



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 04:36 PM EDT

PDB ID : 3OW2  
Title : Crystal Structure of Enhanced Macrolide Bound to 50S Ribosomal Subunit  
Authors : Kanyo, Z.F.  
Deposited on : 2010-09-17  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

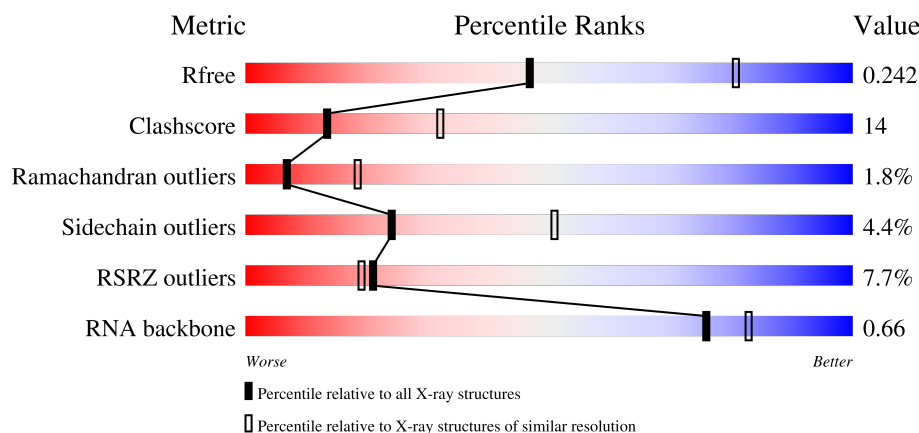
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)
RNA backbone	3690	1028 (2.94-2.46)

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

Mol	Chain	Length	Quality of chain
1	0	2902	<div> <div>5%</div> <div>55% 35% 5% 5%</div> </div>
2	9	122	<div> <div>7%</div> <div>51% 39% 9%</div> </div>
3	A	237	<div> <div>6%</div> <div>67% 28% 5%</div> </div>
4	B	337	<div> <div>5%</div> <div>62% 34%</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	165	
7	E	172	
8	F	119	
9	G	62	
10	H	167	
11	I	142	
12	J	132	
13	K	150	
14	L	194	
15	M	186	
16	N	115	
17	O	143	
18	P	95	
19	Q	150	
20	R	81	
21	S	119	
22	T	53	
23	U	65	
24	V	154	
25	W	82	
26	X	142	
27	Y	73	
28	Z	56	
29	1	48	

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Mol	Chain	Length	Quality of chain
30	2	92	<div> <div></div> <div>%</div> <div>76%</div> <div>24%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	0	8012	-	-	-	X
31	MG	0	8018	-	-	-	X
31	MG	0	8035	-	-	-	X
31	MG	0	8043	-	-	-	X
31	MG	0	8050	-	-	-	X
31	MG	0	8053	-	-	-	X
31	MG	B	401	-	-	-	X
31	MG	S	201	-	-	-	X
33	NA	0	8063	-	-	-	X
33	NA	0	8075	-	-	-	X
33	NA	9	3202	-	-	-	X
36	EMK	0	8163	-	-	X	-

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 90725 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59016	26346	10878	19047	2745			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	?	-	U	deletion	GB 3377779
0	?	-	C	deletion	GB 3377779
0	560	C	U	conflict	GB 3377779
0	2099	A	G	conflict	GB 3377779

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	237	Total	C	N	O	S	0	0	0
			1755	1072	352	326	5			

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 5 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 6 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	140	Total	C	N	O	S	0	0	0
			1095	685	195	211	4			

- Molecule 7 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	172	Total	C	N	O	S	0	0	0
			1358	840	224	290	4			

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	119	Total	C	N	O	S	0	0	0
			886	552	141	192	1			

- Molecule 9 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	29	Total	C	N	O	S	0	0	0
			241	149	39	52	1			

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	156	Total	C	N	O	S	0	0	0
			1216	766	233	213	4			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	145	Total	C	N	O		0	0	0
			1119	670	222	227				

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	194	Total	C	N	O	S	0	0	0
			1606	988	346	267	5			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 16 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	143	Total	C	N	O		0	0	0
			1134	680	230	224				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	71	LYS	TYR	conflict	UNP P14119

- Molecule 18 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	95	Total	C	N	O			
			735	450	141	144	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	150	Total	C	N	O	S		
			1150	713	209	224	4	0	0

- Molecule 20 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	81	Total	C	N	O	S		
			642	389	111	139	3	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	S	119	Total	C	N	O			
			950	568	180	202		0	0

- Molecule 22 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	53	Total	C	N	O	S		
			411	244	75	87	5	0	0

- Molecule 23 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	U	65	Total	C	N	O	S		
			500	304	94	101	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	V	154	Total	C	N	O	S		
			1196	737	209	244	6	0	0

- Molecule 25 is a protein called 50S ribosomal protein L31e.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	82	Total	C	N	O	S	0	0	0
			655	402	129	123	1			

- Molecule 26 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	142	Total	C	N	O		0	0	0
			1131	686	228	217				

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	73	Total	C	N	O	S	0	0	0
			564	359	111	87	7			

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	46	Total	C	N	O	S	0	0	0
			394	238	86	69	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	0	55	Total	Mg	0	0
			55	55		
31	9	1	Total	Mg	0	0
			1	1		
31	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	J	1	Total 1	Mg 1	0	0
31	K	1	Total 1	Mg 1	0	0
31	S	1	Total 1	Mg 1	0	0
31	X	1	Total 1	Mg 1	0	0

- Molecule 32 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	1	Total 1	K 1	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	19	Total 19	Na 19	0	0
33	9	1	Total 1	Na 1	0	0
33	C	1	Total 1	Na 1	0	0
33	I	1	Total 1	Na 1	0	0
33	L	1	Total 1	Na 1	0	0
33	P	1	Total 1	Na 1	0	0
33	Q	2	Total 2	Na 2	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	5	Total 5	Cl 5	0	0
34	A	1	Total 1	Cl 1	0	0
34	D	1	Total 1	Cl 1	0	0

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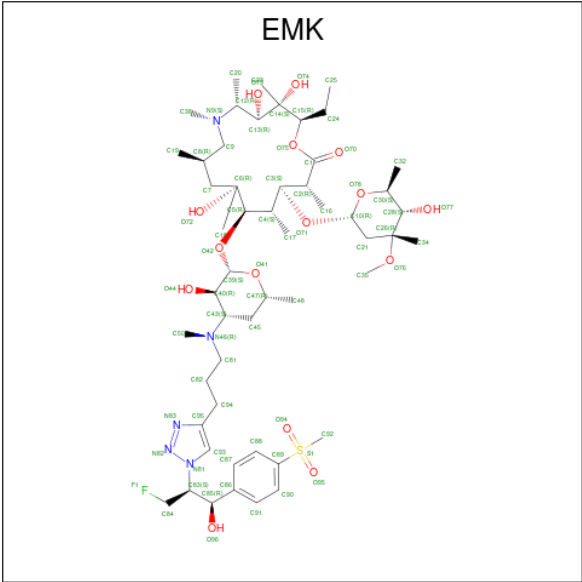
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	I	2	Total	Cl	0	0
			2	2		
34	L	1	Total	Cl	0	0
			1	1		
34	N	1	Total	Cl	0	0
			1	1		
34	Q	1	Total	Cl	0	0
			1	1		
34	X	1	Total	Cl	0	0
			1	1		

- Molecule 35 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	82	Total	Sr	0	0
			82	82		
35	9	3	Total	Sr	0	0
			3	3		
35	A	4	Total	Sr	0	0
			4	4		
35	B	2	Total	Sr	0	0
			2	2		
35	F	1	Total	Sr	0	0
			1	1		
35	Q	1	Total	Sr	0	0
			1	1		
35	R	1	Total	Sr	0	0
			1	1		
35	Z	2	Total	Sr	0	0
			2	2		
35	2	2	Total	Sr	0	0
			2	2		

- Molecule 36 is (2R,3S,4R,5R,8R,10R,11R,12S,13S,14R)-2-ethyl-3,4,10-trihydroxy-3,5,6,8,10,12,14-heptamethyl-15-oxo-11-[(3,4,6-trideoxy-3-{[3-(1-{(1S,2R)-1-(fluoromethyl)-2-hydroxy-2-[4-(methylsulfonyl)phenyl]ethyl}-1H-1,2,3-triazol-4-yl)propyl](methyl)amino}-beta-D-xylo-hexopyranosyl)oxy]-1-oxa-6-azacyclopentadecan-13-yl 2,6-dideoxy-3-C-methyl-3-O-methyl-alpha-L-ribo-hexopyranoside (three-letter code: EMK) (formula: C<sub>52</sub>H<sub>88</sub>FN<sub>5</sub>O<sub>15</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
36	0	1	Total	C	F	N	O	S	0	0
			74	52	1	5	15	1		

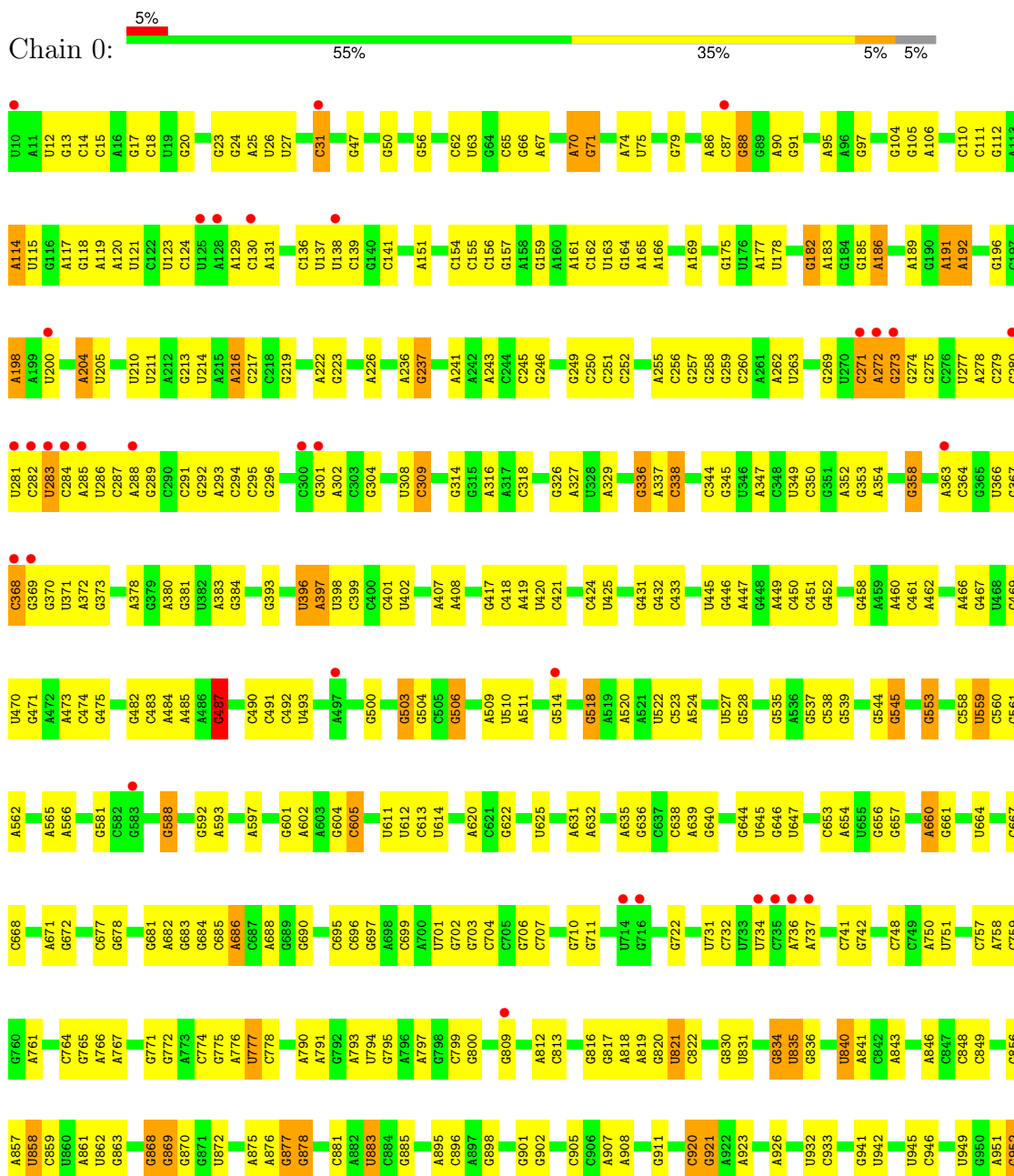
- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

