SPM:H92	2.32	0.44
1:2:1346:C:H2'	1:2:1347:C:H6	1.81	0.44
11:J:66:LEU:HA	11:J:73:ALA:HA	1.99	0.44
12:K:9:ILE:HD12	12:K:22:TYR:CD2	2.52	0.44
13:L:41:LEU:HD13	13:L:71:LYS:HE2	1.99	0.44
26:Y:55:ASN:ND2	26:Y:57:ARG:HG2	2.32	0.44
31:d:24:LEU:HB3	31:d:61:MET:HG2	1.99	0.44
1:2:110:A:H1'	19:R:35:ARG:HD2	1.99	0.44
1:2:476:G:N2	1:2:492:A:OP2	2.47	0.44
1:2:653:A:H4'	14:M:47:ARG:NH2	2.32	0.44
1:2:1059:A:H2'	1:2:1060:OMC:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1097:C:C4	22:U:140:LEU:HB2	2.52	0.44
2:A:127:THR:HA	2:A:182:ARG:HG3	1.99	0.44
6:E:12:PHE:CE1	6:E:104:MET:HE2	2.53	0.44
11:J:83:GLU:OE1	11:J:88:LYS:NZ	2.50	0.44
24:W:50:SER:O	24:W:51:MET:HE2	2.17	0.44
26:Y:24:ARG:HD3	28:3:37:ASN:HB3	2.00	0.44
27:Z:29:ALA:CB	27:Z:55:ILE:HG13	2.48	0.44
28:3:34:LYS:HE2	28:3:92:LEU:CD2	2.45	0.44
30:c:94:VAL:HB	30:c:106:TYR:HB3	1.98	0.44
34:s:814:A:OP1	34:s:814:A:C8	2.71	0.44
1:2:1058:A:H4'	1:2:1059:A:H5'	1.99	0.44
1:2:1490:C:H2'	1:2:1491:A:C8	2.52	0.44
37:2:1589:SPM:N10	37:2:1589:SPM:C6	2.80	0.44
3:B:37:VAL:CG1	3:B:41:THR:HB	2.47	0.44
9:H:11:LYS:HB3	9:H:16:TRP:N	2.33	0.44
9:H:114:VAL:HG23	9:H:126:VAL:C	2.43	0.44
16:O:59:GLU:O	16:O:62:LYS:HG2	2.17	0.44
35:4:27:U:H2'	35:4:28:C:C6	2.52	0.44
1:2:1350:C:H2'	1:2:1351:U:H6	1.81	0.44
8:G:64:ILE:HD13	8:G:102:PHE:CD1	2.53	0.44
18:Q:123:LEU:HD23	18:Q:123:LEU:HA	1.83	0.44
18:Q:124:THR:HG22	18:Q:128:LYS:HE3	2.00	0.44
21:T:90:VAL:CG2	21:T:114:SER:HB2	2.46	0.44
22:U:45:PHE:HB3	22:U:97:VAL:HB	1.99	0.44
23:V:19:ARG:NH1	23:V:21:MET:HE2	2.33	0.44
28:3:34:LYS:HE3	28:3:92:LEU:HD22	1.91	0.44
1:2:1260:C:H4'	1:2:1266:U:O4	2.18	0.44
1:2:1490:C:H42	34:s:813:G:H1	1.66	0.44
4:C:63:LYS:HE3	4:C:63:LYS:HB3	1.84	0.44
8:G:23:VAL:HA	8:G:92:VAL:O	2.17	0.44
9:H:36:VAL:HG23	12:K:106:TYR:OH	2.18	0.44
9:H:90:TYR:HD1	9:H:97:PRO:HD3	1.83	0.44
16:O:46:MET:HE1	16:O:55:LEU:HD21	1.99	0.44
28:3:6:TYR:CZ	28:3:8:LYS:HD2	2.53	0.44
28:3:24:ARG:O	28:3:28:GLU:HG3	2.18	0.44
1:2:246:OMC:HM22	1:2:247:C:H5'	1.98	0.44
1:2:376:C:H3'	37:2:1591:SPM:N1	2.33	0.44
1:2:587:G:OP1	37:2:1566:SPM:H122	2.18	0.44
1:2:990:C:O2'	26:Y:62:LYS:HD3	2.17	0.44
3:B:63:TYR:CE2	3:B:64:ARG:HD3	2.52	0.44
6:E:209:ILE:HD11	6:E:223:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:6:LEU:HD12	9:H:7:GLN:N	2.33	0.44
10:I:91:ASP:OD1	10:I:94:ARG:NH2	2.49	0.44
13:L:21:ILE:O	13:L:24:ILE:HG22	2.17	0.44
22:U:45:PHE:CE1	22:U:46:LYS:HE2	2.53	0.44
27:Z:63:ILE:HD12	27:Z:63:ILE:N	2.28	0.44
27:Z:96:MET:HE3	27:Z:96:MET:HA	1.98	0.44
28:3:83:LYS:NZ	28:3:95:ALA:HB1	2.33	0.44
1:2:2:A:OP1	39:2:1713:HOH:O	2.21	0.44
1:2:270:G:H2'	1:2:272:C:H5	1.81	0.44
1:2:324:G:O6	37:2:1565:SPM:H81	2.18	0.44
1:2:1207:A:H2'	1:2:1208:G:C8	2.53	0.44
14:M:111:GLU:OE2	14:M:113:VAL:HG13	2.18	0.44
17:P:28:VAL:HA	17:P:37:CYS:HA	1.99	0.44
19:R:37:ARG:HD3	19:R:37:ARG:N	2.33	0.44
21:T:72:THR:OG1	21:T:74:VAL:HG12	2.18	0.44
28:3:11:VAL:HA	28:3:79:TYR:CD2	2.53	0.44
29:a:55:ARG:HH11	29:a:55:ARG:HB3	1.83	0.44
1:2:16:G:H22	37:2:1584:SPM:C2	2.31	0.44
1:2:408:A:O5'	5:D:141:PRO:HD2	2.17	0.44
1:2:1206:C:O2'	22:U:48:ARG:HD2	2.18	0.44
3:B:182:LEU:HD22	4:C:35:PRO:HB3	2.00	0.44
9:H:44:ARG:NH2	12:K:114:ASP:OD2	2.49	0.44
9:H:138:LEU:HD23	9:H:142:HIS:NE2	2.33	0.44
13:L:11:SER:HB2	13:L:95:VAL:HG22	2.00	0.44
16:O:87:GLU:O	21:T:16:GLY:N	2.51	0.44
1:2:141:A:H2'	1:2:142:A:O4'	2.18	0.43
1:2:263:G:OP1	11:J:98:ARG:HD3	2.18	0.43
1:2:516:A:H2'	1:2:517:C:O4'	2.17	0.43
1:2:642:G:H2'	1:2:643:A:O4'	2.17	0.43
1:2:1097:C:N4	22:U:140:LEU:HB2	2.33	0.43
1:2:1369:G:H2'	1:2:1370:U:C6	2.53	0.43
5:D:134:ASN:O	5:D:134:ASN:ND2	2.46	0.43
7:F:47:VAL:HG21	7:F:111:LYS:O	2.18	0.43
12:K:51:GLU:HB2	12:K:83:ARG:HH21	1.83	0.43
16:O:75:LEU:HD12	16:O:79:LEU:CD1	2.48	0.43
16:O:96:THR:HG22	16:O:97:SER:N	2.32	0.43
21:T:19:ILE:HD12	21:T:19:ILE:H	1.83	0.43
1:2:1307:C:H2'	1:2:1308:C:C6	2.54	0.43
1:2:1321:A:C5'	17:P:31:LYS:HD3	2.49	0.43
9:H:10:ILE:CG2	9:H:37:TYR:CE1	2.96	0.43
12:K:24:TYR:OH	12:K:67:LYS:HE3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:81:ARG:HA	13:L:84:ARG:NE	2.33	0.43
20:S:17:TYR:HE2	20:S:58:TYR:HA	1.82	0.43
27:Z:25:GLN:HA	27:Z:25:GLN:OE1	2.18	0.43
1:2:749:A:H2'	1:2:750:G:C8	2.53	0.43
1:2:865:OMG:O3'	37:2:1599:SPM:H31	2.19	0.43
1:2:1375:C:HO2'	1:2:1376:C:P	2.40	0.43
14:M:41:MET:HE3	14:M:41:MET:HB3	1.83	0.43
31:d:61:MET:HB2	31:d:61:MET:HE3	1.68	0.43
1:2:58:U:H2'	1:2:59:C:C6	2.54	0.43
1:2:822:C:O2'	4:C:51:GLN:OE1	2.30	0.43
6:E:169:ASP:CG	6:E:231:ARG:HH22	2.25	0.43
8:G:60:LEU:HD21	8:G:111:ALA:HB1	2.00	0.43
9:H:28:LYS:CE	31:d:53:ILE:HG22	2.46	0.43
12:K:42:ILE:HB	12:K:45:VAL:HB	1.99	0.43
20:S:23:GLU:O	20:S:25:LYS:HE2	2.19	0.43
21:T:19:ILE:O	21:T:23:LEU:HD12	2.19	0.43
23:V:80:LYS:HD2	23:V:80:LYS:HA	1.87	0.43
1:2:576:G:N7	37:2:1594:SPM:H122	2.33	0.43
1:2:673:G:H2'	1:2:674:A:C8	2.54	0.43
1:2:823:A:H5''	4:C:47:MET:CE	2.48	0.43
1:2:1015:G:H2'	1:2:1016:C:O4'	2.18	0.43
37:2:1570:SPM:H121	37:2:1570:SPM:H91	1.84	0.43
37:2:1574:SPM:H41	37:2:1574:SPM:H72	1.60	0.43
3:B:199:TRP:CD2	3:B:222:VAL:HG22	2.54	0.43
10:I:2:VAL:O	10:I:4:VAL:N	2.52	0.43
11:J:43:ARG:NE	11:J:119:GLY:O	2.47	0.43
17:P:48:LEU:HD23	27:Z:16:VAL:HG21	1.99	0.43
20:S:8:ASP:OD1	20:S:8:ASP:N	2.50	0.43
30:c:47:ILE:HD11	30:c:87:GLU:HB3	1.99	0.43
1:2:726:A:H2'	1:2:727:A:C8	2.53	0.43
20:S:57:TYR:CZ	20:S:61:MET:HE2	2.53	0.43
1:2:73:C:OP2	1:2:209:U:N3	2.39	0.43
1:2:268:A:H2'	1:2:269:G:C8	2.53	0.43
1:2:1099:G:N2	22:U:5:MET:N	2.67	0.43
1:2:1230:G:N7	22:U:102:HIS:ND1	2.67	0.43
2:A:47:ARG:HB2	2:A:71:ILE:HD12	1.99	0.43
2:A:96:LEU:HB3	2:A:125:LEU:CD1	2.49	0.43
2:A:114:ASP:O	2:A:195:PRO:HG3	2.19	0.43
4:C:26:ARG:HG3	7:F:115:ILE:HG22	2.00	0.43
7:F:139:VAL:HG22	7:F:148:ASP:CG	2.42	0.43
8:G:7:VAL:HB	8:G:209:ASN:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:84:LYS:O	21:T:15:ARG:NH1	2.51	0.43
16:O:142:ILE:HD12	21:T:125:PRO:CG	2.46	0.43
22:U:23:TYR:CD1	22:U:23:TYR:C	2.96	0.43
1:2:806:A:O2'	2:A:178:ILE:O	2.34	0.43
1:2:985:C:C2	1:2:986:U:C5	3.06	0.43
9:H:114:VAL:HG23	9:H:125:TYR:C	2.44	0.43
13:L:27:ILE:HG13	13:L:85:GLN:CD	2.44	0.43
21:T:4:GLU:N	21:T:4:GLU:OE1	2.52	0.43
27:Z:95:VAL:O	27:Z:99:ARG:HG3	2.17	0.43
31:d:65:LEU:C	31:d:65:LEU:CD2	2.90	0.43
1:2:44:C:H3'	1:2:45:U:H5''	2.01	0.43
1:2:570:A:C5	1:2:571:C:C5	3.07	0.43
1:2:886:G:O2'	1:2:1363:C:OP2	2.33	0.43
1:2:976:G:H2'	1:2:977:C:C6	2.54	0.43
1:2:1172:C:H2'	1:2:1173:C:C6	2.53	0.43
1:2:1201:A:C8	1:2:1267:G:H1'	2.53	0.43
1:2:1257:U:OP1	30:c:99:LYS:NZ	2.52	0.43
6:E:127:ILE:HG13	6:E:128:LYS:H	1.84	0.43
10:I:100:LYS:HG3	10:I:101:GLU:OE2	2.19	0.43
11:J:11:LYS:HG2	11:J:17:LYS:HD3	2.01	0.43
14:M:7:ILE:HD12	14:M:106:ILE:HD12	2.01	0.43
23:V:84:TYR:OH	23:V:94:GLU:OE2	2.14	0.43
29:a:54:LYS:HZ2	29:a:54:LYS:HG3	1.75	0.43
31:d:12:ARG:HD3	31:d:13:GLU:O	2.18	0.43
1:2:192:G:O2'	1:2:193:A:H5''	2.19	0.43
1:2:637:U:H2'	1:2:638:C:H6	1.84	0.43
1:2:665:C:N3	14:M:36:ARG:NH1	2.66	0.43
1:2:1121:A:N3	1:2:1144:G:C2	2.87	0.43
8:G:7:VAL:O	8:G:210:THR:OG1	2.31	0.43
9:H:13:PHE:HD2	9:H:79:TYR:CZ	2.37	0.43
9:H:114:VAL:HA	9:H:126:VAL:O	2.19	0.43
11:J:58:LYS:HD2	11:J:58:LYS:HA	1.72	0.43
24:W:18:ARG:HD2	24:W:18:ARG:HA	1.83	0.43
27:Z:88:ASN:HB3	27:Z:91:LEU:HB2	2.00	0.43
28:3:25:LYS:HG3	28:3:26:ALA:N	2.34	0.43
30:c:32:GLY:HA3	30:c:35:LYS:HE3	2.01	0.43
1:2:67:C:C2'	1:2:68:C:H5'	2.49	0.42
1:2:877:A:H5''	37:2:1584:SPM:N5	2.34	0.42
1:2:1350:C:H2'	1:2:1351:U:C6	2.54	0.42
1:2:1448:G:O2'	1:2:1449:A:H5'	2.19	0.42
9:H:24:ASP:OD2	9:H:27:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:44:ARG:NE	12:K:109:THR:HG21	2.34	0.42
28:3:32:ILE:C	28:3:33:LYS:HG3	2.40	0.42
28:3:66:LEU:O	28:3:70:CYS:N	2.52	0.42
1:2:1077:A:H2'	1:2:1078:C:H6	1.84	0.42
3:B:178:ASP:OD1	3:B:178:ASP:N	2.52	0.42
17:P:9:GLU:OE1	29:a:44:LYS:HG3	2.18	0.42
20:S:11:ARG:HH22	20:S:12:ILE:HD12	1.83	0.42
25:X:20:ALA:HB1	25:X:40:VAL:HG22	2.01	0.42
30:c:96:LEU:HD22	30:c:105:ILE:O	2.19	0.42
31:d:35:GLU:N	31:d:35:GLU:OE2	2.52	0.42
31:d:37:LEU:O	31:d:41:LEU:HG	2.18	0.42
1:2:404:C:H2'	1:2:405:C:C6	2.54	0.42
1:2:642:G:H2'	1:2:643:A:C8	2.54	0.42
1:2:831:C:H2'	1:2:832:G:O4'	2.19	0.42
1:2:1343:G:H2'	1:2:1344:OMU:C6	2.48	0.42
2:A:168:ALA:HB1	2:A:184:ALA:O	2.18	0.42
9:H:30:TYR:HE2	9:H:132:PRO:HG2	1.85	0.42
28:3:59:PRO:HG2	28:3:62:ILE:HB	2.02	0.42
1:2:436:C:H2'	1:2:437:U:O4'	2.19	0.42
1:2:794:A:H2'	1:2:795:C:C6	2.55	0.42
1:2:865:OMG:HM22	1:2:866:A:O4'	2.20	0.42
1:2:1096:U:O3'	1:2:1097:C:H6	2.02	0.42
1:2:1101:G:C1'	22:U:5:MET:CE	2.97	0.42
1:2:1173:C:H2'	1:2:1174:G:O4'	2.20	0.42
1:2:1226:C:OP1	22:U:78:LYS:HD3	2.19	0.42
37:2:1570:SPM:C6	37:2:1570:SPM:N1	2.73	0.42
3:B:107:TYR:O	3:B:111:GLN:HG3	2.19	0.42
5:D:162:LYS:HE3	5:D:162:LYS:HB3	1.89	0.42
6:E:169:ASP:OD1	6:E:231:ARG:NH2	2.53	0.42
19:R:26:GLU:OE1	19:R:33:SER:OG	2.31	0.42
26:Y:48:MET:HG3	26:Y:49:ALA:N	2.34	0.42
31:d:65:LEU:HB3	31:d:66:PRO:CD	2.48	0.42
1:2:72:G:H2'	1:2:209:U:O2	2.20	0.42
1:2:655:A:H2'	1:2:656:U:C6	2.55	0.42
1:2:1000:G:H2'	1:2:1001:A:O4'	2.19	0.42
1:2:1071:C:H2'	1:2:1072:C:H6	1.84	0.42
1:2:1085:G:H21	1:2:1110:A:H62	1.68	0.42
1:2:1287:G:H2'	1:2:1288:C:H6	1.85	0.42
7:F:9:ASN:HB2	7:F:12:GLU:CD	2.44	0.42
9:H:131:SER:HB2	25:X:60:VAL:HG22	2.01	0.42
10:I:83:TYR:CE1	10:I:123:ARG:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:41:LEU:HB2	13:L:71:LYS:HB3	2.02	0.42
27:Z:60:GLY:HA2	27:Z:63:ILE:HD13	2.01	0.42
1:2:141:A:OP1	39:2:1714:HOH:O	2.21	0.42
1:2:207:U:H2'	1:2:208:A:H8	1.85	0.42
1:2:738:C:H5''	14:M:124:PRO:HB3	2.01	0.42
1:2:787:A:H2'	1:2:788:G:O4'	2.19	0.42
1:2:886:G:H2'	1:2:887:C:C6	2.55	0.42
1:2:949:U:H2'	1:2:950:A:C8	2.54	0.42
1:2:1001:A:H2'	1:2:1002:G:O4'	2.19	0.42
3:B:81:ARG:HD3	3:B:81:ARG:HA	1.81	0.42
6:E:68:ASP:HA	6:E:162:LEU:HD13	2.01	0.42
8:G:16:PRO:HB2	8:G:112:TYR:HB2	2.01	0.42
9:H:9:ASP:O	9:H:37:TYR:CE2	2.73	0.42
9:H:13:PHE:HB3	9:H:83:LYS:HD3	2.00	0.42
12:K:30:VAL:HA	12:K:66:ALA:O	2.20	0.42
25:X:14:GLU:HG3	25:X:45:GLY:HA2	2.02	0.42
25:X:25:ILE:HD13	25:X:38:VAL:HG23	2.02	0.42
2:A:23:ILE:HG23	2:A:78:ARG:HD2	1.97	0.42
2:A:47:ARG:HD3	14:M:29:THR:HG21	2.01	0.42
3:B:26:LYS:NZ	3:B:75:VAL:H	2.17	0.42
6:E:84:ILE:HD11	6:E:95:ARG:NH1	2.34	0.42
9:H:3:LEU:HD11	12:K:99:LEU:CA	2.49	0.42
9:H:32:SER:HA	31:d:62:TRP:CE2	2.54	0.42
9:H:169:ALA:HA	9:H:179:ILE:CG1	2.50	0.42
9:H:193:ARG:NH1	25:X:73:ARG:HH11	2.18	0.42
18:Q:28:ARG:HB2	18:Q:28:ARG:NH1	2.35	0.42
22:U:76:ILE:HD13	22:U:76:ILE:HA	1.86	0.42
1:2:246:OMC:HM21	15:N:34:ILE:HA	2.02	0.42
1:2:310:G:H5''	1:2:311:A:OP1	2.20	0.42
1:2:337:OMG:N7	37:2:1565:SPM:H21	2.35	0.42
1:2:1077:A:H2'	1:2:1078:C:C6	2.54	0.42
1:2:1216:G:H5'	13:L:47:GLU:OE2	2.20	0.42
11:J:128:ASN:OD1	11:J:128:ASN:N	2.52	0.42
28:3:70:CYS:SG	28:3:77:TYR:HB3	2.60	0.42
31:d:71:LEU:HD22	31:d:71:LEU:HA	1.79	0.42
1:2:7:G:C2'	37:2:1584:SPM:H61	2.50	0.42
1:2:52:OMU:HM22	1:2:53:G:O4'	2.20	0.42
1:2:360:C:H4'	37:2:1564:SPM:HN5	1.84	0.42
1:2:1161:G:O6	37:2:1571:SPM:N1	2.53	0.42
1:2:1228:C:P	22:U:125:ARG:HH22	2.41	0.42
37:2:1570:SPM:H32	37:2:1570:SPM:H61	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:160:ALA:HB1	3:B:165:ILE:HB	2.01	0.42
8:G:31:SER:OG	8:G:35:GLU:OE1	2.35	0.42
9:H:13:PHE:CD2	9:H:79:TYR:CZ	3.07	0.42
9:H:28:LYS:NZ	31:d:58:ALA:HA	2.35	0.42
18:Q:102:GLU:HG3	18:Q:103:TYR:CD2	2.55	0.42
23:V:52:ILE:HD13	23:V:52:ILE:HA	1.91	0.42
31:d:64:PRO:HG2	31:d:67:ILE:CB	2.45	0.42
1:2:376:C:C5	37:2:1591:SPM:H32	2.55	0.42
1:2:1078:C:H2'	1:2:1079:U:C6	2.55	0.42
3:B:61:PHE:CD1	3:B:185:PRO:HG3	2.55	0.42
13:L:94:ASP:OD1	13:L:94:ASP:N	2.49	0.42
21:T:110:LEU:HD13	21:T:110:LEU:HA	1.88	0.42
31:d:65:LEU:HB3	31:d:66:PRO:HD3	2.01	0.42
1:2:716:U:H2'	1:2:717:G:O4'	2.20	0.41
1:2:983:A:C5'	17:P:2:GLY:CA	2.98	0.41
1:2:986:U:C4	1:2:987:U:C4	3.08	0.41
1:2:1470:A:H2'	1:2:1471:G:C8	2.55	0.41
37:2:1586:SPM:H71	39:2:1709:HOH:O	2.20	0.41
2:A:153:LEU:HD23	2:A:153:LEU:HA	1.77	0.41
6:E:49:LEU:HD13	23:V:25:VAL:HG21	2.01	0.41
9:H:13:PHE:HE2	9:H:79:TYR:CD2	2.38	0.41
12:K:98:GLU:O	12:K:101:LYS:HG2	2.20	0.41
28:3:34:LYS:CE	28:3:92:LEU:HD23	2.45	0.41
1:2:9:U:C4	37:2:1585:SPM:H131	2.56	0.41
1:2:25:G:H2'	1:2:26:A:C8	2.55	0.41
1:2:33:U:O4	1:2:506:A:H2'	2.19	0.41
1:2:446:G:H21	23:V:42:THR:CG2	2.34	0.41
1:2:519:C:H5'	1:2:525:G:N2	2.35	0.41
1:2:1101:G:C1'	22:U:5:MET:HE1	2.50	0.41
1:2:1125:C:H2'	1:2:1126:C:C6	2.54	0.41
1:2:1288:C:H4'	1:2:1326:C:H4'	2.02	0.41
6:E:55:GLU:O	6:E:59:ILE:HG23	2.20	0.41
7:F:76:TYR:O	7:F:95:LYS:HA	2.20	0.41
9:H:154:ASN:OD1	9:H:156:LYS:HB3	2.20	0.41
12:K:8:VAL:HG22	12:K:23:ILE:CG2	2.43	0.41
18:Q:76:ARG:HB2	18:Q:78:LEU:HD12	2.02	0.41
27:Z:163:ILE:C	27:Z:163:ILE:CD1	2.87	0.41
29:a:23:ILE:HD11	29:a:57:LEU:HD21	2.02	0.41
1:2:311:A:O2'	1:2:312:G:H5'	2.21	0.41
1:2:642:G:O2'	1:2:643:A:H5'	2.21	0.41
1:2:1121:A:OP2	20:S:32:LYS:NZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1188:G:H2'	21:T:120:VAL:CG2	2.49	0.41
6:E:95:ARG:NH2	6:E:113:GLU:O	2.50	0.41
9:H:113:GLU:CD	25:X:57:LYS:HD3	2.45	0.41
21:T:58:ARG:HG3	21:T:61:ARG:HH22	1.84	0.41
26:Y:57:ARG:HB3	26:Y:68:PHE:CD1	2.53	0.41
28:3:55:GLU:HB2	28:3:80:VAL:HG21	2.01	0.41
29:a:66:THR:HG22	29:a:67:GLU:N	2.35	0.41
1:2:649:G:H2'	1:2:650:G:C8	2.55	0.41
1:2:740:A:OP2	37:2:1568:SPM:H112	2.20	0.41
1:2:807:G:H2'	1:2:808:C:C6	2.56	0.41
1:2:899:A:H2'	1:2:900:C:C6	2.56	0.41
37:2:1585:SPM:H91	37:F:303:SPM:N5	2.35	0.41
3:B:26:LYS:HE2	3:B:63:TYR:CE2	2.56	0.41
8:G:80:LYS:NZ	8:G:147:PRO:HD3	2.34	0.41
8:G:94:ILE:HD12	8:G:98:MET:HB2	2.02	0.41
12:K:30:VAL:O	22:U:156:TYR:OH	2.39	0.41
12:K:121:GLU:HA	12:K:128:ALA:HA	2.01	0.41
16:O:28:MET:HE2	16:O:28:MET:HB3	1.81	0.41
20:S:58:TYR:CZ	20:S:62:LYS:HE2	2.55	0.41
22:U:120:ILE:HG13	22:U:126:SER:OG	2.20	0.41
1:2:601:A:H2'	1:2:602:C:C6	2.55	0.41
1:2:1124:G:C2	1:2:1125:C:C6	3.08	0.41
1:2:1283:A:O2'	1:2:1287:G:N7	2.46	0.41
1:2:1369:G:H2'	1:2:1370:U:H6	1.84	0.41
37:2:1564:SPM:H61	37:2:1564:SPM:H21	2.02	0.41
8:G:142:GLN:HG2	8:G:143:LEU:HD12	2.02	0.41
9:H:33:LEU:H	31:d:62:TRP:CG	2.37	0.41
11:J:127:LYS:HD2	11:J:127:LYS:HA	1.67	0.41
13:L:23:GLN:NE2	13:L:89:VAL:HG22	2.34	0.41
13:L:65:TRP:HB3	17:P:50:PHE:HB3	2.02	0.41
17:P:21:ARG:NE	27:Z:20:GLU:OE1	2.31	0.41
22:U:70:VAL:HG12	22:U:71:ASN:OD1	2.20	0.41
23:V:19:ARG:HH12	23:V:21:MET:HE2	1.86	0.41
27:Z:163:ILE:HD12	27:Z:163:ILE:O	2.21	0.41
27:Z:189:ILE:CG2	27:Z:192:LYS:HG3	2.51	0.41
29:a:57:LEU:N	29:a:57:LEU:CD1	2.82	0.41
1:2:1009:U:H5	39:2:1980:HOH:O	2.04	0.41
2:A:112:THR:HA	2:A:150:ALA:O	2.21	0.41
9:H:31:ILE:O	31:d:62:TRP:NE1	2.53	0.41
9:H:91:LEU:CB	30:c:64:ILE:HD11	2.51	0.41
9:H:115:THR:HG23	9:H:117:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:51:ARG:HB2	17:P:53:TYR:CE1	2.56	0.41
29:a:36:TYR:O	29:a:48:TYR:HA	2.19	0.41
1:2:50:C:OP2	39:2:1716:HOH:O	2.22	0.41
1:2:131:U:H2'	1:2:132:A:C8	2.56	0.41
1:2:167:A:H2'	1:2:168:G:C8	2.54	0.41
1:2:271:G:H3'	19:R:103:LYS:HB2	2.03	0.41
1:2:885:G:N3	1:2:1362:A:H2	2.18	0.41
2:A:94:ARG:HH22	14:M:116:ILE:HD13	1.85	0.41
7:F:97:LYS:HB3	7:F:97:LYS:HE2	1.89	0.41
16:O:88:SER:C	16:O:90:LEU:H	2.28	0.41
22:U:19:ARG:HH22	22:U:141:GLU:CD	2.25	0.41
26:Y:56:GLU:O	26:Y:58:TRP:CD1	2.74	0.41
27:Z:189:ILE:HG21	27:Z:192:LYS:HG3	2.03	0.41
30:c:64:ILE:HD13	30:c:64:ILE:HA	1.78	0.41
1:2:149:G:P	37:2:1589:SPM:H92	2.59	0.41
1:2:538:OMC:HM22	1:2:539:C:O4'	2.20	0.41
1:2:579:C:H2'	1:2:580:A:O4'	2.21	0.41
1:2:1121:A:C2	1:2:1144:G:C4	3.08	0.41
1:2:1284:C:OP2	39:2:1711:HOH:O	2.22	0.41
1:2:1349:G:H2'	1:2:1350:C:C6	2.55	0.41
2:A:183:LYS:HD2	2:A:183:LYS:HA	1.89	0.41
4:C:14:PRO:HB2	4:C:23:ILE:HD12	2.02	0.41
6:E:119:VAL:HG21	6:E:138:ASP:OD1	2.21	0.41
8:G:119:ILE:HG21	8:G:144:ILE:HG12	2.03	0.41
9:H:38:LEU:HD12	9:H:39:PRO:HD2	2.03	0.41
13:L:51:MET:HE2	13:L:51:MET:HB3	1.79	0.41
26:Y:25:THR:HG23	28:3:65:HIS:ND1	2.35	0.41
28:3:43:VAL:HG22	28:3:51:VAL:HG11	2.03	0.41
1:2:18:C:H5''	15:N:112:LEU:HD21	2.01	0.41
1:2:166:G:H4'	11:J:118:ASP:OD1	2.20	0.41
1:2:366:C:H2'	1:2:367:G:O4'	2.20	0.41
1:2:483:G:N2	37:2:1558:SPM:H111	2.35	0.41
1:2:569:G:C5	1:2:570:A:N7	2.89	0.41
1:2:884:U:H2'	1:2:885:G:O4'	2.20	0.41
1:2:974:A:H1'	26:Y:57:ARG:CZ	2.51	0.41
1:2:1043:C:H2'	1:2:1044:C:H6	1.86	0.41
1:2:1293:G:OP1	16:O:36:THR:OG1	2.37	0.41
1:2:1322:U:H3'	1:2:1323:C:C6	2.56	0.41
1:2:1368:5MC:H2'	1:2:1369:G:C8	2.56	0.41
1:2:1444:G:HO2'	1:2:1445:G:H8	1.65	0.41
1:2:1469:U:H2'	1:2:1470:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:34:CYS:HA	4:C:35:PRO:HD3	1.90	0.41
6:E:26:PRO:HG2	6:E:33:ILE:HG12	2.03	0.41
8:G:25:ALA:O	8:G:96:LYS:HE3	2.21	0.41
9:H:98:ILE:O	9:H:102:VAL:HG23	2.20	0.41
9:H:114:VAL:HG21	9:H:125:TYR:HB3	2.03	0.41
9:H:116:ARG:C	9:H:117:ILE:HD12	2.46	0.41
9:H:159:GLU:OE2	30:c:102:ARG:HD2	2.20	0.41
11:J:65:VAL:HG22	11:J:123:ALA:HB3	2.03	0.41
12:K:27:LYS:HA	12:K:62:SER:O	2.21	0.41
20:S:19:ARG:HG2	20:S:20:TYR:CE2	2.56	0.41
21:T:5:ILE:HD12	21:T:5:ILE:C	2.45	0.41
24:W:18:ARG:HH21	24:W:27:GLU:HG3	1.85	0.41
1:2:391:G:OP2	37:2:1573:SPM:H61	2.21	0.41
1:2:1191:C:H1'	16:O:142:ILE:HD11	2.03	0.41
1:2:1283:A:H2'	21:T:37:ARG:HD3	2.03	0.41
37:2:1593:SPM:N14	5:D:6:LYS:HA	2.36	0.41
19:R:37:ARG:HD3	19:R:37:ARG:H	1.86	0.41
22:U:5:MET:O	22:U:6:ILE:CD1	2.48	0.41
22:U:112:GLU:HA	22:U:117:VAL:O	2.21	0.41
25:X:50:ARG:CZ	25:X:52:LEU:HD21	2.51	0.41
28:3:22:ALA:HB1	28:3:111:VAL:HG23	2.02	0.41
1:2:1447:A:H2'	1:2:1448:G:C8	2.52	0.40
2:A:25:PRO:HG3	2:A:81:THR:O	2.21	0.40
6:E:93:TYR:HB2	6:E:109:ILE:O	2.22	0.40
7:F:186:THR:HA	37:F:303:SPM:N10	2.36	0.40
17:P:5:LYS:HE3	17:P:5:LYS:HB2	1.88	0.40
24:W:16:PHE:O	24:W:65:MET:HG2	2.21	0.40
28:3:115:ILE:O	28:3:118:VAL:HG12	2.21	0.40
30:c:43:ARG:HG3	30:c:44:ALA:N	2.36	0.40
30:c:88:LEU:HD23	30:c:88:LEU:HA	1.80	0.40
1:2:210:U:H5''	1:2:211:C:C5'	2.51	0.40
1:2:699:U:H2'	1:2:700:A:C8	2.56	0.40
1:2:924:U:C5	1:2:1188:G:C8	3.09	0.40
1:2:1084:G:H5'	1:2:1244:A:O2'	2.21	0.40
1:2:1252:A:N1	1:2:1335:G:H1'	2.35	0.40
1:2:1317:G:N7	37:2:1572:SPM:H42	2.35	0.40
7:F:82:MET:HE3	7:F:82:MET:HB2	1.90	0.40
8:G:8:ILE:HB	8:G:117:LEU:HD23	2.02	0.40
8:G:60:LEU:HD23	8:G:61:THR:N	2.36	0.40
13:L:16:ASN:ND2	13:L:94:ASP:OD1	2.55	0.40
25:X:18:PHE:HB2	25:X:68:LEU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1336:U:H2'	1:2:1337:G:O4'	2.20	0.40
9:H:13:PHE:HD2	9:H:79:TYR:OH	2.04	0.40
11:J:126:LEU:HD23	11:J:126:LEU:HA	1.92	0.40
12:K:102:ILE:HD11	31:d:66:PRO:O	2.21	0.40
13:L:45:LYS:HA	13:L:67:MET:O	2.21	0.40
16:O:98:ASP:OD1	16:O:98:ASP:N	2.53	0.40
29:a:6:ARG:HD2	29:a:6:ARG:HA	1.95	0.40
31:d:34:LEU:H	31:d:34:LEU:HG	1.74	0.40
1:2:13:C:OP2	37:F:303:SPM:H82	2.22	0.40
1:2:113:OMC:HM22	1:2:114:U:H5'	2.03	0.40
1:2:151:U:O4	37:2:1589:SPM:N14	2.54	0.40
1:2:968:A:H62	1:2:992:G:H21	1.68	0.40
2:A:127:THR:HG21	2:A:180:PRO:HB2	2.04	0.40
3:B:209:ARG:HH11	3:B:209:ARG:HG2	1.86	0.40
16:O:31:GLY:HA3	16:O:95:VAL:HA	2.03	0.40
25:X:53:THR:OG1	25:X:74:GLU:OE2	2.36	0.40
26:Y:39:LYS:HB3	26:Y:39:LYS:HE2	1.76	0.40
29:a:50:CYS:SG	29:a:53:ASP:HB2	2.61	0.40
1:2:864:A:C5	1:2:865:OMG:H1'	2.56	0.40
1:2:989:C:O2'	1:2:990:C:H5'	2.21	0.40
1:2:1278:C:O2'	1:2:1279:U:H5'	2.21	0.40
1:2:1338:A:OP1	9:H:75:LYS:NZ	2.46	0.40
39:2:2103:HOH:O	37:F:303:SPM:H71	2.21	0.40
6:E:120:ARG:NH1	6:E:226:VAL:O	2.55	0.40
6:E:178:TYR:CD1	6:E:234:SER:HB2	2.56	0.40
7:F:91:ILE:HG21	7:F:191:VAL:HG12	2.04	0.40
9:H:44:ARG:NE	12:K:114:ASP:OD2	2.52	0.40
9:H:61:LEU:O	9:H:65:ILE:HG12	2.22	0.40
9:H:114:VAL:CG2	9:H:125:TYR:C	2.94	0.40
17:P:34:ILE:CG1	27:Z:9:LEU:HD21	2.52	0.40
18:Q:89:LEU:HD12	18:Q:123:LEU:HD12	2.04	0.40
26:Y:41:CYS:HA	26:Y:65:TYR:HH	1.86	0.40
27:Z:173:LYS:HA	27:Z:173:LYS:HD2	1.93	0.40
30:c:27:GLU:O	30:c:31:LYS:N	2.55	0.40
30:c:37:GLY:O	30:c:38:LYS:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	184/208 (88%)	181 (98%)	3 (2%)	0	100	100
3	B	213/231 (92%)	209 (98%)	4 (2%)	0	100	100
4	C	56/65 (86%)	55 (98%)	1 (2%)	0	100	100
5	D	164/181 (91%)	162 (99%)	2 (1%)	0	100	100
6	E	236/239 (99%)	229 (97%)	7 (3%)	0	100	100
7	F	208/214 (97%)	201 (97%)	7 (3%)	0	100	100
8	G	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
9	H	190/193 (98%)	181 (95%)	9 (5%)	0	100	100
10	I	130/133 (98%)	128 (98%)	2 (2%)	0	100	100
11	J	125/133 (94%)	116 (93%)	9 (7%)	0	100	100
12	K	131/137 (96%)	125 (95%)	6 (5%)	0	100	100
13	L	99/102 (97%)	95 (96%)	4 (4%)	0	100	100
14	M	125/132 (95%)	118 (94%)	6 (5%)	1 (1%)	16	31
15	N	144/147 (98%)	138 (96%)	5 (4%)	1 (1%)	18	34
16	O	138/165 (84%)	130 (94%)	8 (6%)	0	100	100
17	P	51/54 (94%)	50 (98%)	1 (2%)	0	100	100
18	Q	143/152 (94%)	142 (99%)	1 (1%)	0	100	100
19	R	111/114 (97%)	108 (97%)	3 (3%)	0	100	100
20	S	64/79 (81%)	62 (97%)	2 (3%)	0	100	100
21	T	126/140 (90%)	119 (94%)	7 (6%)	0	100	100
22	U	152/158 (96%)	147 (97%)	5 (3%)	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%)	57 (88%)	8 (12%)	0	100	100
26	Y	47/75 (63%)	40 (85%)	7 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Z	194/229 (85%)	189 (97%)	5 (3%)	0	100	100
28	3	115/127 (91%)	103 (90%)	12 (10%)	0	100	100
29	a	69/72 (96%)	69 (100%)	0	0	100	100
30	c	107/110 (97%)	99 (92%)	8 (8%)	0	100	100
31	d	68/72 (94%)	64 (94%)	4 (6%)	0	100	100
32	e	41/52 (79%)	40 (98%)	1 (2%)	0	100	100
All	All	3875/4197 (92%)	3717 (96%)	156 (4%)	2 (0%)	49	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	N	64	GLN
14	M	119	ASP

