



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 08:08 PM UTC

PDB ID : 5GAD / pdb_00005gad
EMDB ID : EMD-8000
Title : RNC-SRP-SR complex early state
Authors : Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.
Deposited on : 2015-11-24
Resolution : 3.70 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 : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

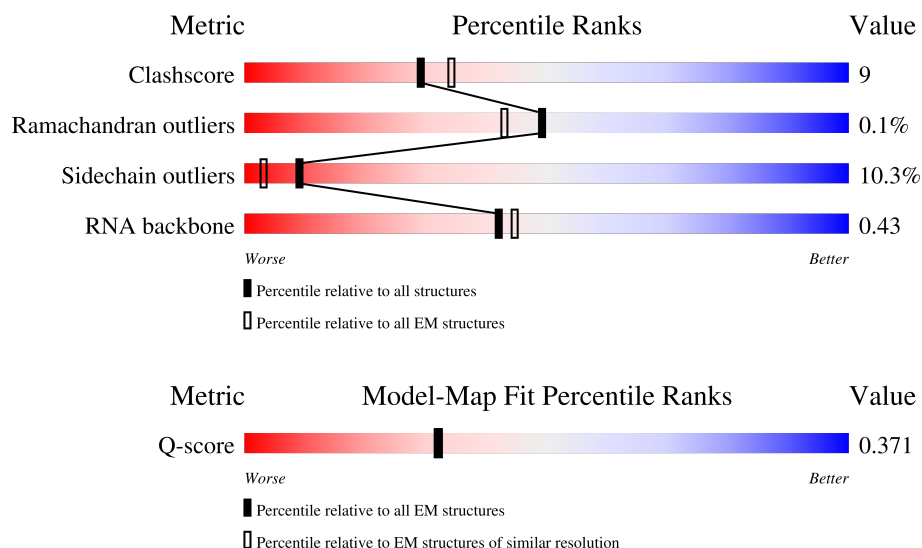
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.



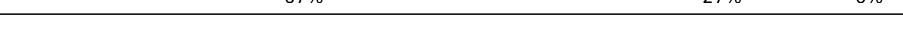
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	1	113	
2	2	3	
3	A	2903	

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Mol	Chain	Length	Quality of chain
4	B	120	
5	C	273	
6	D	209	
7	E	201	
8	F	179	
9	G	177	
10	H	149	
11	I	165	
12	J	142	
13	K	142	
14	L	123	
15	M	144	
16	N	136	
17	O	127	
18	P	117	
19	Q	115	
20	R	118	
21	S	103	
22	T	110	
23	U	100	
24	V	104	
25	W	94	
26	X	85	
27	Y	78	
28	Z	63	

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Mol	Chain	Length	Quality of chain
29	a	59	69%27%
30	b	57	54%33%11%
31	c	55	69%20%7%
32	d	46	67%28%
33	e	65	60%37%
34	f	38	71%21%8%
35	i	450	12%59%38%
36	k	18	11%28%72%
37	l	497	11%24%15%60%

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98006 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 ESRP 4.5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	43	Total	C	N	O	P	0	0
			926	413	174	296	43		

- Molecule 2 is a RNA chain called tRNA CCAend.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	2883	Total	C	N	O	P	0	0
			61902	27613	11397	20009	2883		

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	125	Total	C	N	O	S	0	0
			946	599	169	175	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	85	VAL	SER	conflict	UNP P0A7J3
I	86	THR	MET	conflict	UNP P0A7J3

- Molecule 12 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	134	Total	C	N	O	S	0	0
			979	619	169	185	6		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	V	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	51	Total	C	N	O	0	0
			414	266	76	72		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a protein called Signal recognition particle protein Ffh.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	450	Total	C	N	O	S	0	0
			3337	2109	600	610	18		

- Molecule 36 is a protein called 1A9L SS.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	18	Total	C	N	O	S	0	0
			137	94	20	22	1		

- Molecule 37 is a protein called Signal recognition particle receptor FtsY.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	198	Total	C	N	O	S	0	0
			1492	944	266	277	5		

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	2	1	Total	Mg	0
			1	1	
38	A	412	Total	Mg	0
			412	412	
38	B	11	Total	Mg	0
			11	11	
38	C	2	Total	Mg	0
			2	2	
38	D	1	Total	Mg	0
			1	1	
38	E	1	Total	Mg	0
			1	1	
38	P	1	Total	Mg	0
			1	1	
38	R	1	Total	Mg	0
			1	1	
38	b	1	Total	Mg	0
			1	1	

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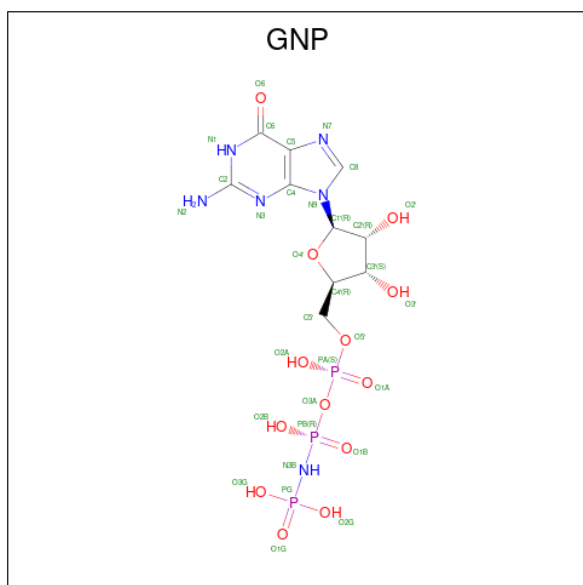
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Mol	Chain	Residues	Atoms		AltConf
38	i	1	Total	Mg	0
			1	1	
38	l	1	Total	Mg	0
			1	1	

- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
39	f	1	Total	Zn	0
			1	1	

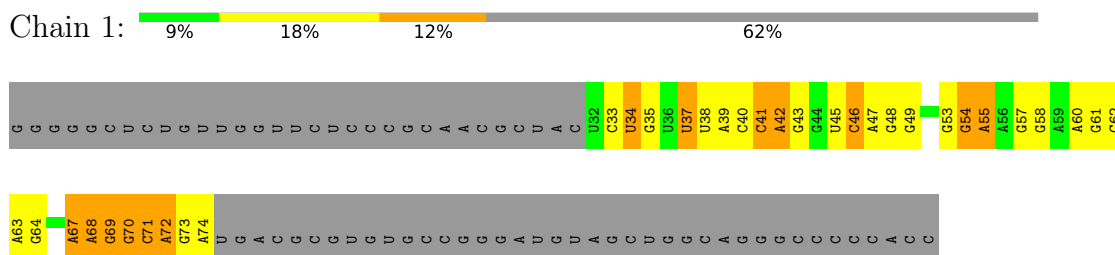
- Molecule 40 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



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.

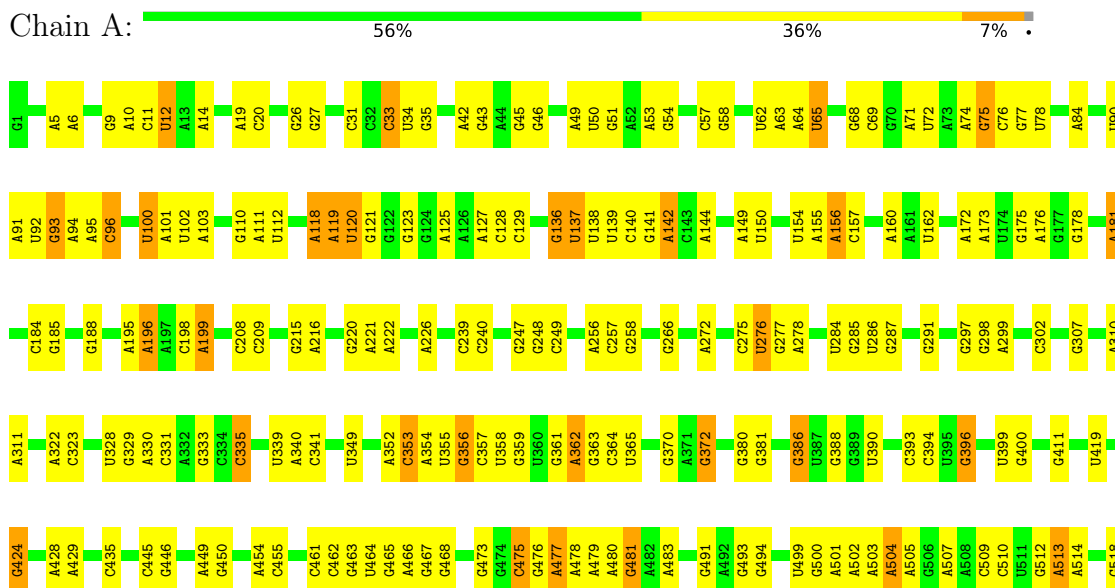
• Molecule 1: ESRP 4.5S RNA



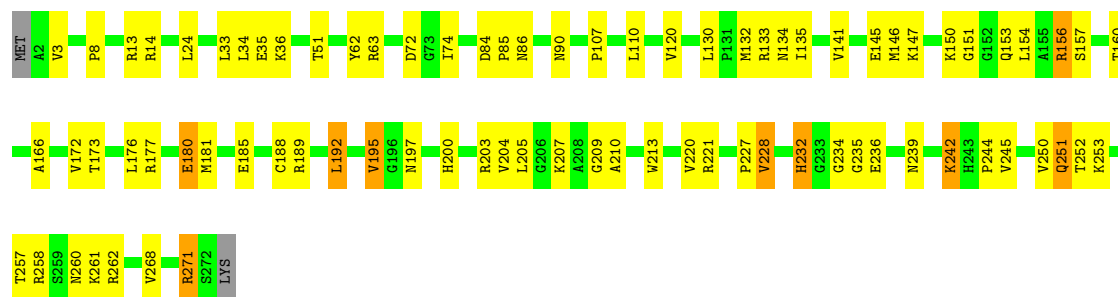
• Molecule 2: tRNA CCAend



• Molecule 3: 23S rRNA

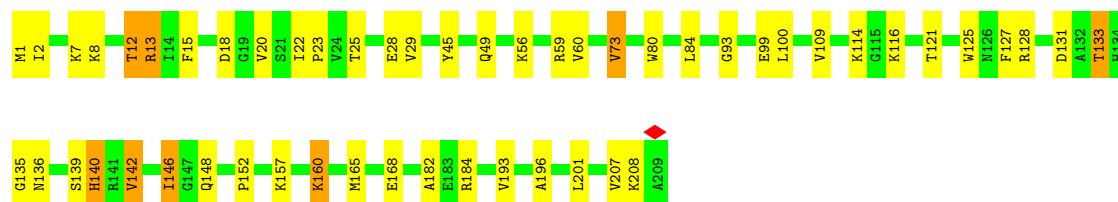






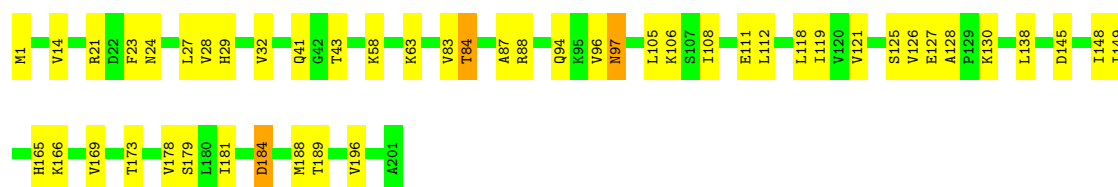
- Molecule 6: 50S ribosomal protein L3

Chain D: 75% 22% .



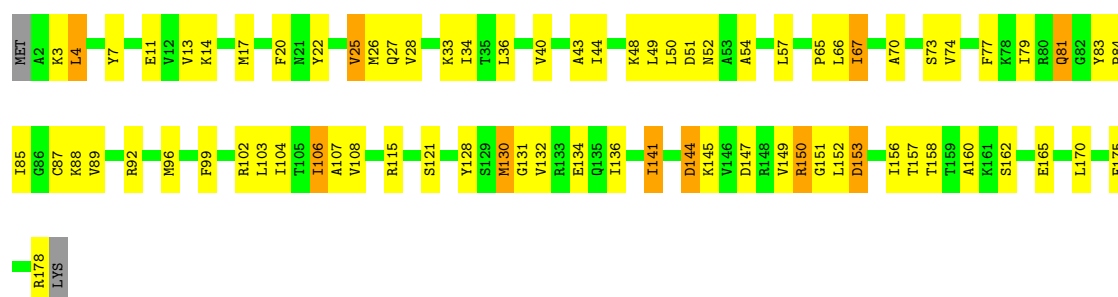
- Molecule 7: 50S ribosomal protein L4

Chain E: 76% 22% .



- Molecule 8: 50S ribosomal protein L5

Chain F: 56% 37% 6% .



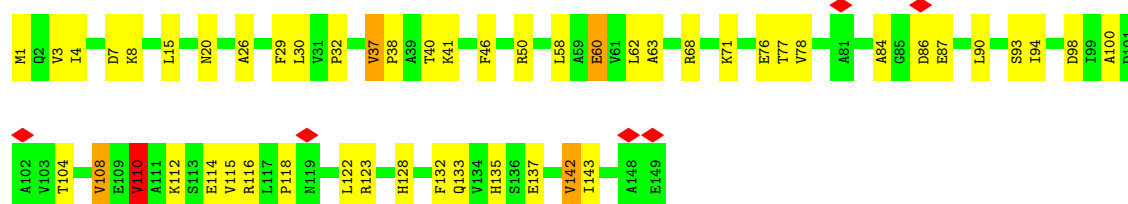
- Molecule 9: 50S ribosomal protein L6

Chain G: 67% 29% .

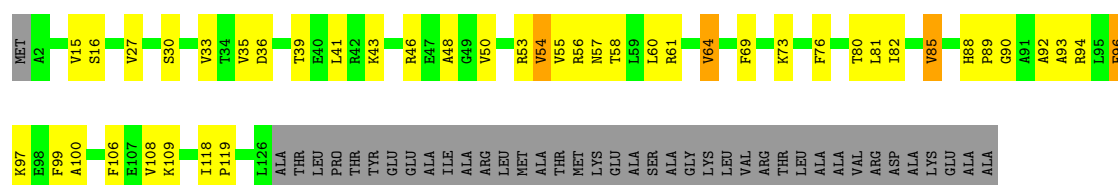




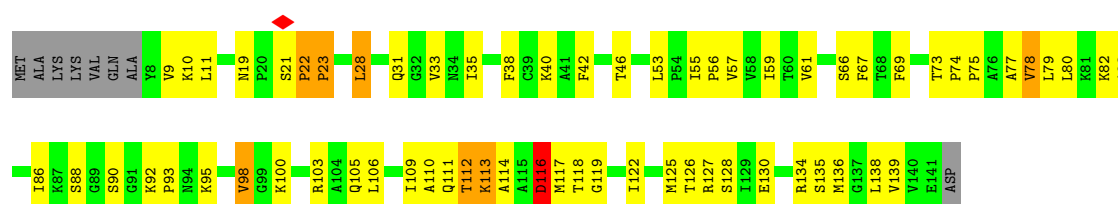
- Molecule 10: 50S ribosomal protein L9



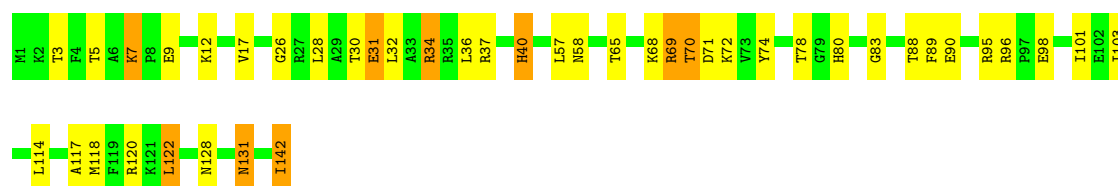
- Molecule 11: 50S ribosomal protein L10



- Molecule 12: 50S ribosomal protein L11

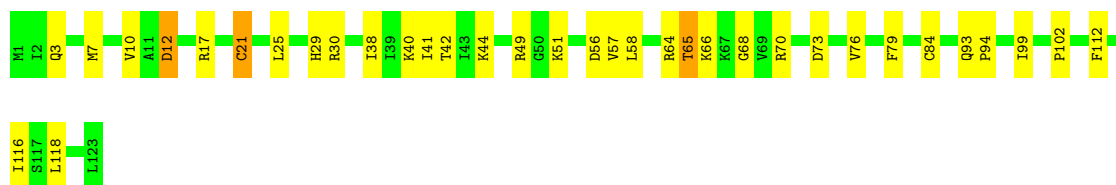


- Molecule 13: 50S ribosomal protein L13



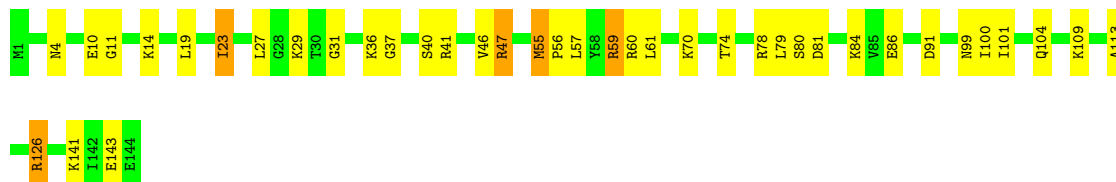
- Molecule 14: 50S ribosomal protein L14





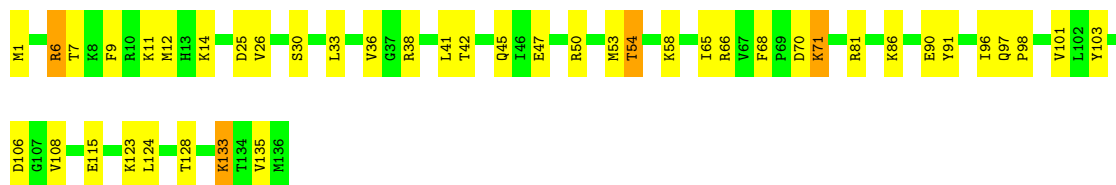
- Molecule 15: 50S ribosomal protein L15

Chain M: 73% 24% .



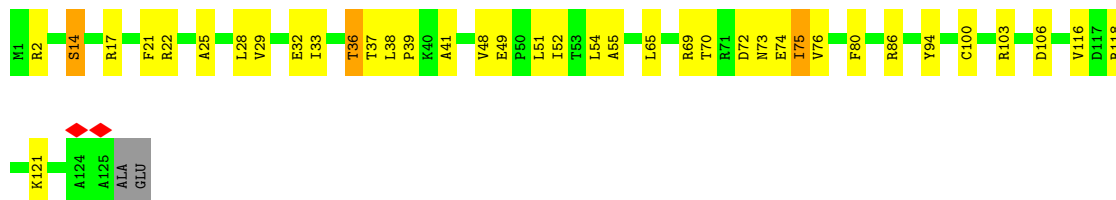
- Molecule 16: 50S ribosomal protein L16

Chain N: 68% 29% .



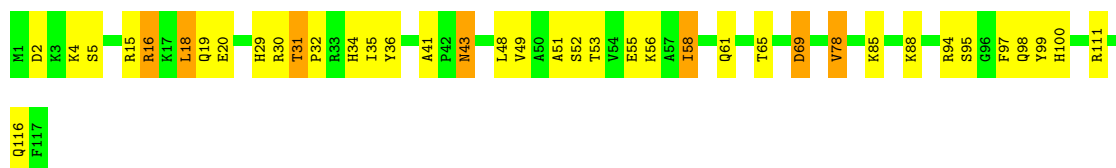
- Molecule 17: 50S ribosomal protein L17

Chain O: 69% 28% . .



- Molecule 18: 50S ribosomal protein L18

Chain P: 67% 27% 6%



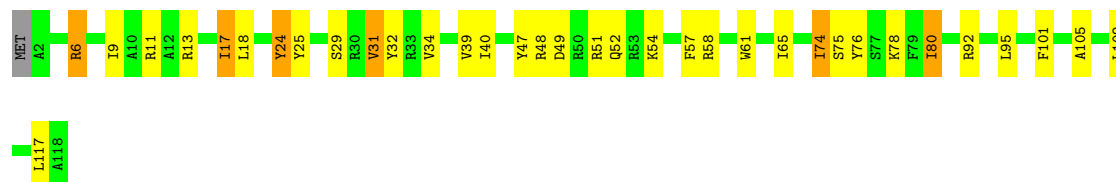
- Molecule 19: 50S ribosomal protein L19

Chain Q: 71% 26% . .



- Molecule 20: 50S ribosomal protein L20

Chain R: 69% 25% 5% .



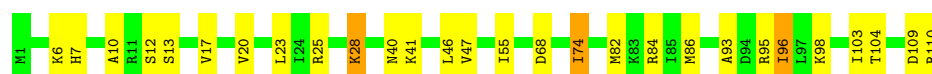
- Molecule 21: 50S ribosomal protein L21

Chain S: 66% 29% 5%



- Molecule 22: 50S ribosomal protein L22

Chain T: 75% 23% .



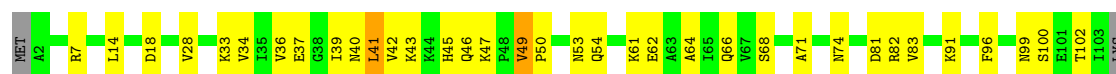
- Molecule 23: 50S ribosomal protein L23

Chain U: 66% 24% 5% 5%



- Molecule 24: 50S ribosomal protein L24

Chain V: 64% 32% . .



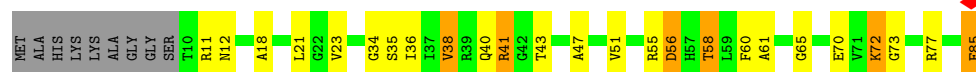
- Molecule 25: 50S ribosomal protein L25

Chain W: 74% 23% .



- Molecule 26: 50S ribosomal protein L27

Chain X: 



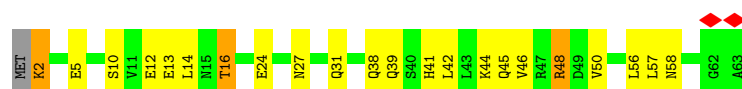
- Molecule 27: 50S ribosomal protein L28

Chain Y: 



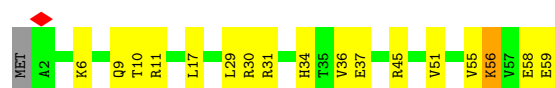
- Molecule 28: 50S ribosomal protein L29

Chain Z: 



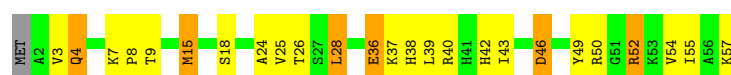
- Molecule 29: 50S ribosomal protein L30

Chain a: 



- Molecule 30: 50S ribosomal protein L32

Chain b: 



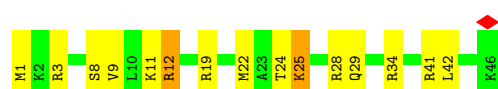
- Molecule 31: 50S ribosomal protein L33

Chain c: 



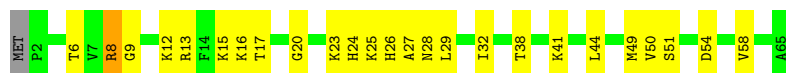
- Molecule 32: 50S ribosomal protein L34

Chain d: 



- Molecule 33: 50S ribosomal protein L35

Chain e:  60% 37% ..



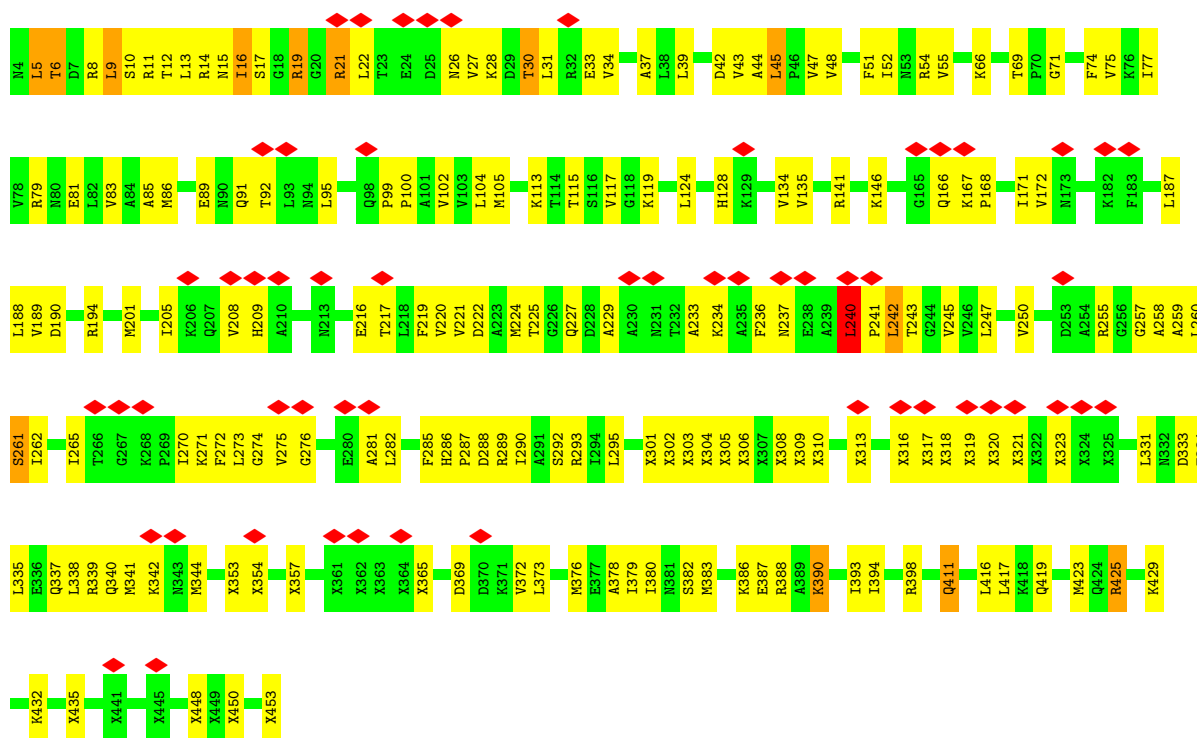
- Molecule 34: 50S ribosomal protein L36

Chain f:  71% 21% 8%



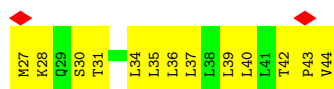
- Molecule 35: Signal recognition particle protein Ffh

Chain i:  12% 59% 38% .