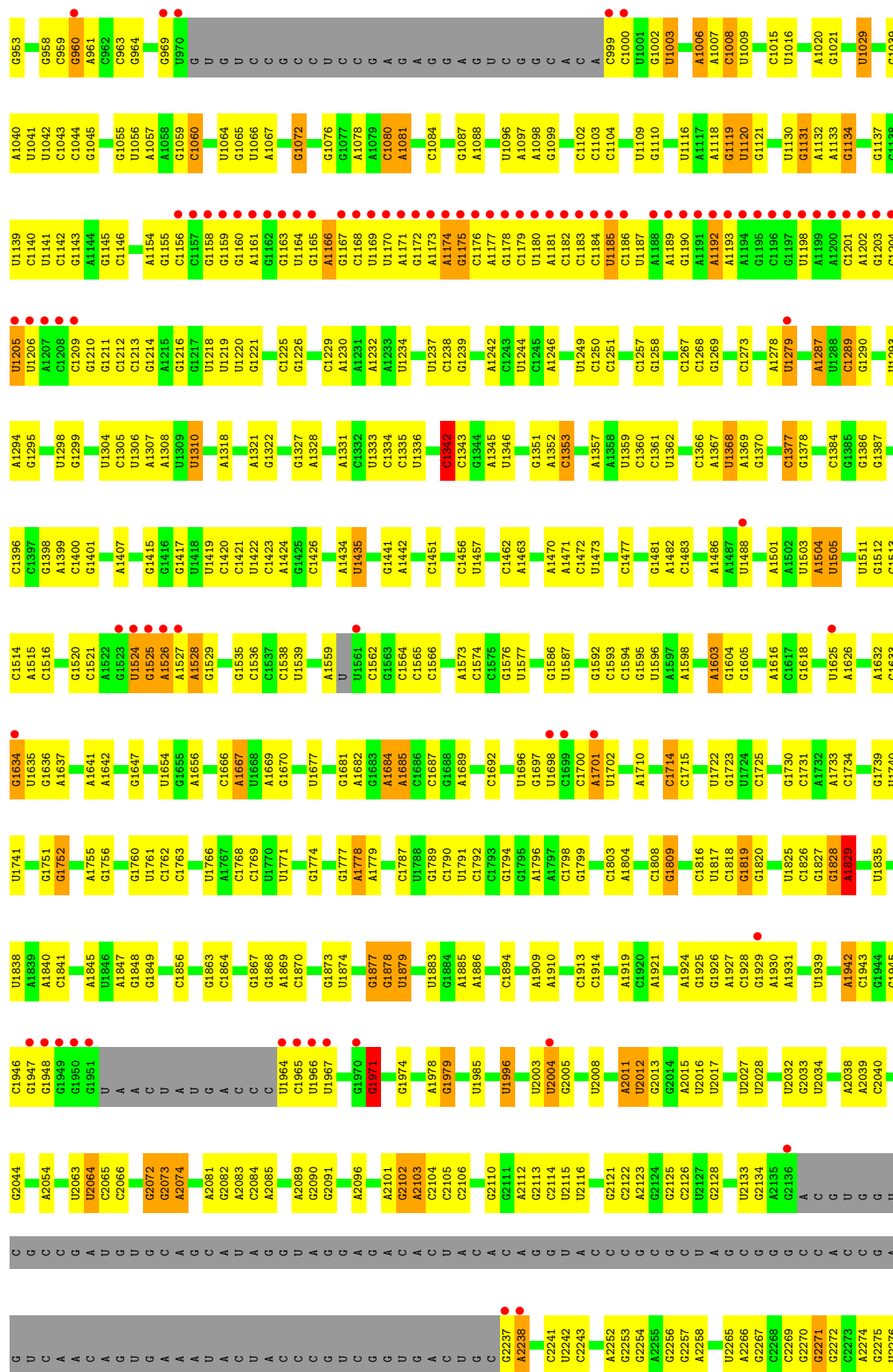
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	T	1	Total	Cd	0	0
			1	1		
37	Y	1	Total	Cd	0	0
			1	1		
37	Z	1	Total	Cd	0	0
			1	1		
37	2	1	Total	Cd	0	0
			1	1		

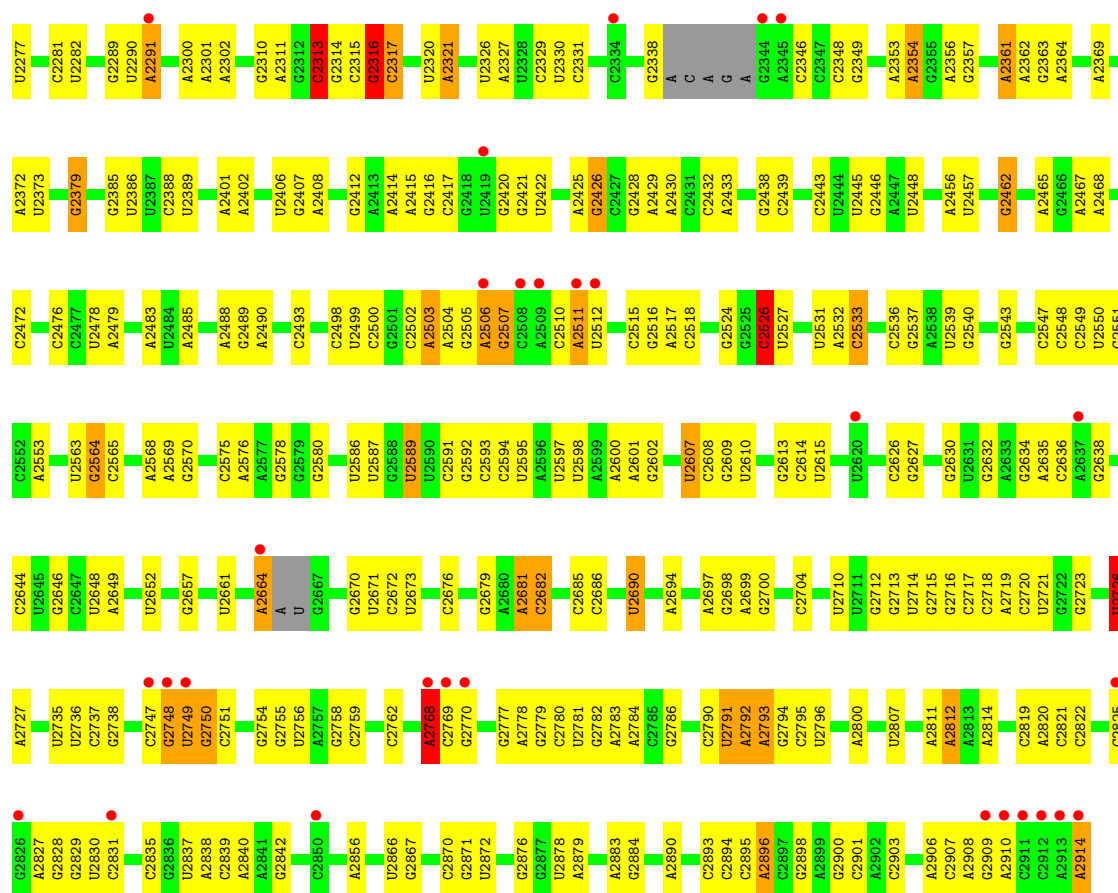
### 3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