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%)	162 (96%)	6 (4%)	31	58
3	B	182/198 (92%)	179 (98%)	3 (2%)	55	79
4	C	51/58 (88%)	47 (92%)	4 (8%)	11	24
5	D	147/158 (93%)	145 (99%)	2 (1%)	59	81
6	E	214/215 (100%)	211 (99%)	3 (1%)	59	81
7	F	180/184 (98%)	179 (99%)	1 (1%)	78	91
8	G	186/187 (100%)	181 (97%)	5 (3%)	39	67
9	H	166/167 (99%)	159 (96%)	7 (4%)	26	52
10	I	113/114 (99%)	112 (99%)	1 (1%)	70	87
11	J	104/110 (94%)	103 (99%)	1 (1%)	68	86
12	K	109/113 (96%)	106 (97%)	3 (3%)	38	66
13	L	93/94 (99%)	92 (99%)	1 (1%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M	93/98 (95%)	89 (96%)	4 (4%)	26	51
15	N	122/123 (99%)	119 (98%)	3 (2%)	42	69
16	O	121/142 (85%)	116 (96%)	5 (4%)	27	53
17	P	45/46 (98%)	45 (100%)	0	100	100
18	Q	125/129 (97%)	125 (100%)	0	100	100
19	R	101/102 (99%)	100 (99%)	1 (1%)	68	86
20	S	63/75 (84%)	62 (98%)	1 (2%)	55	79
21	T	116/126 (92%)	111 (96%)	5 (4%)	26	51
22	U	134/138 (97%)	131 (98%)	3 (2%)	45	73
23	V	92/99 (93%)	90 (98%)	2 (2%)	45	73
24	W	57/58 (98%)	54 (95%)	3 (5%)	20	42
25	X	58/73 (80%)	57 (98%)	1 (2%)	53	78
26	Y	43/65 (66%)	42 (98%)	1 (2%)	44	72
27	Z	163/195 (84%)	159 (98%)	4 (2%)	42	69
28	3	97/105 (92%)	96 (99%)	1 (1%)	68	86
29	a	61/62 (98%)	51 (84%)	10 (16%)	2	4
30	c	95/96 (99%)	89 (94%)	6 (6%)	16	34
31	d	63/65 (97%)	44 (70%)	19 (30%)	0	0
32	e	40/46 (87%)	38 (95%)	2 (5%)	22	44
All	All	3402/3625 (94%)	3294 (97%)	108 (3%)	35	62