- Molecule 36: 1A9L SS

Chain k:  11% 28% 72%



- Molecule 37: Signal recognition particle receptor FtsY

Chain l:  11% 24% 15% 60%

MET	GLU	ALA	ALA	GLU	SER	GLU	ALA	GLU	PHE	PHE	SER	SER	TRP	LEU	GLY	PHE	PHE	GLN	GLN	GLN	THR	PRO	GLY	LYS	GLU	ALA	GLU	GLN	GLN	GLN	GLN	GLU	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81197	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.234	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	443.2, 443.2, 443.2	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.385, 1.385, 1.385	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GNP, ZN

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	1	0.16	0/1037	0.38	0/1616
2	2	0.35	0/68	0.51	0/103
3	A	0.35	0/69329	0.48	1/108152 (0.0%)
4	B	0.27	0/2872	0.40	0/4478
5	C	0.61	0/2121	0.96	1/2852 (0.0%)
6	D	0.61	0/1586	0.95	4/2134 (0.2%)
7	E	0.57	0/1571	0.91	0/2113
8	F	0.52	1/1434 (0.1%)	0.93	5/1926 (0.3%)
9	G	0.51	0/1343	0.97	4/1816 (0.2%)
10	H	0.59	0/1121	0.89	1/1515 (0.1%)
11	I	0.72	0/958	0.95	0/1292
12	J	0.94	1/993 (0.1%)	1.13	8/1341 (0.6%)
13	K	0.58	0/1152	0.88	2/1551 (0.1%)
14	L	0.57	0/955	0.97	2/1279 (0.2%)
15	M	0.57	0/1062	0.98	3/1413 (0.2%)
16	N	0.59	0/1093	0.96	6/1460 (0.4%)
17	O	0.61	0/1006	0.95	1/1345 (0.1%)
18	P	0.50	0/910	0.93	0/1219
19	Q	0.54	0/929	0.94	2/1242 (0.2%)
20	R	0.73	0/960	0.91	1/1278 (0.1%)
21	S	0.57	0/829	0.95	0/1107
22	T	0.66	0/864	1.05	2/1156 (0.2%)
23	U	0.95	5/763 (0.7%)	1.09	3/1021 (0.3%)
24	V	0.45	0/787	0.88	2/1051 (0.2%)
25	W	0.47	0/766	0.92	0/1025
26	X	0.59	0/587	0.98	2/776 (0.3%)
27	Y	0.61	0/635	0.92	0/848
28	Z	0.41	0/500	0.81	0/661
29	a	0.53	0/453	0.87	0/605
30	b	0.54	0/450	0.89	0/599
31	c	0.55	0/421	1.01	2/561 (0.4%)
32	d	0.66	0/380	0.95	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.62	0/513	0.97	0/676
34	f	0.60	0/303	0.99	0/397
35	i	0.42	0/2942	0.85	5/3950 (0.1%)
36	k	0.55	0/137	0.90	0/186
37	l	0.47	0/1511	1.03	3/2040 (0.1%)
All	All	0.43	7/105341 (0.0%)	0.64	60/157282 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	C	0	1
9	G	0	1
12	J	0	1
35	i	0	1
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	U	89	GLU	N-CA	10.73	1.60	1.46
23	U	88	LYS	CA-C	10.06	1.66	1.52
23	U	88	LYS	C-N	9.90	1.47	1.33
8	F	108	VAL	CA-CB	5.57	1.57	1.53
12	J	22	PRO	CA-C	5.50	1.57	1.52
23	U	88	LYS	CA-CB	5.38	1.61	1.53
23	U	88	LYS	N-CA	5.17	1.52	1.46

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	l	476	ARG	NH1-CZ-NH2	19.39	144.50	119.30
37	l	476	ARG	NE-CZ-NH1	-13.72	107.78	121.50
37	l	476	ARG	NE-CZ-NH2	-12.75	107.72	119.20
9	G	155	GLU	CA-C-N	9.36	128.99	119.82
9	G	155	GLU	C-N-CA	9.36	128.99	119.82
12	J	116	ASP	N-CA-C	8.02	123.27	113.17
23	U	88	LYS	CB-CA-C	7.80	122.38	109.89
12	J	98	VAL	N-CA-C	7.62	120.38	112.83
35	i	69	THR	CA-C-N	6.78	126.41	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	69	THR	C-N-CA	6.78	126.41	119.56
12	J	22	PRO	N-CA-C	6.58	118.73	110.70
16	N	71	LYS	CA-C-N	6.48	126.70	119.90
16	N	71	LYS	C-N-CA	6.48	126.70	119.90
6	D	142	VAL	CA-C-N	6.31	126.22	119.28
6	D	142	VAL	C-N-CA	6.31	126.22	119.28
8	F	175	PHE	CA-C-N	6.25	126.62	119.93
8	F	175	PHE	C-N-CA	6.25	126.62	119.93
14	L	12	ASP	N-CA-C	6.25	117.67	108.86
6	D	140	HIS	N-CA-C	-6.24	103.76	112.12
16	N	108	VAL	CA-C-N	6.18	126.13	119.76
16	N	108	VAL	C-N-CA	6.18	126.13	119.76
13	K	7	LYS	CA-C-N	6.11	126.56	119.47
13	K	7	LYS	C-N-CA	6.11	126.56	119.47
17	O	70	THR	N-CA-C	6.04	120.81	113.38
23	U	93	LEU	N-CA-C	6.03	118.48	109.25
15	M	23	ILE	N-CA-C	5.84	117.28	110.62
14	L	51	LYS	N-CA-C	-5.80	105.97	113.16
15	M	61	LEU	N-CA-C	5.73	117.29	110.07
6	D	146	ILE	N-CA-C	5.72	118.49	112.83
9	G	47	ASP	CB-CA-C	-5.62	110.11	116.63
12	J	92	LYS	CA-C-N	5.50	125.78	119.83
12	J	92	LYS	C-N-CA	5.50	125.78	119.83
31	c	40	ASP	CA-C-N	5.49	125.01	119.19
31	c	40	ASP	C-N-CA	5.49	125.01	119.19
23	U	88	LYS	CA-C-O	-5.37	114.63	120.81
3	A	2423	U	N1-C1'-C2'	5.37	120.05	112.00
35	i	390	LYS	CA-C-N	5.34	124.95	119.56
35	i	390	LYS	C-N-CA	5.34	124.95	119.56
35	i	240	LEU	N-CA-C	5.32	121.58	109.81
16	N	124	LEU	CA-C-N	5.30	124.92	119.56
16	N	124	LEU	C-N-CA	5.30	124.92	119.56
26	X	73	GLY	CA-C-N	5.29	124.95	119.56
26	X	73	GLY	C-N-CA	5.29	124.95	119.56
12	J	119	GLY	N-CA-C	5.25	117.96	111.93
19	Q	21	ARG	CA-C-N	-5.24	114.84	120.03
19	Q	21	ARG	C-N-CA	-5.24	114.84	120.03
10	H	110	VAL	N-CA-C	5.22	116.14	109.30
20	R	101	PHE	N-CA-C	5.17	117.00	111.36
12	J	23	PRO	N-CA-C	5.11	120.25	113.40
24	V	49	VAL	CA-C-N	5.11	124.61	119.19
24	V	49	VAL	C-N-CA	5.11	124.61	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	59	ARG	N-CA-C	-5.11	105.89	112.68
12	J	100	LYS	N-CA-C	5.07	117.42	108.75
8	F	83	TYR	CA-C-N	-5.04	114.13	119.98
8	F	83	TYR	C-N-CA	-5.04	114.13	119.98
22	T	86	MET	CA-C-N	5.02	125.30	119.93
22	T	86	MET	C-N-CA	5.02	125.30	119.93
5	C	154	LEU	N-CA-C	5.02	117.50	110.23
9	G	156	PRO	N-CA-C	5.01	120.45	113.98
8	F	106	ILE	CB-CA-C	-5.01	107.45	111.71

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide
12	J	19	ASN	Peptide
35	i	240	LEU	Peptide

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	1	926	0	467	35	0
2	2	62	0	34	1	0
3	A	61902	0	31133	714	0
4	B	2569	0	1301	21	0
5	C	2082	0	2154	50	0
6	D	1565	0	1616	35	0
7	E	1552	0	1619	26	0
8	F	1410	0	1444	45	0
9	G	1323	0	1371	33	0
10	H	1110	0	1148	25	0
11	I	946	0	978	31	0
12	J	979	0	1028	40	0
13	K	1129	0	1162	25	0
14	L	946	0	1023	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	M	1053	0	1129	28	0
16	N	1074	0	1157	25	0
17	O	993	0	1034	26	0
18	P	900	0	935	20	0
19	Q	917	0	962	19	0
20	R	947	0	1019	25	0
21	S	816	0	839	23	0
22	T	857	0	922	15	0
23	U	756	0	817	27	0
24	V	779	0	831	20	0
25	W	753	0	780	16	0
26	X	580	0	594	16	0
27	Y	625	0	652	17	0
28	Z	501	0	529	17	0
29	a	449	0	488	11	0
30	b	444	0	458	18	0
31	c	414	0	442	6	0
32	d	377	0	418	8	0
33	e	504	0	572	14	0
34	f	302	0	340	12	0
35	i	3337	0	3457	163	0
36	k	137	0	168	18	0
37	l	1492	0	1544	70	0
38	2	1	0	0	0	0
38	A	412	0	0	0	0
38	B	11	0	0	0	0
38	C	2	0	0	0	0
38	D	1	0	0	0	0
38	E	1	0	0	0	0
38	P	1	0	0	0	0
38	R	1	0	0	0	0
38	b	1	0	0	0	0
38	i	1	0	0	0	0
38	l	1	0	0	0	0
39	f	1	0	0	0	0
40	i	32	0	13	1	0
40	l	32	0	13	0	0
All	All	98006	0	66591	1513	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 9.