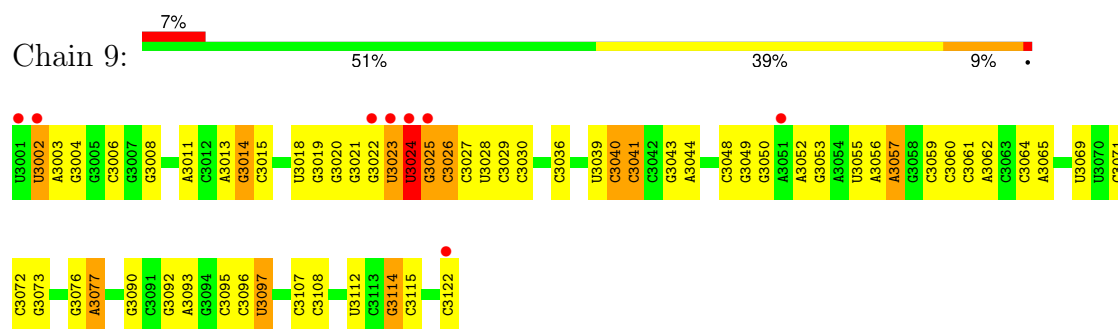
#### • Molecule 1: 23S RIBOSOMAL RNA



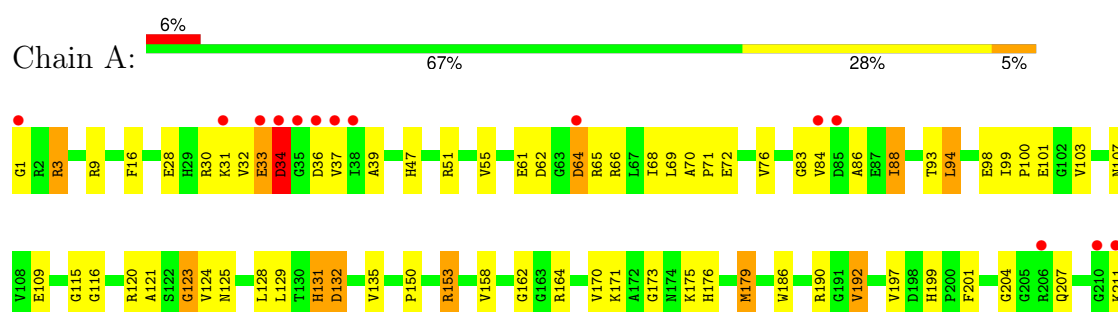




- Molecule 2: 5S RIBOSOMAL RNA

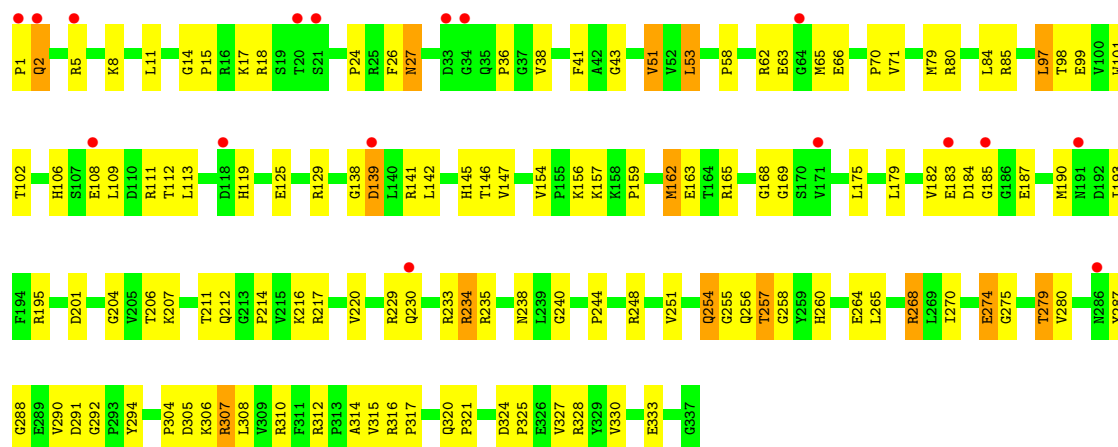


- Molecule 3: 50S ribosomal protein L2P

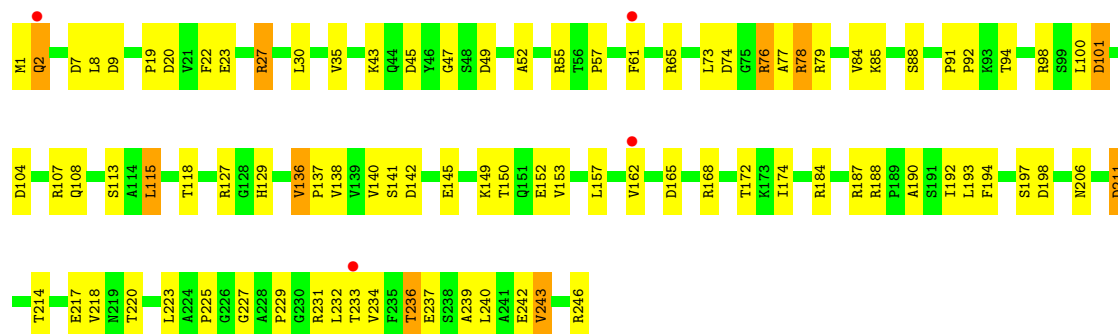




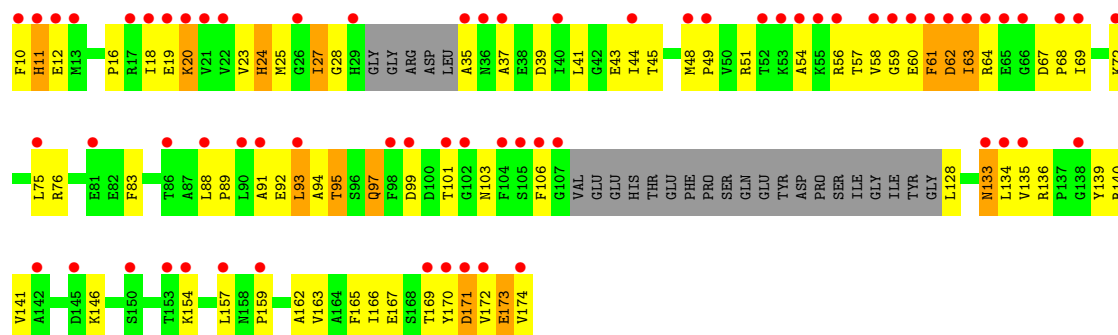
• Molecule 4: 50S ribosomal protein L3P



• Molecule 5: 50S ribosomal protein L4P

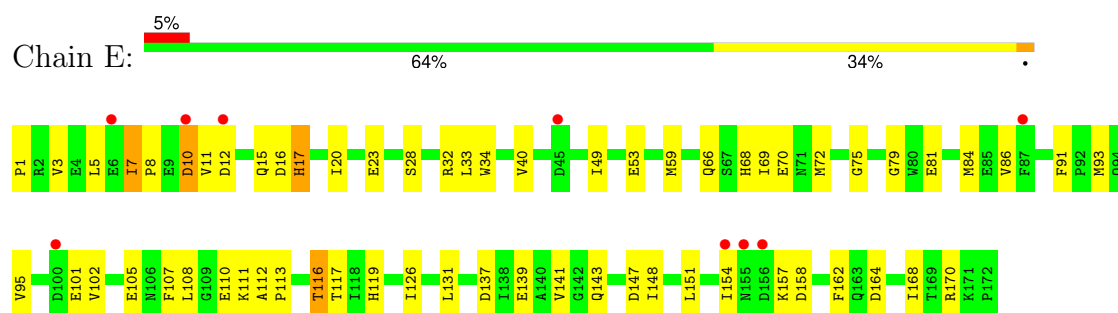


• Molecule 6: 50S ribosomal protein L5P

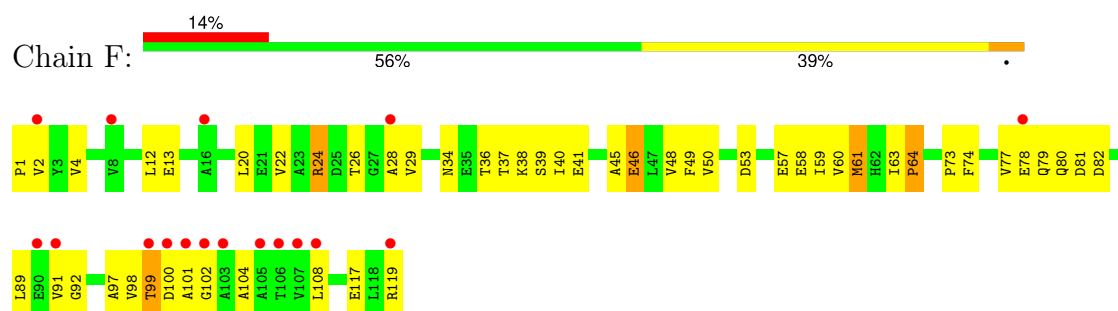




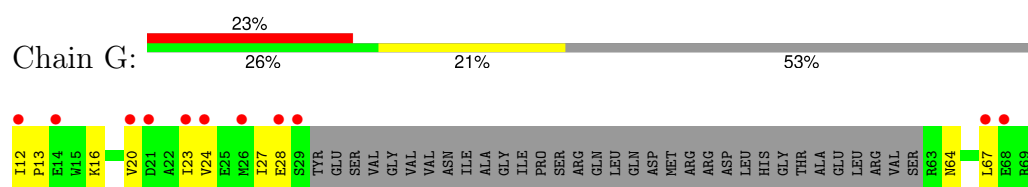
- Molecule 7: 50S ribosomal protein L6P



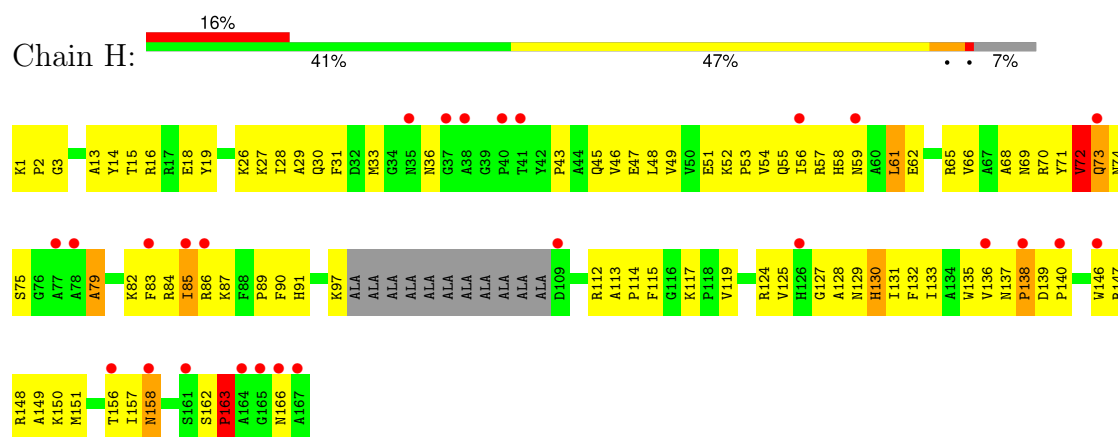
- Molecule 8: 50S ribosomal protein L7Ae



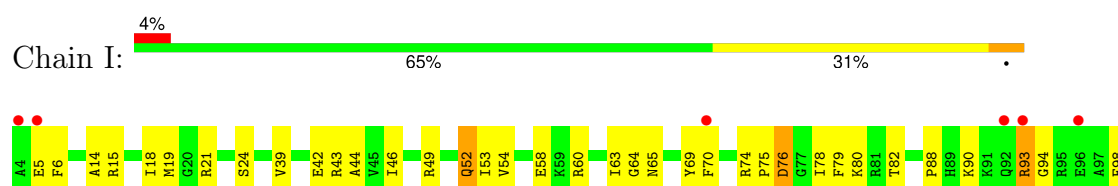
- Molecule 9: 50S ribosomal protein L10E



- Molecule 10: 50S ribosomal protein L10e

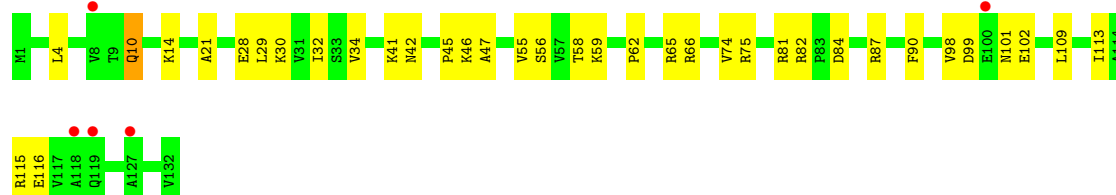


- Molecule 11: 50S ribosomal protein L13P

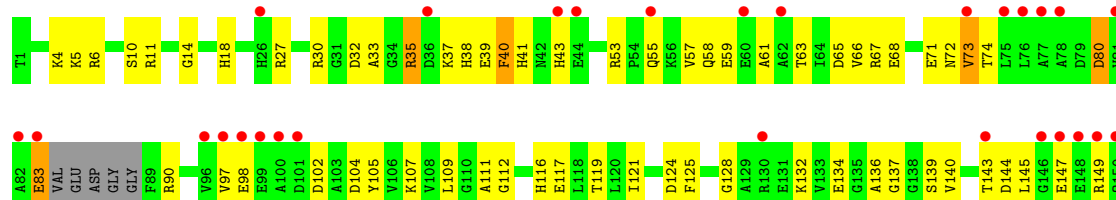




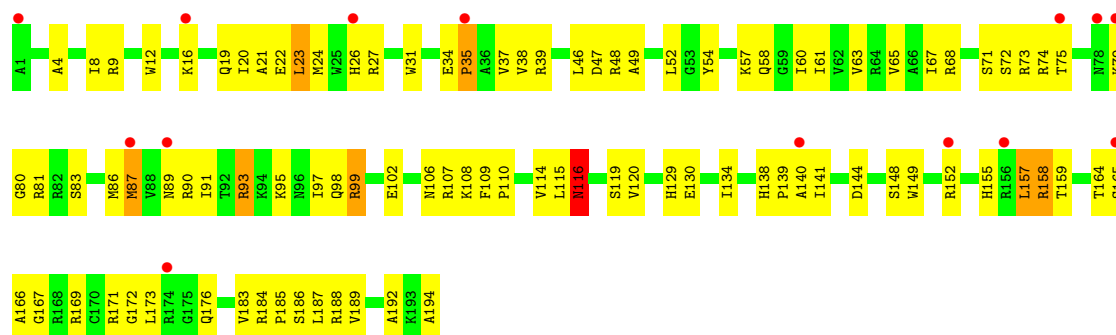
• Molecule 12: 50S ribosomal protein L14P



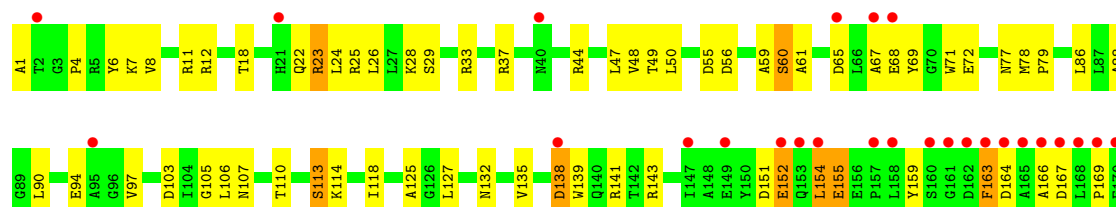
• Molecule 13: 50S ribosomal protein L15P

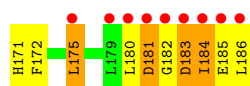


• Molecule 14: 50S ribosomal protein L15e

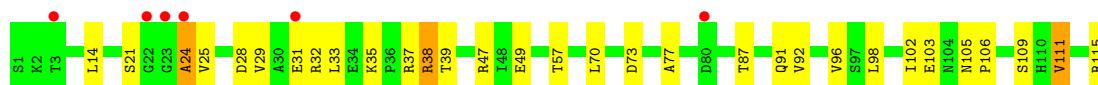
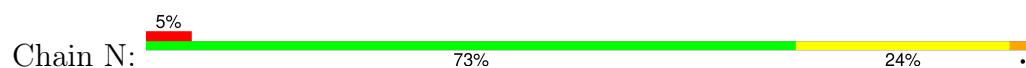