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	49	VAL
2	A	77	ASP
2	A	114	ASP
2	A	127	THR
2	A	169	ASN
2	A	194	VAL
3	B	37	VAL
3	B	177	ILE
3	B	211	VAL
4	C	10	GLU
4	C	21	LYS

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Mol	Chain	Res	Type
4	C	47	MET
4	C	60	CYS
5	D	134	ASN
5	D	162	LYS
6	E	8	GLU
6	E	59	ILE
6	E	168	LEU
7	F	174	LYS
8	G	32	ILE
8	G	41	VAL
8	G	46	VAL
8	G	50	THR
8	G	206	VAL
9	H	6	LEU
9	H	10	ILE
9	H	12	VAL
9	H	15	LYS
9	H	89	ILE
9	H	136	ILE
9	H	192	SER
10	I	24	GLN
11	J	108	LEU
12	K	20	THR
12	K	49	ILE
12	K	99	LEU
13	L	100	GLN
14	M	23	LEU
14	M	28	LEU
14	M	84	TYR
14	M	119	ASP
15	N	21	LEU
15	N	29	LYS
15	N	111	THR
16	O	16	VAL
16	O	30	LYS
16	O	36	THR
16	O	72	ILE
16	O	98	ASP
19	R	94	ILE
20	S	3	ASN
21	T	67	ASN
21	T	76	ASN

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Mol	Chain	Res	Type
21	T	88	MET
21	T	102	THR
21	T	130	THR
22	U	9	GLU
22	U	106	LEU
22	U	120	ILE
23	V	64	VAL
23	V	92	LYS
24	W	17	LEU
24	W	48	VAL
24	W	62	VAL
25	X	71	THR
26	Y	32	ASN
27	Z	20	GLU
27	Z	69	ILE
27	Z	84	THR
27	Z	190	GLU
28	3	118	VAL
29	a	14	LEU
29	a	17	LEU
29	a	37	LYS
29	a	40	LYS
29	a	54	LYS
29	a	58	LYS
29	a	60	LYS
29	a	61	CYS
29	a	71	ILE
29	a	72	LEU
30	c	9	ILE
30	c	11	THR
30	c	35	LYS
30	c	48	ASP
30	c	74	SER
30	c	92	ASN
31	d	4	LEU
31	d	5	LYS
31	d	6	ILE
31	d	7	LYS
31	d	8	LEU
31	d	9	SER
31	d	10	SER
31	d	12	ARG

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Mol	Chain	Res	Type
31	d	13	GLU
31	d	14	VAL
31	d	15	GLU
31	d	30	THR
31	d	33	THR
31	d	34	LEU
31	d	52	LEU
31	d	56	VAL
31	d	65	LEU
31	d	70	LYS
31	d	71	LEU
32	e	17	THR
32	e	29	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	74	ASN
4	C	46	HIS
4	C	59	ASN
5	D	53	HIS
5	D	54	GLN
8	G	186	ASN
9	H	71	ASN
9	H	76	HIS
10	I	42	GLN
11	J	5	GLN
11	J	52	ASN
13	L	23	GLN
14	M	13	HIS
14	M	18	GLN
14	M	60	ASN
14	M	94	GLN
15	N	27	GLN
15	N	100	HIS
16	O	3	GLN
18	Q	2	ASN
26	Y	51	HIS
27	Z	62	ASN
27	Z	68	GLN
29	a	25	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1428/1497 (95%)	227 (15%)	7 (0%)
33	5	1/15 (6%)	0	0
34	s	9/15 (60%)	8 (88%)	0
35	4	16/77 (20%)	0	0
All	All	1454/1604 (90%)	235 (16%)	7 (0%)

All (235) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	U
1	2	14	C
1	2	33	U
1	2	34	C
1	2	45	U
1	2	46	A
1	2	47	A
1	2	60	G
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	100	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	126	G
1	2	138	G
1	2	144	C
1	2	181	G
1	2	193	A
1	2	195	A
1	2	196	G
1	2	208	A
1	2	209	U

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Mol	Chain	Res	Type
1	2	211	C
1	2	212	C
1	2	213	C
1	2	214	C
1	2	215	G
1	2	225	G
1	2	245	C
1	2	246	OMC
1	2	248	A
1	2	249	U
1	2	250	C
1	2	251	A
1	2	252	G
1	2	256	G
1	2	257	U
1	2	258	U
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	321	U
1	2	333	C
1	2	334	A
1	2	335	A
1	2	336	G
1	2	349	A
1	2	357	C
1	2	358	A
1	2	359	C
1	2	372	G
1	2	377	C
1	2	378	A
1	2	389	G
1	2	395	G
1	2	398	C
1	2	402	A
1	2	408	A
1	2	411	G
1	2	417	G

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Mol	Chain	Res	Type
1	2	418	U
1	2	420	A
1	2	453	A
1	2	470	U
1	2	471	C
1	2	476	G
1	2	477	U
1	2	480	G
1	2	489	G
1	2	490	U
1	2	491	A
1	2	506	A
1	2	522	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	601	A
1	2	609	G
1	2	612	A
1	2	624	A
1	2	634	U
1	2	682	U
1	2	683	G
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	751	A
1	2	752	U
1	2	753	A
1	2	774	A
1	2	776	C
1	2	780	G
1	2	802	U
1	2	804	A
1	2	805	G
1	2	806	A

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Mol	Chain	Res	Type
1	2	828	A
1	2	835	A
1	2	853	G
1	2	865	OMG
1	2	877	A
1	2	889	G
1	2	897	C
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	957	A
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	1091	U
1	2	1094	U
1	2	1095	C

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Mol	Chain	Res	Type
1	2	1096	U
1	2	1097	C
1	2	1098	C
1	2	1099	G
1	2	1101	G
1	2	1103	C
1	2	1106	G
1	2	1107	A
1	2	1118	G
1	2	1120	G
1	2	1121	A
1	2	1123	U
1	2	1147	G
1	2	1157	G
1	2	1159	A
1	2	1160	G
1	2	1175	A
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	1217	G
1	2	1219	A
1	2	1220	U
1	2	1221	U
1	2	1222	C
1	2	1224	G
1	2	1226	C
1	2	1243	A
1	2	1244	A
1	2	1248	C
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

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Mol	Chain	Res	Type
1	2	1286	C
1	2	1300	A
1	2	1309	U
1	2	1328	A
1	2	1334	G
1	2	1338	A
1	2	1358	A
1	2	1361	C
1	2	1376	C
1	2	1445	G
1	2	1448	G
1	2	1449	A
1	2	1450	A
1	2	1452	U
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	1476	A
1	2	1477	4AC
1	2	1478	4AC
1	2	1483	G
1	2	1486	G
1	2	1487	G
34	s	807	G
34	s	809	G
34	s	810	G
34	s	811	A
34	s	812	U
34	s	813	G
34	s	814	A
34	s	815	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	45	U
1	2	490	U
1	2	522	A