All (1513) 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)
3:A:1318:U:OP1	35:i:432:LYS:NZ	1.86	1.08
23:U:96:VAL:HG23	35:i:66:LYS:HD3	1.42	0.99
3:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
37:l:330:ASP:OD2	37:l:336:ALA:HB1	1.67	0.94
35:i:10:SER:O	35:i:14:ARG:HB2	1.68	0.93
35:i:250:VAL:HG22	35:i:274:GLY:O	1.70	0.91
37:l:330:ASP:CG	37:l:336:ALA:HB1	1.96	0.90
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90
23:U:53:VAL:HG21	23:U:93:LEU:HD11	1.53	0.89
35:i:47:VAL:HG21	35:i:261:SER:HB3	1.55	0.88
3:A:276:U:O2	3:A:278:A:N6	2.07	0.87
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.57	0.86
3:A:1827:U:OP2	5:C:221:ARG:NH1	2.08	0.86
37:l:432:LYS:HG2	37:l:464:PHE:HZ	1.40	0.85
35:i:79:ARG:NH1	35:i:288:ASP:OD1	2.09	0.85
5:C:107:PRO:HD2	5:C:110:LEU:HD22	1.59	0.84
3:A:287:G:O6	3:A:352:A:N6	2.10	0.84
3:A:2135:A:N6	3:A:2156:G:O2'	2.10	0.83
3:A:2107:G:H1	3:A:2182:U:H3	1.22	0.82
37:l:361:ALA:HB1	37:l:403:VAL:HG21	1.60	0.81
3:A:807:U:OP2	15:M:41:ARG:NH1	2.14	0.81
3:A:2478:A:H5'	34:f:32:LYS:HD3	1.62	0.81
23:U:53:VAL:HG11	23:U:93:LEU:HD21	1.61	0.81
37:l:330:ASP:OD2	37:l:336:ALA:CB	2.29	0.80
1:l:49:G:H1	1:l:60:A:H61	1.30	0.80
15:M:109:LYS:HG2	15:M:126:ARG:HB2	1.64	0.80
3:A:2128:G:N3	3:A:2173:A:O2'	2.14	0.79
35:i:119:LYS:HB3	35:i:282:LEU:HB2	1.64	0.78
35:i:317:UNK:HG1	36:k:30:SER:OG	1.82	0.78
3:A:994:C:O2	21:S:10:LYS:NZ	2.16	0.78
23:U:87:LEU:HD13	23:U:93:LEU:HD12	1.66	0.77
18:P:15:ARG:NH2	18:P:95:SER:OG	2.18	0.77
11:I:41:LEU:HD21	11:I:96:PHE:HE1	1.50	0.77
30:b:43:ILE:HG22	30:b:49:TYR:HB2	1.66	0.77
3:A:614:A:O2'	3:A:616:A:N7	2.18	0.76
5:C:245:VAL:HG12	5:C:251:GLN:HA	1.67	0.76
35:i:6:THR:O	35:i:10:SER:HB2	1.86	0.76
29:a:6:LYS:HG2	29:a:37:GLU:HG2	1.68	0.75
1:l:71:C:H2'	1:l:72:A:C8	2.21	0.75
23:U:96:VAL:CG2	35:i:66:LYS:HD3	2.17	0.75
35:i:257:GLY:O	35:i:260:LEU:HB3	1.86	0.74
5:C:181:MET:HB2	5:C:268:VAL:HB	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:18:LYS:HE2	34:f:21:GLY:HA2	1.69	0.74
3:A:2599:G:N7	5:C:236:GLU:HB2	2.02	0.74
3:A:2848:G:O2'	3:A:2867:G:N2	2.19	0.74
35:i:250:VAL:CG2	35:i:275:VAL:HG12	2.18	0.74
37:l:330:ASP:CG	37:l:336:ALA:CB	2.61	0.73
3:A:2135:A:O2'	3:A:2159:G:O2'	2.06	0.73
3:A:95:A:HO2'	28:Z:41:HIS:N	1.85	0.73
36:k:36:LEU:O	36:k:40:LEU:HB3	1.89	0.73
3:A:331:C:H41	3:A:1210:G:H22	1.37	0.72
3:A:2119:A:N6	3:A:2167:U:O2	2.22	0.72
3:A:545:U:O2	3:A:548:G:N1	2.19	0.72
7:E:1:MET:HG3	7:E:14:VAL:HG23	1.71	0.72
13:K:70:THR:OG1	13:K:71:ASP:OD1	2.08	0.72
35:i:250:VAL:HG23	35:i:275:VAL:HG12	1.71	0.71
3:A:331:C:H41	3:A:1210:G:N2	1.88	0.71
3:A:1069:A:H4'	3:A:1070:A:H5''	1.71	0.71
3:A:720:U:H2'	3:A:721:A:C8	2.24	0.71
1:l:42:A:H61	1:l:67:A:H62	1.36	0.71
23:U:87:LEU:CD1	23:U:93:LEU:HD12	2.21	0.71
3:A:2423:U:H2'	3:A:2424:C:O4'	1.89	0.71
36:k:36:LEU:O	36:k:40:LEU:CB	2.39	0.71
13:K:131:ASN:OD1	13:K:131:ASN:N	2.22	0.71
11:I:50:VAL:HG22	11:I:85:VAL:HG13	1.73	0.70
3:A:2163:A:OP1	3:A:2170:A:O2'	2.08	0.70
35:i:75:VAL:HG13	35:i:295:LEU:HD13	1.71	0.70
37:l:386:ARG:HD3	37:l:393:LEU:HB3	1.71	0.70
37:l:423:THR:HG22	37:l:424:GLY:H	1.56	0.70
3:A:258:G:H1'	15:M:104:GLN:HE22	1.56	0.70
1:l:68:A:H2'	1:l:69:G:C8	2.26	0.70
35:i:354:UNK:HG1	36:k:39:LEU:HD21	1.73	0.70
3:A:1801:A:OP2	5:C:150:LYS:NZ	2.18	0.70
3:A:2310:C:H2'	8:F:77:PHE:HE2	1.54	0.70
35:i:6:THR:O	35:i:10:SER:CB	2.40	0.70
35:i:342:LYS:HA	35:i:373:LEU:HD13	1.74	0.69
3:A:971:G:H2'	3:A:972:A:O4'	1.92	0.69
3:A:1340:U:OP1	23:U:19:LYS:NZ	2.26	0.69
14:L:70:ARG:HD3	14:L:76:VAL:HG22	1.72	0.69
35:i:134:VAL:HG12	35:i:188:LEU:HB2	1.74	0.69
35:i:27:VAL:HG13	35:i:74:PHE:HZ	1.58	0.69
35:i:289:ARG:NH2	35:i:304:UNK:HG1	2.07	0.69
3:A:249:C:O2	33:e:12:LYS:NZ	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1536:C:H4'	3:A:1537:G:H5''	1.75	0.69
21:S:40:MET:HE2	21:S:42:ALA:HB2	1.74	0.69
37:l:352:ILE:HG13	37:l:367:ALA:HA	1.73	0.69
1:l:68:A:H2'	1:l:69:G:H8	1.58	0.69
3:A:2830:C:H5''	6:D:56:LYS:HE3	1.75	0.68
9:G:35:ARG:HD3	9:G:71:LEU:HD13	1.74	0.68
3:A:513:A:O2'	20:R:11:ARG:NH1	2.26	0.68
14:L:21:CYS:HA	14:L:41:ILE:HG22	1.76	0.68
36:k:39:LEU:O	36:k:43:PRO:HD2	1.93	0.68
3:A:362:A:H3'	3:A:363:G:H8	1.59	0.68
3:A:2122:U:OP1	3:A:2168:G:N2	2.26	0.68
11:I:43:LYS:HG2	11:I:46:ARG:HH22	1.56	0.68
4:B:54:G:H21	8:F:26:MET:HE3	1.58	0.68
14:L:79:PHE:HD1	19:Q:70:VAL:HG22	1.58	0.67
37:l:368:ILE:HB	37:l:407:LEU:HD23	1.75	0.67
3:A:358:U:H2'	3:A:359:G:H8	1.60	0.67
3:A:878:A:H3'	3:A:879:G:H8	1.60	0.67
18:P:31:THR:HG22	18:P:34:HIS:H	1.59	0.67
35:i:205:ILE:HG22	35:i:240:LEU:HD11	1.75	0.67
37:l:315:ARG:HB2	37:l:477:ILE:HG13	1.75	0.67
3:A:2103:C:O2	3:A:2186:G:N1	2.27	0.67
3:A:370:G:O2'	3:A:424:G:OP1	2.11	0.66
3:A:2303:G:O2'	8:F:121:SER:O	2.13	0.66
3:A:2713:U:H3'	3:A:2714:G:H5''	1.77	0.66
12:J:79:LEU:HB3	12:J:109:ILE:HG12	1.76	0.66
13:K:31:GLU:HG3	13:K:142:ILE:HG13	1.77	0.66
35:i:319:UNK:O	35:i:323:UNK:HG3	1.94	0.66
37:l:327:ALA:HB3	37:l:381:ALA:HA	1.77	0.66
3:A:572:A:OP2	21:S:80:ARG:NH2	2.27	0.66
3:A:196:A:OP2	15:M:47:ARG:NH1	2.29	0.66
3:A:286:U:H2'	3:A:287:G:H8	1.60	0.66
3:A:1105:U:H2'	3:A:1106:G:C8	2.29	0.66
3:A:2216:G:H2'	3:A:2217:G:H8	1.60	0.66
27:Y:32:ASN:O	27:Y:52:SER:HA	1.95	0.66
3:A:2305:U:C2	8:F:151:GLY:HA3	2.31	0.66
28:Z:10:SER:N	28:Z:13:GLU:OE1	2.26	0.66
37:l:404:MET:HB2	37:l:412:PRO:HD3	1.77	0.66
37:l:388:GLN:HG2	37:l:433:LEU:HD12	1.76	0.66
3:A:286:U:H2'	3:A:287:G:C8	2.31	0.66
3:A:2209:G:H1	3:A:2215:C:H42	1.44	0.66
3:A:2590:A:H2'	3:A:2591:C:H6	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:432:LYS:HG2	37:l:464:PHE:CZ	2.27	0.66
3:A:1344:U:O2'	3:A:1345:C:OP1	2.14	0.66
10:H:84:ALA:HA	10:H:90:LEU:HA	1.78	0.66
16:N:50:ARG:O	16:N:54:THR:OG1	2.13	0.66
3:A:1597:A:H5''	3:A:1598:A:H5'	1.78	0.65
9:G:9:VAL:HG22	9:G:69:ARG:HE	1.61	0.65
4:B:43:C:O2	8:F:92:ARG:NH2	2.28	0.65
35:i:42:ASP:OD2	37:l:424:GLY:HA3	1.97	0.65
37:l:312:LYS:HB3	37:l:480:LEU:HB2	1.79	0.65
3:A:1794:A:H2'	3:A:1795:C:H6	1.61	0.65
7:E:87:ALA:O	7:E:88:ARG:NH2	2.30	0.65
3:A:2788:C:O2'	3:A:2809:A:N3	2.28	0.65
23:U:96:VAL:HG23	35:i:66:LYS:CD	2.24	0.65
26:X:65:GLY:HA2	26:X:85:GLU:HG2	1.78	0.65
35:i:448:UNK:HG2	35:i:450:UNK:HG3	1.79	0.65
37:l:329:GLY:H	37:l:382:ASP:HB3	1.61	0.65
37:l:388:GLN:HG3	37:l:430:GLN:HA	1.78	0.65
3:A:322:A:H5'	3:A:340:A:H1'	1.78	0.65
3:A:1007:C:OP1	13:K:37:ARG:NH2	2.29	0.65
3:A:1869:G:N2	3:A:1871:A:O2'	2.30	0.65
30:b:28:LEU:HD13	30:b:37:LYS:HB3	1.78	0.65
35:i:340:GLN:HE21	36:k:34:LEU:HD21	1.62	0.65
8:F:158:THR:HG22	8:F:160:ALA:H	1.62	0.64
25:W:2:PHE:HB3	25:W:50:MET:HE3	1.77	0.64
3:A:860:U:H1'	3:A:2268:A:H5'	1.78	0.64
3:A:284:U:H3	3:A:356:G:H1	1.44	0.64
8:F:144:ASP:N	8:F:144:ASP:OD1	2.30	0.64
3:A:2116:G:N7	3:A:2165:C:N4	2.44	0.64
35:i:234:LYS:HB2	35:i:265:ILE:HG21	1.78	0.64
3:A:1105:U:H2'	3:A:1106:G:H8	1.63	0.64
3:A:1510:G:H2'	3:A:1511:G:C8	2.32	0.64
3:A:1980:G:O2'	3:A:1982:U:OP2	2.16	0.64
3:A:2674:G:H4'	14:L:30:ARG:HG3	1.78	0.64
35:i:369:ASP:O	35:i:373:LEU:HB2	1.98	0.64
3:A:825:A:H2'	3:A:826:U:O4'	1.98	0.63
3:A:968:C:H2'	3:A:969:G:H8	1.62	0.63
3:A:1094:U:N3	3:A:1097:U:OP2	2.30	0.63
19:Q:91:ALA:HB2	19:Q:113:ARG:HA	1.80	0.63
25:W:21:ARG:NH2	25:W:87:GLN:O	2.28	0.63
35:i:42:ASP:HB2	37:l:425:GLN:H	1.64	0.63
3:A:1614:A:N1	22:T:93:ALA:HB2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2151:U:H2'	3:A:2152:G:C8	2.34	0.63
20:R:58:ARG:HA	20:R:61:TRP:CE3	2.34	0.63
35:i:5:LEU:HB2	35:i:255:ARG:HD2	1.81	0.63
35:i:5:LEU:O	35:i:9:LEU:N	2.22	0.63
3:A:2424:C:H5''	3:A:2425:A:H5'	1.79	0.62
13:K:117:ALA:HA	13:K:120:ARG:HH21	1.63	0.62
16:N:14:LYS:O	16:N:71:LYS:NZ	2.32	0.62
35:i:83:VAL:HA	35:i:287:PRO:HB2	1.81	0.62
1:1:63:A:O2'	35:i:388:ARG:NH2	2.32	0.62
20:R:74:ILE:HD11	20:R:78:LYS:HB3	1.80	0.62
3:A:1433:A:N1	3:A:1434:A:N6	2.47	0.62
3:A:2822:G:O6	17:O:2:ARG:NH1	2.32	0.62
22:T:82:MET:HB3	22:T:84:ARG:HH22	1.63	0.62
35:i:8:ARG:O	35:i:12:THR:OG1	2.15	0.62
35:i:124:LEU:O	35:i:128:HIS:HB2	2.00	0.62
3:A:2809:A:H2'	3:A:2810:A:C8	2.34	0.62
8:F:74:VAL:HG22	8:F:79:ILE:HD11	1.79	0.62
19:Q:4:ILE:HD12	19:Q:4:ILE:H	1.65	0.62
3:A:514:A:N3	3:A:581:C:O2'	2.32	0.62
10:H:68:ARG:HA	10:H:71:LYS:HD2	1.81	0.62
11:I:41:LEU:HD21	11:I:96:PHE:CE1	2.34	0.62
17:O:49:GLU:HA	17:O:52:ILE:HD12	1.80	0.62
21:S:41:ILE:HB	21:S:48:LYS:HD2	1.79	0.62
3:A:784:G:C6	5:C:228:VAL:HG11	2.35	0.62
11:I:57:ASN:ND2	11:I:76:PHE:O	2.33	0.62
16:N:50:ARG:HA	16:N:53:MET:HE3	1.82	0.62
35:i:337:GLN:O	35:i:341:MET:HB2	2.00	0.61
3:A:503:A:H4'	3:A:504:A:H5'	1.82	0.61
3:A:2742:G:OP2	34:f:24:ARG:NH1	2.32	0.61
3:A:2590:A:H2'	3:A:2591:C:C6	2.35	0.61
35:i:11:ARG:O	35:i:15:ASN:HB2	2.01	0.61
3:A:2639:A:H2'	3:A:2640:G:O4'	2.01	0.61
9:G:137:ASP:O	9:G:141:ILE:HG22	2.01	0.61
12:J:53:LEU:HD11	12:J:82:LYS:HD2	1.83	0.61
15:M:57:LEU:HD13	15:M:60:ARG:HH11	1.65	0.61
3:A:1079:C:O2'	12:J:134:ARG:NH1	2.33	0.61
22:T:6:LYS:HG2	22:T:104:THR:HG23	1.82	0.61
28:Z:24:GLU:HG2	35:i:21:ARG:HB2	1.83	0.61
30:b:52:ARG:HB2	30:b:52:ARG:NH2	2.16	0.61
3:A:1001:A:H2'	3:A:1002:G:O4'	2.01	0.60
3:A:585:G:N7	20:R:6:ARG:NH1	2.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:50:ARG:HB2	30:b:52:ARG:HH12	1.65	0.60
3:A:1076:C:H2'	3:A:1077:A:C8	2.37	0.60
30:b:38:HIS:ND1	30:b:39:LEU:O	2.30	0.60
5:C:235:GLY:HA3	5:C:239:ASN:HB2	1.83	0.60
9:G:170:ARG:NH1	34:f:29:ALA:O	2.24	0.60
3:A:2310:C:H2'	8:F:77:PHE:CE2	2.35	0.60
35:i:42:ASP:CG	37:l:424:GLY:HA3	2.26	0.60
3:A:570:G:H2'	3:A:2030:A:N7	2.16	0.60
3:A:1363:C:O2'	3:A:1809:A:N3	2.33	0.60
11:I:27:VAL:HG22	11:I:82:ILE:HG22	1.83	0.60
3:A:299:A:N1	3:A:322:A:O2'	2.27	0.60
17:O:54:LEU:HD21	17:O:65:LEU:HD23	1.82	0.60
23:U:96:VAL:CG2	35:i:66:LYS:CD	2.80	0.60
3:A:355:U:H2'	3:A:356:G:C8	2.37	0.60
3:A:1170:C:O2	3:A:1179:G:N2	2.34	0.60
3:A:2102:G:N2	3:A:2187:U:O2	2.31	0.60
35:i:39:LEU:HD13	35:i:45:LEU:HD13	1.83	0.60
3:A:1342:A:O2'	3:A:1344:U:OP2	2.16	0.59
8:F:44:ILE:HG21	8:F:79:ILE:HG22	1.83	0.59
15:M:81:ASP:HA	15:M:84:LYS:HD2	1.82	0.59
35:i:5:LEU:HD13	35:i:255:ARG:HG3	1.82	0.59
3:A:1251:C:OP2	20:R:6:ARG:NH2	2.35	0.59
6:D:2:ILE:HG13	6:D:100:LEU:HD21	1.83	0.59
9:G:27:LYS:NZ	9:G:27:LYS:HB3	2.17	0.59
23:U:88:LYS:C	23:U:90:GLY:H	2.08	0.59
3:A:1794:A:H2'	3:A:1795:C:C6	2.37	0.59
11:I:64:VAL:HG22	11:I:69:PHE:HB2	1.84	0.59
1:1:38:U:OP2	35:i:386:LYS:NZ	2.31	0.59
1:1:69:G:H2'	1:1:70:G:H1'	1.85	0.59
3:A:2636:C:HO2'	6:D:45:TYR:HH	1.46	0.59
24:V:81:ASP:OD1	24:V:82:ARG:N	2.35	0.59
3:A:2819:G:H2'	3:A:2821:A:N7	2.17	0.59
7:E:97:ASN:N	7:E:97:ASN:OD1	2.34	0.59
13:K:36:LEU:HD11	13:K:122:LEU:HB2	1.83	0.59
37:l:398:LYS:HE2	37:l:437:ALA:HA	1.84	0.59
1:1:70:G:H3'	1:1:71:C:H6	1.66	0.59
6:D:116:LYS:HG3	6:D:165:MET:HE2	1.83	0.59
3:A:1808:A:H3'	3:A:1809:A:C8	2.38	0.59
3:A:2584:U:H3'	3:A:2585:U:H5''	1.84	0.59
25:W:4:ILE:HG12	25:W:50:MET:HE1	1.85	0.59
3:A:2615:U:C2	30:b:4:GLN:HA	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:e:15:LYS:HB2	33:e:23:LYS:HE3	1.84	0.59
35:i:289:ARG:CZ	35:i:304:UNK:HG1	2.32	0.59
3:A:396:G:OP2	27:Y:10:LYS:NZ	2.36	0.59
3:A:878:A:H3'	3:A:879:G:C8	2.38	0.59
3:A:776:G:O2'	3:A:777:G:OP1	2.19	0.59
3:A:2127:G:O2'	3:A:2128:G:O5'	2.19	0.59
3:A:2831:G:OP1	6:D:56:LYS:NZ	2.35	0.59
37:l:350:PRO:HG3	37:l:374:ARG:NH1	2.17	0.58
18:P:99:TYR:OH	18:P:111:ARG:NH1	2.36	0.58
30:b:52:ARG:HB2	30:b:52:ARG:HH21	1.66	0.58
37:l:424:GLY:O	37:l:427:ALA:N	2.33	0.58
21:S:37:GLU:HB3	21:S:53:PHE:CE1	2.39	0.58
3:A:1796:U:H2'	3:A:1797:G:H8	1.67	0.58
12:J:106:LEU:HB3	12:J:126:THR:HG23	1.85	0.58
3:A:2127:G:O2'	3:A:2128:G:O4'	2.20	0.58
3:A:2205:A:H61	3:A:2219:U:H3	1.50	0.58
17:O:73:ASN:HA	17:O:76:VAL:HG22	1.86	0.58
25:W:76:ASP:OD1	25:W:77:VAL:N	2.37	0.58
35:i:310:UNK:HA	35:i:313:UNK:HG3	1.84	0.58
3:A:1130:U:O2'	3:A:1131:G:H8	1.87	0.58
3:A:2060:A:H3'	7:E:63:LYS:HZ3	1.67	0.58
17:O:118:ARG:NH2	30:b:54:VAL:O	2.37	0.58
35:i:335:LEU:HD13	35:i:380:ILE:HB	1.85	0.58
3:A:2291:U:H2'	3:A:2292:U:C6	2.38	0.58
35:i:44:ALA:HA	35:i:227:GLN:HA	1.84	0.58
3:A:2021:C:OP1	20:R:25:TYR:OH	2.21	0.58
1:l:48:G:N2	35:i:378:ALA:O	2.36	0.58
3:A:833:A:H2'	3:A:834:G:C8	2.38	0.58
3:A:2412:A:H2'	3:A:2413:G:O4'	2.04	0.58
6:D:13:ARG:HD2	6:D:15:PHE:CZ	2.38	0.58
37:l:355:HIS:ND1	37:l:356:THR:O	2.37	0.58
5:C:227:PRO:HG3	5:C:234:GLY:H	1.69	0.57
6:D:12:THR:OG1	6:D:13:ARG:N	2.34	0.57
12:J:59:ILE:HD13	12:J:69:PHE:HB3	1.86	0.57
19:Q:16:ASP:OD1	19:Q:16:ASP:N	2.32	0.57
37:l:416:MET:SD	37:l:444:THR:OG1	2.58	0.57
3:A:340:A:H2'	3:A:341:C:O4'	2.05	0.57
3:A:1187:G:OP1	21:S:85:LYS:NZ	2.31	0.57
7:E:21:ARG:HD3	7:E:106:LYS:HB3	1.85	0.57
35:i:91:GLN:HB2	35:i:286:HIS:CG	2.39	0.57
18:P:41:ALA:HB2	18:P:48:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1715:G:O2'	3:A:1743:G:O6	2.17	0.57
3:A:2447:G:N2	3:A:2450:A:OP2	2.37	0.57
6:D:157:LYS:HD2	13:K:80:HIS:CE1	2.40	0.57
25:W:55:GLU:H	25:W:55:GLU:CD	2.13	0.57
35:i:42:ASP:HB2	37:l:425:GLN:N	2.20	0.57
3:A:876:C:H2'	3:A:877:A:O4'	2.05	0.57
3:A:1063:G:H5'	12:J:77:ALA:HB1	1.87	0.57
17:O:94:TYR:O	17:O:116:VAL:HG23	2.05	0.57
35:i:117:VAL:HG21	35:i:190:ASP:HB2	1.87	0.57
3:A:849:A:H2'	3:A:850:U:H6	1.69	0.57
5:C:166:ALA:HB3	5:C:173:THR:HB	1.86	0.57
3:A:1645:G:H5''	3:A:1646:C:H5'	1.85	0.57
3:A:2216:G:H2'	3:A:2217:G:C8	2.40	0.57
24:V:18:ASP:OD2	24:V:40:ASN:N	2.37	0.57
3:A:839:U:H2'	3:A:840:C:C6	2.40	0.57
1:1:49:G:H1	1:1:60:A:N6	1.99	0.56
3:A:2602:A:H4'	3:A:2603:G:O5'	2.04	0.56
3:A:849:A:H2'	3:A:850:U:C6	2.39	0.56
3:A:1905:C:H2'	3:A:1930:G:C8	2.40	0.56
3:A:2430:A:N3	3:A:2430:A:H2'	2.21	0.56
6:D:148:GLN:HB2	6:D:152:PRO:HD2	1.85	0.56
7:E:112:LEU:HB3	7:E:118:LEU:HB2	1.87	0.56
35:i:22:LEU:HD11	35:i:26:ASN:HB2	1.86	0.56
37:l:420:ASP:HB3	37:l:423:THR:OG1	2.05	0.56
3:A:1790:C:H3'	3:A:1828:G:N2	2.21	0.56
9:G:30:ASN:HB3	9:G:79:VAL:HA	1.88	0.56
13:K:72:LYS:HE3	13:K:74:TYR:CE1	2.39	0.56
35:i:99:PRO:HB2	35:i:100:PRO:HD3	1.87	0.56
35:i:313:UNK:HG1	36:k:34:LEU:HD13	1.88	0.56
3:A:812:C:H4'	20:R:13:ARG:NH1	2.21	0.56
3:A:2491:U:H5''	3:A:2570:G:H5''	1.88	0.56
6:D:1:MET:HG2	6:D:2:ILE:H	1.70	0.56
8:F:33:LYS:HG2	8:F:157:THR:HB	1.87	0.56
4:B:42:C:C5	8:F:66:LEU:HD22	2.41	0.56
11:I:60:LEU:O	11:I:64:VAL:HB	2.06	0.56
1:1:60:A:H2'	1:1:61:G:O4'	2.06	0.56
3:A:26:G:C6	3:A:27:G:N1	2.73	0.56
3:A:721:A:H2'	3:A:722:A:C8	2.41	0.56
3:A:1076:C:H2'	3:A:1077:A:H8	1.69	0.56
3:A:1796:U:H2'	3:A:1797:G:C8	2.40	0.56
3:A:2298:A:H2'	3:A:2299:U:O4'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:73:THR:HB	12:J:112:THR:HG22	1.87	0.56
35:i:86:MET:HB2	35:i:287:PRO:HB3	1.88	0.56
3:A:388:G:N7	3:A:390:U:H2'	2.21	0.56
10:H:37:VAL:HG22	10:H:38:PRO:HD2	1.86	0.56
17:O:48:VAL:O	17:O:51:LEU:HB2	2.06	0.56
37:l:294:PHE:N	37:l:377:ASP:O	2.23	0.56
3:A:591:U:H2'	3:A:592:A:H8	1.71	0.56
3:A:2584:U:H3'	3:A:2585:U:C5'	2.36	0.56
18:P:16:ARG:HA	18:P:16:ARG:HH21	1.71	0.56
30:b:49:TYR:O	30:b:52:ARG:NH2	2.39	0.56
3:A:19:A:H2'	3:A:20:C:C6	2.41	0.55
8:F:132:VAL:HG22	8:F:152:LEU:HB3	1.88	0.55
24:V:33:LYS:HB3	24:V:64:ALA:HB1	1.87	0.55
35:i:222:ASP:OD2	35:i:224:MET:HE2	2.06	0.55
37:l:294:PHE:O	37:l:378:VAL:HA	2.06	0.55
12:J:53:LEU:HD22	12:J:78:VAL:HG13	1.87	0.55
23:U:56:GLU:HG3	23:U:88:LYS:HG2	1.88	0.55
25:W:62:THR:HG22	25:W:71:LYS:HG2	1.88	0.55
3:A:1442:U:H2'	3:A:1443:U:C6	2.41	0.55
35:i:54:ARG:HH12	35:i:85:ALA:HB2	1.71	0.55
3:A:859:G:O2'	3:A:916:G:O6	2.22	0.55
3:A:882:G:H1	3:A:894:U:H3	1.54	0.55
12:J:79:LEU:HA	12:J:82:LYS:HG2	1.88	0.55
17:O:2:ARG:NH1	17:O:2:ARG:HB3	2.21	0.55
33:e:17:THR:HG21	33:e:49:MET:HE1	1.87	0.55
35:i:317:UNK:HA	35:i:320:UNK:HG3	1.89	0.55
3:A:184:C:H2'	3:A:185:G:C8	2.41	0.55
3:A:2783:U:H2'	3:A:2784:U:C6	2.42	0.55
5:C:160:THR:HG22	5:C:177:ARG:HG2	1.89	0.55
10:H:7:ASP:OD1	10:H:8:LYS:N	2.40	0.55
3:A:2162:G:H5''	3:A:2171:A:H2'	1.86	0.55
12:J:127:ARG:HA	12:J:130:GLU:HB2	1.89	0.55
3:A:621:A:OP2	15:M:99:ASN:ND2	2.40	0.55
3:A:2171:A:H3'	3:A:2173:A:C8	2.42	0.55
18:P:69:ASP:N	18:P:69:ASP:OD1	2.40	0.55
35:i:102:VAL:HG22	35:i:187:LEU:HD12	1.88	0.55
3:A:996:A:OP2	21:S:10:LYS:HD3	2.07	0.55
3:A:2070:A:H2'	3:A:2071:A:C8	2.42	0.55
3:A:2133:G:H2'	3:A:2157:G:H1	1.70	0.55
8:F:134:GLU:HB3	8:F:136:ILE:HG12	1.89	0.55
35:i:194:ARG:CZ	35:i:205:ILE:HG13	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:i:383:MET:O	35:i:388:ARG:NH2	2.40	0.55
3:A:609:A:H2'	3:A:610:C:O4'	2.07	0.55
3:A:833:A:H2'	3:A:834:G:H8	1.72	0.55
3:A:968:C:H2'	3:A:969:G:C8	2.42	0.55
3:A:2262:U:H2'	3:A:2263:C:H6	1.72	0.55
35:i:194:ARG:NH1	35:i:201:MET:HE3	2.22	0.55
3:A:2576:G:O2'	3:A:2579:C:OP2	2.23	0.54
3:A:2591:C:H2'	3:A:2592:G:C8	2.41	0.54
33:e:29:LEU:HD22	33:e:44:LEU:HB3	1.89	0.54
37:l:364:ILE:O	37:l:368:ILE:HG13	2.07	0.54
32:d:25:LYS:HG3	32:d:29:GLN:HE21	1.72	0.54
6:D:8:LYS:HB2	6:D:201:LEU:HD11	1.88	0.54
21:S:20:VAL:HG13	21:S:96:VAL:HG23	1.89	0.54
3:A:586:A:H5'	7:E:84:THR:HG21	1.90	0.54
3:A:1800:C:H5'	5:C:146:MET:HE1	1.89	0.54
3:A:1837:C:H2'	3:A:1899:A:H61	1.73	0.54
3:A:2267:A:H5''	3:A:2268:A:H5''	1.89	0.54
1:l:72:A:H2'	1:l:73:G:H8	1.72	0.54
3:A:172:A:H2'	3:A:173:A:C8	2.43	0.54
3:A:645:C:O2'	3:A:646:U:OP1	2.24	0.54
35:i:305:UNK:HA	35:i:308:UNK:HG3	1.90	0.54
1:l:45:U:H3	1:l:64:G:H1	1.54	0.54
3:A:2619:C:H5''	6:D:157:LYS:HG3	1.89	0.54
7:E:88:ARG:HA	7:E:88:ARG:HH21	1.72	0.54
12:J:56:PRO:HD3	12:J:75:PRO:HD3	1.90	0.54
13:K:34:ARG:HH22	13:K:40:HIS:HB3	1.71	0.54
30:b:50:ARG:CB	30:b:52:ARG:HH12	2.21	0.54
33:e:54:ASP:O	33:e:58:VAL:HG23	2.08	0.54
3:A:284:U:O2	3:A:356:G:N2	2.37	0.54
3:A:639:U:H2'	3:A:640:C:C6	2.42	0.54
3:A:2424:C:H5''	3:A:2425:A:C5'	2.37	0.54
3:A:2845:U:H5''	19:Q:52:ASN:O	2.08	0.54
33:e:27:ALA:O	33:e:28:ASN:HB2	2.07	0.54
35:i:233:ALA:HB2	35:i:262:ILE:HG12	1.90	0.54
3:A:2834:G:O6	3:A:2879:A:H2'	2.08	0.54
23:U:88:LYS:O	23:U:90:GLY:N	2.41	0.54
26:X:56:ASP:OD1	26:X:56:ASP:N	2.28	0.54
32:d:25:LYS:HB2	32:d:25:LYS:NZ	2.22	0.54
3:A:1056:G:O2'	3:A:1103:A:N6	2.41	0.54
3:A:2443:C:H2'	3:A:2444:G:C8	2.43	0.54
5:C:62:TYR:HA	5:C:86:ASN:HD21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:93:C:OP2	25:W:18:ARG:NH1	2.42	0.53
11:I:54:VAL:HG22	11:I:81:LEU:HD13	1.90	0.53
14:L:38:ILE:HD11	14:L:112:PHE:HZ	1.73	0.53
3:A:608:A:H2'	3:A:609:A:C8	2.44	0.53
3:A:720:U:H2'	3:A:721:A:H8	1.72	0.53
17:O:36:THR:OG1	17:O:37:THR:N	2.42	0.53
5:C:145:GLU:HB2	5:C:188:CYS:HB3	1.89	0.53
17:O:36:THR:HG23	17:O:41:ALA:HB2	1.90	0.53
1:I:63:A:HO2'	35:i:388:ARG:NH2	2.06	0.53
3:A:2547:A:H4'	14:L:29:HIS:CD2	2.44	0.53
3:A:2579:C:O2'	6:D:136:ASN:ND2	2.41	0.53
13:K:98:GLU:OE1	13:K:98:GLU:N	2.41	0.53
21:S:48:LYS:HE3	21:S:103:ALA:HB1	1.90	0.53
23:U:68:LYS:HG3	23:U:77:ARG:NH2	2.23	0.53
3:A:120:U:H4'	3:A:121:G:H5''	1.89	0.53
3:A:1923:U:H2'	3:A:1924:C:C6	2.43	0.53
9:G:104:ASN:ND2	9:G:114:ASP:OD1	2.41	0.53
14:L:40:LYS:HE3	14:L:57:VAL:HG12	1.91	0.53
35:i:217:THR:HB	35:i:242:LEU:HA	1.90	0.53
5:C:145:GLU:HG2	5:C:151:GLY:C	2.34	0.53
11:I:88:HIS:ND1	11:I:89:PRO:O	2.42	0.53
13:K:37:ARG:HG3	13:K:118:MET:HE1	1.90	0.53
33:e:9:GLY:O	33:e:13:ARG:NH2	2.40	0.53
3:A:653:U:H1'	3:A:654:A:H5''	1.91	0.53
35:i:83:VAL:HA	35:i:287:PRO:CB	2.39	0.53
36:k:35:LEU:O	36:k:39:LEU:HB2	2.09	0.53
3:A:2210:U:H4'	3:A:2211:A:H5'	1.91	0.53
1:I:62:C:O2'	35:i:382:SER:O	2.24	0.53
3:A:2171:A:H3'	3:A:2173:A:H8	1.74	0.53
30:b:39:LEU:HB2	30:b:42:HIS:HB2	1.89	0.53
3:A:9:G:O2'	3:A:2800:A:N6	2.42	0.52
3:A:1056:G:H5''	3:A:1057:A:H5'	1.90	0.52
3:A:2086:U:H2'	3:A:2087:G:C8	2.45	0.52
3:A:2637:U:C2'	3:A:2638:G:H5'	2.39	0.52
7:E:28:VAL:O	7:E:32:VAL:HG13	2.09	0.52
10:H:116:ARG:HH21	10:H:133:GLN:HB3	1.74	0.52
35:i:237:ASN:O	35:i:241:PRO:HB3	2.09	0.52
3:A:2808:G:O2'	3:A:2890:G:O6	2.21	0.52
13:K:3:THR:HB	20:R:57:PHE:HE1	1.75	0.52
35:i:273:LEU:HG	35:i:285:PHE:HA	1.91	0.52
35:i:275:VAL:HG22	35:i:281:ALA:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:90:U:H3'	3:A:91:A:H8	1.74	0.52
3:A:1069:A:C2	3:A:1096:A:H5''	2.44	0.52
3:A:2127:G:H2'	3:A:2128:G:C8	2.45	0.52
1:1:68:A:O2'	1:1:69:G:OP1	2.27	0.52
8:F:99:PHE:HD1	8:F:102:ARG:HH22	1.57	0.52
3:A:671:C:H2'	3:A:672:C:H6	1.74	0.52
3:A:1791:A:N6	3:A:1828:G:O2'	2.42	0.52
35:i:146:LYS:HG2	37:l:338:GLU:OE1	2.10	0.52
3:A:1428:C:C5	3:A:1569:A:H5''	2.45	0.52
3:A:1798:U:H5''	5:C:258:ARG:HB2	1.92	0.52
21:S:52:PRO:HG2	21:S:53:PHE:CD2	2.45	0.52
32:d:8:SER:HB3	32:d:11:LYS:HB2	1.92	0.52
35:i:302:UNK:HB2	35:i:353:UNK:O	2.10	0.52
1:1:42:A:N6	1:1:67:A:H62	2.05	0.52
3:A:256:A:H2'	3:A:257:C:H6	1.74	0.52
3:A:679:C:H2'	3:A:680:C:C6	2.44	0.52
3:A:1425:G:H2'	3:A:1426:G:O4'	2.09	0.52
3:A:1993:U:H4'	6:D:133:THR:OG1	2.10	0.52
28:Z:38:GLN:HG3	28:Z:39:GLN:H	1.75	0.52
37:l:298:MET:HG3	37:l:310:ILE:HG12	1.92	0.52
3:A:68:G:H2'	3:A:69:C:O4'	2.10	0.52
3:A:2564:A:OP1	3:A:2648:G:O2'	2.20	0.52
6:D:114:LYS:HD3	6:D:196:ALA:HB2	1.92	0.52
34:f:12:ARG:HB2	34:f:12:ARG:NH1	2.25	0.52
17:O:55:ALA:HA	17:O:80:PHE:CE2	2.45	0.52
35:i:306:UNK:HA	35:i:309:UNK:HG3	1.91	0.52
37:l:326:LEU:HB2	37:l:351:VAL:HG22	1.92	0.52
3:A:1115:G:O2'	3:A:1116:G:H5''	2.10	0.51
8:F:128:TYR:HE2	8:F:130:MET:HG2	1.76	0.51
3:A:364:C:H2'	3:A:365:U:C6	2.45	0.51
3:A:788:A:OP1	3:A:791:C:N4	2.41	0.51
3:A:845:A:H61	3:A:932:U:H3	1.58	0.51
3:A:1421:G:C2	3:A:1422:G:C8	2.98	0.51
3:A:1790:C:H2'	3:A:1791:A:C5	2.45	0.51
7:E:41:GLN:HG2	7:E:43:THR:HG23	1.92	0.51
14:L:7:MET:HE1	14:L:44:LYS:HG3	1.91	0.51
3:A:1289:C:H2'	3:A:1290:C:C6	2.45	0.51
3:A:2720:U:OP1	19:Q:53:ARG:NH2	2.41	0.51
16:N:30:SER:H	16:N:106:ASP:HB3	1.75	0.51
30:b:55:ILE:HG22	30:b:57:LYS:HB2	1.92	0.51
37:l:314:ALA:HB1	37:l:349:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1410:G:H1	3:A:1592:C:H42	1.57	0.51
3:A:1451:C:H1'	3:A:1452:G:C2	2.45	0.51
3:A:2133:G:H21	3:A:2158:A:H62	1.58	0.51
3:A:2439:A:H4'	3:A:2440:C:H5''	1.91	0.51
3:A:2647:U:H2'	3:A:2648:G:H8	1.76	0.51
6:D:184:ARG:NH1	19:Q:7:GLN:OE1	2.40	0.51
7:E:145:ASP:HA	7:E:166:LYS:HB3	1.93	0.51
15:M:4:ASN:OD1	15:M:4:ASN:N	2.39	0.51
21:S:28:ALA:HB3	21:S:31:GLU:HG3	1.93	0.51
22:T:40:ASN:O	22:T:41:LYS:HG2	2.10	0.51
24:V:74:ASN:HD21	24:V:99:ASN:HD21	1.58	0.51
3:A:576:U:H2'	3:A:577:G:C8	2.46	0.51
3:A:1437:C:H2'	3:A:1438:U:C6	2.46	0.51
3:A:1681:G:H21	3:A:1762:A:H3'	1.75	0.51
20:R:76:TYR:CZ	20:R:80:ILE:HG13	2.46	0.51
3:A:499:U:H2'	3:A:500:G:O4'	2.10	0.51
3:A:1405:U:H2'	3:A:1406:U:C6	2.46	0.51
3:A:1825:U:O2	5:C:253:LYS:NZ	2.31	0.51
3:A:1873:G:H2'	3:A:1874:C:H6	1.74	0.51
7:E:24:ASN:ND2	7:E:27:LEU:HB2	2.25	0.51
28:Z:2:LYS:HG3	28:Z:5:GLU:OE1	2.10	0.51
3:A:1000:A:OP2	3:A:1154:G:N1	2.32	0.51
3:A:1414:C:H2'	3:A:1415:U:O4'	2.11	0.51
3:A:2045:C:H4'	30:b:15:MET:HG2	1.93	0.51
33:e:26:HIS:HB3	33:e:44:LEU:HD22	1.93	0.51
35:i:301:UNK:HA	35:i:304:UNK:HG3	1.93	0.51
3:A:898:C:H2'	3:A:899:A:O4'	2.10	0.51
3:A:1132:U:H2'	3:A:1133:A:C8	2.46	0.51
3:A:2271:G:H5''	26:X:18:ALA:HB1	1.93	0.51
8:F:40:VAL:HG11	8:F:43:ALA:HB2	1.92	0.51
37:l:365:PHE:CE2	37:l:407:LEU:HD22	2.45	0.51
3:A:2502:G:H5''	3:A:2503:A:H5''	1.93	0.51
12:J:73:THR:OG1	12:J:113:LYS:NZ	2.40	0.51
3:A:948:C:H2'	3:A:949:G:C8	2.45	0.51
3:A:2024:G:H2'	3:A:2025:C:H6	1.76	0.51
3:A:141:G:H2'	3:A:142:A:O4'	2.11	0.50
3:A:1344:U:HO2'	3:A:1345:C:P	2.34	0.50
8:F:50:LEU:O	8:F:54:ALA:N	2.38	0.50
22:T:23:LEU:HD22	30:b:24:ALA:HB2	1.92	0.50
23:U:7:LEU:HD13	23:U:46:ALA:HA	1.92	0.50
35:i:316:UNK:HG1	35:i:340:GLN:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:i:354:UNK:HG1	36:k:39:LEU:CD2	2.40	0.50
3:A:95:A:O2'	28:Z:41:HIS:N	2.43	0.50
3:A:256:A:H2'	3:A:257:C:C6	2.46	0.50
3:A:1394:U:H4'	3:A:1603:A:H4'	1.92	0.50
12:J:113:LYS:HE3	12:J:116:ASP:HB3	1.92	0.50
16:N:1:MET:HA	16:N:47:GLU:HG3	1.94	0.50
29:a:10:THR:HG22	29:a:11:ARG:HG3	1.93	0.50
33:e:16:LYS:HE3	33:e:20:GLY:HA2	1.93	0.50
3:A:1939:U:OP1	3:A:2604:U:O2'	2.28	0.50
35:i:13:LEU:HD22	35:i:74:PHE:HB3	1.94	0.50
3:A:128:C:H2'	3:A:129:C:C6	2.46	0.50
3:A:2282:G:C6	3:A:2425:A:C2	3.00	0.50
6:D:184:ARG:HH11	19:Q:7:GLN:CD	2.20	0.50
13:K:32:LEU:O	13:K:36:LEU:HB2	2.12	0.50
20:R:65:ILE:HD11	20:R:95:LEU:HB2	1.93	0.50
27:Y:6:GLN:NE2	27:Y:76:GLU:OE2	2.39	0.50
35:i:376:MET:HG2	35:i:416:LEU:HD22	1.93	0.50
35:i:429:LYS:HA	35:i:432:LYS:HE2	1.93	0.50
3:A:90:U:C2	3:A:91:A:N7	2.80	0.50
3:A:1048:A:N1	3:A:1112:G:O2'	2.36	0.50
3:A:2333:A:P	26:X:77:ARG:HH22	2.34	0.50
35:i:259:ALA:HA	35:i:262:ILE:HD12	1.94	0.50
9:G:83:PHE:O	9:G:134:LYS:HA	2.12	0.50
3:A:93:G:H1'	35:i:453:UNK:HB2	1.94	0.50
3:A:239:C:HO2'	3:A:622:G:HO2'	1.58	0.50
3:A:738:G:H1'	3:A:759:G:N2	2.27	0.50
3:A:1927:A:H2'	3:A:1928:A:C8	2.46	0.50
4:B:2:G:H2'	4:B:3:C:C6	2.47	0.50
14:L:64:ARG:NH1	14:L:102:PRO:O	2.44	0.50
15:M:36:LYS:O	15:M:40:SER:HB3	2.11	0.50
1:1:37:U:H2'	1:1:38:U:C6	2.47	0.50
3:A:357:C:H2'	3:A:358:U:C6	2.47	0.50
3:A:878:A:N6	3:A:899:A:O2'	2.45	0.50
3:A:1327:A:N6	3:A:1647:U:O2	2.45	0.50
12:J:83:ALA:O	12:J:105:GLN:NE2	2.45	0.50
19:Q:23:GLY:O	19:Q:90:GLY:HA3	2.11	0.50
24:V:46:GLN:OE1	24:V:54:GLN:NE2	2.44	0.50
37:l:388:GLN:OE1	37:l:388:GLN:N	2.45	0.50
3:A:1088:A:N6	12:J:135:SER:HB3	2.26	0.50
3:A:1638:C:H1'	3:A:2698:U:O2'	2.12	0.50
3:A:2171:A:H5'	3:A:2173:A:N7	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:127:THR:HG22	9:G:128:GLN:H	1.77	0.50
35:i:19:ARG:HD3	35:i:22:LEU:HD13	1.92	0.50
35:i:221:VAL:HG21	35:i:262:ILE:HD13	1.93	0.50
7:E:184:ASP:OD1	7:E:184:ASP:N	2.44	0.49
9:G:8:PRO:HB3	9:G:51:THR:HG22	1.94	0.49
26:X:34:GLY:N	26:X:61:ALA:O	2.37	0.49
3:A:981:A:N1	3:A:2027:G:O2'	2.42	0.49
3:A:1028:A:N3	3:A:2486:C:O2'	2.42	0.49
3:A:2626:C:H2'	3:A:2627:G:O4'	2.12	0.49
3:A:2755:C:C4	34:f:19:ARG:NH1	2.79	0.49
15:M:23:ILE:HG12	21:S:82:HIS:CD2	2.47	0.49
35:i:272:PHE:HB3	35:i:282:LEU:HD11	1.94	0.49
3:A:1506:U:H2'	3:A:1507:C:C6	2.48	0.49
1:l:46:C:H42	1:l:61:G:H3'	1.77	0.49
3:A:2183:A:H2'	3:A:2184:A:C8	2.46	0.49
3:A:2290:G:H2'	3:A:2291:U:O4'	2.12	0.49
10:H:94:ILE:HB	10:H:122:LEU:HB2	1.94	0.49
18:P:30:ARG:HG3	18:P:35:ILE:HD12	1.94	0.49
25:W:75:GLN:HB2	25:W:92:VAL:HG12	1.94	0.49
3:A:27:G:N2	3:A:512:G:H1'	2.28	0.49
3:A:563:A:C4	3:A:2018:G:C2	3.01	0.49
3:A:1790:C:H3'	3:A:1828:G:H22	1.77	0.49
3:A:2151:U:H2'	3:A:2152:G:H8	1.77	0.49
8:F:17:MET:SD	8:F:22:TYR:HB2	2.52	0.49
15:M:19:LEU:HD23	15:M:27:LEU:HD13	1.95	0.49
36:k:36:LEU:O	36:k:40:LEU:HB2	2.12	0.49
37:l:312:LYS:NZ	37:l:474:GLY:O	2.36	0.49
3:A:247:G:O6	33:e:12:LYS:NZ	2.37	0.49
21:S:65:ALA:HB3	21:S:95:ASP:HB2	1.94	0.49
35:i:117:VAL:HG13	35:i:188:LEU:HB3	1.93	0.49
35:i:250:VAL:HG11	35:i:273:LEU:HD22	1.93	0.49
36:k:31:THR:O	36:k:35:LEU:CB	2.61	0.49
3:A:987:C:O2'	3:A:1000:A:N3	2.44	0.49
3:A:2308:G:H3'	3:A:2310:C:OP2	2.11	0.49
5:C:132:MET:HG2	5:C:135:ILE:HD12	1.94	0.49
17:O:14:SER:HA	17:O:17:ARG:NH1	2.27	0.49
3:A:1005:C:H2'	3:A:1006:C:C6	2.47	0.49
3:A:1021:A:H3'	3:A:1021:A:N3	2.27	0.49
3:A:1243:C:H1'	15:M:4:ASN:O	2.13	0.49
3:A:2280:G:O2'	3:A:2388:A:N1	2.37	0.49
3:A:2747:G:O2'	9:G:67:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:101:ASN:ND2	9:G:116:GLN:OE1	2.46	0.49
35:i:276:GLY:N	35:i:281:ALA:HB1	2.27	0.49
3:A:613:A:O2'	3:A:614:A:O5'	2.30	0.49
3:A:1093:G:C2'	3:A:1098:A:H61	2.26	0.49
3:A:1903:G:C2	3:A:1904:G:C8	3.00	0.49
20:R:24:TYR:N	20:R:24:TYR:CD1	2.78	0.49
3:A:136:G:H2'	3:A:137:U:O4'	2.12	0.49
3:A:1179:G:H2'	3:A:1180:U:C6	2.48	0.49
3:A:1535:A:N6	36:k:28:LYS:NZ	2.60	0.49
27:Y:17:ASN:OD1	27:Y:27:ARG:HD2	2.13	0.49
37:l:399:LYS:O	37:l:403:VAL:HG23	2.13	0.49
3:A:467:G:H2'	3:A:468:G:O4'	2.13	0.48
3:A:671:C:H2'	3:A:672:C:C6	2.48	0.48
3:A:1773:A:N7	3:A:1829:A:H1'	2.28	0.48
11:I:33:VAL:HG21	11:I:106:PHE:CE2	2.47	0.48
35:i:337:GLN:HA	35:i:340:GLN:CD	2.38	0.48
3:A:719:C:H2'	3:A:720:U:H6	1.78	0.48
3:A:1132:U:H3'	3:A:1133:A:H5''	1.95	0.48
4:B:116:G:H2'	4:B:117:G:C8	2.49	0.48
8:F:7:TYR:CD1	8:F:11:GLU:HG3	2.48	0.48
12:J:113:LYS:O	12:J:117:MET:N	2.46	0.48
26:X:55:ARG:HE	26:X:55:ARG:HB2	1.45	0.48
3:A:156:A:H2'	3:A:157:C:O4'	2.13	0.48
3:A:184:C:H2'	3:A:185:G:H8	1.77	0.48
1:l:72:A:H2'	1:l:73:G:C8	2.48	0.48
3:A:140:C:H4'	3:A:141:G:OP1	2.13	0.48
3:A:1535:A:N6	36:k:28:LYS:HZ2	2.12	0.48
5:C:260:ASN:OD1	5:C:262:ARG:N	2.37	0.48
13:K:78:THR:HG23	13:K:83:GLY:O	2.13	0.48
14:L:10:VAL:HG12	14:L:12:ASP:H	1.78	0.48
14:L:73:ASP:OD1	14:L:73:ASP:N	2.39	0.48
35:i:369:ASP:HB3	35:i:373:LEU:HD12	1.96	0.48
36:k:34:LEU:HA	36:k:37:LEU:HB2	1.95	0.48
3:A:910:A:H2'	3:A:911:A:C8	2.49	0.48
3:A:911:A:H2'	16:N:9:PHE:HZ	1.78	0.48
3:A:957:C:C5	3:A:959:A:C5	3.01	0.48
3:A:2226:C:H2'	3:A:2227:A:O4'	2.13	0.48
3:A:2834:G:H2'	3:A:2879:A:N6	2.29	0.48
6:D:25:THR:HG21	6:D:193:VAL:HG22	1.95	0.48
8:F:73:SER:OG	8:F:81:GLN:N	2.33	0.48
10:H:115:VAL:HG22	10:H:132:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:31:THR:O	36:k:35:LEU:HB3	2.14	0.48
3:A:208:C:H2'	3:A:209:C:H6	1.78	0.48
3:A:784:G:H5'	3:A:785:G:OP1	2.13	0.48
3:A:1268:A:H2'	3:A:1269:A:O4'	2.13	0.48
3:A:1386:C:H2'	3:A:1387:A:C8	2.49	0.48
3:A:1654:A:H2'	3:A:1655:A:H8	1.79	0.48
7:E:23:PHE:CD1	7:E:111:GLU:HG3	2.48	0.48
9:G:86:LYS:HG2	9:G:132:VAL:HG22	1.96	0.48
16:N:41:LEU:HG	16:N:96:ILE:HG13	1.95	0.48
37:l:420:ASP:CG	37:l:447:LYS:HD2	2.39	0.48
3:A:813:U:H2'	3:A:814:C:C6	2.49	0.48
3:A:995:C:OP2	20:R:54:LYS:NZ	2.44	0.48
3:A:2433:A:H2	27:Y:21:ALA:HB1	1.79	0.48
4:B:7:G:OP1	18:P:4:LYS:NZ	2.27	0.48
13:K:72:LYS:HE3	13:K:74:TYR:CZ	2.49	0.48
27:Y:17:ASN:HB2	27:Y:25:THR:OG1	2.13	0.48
3:A:175:G:N2	3:A:176:A:N3	2.62	0.48
3:A:1527:G:N1	3:A:1544:A:OP2	2.32	0.48
3:A:2483:C:N3	16:N:123:LYS:NZ	2.60	0.48
10:H:110:VAL:HG12	10:H:114:GLU:HB2	1.94	0.48
16:N:11:LYS:HD3	16:N:86:LYS:HD3	1.96	0.48
28:Z:14:LEU:HB3	28:Z:57:LEU:HD21	1.96	0.48
3:A:477:A:H2'	3:A:478:A:C8	2.49	0.48
3:A:1007:C:H5''	13:K:37:ARG:NH2	2.28	0.48
3:A:1085:A:H61	11:I:35:VAL:HG22	1.78	0.48
3:A:2060:A:H3'	7:E:63:LYS:NZ	2.29	0.48
3:A:2073:C:H2'	3:A:2074:U:H6	1.77	0.48
3:A:2158:A:H4'	3:A:2159:G:O5'	2.14	0.48
3:A:2305:U:H5''	8:F:131:GLY:HA3	1.96	0.48
3:A:2809:A:H2'	3:A:2810:A:H8	1.75	0.48
9:G:80:THR:OG1	9:G:81:GLU:N	2.46	0.48
10:H:93:SER:HB3	10:H:123:ARG:HG2	1.95	0.48
35:i:247:LEU:HD13	35:i:259:ALA:HB2	1.95	0.48
3:A:1027:A:C6	3:A:1126:A:C4	3.02	0.48
3:A:1873:G:H2'	3:A:1874:C:C6	2.49	0.48
9:G:102:VAL:HG22	9:G:116:GLN:HE22	1.78	0.48
13:K:58:ASN:ND2	13:K:128:ASN:OD1	2.42	0.48
18:P:51:ALA:HB3	18:P:78:VAL:HG13	1.95	0.48
22:T:7:HIS:CE1	22:T:10:ALA:HB2	2.49	0.48
26:X:40:GLN:NE2	26:X:43:THR:HA	2.29	0.48
35:i:380:ILE:HG22	35:i:388:ARG:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1846:G:H5''	3:A:1847:A:OP2	2.14	0.47
8:F:25:VAL:O	8:F:28:VAL:HG12	2.14	0.47
35:i:43:VAL:O	35:i:48:VAL:HG23	2.15	0.47
3:A:1819:A:H5''	5:C:160:THR:HG21	1.94	0.47
3:A:2116:G:C5	3:A:2165:C:N4	2.82	0.47
3:A:2428:G:H21	15:M:60:ARG:NH2	2.12	0.47
12:J:42:PHE:O	12:J:46:THR:OG1	2.32	0.47
24:V:14:LEU:HD11	24:V:71:ALA:HB2	1.95	0.47
3:A:1446:C:H2'	3:A:1447:C:C6	2.49	0.47
3:A:1606:C:H5'	3:A:1607:C:OP1	2.13	0.47
18:P:31:THR:HG23	18:P:32:PRO:HD2	1.96	0.47
23:U:68:LYS:HG3	23:U:77:ARG:HH21	1.79	0.47
31:c:9:ILE:HD13	31:c:25:LYS:HB2	1.95	0.47
35:i:331:LEU:HD22	35:i:380:ILE:HD13	1.95	0.47
3:A:160:A:N3	3:A:2208:C:O2'	2.42	0.47
3:A:428:A:H2'	3:A:429:A:C8	2.49	0.47
3:A:483:A:O4'	24:V:45:HIS:HB3	2.14	0.47
3:A:914:G:H5'	3:A:915:C:OP2	2.14	0.47
15:M:55:MET:SD	15:M:56:PRO:HD2	2.55	0.47
17:O:38:LEU:HB3	17:O:39:PRO:HD3	1.96	0.47
23:U:58:VAL:HG22	23:U:85:VAL:HG22	1.96	0.47
36:k:39:LEU:O	36:k:42:THR:N	2.46	0.47
37:l:429:SER:HA	37:l:432:LYS:HG3	1.97	0.47
3:A:358:U:H2'	3:A:359:G:C8	2.44	0.47
3:A:481:G:O2'	3:A:507:A:N1	2.45	0.47
3:A:782:A:N7	5:C:220:VAL:HG21	2.29	0.47
3:A:1110:G:HO2'	3:A:1111:A:P	2.38	0.47
3:A:2570:G:H2'	3:A:2571:U:O4'	2.14	0.47
9:G:35:ARG:CD	9:G:71:LEU:HD13	2.43	0.47
1:1:53:G:C6	1:1:55:A:OP2	2.68	0.47
1:1:54:G:P	37:l:406:LYS:HD2	2.55	0.47
3:A:2419:U:O2'	3:A:2420:C:H5'	2.15	0.47
3:A:2431:U:H5	3:A:2433:A:H5''	1.79	0.47
5:C:200:HIS:C	5:C:200:HIS:CD2	2.92	0.47
11:I:85:VAL:HG22	11:I:92:ALA:HB2	1.96	0.47
18:P:30:ARG:HB3	18:P:97:PHE:CE1	2.50	0.47
3:A:1438:U:H2'	3:A:1439:A:H8	1.79	0.47
3:A:1672:A:C6	3:A:1673:G:C6	3.03	0.47
3:A:1808:A:H3'	3:A:1809:A:H8	1.79	0.47
3:A:2347:C:O2'	31:c:39:PHE:HB3	2.14	0.47
3:A:2592:G:C6	3:A:2593:U:N3	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2786:U:H2'	3:A:2787:C:H6	1.79	0.47
6:D:121:THR:HB	6:D:127:PHE:CD2	2.50	0.47
10:H:142:VAL:HG12	10:H:143:ILE:H	1.79	0.47
12:J:28:LEU:HD11	12:J:33:VAL:HG11	1.97	0.47
12:J:40:LYS:N	12:J:40:LYS:HD2	2.30	0.47
19:Q:106:LYS:O	19:Q:109:ARG:NH2	2.45	0.47
24:V:41:LEU:HD22	24:V:62:GLU:HG2	1.96	0.47
35:i:115:THR:HG22	35:i:119:LYS:HE3	1.97	0.47
35:i:172:VAL:HG21	35:i:208:VAL:HG13	1.96	0.47
3:A:75:G:H4'	28:Z:48:ARG:CZ	2.45	0.47
3:A:1387:A:H5'	3:A:1469:A:H1'	1.97	0.47
3:A:1420:A:N7	3:A:2211:A:N6	2.62	0.47
3:A:2209:G:H1	3:A:2215:C:N4	2.11	0.47
4:B:116:G:H2'	4:B:117:G:H8	1.80	0.47
6:D:56:LYS:HB2	6:D:59:ARG:HB2	1.96	0.47
8:F:4:LEU:HD23	8:F:4:LEU:HA	1.73	0.47
25:W:25:LYS:HE2	25:W:25:LYS:HB3	1.71	0.47
27:Y:40:VAL:HG12	27:Y:43:GLU:H	1.80	0.47
3:A:112:U:H5'	28:Z:58:ASN:HD21	1.80	0.47
3:A:247:G:H4'	3:A:386:G:C5	2.50	0.47
3:A:871:U:H2'	3:A:872:U:C6	2.50	0.47
3:A:998:C:H2'	3:A:999:U:O4'	2.14	0.47
3:A:1097:U:H2'	3:A:1098:A:O4'	2.15	0.47
3:A:2444:G:OP2	7:E:63:LYS:HD2	2.14	0.47
7:E:149:ILE:HB	7:E:188:MET:HG2	1.96	0.47
12:J:10:LYS:O	12:J:11:LEU:HD12	2.15	0.47
17:O:25:ALA:O	17:O:29:VAL:HG23	2.15	0.47