• Molecule 15: 50S ribosomal protein L18P

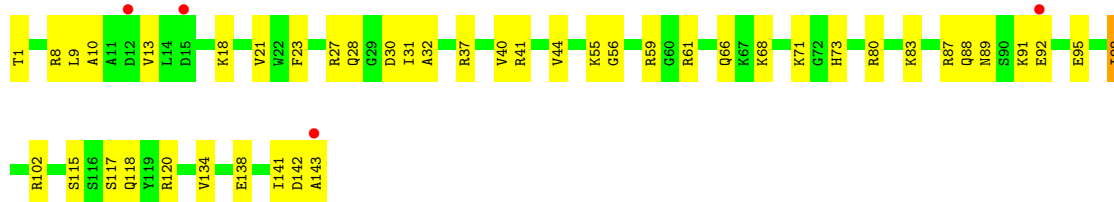




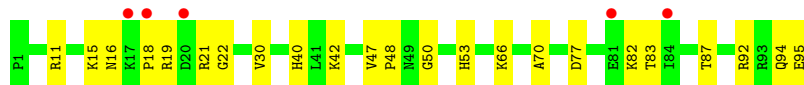
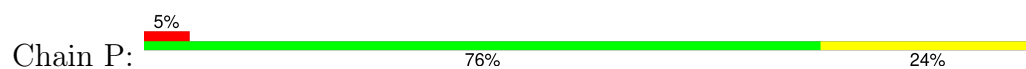
- Molecule 16: 50S ribosomal protein L18e



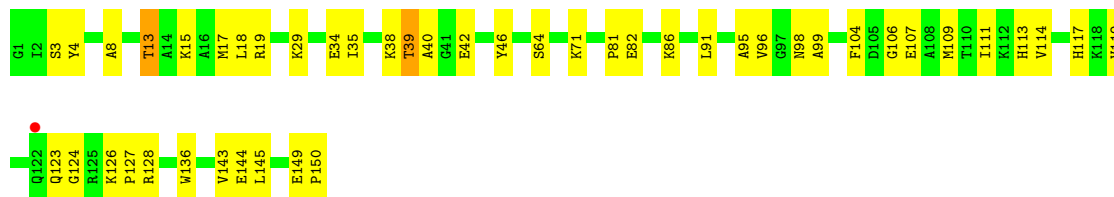
- Molecule 17: 50S ribosomal protein L19e



- Molecule 18: 50S ribosomal protein L21e



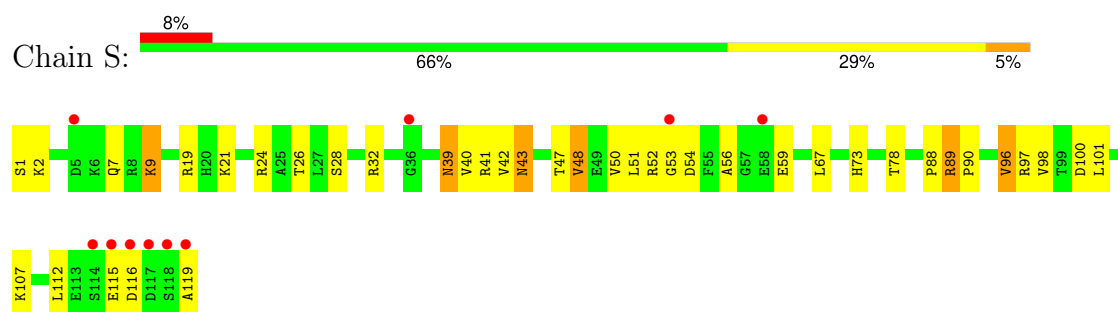
- Molecule 19: 50S ribosomal protein L22P



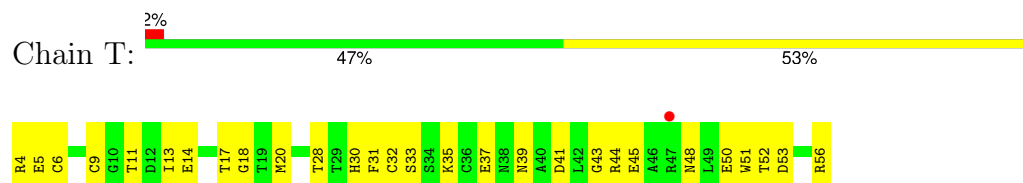
- Molecule 20: 50S ribosomal protein L23P



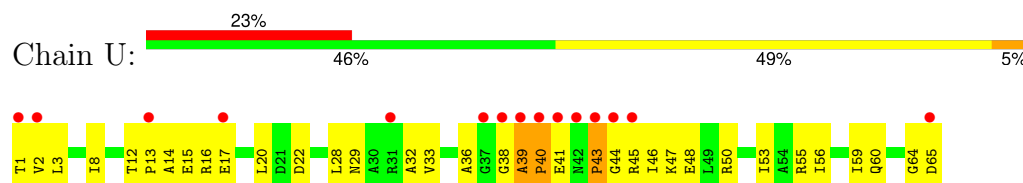
- Molecule 21: 50S ribosomal protein L24P



- Molecule 22: 50S ribosomal protein L24e



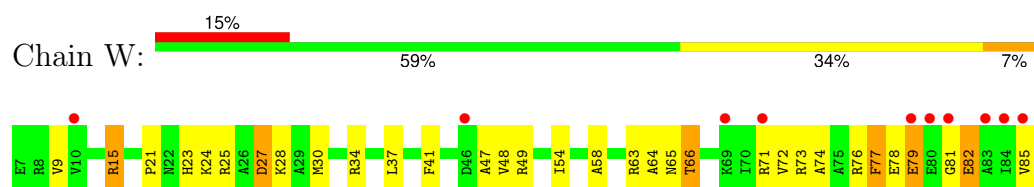
- Molecule 23: 50S ribosomal protein L29P



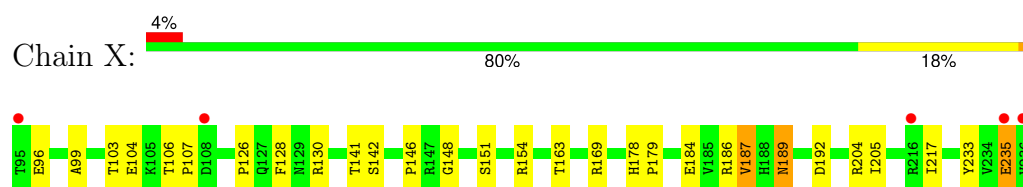
- Molecule 24: 50S ribosomal protein L30P



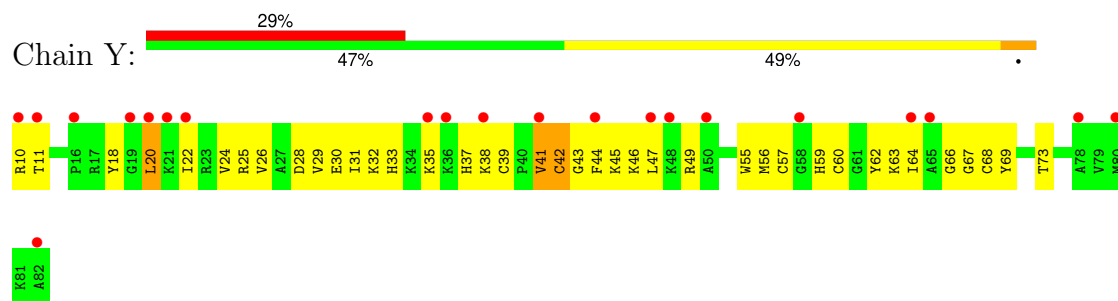
- Molecule 25: 50S ribosomal protein L31e



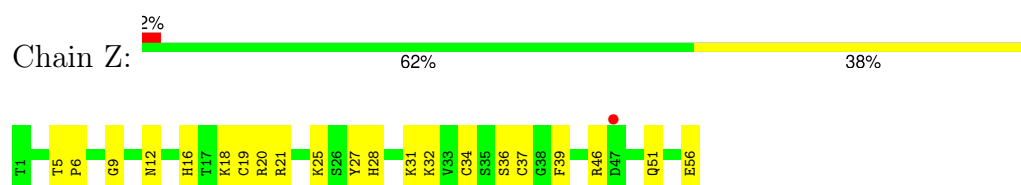
- Molecule 26: 50S ribosomal protein L32e



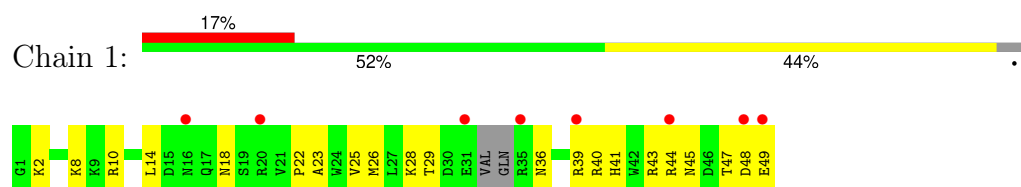
- Molecule 27: 50S ribosomal protein L37Ae



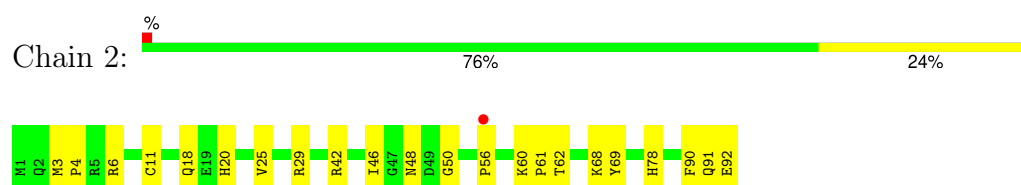
- Molecule 28: 50S ribosomal protein L37e



- Molecule 29: 50S ribosomal protein L39e



- Molecule 30: 50S ribosomal protein L44E



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.85Å 298.00Å 574.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.71	Depositor EDS
% Data completeness (in resolution range)	92.9 (50.00-2.70) 90.9 (50.00-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.73Å)	Xtriage
Refinement program	CNS, CNX	Depositor
R, $R_{free}$	0.222 , 0.253 0.207 , 0.242	Depositor DCC
$R_{free}$ test set	4458 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	90725	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EMK, NA, CD, K, SR, CL

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	0	0.41	0/66075	0.69	18/103050 (0.0%)
2	9	0.37	0/2905	0.72	2/4528 (0.0%)
3	A	0.36	0/1788	0.66	0/2409
4	B	0.39	0/2690	0.67	0/3652
5	C	0.39	0/1884	0.65	0/2551
6	D	0.32	0/1112	0.58	0/1498
7	E	0.35	0/1383	0.59	0/1880
8	F	0.37	0/897	0.58	0/1219
9	G	0.30	0/242	0.45	0/324
10	H	0.40	0/1247	0.74	1/1686 (0.1%)
11	I	0.38	0/1136	0.63	0/1530
12	J	0.39	0/1004	0.70	0/1351
13	K	0.39	0/1131	0.68	0/1509
14	L	0.39	0/1634	0.69	1/2180 (0.0%)
15	M	0.32	0/1474	0.61	0/1999
16	N	0.33	0/874	0.62	0/1181
17	O	0.37	0/1144	0.57	0/1521
18	P	0.38	0/749	0.72	0/1005
19	Q	0.36	0/1173	0.63	0/1578
20	R	0.36	0/649	0.58	0/875
21	S	0.35	0/958	0.65	0/1289
22	T	0.39	0/418	0.59	0/562
23	U	0.31	0/503	0.52	0/675
24	V	0.36	0/1219	0.65	0/1655
25	W	0.36	0/665	0.60	0/895
26	X	0.38	0/1147	0.66	0/1536
27	Y	0.40	0/576	0.71	0/763
28	Z	0.49	0/438	0.70	0/578
29	1	0.37	0/399	0.60	0/527
30	2	0.41	0/771	0.60	0/1024
All	All	0.40	0/98285	0.68	22/147030 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	75
2	9	1	2
24	V	0	1
All	All	1	78