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Mol	Chain	Res	Type
1	2	804	A
1	2	1188	G
1	2	1455	U
1	2	1477	4AC

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

34 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	OMU	2	1344	1	19,22,23	1.24	3 (15%)	26,31,34	1.75	5 (19%)
1	OMU	2	15	1	19,22,23	1.41	3 (15%)	26,31,34	1.78	4 (15%)
1	OMG	2	1194	1	23,26,27	1.22	3 (13%)	33,38,41	2.04	7 (21%)
1	OMC	2	481	1	19,22,23	1.10	2 (10%)	26,31,34	1.84	6 (23%)
1	A2M	2	494	1	22,25,26	1.46	4 (18%)	31,36,39	2.11	9 (29%)
1	OMU	2	52	1	19,22,23	1.25	3 (15%)	26,31,34	1.72	4 (15%)
1	OMG	2	546	1	23,26,27	1.23	4 (17%)	33,38,41	1.91	6 (18%)
1	4AC	2	1477	1	21,24,25	1.08	2 (9%)	29,34,37	1.48	4 (13%)
1	OMG	2	1018	1	23,26,27	1.20	3 (13%)	33,38,41	2.01	7 (21%)
1	OMG	2	672	1	23,26,27	1.21	3 (13%)	33,38,41	1.94	5 (15%)
1	MA6	2	1475	1	23,26,27	1.44	4 (17%)	34,38,41	2.25	11 (32%)
1	5MC	2	1368	1	18,22,23	0.91	2 (11%)	26,32,35	1.10	2 (7%)
1	OMG	2	905	1	23,26,27	1.19	3 (13%)	33,38,41	1.99	8 (24%)
1	OMG	2	1061	1	23,26,27	1.19	4 (17%)	33,38,41	1.89	6 (18%)
1	OMC	2	113	1	19,22,23	0.79	0	26,31,34	0.91	0
1	OMC	2	1366	1	19,22,23	0.80	0	26,31,34	0.83	1 (3%)
1	4AC	2	1478	1	21,24,25	1.05	2 (9%)	29,34,37	1.28	4 (13%)
1	OMG	2	337	1	23,26,27	1.24	4 (17%)	33,38,41	1.98	7 (21%)
1	OMG	2	399	1	23,26,27	1.21	3 (13%)	33,38,41	1.95	6 (18%)
1	OMG	2	865	1	23,26,27	1.25	3 (13%)	33,38,41	1.95	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	2	710	1	19,22,23	0.82	0	26,31,34	0.78	1 (3%)
1	C4J	2	930	1	24,29,30	0.23	0	29,42,45	0.54	0
1	4AC	2	1466	1	21,24,25	1.01	2 (9%)	29,34,37	1.16	3 (10%)
1	6MZ	2	1457	36,1	22,25,26	1.42	4 (18%)	30,36,39	2.23	10 (33%)
1	OMC	2	1060	1	19,22,23	0.81	0	26,31,34	0.75	0
1	OMG	2	926	1	23,26,27	1.23	3 (13%)	33,38,41	1.96	6 (18%)
1	OMC	2	313	1	19,22,23	0.83	0	26,31,34	0.79	0
1	OMU	2	1032	1	19,22,23	1.33	3 (15%)	26,31,34	1.71	4 (15%)
1	OMC	2	246	1	19,22,23	0.87	1 (5%)	26,31,34	1.00	1 (3%)
1	4AC	2	843	1	21,24,25	1.09	2 (9%)	29,34,37	1.40	4 (13%)
1	OMC	2	538	1	19,22,23	0.81	0	26,31,34	0.83	1 (3%)
1	4AC	2	1467	1	21,24,25	1.10	3 (14%)	29,34,37	1.22	4 (13%)
35	OMC	4	32	35	19,22,23	0.88	1 (5%)	26,31,34	1.12	2 (7%)
1	OMC	2	512	1	19,22,23	0.81	0	26,31,34	0.86	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
1	OMU	2	1344	1	-	0/9/27/28	0/2/2/2
1	OMU	2	15	1	-	0/9/27/28	0/2/2/2
1	OMG	2	1194	1	-	0/9/27/28	0/3/3/3
1	OMC	2	481	1	-	0/9/27/28	0/2/2/2
1	A2M	2	494	1	-	1/9/27/28	0/3/3/3
1	OMU	2	52	1	-	0/9/27/28	0/2/2/2
1	OMG	2	546	1	-	0/9/27/28	0/3/3/3
1	4AC	2	1477	1	-	0/11/29/30	0/2/2/2
1	OMG	2	1018	1	-	0/9/27/28	0/3/3/3
1	OMG	2	672	1	-	0/9/27/28	0/3/3/3
1	MA6	2	1475	1	-	0/11/29/30	0/3/3/3
1	5MC	2	1368	1	-	0/7/25/26	0/2/2/2
1	OMG	2	905	1	-	0/9/27/28	0/3/3/3
1	OMG	2	1061	1	-	0/9/27/28	0/3/3/3
1	OMC	2	113	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	1478	1	-	0/11/29/30	0/2/2/2
1	OMG	2	337	1	-	1/9/27/28	0/3/3/3
1	OMG	2	399	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	2	865	1	-	2/9/27/28	0/3/3/3
1	OMC	2	710	1	-	0/9/27/28	0/2/2/2
1	C4J	2	930	1	-	3/16/34/35	0/2/2/2
1	4AC	2	1466	1	-	0/11/29/30	0/2/2/2
1	6MZ	2	1457	36,1	-	0/9/27/28	0/3/3/3
1	OMC	2	1060	1	-	0/9/27/28	0/2/2/2
1	OMG	2	926	1	-	0/9/27/28	0/3/3/3
1	OMC	2	313	1	-	0/9/27/28	0/2/2/2
1	OMU	2	1032	1	-	0/9/27/28	0/2/2/2
1	OMC	2	246	1	-	3/9/27/28	0/2/2/2
1	4AC	2	843	1	-	0/11/29/30	0/2/2/2
1	OMC	2	538	1	-	0/9/27/28	0/2/2/2
1	4AC	2	1467	1	-	0/11/29/30	0/2/2/2
35	OMC	4	32	35	-	3/9/27/28	0/2/2/2
1	OMC	2	512	1	-	0/9/27/28	0/2/2/2

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	494	A2M	C5-C4	4.44	1.47	1.39
1	2	1475	MA6	C5-C4	4.38	1.47	1.39
1	2	1457	6MZ	C5-C4	4.08	1.46	1.39
1	2	15	OMU	C4-N3	-3.47	1.32	1.38
1	2	15	OMU	C2-N3	-3.22	1.32	1.38
1	2	1032	OMU	C4-N3	-3.13	1.33	1.38
1	2	481	OMC	C6-C5	3.13	1.42	1.35
1	2	1478	4AC	C5-C4	2.95	1.47	1.40
1	2	926	OMG	C5-C4	2.93	1.46	1.38
1	2	1477	4AC	C5-C4	2.93	1.47	1.40
1	2	546	OMG	C5-C4	2.93	1.46	1.38
1	2	865	OMG	C5-C4	2.88	1.46	1.38
1	2	337	OMG	C6-N1	-2.85	1.33	1.38
1	2	843	4AC	C5-C4	2.84	1.46	1.40
1	2	672	OMG	C5-C4	2.83	1.46	1.38
1	2	865	OMG	C6-N1	-2.83	1.33	1.38
1	2	1467	4AC	C4-N3	-2.83	1.27	1.32
1	2	905	OMG	C5-C4	2.82	1.46	1.38
1	2	926	OMG	C6-N1	-2.78	1.33	1.38
1	2	399	OMG	C6-N1	-2.77	1.33	1.38
1	2	1061	OMG	C5-C4	2.77	1.46	1.38
1	2	1467	4AC	C5-C4	2.76	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	337	OMG	C5-C4	2.75	1.46	1.38
1	2	1032	OMU	C2-N3	-2.75	1.33	1.38
1	2	52	OMU	C4-N3	-2.72	1.33	1.38
1	2	672	OMG	C6-N1	-2.71	1.33	1.38
1	2	1194	OMG	C5-C4	2.69	1.46	1.38
1	2	494	A2M	C5-C6	2.69	1.48	1.41
1	2	1344	OMU	C4-N3	-2.69	1.33	1.38
1	2	1018	OMG	C6-N1	-2.68	1.33	1.38
1	2	1194	OMG	C5-N7	-2.68	1.33	1.39
1	2	1018	OMG	C5-C4	2.67	1.46	1.38
1	2	1457	6MZ	C5-C6	2.66	1.48	1.41
1	2	1466	4AC	C5-C4	2.65	1.46	1.40
1	2	905	OMG	C6-N1	-2.65	1.33	1.38
1	2	1194	OMG	C6-N1	-2.63	1.34	1.38
1	2	399	OMG	C5-C4	2.62	1.46	1.38
1	2	1475	MA6	C5-C6	2.61	1.48	1.41
1	2	843	4AC	C4-N3	-2.61	1.28	1.32
1	2	1368	5MC	C6-N1	-2.59	1.33	1.38
1	2	546	OMG	C6-N1	-2.52	1.34	1.38
1	2	865	OMG	C5-N7	-2.52	1.34	1.39
1	2	1466	4AC	C4-N3	-2.51	1.28	1.32
1	2	52	OMU	C2-N3	-2.50	1.33	1.38
1	2	1061	OMG	C6-N1	-2.49	1.34	1.38
1	2	337	OMG	C5-N7	-2.44	1.34	1.39
1	2	1018	OMG	C5-N7	-2.43	1.34	1.39
1	2	494	A2M	C8-N7	2.43	1.36	1.31
1	2	399	OMG	C5-N7	-2.41	1.34	1.39
1	2	1344	OMU	C2-N3	-2.40	1.33	1.38
1	2	672	OMG	C5-N7	-2.38	1.34	1.39
1	2	546	OMG	C5-N7	-2.35	1.34	1.39
1	2	926	OMG	C5-N7	-2.35	1.34	1.39
1	2	1478	4AC	C4-N3	-2.35	1.28	1.32
1	2	1061	OMG	C5-N7	-2.34	1.34	1.39
1	2	1457	6MZ	C5-N7	-2.30	1.34	1.39
1	2	52	OMU	C5-C4	-2.27	1.38	1.43
1	2	15	OMU	C5-C4	-2.27	1.38	1.43
1	2	905	OMG	C5-N7	-2.26	1.34	1.39
1	2	1457	6MZ	C4-N9	-2.24	1.32	1.37
1	2	1475	MA6	C8-N7	2.24	1.35	1.31
1	2	546	OMG	C4-N9	-2.23	1.32	1.38
1	2	1344	OMU	C5-C4	-2.22	1.38	1.43
1	2	1032	OMU	C5-C4	-2.20	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1368	5MC	C6-C5	2.19	1.38	1.34
1	2	1475	MA6	C5-N7	-2.18	1.34	1.39
1	2	1477	4AC	C4-N3	-2.17	1.29	1.32
1	2	494	A2M	C5-N7	-2.17	1.34	1.39
1	2	481	OMC	C4-N4	2.16	1.39	1.33
1	2	246	OMC	C5-C4	-2.07	1.38	1.42
1	2	1061	OMG	C4-N9	-2.05	1.32	1.38
35	4	32	OMC	C6-N1	-2.04	1.33	1.38
1	2	1467	4AC	C4-N4	-2.02	1.36	1.39
1	2	337	OMG	C4-N9	-2.02	1.32	1.38