18:P:43:ASN:ND2	18:P:43:ASN:H	2.13	0.47
29:a:31:ARG:HG2	29:a:34:HIS:HB2	1.97	0.47
35:i:258:ALA:O	35:i:261:SER:OG	2.18	0.47
35:i:354:UNK:HB2	35:i:357:UNK:HG3	1.95	0.47
3:A:630:G:N2	3:A:633:A:OP2	2.43	0.47
3:A:713:G:H2'	3:A:714:U:C6	2.50	0.47
3:A:795:C:H2'	3:A:796:C:C6	2.49	0.47
3:A:1028:A:N6	3:A:1125:G:H2'	2.30	0.47
3:A:1060:U:C2	3:A:1062:G:H5'	2.50	0.47
3:A:1416:G:N2	3:A:1582:C:O2	2.33	0.47
3:A:2788:C:H2'	3:A:2789:C:C6	2.50	0.47
5:C:252:THR:OG1	5:C:253:LYS:N	2.48	0.47
13:K:114:LEU:O	13:K:118:MET:HG3	2.14	0.47
20:R:18:LEU:HD11	20:R:32:TYR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:38:VAL:O	21:S:54:VAL:HG23	2.15	0.47
33:e:29:LEU:HD12	33:e:29:LEU:HA	1.57	0.47
3:A:323:C:C4	3:A:333:G:C8	3.03	0.46
3:A:911:A:H2'	16:N:9:PHE:CZ	2.50	0.46
3:A:2392:A:H2	15:M:55:MET:HE3	1.81	0.46
7:E:125:SER:OG	7:E:126:VAL:N	2.46	0.46
10:H:29:PHE:O	10:H:32:PRO:HD2	2.15	0.46
11:I:27:VAL:HG13	11:I:80:THR:HG23	1.97	0.46
27:Y:62:LYS:HE3	27:Y:66:THR:HG21	1.96	0.46
35:i:6:THR:O	35:i:10:SER:OG	2.32	0.46
3:A:125:A:OP2	32:d:19:ARG:HD3	2.15	0.46
3:A:127:A:H5''	3:A:128:C:O4'	2.14	0.46
3:A:796:C:H2'	3:A:797:G:C8	2.51	0.46
3:A:825:A:C2	3:A:833:A:C2	3.03	0.46
3:A:975:A:H1'	3:A:990:A:C2	2.50	0.46
3:A:1341:G:O2'	23:U:59:ASN:ND2	2.47	0.46
30:b:36:GLU:OE2	30:b:46:ASP:HB2	2.15	0.46
1:l:47:A:OP2	1:l:61:G:N1	2.48	0.46
3:A:532:A:N3	3:A:532:A:H2'	2.31	0.46
3:A:1149:G:H2'	3:A:1150:C:C6	2.50	0.46
3:A:2126:A:H61	3:A:2163:A:H5'	1.80	0.46
3:A:2339:C:H2'	3:A:2340:A:H8	1.81	0.46
11:I:39:THR:HG22	11:I:43:LYS:HE3	1.98	0.46
15:M:70:LYS:O	15:M:74:THR:OG1	2.31	0.46
25:W:2:PHE:HB3	25:W:50:MET:CE	2.44	0.46
26:X:41:ARG:HD3	26:X:41:ARG:HA	1.53	0.46
29:a:17:LEU:HD23	29:a:17:LEU:HA	1.76	0.46
31:c:17:THR:HG21	31:c:42:VAL:HB	1.98	0.46
33:e:24:HIS:ND1	33:e:25:LYS:O	2.43	0.46
35:i:95:LEU:HD23	35:i:271:LYS:HE3	1.97	0.46
37:l:365:PHE:CE1	37:l:407:LEU:HB2	2.49	0.46
3:A:857:G:H2'	3:A:858:G:O4'	2.16	0.46
3:A:861:A:C6	3:A:917:A:C8	3.03	0.46
3:A:1038:G:H2'	3:A:1039:A:C8	2.50	0.46
3:A:1062:G:N2	12:J:93:PRO:HG2	2.30	0.46
3:A:1689:A:C6	3:A:1700:A:C2	3.03	0.46
3:A:1799:G:C5	5:C:176:LEU:HD13	2.50	0.46
3:A:2039:U:H2'	3:A:2040:G:C8	2.50	0.46
3:A:2557:G:H2'	3:A:2558:C:C6	2.49	0.46
5:C:232:HIS:NE2	5:C:244:PRO:HA	2.30	0.46
12:J:75:PRO:HD2	12:J:78:VAL:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:122:ILE:O	12:J:126:THR:OG1	2.22	0.46
13:K:95:ARG:HG2	13:K:96:ARG:N	2.29	0.46
19:Q:88:ARG:NH2	19:Q:112:GLU:HB2	2.31	0.46
20:R:49:ASP:HA	20:R:52:GLN:HB2	1.96	0.46
35:i:16:ILE:HA	35:i:19:ARG:HH11	1.80	0.46
35:i:372:VAL:O	35:i:376:MET:HG3	2.16	0.46
3:A:880:G:N2	3:A:898:C:C2	2.84	0.46
3:A:1709:U:H2'	3:A:1710:G:H8	1.80	0.46
14:L:25:LEU:HA	14:L:25:LEU:HD23	1.67	0.46
22:T:25:ARG:NH2	22:T:74:ILE:O	2.49	0.46
35:i:222:ASP:O	35:i:225:THR:OG1	2.33	0.46
35:i:310:UNK:HA	35:i:313:UNK:CG	2.46	0.46
3:A:144:A:H1'	23:U:3:ARG:HH22	1.80	0.46
3:A:1848:A:H3'	3:A:1849:G:H8	1.80	0.46
3:A:1946:U:H2'	3:A:1947:C:C6	2.51	0.46
9:G:148:LEU:HD23	9:G:148:LEU:HA	1.71	0.46
18:P:53:THR:HB	18:P:65:THR:HB	1.98	0.46
30:b:52:ARG:HB3	30:b:54:VAL:HG13	1.98	0.46
35:i:205:ILE:HD13	35:i:208:VAL:HG21	1.96	0.46
3:A:96:C:H4'	28:Z:41:HIS:CD2	2.50	0.46
3:A:1342:A:C6	3:A:1397:U:C5	3.04	0.46
11:I:30:SER:HB3	11:I:81:LEU:HB2	1.98	0.46
16:N:133:LYS:HB3	16:N:133:LYS:HE3	1.42	0.46
18:P:18:LEU:HA	18:P:18:LEU:HD23	1.71	0.46
23:U:87:LEU:HD13	23:U:93:LEU:CD1	2.42	0.46
35:i:394:ILE:HA	35:i:398:ARG:HD2	1.98	0.46
3:A:92:U:H3	35:i:453:UNK:HB1	1.80	0.46
3:A:1510:G:H2'	3:A:1511:G:H8	1.79	0.46
3:A:2821:A:H2'	3:A:2822:G:C8	2.51	0.46
5:C:33:LEU:HD23	5:C:33:LEU:HA	1.58	0.46
35:i:28:LYS:HA	35:i:31:LEU:HD12	1.97	0.46
35:i:39:LEU:O	37:l:425:GLN:HG3	2.16	0.46
3:A:789:A:C4	32:d:3:ARG:NH1	2.84	0.46
3:A:861:A:H2'	3:A:862:G:O4'	2.15	0.46
3:A:2069:G:N2	3:A:2443:C:C2	2.83	0.46
3:A:2524:G:H2'	3:A:2525:G:O4'	2.16	0.46
6:D:207:VAL:HG13	6:D:208:LYS:HG3	1.98	0.46
10:H:40:THR:HG22	10:H:41:LYS:H	1.80	0.46
18:P:88:LYS:HG2	18:P:116:GLN:HB2	1.98	0.46
29:a:56:LYS:NZ	29:a:58:GLU:HG2	2.31	0.46
35:i:33:GLU:O	35:i:37:ALA:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:419:ILE:O	37:l:445:LEU:HD12	2.16	0.46
3:A:1022:G:O2'	3:A:1024:G:O6	2.27	0.46
3:A:1508:A:O2'	3:A:1509:A:O4'	2.19	0.46
4:B:95:U:H2'	4:B:96:G:H8	1.81	0.46
9:G:42:GLU:CG	9:G:55:ARG:HH21	2.29	0.46
11:I:53:ARG:O	11:I:81:LEU:HD12	2.16	0.46
20:R:17:ILE:HA	20:R:17:ILE:HD13	1.63	0.46
24:V:81:ASP:OD2	24:V:96:PHE:HB3	2.16	0.46
35:i:259:ALA:HA	35:i:262:ILE:HB	1.98	0.46
35:i:316:UNK:HB2	35:i:340:GLN:OE1	2.16	0.46
3:A:1570:A:H5'	5:C:36:LYS:HB2	1.98	0.45
3:A:1869:G:N2	3:A:1873:G:C5	2.83	0.45
3:A:2327:A:H2'	3:A:2328:A:C8	2.51	0.45
5:C:160:THR:O	5:C:195:VAL:HG23	2.17	0.45
14:L:66:LYS:HE2	14:L:66:LYS:HB3	1.64	0.45
14:L:79:PHE:CD1	19:Q:70:VAL:HG22	2.46	0.45
16:N:66:ARG:HB2	16:N:101:VAL:O	2.16	0.45
35:i:289:ARG:O	35:i:293:ARG:HB2	2.16	0.45
37:l:301:VAL:HA	37:l:386:ARG:O	2.16	0.45
3:A:141:G:C8	3:A:141:G:H3'	2.51	0.45
3:A:483:A:H5''	24:V:47:LYS:HG2	1.97	0.45
3:A:594:U:H2'	3:A:595:C:C6	2.51	0.45
3:A:2344:U:OP1	31:c:37:LYS:HD2	2.16	0.45
9:G:121:ILE:HD13	9:G:135:GLY:HA3	1.98	0.45
15:M:27:LEU:O	15:M:31:GLY:HA2	2.17	0.45
37:l:325:MET:O	37:l:379:LEU:HD12	2.16	0.45
3:A:629:G:H5''	3:A:650:C:O2'	2.16	0.45
3:A:772:C:H2'	3:A:773:U:C6	2.52	0.45
3:A:1545:A:H2'	3:A:1546:G:O4'	2.17	0.45
3:A:1653:G:H3'	17:O:2:ARG:HG3	1.98	0.45
3:A:2052:A:OP1	6:D:146:ILE:HG12	2.17	0.45
8:F:20:PHE:CZ	8:F:165:GLU:HA	2.51	0.45
27:Y:77:LYS:HD2	27:Y:77:LYS:HA	1.66	0.45
1:l:42:A:H61	1:l:67:A:N6	2.10	0.45
3:A:111:A:H2'	3:A:112:U:O4'	2.16	0.45
3:A:706:A:C2	3:A:707:G:H1'	2.52	0.45
3:A:878:A:H5'	3:A:879:G:OP2	2.16	0.45
3:A:1313:U:H2'	3:A:1610:A:C2	2.51	0.45
3:A:1785:A:O2'	3:A:1786:A:H2'	2.16	0.45
22:T:13:SER:O	22:T:17:VAL:HG23	2.17	0.45
35:i:303:UNK:HA	35:i:306:UNK:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:425:GLN:H	37:l:425:GLN:HG2	1.51	0.45
3:A:77:G:H2'	3:A:78:U:O4'	2.16	0.45
3:A:718:A:H2'	3:A:719:C:O4'	2.16	0.45
3:A:831:G:H5''	15:M:37:GLY:HA2	1.97	0.45
3:A:1706:C:O2'	3:A:1757:A:H5'	2.17	0.45
3:A:2229:U:H2'	3:A:2230:G:C8	2.51	0.45
3:A:2230:G:H2'	3:A:2231:U:C6	2.51	0.45
3:A:2313:C:H5''	8:F:88:LYS:HD3	1.98	0.45
34:f:1:MET:HE2	34:f:1:MET:HB2	1.75	0.45
35:i:272:PHE:HA	35:i:285:PHE:H	1.82	0.45
35:i:419:GLN:O	35:i:423:MET:HG2	2.17	0.45
1:l:40:C:H3'	1:l:41:C:H5''	1.98	0.45
3:A:764:A:H5'	5:C:209:GLY:HA2	1.98	0.45
3:A:1086:A:H4'	3:A:1103:A:C2	2.52	0.45
3:A:1972:G:H2'	3:A:1973:G:H8	1.81	0.45
3:A:2646:C:OP2	3:A:2732:G:O2'	2.35	0.45
3:A:2667:C:H1'	9:G:109:PHE:CD1	2.52	0.45
6:D:7:LYS:HB3	6:D:7:LYS:HE2	1.78	0.45
6:D:49:GLN:HA	6:D:80:TRP:O	2.16	0.45
6:D:99:GLU:OE2	6:D:182:ALA:HB2	2.15	0.45
8:F:136:ILE:HG22	8:F:141:ILE:HG21	1.98	0.45
13:K:65:THR:O	13:K:68:LYS:HB2	2.17	0.45
26:X:23:VAL:HG22	26:X:38:VAL:HB	1.99	0.45
35:i:89:GLU:HA	35:i:286:HIS:CD2	2.51	0.45
35:i:166:GLN:HB2	35:i:171:ILE:HD11	1.99	0.45
3:A:2683:C:H4'	6:D:13:ARG:HH12	1.81	0.45
17:O:2:ARG:HB3	17:O:2:ARG:CZ	2.46	0.45
21:S:4:VAL:HA	21:S:12:HIS:O	2.17	0.45
28:Z:27:ASN:O	28:Z:31:GLN:HG3	2.16	0.45
31:c:33:LYS:HA	31:c:33:LYS:HD3	1.74	0.45
35:i:245:VAL:HB	35:i:270:ILE:HG12	1.99	0.45
37:l:286:LEU:HD23	37:l:317:PHE:HZ	1.82	0.45
3:A:208:C:H2'	3:A:209:C:C6	2.52	0.45
3:A:1287:A:H3'	3:A:1288:G:N2	2.32	0.45
3:A:2165:C:H2'	3:A:2166:U:O4'	2.16	0.45
3:A:2396:G:N3	3:A:2421:G:N2	2.64	0.45
12:J:80:LEU:HB3	12:J:138:LEU:CD1	2.46	0.45
20:R:105:ALA:HB1	21:S:40:MET:HE1	1.98	0.45
25:W:83:LYS:HB3	25:W:85:LYS:HG3	1.98	0.45
3:A:181:A:H1'	3:A:435:C:O4'	2.17	0.45
3:A:1177:G:H2'	3:A:1178:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1848:A:N3	3:A:1849:G:C8	2.85	0.45
3:A:2318:G:C6	3:A:2319:G:N1	2.85	0.45
10:H:62:LEU:HD23	10:H:135:HIS:CD2	2.52	0.45
11:I:41:LEU:HB2	11:I:99:PHE:CE1	2.52	0.45
12:J:117:MET:HB2	12:J:125:MET:HG2	1.99	0.45
19:Q:53:ARG:HB2	19:Q:56:HIS:HB2	1.99	0.45
22:T:28:LYS:HB2	22:T:28:LYS:HE2	1.41	0.45
1:I:54:G:H2'	1:I:55:A:O4'	2.17	0.45
3:A:499:U:H5''	24:V:43:LYS:HE3	1.99	0.45
3:A:1466:U:H5''	3:A:1467:U:H5'	1.98	0.45
3:A:1918:A:O2'	3:A:1920:C:N4	2.50	0.45
3:A:2569:G:C2	3:A:2570:G:C8	3.05	0.45
12:J:86:ILE:CD1	12:J:138:LEU:HD21	2.46	0.45
13:K:69:ARG:O	13:K:89:PHE:HB3	2.17	0.45
15:M:10:GLU:OE2	15:M:11:GLY:N	2.50	0.45
16:N:65:ILE:HG12	16:N:103:TYR:CD2	2.51	0.45
17:O:17:ARG:HG2	17:O:21:PHE:HE2	1.82	0.45
21:S:27:ILE:HG22	21:S:28:ALA:O	2.17	0.45
35:i:341:MET:HA	35:i:344:MET:HE3	1.98	0.45
3:A:239:C:H2'	3:A:240:C:O4'	2.16	0.44
3:A:257:C:H2'	3:A:258:G:O4'	2.15	0.44
3:A:356:G:H2'	3:A:357:C:O4'	2.18	0.44
3:A:657:U:H2'	3:A:658:U:C6	2.52	0.44
3:A:1563:U:H2'	3:A:1564:C:C6	2.51	0.44
3:A:2273:A:H2'	3:A:2274:A:C8	2.52	0.44
9:G:42:GLU:HG3	9:G:55:ARG:HH21	1.83	0.44
10:H:100:ALA:O	10:H:104:THR:HG23	2.17	0.44
19:Q:100:LEU:HA	19:Q:100:LEU:HD23	1.67	0.44
21:S:40:MET:HE3	21:S:47:VAL:HG13	1.99	0.44
23:U:34:VAL:HG21	23:U:43:ILE:HD11	1.99	0.44
3:A:2396:G:C2	3:A:2421:G:C2	3.05	0.44
5:C:141:VAL:HG12	5:C:192:LEU:HA	1.99	0.44
9:G:155:GLU:OE1	9:G:157:TYR:N	2.45	0.44
9:G:155:GLU:OE2	9:G:158:LYS:N	2.48	0.44
14:L:99:ILE:HG12	14:L:118:LEU:HB2	1.98	0.44
25:W:21:ARG:HE	25:W:87:GLN:HA	1.83	0.44
26:X:36:ILE:HG23	26:X:58:THR:HG23	2.00	0.44
3:A:93:G:N2	35:i:450:UNK:HG2	2.32	0.44
3:A:154:U:H2'	3:A:155:A:C8	2.52	0.44
3:A:198:C:O2'	3:A:199:A:H5'	2.17	0.44
3:A:1858:A:H2'	3:A:1859:U:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2130:U:O2'	3:A:2133:G:O2'	2.32	0.44
9:G:117:LEU:HD13	9:G:121:ILE:HG22	1.99	0.44
12:J:130:GLU:HB3	12:J:134:ARG:NH2	2.32	0.44
19:Q:89:ARG:HB3	19:Q:113:ARG:NH1	2.32	0.44
24:V:37:GLU:O	24:V:39:ILE:HG12	2.17	0.44
3:A:593:U:H2'	3:A:594:U:C6	2.52	0.44
16:N:90:GLU:HB3	16:N:91:TYR:CD1	2.52	0.44
35:i:10:SER:O	35:i:14:ARG:CB	2.54	0.44
35:i:387:GLU:HG2	35:i:398:ARG:HH11	1.82	0.44
1:1:34:U:H2'	1:1:35:G:C8	2.52	0.44
3:A:2134:A:H1'	3:A:2159:G:H21	1.82	0.44
3:A:2489:U:C4	3:A:2490:G:C6	3.06	0.44
3:A:2776:A:C8	3:A:2782:G:C5	3.05	0.44
7:E:1:MET:HE3	7:E:1:MET:HB2	1.88	0.44
35:i:5:LEU:HG	35:i:9:LEU:HG	2.00	0.44
35:i:209:HIS:CE1	35:i:240:LEU:HG	2.53	0.44
3:A:149:A:C2	3:A:150:U:C2	3.06	0.44
3:A:1450:G:C6	3:A:1451:C:N4	2.86	0.44
3:A:1962:C:H4'	3:A:1963:U:C5	2.52	0.44
3:A:2038:G:H2'	3:A:2039:U:O4'	2.17	0.44
17:O:86:ARG:HD3	17:O:121:LYS:HG3	1.98	0.44
23:U:31:VAL:O	23:U:32:LEU:HD23	2.18	0.44
35:i:288:ASP:O	35:i:292:SER:OG	2.35	0.44
37:l:421:ALA:HA	37:l:445:LEU:HD11	1.99	0.44
3:A:172:A:H2'	3:A:173:A:H8	1.81	0.44
3:A:566:U:H5''	15:M:29:LYS:HE3	1.99	0.44
3:A:620:G:H4'	3:A:621:A:O5'	2.17	0.44
3:A:1082:U:O2'	11:I:39:THR:HG23	2.18	0.44
3:A:1205:A:H2'	7:E:165:HIS:HE1	1.83	0.44
3:A:1420:A:N7	3:A:2211:A:C6	2.86	0.44
3:A:1542:U:H2'	3:A:1543:G:O4'	2.18	0.44
3:A:2433:A:H5'	3:A:2434:A:P	2.57	0.44
3:A:2667:C:H1'	9:G:109:PHE:HD1	1.82	0.44
3:A:2683:C:H4'	6:D:13:ARG:NH1	2.33	0.44
8:F:48:LYS:HE2	8:F:48:LYS:HB2	1.85	0.44
3:A:57:C:H2'	3:A:58:G:O4'	2.18	0.44
3:A:277:G:H4'	3:A:278:A:N7	2.33	0.44
3:A:2377:A:H2'	3:A:2378:A:C8	2.53	0.44
3:A:2443:C:H2'	3:A:2444:G:H8	1.82	0.44
10:H:26:ALA:HA	10:H:30:LEU:HB2	1.98	0.44
18:P:52:SER:O	18:P:58:ILE:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:463:G:N1	3:A:467:G:C6	2.86	0.44
3:A:948:C:H1'	3:A:984:A:C8	2.52	0.44
3:A:1056:G:H1'	3:A:1103:A:N6	2.33	0.44
3:A:1198:U:H2'	3:A:1199:U:C6	2.52	0.44
3:A:1591:A:H2'	3:A:1592:C:C6	2.53	0.44
3:A:2230:G:H1'	27:Y:32:ASN:HB2	1.99	0.44
3:A:2292:U:H2'	3:A:2293:G:C8	2.52	0.44
3:A:2654:A:OP1	3:A:2654:A:H8	2.01	0.44
3:A:2678:C:H2'	3:A:2679:A:O4'	2.18	0.44
3:A:2704:C:H2'	3:A:2705:A:O4'	2.17	0.44
3:A:2742:G:P	34:f:24:ARG:HH12	2.40	0.44
12:J:90:SER:HB2	12:J:136:MET:O	2.18	0.44
14:L:17:ARG:HA	14:L:17:ARG:HD3	1.77	0.44
16:N:97:GLN:CD	16:N:97:GLN:N	2.76	0.44
21:S:91:GLN:NE2	21:S:92:TRP:H	2.16	0.44
23:U:88:LYS:C	23:U:90:GLY:N	2.76	0.44
29:a:9:GLN:HB2	29:a:29:LEU:HD13	2.00	0.44
3:A:372:G:O2'	3:A:400:G:O6	2.31	0.43
3:A:870:U:OP1	16:N:6:ARG:NH1	2.51	0.43
3:A:1093:G:H1'	3:A:1099:G:N1	2.32	0.43
3:A:1710:G:H2'	3:A:1711:A:C8	2.53	0.43
3:A:2387:U:H1'	26:X:41:ARG:NH1	2.33	0.43
3:A:2786:U:H2'	3:A:2787:C:C6	2.53	0.43
7:E:121:VAL:O	7:E:189:THR:HA	2.18	0.43
7:E:128:ALA:O	7:E:130:LYS:N	2.51	0.43
10:H:46:PHE:HD1	10:H:50:ARG:NH2	2.16	0.43
17:O:28:LEU:O	17:O:32:GLU:N	2.45	0.43
3:A:1853:A:N6	3:A:1888:G:O2'	2.51	0.43
3:A:2533:U:OP1	3:A:2665:A:O2'	2.34	0.43
8:F:67:ILE:HD12	8:F:84:PRO:HB3	2.00	0.43
17:O:72:ASP:OD1	17:O:73:ASN:N	2.51	0.43
21:S:4:VAL:HG12	21:S:39:LEU:HB2	2.00	0.43
37:l:435:HIS:HA	37:l:440:LEU:HG	2.00	0.43
3:A:11:C:H2'	3:A:12:U:H5'	2.00	0.43
3:A:14:A:C6	3:A:526:A:C2	3.07	0.43
3:A:677:A:O2'	3:A:2071:A:H5'	2.17	0.43
3:A:783:A:C5	3:A:785:G:H1'	2.53	0.43
3:A:1082:U:H4'	11:I:46:ARG:NH1	2.32	0.43
3:A:1287:A:H5'	17:O:103:ARG:HD2	1.98	0.43
3:A:1517:G:C2	3:A:1732:C:N3	2.86	0.43
3:A:2024:G:H2'	3:A:2025:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2172:U:H4'	3:A:2173:A:H5'	2.00	0.43
3:A:2512:C:H5''	3:A:2513:A:OP2	2.17	0.43
5:C:205:LEU:HA	5:C:205:LEU:HD23	1.68	0.43
6:D:131:ASP:O	6:D:140:HIS:HD2	2.02	0.43
19:Q:62:ARG:NH2	19:Q:101:ARG:HG2	2.32	0.43
24:V:49:VAL:HA	24:V:50:PRO:HD3	1.84	0.43
27:Y:59:ILE:HG12	27:Y:67:VAL:HG21	1.99	0.43
37:l:420:ASP:OD2	37:l:447:LYS:HD2	2.19	0.43
3:A:834:G:C2	3:A:835:C:C2	3.06	0.43
3:A:997:G:H5''	20:R:92:ARG:NH1	2.33	0.43
3:A:1266:G:N2	3:A:2012:G:H2'	2.33	0.43
3:A:1301:A:H2'	3:A:1301:A:N3	2.33	0.43
3:A:1354:A:H2'	3:A:1355:G:O4'	2.19	0.43
3:A:1614:A:C2	22:T:93:ALA:HB2	2.52	0.43
5:C:176:LEU:HD23	5:C:176:LEU:HA	1.80	0.43
8:F:128:TYR:CE2	8:F:130:MET:HG2	2.53	0.43
8:F:147:ASP:OD1	8:F:150:ARG:NH2	2.51	0.43
11:I:93:ALA:O	11:I:97:LYS:NZ	2.41	0.43
13:K:26:GLY:O	13:K:30:THR:HG23	2.18	0.43
20:R:24:TYR:O	20:R:29:SER:HB3	2.19	0.43
35:i:86:MET:HE1	35:i:259:ALA:HB3	2.00	0.43
35:i:285:PHE:CG	35:i:286:HIS:N	2.86	0.43
37:l:425:GLN:O	37:l:428:VAL:HB	2.18	0.43
3:A:195:A:H5''	15:M:47:ARG:HH22	1.84	0.43
3:A:464:U:C2	3:A:788:A:C6	3.07	0.43
3:A:493:G:H2'	3:A:494:G:O4'	2.19	0.43
3:A:819:A:N3	3:A:819:A:H2'	2.34	0.43
3:A:969:G:H2'	3:A:970:U:C6	2.53	0.43
3:A:1627:G:C2	3:A:1628:G:C8	3.07	0.43
3:A:2144:G:N2	3:A:2148:G:O6	2.52	0.43
5:C:251:GLN:HE21	5:C:251:GLN:HB2	1.58	0.43
11:I:118:ILE:HA	11:I:119:PRO:HD2	1.84	0.43
15:M:80:SER:O	15:M:84:LYS:HE3	2.19	0.43
19:Q:25:THR:HB	19:Q:88:ARG:HG2	1.99	0.43
23:U:34:VAL:HG11	23:U:43:ILE:HD13	2.01	0.43
34:f:22:VAL:HG12	34:f:24:ARG:HG3	2.00	0.43
1:l:69:G:H2'	1:l:70:G:C1'	2.48	0.43
3:A:112:U:H5'	28:Z:58:ASN:ND2	2.34	0.43
3:A:307:G:N1	3:A:310:A:OP2	2.51	0.43
3:A:543:G:H5'	3:A:544:C:OP2	2.18	0.43
3:A:1327:A:H2'	3:A:1328:A:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1494:A:H2'	3:A:1495:A:H8	1.83	0.43
3:A:2047:C:O2'	3:A:2823:A:N1	2.42	0.43
3:A:2114:A:C2	3:A:2166:U:H2'	2.54	0.43
5:C:153:GLN:O	5:C:156:ARG:HG3	2.18	0.43
10:H:104:THR:HA	10:H:108:VAL:O	2.18	0.43
12:J:110:ALA:O	12:J:114:ALA:HB2	2.18	0.43
16:N:26:VAL:HB	16:N:133:LYS:HB2	2.00	0.43
20:R:117:LEU:HD23	20:R:117:LEU:HA	1.77	0.43
22:T:7:HIS:CD2	22:T:7:HIS:C	2.96	0.43
28:Z:42:LEU:HA	28:Z:42:LEU:HD23	1.81	0.43
35:i:77:ILE:O	35:i:81:GLU:HB2	2.19	0.43
37:l:330:ASP:OD2	37:l:336:ALA:HB2	2.16	0.43
3:A:93:G:H2'	3:A:94:A:H8	1.84	0.43
3:A:141:G:C8	3:A:142:A:O4'	2.72	0.43
3:A:686:U:O4	32:d:12:ARG:NH1	2.52	0.43
3:A:1230:A:H2'	3:A:1231:U:O4'	2.18	0.43
3:A:1387:A:H2'	3:A:1388:G:O4'	2.18	0.43
3:A:1434:A:C2	3:A:1435:G:C5	3.07	0.43
3:A:1515:A:H3'	3:A:1516:G:H8	1.84	0.43
3:A:1667:G:N2	3:A:1992:G:OP2	2.44	0.43
5:C:8:PRO:HB3	5:C:14:ARG:HG3	1.99	0.43
5:C:90:ASN:ND2	5:C:197:ASN:HB2	2.34	0.43
10:H:8:LYS:HE3	10:H:8:LYS:HB3	1.87	0.43
17:O:22:ARG:HE	17:O:22:ARG:HB2	1.49	0.43
22:T:47:VAL:HG22	22:T:103:ILE:HD13	2.00	0.43
25:W:21:ARG:HH21	25:W:87:GLN:C	2.22	0.43
3:A:973:A:OP2	21:S:81:LYS:HE3	2.18	0.43
3:A:1400:U:H2'	3:A:1401:G:O4'	2.19	0.43
3:A:1735:A:H2'	3:A:1736:U:O4'	2.18	0.43
3:A:1759:A:C2	3:A:2697:G:H1'	2.54	0.43
3:A:2518:A:H2'	3:A:2518:A:N3	2.34	0.43
3:A:2790:U:H5'	3:A:2893:A:N7	2.34	0.43
3:A:2847:U:H2'	3:A:2848:G:O4'	2.18	0.43
20:R:24:TYR:N	20:R:24:TYR:HD1	2.17	0.43
3:A:76:C:H6	3:A:76:C:O5'	2.02	0.43
3:A:475:C:N4	3:A:476:G:C6	2.87	0.43
3:A:558:U:OP1	13:K:114:LEU:N	2.46	0.43
3:A:1351:C:H4'	3:A:1572:A:O4'	2.18	0.43
3:A:1501:G:H2'	3:A:1502:A:H8	1.84	0.43
3:A:2184:A:H2'	3:A:2185:U:C6	2.53	0.43
3:A:2292:U:H2'	3:A:2293:G:H8	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2588:G:O6	3:A:2607:G:C6	2.72	0.43
5:C:245:VAL:HA	5:C:252:THR:HG22	2.01	0.43
25:W:29:ILE:O	25:W:91:PHE:HB2	2.19	0.43
31:c:40:ASP:HA	31:c:41:PRO:HD2	1.89	0.43
34:f:2:LYS:HD3	34:f:4:ARG:NH2	2.33	0.43
35:i:51:PHE:O	35:i:55:VAL:HG23	2.18	0.43
35:i:425:ARG:O	35:i:429:LYS:HG2	2.18	0.43
3:A:675:A:OP1	7:E:58:LYS:NZ	2.52	0.43
3:A:976:G:HO2'	3:A:1155:A:HO2'	1.61	0.43
3:A:1047:G:OP1	11:I:56:ARG:NH1	2.52	0.43
3:A:1088:A:H61	12:J:135:SER:HB3	1.82	0.43
3:A:2304:G:H22	3:A:2312:U:H3	1.67	0.43
4:B:49:C:H2'	4:B:50:A:C8	2.54	0.43
7:E:108:ILE:O	7:E:112:LEU:HG	2.18	0.43
10:H:62:LEU:HD22	10:H:137:GLU:OE1	2.19	0.43
12:J:103:ARG:H	12:J:103:ARG:HD2	1.83	0.43
12:J:113:LYS:HA	12:J:116:ASP:HB2	2.01	0.43
34:f:2:LYS:HE2	34:f:2:LYS:HB3	1.77	0.43
35:i:12:THR:HG22	35:i:30:THR:HG23	2.01	0.43
35:i:313:UNK:HG1	36:k:34:LEU:CD1	2.49	0.43
3:A:5:A:H2'	3:A:6:A:C8	2.54	0.42
3:A:1751:U:H2'	3:A:1752:C:C6	2.54	0.42
3:A:2700:A:H2'	3:A:2701:U:C6	2.54	0.42
3:A:2843:G:H2'	3:A:2844:G:C8	2.54	0.42
4:B:114:C:H2'	4:B:115:A:H8	1.83	0.42
7:E:29:HIS:O	7:E:32:VAL:HG22	2.19	0.42
8:F:170:LEU:HA	8:F:170:LEU:HD23	1.75	0.42
12:J:38:PHE:CD1	12:J:59:ILE:HD11	2.54	0.42
12:J:74:PRO:HA	12:J:75:PRO:HD3	1.89	0.42
20:R:9:ILE:H	20:R:9:ILE:HD12	1.84	0.42
22:T:46:LEU:HA	22:T:46:LEU:HD23	1.82	0.42
29:a:51:VAL:HG23	29:a:55:VAL:HG21	2.00	0.42
3:A:380:G:H2'	3:A:381:G:O4'	2.18	0.42
3:A:461:C:H2'	3:A:462:C:H6	1.84	0.42
3:A:1736:U:H2'	3:A:1737:G:O4'	2.18	0.42
3:A:1759:A:H2'	3:A:1760:C:C6	2.54	0.42
3:A:1780:A:H3'	3:A:1781:U:H2'	2.01	0.42
3:A:2293:G:OP1	18:P:94:ARG:NH1	2.46	0.42
4:B:106:G:H2'	4:B:107:G:O4'	2.19	0.42
8:F:130:MET:HB2	8:F:130:MET:HE3	1.81	0.42
9:G:149:ARG:HG3	9:G:162:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:12:GLU:O	28:Z:16:THR:N	2.53	0.42
3:A:674:G:H2'	3:A:804:A:H61	1.83	0.42
3:A:794:A:H2'	3:A:795:C:C6	2.55	0.42
3:A:1473:G:H2'	3:A:1474:U:O4'	2.19	0.42
3:A:1614:A:H8	3:A:1614:A:O5'	2.02	0.42
3:A:1922:G:H2'	3:A:1923:U:O4'	2.18	0.42
3:A:2079:U:O2'	27:Y:23:ASN:OD1	2.31	0.42
3:A:2339:C:O3'	4:B:41:G:N2	2.53	0.42
3:A:2586:U:OP2	3:A:2608:G:N1	2.48	0.42
3:A:2776:A:C2	3:A:2778:A:C4	3.07	0.42
4:B:66:A:H61	4:B:107:G:H2'	1.84	0.42
8:F:145:LYS:HA	8:F:145:LYS:HD3	1.89	0.42
10:H:94:ILE:HG23	10:H:98:ASP:HB2	2.01	0.42
12:J:33:VAL:HG13	12:J:67:PHE:CD2	2.54	0.42
16:N:33:LEU:HD11	16:N:128:THR:HB	2.00	0.42
16:N:42:THR:N	16:N:45:GLN:OE1	2.47	0.42
19:Q:34:GLU:CD	19:Q:39:ARG:HB2	2.44	0.42
23:U:24:MET:HE2	23:U:24:MET:HB3	1.89	0.42
35:i:30:THR:O	35:i:34:VAL:HG23	2.19	0.42
37:l:293:PRO:HD3	37:l:372:LYS:HG3	2.01	0.42
37:l:315:ARG:CB	37:l:477:ILE:HG13	2.45	0.42
3:A:669:G:N2	3:A:670:A:C2	2.88	0.42
3:A:729:G:C5	5:C:207:LYS:HB2	2.55	0.42
3:A:1064:C:H5''	12:J:88:SER:HB2	2.02	0.42
3:A:1141:U:H4'	3:A:1142:A:O4'	2.19	0.42
3:A:1524:G:H2'	3:A:1525:A:O4'	2.20	0.42
4:B:57:A:C4	8:F:26:MET:HB3	2.54	0.42
6:D:148:GLN:OE1	6:D:148:GLN:N	2.51	0.42
17:O:75:ILE:HD12	17:O:75:ILE:HA	1.82	0.42
20:R:47:TYR:CD2	20:R:47:TYR:C	2.98	0.42
24:V:61:LYS:HG2	24:V:62:GLU:H	1.85	0.42
25:W:2:PHE:HE1	25:W:53:LYS:HD2	1.84	0.42
35:i:104:LEU:HD13	35:i:209:HIS:CD2	2.55	0.42
35:i:448:UNK:CG	35:i:450:UNK:HG3	2.48	0.42
3:A:123:G:N2	3:A:129:C:C2	2.87	0.42
3:A:1039:A:H2'	3:A:1040:A:O4'	2.20	0.42
3:A:1637:A:H2'	3:A:1638:C:C6	2.54	0.42
3:A:2119:A:H62	3:A:2167:U:H1'	1.85	0.42
4:B:48:U:H4'	18:P:100:HIS:HD2	1.84	0.42
8:F:79:ILE:HG21	8:F:85:ILE:HD11	2.01	0.42
9:G:44:LYS:HB2	9:G:44:LYS:HE3	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:1:MET:O	10:H:20:ASN:HA	2.20	0.42
12:J:22:PRO:HB2	12:J:23:PRO:HD3	2.02	0.42
14:L:3:GLN:HE21	14:L:3:GLN:HB3	1.65	0.42
26:X:47:ALA:HB1	26:X:51:VAL:O	2.19	0.42
35:i:43:VAL:O	35:i:44:ALA:C	2.61	0.42
35:i:339:ARG:O	35:i:342:LYS:HG2	2.19	0.42
37:l:298:MET:HG3	37:l:310:ILE:CG1	2.49	0.42
1:l:54:G:OP2	37:l:406:LYS:NZ	2.41	0.42
3:A:393:C:H2'	3:A:394:C:H6	1.85	0.42
3:A:571:U:H3'	21:S:80:ARG:NH2	2.33	0.42
3:A:812:C:C2	3:A:1250:G:N1	2.87	0.42
3:A:1463:C:H2'	3:A:1464:G:H8	1.85	0.42
3:A:1880:U:H2'	3:A:1881:C:C6	2.55	0.42
3:A:2138:G:C6	3:A:2154:A:C2	3.06	0.42
3:A:2322:A:C4	3:A:2323:G:C8	3.07	0.42
9:G:73:ASN:O	9:G:77:ILE:HG13	2.20	0.42
35:i:113:LYS:HG2	35:i:220:VAL:HG21	2.01	0.42
35:i:167:LYS:HA	35:i:168:PRO:HD3	1.94	0.42
35:i:216:GLU:OE1	35:i:243:THR:OG1	2.37	0.42
35:i:309:UNK:O	35:i:313:UNK:HG3	2.19	0.42
35:i:334:PHE:O	35:i:338:LEU:HG	2.20	0.42
3:A:647:G:H2'	3:A:648:G:C8	2.55	0.42
3:A:729:G:H2'	3:A:1775:U:H1'	2.01	0.42
3:A:910:A:C6	3:A:911:A:C6	3.08	0.42
3:A:1590:A:H2'	3:A:1591:A:C8	2.54	0.42
5:C:210:ALA:HA	5:C:213:TRP:CE3	2.53	0.42
14:L:65:THR:HB	14:L:68:GLY:H	1.84	0.42
16:N:36:VAL:HG13	25:W:82:TYR:CD2	2.55	0.42
23:U:88:LYS:H	23:U:91:GLN:HE22	1.67	0.42
3:A:1482:G:H2'	3:A:1483:G:H8	1.83	0.42
5:C:133:ARG:HD2	10:H:123:ARG:NH1	2.35	0.42
6:D:109:VAL:HG12	6:D:201:LEU:HD22	2.01	0.42
9:G:97:ALA:HB3	9:G:104:ASN:HB2	2.01	0.42
20:R:74:ILE:HG12	20:R:75:SER:N	2.34	0.42
3:A:799:G:C6	3:A:800:A:C6	3.08	0.42
3:A:1057:A:N7	3:A:1086:A:H2'	2.35	0.42
3:A:1417:C:H2'	3:A:1418:G:C8	2.55	0.42
3:A:1509:A:O2'	3:A:1510:G:H8	2.03	0.42
3:A:1631:G:N2	3:A:1634:A:OP2	2.32	0.42
3:A:1709:U:H2'	3:A:1710:G:C8	2.55	0.42
3:A:1821:A:H2'	3:A:1822:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2771:C:H2'	3:A:2772:C:C6	2.54	0.42
15:M:41:ARG:H	15:M:41:ARG:HG2	1.62	0.42
35:i:219:PHE:HB2	35:i:242:LEU:HD13	2.01	0.42
3:A:297:G:H2'	3:A:298:G:O4'	2.20	0.42
3:A:1065:U:H2'	3:A:1066:U:O4'	2.19	0.42
3:A:1902:C:H4'	5:C:242:LYS:O	2.19	0.42
3:A:1946:U:H2'	3:A:1947:C:H6	1.84	0.42
3:A:2209:G:C2	3:A:2216:G:C2	3.08	0.42
3:A:2286:G:C8	3:A:2287:A:N6	2.88	0.42
3:A:2706:A:C2	3:A:2707:U:C2	3.08	0.42
8:F:70:ALA:HB3	8:F:81:GLN:HA	2.02	0.42
11:I:15:VAL:HG11	11:I:60:LEU:CD2	2.50	0.42
11:I:43:LYS:HE2	12:J:118:THR:HA	2.02	0.42
19:Q:106:LYS:O	19:Q:109:ARG:HD3	2.20	0.42
24:V:53:ASN:HD21	35:i:365:UNK:HB2	1.85	0.42
29:a:51:VAL:O	29:a:55:VAL:HG22	2.20	0.42
3:A:100:U:O2	24:V:91:LYS:NZ	2.43	0.41
3:A:848:C:H42	3:A:930:G:H1	1.68	0.41
3:A:1597:A:C5'	3:A:1598:A:H5'	2.47	0.41
3:A:2365:G:H4'	26:X:60:PHE:CE2	2.55	0.41
3:A:2433:A:H5'	3:A:2434:A:OP2	2.19	0.41
3:A:2812:G:H2'	3:A:2813:A:O4'	2.20	0.41
6:D:73:VAL:HG11	6:D:93:GLY:HA2	2.02	0.41
13:K:12:LYS:HD2	13:K:12:LYS:HA	1.81	0.41
17:O:103:ARG:HB3	17:O:106:ASP:OD1	2.20	0.41
28:Z:14:LEU:HD23	28:Z:14:LEU:HA	1.79	0.41
32:d:22:MET:O	32:d:28:ARG:NH1	2.53	0.41
35:i:383:MET:HE1	35:i:417:LEU:HD21	2.02	0.41
3:A:335:C:H5''	24:V:82:ARG:HD2	2.02	0.41
3:A:678:C:H2'	3:A:679:C:H6	1.84	0.41
3:A:877:A:C6	3:A:899:A:C6	3.08	0.41
3:A:908:C:O2'	16:N:70:ASP:OD2	2.30	0.41
3:A:1056:G:H5'	11:I:35:VAL:HG21	2.02	0.41
3:A:1068:G:N2	3:A:1095:A:O3'	2.44	0.41
3:A:1078:U:O2	3:A:1088:A:H3'	2.20	0.41
3:A:1432:G:H2'	3:A:1433:A:C8	2.55	0.41
3:A:1535:A:C8	35:i:435:UNK:HB1	2.56	0.41
8:F:57:LEU:HD12	8:F:87:CYS:SG	2.61	0.41
8:F:79:ILE:HD12	8:F:79:ILE:O	2.20	0.41
23:U:87:LEU:HD11	23:U:93:LEU:HD12	2.01	0.41
35:i:411:GLN:H	35:i:411:GLN:HG3	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:573:U:O4	3:A:2029:G:O2'	2.36	0.41
3:A:1324:G:C4	3:A:1328:A:N6	2.88	0.41
3:A:1449:G:N2	3:A:1463:C:C2	2.88	0.41
3:A:1463:C:H2'	3:A:1464:G:C8	2.55	0.41
3:A:1877:A:H2'	3:A:1878:G:O4'	2.19	0.41
18:P:85:LYS:HE2	18:P:85:LYS:HB3	1.79	0.41
35:i:302:UNK:HA	35:i:353:UNK:HA	2.02	0.41
1:l:54:G:H1'	37:l:403:VAL:HG13	2.02	0.41
1:l:55:A:H4'	37:l:362:SER:HB3	2.03	0.41
3:A:328:U:H4'	24:V:66:GLN:HE21	1.86	0.41
3:A:648:G:C2	3:A:649:G:C5	3.08	0.41
3:A:1365:A:N3	3:A:1365:A:H2'	2.36	0.41
3:A:1484:U:H2'	3:A:1485:U:C6	2.55	0.41
3:A:2343:U:H2'	3:A:2344:U:C6	2.55	0.41
3:A:2352:A:N1	26:X:34:GLY:HA3	2.35	0.41
3:A:2578:G:OP2	3:A:2578:G:H4'	2.19	0.41
3:A:2895:G:H2'	3:A:2896:C:C6	2.56	0.41
7:E:181:ILE:H	7:E:181:ILE:HG13	1.70	0.41
10:H:128:HIS:O	10:H:143:ILE:HA	2.20	0.41
3:A:465:G:C6	3:A:466:A:N6	2.89	0.41
3:A:653:U:C1'	3:A:654:A:H5''	2.49	0.41
3:A:948:C:H2'	3:A:949:G:H8	1.85	0.41
3:A:1499:C:H2'	3:A:1500:G:H8	1.85	0.41
3:A:1798:U:OP2	5:C:271:ARG:NH2	2.52	0.41
3:A:2229:U:H2'	3:A:2230:G:H8	1.85	0.41
5:C:176:LEU:HB2	5:C:180:GLU:O	2.20	0.41
15:M:78:ARG:HG2	15:M:113:ALA:HB3	2.03	0.41
35:i:17:SER:HB3	35:i:71:GLY:HA3	2.02	0.41
35:i:236:PHE:HB3	35:i:242:LEU:HD21	2.03	0.41
3:A:75:G:H4'	28:Z:48:ARG:NH2	2.35	0.41
3:A:561:G:H4'	20:R:48:ARG:HH22	1.86	0.41
3:A:1972:G:H2'	3:A:1973:G:C8	2.55	0.41
3:A:2466:C:OP1	34:f:4:ARG:HB2	2.19	0.41
4:B:71:C:C2	4:B:106:G:C2	3.08	0.41
9:G:83:PHE:HB2	9:G:135:GLY:O	2.20	0.41
20:R:31:VAL:HG12	20:R:34:VAL:H	1.85	0.41
27:Y:3:ARG:NE	27:Y:30:LEU:HD13	2.35	0.41
27:Y:54:LYS:O	27:Y:58:VAL:HG23	2.19	0.41
35:i:135:VAL:HG13	35:i:189:VAL:HG13	2.03	0.41
3:A:118:A:N3	3:A:178:G:H1'	2.36	0.41
3:A:449:A:C4	3:A:450:G:C8	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:565:C:H4'	3:A:1253:A:C6	2.55	0.41
3:A:681:G:C2	3:A:797:G:C2	3.09	0.41
3:A:779:U:H2'	3:A:780:G:C8	2.56	0.41
3:A:1770:G:C6	3:A:1983:G:C6	3.07	0.41
3:A:2102:G:C2	3:A:2187:U:O2	2.74	0.41
3:A:2209:G:N2	3:A:2215:C:N3	2.60	0.41
3:A:2627:G:H1'	3:A:2777:G:N2	2.36	0.41
3:A:2785:C:H2'	3:A:2786:U:H6	1.85	0.41
4:B:7:G:H5''	18:P:29:HIS:CE1	2.56	0.41
11:I:100:ALA:HB2	11:I:106:PHE:CE1	2.56	0.41
17:O:65:LEU:HD12	17:O:65:LEU:HA	1.85	0.41
33:e:6:THR:O	33:e:8:ARG:HG2	2.21	0.41
35:i:31:LEU:O	35:i:52:ILE:HG12	2.21	0.41
37:l:368:ILE:O	37:l:372:LYS:HG3	2.21	0.41
1:l:72:A:C4	1:l:73:G:C8	3.08	0.41
3:A:1275:A:OP2	3:A:1646:C:N4	2.53	0.41
3:A:1807:G:N2	3:A:1811:G:C5	2.89	0.41
4:B:95:U:H2'	4:B:96:G:C8	2.56	0.41
5:C:84:ASP:HA	5:C:85:PRO:HD2	1.85	0.41
8:F:34:ILE:HB	8:F:96:MET:HG3	2.02	0.41
8:F:36:LEU:HA	8:F:153:ASP:O	2.21	0.41
11:I:85:VAL:HG21	11:I:90:GLY:O	2.20	0.41
14:L:93:GLN:HA	14:L:94:PRO:HD3	1.88	0.41
16:N:6:ARG:CZ	16:N:6:ARG:HB2	2.50	0.41
22:T:109:ASP:OD1	22:T:110:ARG:N	2.54	0.41
28:Z:46:VAL:O	28:Z:50:VAL:HG23	2.21	0.41
35:i:42:ASP:HB2	37:l:425:GLN:HG2	2.01	0.41
1:l:42:A:OP1	1:l:42:A:H4'	2.20	0.41
1:l:67:A:C4	1:l:68:A:C8	3.08	0.41
3:A:31:C:O3'	3:A:1238:G:H5'	2.21	0.41
3:A:53:A:H2'	3:A:54:G:O4'	2.21	0.41
3:A:528:A:C8	3:A:2042:A:C2	3.09	0.41
3:A:601:C:O2'	3:A:605:G:H5''	2.21	0.41
3:A:811:U:C2	3:A:1251:C:C5	3.09	0.41
3:A:1071:G:O2'	3:A:1089:A:OP2	2.36	0.41
3:A:1073:A:H2'	3:A:1074:G:O4'	2.21	0.41
3:A:1374:G:H8	3:A:1374:G:OP2	2.04	0.41
3:A:1672:A:N6	3:A:1673:G:C6	2.89	0.41
3:A:1789:A:H2'	3:A:1790:C:O4'	2.21	0.41
3:A:2061:G:H2'	3:A:2501:C:O2'	2.21	0.41
3:A:2267:A:H5''	3:A:2268:A:C5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2431:U:O2	3:A:2431:U:O4'	2.39	0.41
3:A:2663:G:H2'	3:A:2664:G:O4'	2.21	0.41
3:A:2847:U:C5	3:A:2848:G:C5	3.09	0.41
3:A:2860:A:H5''	3:A:2861:U:OP2	2.21	0.41
8:F:65:PRO:HA	8:F:89:VAL:HG22	2.02	0.41
9:G:76:VAL:O	9:G:80:THR:HG23	2.20	0.41
9:G:154:PRO:HA	9:G:160:LYS:O	2.21	0.41
11:I:48:ALA:HB3	11:I:50:VAL:HG23	2.02	0.41
12:J:42:PHE:CE1	12:J:57:VAL:HB	2.56	0.41
12:J:93:PRO:C	12:J:95:LYS:H	2.29	0.41
17:O:72:ASP:O	17:O:76:VAL:HG13	2.21	0.41
22:T:96:ILE:HD13	22:T:96:ILE:HA	1.73	0.41
29:a:6:LYS:HB3	29:a:6:LYS:HE2	1.94	0.41
29:a:45:ARG:HH12	29:a:59:GLU:CD	2.29	0.41
35:i:105:MET:HG3	35:i:117:VAL:HG22	2.03	0.41
35:i:331:LEU:HD12	35:i:388:ARG:HA	2.03	0.41
37:l:400:ILE:O	37:l:403:VAL:HB	2.21	0.41
3:A:339:U:H6	3:A:339:U:O5'	2.04	0.41
3:A:743:A:OP1	6:D:135:GLY:HA2	2.21	0.41
3:A:807:U:H2'	3:A:808:G:H8	1.85	0.41
3:A:1024:G:C6	3:A:1025:G:C6	3.09	0.41
3:A:1127:A:N7	3:A:2488:G:O2'	2.55	0.41
3:A:1341:G:C2	3:A:1398:C:H4'	2.56	0.41
3:A:1366:A:H2'	3:A:1367:A:O4'	2.21	0.41
3:A:1838:C:H4'	3:A:1839:G:H8	1.85	0.41
3:A:2143:C:H2'	3:A:2144:G:O4'	2.21	0.41
3:A:2550:G:C6	3:A:2551:C:C4	3.09	0.41
3:A:2838:G:H2'	3:A:2839:G:O4'	2.20	0.41
16:N:65:ILE:HG12	16:N:103:TYR:HD2	1.86	0.41
35:i:354:UNK:CG	36:k:39:LEU:HD21	2.46	0.41
3:A:64:A:C6	3:A:65:U:C4	3.09	0.40
3:A:118:A:C8	3:A:119:A:C8	3.09	0.40
3:A:396:G:H1'	27:Y:29:PHE:HB3	2.02	0.40
3:A:520:G:H2'	3:A:521:U:C6	2.56	0.40
3:A:729:G:C6	5:C:207:LYS:HB2	2.56	0.40
3:A:1869:G:C2	3:A:1873:G:C6	3.09	0.40
3:A:2682:A:C2	6:D:23:PRO:HB3	2.56	0.40
5:C:157:SER:O	5:C:160:THR:OG1	2.38	0.40
6:D:13:ARG:HD2	6:D:15:PHE:CE2	2.57	0.40
8:F:13:VAL:O	8:F:17:MET:HB2	2.21	0.40
11:I:99:PHE:HD2	11:I:106:PHE:HZ	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:96:PHE:O	24:V:100:SER:HA	2.21	0.40
35:i:320:UNK:HG1	35:i:337:GLN:HE21	1.86	0.40
3:A:33:C:N4	3:A:446:G:O2'	2.45	0.40
3:A:247:G:H4'	3:A:386:G:C4	2.57	0.40
3:A:501:A:H2'	3:A:502:A:C8	2.56	0.40
3:A:717:C:C5	3:A:718:A:C8	3.10	0.40
3:A:1005:C:H2'	3:A:1006:C:H6	1.84	0.40
3:A:1423:G:N2	3:A:1576:U:O2	2.54	0.40
3:A:2365:G:P	26:X:55:ARG:HG2	2.61	0.40
3:A:2603:G:C6	3:A:2604:U:C4	3.10	0.40
3:A:2667:C:H6	3:A:2667:C:O5'	2.04	0.40
4:B:68:C:H2'	4:B:69:G:O4'	2.21	0.40
6:D:125:TRP:CE2	6:D:160:LYS:HB3	2.57	0.40
13:K:9:GLU:H	13:K:9:GLU:HG2	1.66	0.40
15:M:79:LEU:HB2	15:M:113:ALA:O	2.21	0.40
16:N:38:ARG:HB2	16:N:98:PRO:HD3	2.02	0.40
23:U:49:LYS:HG3	23:U:50:LEU:HD23	2.03	0.40
27:Y:3:ARG:O	27:Y:12:PRO:HD3	2.21	0.40
27:Y:36:HIS:O	27:Y:48:THR:HA	2.21	0.40
33:e:38:THR:HA	33:e:41:LYS:HE3	2.03	0.40
35:i:168:PRO:O	35:i:172:VAL:HG22	2.21	0.40
37:l:286:LEU:HD22	37:l:469:ARG:NH2	2.36	0.40
37:l:330:ASP:CB	37:l:336:ALA:HB1	2.51	0.40
3:A:125:A:H2	32:d:9:VAL:HG12	1.86	0.40
3:A:199:A:N6	3:A:2434:A:C5	2.90	0.40
3:A:258:G:H1'	15:M:104:GLN:NE2	2.31	0.40
3:A:445:C:H2'	3:A:446:G:O4'	2.22	0.40
3:A:776:G:HO2'	3:A:777:G:P	2.42	0.40
3:A:2394:C:H42	3:A:2422:C:N4	2.19	0.40
3:A:2563:U:O2	3:A:2566:A:C5	2.75	0.40
3:A:2647:U:H2'	3:A:2648:G:C8	2.54	0.40
3:A:2796:U:HO2'	3:A:2797:U:H6	1.65	0.40
5:C:13:ARG:HA	5:C:13:ARG:HD2	1.82	0.40
5:C:34:LEU:HD21	5:C:63:ARG:HG3	2.04	0.40
8:F:22:TYR:HB3	8:F:27:GLN:HB2	2.04	0.40
8:F:103:LEU:HA	8:F:107:ALA:HB3	2.02	0.40
15:M:27:LEU:HA	15:M:27:LEU:HD23	1.66	0.40
21:S:22:LEU:HD23	21:S:22:LEU:HA	1.94	0.40
24:V:36:VAL:HB	24:V:39:ILE:HB	2.03	0.40
35:i:229:ALA:HB1	35:i:262:ILE:HD11	2.04	0.40
35:i:301:UNK:O	35:i:304:UNK:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:i:390:LYS:O	35:i:393:ILE:HG12	2.21	0.40
37:l:394:MET:HE1	37:l:434:PHE:CE1	2.56	0.40
37:l:424:GLY:C	37:l:456:VAL:HG21	2.47	0.40
3:A:42:A:C6	3:A:43:G:C5	3.10	0.40
3:A:277:G:H4'	3:A:278:A:C5	2.56	0.40
3:A:778:G:H5''	3:A:779:U:OP2	2.21	0.40
3:A:871:U:H4'	16:N:68:PHE:CD2	2.57	0.40
3:A:1139:G:H8	3:A:1139:G:OP2	2.05	0.40
3:A:1607:C:O2'	3:A:1608:A:OP1	2.37	0.40
3:A:1681:G:O2'	3:A:1762:A:N3	2.52	0.40
3:A:1803:A:C8	3:A:1804:C:C6	3.10	0.40
3:A:1818:U:C5	5:C:156:ARG:NH2	2.90	0.40
3:A:1869:G:C6	3:A:1871:A:OP2	2.75	0.40
3:A:2052:A:C6	3:A:2053:G:N7	2.90	0.40
3:A:2804:U:H2'	3:A:2805:C:C6	2.56	0.40
4:B:49:C:H2'	4:B:50:A:H8	1.87	0.40
10:H:60:GLU:HA	10:H:63:ALA:HB3	2.04	0.40
11:I:61:ARG:HG2	11:I:73:LYS:HG2	2.02	0.40
26:X:70:GLU:HG3	26:X:72:LYS:HE2	2.04	0.40
30:b:7:LYS:HA	30:b:8:PRO:HD3	1.91	0.40
37:l:477:ILE:HD12	37:l:477:ILE:HA	1.90	0.40
2:2:74:C:H6	2:2:74:C:O5'	2.04	0.40
3:A:353:C:H2'	3:A:354:A:O4'	2.22	0.40
3:A:822:G:H2'	3:A:823:C:C6	2.57	0.40
3:A:856:G:H2'	3:A:857:G:C8	2.57	0.40
3:A:1113:U:H2'	3:A:1114:C:H6	1.86	0.40
3:A:1258:U:C2	3:A:1259:G:C8	3.09	0.40
3:A:1707:G:C5	3:A:1756:G:C6	3.10	0.40
3:A:2015:A:C2	30:b:3:VAL:HB	2.57	0.40
3:A:2048:G:H2'	3:A:2049:G:O4'	2.22	0.40
9:G:90:VAL:HG21	9:G:163:ARG:NH1	2.37	0.40
15:M:81:ASP:HB3	15:M:100:ILE:HD13	2.02	0.40
29:a:45:ARG:HD2	29:a:45:ARG:HA	1.80	0.40
35:i:318:UNK:HA	35:i:321:UNK:HG3	2.04	0.40
40:i:1400:GNP:O4'	37:l:302:ASN:HB3	2.22	0.40
37:l:368:ILE:HD11	37:l:404:MET:HG2	2.04	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	
5	C	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
9	G	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
10	H	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	18	50
11	I	123/165 (74%)	113 (92%)	9 (7%)	1 (1%)	16	48
12	J	132/142 (93%)	126 (96%)	6 (4%)	0	100	100
13	K	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/127 (97%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
20	R	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
23	U	93/100 (93%)	89 (96%)	3 (3%)	1 (1%)	11	42
24	V	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
28	Z	56/63 (89%)	54 (96%)	2 (4%)	0	100	100
29	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	b	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
31	c	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
33	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
34	f	36/38 (95%)	36 (100%)	0	0	100	100
35	i	378/450 (84%)	361 (96%)	17 (4%)	0	100	100
36	k	16/18 (89%)	11 (69%)	5 (31%)	0	100	100
37	l	196/497 (39%)	189 (96%)	7 (4%)	0	100	100
All	All	4018/4539 (88%)	3876 (96%)	139 (4%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	U	89	GLU
10	H	118	PRO
11	I	108	VAL