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	3024	U	C2'-C3'-O3'	9.36	130.09	109.50
1	0	1559	A	C2'-C3'-O3'	8.36	127.88	109.50
1	0	2338	G	C2'-C3'-O3'	7.19	125.32	109.50
1	0	1120	U	C5'-C4'-C3'	-6.74	105.22	116.00
1	0	777	U	O4'-C1'-N1	6.46	113.37	108.20
1	0	1829	A	N9-C1'-C2'	-6.38	104.98	112.00
1	0	2316	G	O4'-C1'-N9	5.97	112.97	108.20
1	0	1504	A	N9-C1'-C2'	5.85	121.60	114.00
14	L	157	LEU	CB-CG-CD1	-5.60	101.49	111.00
1	0	2914	A	C2'-C3'-O3'	5.57	122.62	113.70
1	0	2313	C	C5'-C4'-O4'	5.56	115.77	109.10
1	0	2526	C	N1-C1'-C2'	5.33	120.94	114.00
1	0	2726	U	N1-C1'-C2'	5.32	120.92	114.00
1	0	1971	G	N9-C1'-C2'	5.32	120.92	114.00
1	0	2607	U	N1-C1'-C2'	5.20	120.77	114.00
1	0	2316	G	C5'-C4'-C3'	-5.20	107.69	116.00
2	9	3024	U	C4'-C3'-O3'	5.16	123.32	113.00
10	H	74	ASN	N-CA-C	-5.13	97.15	111.00
1	0	883	U	N1-C1'-C2'	5.10	120.63	114.00
1	0	2313	C	C5'-C4'-C3'	5.09	124.14	116.00
1	0	535	G	N9-C1'-C2'	5.09	120.61	114.00
1	0	2664	A	N9-C1'-C2'	5.04	120.55	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	9	3024	U	C3'

All (78) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	0	1055	G	Sidechain
1	0	1078	A	Sidechain
1	0	1134	G	Sidechain
1	0	1310	U	Sidechain
1	0	1327	G	Sidechain
1	0	1342	C	Sidechain
1	0	1359	U	Sidechain
1	0	1368	U	Sidechain
1	0	1417	G	Sidechain
1	0	1435	U	Sidechain
1	0	1473	U	Sidechain
1	0	1647	G	Sidechain
1	0	1681	G	Sidechain
1	0	1696	U	Sidechain
1	0	1714	C	Sidechain
1	0	1771	U	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	182	G	Sidechain
1	0	1828	G	Sidechain
1	0	1829	A	Sidechain
1	0	1848	G	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1885	A	Sidechain
1	0	1979	G	Sidechain
1	0	2102	G	Sidechain
1	0	2103	A	Sidechain
1	0	216	A	Sidechain
1	0	2313	C	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2426	G	Sidechain
1	0	2448	U	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2543	G	Sidechain
1	0	2607	U	Sidechain
1	0	2610	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2679	G	Sidechain
1	0	2690	U	Sidechain
1	0	2710	U	Sidechain
1	0	2768	A	Sidechain
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	314	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	460	A	Sidechain
1	0	462	A	Sidechain
1	0	469	G	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	487	G	Sidechain
1	0	50	G	Sidechain
1	0	503	G	Sidechain
1	0	506	G	Sidechain
1	0	518	G	Sidechain
1	0	686	A	Sidechain
1	0	722	G	Sidechain
1	0	742	G	Sidechain
1	0	761	A	Sidechain
1	0	774	C	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	818	A	Sidechain
1	0	868	G	Sidechain
1	0	872	U	Sidechain
1	0	952	G	Sidechain
2	9	3090	G	Sidechain
2	9	3097	U	Sidechain
24	V	90	TYR	Sidechain

## 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	0	59016	0	29808	892	0
2	9	2600	0	1326	67	0
3	A	1755	0	1763	77	0
4	B	2625	0	2533	124	0
5	C	1859	0	1816	85	0
6	D	1095	0	1085	84	0
7	E	1358	0	1266	53	0
8	F	886	0	854	50	0
9	G	241	0	231	8	0
10	H	1216	0	1215	132	0
11	I	1120	0	1098	57	0
12	J	994	0	1027	37	0
13	K	1119	0	1076	57	0
14	L	1606	0	1676	123	0
15	M	1445	0	1401	69	0
16	N	865	0	873	23	0
17	O	1134	0	1127	42	0
18	P	735	0	729	17	0
19	Q	1150	0	1122	53	0
20	R	642	0	605	25	0
21	S	950	0	924	31	0
22	T	411	0	364	22	0
23	U	500	0	511	32	0
24	V	1196	0	1137	69	0
25	W	655	0	653	35	0
26	X	1131	0	1133	26	0
27	Y	564	0	598	46	0
28	Z	431	0	426	24	0
29	1	394	0	406	24	0
30	2	755	0	729	22	0
31	0	55	0	0	0	0
31	9	1	0	0	0	0
31	B	1	0	0	0	0
31	J	1	0	0	0	0
31	K	1	0	0	0	0
31	S	1	0	0	0	0
31	X	1	0	0	0	0
32	0	1	0	0	0	0
33	0	19	0	0	0	0
33	9	1	0	0	0	0
33	C	1	0	0	0	0
33	I	1	0	0	0	0
33	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	P	1	0	0	0	0
33	Q	2	0	0	0	0
34	0	5	0	0	0	0
34	A	1	0	0	0	0
34	D	1	0	0	0	0
34	I	2	0	0	0	0
34	L	1	0	0	1	0
34	N	1	0	0	0	0
34	Q	1	0	0	0	0
34	X	1	0	0	0	0
35	0	82	0	0	0	0
35	2	2	0	0	0	0
35	9	3	0	0	0	0
35	A	4	0	0	0	0
35	B	2	0	0	0	0
35	F	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	Z	2	0	0	0	0
36	0	74	0	88	30	0
37	2	1	0	0	0	0
37	T	1	0	0	0	0
37	Y	1	0	0	0	0
37	Z	1	0	0	0	0
All	All	90725	0	59600	2169	0