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1475	MA6	C5-C4-N3	-6.28	118.56	126.75
1	2	926	OMG	C5-C4-N3	-6.18	118.43	128.46
1	2	494	A2M	C5-C4-N3	-6.16	118.71	126.75
1	2	1018	OMG	C5-C4-N3	-6.13	118.51	128.46
1	2	865	OMG	C5-C4-N3	-6.11	118.55	128.46
1	2	1194	OMG	C5-C4-N3	-6.04	118.66	128.46
1	2	672	OMG	C5-C4-N3	-6.01	118.70	128.46
1	2	337	OMG	C5-C4-N3	-5.86	118.95	128.46
1	2	399	OMG	C5-C4-N3	-5.79	119.06	128.46
1	2	546	OMG	C5-C4-N3	-5.63	119.33	128.46
1	2	905	OMG	C5-C4-N3	-5.61	119.35	128.46
1	2	1061	OMG	C5-C4-N3	-5.58	119.40	128.46
1	2	1018	OMG	C2-N3-C4	5.29	121.72	112.30
1	2	1457	6MZ	C5-C4-N3	-5.25	119.90	126.75
1	2	1194	OMG	C2-N3-C4	4.99	121.18	112.30
1	2	672	OMG	C2-N3-C4	4.96	121.14	112.30
1	2	905	OMG	C2-N3-C4	4.95	121.12	112.30
1	2	1457	6MZ	C6-C5-N7	4.92	137.71	132.39
1	2	843	4AC	O7-C7-N4	4.90	129.75	121.82
1	2	1475	MA6	N3-C4-N9	4.90	135.15	127.08
1	2	399	OMG	C2-N3-C4	4.89	121.02	112.30
1	2	926	OMG	C2-N3-C4	4.89	121.02	112.30
1	2	337	OMG	C2-N3-C4	4.87	120.97	112.30
1	2	865	OMG	C2-N3-C4	4.81	120.88	112.30
1	2	494	A2M	N3-C4-N9	4.77	134.94	127.08
1	2	1061	OMG	C2-N3-C4	4.74	120.74	112.30
1	2	15	OMU	C4-N3-C2	-4.72	120.35	126.58
1	2	865	OMG	N9-C4-N3	4.67	135.32	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	15	OMU	C5-C4-N3	4.65	121.80	114.84
1	2	546	OMG	C2-N3-C4	4.64	120.58	112.30
1	2	1018	OMG	N9-C4-N3	4.62	135.22	125.94
1	2	481	OMC	C6-C5-C4	4.61	124.95	117.50
1	2	926	OMG	N9-C4-N3	4.60	135.17	125.94
1	2	1478	4AC	O7-C7-N4	4.50	129.09	121.82
1	2	52	OMU	C4-N3-C2	-4.47	120.68	126.58
1	2	1194	OMG	N9-C4-N3	4.45	134.87	125.94
1	2	1032	OMU	C4-N3-C2	-4.44	120.72	126.58
1	2	1344	OMU	C4-N3-C2	-4.39	120.79	126.58
1	2	399	OMG	N9-C4-N3	4.39	134.75	125.94
1	2	672	OMG	N9-C4-N3	4.36	134.70	125.94
1	2	337	OMG	N9-C4-N3	4.25	134.47	125.94
1	2	905	OMG	N9-C4-N3	4.25	134.47	125.94
1	2	1475	MA6	C2-N1-C6	4.23	121.73	111.75
1	2	1061	OMG	N9-C4-N3	4.21	134.40	125.94
1	2	481	OMC	C5-C4-N3	-4.18	114.21	121.33
1	2	1032	OMU	N3-C2-N1	4.18	120.44	114.89
1	2	546	OMG	N9-C4-N3	4.10	134.18	125.94
1	2	52	OMU	N3-C2-N1	4.08	120.30	114.89
1	2	1457	6MZ	N1-C2-N3	-4.07	122.24	128.60
1	2	1467	4AC	O7-C7-N4	4.03	128.34	121.82
1	2	1457	6MZ	N3-C4-N9	3.98	133.64	127.08
1	2	15	OMU	N3-C2-N1	3.93	120.11	114.89
1	2	1457	6MZ	C2-N3-C4	3.92	121.02	111.75
1	2	1475	MA6	C2-N3-C4	3.91	120.99	111.75
1	2	1344	OMU	N3-C2-N1	3.89	120.05	114.89
1	2	1475	MA6	N1-C6-N6	3.88	121.33	117.08
1	2	494	A2M	C2-N3-C4	3.87	120.89	111.75
1	2	1466	4AC	O7-C7-N4	3.86	128.07	121.82
1	2	1344	OMU	C5-C4-N3	3.77	120.48	114.84
1	2	52	OMU	C5-C4-N3	3.73	120.41	114.84
1	2	1032	OMU	C5-C4-N3	3.71	120.40	114.84
1	2	1457	6MZ	C4-C5-N7	-3.67	106.15	110.62
1	2	1477	4AC	C5-C4-N4	-3.64	116.59	122.92
1	2	905	OMG	C6-C5-N7	3.58	136.91	130.25
1	2	337	OMG	C6-C5-N7	3.56	136.86	130.25
1	2	1477	4AC	O7-C7-N4	3.51	127.50	121.82
1	2	672	OMG	C6-C5-N7	3.46	136.68	130.25
1	2	1477	4AC	N4-C4-N3	3.45	119.65	113.85
1	2	546	OMG	C6-C5-N7	3.45	136.66	130.25
1	2	399	OMG	C6-C5-N7	3.40	136.57	130.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1194	OMG	C6-C5-N7	3.39	136.56	130.25
1	2	1018	OMG	C6-C5-N7	3.36	136.50	130.25
1	2	494	A2M	C4-C5-N7	-3.32	106.58	110.62
1	2	1061	OMG	C6-C5-N7	3.30	136.39	130.25
1	2	1344	OMU	O4-C4-C5	-3.30	119.36	125.16
1	2	1475	MA6	C4-C5-N7	-3.23	106.69	110.62
1	2	52	OMU	O4-C4-C5	-3.21	119.52	125.16
1	2	1475	MA6	N1-C2-N3	-3.18	123.62	128.60
1	2	494	A2M	N3-C2-N1	-3.16	123.66	128.60
1	2	926	OMG	C6-C5-N7	3.15	136.10	130.25
1	2	865	OMG	C6-C5-N7	3.14	136.09	130.25
1	2	1457	6MZ	C5-N7-C8	3.04	107.83	103.51
1	2	481	OMC	N1-C2-N3	2.93	124.15	118.81
1	2	481	OMC	O2-C2-N3	-2.91	117.60	122.33
1	2	1368	5MC	C5-C6-N1	-2.87	120.38	123.34
1	2	1466	4AC	N4-C4-N3	2.85	118.64	113.85
1	2	337	OMG	C4-C5-N7	-2.83	106.24	110.72
1	2	246	OMC	O2-C2-N3	-2.83	117.74	122.33
1	2	494	A2M	C5-N7-C8	2.82	107.52	103.51
1	2	1457	6MZ	C4-N9-C8	2.82	108.79	105.73
1	2	1194	OMG	C4-C5-N7	-2.82	106.26	110.72
1	2	1478	4AC	CM7-C7-N4	-2.77	110.51	115.29
1	2	481	OMC	C6-N1-C2	-2.76	115.71	120.49
1	2	481	OMC	N4-C4-N3	2.75	122.80	117.97
1	2	672	OMG	C4-C5-N7	-2.74	106.39	110.72
35	4	32	OMC	O2-C2-N3	-2.73	117.88	122.33
1	2	1475	MA6	C5-N7-C8	2.72	107.38	103.51
1	2	1344	OMU	C1'-N1-C2	2.71	122.48	117.57
1	2	926	OMG	C4-C5-N7	-2.68	106.48	110.72
1	2	1032	OMU	O4-C4-C5	-2.67	120.46	125.16
1	2	1467	4AC	CM7-C7-N4	-2.64	110.72	115.29
1	2	843	4AC	CM7-C7-N4	-2.64	110.73	115.29
1	2	399	OMG	C4-C5-N7	-2.64	106.55	110.72
1	2	546	OMG	C4-C5-N7	-2.63	106.55	110.72
1	2	494	A2M	C4-N9-C8	2.62	108.56	105.73
1	2	843	4AC	N4-C4-N3	2.62	118.24	113.85
1	2	843	4AC	C5-C4-N4	-2.59	118.42	122.92
1	2	905	OMG	C2'-C1'-N9	-2.58	109.21	114.22
1	2	1368	5MC	C5-C4-N3	-2.55	118.92	121.67
1	2	1194	OMG	O6-C6-C5	-2.55	119.84	126.60
1	2	865	OMG	C4-C5-N7	-2.53	106.71	110.72
1	2	1457	6MZ	C2-N1-C6	2.52	123.72	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	1475	MA6	C5-C6-N6	-2.52	120.92	125.30
1	2	1018	OMG	C4-C5-N7	-2.51	106.74	110.72
1	2	1061	OMG	C4-C5-N7	-2.49	106.78	110.72
1	2	1478	4AC	N4-C4-N3	2.48	118.01	113.85
1	2	905	OMG	C4-C5-N7	-2.47	106.81	110.72
1	2	1475	MA6	C4-N9-C8	2.47	108.41	105.73
1	2	15	OMU	O4-C4-C5	-2.46	120.84	125.16
1	2	1018	OMG	O6-C6-C5	-2.45	120.10	126.60
1	2	1467	4AC	C5-C4-N4	-2.43	118.69	122.92
1	2	1466	4AC	C5-C4-N4	-2.41	118.73	122.92
35	4	32	OMC	C1'-N1-C2	2.38	123.73	118.42
1	2	1477	4AC	CM7-C7-N4	-2.37	111.20	115.29
1	2	1478	4AC	C5-C4-N4	-2.32	118.89	122.92
1	2	1457	6MZ	N9-C8-N7	-2.30	110.77	113.91
1	2	865	OMG	O6-C6-C5	-2.29	120.52	126.60
1	2	1061	OMG	O6-C6-C5	-2.27	120.58	126.60
1	2	494	A2M	C6-C5-N7	2.23	136.17	132.02
1	2	546	OMG	O6-C6-C5	-2.18	120.82	126.60
1	2	905	OMG	O6-C6-C5	-2.18	120.82	126.60
1	2	1018	OMG	C5-C6-N1	2.16	118.67	113.19
1	2	494	A2M	N9-C8-N7	-2.13	111.00	113.91
1	2	337	OMG	C2'-C1'-N9	-2.13	110.09	114.22
1	2	926	OMG	O6-C6-C5	-2.13	120.96	126.60
1	2	1467	4AC	N4-C4-N3	2.12	117.42	113.85
1	2	1194	OMG	C8-N7-C5	2.10	108.04	104.24
1	2	399	OMG	O6-C6-C5	-2.09	121.05	126.60
1	2	1366	OMC	O2-C2-N3	-2.07	118.97	122.33
1	2	337	OMG	O6-C6-C5	-2.06	121.12	126.60
1	2	710	OMC	O2-C2-N3	-2.05	119.00	122.33
1	2	538	OMC	O2-C2-N3	-2.04	119.01	122.33
1	2	905	OMG	C5-C6-N1	2.03	118.33	113.19
1	2	1475	MA6	C2'-C1'-N9	-2.03	108.17	113.30

There are no chirality outliers.

All (13) 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'
1	2	930	C4J	C4'-C5'-O5'-P
1	2	930	C4J	C3'-C4'-C5'-O5'
1	2	930	C4J	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	2	865	OMG	C4'-C5'-O5'-P
1	2	337	OMG	C4'-C5'-O5'-P
35	4	32	OMC	C2'-C1'-N1-C6
1	2	865	OMG	C3'-C4'-C5'-O5'
1	2	494	A2M	C3'-C2'-O2'-CM'
35	4	32	OMC	C2'-C1'-N1-C2
35	4	32	OMC	C3'-C2'-O2'-CM2
1	2	246	OMC	C2'-C1'-N1-C2

There are no ring outliers.

21 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1344	OMU	3	0
1	2	481	OMC	3	0
1	2	52	OMU	1	0
1	2	1477	4AC	2	0
1	2	672	OMG	1	0
1	2	1475	MA6	1	0
1	2	1368	5MC	1	0
1	2	905	OMG	2	0
1	2	113	OMC	2	0
1	2	1478	4AC	2	0
1	2	337	OMG	3	0
1	2	865	OMG	3	0
1	2	930	C4J	2	0
1	2	1466	4AC	1	0
1	2	1060	OMC	2	0
1	2	1032	OMU	1	0
1	2	246	OMC	2	0
1	2	843	4AC	1	0
1	2	538	OMC	2	0
1	2	1467	4AC	1	0
35	4	32	OMC	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 111 ligands modelled in this entry, 67 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	$\# Z > 2$
37	SPM	2	1589	-	13,13,13	0.11	0	12,12,12	0.08	0
37	SPM	2	1560	-	13,13,13	0.12	0	12,12,12	0.11	0
37	SPM	2	1575	-	13,13,13	0.12	0	12,12,12	0.07	0
37	SPM	2	1576	-	13,13,13	0.11	0	12,12,12	0.07	0
37	SPM	2	1599	-	13,13,13	0.10	0	12,12,12	0.21	0
37	SPM	2	1598	-	13,13,13	0.12	0	12,12,12	0.07	0
37	SPM	F	303	-	13,13,13	0.09	0	12,12,12	0.21	0
37	SPM	2	1580	-	13,13,13	0.11	0	12,12,12	0.13	0
37	SPM	2	1597	-	13,13,13	0.16	0	12,12,12	0.14	0
37	SPM	2	1581	-	13,13,13	0.10	0	12,12,12	0.07	0
37	SPM	2	1591	-	13,13,13	0.06	0	12,12,12	0.13	0
37	SPM	2	1565	-	13,13,13	0.07	0	12,12,12	0.22	0
37	SPM	2	1566	-	13,13,13	0.09	0	12,12,12	0.08	0
37	SPM	2	1571	-	13,13,13	0.09	0	12,12,12	0.13	0
37	SPM	2	1573	-	13,13,13	0.07	0	12,12,12	0.13	0
37	SPM	2	1559	-	13,13,13	0.08	0	12,12,12	0.30	0
37	SPM	2	1578	-	13,13,13	0.10	0	12,12,12	0.09	0
37	SPM	2	1574	-	13,13,13	0.07	0	12,12,12	0.23	0
37	SPM	2	1588	1	13,13,13	0.12	0	12,12,12	0.14	0
37	SPM	2	1568	-	13,13,13	0.11	0	12,12,12	0.08	0
37	SPM	2	1594	-	13,13,13	0.11	0	12,12,12	0.05	0
37	SPM	2	1570	-	13,13,13	0.10	0	12,12,12	0.07	0
37	SPM	2	1561	-	13,13,13	0.07	0	12,12,12	0.11	0
37	SPM	2	1562	-	13,13,13	0.06	0	12,12,12	0.11	0
37	SPM	2	1587	-	13,13,13	0.11	0	12,12,12	0.10	0
37	SPM	2	1584	-	13,13,13	0.16	0	12,12,12	0.30	0
37	SPM	2	1586	-	13,13,13	0.10	0	12,12,12	0.08	0
37	SPM	2	1569	-	13,13,13	0.12	0	12,12,12	0.32	0
37	SPM	2	1557	-	13,13,13	0.11	0	12,12,12	0.14	0
37	SPM	2	1579	-	13,13,13	0.12	0	12,12,12	0.29	0
37	SPM	2	1590	-	13,13,13	0.10	0	12,12,12	0.17	0
37	SPM	2	1582	-	13,13,13	0.10	0	12,12,12	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	SPM	2	1564	-	13,13,13	0.06	0	12,12,12	0.13	0
37	SPM	2	1567	-	13,13,13	0.06	0	12,12,12	0.18	0
37	SPM	2	1558	-	13,13,13	0.13	0	12,12,12	0.06	0
37	SPM	2	1592	-	13,13,13	0.12	0	12,12,12	0.06	0
37	SPM	2	1595	-	13,13,13	0.12	0	12,12,12	0.06	0
37	SPM	2	1572	-	13,13,13	0.10	0	12,12,12	0.28	0
37	SPM	2	1563	-	13,13,13	0.09	0	12,12,12	0.08	0
37	SPM	2	1596	-	13,13,13	0.10	0	12,12,12	0.08	0
37	SPM	2	1577	-	13,13,13	0.09	0	12,12,12	0.11	0
37	SPM	2	1583	-	13,13,13	0.11	0	12,12,12	0.08	0
37	SPM	2	1593	-	13,13,13	0.10	0	12,12,12	0.16	0
37	SPM	2	1585	-	13,13,13	0.09	0	12,12,12	0.12	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
37	SPM	2	1589	-	-	3/11/11/11	-
37	SPM	2	1560	-	-	3/11/11/11	-
37	SPM	2	1575	-	-	3/11/11/11	-
37	SPM	2	1576	-	-	4/11/11/11	-
37	SPM	2	1599	-	-	6/11/11/11	-
37	SPM	2	1598	-	-	3/11/11/11	-
37	SPM	F	303	-	-	3/11/11/11	-
37	SPM	2	1580	-	-	4/11/11/11	-
37	SPM	2	1597	-	-	2/11/11/11	-
37	SPM	2	1581	-	-	3/11/11/11	-
37	SPM	2	1591	-	-	3/11/11/11	-
37	SPM	2	1565	-	-	3/11/11/11	-
37	SPM	2	1566	-	-	2/11/11/11	-
37	SPM	2	1571	-	-	1/11/11/11	-
37	SPM	2	1573	-	-	5/11/11/11	-
37	SPM	2	1559	-	-	4/11/11/11	-
37	SPM	2	1578	-	-	4/11/11/11	-
37	SPM	2	1574	-	-	4/11/11/11	-
37	SPM	2	1588	1	-	4/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	SPM	2	1568	-	-	2/11/11/11	-
37	SPM	2	1594	-	-	3/11/11/11	-
37	SPM	2	1570	-	-	4/11/11/11	-
37	SPM	2	1561	-	-	5/11/11/11	-
37	SPM	2	1562	-	-	3/11/11/11	-
37	SPM	2	1587	-	-	2/11/11/11	-
37	SPM	2	1584	-	-	5/11/11/11	-
37	SPM	2	1586	-	-	3/11/11/11	-
37	SPM	2	1569	-	-	2/11/11/11	-
37	SPM	2	1557	-	-	2/11/11/11	-
37	SPM	2	1579	-	-	6/11/11/11	-
37	SPM	2	1590	-	-	4/11/11/11	-
37	SPM	2	1582	-	-	3/11/11/11	-
37	SPM	2	1564	-	-	3/11/11/11	-
37	SPM	2	1567	-	-	3/11/11/11	-
37	SPM	2	1558	-	-	3/11/11/11	-
37	SPM	2	1592	-	-	4/11/11/11	-
37	SPM	2	1595	-	-	0/11/11/11	-
37	SPM	2	1572	-	-	2/11/11/11	-
37	SPM	2	1563	-	-	3/11/11/11	-
37	SPM	2	1596	-	-	2/11/11/11	-
37	SPM	2	1577	-	-	3/11/11/11	-
37	SPM	2	1583	-	-	2/11/11/11	-
37	SPM	2	1593	-	-	4/11/11/11	-
37	SPM	2	1585	-	-	3/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (140) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	2	1562	SPM	C3-C4-N5-C6
37	2	1568	SPM	C8-C9-N10-C11
37	2	1574	SPM	C7-C6-N5-C4

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Mol	Chain	Res	Type	Atoms
37	2	1575	SPM	C3-C4-N5-C6
37	2	1576	SPM	C8-C9-N10-C11
37	2	1580	SPM	C3-C4-N5-C6
37	2	1581	SPM	C8-C9-N10-C11
37	2	1591	SPM	C3-C4-N5-C6
37	F	303	SPM	C7-C6-N5-C4
37	2	1599	SPM	N5-C6-C7-C8
37	2	1573	SPM	N10-C11-C12-C13
37	2	1560	SPM	C3-C4-N5-C6
37	2	1565	SPM	C8-C9-N10-C11
37	2	1567	SPM	C3-C4-N5-C6
37	2	1570	SPM	C3-C4-N5-C6
37	2	1575	SPM	C12-C11-N10-C9
37	2	1578	SPM	C8-C9-N10-C11
37	2	1579	SPM	C8-C9-N10-C11
37	2	1585	SPM	C7-C6-N5-C4
37	2	1592	SPM	C3-C4-N5-C6
37	2	1590	SPM	C2-C3-C4-N5
37	2	1562	SPM	C12-C11-N10-C9
37	2	1566	SPM	C7-C6-N5-C4
37	2	1582	SPM	C12-C11-N10-C9
37	2	1586	SPM	C7-C6-N5-C4
37	2	1587	SPM	C12-C11-N10-C9
37	2	1589	SPM	C8-C9-N10-C11
37	2	1598	SPM	C3-C4-N5-C6
37	2	1599	SPM	C3-C4-N5-C6
37	2	1599	SPM	C12-C11-N10-C9
37	2	1579	SPM	C6-C7-C8-C9
37	2	1558	SPM	C12-C11-N10-C9
37	2	1559	SPM	C7-C6-N5-C4
37	2	1559	SPM	C12-C11-N10-C9
37	2	1590	SPM	C7-C6-N5-C4
37	2	1592	SPM	C12-C11-N10-C9
37	2	1596	SPM	C12-C11-N10-C9
37	2	1557	SPM	C8-C9-N10-C11
37	2	1570	SPM	C7-C6-N5-C4
37	2	1575	SPM	C7-C6-N5-C4
37	2	1576	SPM	C12-C11-N10-C9
37	2	1578	SPM	C7-C6-N5-C4
37	2	1582	SPM	C7-C6-N5-C4
37	2	1583	SPM	C3-C4-N5-C6
37	2	1584	SPM	C8-C9-N10-C11