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	
5	C	216/218 (99%)	190 (88%)	26 (12%)	5	23
6	D	164/164 (100%)	148 (90%)	16 (10%)	7	30
7	E	165/165 (100%)	149 (90%)	16 (10%)	8	31
8	F	148/150 (99%)	127 (86%)	21 (14%)	3	18
9	G	137/138 (99%)	126 (92%)	11 (8%)	11	37
10	H	114/114 (100%)	100 (88%)	14 (12%)	4	22
11	I	95/123 (77%)	85 (90%)	10 (10%)	6	28
12	J	104/110 (94%)	88 (85%)	16 (15%)	2	16
13	K	116/116 (100%)	99 (85%)	17 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	L	104/104 (100%)	96 (92%)	8 (8%)	12	38
15	M	103/103 (100%)	92 (89%)	11 (11%)	6	27
16	N	109/109 (100%)	99 (91%)	10 (9%)	8	32
17	O	102/103 (99%)	95 (93%)	7 (7%)	14	41
18	P	87/87 (100%)	70 (80%)	17 (20%)	1	9
19	Q	99/100 (99%)	88 (89%)	11 (11%)	6	25
20	R	89/90 (99%)	79 (89%)	10 (11%)	6	25
21	S	84/84 (100%)	73 (87%)	11 (13%)	4	20
22	T	93/93 (100%)	84 (90%)	9 (10%)	8	31
23	U	82/84 (98%)	76 (93%)	6 (7%)	13	40
24	V	83/85 (98%)	75 (90%)	8 (10%)	8	31
25	W	78/78 (100%)	72 (92%)	6 (8%)	12	38
26	X	57/63 (90%)	47 (82%)	10 (18%)	2	12
27	Y	67/68 (98%)	59 (88%)	8 (12%)	5	23
28	Z	54/55 (98%)	48 (89%)	6 (11%)	6	25
29	a	48/49 (98%)	45 (94%)	3 (6%)	16	43
30	b	47/48 (98%)	36 (77%)	11 (23%)	1	6
31	c	45/49 (92%)	40 (89%)	5 (11%)	6	25
32	d	38/38 (100%)	31 (82%)	7 (18%)	1	11
33	e	51/52 (98%)	47 (92%)	4 (8%)	11	37
34	f	34/34 (100%)	31 (91%)	3 (9%)	9	33
35	i	311/313 (99%)	293 (94%)	18 (6%)	18	45
36	k	17/17 (100%)	15 (88%)	2 (12%)	5	23
37	l	156/405 (38%)	153 (98%)	3 (2%)	50	65
All	All	3297/3609 (91%)	2956 (90%)	341 (10%)	9	29