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

All (2169) 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)
36:0:8163:EMK:C14	36:0:8163:EMK:C15	1.75	1.63
36:0:8163:EMK:C12	36:0:8163:EMK:C20	1.76	1.58
36:0:8163:EMK:C14	36:0:8163:EMK:C13	1.78	1.58
36:0:8163:EMK:C8	36:0:8163:EMK:C9	1.75	1.57
36:0:8163:EMK:C12	36:0:8163:EMK:N9	1.71	1.49
36:0:8163:EMK:C26	36:0:8163:EMK:O76	1.63	1.47
36:0:8163:EMK:O78	36:0:8163:EMK:C10	1.66	1.42
1:0:1160:G:H5'	1:0:1161:A:H5'	1.28	1.14
2:9:3023:U:H3'	2:9:3024:U:H5''	1.20	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3056:A:H2'	2:9:3057:A:H5''	1.35	1.06
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.40	1.03
3:A:153:ARG:HB2	3:A:153:ARG:HH11	1.24	1.02
12:J:29:LEU:HB3	12:J:55:VAL:HG11	1.36	1.02
1:0:1451:C:H5'	1:0:1505:U:H3	1.17	1.02
10:H:27:LYS:H	10:H:58:HIS:HD2	1.03	1.02
1:0:1242:A:H5'	11:I:82:THR:HG23	1.39	1.01
10:H:55:GLN:NE2	10:H:124:ARG:HE	1.59	1.01
36:0:8163:EMK:C9	36:0:8163:EMK:C7	2.39	1.00
1:0:156:C:H5''	14:L:171:ARG:HD3	1.45	0.99
10:H:86:ARG:NH1	10:H:133:ILE:HG13	1.79	0.98
1:0:1666:C:C2'	1:0:1667:A:H5''	1.95	0.97
2:9:3076:G:H3'	2:9:3077:A:H5''	1.47	0.96
5:C:236:THR:HG22	5:C:239:ALA:H	1.27	0.96
28:Z:25:LYS:HD2	29:1:49:GLU:H	1.30	0.96
20:R:51:GLN:HE21	20:R:53:ASN:HD21	1.07	0.95
4:B:162:MET:HE2	4:B:310:ARG:HD3	1.47	0.94
19:Q:99:ALA:HB1	19:Q:109:MET:HE1	1.48	0.93
12:J:10:GLN:H	12:J:10:GLN:HE21	0.98	0.93
1:0:2812:A:H2	1:0:2814:A:H62	1.18	0.92
15:M:184:ILE:HG22	15:M:185:GLU:H	1.34	0.92
24:V:137:GLN:HE21	24:V:141:HIS:HE1	1.14	0.91
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.50	0.91
12:J:10:GLN:H	12:J:10:GLN:NE2	1.68	0.90
19:Q:39:THR:HG22	19:Q:42:GLU:H	1.36	0.90
10:H:55:GLN:HE21	10:H:124:ARG:HE	1.13	0.90
10:H:86:ARG:HH11	10:H:133:ILE:HG13	1.33	0.90
14:L:107:ARG:HH11	14:L:107:ARG:HG3	1.34	0.90
10:H:47:GLU:HB3	10:H:133:ILE:HD13	1.54	0.90
10:H:14:TYR:H	10:H:91:HIS:CE1	1.89	0.90
23:U:12:THR:HB	23:U:15:GLU:HG3	1.53	0.90
1:0:288:A:H61	1:0:364:C:H42	1.21	0.89
17:O:59:ARG:NH2	17:O:66:GLN:HE22	1.70	0.89
27:Y:38:LYS:HE3	27:Y:45:LYS:HE2	1.54	0.89
24:V:4:LEU:HD13	24:V:52:VAL:HG21	1.52	0.89
1:0:1666:C:H2'	1:0:1667:A:H5''	1.51	0.89
2:9:3025:G:H3'	2:9:3026:C:H5'	1.55	0.88
2:9:3023:U:C3'	2:9:3024:U:H5''	2.03	0.88
25:W:37:LEU:HD13	25:W:85:VAL:HG11	1.56	0.88
3:A:199:HIS:HD2	3:A:201:PHE:H	1.16	0.88
10:H:13:ALA:HA	10:H:91:HIS:HE1	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.58	0.86
1:O:289:G:H22	1:O:363:A:H2	1.22	0.86
6:D:28:GLY:HA2	6:D:69:ILE:HG23	1.57	0.86
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.57	0.86
1:O:1119:G:H2'	11:I:52:GLN:NE2	1.91	0.86
17:O:59:ARG:HH22	17:O:66:GLN:HE22	1.24	0.85
10:H:139:ASP:N	10:H:140:PRO:HD3	1.91	0.85
14:L:102:GLU:OE1	14:L:164:THR:HG21	1.76	0.85
30:2:60:LYS:HG3	30:2:61:PRO:HD2	1.59	0.85
7:E:15:GLN:HE21	7:E:20:ILE:HG12	1.41	0.84
14:L:87:MET:HB3	30:2:46:ILE:HD13	1.58	0.84
5:C:1:MET:HG2	5:C:2:GLN:H	1.41	0.84
1:O:2506:A:O2'	1:O:2507:G:H8	1.59	0.84
2:9:3056:A:C2'	2:9:3057:A:H5''	2.08	0.84
1:O:1451:C:H5'	1:O:1505:U:N3	1.93	0.84
1:O:2502:C:H4'	10:H:151:MET:HG3	1.60	0.83
1:O:558:C:C2'	1:O:559:U:H5''	2.09	0.83
1:O:2506:A:HO2'	1:O:2507:G:H8	0.84	0.83
19:Q:18:LEU:HB2	19:Q:143:VAL:HG12	1.61	0.83
29:1:41:HIS:H	29:1:45:ASN:HD22	1.24	0.83
1:O:1701:A:H4'	1:O:1702:U:H5''	1.57	0.83
10:H:36:ASN:HA	10:H:82:LYS:NZ	1.93	0.83
5:C:162:VAL:HG12	5:C:192:ILE:HD11	1.59	0.83
24:V:88:THR:HG22	24:V:90:TYR:HD1	1.42	0.83
24:V:21:LEU:HD21	24:V:48:VAL:HG11	1.60	0.82
12:J:98:VAL:CG1	12:J:102:GLU:HA	2.08	0.82
12:J:10:GLN:HE21	12:J:10:GLN:N	1.76	0.82
1:O:1160:G:H5'	1:O:1161:A:C5'	2.09	0.82
26:X:235:GLU:H	26:X:235:GLU:CD	1.82	0.82
3:A:199:HIS:CD2	3:A:201:PHE:H	1.96	0.81
1:O:282:C:O2'	1:O:283:U:H4'	1.80	0.81
1:O:2003:U:H4'	1:O:2004:U:H5	1.46	0.81
19:Q:8:ALA:HB1	19:Q:13:THR:HG21	1.62	0.81
14:L:106:ASN:ND2	34:L:202:CL:CL	2.51	0.81
1:O:545:G:H5'	1:O:545:G:H8	1.45	0.81
1:O:2586:U:H3	1:O:2592:G:H22	1.24	0.81
10:H:86:ARG:HH11	10:H:133:ILE:CG1	1.93	0.81
1:O:182:G:H4'	14:L:157:LEU:HD13	1.62	0.81
1:O:1116:U:HO2'	1:O:1118:A:H2	0.84	0.81
23:U:56:ILE:O	23:U:60:GLN:HG3	1.80	0.80
27:Y:29:VAL:O	27:Y:33:HIS:HB2	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.62	0.80
13:K:73:VAL:HG23	13:K:74:THR:H	1.46	0.80
15:M:94:GLU:HG3	15:M:186:LEU:O	1.82	0.80
26:X:187:VAL:HG12	26:X:205:ILE:HA	1.64	0.80
27:Y:38:LYS:HE3	27:Y:45:LYS:CE	2.11	0.80
10:H:26:LYS:HD2	10:H:28:ILE:HD12	1.62	0.80
1:O:1002:G:H2'	1:O:1003:U:H5''	1.62	0.80
4:B:217:ARG:HG3	4:B:257:THR:HB	1.64	0.79
1:O:949:U:H4'	18:P:95:GLU:HA	1.62	0.79
1:O:1119:G:H2'	11:I:52:GLN:HE22	1.47	0.79
10:H:26:LYS:HG2	10:H:28:ILE:H	1.47	0.79
10:H:27:LYS:H	10:H:58:HIS:CD2	1.96	0.79
1:O:1160:G:C5'	1:O:1161:A:H5'	2.10	0.79
1:O:2271:G:H5'	3:A:223:ARG:HH21	1.48	0.79
10:H:29:ALA:HB3	10:H:65:ARG:HH12	1.48	0.79
1:O:877:G:H5'	1:O:878:G:OP1	1.81	0.79
3:A:153:ARG:HH11	3:A:153:ARG:CB	1.96	0.79
2:9:3025:G:H3'	2:9:3026:C:C5'	2.11	0.79
26:X:189:ASN:HA	26:X:217:ILE:HD11	1.65	0.79
1:O:1603:A:H5'	1:O:1605:G:O4'	1.83	0.78
19:Q:99:ALA:HB1	19:Q:109:MET:CE	2.13	0.78
1:O:111:C:O2'	28:Z:20:ARG:HG2	1.84	0.78
1:O:1119:G:N2	1:O:1246:A:C2	2.52	0.78
1:O:2661:U:H3	1:O:2812:A:H62	1.31	0.78
10:H:13:ALA:HA	10:H:91:HIS:CE1	2.18	0.78
8:F:13:GLU:OE2	8:F:78:GLU:HG2	1.83	0.78
1:O:1118:A:C8	1:O:1118:A:H3'	2.18	0.78
1:O:2005:G:H3'	1:O:2005:G:OP2	1.83	0.78
17:O:115:SER:H	17:O:118:GLN:NE2	1.81	0.77
1:O:1118:A:H3'	1:O:1118:A:H8	1.47	0.77
4:B:125:GLU:O	4:B:129:ARG:HG3	1.83	0.77
1:O:1209:C:H2'	1:O:1210:G:H8	1.50	0.77
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.20	0.76
1:O:560:C:H42	1:O:597:A:H61	1.31	0.76
36:O:8163:EMK:C12	36:O:8163:EMK:C9	2.63	0.76
10:H:137:ASN:O	10:H:139:ASP:N	2.17	0.76
19:Q:18:LEU:HB2	19:Q:143:VAL:CG1	2.15	0.76
22:T:14:GLU:O	22:T:17:THR:HB	1.84	0.76
10:H:56:ILE:HG21	10:H:61:LEU:HD13	1.68	0.76
10:H:53:PRO:HG3	10:H:127:GLY:H	1.51	0.76
1:O:2533:C:H5'	1:O:2533:C:H6	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:25:VAL:HG22	30:2:68:LYS:HG3	1.67	0.76
1:0:1835:U:H5	1:0:1840:A:N7	1.84	0.76
4:B:265:LEU:HD21	4:B:316:ARG:HD3	1.66	0.75
14:L:35:PRO:HD2	14:L:38:VAL:HG21	1.68	0.75
1:0:861:A:H4'	1:0:1697:G:H4'	1.68	0.75
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.68	0.75
12:J:28:GLU:HB3	12:J:59:LYS:HB2	1.67	0.75
1:0:1669:A:H2'	1:0:1670:G:C8	2.21	0.75
24:V:6:GLN:HB2	24:V:26:ILE:HD12	1.69	0.75
2:9:3023:U:H3'	2:9:3024:U:C5'	2.11	0.75
3:A:109:GLU:HG2	3:A:116:GLY:H	1.52	0.75
14:L:37:VAL:HG13	14:L:63:VAL:HG11	1.68	0.75
29:1:36:ASN:H	29:1:39:ARG:HH21	1.35	0.75
6:D:19:GLU:O	6:D:20:LYS:HB3	1.86	0.74
24:V:149:LEU:HG	24:V:153:MET:HE2	1.67	0.74
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.68	0.74
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.69	0.74
14:L:99:ARG:HD2	14:L:167:GLY:HA2	1.67	0.74
12:J:74:VAL:HG11	12:J:113:ILE:HG12	1.70	0.73
17:O:91:LYS:O	17:O:95:GLU:HG3	1.88	0.73
24:V:21:LEU:HD22	24:V:26:ILE:HD11	1.68	0.73
10:H:82:LYS:HB2	10:H:135:TRP:HB2	1.70	0.73
4:B:51:VAL:CG1	4:B:53:LEU:HD13	2.18	0.73
15:M:71:TRP:CE3	15:M:175:LEU:HD22	2.24	0.73
1:0:1666:C:O2'	1:0:1667:A:H5''	1.87	0.73
1:0:282:C:H1'	1:0:368:C:N4	2.03	0.73
27:Y:37:HIS:HB2	27:Y:47:LEU:HB2	1.70	0.73
14:L:87:MET:HG2	30:2:46:ILE:HG21	1.71	0.72
15:M:184:ILE:HG22	15:M:185:GLU:N	2.03	0.72
10:H:55:GLN:HE21	10:H:124:ARG:NE	1.87	0.72
1:0:2635:A:O2'	1:0:2636:C:H5'	1.88	0.72
1:0:1666:C:H2'	1:0:1667:A:C5'	2.18	0.72
10:H:47:GLU:HB3	10:H:133:ILE:CD1	2.19	0.72
2:9:3029:C:H2'	2:9:3030:C:H5'	1.72	0.72
1:0:289:G:N2	1:0:363:A:H2	1.86	0.72
1:0:2468:A:H61	30:2:48:ASN:HD21	1.38	0.72
1:0:559:U:H6	1:0:559:U:H5'	1.54	0.71
22:T:45:GLU:HB2	22:T:48:ASN:ND2	2.05	0.71
1:0:2769:C:O2'	1:0:2770:G:H5'	1.88	0.71