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Mol	Chain	Res	Type	Atoms
37	2	1590	SPM	C8-C9-N10-C11
37	2	1592	SPM	C7-C6-N5-C4
37	2	1559	SPM	N1-C2-C3-C4
37	2	1564	SPM	N1-C2-C3-C4
37	2	1569	SPM	C11-C12-C13-N14
37	2	1579	SPM	C11-C12-C13-N14
37	2	1593	SPM	C11-C12-C13-N14
37	2	1593	SPM	N5-C6-C7-C8
37	2	1560	SPM	C8-C9-N10-C11
37	2	1586	SPM	C3-C4-N5-C6
37	2	1586	SPM	C8-C9-N10-C11
37	2	1590	SPM	C6-C7-C8-C9
37	2	1572	SPM	C3-C4-N5-C6
37	2	1579	SPM	C3-C4-N5-C6
37	2	1593	SPM	C8-C9-N10-C11
37	2	1561	SPM	C8-C9-N10-C11
37	2	1563	SPM	C12-C11-N10-C9
37	2	1598	SPM	C7-C6-N5-C4
37	2	1562	SPM	C6-C7-C8-C9
37	2	1574	SPM	C3-C4-N5-C6
37	2	1560	SPM	C12-C11-N10-C9
37	2	1563	SPM	C3-C4-N5-C6
37	2	1573	SPM	C7-C6-N5-C4
37	2	1577	SPM	C3-C4-N5-C6
37	2	1580	SPM	C8-C9-N10-C11
37	2	1580	SPM	C12-C11-N10-C9
37	2	1583	SPM	C8-C9-N10-C11
37	2	1596	SPM	C3-C4-N5-C6
37	2	1584	SPM	C11-C12-C13-N14
37	2	1581	SPM	C3-C4-N5-C6
37	2	1584	SPM	C7-C6-N5-C4
37	2	1594	SPM	C8-C9-N10-C11
37	2	1561	SPM	C7-C6-N5-C4
37	2	1568	SPM	C7-C6-N5-C4
37	2	1570	SPM	C8-C9-N10-C11
37	2	1576	SPM	C3-C4-N5-C6
37	2	1577	SPM	C7-C6-N5-C4
37	2	1580	SPM	C7-C6-N5-C4
37	2	1582	SPM	C3-C4-N5-C6
37	2	1587	SPM	C3-C4-N5-C6
37	2	1565	SPM	C12-C11-N10-C9
37	2	1574	SPM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
37	2	1593	SPM	C6-C7-C8-C9
37	2	1585	SPM	C12-C11-N10-C9
37	2	1576	SPM	C6-C7-C8-C9
37	2	1599	SPM	N10-C11-C12-C13
37	2	1573	SPM	C3-C4-N5-C6
37	2	1574	SPM	C8-C9-N10-C11
37	2	1570	SPM	C12-C11-N10-C9
37	2	1588	SPM	C6-C7-C8-C9
37	2	1558	SPM	C8-C9-N10-C11
37	2	1564	SPM	C8-C9-N10-C11
37	2	1597	SPM	C12-C11-N10-C9
37	2	1598	SPM	C12-C11-N10-C9
37	2	1588	SPM	C7-C8-C9-N10
37	2	1561	SPM	N10-C11-C12-C13
37	2	1594	SPM	C6-C7-C8-C9
37	2	1573	SPM	C8-C9-N10-C11
37	2	1578	SPM	C3-C4-N5-C6
37	2	1581	SPM	C7-C6-N5-C4
37	2	1584	SPM	C12-C11-N10-C9
37	2	1592	SPM	C8-C9-N10-C11
37	2	1599	SPM	C8-C9-N10-C11
37	2	1558	SPM	C3-C4-N5-C6
37	2	1559	SPM	C3-C4-N5-C6
37	2	1567	SPM	C8-C9-N10-C11
37	2	1571	SPM	C7-C6-N5-C4
37	2	1561	SPM	C12-C11-N10-C9
37	2	1564	SPM	C3-C4-N5-C6
37	2	1565	SPM	C3-C4-N5-C6
37	2	1567	SPM	C7-C6-N5-C4
37	2	1578	SPM	C12-C11-N10-C9
37	2	1588	SPM	C7-C6-N5-C4
37	2	1589	SPM	C7-C6-N5-C4
37	2	1591	SPM	C7-C6-N5-C4
37	2	1591	SPM	C8-C9-N10-C11
37	2	1597	SPM	C7-C6-N5-C4
37	2	1579	SPM	N1-C2-C3-C4
37	2	1569	SPM	C8-C9-N10-C11
37	2	1584	SPM	C3-C4-N5-C6
37	2	1594	SPM	C12-C11-N10-C9
37	2	1599	SPM	C7-C6-N5-C4
37	F	303	SPM	C12-C11-N10-C9
37	2	1557	SPM	C7-C8-C9-N10

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Mol	Chain	Res	Type	Atoms
37	2	1589	SPM	C6-C7-C8-C9
37	2	1561	SPM	C3-C4-N5-C6
37	2	1563	SPM	C8-C9-N10-C11
37	2	1572	SPM	C12-C11-N10-C9
37	2	1573	SPM	C12-C11-N10-C9
37	2	1577	SPM	C8-C9-N10-C11
37	2	1579	SPM	C12-C11-N10-C9
37	2	1585	SPM	C3-C4-N5-C6
37	2	1588	SPM	C3-C4-N5-C6
37	2	1566	SPM	C12-C11-N10-C9
37	F	303	SPM	C7-C8-C9-N10

There are no ring outliers.

37 monomers are involved in 160 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	2	1589	SPM	10	0
37	2	1560	SPM	2	0
37	2	1575	SPM	5	0
37	2	1576	SPM	2	0
37	2	1599	SPM	3	0
37	F	303	SPM	11	0
37	2	1580	SPM	1	0
37	2	1597	SPM	2	0
37	2	1581	SPM	11	0
37	2	1591	SPM	3	0
37	2	1565	SPM	2	0
37	2	1566	SPM	6	0
37	2	1571	SPM	4	0
37	2	1573	SPM	2	0
37	2	1578	SPM	1	0
37	2	1574	SPM	1	0
37	2	1588	SPM	5	0
37	2	1568	SPM	5	0
37	2	1594	SPM	11	0
37	2	1570	SPM	11	0
37	2	1587	SPM	5	0
37	2	1584	SPM	14	0
37	2	1586	SPM	8	0
37	2	1569	SPM	3	0
37	2	1579	SPM	1	0
37	2	1582	SPM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	2	1564	SPM	2	0
37	2	1567	SPM	1	0
37	2	1558	SPM	8	0
37	2	1595	SPM	2	0
37	2	1572	SPM	5	0
37	2	1563	SPM	1	0
37	2	1596	SPM	1	0
37	2	1577	SPM	3	0
37	2	1583	SPM	8	0
37	2	1593	SPM	2	0
37	2	1585	SPM	4	0

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.

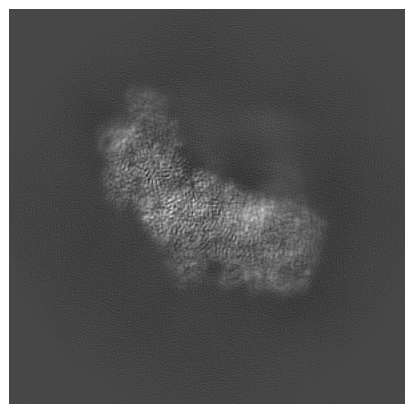
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50445. These allow visual inspection of the internal detail of the map and identification of artifacts.

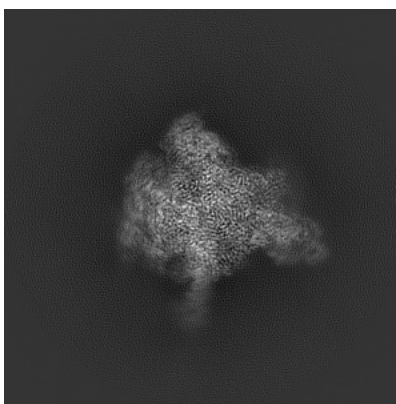
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

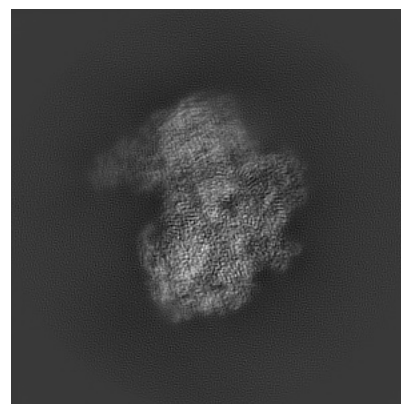
6.1.1 Primary map



X

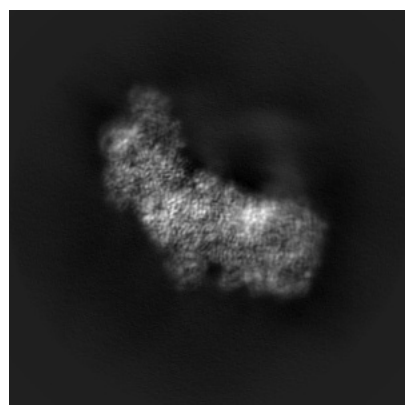


Y

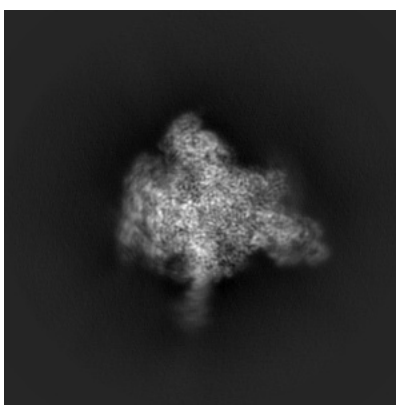


Z

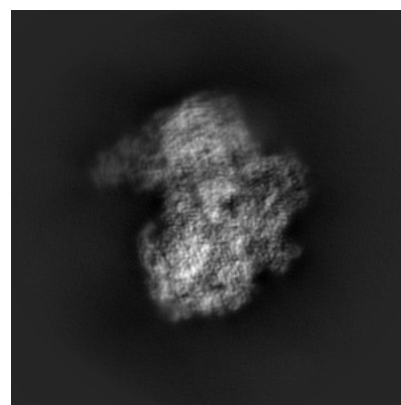
6.1.2 Raw map



X



Y

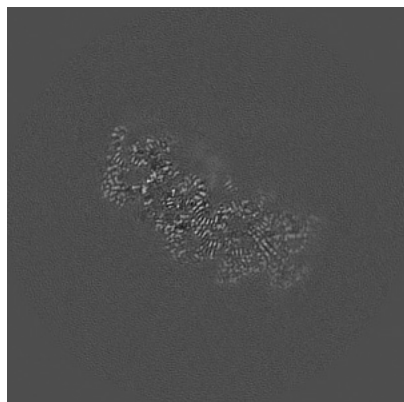


Z

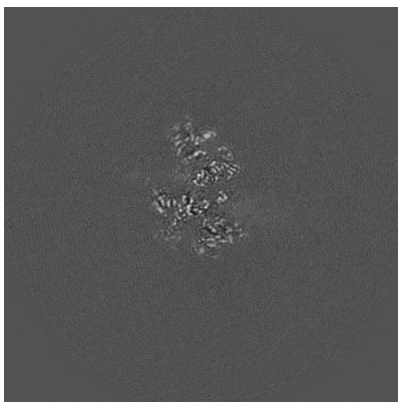
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

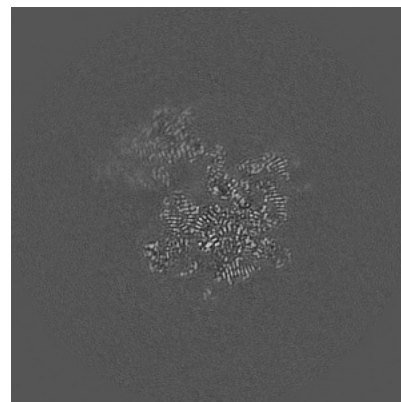
6.2.1 Primary map



X Index: 219

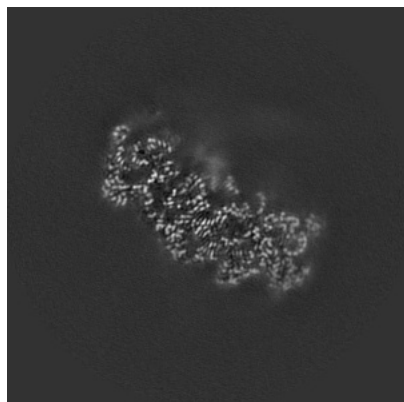


Y Index: 219

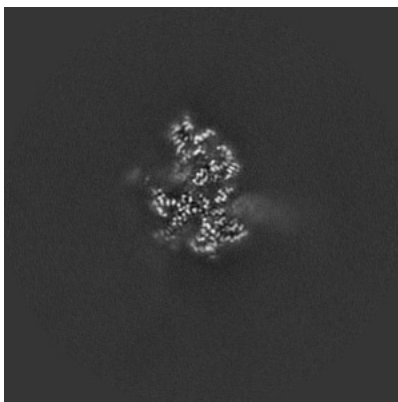


Z Index: 219

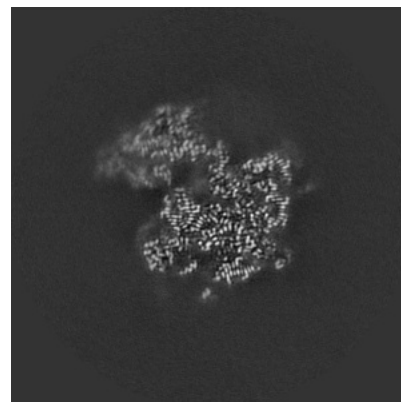
6.2.2 Raw map



X Index: 219



Y Index: 219

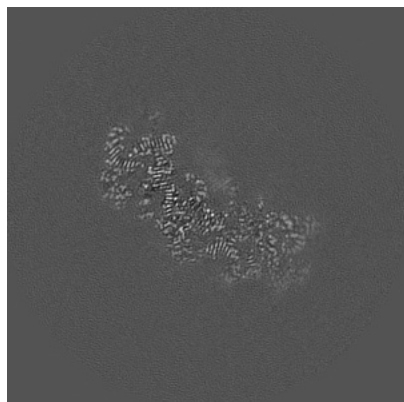


Z Index: 219

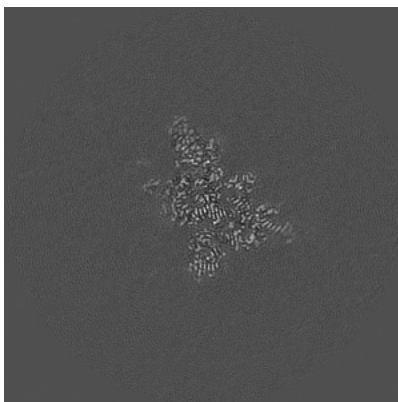
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