All (341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	C	3	VAL
5	C	24	LEU
5	C	35	GLU
5	C	51	THR
5	C	72	ASP

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Mol	Chain	Res	Type
5	C	74	ILE
5	C	120	VAL
5	C	130	LEU
5	C	134	ASN
5	C	147	LYS
5	C	156	ARG
5	C	172	VAL
5	C	180	GLU
5	C	185	GLU
5	C	189	ARG
5	C	192	LEU
5	C	195	VAL
5	C	203	ARG
5	C	204	VAL
5	C	228	VAL
5	C	242	LYS
5	C	250	VAL
5	C	251	GLN
5	C	257	THR
5	C	261	LYS
5	C	271	ARG
6	D	12	THR
6	D	13	ARG
6	D	18	ASP
6	D	20	VAL
6	D	22	ILE
6	D	28	GLU
6	D	29	VAL
6	D	60	VAL
6	D	73	VAL
6	D	84	LEU
6	D	128	ARG
6	D	133	THR
6	D	139	SER
6	D	142	VAL
6	D	160	LYS
6	D	168	GLU
7	E	83	VAL
7	E	84	THR
7	E	94	GLN
7	E	96	VAL
7	E	97	ASN

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Mol	Chain	Res	Type
7	E	105	LEU
7	E	119	ILE
7	E	127	GLU
7	E	138	LEU
7	E	148	ILE
7	E	169	VAL
7	E	173	THR
7	E	178	VAL
7	E	179	SER
7	E	184	ASP
7	E	196	VAL
8	F	3	LYS
8	F	4	LEU
8	F	14	LYS
8	F	25	VAL
8	F	49	LEU
8	F	51	ASP
8	F	52	ASN
8	F	67	ILE
8	F	81	GLN
8	F	104	ILE
8	F	106	ILE
8	F	115	ARG
8	F	130	MET
8	F	141	ILE
8	F	144	ASP
8	F	149	VAL
8	F	150	ARG
8	F	153	ASP
8	F	156	ILE
8	F	162	SER
8	F	178	ARG
9	G	10	VAL
9	G	11	VAL
9	G	43	VAL
9	G	49	THR
9	G	87	LEU
9	G	114	ASP
9	G	124	GLU
9	G	125	CYS
9	G	127	THR
9	G	141	ILE

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Mol	Chain	Res	Type
9	G	153	ARG
10	H	4	ILE
10	H	15	LEU
10	H	37	VAL
10	H	58	LEU
10	H	60	GLU
10	H	76	GLU
10	H	77	THR
10	H	78	VAL
10	H	86	ASP
10	H	87	GLU
10	H	108	VAL
10	H	110	VAL
10	H	112	LYS
10	H	142	VAL
11	I	16	SER
11	I	36	ASP
11	I	54	VAL
11	I	55	VAL
11	I	58	THR
11	I	64	VAL
11	I	85	VAL
11	I	94	ARG
11	I	96	PHE
11	I	109	LYS
12	J	9	VAL
12	J	21	SER
12	J	28	LEU
12	J	31	GLN
12	J	35	ILE
12	J	55	ILE
12	J	61	VAL
12	J	66	SER
12	J	78	VAL
12	J	98	VAL
12	J	111	GLN
12	J	112	THR
12	J	113	LYS
12	J	116	ASP
12	J	128	SER
12	J	139	VAL
13	K	5	THR

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Mol	Chain	Res	Type
13	K	7	LYS
13	K	17	VAL
13	K	28	LEU
13	K	31	GLU
13	K	34	ARG
13	K	40	HIS
13	K	57	LEU
13	K	69	ARG
13	K	70	THR
13	K	88	THR
13	K	90	GLU
13	K	101	ILE
13	K	103	ILE
13	K	122	LEU
13	K	131	ASN
13	K	142	ILE
14	L	21	CYS
14	L	42	THR
14	L	49	ARG
14	L	56	ASP
14	L	58	LEU
14	L	65	THR
14	L	84	CYS
14	L	116	ILE
15	M	14	LYS
15	M	46	VAL
15	M	47	ARG
15	M	55	MET
15	M	59	ARG
15	M	86	GLU
15	M	91	ASP
15	M	101	ILE
15	M	126	ARG
15	M	141	LYS
15	M	143	GLU
16	N	6	ARG
16	N	7	THR
16	N	12	MET
16	N	25	ASP
16	N	54	THR
16	N	58	LYS
16	N	81	ARG

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Mol	Chain	Res	Type
16	N	115	GLU
16	N	133	LYS
16	N	135	VAL
17	O	14	SER
17	O	33	ILE
17	O	36	THR
17	O	69	ARG
17	O	74	GLU
17	O	75	ILE
17	O	100	CYS
18	P	2	ASP
18	P	5	SER
18	P	16	ARG
18	P	18	LEU
18	P	19	GLN
18	P	20	GLU
18	P	31	THR
18	P	36	TYR
18	P	43	ASN
18	P	49	VAL
18	P	55	GLU
18	P	56	LYS
18	P	58	ILE
18	P	61	GLN
18	P	69	ASP
18	P	78	VAL
18	P	98	GLN
19	Q	3	ASN
19	Q	7	GLN
19	Q	21	ARG
19	Q	26	VAL
19	Q	51	ARG
19	Q	65	SER
19	Q	68	GLU
19	Q	92	VAL
19	Q	94	LYS
19	Q	102	GLU
19	Q	115	ASN
20	R	6	ARG
20	R	17	ILE
20	R	24	TYR
20	R	31	VAL

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Mol	Chain	Res	Type
20	R	39	VAL
20	R	40	ILE
20	R	51	ARG
20	R	74	ILE
20	R	80	ILE
20	R	109	LEU
21	S	4	VAL
21	S	10	LYS
21	S	20	VAL
21	S	25	LEU
21	S	38	VAL
21	S	45	GLU
21	S	60	LYS
21	S	72	VAL
21	S	83	TYR
21	S	85	LYS
21	S	101	ILE
22	T	12	SER
22	T	20	VAL
22	T	28	LYS
22	T	55	ILE
22	T	68	ASP
22	T	74	ILE
22	T	95	ARG
22	T	96	ILE
22	T	98	LYS
23	U	7	LEU
23	U	16	VAL
23	U	17	SER
23	U	48	GLN
23	U	72	GLN
23	U	91	GLN
24	V	7	ARG
24	V	28	VAL
24	V	34	VAL
24	V	41	LEU
24	V	42	VAL
24	V	68	SER
24	V	83	VAL
24	V	102	THR
25	W	7	GLU
25	W	12	GLN

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Mol	Chain	Res	Type
25	W	61	LEU
25	W	77	VAL
25	W	78	GLN
25	W	92	VAL
26	X	11	ARG
26	X	12	ASN
26	X	21	LEU
26	X	35	SER
26	X	38	VAL
26	X	41	ARG
26	X	56	ASP
26	X	58	THR
26	X	72	LYS
26	X	85	GLU
27	Y	2	SER
27	Y	4	VAL
27	Y	13	VAL
27	Y	42	SER
27	Y	44	LYS
27	Y	71	LEU
27	Y	74	ARG
27	Y	77	LYS
28	Z	2	LYS
28	Z	16	THR
28	Z	44	LYS
28	Z	45	GLN
28	Z	48	ARG
28	Z	56	LEU
29	a	30	ARG
29	a	36	VAL
29	a	56	LYS
30	b	4	GLN
30	b	9	THR
30	b	15	MET
30	b	18	SER
30	b	25	VAL
30	b	26	THR
30	b	28	LEU
30	b	36	GLU
30	b	40	ARG
30	b	46	ASP
30	b	52	ARG