19:Q:18:LEU:HD12	19:Q:143:VAL:HG11	1.71	0.71
15:M:169:PRO:O	15:M:172:PHE:HB3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:32:ARG:HE	16:N:35:LYS:HD2	1.54	0.71
1:O:2721:U:H4'	12:J:87:ARG:HG3	1.71	0.71
9:G:12:ILE:N	9:G:13:PRO:HD3	2.05	0.71
15:M:48:VAL:CG1	15:M:55:ASP:HB3	2.21	0.71
8:F:37:THR:O	8:F:41:GLU:HG3	1.90	0.71
1:O:1116:U:O2'	1:O:1118:A:H2	1.66	0.71
1:O:1877:G:OP1	3:A:164:ARG:NH2	2.22	0.71
12:J:32:ILE:HD11	12:J:56:SER:HB3	1.72	0.71
25:W:78:GLU:HG2	25:W:79:GLU:H	1.56	0.71
3:A:153:ARG:HB2	3:A:153:ARG:NH1	2.02	0.71
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.72	0.71
6:D:25:MET:HE1	6:D:37:ALA:HB1	1.73	0.71
10:H:49:VAL:O	10:H:157:ILE:HG23	1.90	0.71
13:K:53:ARG:NH2	13:K:57:VAL:HG12	2.06	0.71
14:L:172:GLY:O	14:L:183:VAL:HG11	1.88	0.71
15:M:110:THR:HB	15:M:113:SER:OG	1.91	0.71
24:V:88:THR:HG23	24:V:110:GLN:NE2	2.06	0.71
2:9:3014:G:H5'	2:9:3014:G:H8	1.54	0.71
10:H:33:MET:HB2	10:H:83:PHE:HB3	1.72	0.70
1:O:396:U:O2'	1:O:418:C:H4'	1.90	0.70
1:O:1204:C:H3'	1:O:1205:U:H5''	1.74	0.70
1:O:2716:G:H5''	4:B:206:THR:HG21	1.72	0.70
1:O:2840:A:OP1	4:B:211:THR:HG23	1.90	0.70
24:V:137:GLN:HE21	24:V:141:HIS:CE1	2.03	0.70
26:X:186:ARG:HH11	26:X:186:ARG:HG2	1.57	0.70
3:A:86:ALA:HB3	3:A:94:LEU:HD22	1.72	0.70
1:O:2420:G:O2'	1:O:2421:G:H5'	1.91	0.70
6:D:25:MET:HE2	6:D:41:LEU:HG	1.72	0.70
25:W:15:ARG:HB3	25:W:15:ARG:HH11	1.55	0.70
36:O:8163:EMK:C10	36:O:8163:EMK:C30	2.70	0.70
1:O:558:C:H2'	1:O:559:U:H5''	1.72	0.70
21:S:50:VAL:HG12	21:S:56:ALA:HA	1.73	0.70
1:O:470:U:O2'	28:Z:16:HIS:HD2	1.75	0.70
1:O:1377:C:H5'	1:O:1377:C:H6	1.57	0.70
6:D:170:TYR:O	6:D:171:ASP:HB3	1.91	0.70
14:L:80:GLY:O	14:L:81:ARG:HD2	1.91	0.69
1:O:657:G:OP1	5:C:27:ARG:NH2	2.24	0.69
1:O:2372:A:H2'	1:O:2373:U:C6	2.27	0.69
10:H:48:LEU:HG	10:H:157:ILE:HG21	1.73	0.69
4:B:162:MET:CE	4:B:310:ARG:HD3	2.19	0.69
4:B:212:GLN:CB	4:B:257:THR:HG21	2.19	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:52:VAL:HG22	24:V:53:ALA:N	2.08	0.69
14:L:139:PRO:C	14:L:141:ILE:H	1.96	0.69
1:0:2578:G:H5'	1:0:2578:G:H8	1.58	0.69
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.74	0.69
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.57	0.69
12:J:4:LEU:HD22	12:J:116:GLU:HB3	1.74	0.69
25:W:65:ASN:O	25:W:66:THR:HB	1.92	0.69
4:B:109:LEU:HG	4:B:113:LEU:HD11	1.75	0.69
17:O:80:ARG:HG2	17:O:87:ARG:CZ	2.23	0.69
19:Q:18:LEU:HG	19:Q:91:LEU:HD13	1.75	0.69
12:J:29:LEU:HB3	12:J:55:VAL:CG1	2.18	0.69
14:L:139:PRO:O	14:L:140:ALA:HB3	1.91	0.69
1:0:1180:U:H2'	1:0:1181:A:C8	2.27	0.68
1:0:1462:C:H2'	1:0:1463:A:C8	2.28	0.68
27:Y:26:VAL:O	27:Y:30:GLU:HB2	1.92	0.68
20:R:33:SER:O	20:R:37:VAL:HG23	1.93	0.68
26:X:146:PRO:O	26:X:154:ARG:HG3	1.93	0.68
1:0:289:G:H1	1:0:363:A:H2	1.40	0.68
1:0:500:G:H21	19:Q:98:ASN:HD21	1.41	0.68
7:E:23:GLU:HG2	7:E:28:SER:HB2	1.75	0.68
8:F:22:VAL:HG23	8:F:104:ALA:HB2	1.76	0.68
11:I:107:ASN:ND2	11:I:109:TYR:H	1.91	0.68
14:L:87:MET:HB2	14:L:91:ILE:HD11	1.76	0.68
27:Y:38:LYS:HA	27:Y:45:LYS:HA	1.76	0.68
14:L:72:SER:HB2	14:L:93:ARG:HG2	1.75	0.68
30:2:11:CYS:HB2	30:2:20:HIS:CE1	2.29	0.68
1:0:1751:G:H2'	1:0:1752:G:H5''	1.76	0.68
10:H:36:ASN:HA	10:H:82:LYS:HZ3	1.56	0.68
1:0:2054:A:N3	19:Q:128:ARG:NH2	2.40	0.68
10:H:136:VAL:HG22	10:H:137:ASN:N	2.09	0.68
15:M:90:LEU:HB3	15:M:186:LEU:HD11	1.75	0.68
36:0:8163:EMK:C14	36:0:8163:EMK:O73	2.41	0.68
2:9:3006:C:H5''	15:M:37:ARG:NH1	2.09	0.68
1:0:544:G:H2'	1:0:545:G:H5''	1.76	0.67
1:0:1209:C:H2'	1:0:1210:G:C8	2.29	0.67
1:0:1641:A:H2'	1:0:1642:A:H5'	1.77	0.67
1:0:259:G:H21	14:L:58:GLN:HE22	1.41	0.67
36:0:8163:EMK:C14	36:0:8163:EMK:C12	2.71	0.67
10:H:27:LYS:N	10:H:58:HIS:HD2	1.85	0.67
11:I:131:THR:HB	11:I:134:GLU:OE1	1.94	0.67
1:0:450:C:OP1	5:C:184:ARG:NH2	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:30:GLN:H	10:H:65:ARG:NH1	1.92	0.67
2:9:3024:U:O2'	2:9:3025:G:H4'	1.95	0.67
10:H:162:SER:HB2	10:H:163:PRO:HD3	1.76	0.67
1:0:1947:G:H2'	1:0:1948:G:H8	1.58	0.67
1:0:2748:G:OP1	1:0:2749:U:H5''	1.95	0.67
4:B:275:GLY:O	4:B:291:ASP:HA	1.94	0.67
1:0:1118:A:H8	1:0:1119:G:H5''	1.58	0.67
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.76	0.67
11:I:39:VAL:HG13	11:I:106:GLY:O	1.95	0.66
28:Z:28:HIS:CD2	28:Z:31:LYS:HG3	2.30	0.66
1:0:2502:C:C2'	1:0:2503:A:H5'	2.25	0.66
1:0:2539:U:C4	36:0:8163:EMK:H84	2.30	0.66
3:A:109:GLU:HG2	3:A:116:GLY:N	2.11	0.66
1:0:558:C:O2'	1:0:559:U:H5''	1.94	0.66
24:V:4:LEU:CD1	24:V:52:VAL:HG21	2.23	0.66
25:W:9:VAL:HG22	25:W:88:GLU:OE2	1.95	0.66
1:0:2769:C:H2'	1:0:2770:G:O4'	1.95	0.66
36:0:8163:EMK:C15	36:0:8163:EMK:C13	2.73	0.66
4:B:279:THR:HG23	4:B:290:VAL:H	1.60	0.66
2:9:3028:U:H2'	2:9:3029:C:C6	2.31	0.66
2:9:3092:G:H22	10:H:52:LYS:HE2	1.59	0.66
36:0:8163:EMK:C12	36:0:8163:EMK:C38	2.73	0.66
10:H:46:VAL:HG12	10:H:146:TRP:HZ3	1.61	0.66
13:K:119:THR:HG23	13:K:139:SER:OG	1.95	0.66
14:L:37:VAL:CG1	14:L:63:VAL:HG11	2.24	0.66
14:L:187:LEU:CD2	14:L:194:ALA:HB3	2.25	0.66
19:Q:106:GLY:HA2	19:Q:109:MET:HE3	1.77	0.66
23:U:39:ALA:H	23:U:40:PRO:HD2	1.60	0.66
1:0:544:G:C2'	1:0:545:G:H5''	2.25	0.66
1:0:1218:U:H2'	1:0:1219:U:C6	2.30	0.66
1:0:1701:A:H5''	1:0:1702:U:H3'	1.77	0.66
4:B:18:ARG:HE	4:B:256:GLN:NE2	1.94	0.66
8:F:58:GLU:HB3	14:L:8:ILE:HG23	1.76	0.66
23:U:56:ILE:HG22	23:U:60:GLN:HE21	1.59	0.66
11:I:131:THR:HG22	11:I:134:GLU:H	1.60	0.66
1:0:1669:A:H2'	1:0:1670:G:H8	1.60	0.66
8:F:58:GLU:HA	8:F:61:MET:HE2	1.78	0.66
10:H:47:GLU:CB	10:H:133:ILE:HD13	2.25	0.66
10:H:147:ARG:O	10:H:151:MET:HG2	1.95	0.66
1:0:1003:U:HO2'	10:H:90:PHE:HE1	1.44	0.65
36:0:8163:EMK:C20	36:0:8163:EMK:C13	2.73	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:289:G:N1	1:0:363:A:C2	2.63	0.65
4:B:179:LEU:O	4:B:183:GLU:HG2	1.97	0.65
6:D:25:MET:HG3	6:D:41:LEU:HD11	1.76	0.65
11:I:75:PRO:HG2	11:I:105:LEU:HD21	1.78	0.65
2:9:3002:U:OP2	2:9:3003:A:H5'	1.95	0.65
2:9:3025:G:C3'	2:9:3026:C:H5'	2.27	0.65
12:J:14:LYS:HB2	12:J:45:PRO:HG2	1.79	0.65
29:1:36:ASN:HB3	29:1:39:ARG:HE	1.61	0.65
3:A:36:ASP:CG	3:A:37:VAL:N	2.48	0.65
4:B:53:LEU:HD11	4:B:327:VAL:HG22	1.79	0.65
11:I:107:ASN:HD21	11:I:109:TYR:HB2	1.61	0.65
12:J:74:VAL:CG1	12:J:113:ILE:HG12	2.27	0.65
20:R:57:THR:HG22	20:R:58:MET:N	2.11	0.65
1:0:485:A:N3	1:0:487:G:H5''	2.11	0.65
1:0:2908:A:C2'	1:0:2909:G:H5'	2.26	0.65
36:0:8163:EMK:C9	36:0:8163:EMK:H7	2.26	0.65
5:C:1:MET:HG2	5:C:2:GLN:N	2.11	0.65
10:H:57:ARG:HB3	10:H:59:ASN:HD22	1.62	0.65
1:0:183:A:H5'	14:L:157:LEU:HD12	1.78	0.65
1:0:926:A:O2'	13:K:41:HIS:HD2	1.80	0.65
19:Q:39:THR:HG23	19:Q:107:GLU:O	1.97	0.65
24:V:21:LEU:HD21	24:V:48:VAL:CG1	2.26	0.65
16:N:32:ARG:HH21	16:N:35:LYS:NZ	1.94	0.65
25:W:74:ALA:HB2	25:W:85:VAL:HG12	1.78	0.65
1:0:553:G:P	26:X:204:ARG:HH22	2.20	0.65
4:B:58:PRO:HA	4:B:63:GLU:OE1	1.96	0.65
5:C:127:ARG:HD2	5:C:229:PRO:O	1.97	0.65
6:D:91:ALA:HB2	6:D:106:PHE:CD2	2.32	0.65
16:N:47:ARG:HG3	16:N:47:ARG:HH11	1.62	0.65
11:I:107:ASN:HD22	11:I:107:ASN:C	2.00	0.65
25:W:30:MET:HE1	25:W:58:ALA:HB3	1.79	0.64
29:1:23:ALA:HA	29:1:26:MET:CE	2.28	0.64
10:H:71:TYR:C	10:H:73:GLN:H	2.01	0.64
14:L:87:MET:HB3	30:2:46:ILE:HG21	1.79	0.64
24:V:88:THR:HG22	24:V:89:ASP:N	2.11	0.64
1:0:1204:C:C3'	1:0:1205:U:H5''	2.28	0.64
1:0:2515:C:H2'	1:0:2516:G:O4'	1.96	0.64
10:H:45:GLN:H	10:H:163:PRO:HD2	1.62	0.64
14:L:35:PRO:HD2	14:L:38:VAL:CG2	2.27	0.64
15:M:132:ASN:O	15:M:135:VAL:HG12	1.98	0.64
2:9:3049:G:O2'	2:9:3050:G:H5'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1185:U:H2'	1:0:1186:C:C6	2.32	0.64
6:D:99:ASP:HB3	6:D:103:ASN:HB2	1.78	0.64
24:V:119:HIS:HD2	24:V:120:PRO:O	1.79	0.64
30:2:48:ASN:ND2	30:2:50:GLY:H	1.95	0.64
5:C:76:ARG:HB3	5:C:76:ARG:HH11	1.63	0.64
14:L:184:ARG:HG3	14:L:185:PRO:HA	1.79	0.64
15:M:12:ARG:HD3	15:M:18:THR:OG1	1.98	0.64