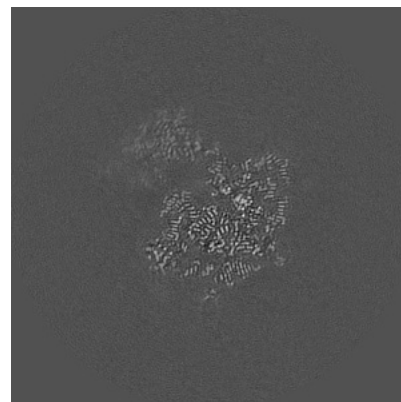
6.3.1 Primary map



X Index: 214

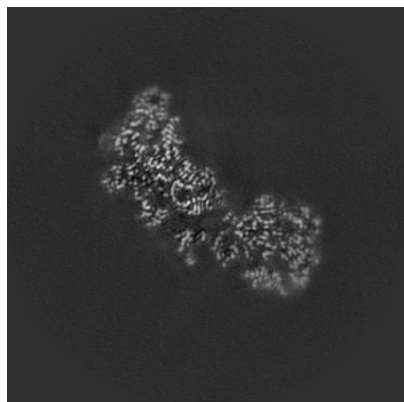


Y Index: 176

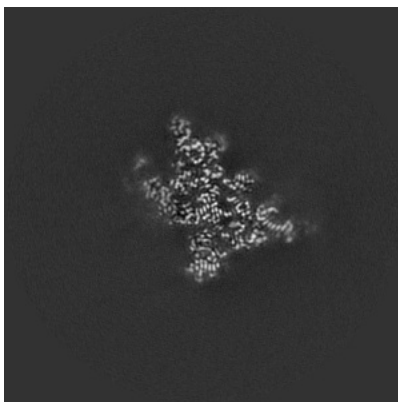


Z Index: 222

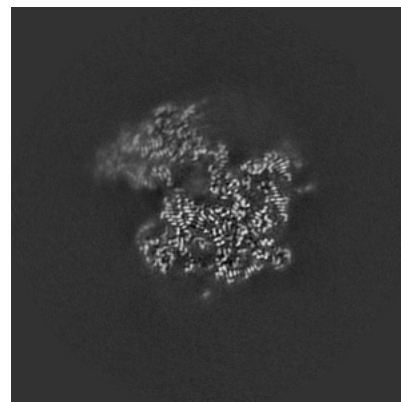
6.3.2 Raw map



X Index: 197



Y Index: 179

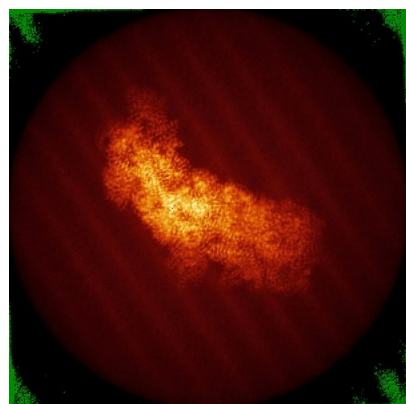


Z Index: 217

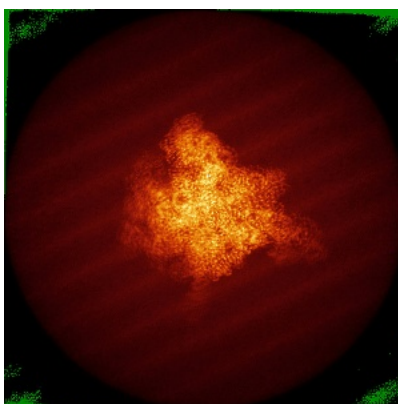
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

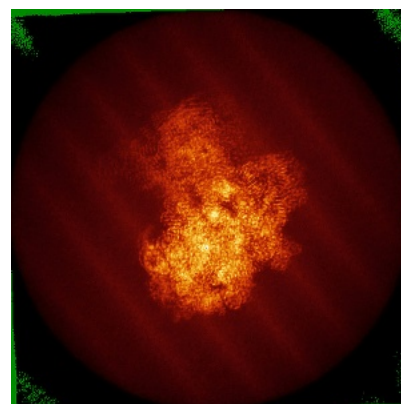
6.4.1 Primary map



X



Y

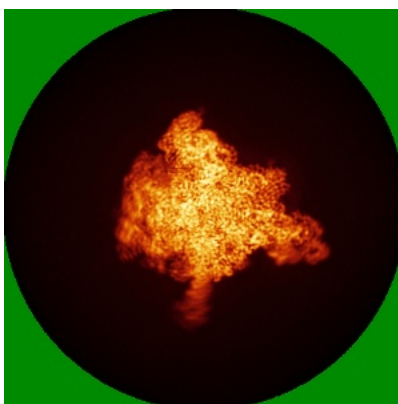


Z

6.4.2 Raw map



X



Y

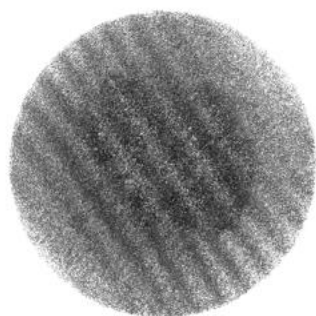


Z

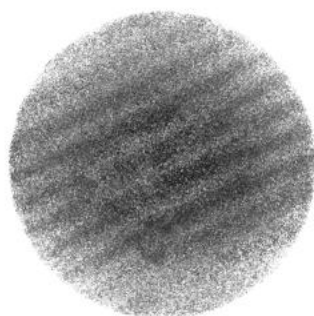
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

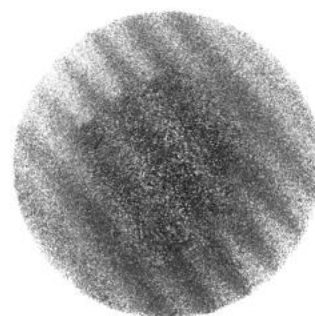
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. 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



X



Y



Z

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

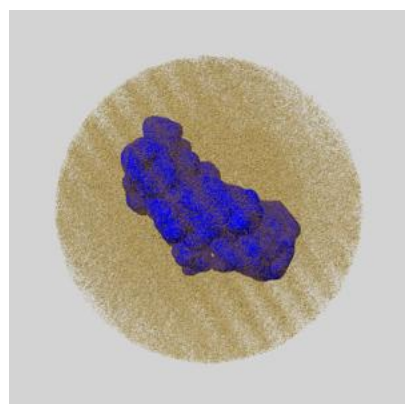
6.6 Mask visualisation [i](#)

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

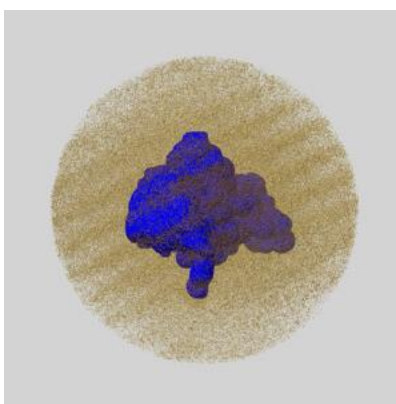
A mask typically either:

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

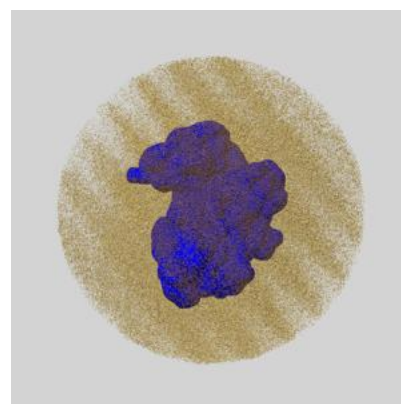
6.6.1 emd_50445_msk_1.map [i](#)



X



Y

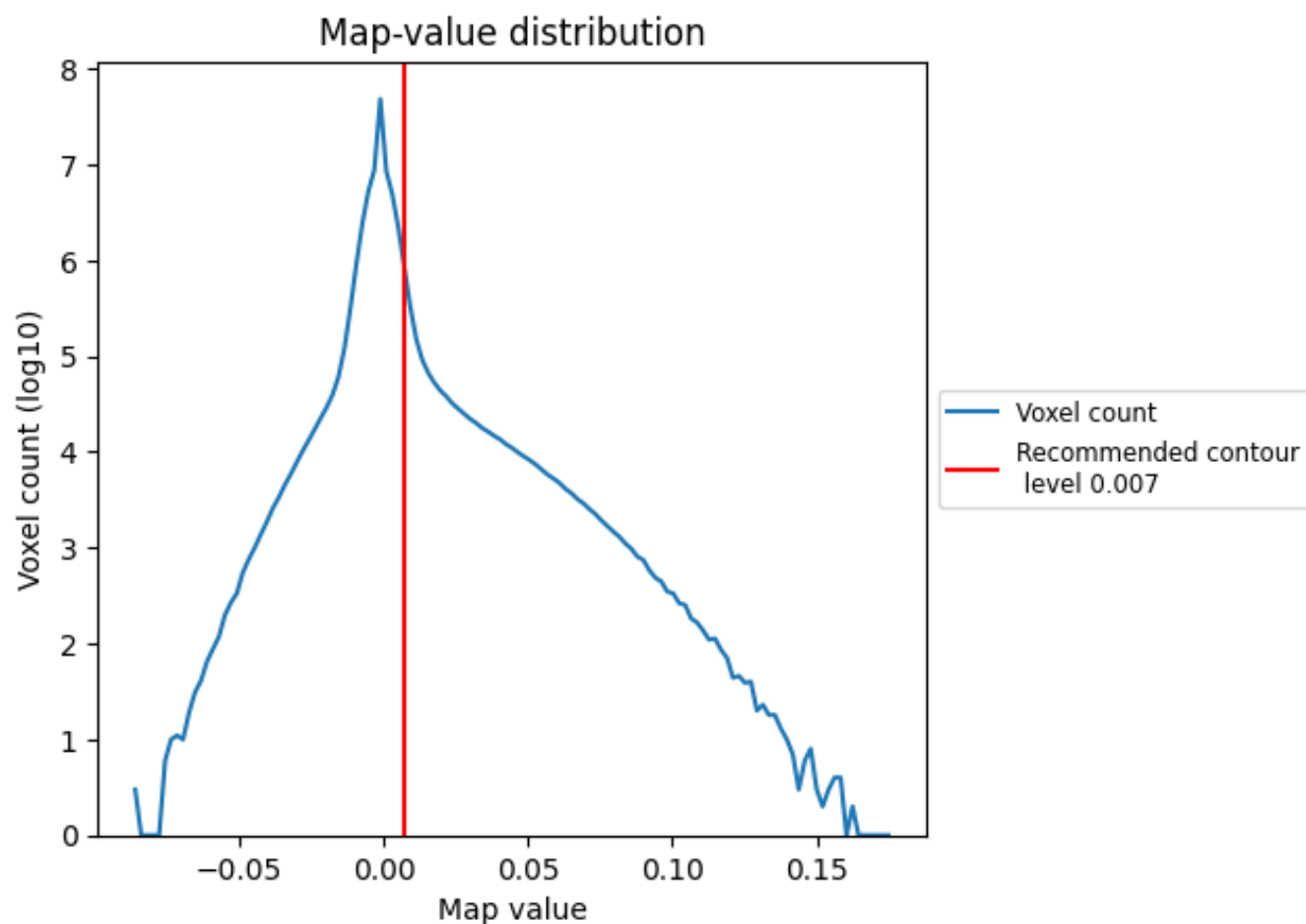


Z

7 Map analysis [i](#)

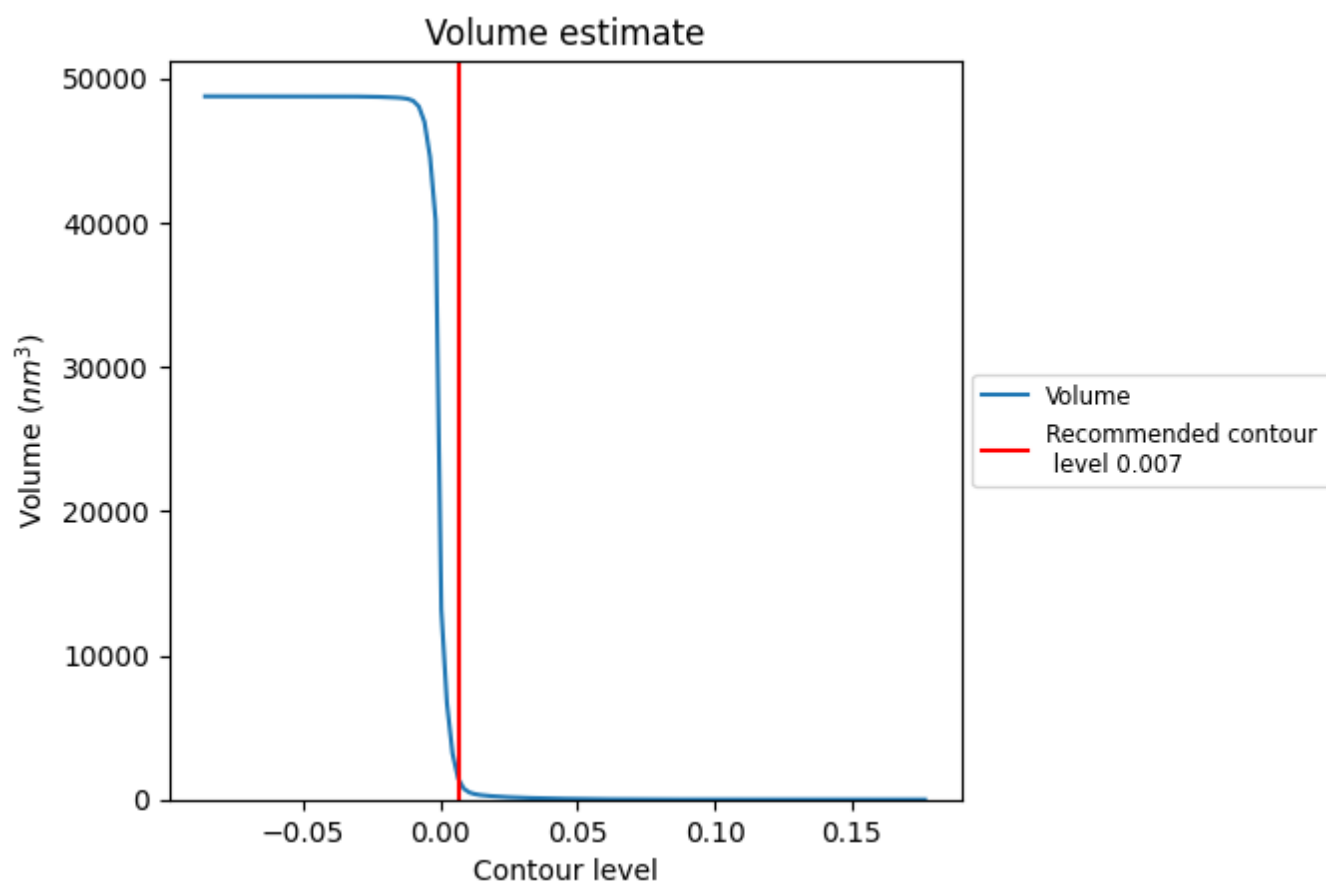
This section contains the results of statistical analysis of the map.

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.