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Mol	Chain	Res	Type
31	c	5	ILE
31	c	6	ARG
31	c	22	THR
31	c	42	VAL
31	c	47	VAL
32	d	1	MET
32	d	12	ARG
32	d	24	THR
32	d	25	LYS
32	d	34	ARG
32	d	41	ARG
32	d	42	LEU
33	e	8	ARG
33	e	32	ILE
33	e	50	VAL
33	e	51	SER
34	f	1	MET
34	f	2	LYS
34	f	12	ARG
35	i	5	LEU
35	i	6	THR
35	i	9	LEU
35	i	16	ILE
35	i	19	ARG
35	i	21	ARG
35	i	30	THR
35	i	45	LEU
35	i	92	THR
35	i	141	ARG
35	i	240	LEU
35	i	242	LEU
35	i	261	SER
35	i	290	ILE
35	i	333	ASP
35	i	379	ILE
35	i	411	GLN
35	i	425	ARG
36	k	27	MET
36	k	44	VAL
37	l	295	VAL
37	l	359	ASP
37	l	394	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
5	C	86	ASN
5	C	90	ASN
5	C	251	GLN
6	D	136	ASN
6	D	140	HIS
7	E	24	ASN
7	E	165	HIS
8	F	37	ASN
8	F	63	GLN
8	F	81	GLN
8	F	127	ASN
9	G	30	ASN
9	G	48	ASN
10	H	33	GLN
12	J	31	GLN
13	K	76	HIS
13	K	80	HIS
13	K	86	GLN
14	L	3	GLN
14	L	89	ASN
14	L	93	GLN
15	M	104	GLN
16	N	3	GLN
18	P	43	ASN
18	P	100	HIS
19	Q	3	ASN
19	Q	52	ASN
19	Q	56	HIS
19	Q	75	GLN
20	R	37	GLN
20	R	81	ASN
21	S	82	HIS
22	T	7	HIS
22	T	102	HIS
23	U	28	ASN
23	U	48	GLN
23	U	59	ASN
24	V	53	ASN
25	W	12	GLN
26	X	46	HIS
27	Y	20	HIS

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Mol	Chain	Res	Type
28	Z	39	GLN
28	Z	58	ASN
29	a	20	HIS
30	b	6	ASN
32	d	26	ASN
32	d	29	GLN
35	i	62	HIS
35	i	72	GLN
35	i	209	HIS
35	i	337	GLN
35	i	411	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	42/113 (37%)	18 (42%)	1 (2%)
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	521 (18%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3041/3139 (96%)	553 (18%)	20 (0%)

All (553) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	C
1	1	34	U
1	1	37	U
1	1	39	A
1	1	41	C
1	1	42	A
1	1	43	G
1	1	46	C
1	1	54	G
1	1	55	A
1	1	57	G
1	1	58	G
1	1	67	A
1	1	69	G
1	1	70	G
1	1	71	C
1	1	72	A

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Mol	Chain	Res	Type
1	1	74	A
2	2	76	A
3	A	10	A
3	A	12	U
3	A	33	C
3	A	34	U
3	A	35	G
3	A	45	G
3	A	46	G
3	A	49	A
3	A	50	U
3	A	51	G
3	A	62	U
3	A	63	A
3	A	65	U
3	A	71	A
3	A	72	U
3	A	74	A
3	A	75	G
3	A	84	A
3	A	93	G
3	A	96	C
3	A	101	A
3	A	102	U
3	A	103	A
3	A	110	G
3	A	118	A
3	A	119	A
3	A	120	U
3	A	136	G
3	A	137	U
3	A	138	U
3	A	139	U
3	A	142	A
3	A	156	A
3	A	162	U
3	A	181	A
3	A	188	G
3	A	196	A
3	A	199	A
3	A	215	G
3	A	216	A

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Mol	Chain	Res	Type
3	A	220	G
3	A	221	A
3	A	222	A
3	A	226	A
3	A	248	G
3	A	266	G
3	A	272	A
3	A	275	C
3	A	276	U
3	A	285	G
3	A	291	G
3	A	302	C
3	A	311	A
3	A	329	G
3	A	330	A
3	A	335	C
3	A	349	U
3	A	353	C
3	A	356	G
3	A	361	G
3	A	362	A
3	A	372	G
3	A	386	G
3	A	396	G
3	A	399	U
3	A	411	G
3	A	419	U
3	A	424	G
3	A	454	A
3	A	455	C
3	A	473	G
3	A	475	C
3	A	477	A
3	A	479	A
3	A	480	A
3	A	481	G
3	A	491	G
3	A	504	A
3	A	505	A
3	A	509	C
3	A	510	C
3	A	513	A

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Mol	Chain	Res	Type
3	A	518	G
3	A	529	A
3	A	531	C
3	A	532	A
3	A	533	G
3	A	543	G
3	A	544	C
3	A	550	C
3	A	552	U
3	A	558	U
3	A	563	A
3	A	567	U
3	A	568	U
3	A	573	U
3	A	575	A
3	A	586	A
3	A	603	A
3	A	613	A
3	A	614	A
3	A	615	U
3	A	627	A
3	A	632	A
3	A	634	C
3	A	637	A
3	A	645	C
3	A	646	U
3	A	647	G
3	A	653	U
3	A	654	A
3	A	655	A
3	A	668	A
3	A	669	G
3	A	685	A
3	A	686	U
3	A	711	G
3	A	712	G
3	A	713	G
3	A	718	A
3	A	730	A
3	A	747	U
3	A	753	A
3	A	757	G

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Mol	Chain	Res	Type
3	A	763	G
3	A	764	A
3	A	765	C
3	A	775	G
3	A	777	G
3	A	782	A
3	A	784	G
3	A	785	G
3	A	788	A
3	A	789	A
3	A	790	U
3	A	791	C
3	A	793	A
3	A	794	A
3	A	801	G
3	A	805	G
3	A	812	C
3	A	827	U
3	A	828	U
3	A	831	G
3	A	846	U
3	A	859	G
3	A	865	C
3	A	869	G
3	A	878	A
3	A	896	A
3	A	897	C
3	A	899	A
3	A	907	G
3	A	910	A
3	A	914	G
3	A	915	C
3	A	932	U
3	A	933	A
3	A	946	C
3	A	953	G
3	A	957	C
3	A	961	C
3	A	974	G
3	A	983	A
3	A	990	A
3	A	996	A

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Mol	Chain	Res	Type
3	A	999	U
3	A	1005	C
3	A	1009	A
3	A	1012	U
3	A	1013	C
3	A	1022	G
3	A	1023	U
3	A	1027	A
3	A	1033	U
3	A	1040	A
3	A	1046	A
3	A	1056	G
3	A	1057	A
3	A	1070	A
3	A	1071	G
3	A	1073	A
3	A	1083	U
3	A	1087	G
3	A	1088	A
3	A	1090	A
3	A	1101	U
3	A	1111	A
3	A	1112	G
3	A	1116	G
3	A	1129	A
3	A	1130	U
3	A	1132	U
3	A	1133	A
3	A	1135	C
3	A	1136	G
3	A	1139	G
3	A	1142	A
3	A	1143	A
3	A	1155	A
3	A	1173	U
3	A	1179	G
3	A	1182	G
3	A	1206	G
3	A	1212	G
3	A	1218	G
3	A	1236	G
3	A	1238	G

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Mol	Chain	Res	Type
3	A	1247	A
3	A	1249	U
3	A	1252	G
3	A	1253	A
3	A	1256	G
3	A	1262	A
3	A	1271	G
3	A	1272	A
3	A	1294	U
3	A	1300	G
3	A	1301	A
3	A	1302	A
3	A	1308	A
3	A	1329	U
3	A	1332	G
3	A	1337	G
3	A	1338	G
3	A	1345	C
3	A	1346	G
3	A	1365	A
3	A	1379	U
3	A	1383	A
3	A	1395	A
3	A	1403	A
3	A	1416	G
3	A	1417	C
3	A	1424	G
3	A	1428	C
3	A	1434	A
3	A	1437	C
3	A	1449	G
3	A	1451	C
3	A	1452	G
3	A	1453	A
3	A	1482	G
3	A	1489	C
3	A	1491	G
3	A	1493	C
3	A	1494	A
3	A	1495	A
3	A	1497	U
3	A	1498	C

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Mol	Chain	Res	Type
3	A	1509	A
3	A	1510	G
3	A	1515	A
3	A	1524	G
3	A	1529	G
3	A	1533	C
3	A	1535	A
3	A	1536	C
3	A	1537	G
3	A	1554	U
3	A	1560	G
3	A	1566	A
3	A	1569	A
3	A	1576	U
3	A	1578	U
3	A	1581	G
3	A	1583	A
3	A	1585	C
3	A	1606	C
3	A	1607	C
3	A	1608	A
3	A	1616	A
3	A	1634	A
3	A	1639	C
3	A	1647	U
3	A	1648	U
3	A	1649	G
3	A	1660	G
3	A	1674	G
3	A	1677	A
3	A	1715	G
3	A	1722	A
3	A	1725	U
3	A	1729	U
3	A	1730	C
3	A	1738	G
3	A	1744	A
3	A	1757	A
3	A	1764	C
3	A	1773	A
3	A	1782	U
3	A	1786	A

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Mol	Chain	Res	Type
3	A	1791	A
3	A	1800	C
3	A	1801	A
3	A	1802	A
3	A	1808	A
3	A	1809	A
3	A	1811	G
3	A	1816	C
3	A	1829	A
3	A	1847	A
3	A	1849	G
3	A	1850	G
3	A	1870	C
3	A	1871	A
3	A	1872	A
3	A	1876	A
3	A	1896	G
3	A	1906	G
3	A	1920	C
3	A	1927	A
3	A	1929	G
3	A	1930	G
3	A	1931	U
3	A	1934	C
3	A	1936	A
3	A	1937	A
3	A	1939	U
3	A	1955	U
3	A	1956	U
3	A	1960	A
3	A	1962	C
3	A	1966	A
3	A	1967	C
3	A	1970	A
3	A	1971	U
3	A	1972	G
3	A	1974	C
3	A	1982	U
3	A	1991	U
3	A	1992	G
3	A	1993	U
3	A	1997	C

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Mol	Chain	Res	Type
3	A	2021	C
3	A	2023	C
3	A	2030	A
3	A	2031	A
3	A	2033	A
3	A	2043	C
3	A	2050	C
3	A	2054	A
3	A	2055	C
3	A	2056	G
3	A	2060	A
3	A	2061	G
3	A	2062	A
3	A	2069	G
3	A	2072	C
3	A	2093	G
3	A	2097	A
3	A	2101	A
3	A	2103	C
3	A	2104	C
3	A	2105	U
3	A	2106	U
3	A	2111	U
3	A	2112	G
3	A	2113	U
3	A	2116	G
3	A	2117	A
3	A	2118	U
3	A	2119	A
3	A	2120	G
3	A	2123	G
3	A	2126	A
3	A	2128	G
3	A	2131	U
3	A	2132	U
3	A	2133	G
3	A	2134	A
3	A	2145	C
3	A	2146	C
3	A	2147	A
3	A	2148	G
3	A	2159	G

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Mol	Chain	Res	Type
3	A	2160	C
3	A	2161	C
3	A	2163	A
3	A	2164	C
3	A	2165	C
3	A	2167	U
3	A	2168	G
3	A	2169	A
3	A	2170	A
3	A	2171	A
3	A	2172	U
3	A	2173	A
3	A	2174	C
3	A	2177	C
3	A	2178	C
3	A	2185	U
3	A	2187	U
3	A	2190	G
3	A	2198	A
3	A	2203	U
3	A	2204	G
3	A	2211	A
3	A	2212	A
3	A	2225	A
3	A	2238	G
3	A	2239	G
3	A	2250	G
3	A	2268	A
3	A	2278	A
3	A	2280	G
3	A	2283	C
3	A	2287	A
3	A	2288	A
3	A	2297	A
3	A	2305	U
3	A	2308	G
3	A	2322	A
3	A	2325	G
3	A	2331	G
3	A	2336	A
3	A	2345	G
3	A	2347	C

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Mol	Chain	Res	Type
3	A	2350	C
3	A	2354	C
3	A	2357	G
3	A	2366	A
3	A	2383	G
3	A	2385	C
3	A	2402	U
3	A	2403	C
3	A	2406	A
3	A	2420	C
3	A	2421	G
3	A	2422	C
3	A	2423	U
3	A	2424	C
3	A	2425	A
3	A	2427	C
3	A	2429	G
3	A	2430	A
3	A	2431	U
3	A	2432	A
3	A	2434	A
3	A	2435	A
3	A	2440	C
3	A	2441	U
3	A	2445	G
3	A	2448	A
3	A	2464	G
3	A	2475	C
3	A	2476	A
3	A	2478	A
3	A	2491	U
3	A	2492	U
3	A	2497	A
3	A	2502	G
3	A	2504	U
3	A	2505	G
3	A	2506	U
3	A	2507	C
3	A	2513	A
3	A	2514	U
3	A	2518	A
3	A	2520	C

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Mol	Chain	Res	Type
3	A	2529	G
3	A	2566	A
3	A	2567	G
3	A	2578	G
3	A	2582	G
3	A	2585	U
3	A	2586	U
3	A	2602	A
3	A	2603	G
3	A	2609	U
3	A	2613	U
3	A	2615	U
3	A	2621	G
3	A	2623	G
3	A	2624	G
3	A	2629	U
3	A	2630	G
3	A	2636	C
3	A	2638	G
3	A	2669	G
3	A	2682	A
3	A	2689	U
3	A	2690	U
3	A	2714	G
3	A	2716	C
3	A	2726	A
3	A	2733	A
3	A	2739	U
3	A	2744	G
3	A	2748	A
3	A	2757	A
3	A	2765	A
3	A	2778	A
3	A	2779	U
3	A	2780	G
3	A	2787	C
3	A	2791	G
3	A	2792	A
3	A	2798	U
3	A	2799	A
3	A	2801	G
3	A	2820	A

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Mol	Chain	Res	Type
3	A	2821	A
3	A	2825	G
3	A	2833	U
3	A	2835	A
3	A	2836	U
3	A	2849	U
3	A	2860	A
3	A	2861	U
3	A	2867	G
3	A	2870	C
3	A	2873	A
3	A	2879	A
3	A	2880	C
3	A	2883	A
3	A	2884	U
3	A	2885	G
3	A	2886	A
3	A	2888	C
3	A	2891	U
4	B	24	G
4	B	25	U
4	B	35	C
4	B	41	G
4	B	45	A
4	B	56	G
4	B	66	A
4	B	67	G
4	B	71	C
4	B	88	C
4	B	89	U
4	B	90	C
4	B	109	A

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	68	A
3	A	100	U
3	A	613	A
3	A	645	C
3	A	653	U
3	A	784	G

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Mol	Chain	Res	Type
3	A	827	U
3	A	830	G
3	A	1110	G
3	A	1344	U
3	A	1494	A
3	A	1721	G
3	A	1939	U
3	A	2127	G
3	A	2158	A
3	A	2422	C
3	A	2424	C
3	A	2430	A
3	A	2602	A
3	A	2756	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 436 ligands modelled in this entry, 434 are monoatomic - leaving 2 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	$\# Z > 2$
40	GNP	l	1400	38	34,34,34	1.68	9 (26%)	47,54,54	1.97	15 (31%)
40	GNP	i	1400	38	34,34,34	1.79	8 (23%)	47,54,54	2.06	15 (31%)

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
40	GNP	l	1400	38	-	3/18/38/38	0/3/3/3
40	GNP	i	1400	38	-	3/18/38/38	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	i	1400	GNP	C4-N3	4.72	1.45	1.34
40	l	1400	GNP	C4-N3	4.26	1.44	1.34
40	l	1400	GNP	PB-O1B	3.34	1.51	1.46
40	i	1400	GNP	PB-O1B	3.11	1.50	1.46
40	i	1400	GNP	PG-O3G	-3.06	1.48	1.56
40	i	1400	GNP	PB-O2B	-3.05	1.48	1.56
40	i	1400	GNP	PG-O1G	2.93	1.50	1.46
40	l	1400	GNP	C4-N9	-2.64	1.31	1.38
40	l	1400	GNP	PG-O3G	-2.63	1.49	1.56
40	i	1400	GNP	C4-N9	-2.60	1.31	1.38
40	i	1400	GNP	PG-O2G	-2.59	1.49	1.56
40	l	1400	GNP	PG-O2G	-2.50	1.50	1.56
40	i	1400	GNP	C5-N7	-2.39	1.34	1.39
40	l	1400	GNP	PG-N3B	2.34	1.69	1.63
40	l	1400	GNP	PB-O2B	-2.32	1.50	1.56
40	l	1400	GNP	PG-O1G	2.30	1.49	1.46
40	l	1400	GNP	C6-N1	-2.01	1.35	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	l	1400	GNP	C6-C5-N7	4.52	138.51	130.29
40	i	1400	GNP	C6-C5-N7	4.47	138.43	130.29
40	i	1400	GNP	O3'-C3'-C4'	-4.37	98.54	111.08
40	l	1400	GNP	O2B-PB-O1B	4.23	118.94	109.87
40	l	1400	GNP	C5-C4-N3	-3.77	122.39	128.39
40	i	1400	GNP	C5-C4-N3	-3.75	122.41	128.39
40	i	1400	GNP	O6-C6-C5	-3.74	116.65	126.53
40	l	1400	GNP	O1G-PG-N3B	-3.72	106.29	111.77
40	i	1400	GNP	C2'-C3'-C4'	3.72	109.80	102.61
40	l	1400	GNP	O3'-C3'-C2'	-3.63	100.19	111.82
40	i	1400	GNP	O2B-PB-O1B	3.59	117.56	109.87
40	i	1400	GNP	C2-N3-C4	3.25	117.89	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	i	1400	GNP	O1G-PG-N3B	-3.04	107.29	111.77
40	l	1400	GNP	O4'-C1'-N9	3.01	115.17	108.36
40	i	1400	GNP	C2'-C1'-N9	2.99	121.56	113.25
40	l	1400	GNP	O6-C6-C5	-2.98	118.68	126.53
40	i	1400	GNP	C6-C5-C4	-2.87	114.51	118.83
40	i	1400	GNP	O3'-C3'-C2'	-2.86	102.65	111.82
40	l	1400	GNP	C2-N3-C4	2.81	117.13	112.30
40	l	1400	GNP	C2'-C3'-C4'	2.72	107.87	102.61
40	i	1400	GNP	O2'-C2'-C1'	2.72	119.45	110.10
40	l	1400	GNP	C6-C5-C4	-2.61	114.91	118.83
40	l	1400	GNP	C4-C5-N7	-2.58	106.58	110.67
40	i	1400	GNP	O2'-C2'-C3'	2.55	119.99	111.82
40	i	1400	GNP	C5-C6-N1	2.54	119.72	113.25
40	l	1400	GNP	C5-C6-N1	2.44	119.45	113.25
40	i	1400	GNP	C4-C5-N7	-2.28	107.05	110.67
40	l	1400	GNP	O2'-C2'-C1'	2.28	117.95	110.10
40	l	1400	GNP	C2'-C1'-N9	2.14	119.19	113.25
40	l	1400	GNP	O3'-C3'-C4'	-2.05	105.19	111.08

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	i	1400	GNP	PB-N3B-PG-O1G
40	i	1400	GNP	PG-N3B-PB-O1B
40	i	1400	GNP	PG-N3B-PB-O3A
40	l	1400	GNP	PB-N3B-PG-O1G
40	l	1400	GNP	PG-N3B-PB-O1B
40	l	1400	GNP	PG-N3B-PB-O3A

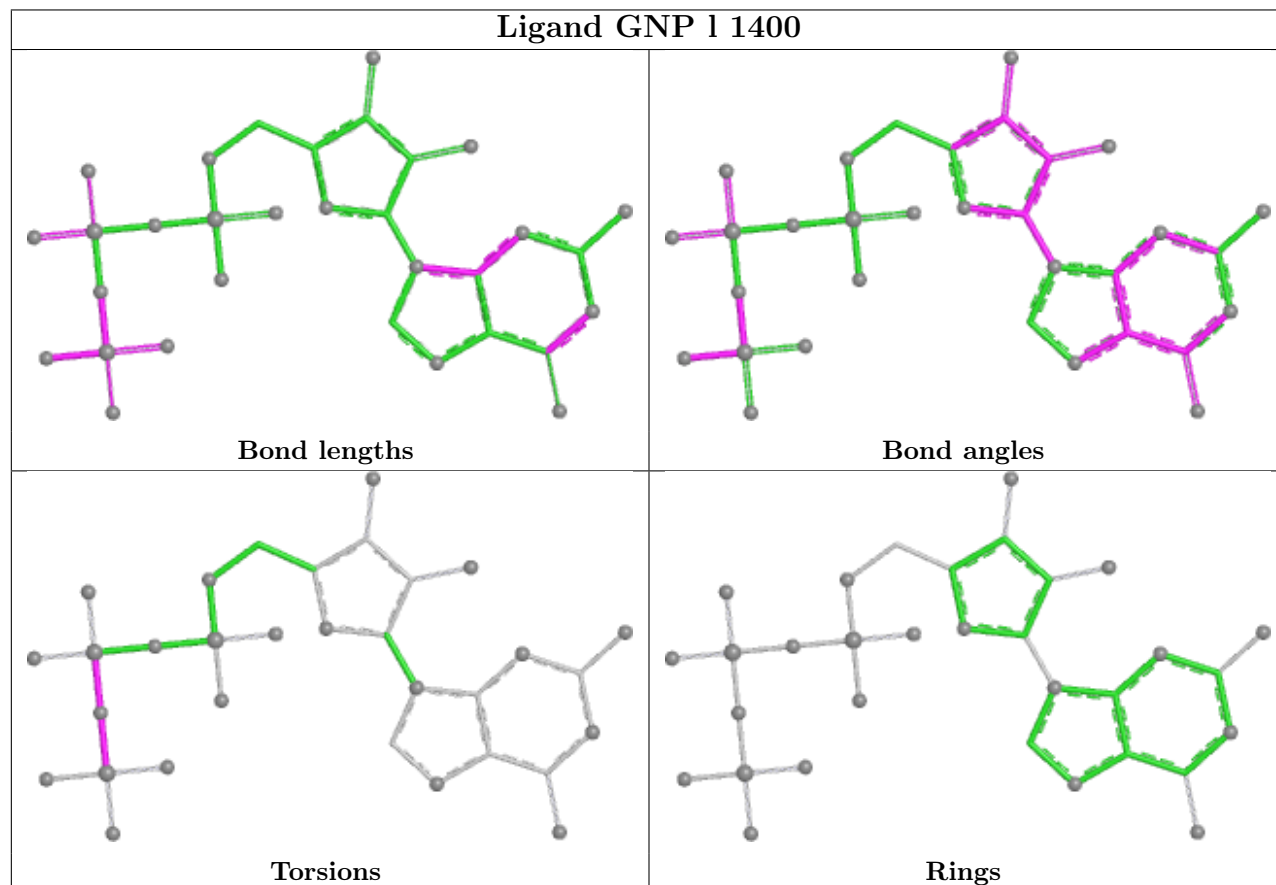
There are no ring outliers.

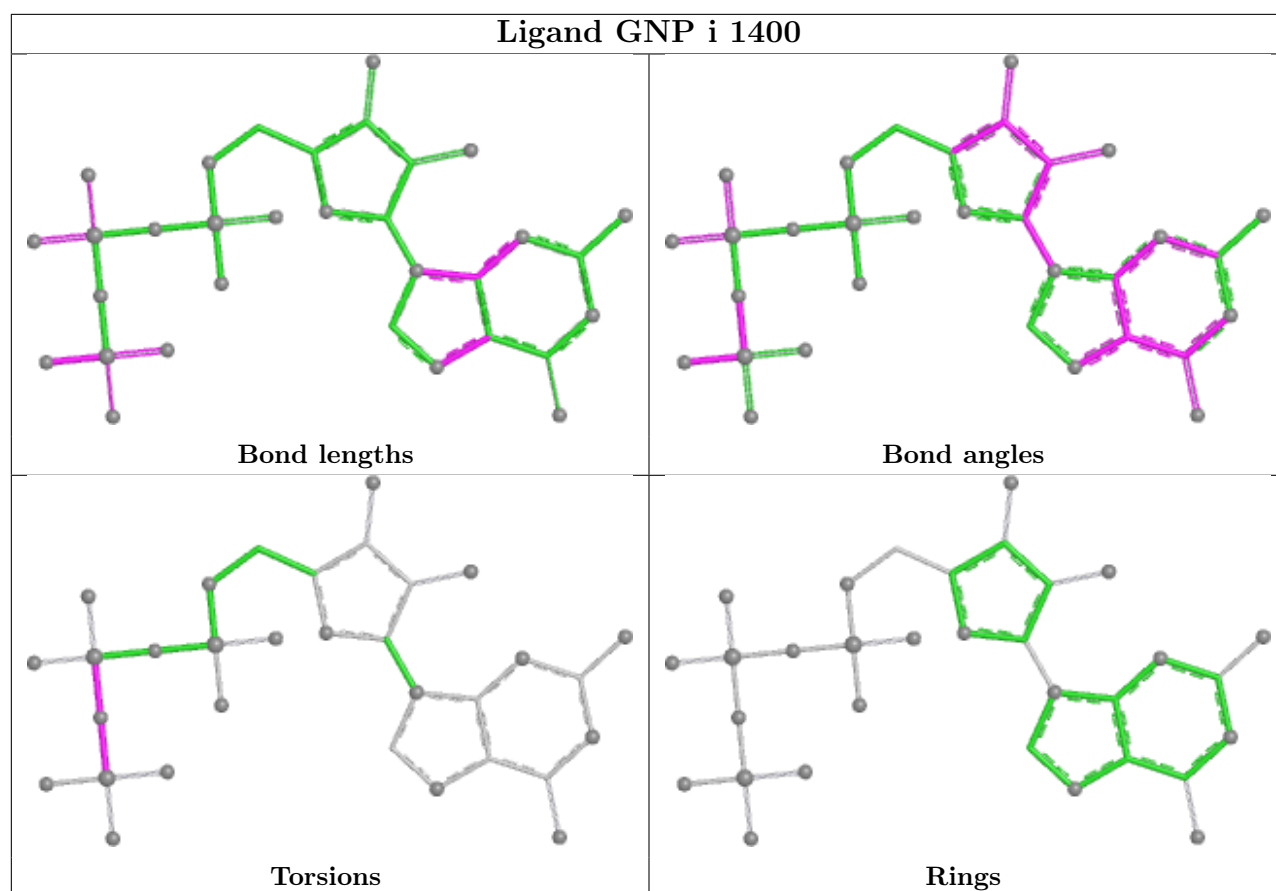
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	i	1400	GNP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	Z	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	15:ASN	C	16:THR	N	3.07
1	Z	40:SER	C	41:HIS	N	2.90

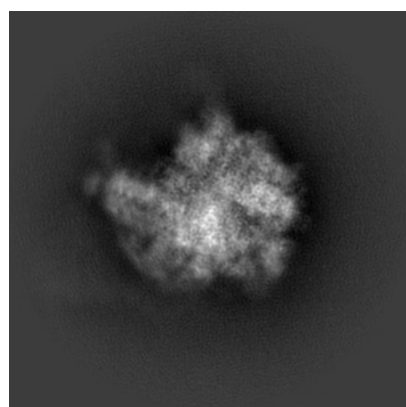
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8000. These allow visual inspection of the internal detail of the map and identification of artifacts.

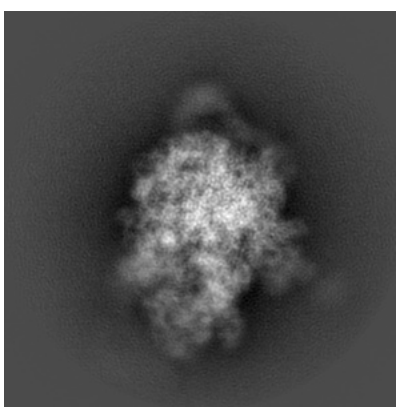
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

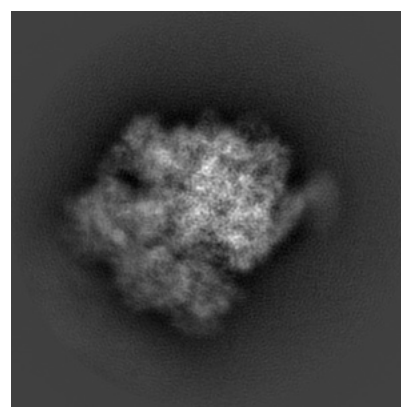
6.1.1 Primary map



X



Y

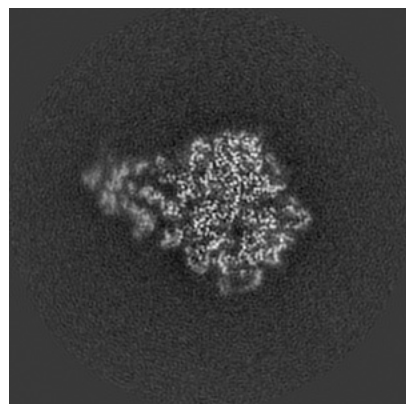


Z

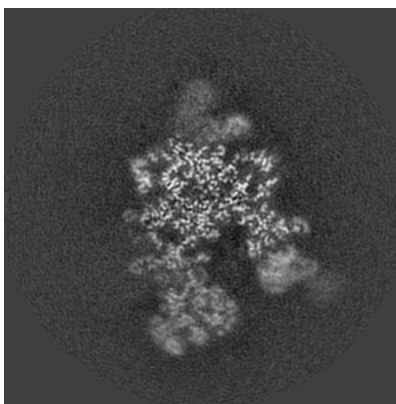
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

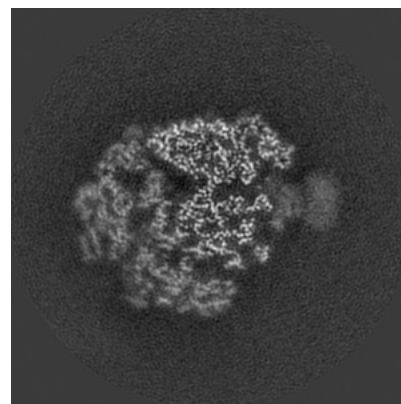
6.2.1 Primary map



X Index: 160



Y Index: 160

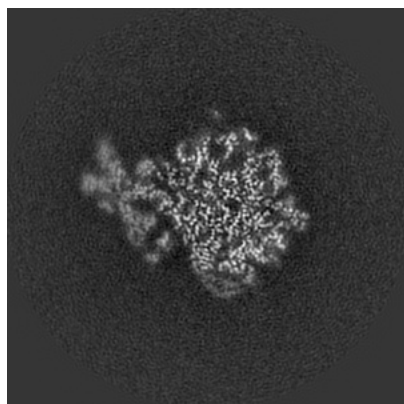


Z Index: 160

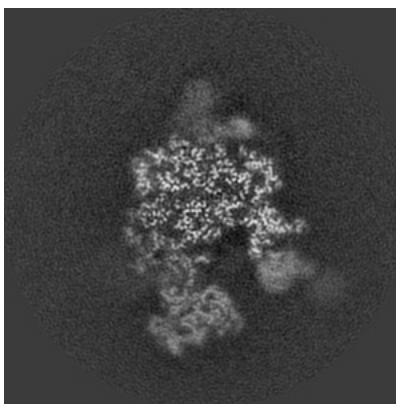
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

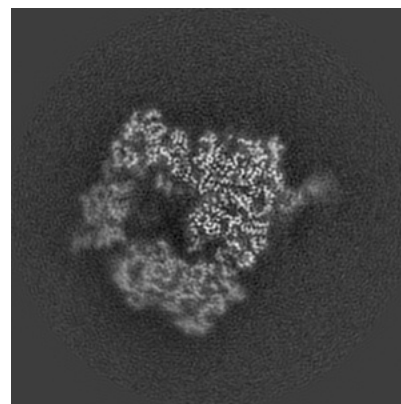
6.3.1 Primary map



X Index: 154



Y Index: 157

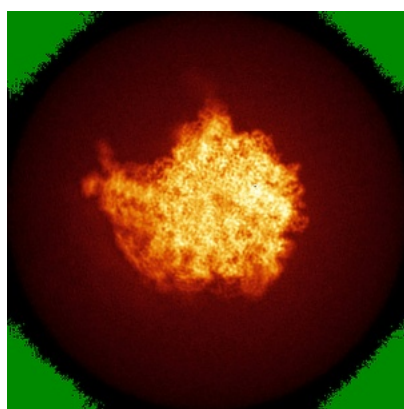


Z Index: 175

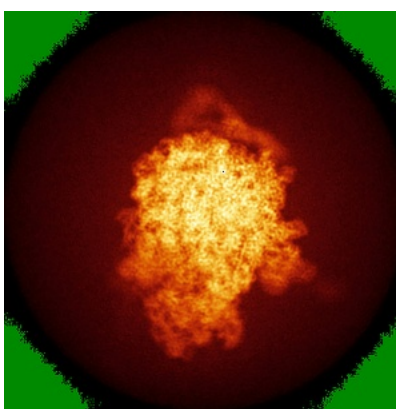
The images above show the largest variance slices of the map in three orthogonal directions.

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

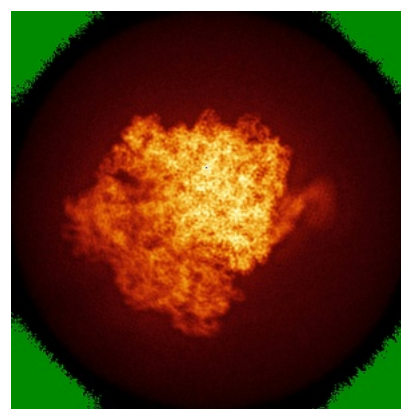
6.4.1 Primary map



X



Y

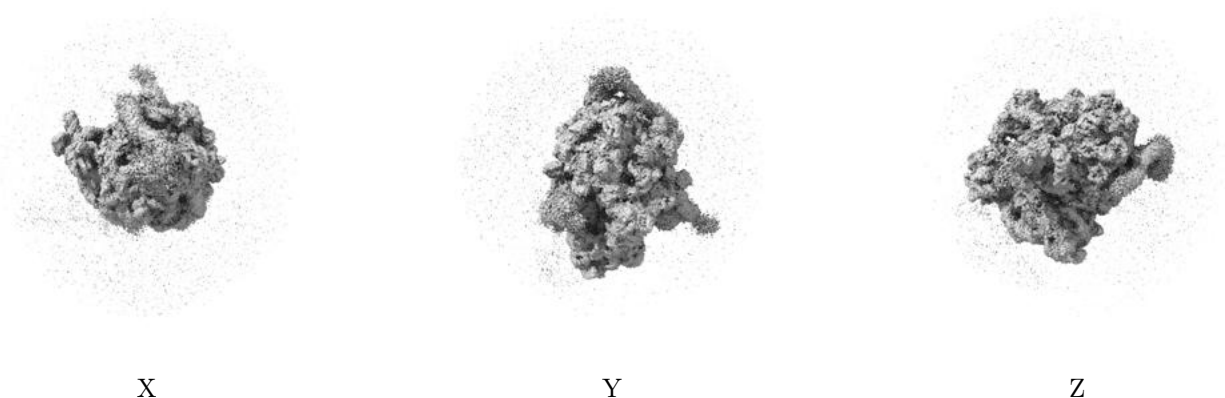


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

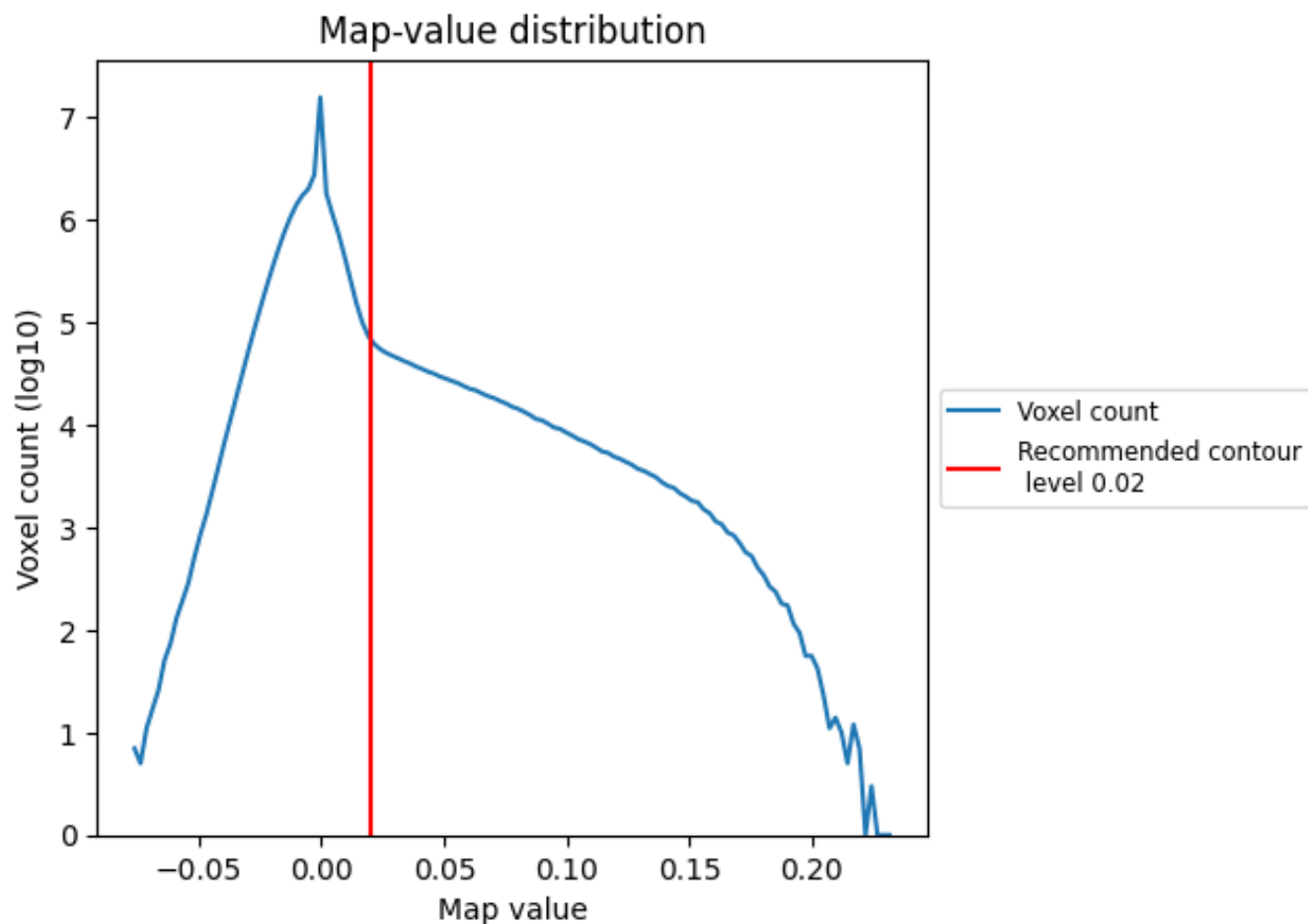
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

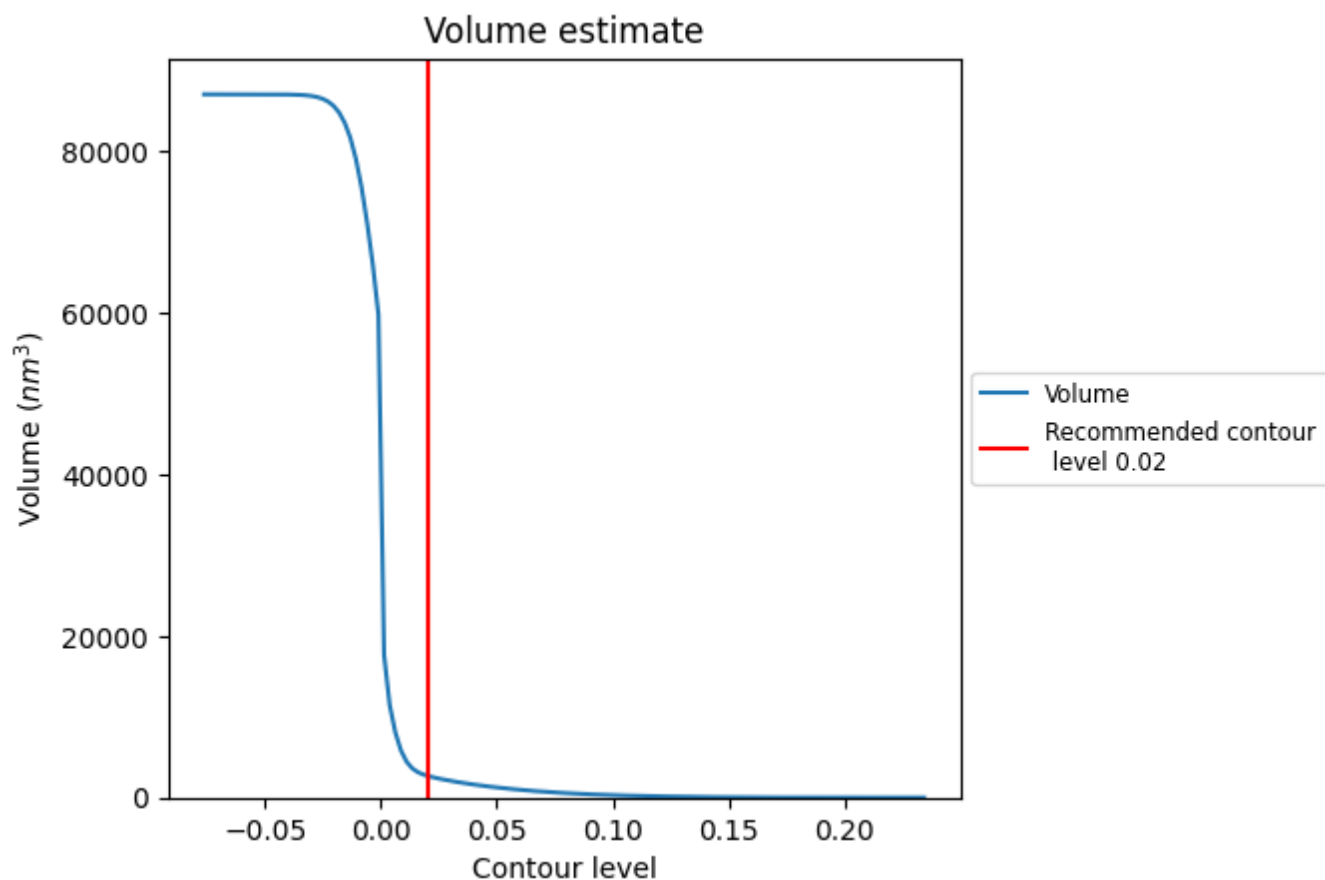
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

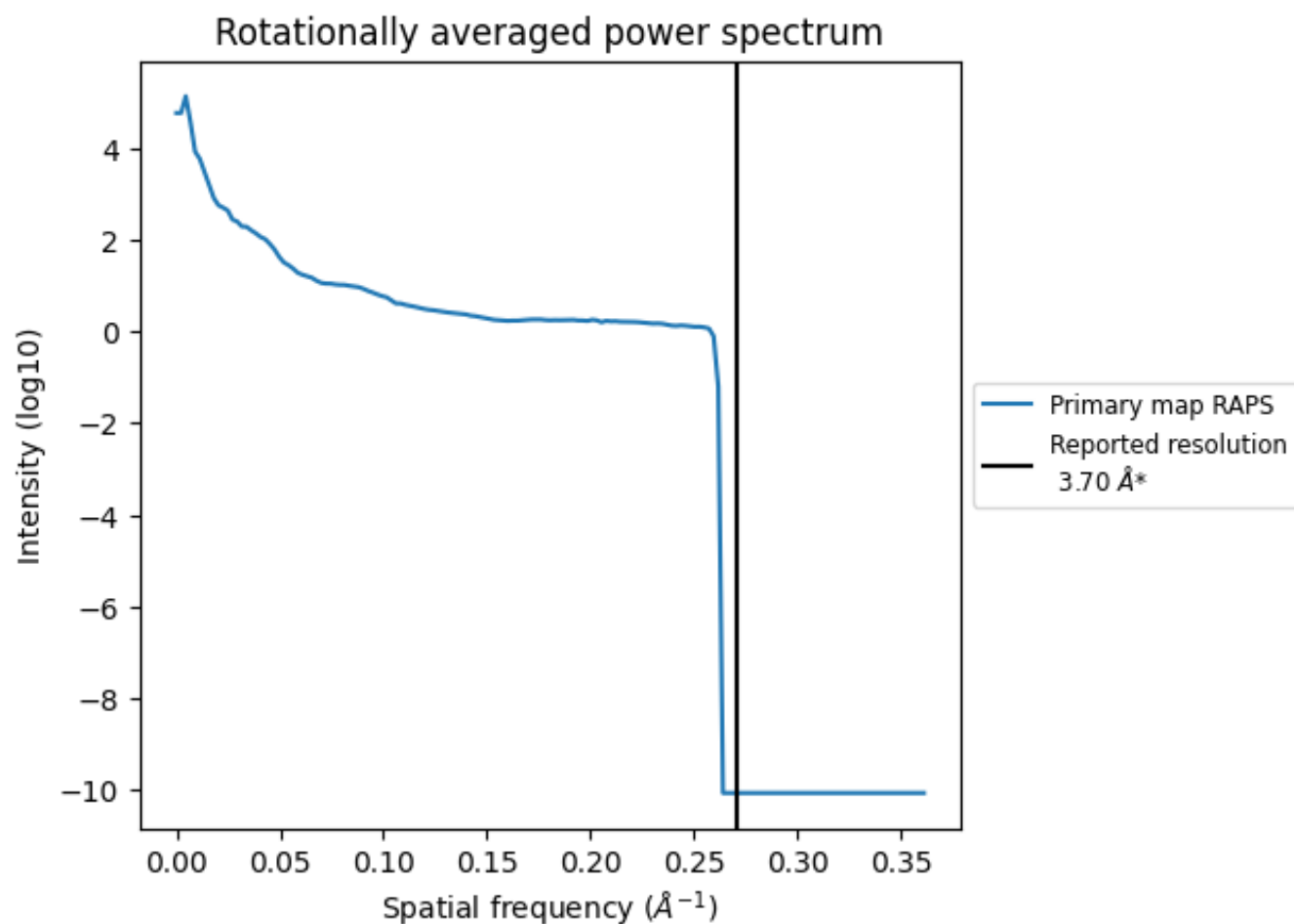
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2699 nm³; this corresponds to an approximate mass of 2438 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 0.270 Å⁻¹

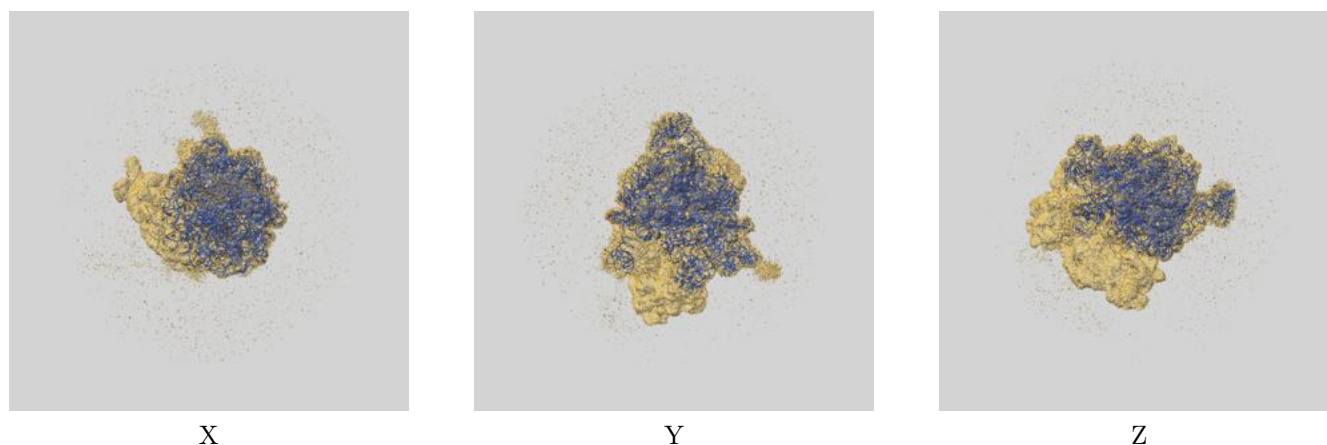
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

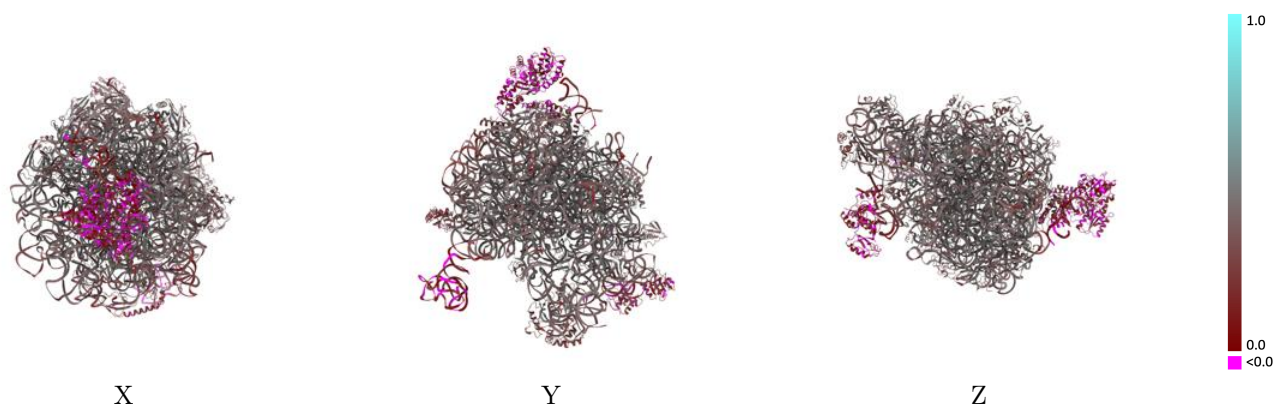
This section contains information regarding the fit between EMDB map EMD-8000 and PDB model 5GAD. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



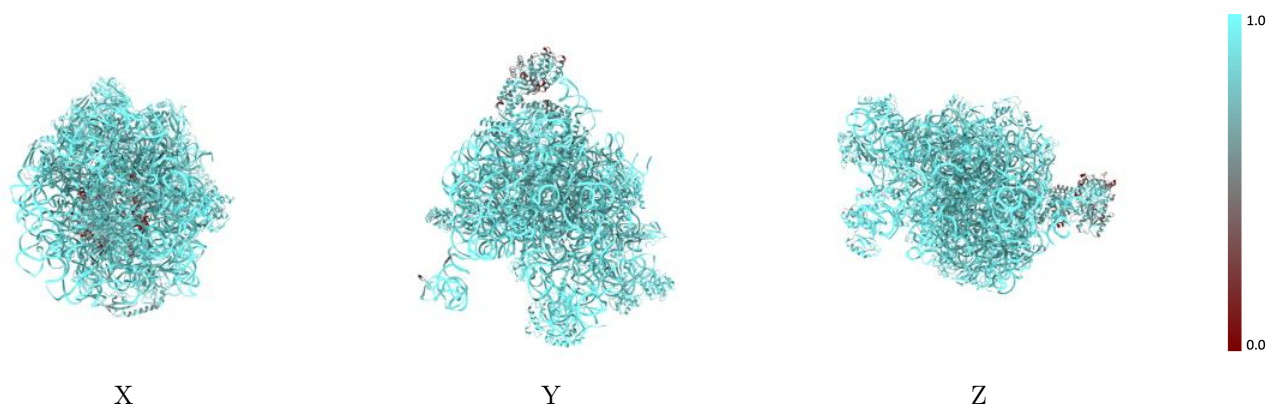
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



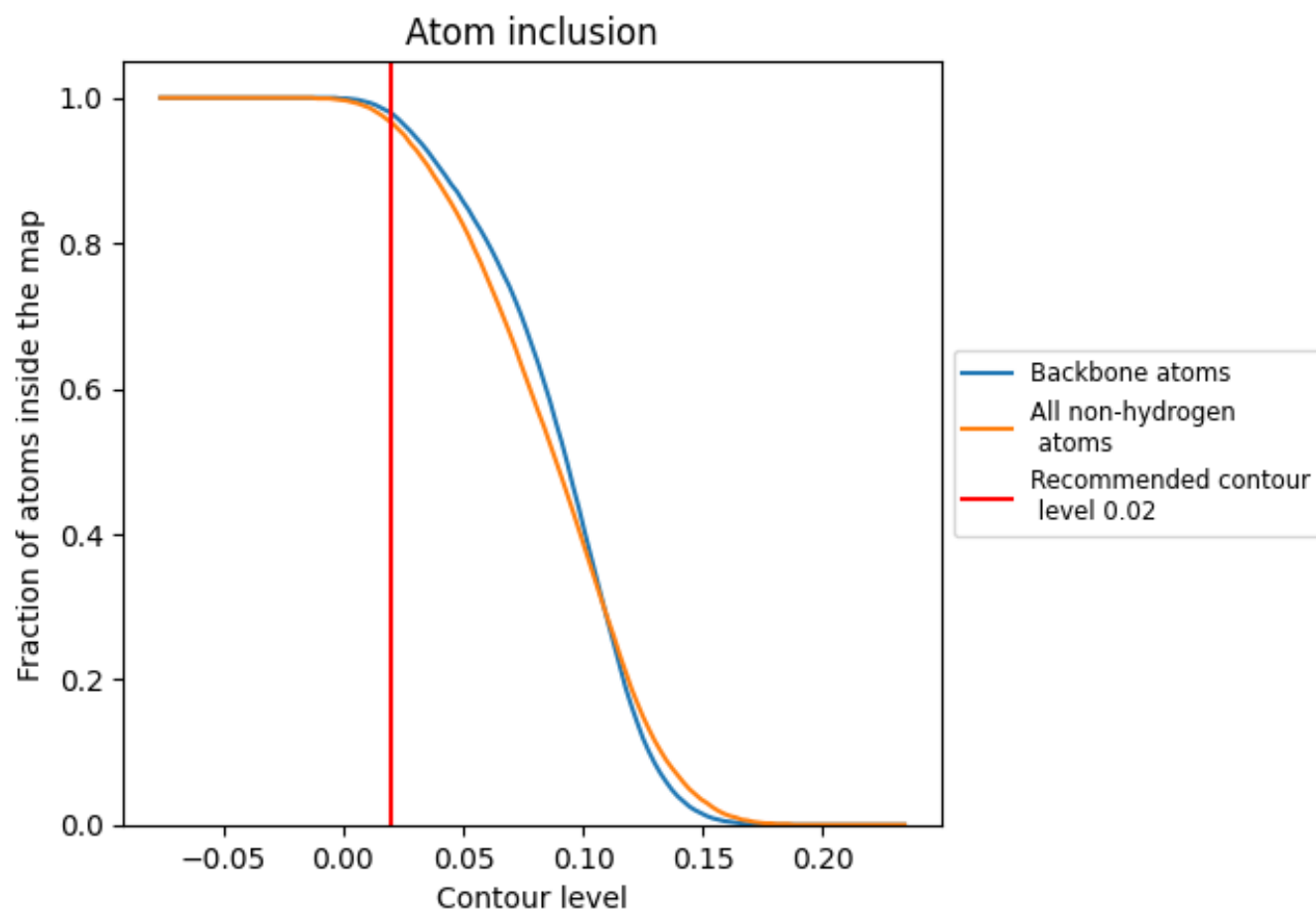
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 97% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9660	 0.3710
1	 0.9890	 0.1330
2	 0.9840	 0.4410
A	 0.9950	 0.3960
B	 1.0000	 0.3890
C	 0.9490	 0.4340
D	 0.9520	 0.4300
E	 0.9330	 0.3940
F	 0.9560	 0.3290
G	 0.9450	 0.3680
H	 0.8110	 0.2610
I	 0.9240	 0.1510
J	 0.9110	 0.0770
K	 0.9660	 0.4150
L	 0.9030	 0.4160
M	 0.9510	 0.4030
N	 0.9500	 0.4270
O	 0.9500	 0.4190
P	 0.9630	 0.3720
Q	 0.9310	 0.4000
R	 0.9770	 0.4220
S	 0.9440	 0.4150
T	 0.9140	 0.4170
U	 0.9220	 0.3880
V	 0.9320	 0.3900
W	 0.9390	 0.3980
X	 0.9520	 0.4230
Y	 0.9480	 0.4100
Z	 0.9020	 0.3350
a	 0.9470	 0.4160
b	 0.9490	 0.4200
c	 0.9290	 0.3880
d	 0.9440	 0.4280
e	 0.9390	 0.4390
f	 0.9730	 0.4150



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Chain	Atom inclusion	Q-score
i	 0.7650	 0.0780
k	 0.7740	 0.1020
l	 0.6490	 0.0230