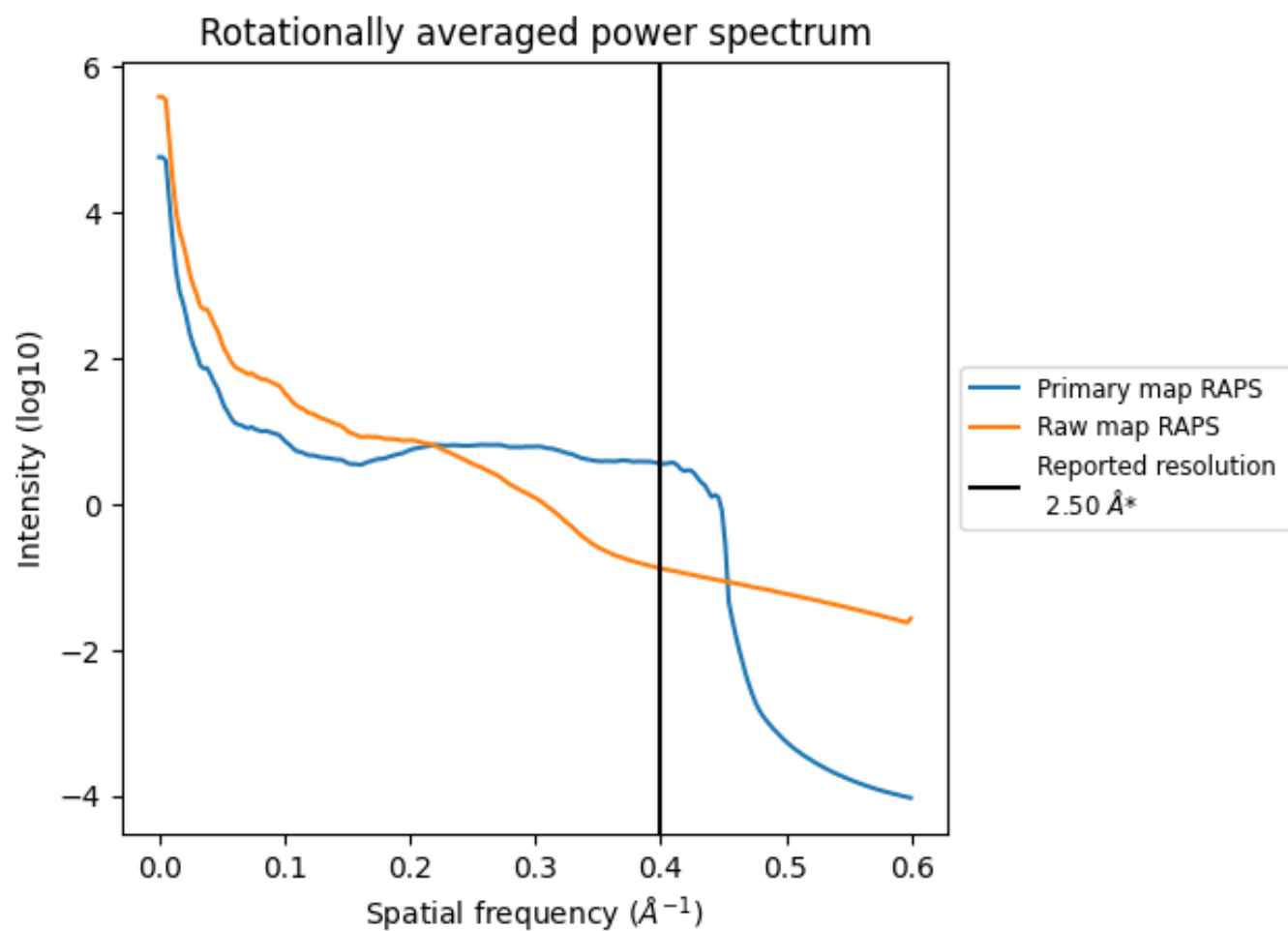
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1269 nm^3 ; this corresponds to an approximate mass of 1146 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 ⓘ

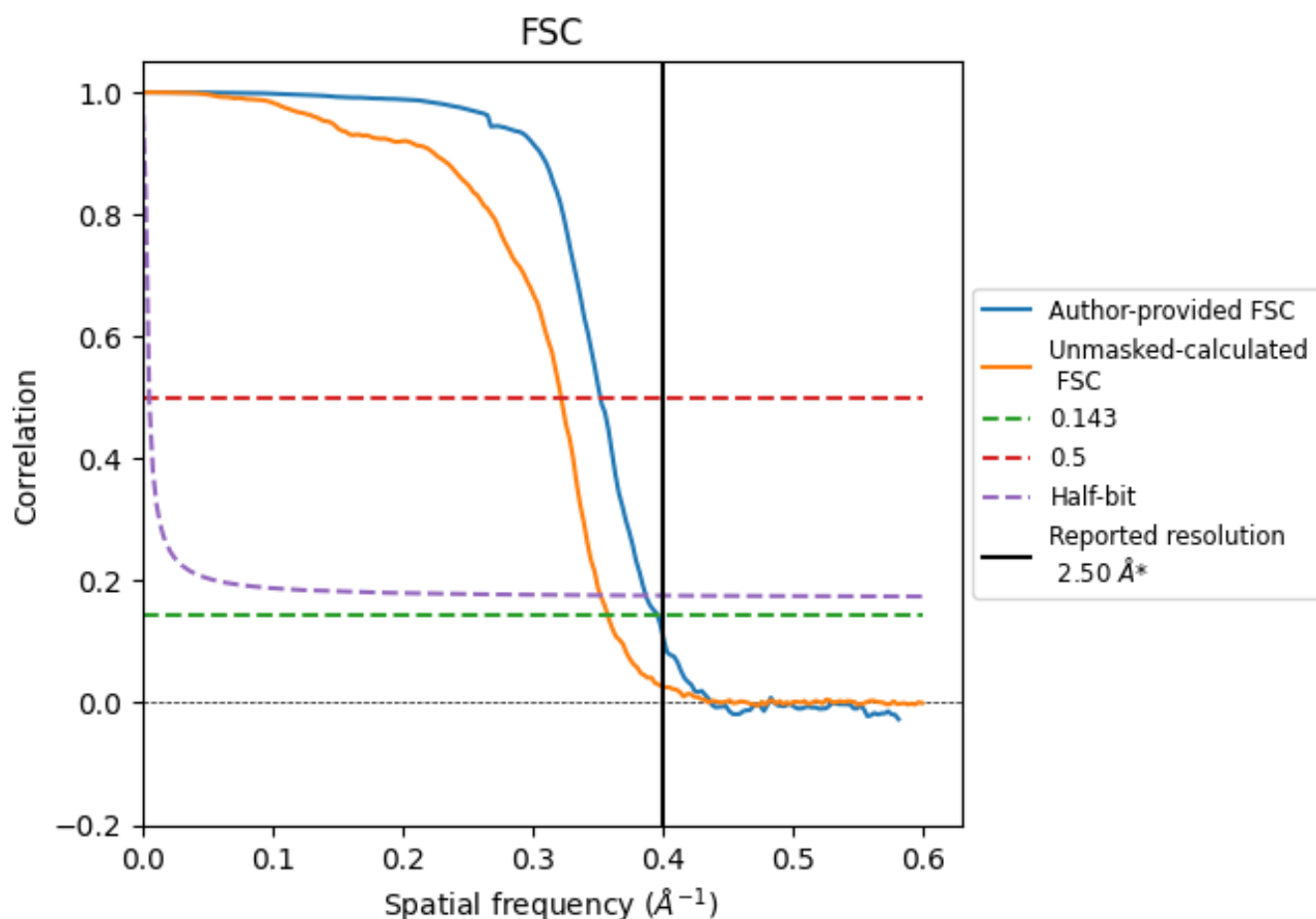


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

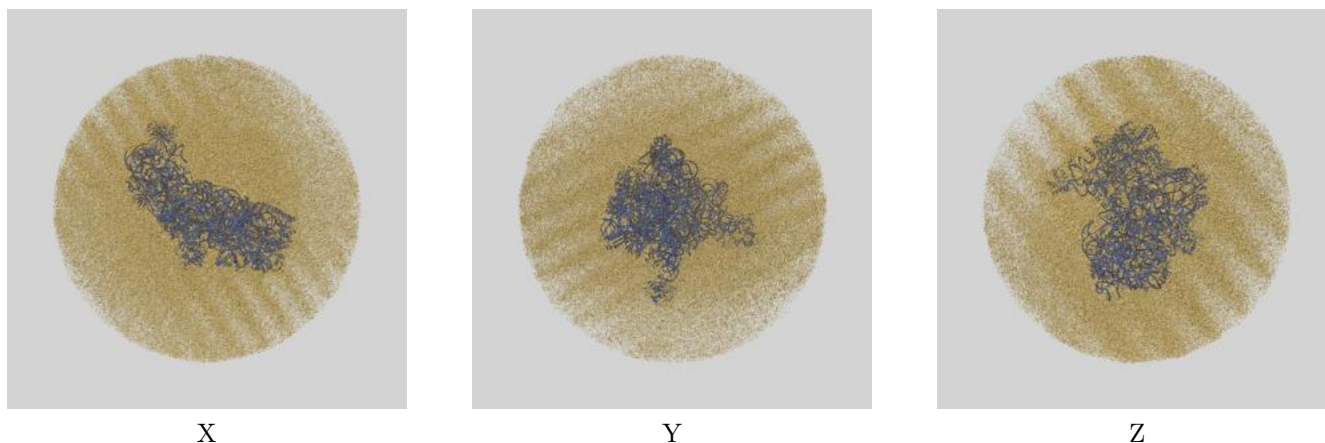
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.53	2.84	2.58
Unmasked-calculated*	2.79	3.10	2.84

*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 2.79 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

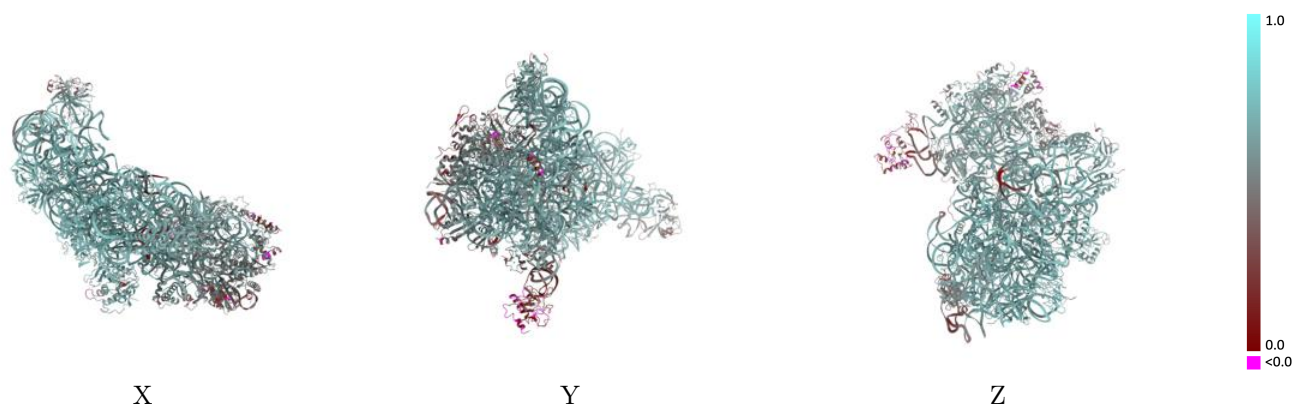
This section contains information regarding the fit between EMDB map EMD-50445 and PDB model 9FHL. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



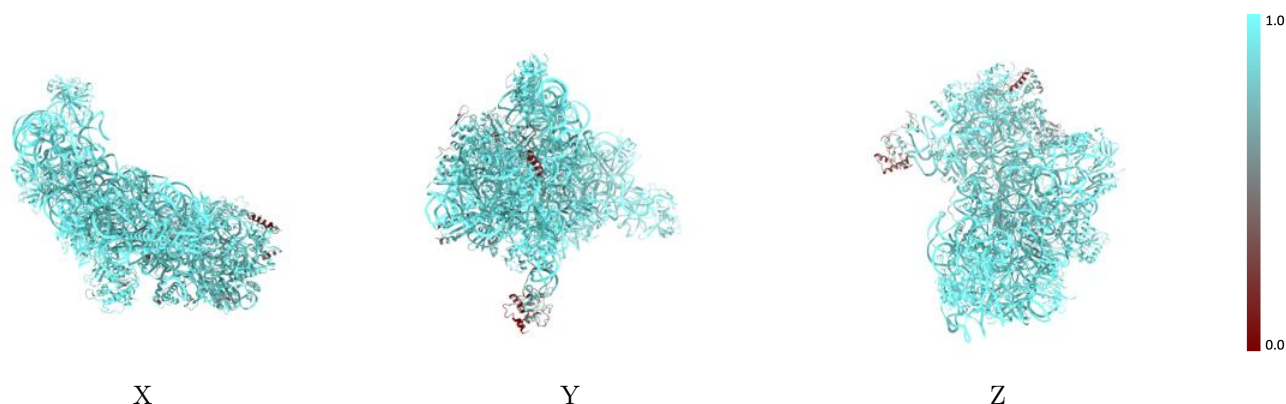
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



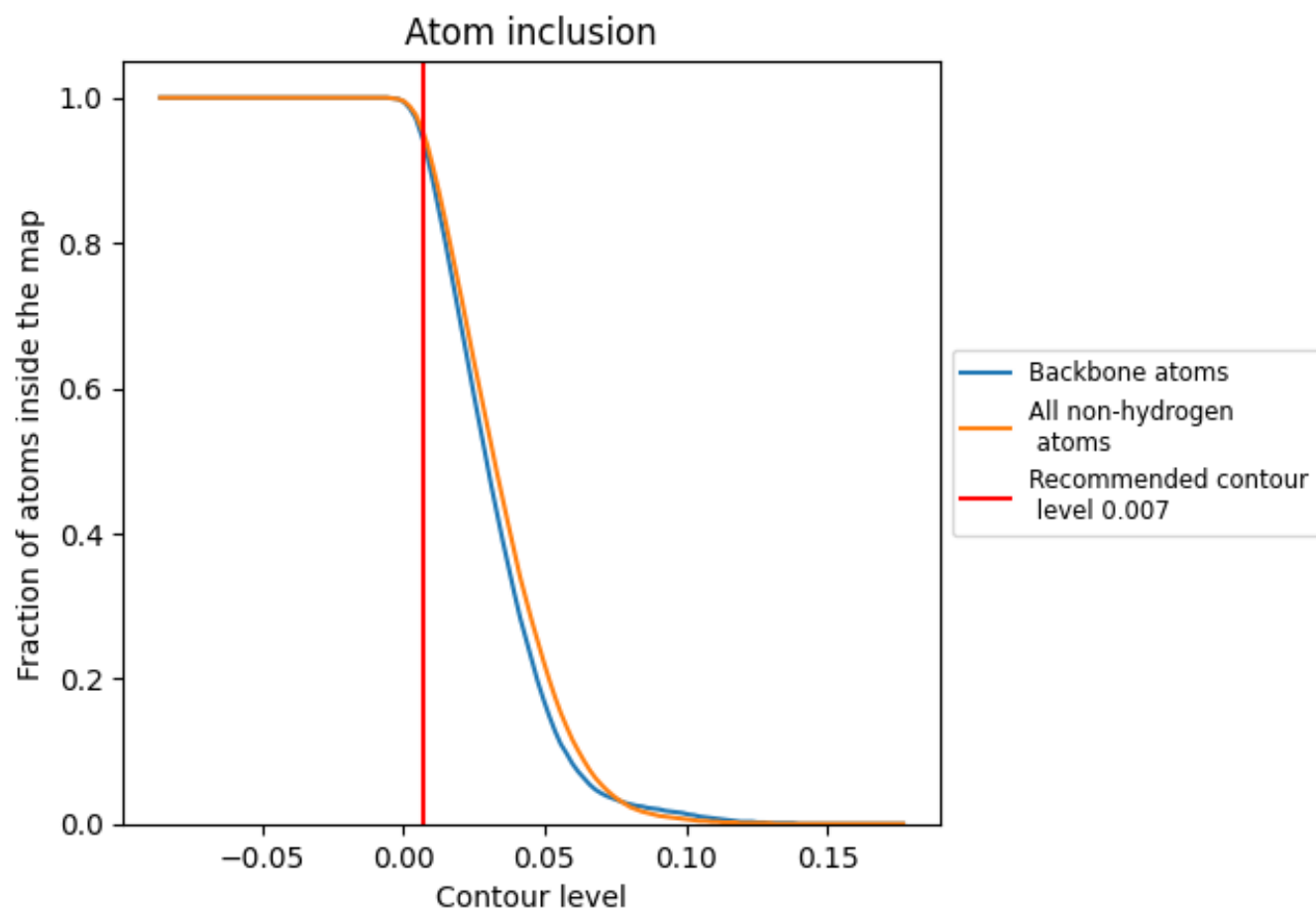
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.6120
2	 0.9880	 0.6460
3	 0.3310	 0.1370
4	 0.9950	 0.6270
5	 0.9870	 0.6710
A	 0.9710	 0.6080
B	 0.9610	 0.6180
C	 0.9840	 0.6550
D	 0.9890	 0.6810
E	 0.9960	 0.6880
F	 0.9870	 0.6870
G	 0.9310	 0.5190
H	 0.8860	 0.5060
I	 0.9950	 0.6990
J	 0.9840	 0.6660
K	 0.9260	 0.5510
L	 0.8730	 0.5130
M	 0.9730	 0.6110
N	 0.9790	 0.6690
O	 0.9490	 0.5800
P	 0.9760	 0.6480
Q	 0.9820	 0.6590
R	 0.9900	 0.6860
S	 0.9360	 0.5700
T	 0.9290	 0.5520
U	 0.9700	 0.5900
V	 0.9760	 0.6520
W	 0.9940	 0.6540
X	 0.8210	 0.4370
Y	 0.5090	 0.1660
Z	 0.9460	 0.5940
a	 0.9130	 0.5270
c	 0.6350	 0.3770
d	 0.7830	 0.3710
e	 0.8660	 0.5770
s	 0.5910	 0.1810