26:X:187:VAL:HG22	26:X:192:ASP:HB2	1.80	0.64
36:0:8163:EMK:C26	36:0:8163:EMK:C35	2.75	0.64
10:H:62:GLU:O	10:H:66:VAL:HG23	1.97	0.64
3:A:33:GLU:H	3:A:33:GLU:CD	2.00	0.64
3:A:72:GLU:HG3	27:Y:66:GLY:HA2	1.79	0.64
10:H:69:ASN:O	10:H:72:VAL:HG12	1.98	0.63
14:L:60:ILE:C	14:L:61:ILE:HD12	2.17	0.63
14:L:99:ARG:CD	14:L:167:GLY:HA2	2.29	0.63
21:S:112:LEU:HD23	21:S:119:ALA:HB3	1.80	0.63
1:0:734:U:H2'	1:0:736:A:OP2	1.99	0.63
1:0:2289:G:O2'	1:0:2290:U:H5'	1.98	0.63
1:0:2414:A:H2'	1:0:2415:A:C8	2.33	0.63
15:M:164:ASP:OD2	15:M:167:ASP:HA	1.97	0.63
24:V:21:LEU:HD22	24:V:26:ILE:CD1	2.28	0.63
1:0:506:G:H22	1:0:509:A:H5'	1.62	0.63
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.80	0.63
5:C:127:ARG:NH2	5:C:225:PRO:HB2	2.14	0.63
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.80	0.63
13:K:143:THR:HG22	13:K:144:ASP:N	2.12	0.63
1:0:1098:A:H2'	1:0:1099:G:O4'	1.99	0.63
3:A:192:VAL:HG13	3:A:207:GLN:HB3	1.79	0.63
19:Q:18:LEU:HD12	19:Q:143:VAL:CG1	2.29	0.63
1:0:475:G:H5'	5:C:73:LEU:HD23	1.81	0.63
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.98	0.63
28:Z:21:ARG:HD2	28:Z:39:PHE:HB2	1.81	0.63
15:M:90:LEU:CB	15:M:186:LEU:HD11	2.29	0.63
5:C:214:THR:HG23	5:C:217:GLU:HG2	1.80	0.63
6:D:62:ASP:C	6:D:64:ARG:H	2.01	0.63
10:H:36:ASN:HA	10:H:82:LYS:HZ2	1.62	0.63
14:L:71:SER:O	14:L:73:ARG:NH1	2.30	0.63
1:0:2320:U:H4'	1:0:2321:A:O4'	1.99	0.62
4:B:85:ARG:HB2	4:B:99:GLU:HG2	1.79	0.62
14:L:87:MET:CB	30:2:46:ILE:HG21	2.30	0.62
14:L:186:SER:O	14:L:189:VAL:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:103:THR:HG22	26:X:104:GLU:OE2	1.99	0.62
1:0:156:C:H5''	14:L:171:ARG:CD	2.26	0.62
1:0:1864:C:OP1	14:L:75:THR:HG23	2.00	0.62
1:0:1947:G:H2'	1:0:1948:G:C8	2.33	0.62
7:E:107:PHE:O	7:E:110:GLU:HG3	1.98	0.62
14:L:107:ARG:HG3	14:L:107:ARG:NH1	2.05	0.62
1:0:259:G:H21	14:L:58:GLN:NE2	1.97	0.62
1:0:1242:A:H5'	11:I:82:THR:CG2	2.23	0.62
1:0:2615:U:OP1	4:B:230:GLN:NE2	2.32	0.62
6:D:165:PHE:HD2	6:D:166:ILE:HD12	1.64	0.62
17:O:115:SER:H	17:O:118:GLN:HE21	1.45	0.62
1:0:645:U:OP2	13:K:4:LYS:HE2	1.98	0.62
14:L:39:ARG:HA	14:L:63:VAL:HG22	1.80	0.62
1:0:2502:C:H2'	1:0:2503:A:H5'	1.81	0.62
6:D:51:ARG:HH11	6:D:68:PRO:HG2	1.65	0.62
6:D:146:LYS:NZ	15:M:107:ASN:HD21	1.98	0.62
14:L:114:VAL:HB	14:L:159:THR:CG2	2.29	0.62
25:W:74:ALA:CB	25:W:85:VAL:HG12	2.29	0.62
1:0:960:G:N3	1:0:960:G:H2'	2.15	0.62
1:0:1118:A:C8	1:0:1119:G:H5''	2.34	0.62
1:0:2265:U:H2'	1:0:2266:A:C8	2.35	0.62
1:0:2908:A:H2'	1:0:2909:G:O4'	2.00	0.62
1:0:506:G:H22	1:0:509:A:C5'	2.11	0.62
1:0:1118:A:H62	1:0:1244:U:H3	1.46	0.62
1:0:1701:A:H4'	1:0:1702:U:C5'	2.27	0.62
8:F:91:VAL:HG12	8:F:92:GLY:N	2.15	0.61
17:O:9:LEU:O	17:O:13:VAL:HG12	2.00	0.61
1:0:545:G:H5'	1:0:545:G:C8	2.32	0.61
36:0:8163:EMK:C9	36:0:8163:EMK:C19	2.73	0.61
4:B:62:ARG:HA	4:B:65:MET:CE	2.30	0.61
27:Y:38:LYS:HE3	27:Y:45:LYS:NZ	2.15	0.61
12:J:82:ARG:NH2	12:J:115:ARG:HG2	2.15	0.61
1:0:1789:G:O6	17:O:73:HIS:HE1	1.83	0.61
1:0:2896:A:N3	1:0:2896:A:H2'	2.16	0.61
16:N:39:THR:O	16:N:115:ARG:NH2	2.34	0.61
1:0:635:A:H2'	1:0:636:G:H5''	1.81	0.61
1:0:1299:G:O6	13:K:6:ARG:HD3	2.01	0.61
5:C:168:ARG:NH2	5:C:190:ALA:O	2.33	0.61
1:0:1120:U:H5'	1:0:1121:G:OP2	2.01	0.61
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.81	0.61
14:L:63:VAL:HG21	14:L:109:PHE:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:149:LEU:HG	24:V:153:MET:CE	2.30	0.61
11:I:18:ILE:HG22	11:I:21:ARG:H	1.65	0.61
11:I:75:PRO:HD3	11:I:136:SER:OG	2.00	0.61
24:V:72:PRO:HG2	24:V:77:ALA:HB3	1.82	0.61
24:V:4:LEU:HB3	24:V:33:THR:HG22	1.83	0.61
1:O:1687:C:O2	28:Z:9:GLY:HA2	2.01	0.61
2:9:3039:U:H3'	2:9:3040:C:H5''	1.82	0.61
4:B:66:GLU:OE1	4:B:328:ARG:HD2	2.00	0.61
14:L:87:MET:CB	30:2:46:ILE:HD13	2.30	0.61
15:M:22:GLN:HA	15:M:25:ARG:HH21	1.66	0.61
19:Q:82:GLU:OE1	19:Q:86:LYS:HE3	2.01	0.61
21:S:89:ARG:HG3	21:S:89:ARG:O	1.99	0.61
27:Y:42:CYS:SG	27:Y:43:GLY:N	2.74	0.61
1:O:1766:U:O2	1:O:1778:A:H5'	2.01	0.61
7:E:34:TRP:O	11:I:127:ILE:HD11	2.00	0.61
10:H:131:ILE:HG23	10:H:132:PHE:CD1	2.35	0.61
23:U:64:GLY:O	23:U:65:ASP:HB2	1.99	0.61
28:Z:36:SER:O	28:Z:46:ARG:HD3	2.01	0.60
1:O:2615:U:OP1	4:B:230:GLN:CD	2.39	0.60
6:D:25:MET:CE	6:D:37:ALA:HB1	2.29	0.60
1:O:256:C:H2'	1:O:257:G:O4'	2.01	0.60
1:O:431:G:P	14:L:48:ARG:HH12	2.24	0.60
25:W:15:ARG:HB3	25:W:15:ARG:NH1	2.16	0.60
2:9:3004:G:H21	15:M:44:ARG:NH1	2.00	0.60
3:A:121:ALA:O	3:A:124:VAL:HG22	2.01	0.60
7:E:20:ILE:HD11	7:E:40:VAL:CG1	2.26	0.60
10:H:136:VAL:HG22	10:H:137:ASN:H	1.64	0.60
12:J:74:VAL:HG13	12:J:113:ILE:HG23	1.84	0.60
14:L:57:LYS:HD3	14:L:140:ALA:O	2.01	0.60
1:O:12:U:H2'	1:O:13:G:H5'	1.82	0.60
1:O:432:G:OP1	14:L:165:SER:HB3	2.01	0.60
1:O:949:U:O2'	18:P:40:HIS:HE1	1.85	0.60
1:O:1966:U:H2'	1:O:1967:U:H2'	1.83	0.60
6:D:20:LYS:HA	6:D:75:LEU:O	2.01	0.60
10:H:57:ARG:CB	10:H:59:ASN:HD22	2.15	0.60
23:U:1:THR:HB	23:U:48:GLU:OE1	2.02	0.60
24:V:41:TYR:O	24:V:45:VAL:HG12	2.01	0.60
1:O:902:G:N7	13:K:18:HIS:HD2	2.00	0.60
1:O:926:A:O2'	13:K:41:HIS:CD2	2.55	0.60
1:O:2626:C:H2'	1:O:2627:G:C8	2.37	0.60
5:C:236:THR:HG22	5:C:239:ALA:N	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:42:CYS:SG	27:Y:44:PHE:HB2	2.41	0.60
10:H:86:ARG:HH11	10:H:133:ILE:CD1	2.13	0.60
12:J:98:VAL:HG11	12:J:102:GLU:HA	1.83	0.60
1:0:558:C:H2'	1:0:559:U:C5'	2.31	0.60
1:0:1778:A:H2'	1:0:1779:A:H5'	1.83	0.60
12:J:58:THR:HG22	12:J:59:LYS:HG3	1.84	0.60
1:0:185:G:H4'	1:0:186:A:H4'	1.83	0.60
1:0:1118:A:C8	1:0:1118:A:C3'	2.82	0.60
15:M:72:GLU:H	15:M:171:HIS:CE1	2.20	0.60
1:0:1175:G:H2'	1:0:1176:C:C6	2.37	0.59
1:0:2609:G:N2	4:B:238:ASN:HD21	2.00	0.59
2:9:3092:G:H22	10:H:52:LYS:CE	2.15	0.59
3:A:36:ASP:CG	3:A:37:VAL:H	2.04	0.59
4:B:14:GLY:HA2	4:B:15:PRO:C	2.23	0.59
10:H:45:GLN:HB3	10:H:163:PRO:HG3	1.84	0.59
10:H:57:ARG:HG3	10:H:57:ARG:HH11	1.67	0.59
17:O:10:ALA:HA	17:O:13:VAL:CG1	2.31	0.59
1:0:475:G:OP1	5:C:73:LEU:HD22	2.01	0.59
2:9:3014:G:H5'	2:9:3014:G:C8	2.37	0.59
3:A:131:HIS:O	3:A:132:ASP:HB2	2.03	0.59
14:L:149:TRP:O	14:L:152:ARG:HG2	2.01	0.59
1:0:646:G:H2'	1:0:647:U:C6	2.37	0.59
6:D:24:HIS:HB2	6:D:72:LYS:CB	2.33	0.59
25:W:47:ALA:HB1	25:W:82:GLU:HB3	1.85	0.59
26:X:106:THR:HG23	26:X:107:PRO:HD2	1.84	0.59
1:0:2505:G:O2'	1:0:2506:A:H5'	2.02	0.59
1:0:2795:C:O2'	1:0:2796:U:H5'	2.01	0.59
5:C:76:ARG:HB3	5:C:76:ARG:NH1	2.16	0.59
17:O:59:ARG:HH22	17:O:66:GLN:NE2	1.97	0.59
36:O:8163:EMK:C13	36:O:8163:EMK:C23	2.80	0.59
4:B:280:VAL:HG13	4:B:333:GLU:O	2.01	0.59
24:V:88:THR:CG2	24:V:90:TYR:HD1	2.13	0.59
27:Y:62:TYR:CE2	27:Y:64:ILE:HG23	2.38	0.59
1:0:2698:G:H2'	1:0:2699:A:C8	2.38	0.59
8:F:22:VAL:CG2	8:F:104:ALA:HB2	2.33	0.59
10:H:139:ASP:N	10:H:140:PRO:CD	2.65	0.59
13:K:97:VAL:HG12	13:K:98:GLU:O	2.02	0.59
22:T:6:CYS:HA	22:T:13:ILE:HD11	1.84	0.59
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.38	0.59
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.84	0.59
1:0:1926:G:H2'	1:0:1927:A:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3114:G:O6	15:M:11:ARG:HD3	2.03	0.59
6:D:58:VAL:HG12	6:D:60:GLU:H	1.67	0.59
15:M:72:GLU:H	15:M:171:HIS:HE1	1.50	0.59
1:0:2253:G:O2'	1:0:2254:G:H5'	2.03	0.59
1:0:2547:C:OP2	4:B:5:ARG:NH1	2.36	0.59
1:0:671:A:O2'	1:0:672:G:H2'	2.03	0.58
8:F:63:ILE:HB	8:F:64:PRO:CD	2.31	0.58
23:U:12:THR:HG22	23:U:14:ALA:H	1.67	0.58
24:V:38:THR:HG22	24:V:40:ALA:H	1.68	0.58
13:K:67:ARG:O	13:K:71:GLU:HG3	2.02	0.58
25:W:73:ARG:HB2	25:W:88:GLU:OE2	2.02	0.58
1:0:182:G:O3'	14:L:157:LEU:CD1	2.51	0.58
6:D:154:LYS:H	6:D:154:LYS:HD2	1.67	0.58
9:G:12:ILE:N	9:G:13:PRO:CD	2.66	0.58
15:M:77:ASN:OD1	15:M:79:PRO:HD2	2.03	0.58
27:Y:33:HIS:CE1	27:Y:49:ARG:HD2	2.38	0.58
1:0:285:A:H2'	1:0:286:U:O4'	2.02	0.58
13:K:61:ALA:HB2	13:K:105:TYR:CZ	2.39	0.58
14:L:37:VAL:HG11	14:L:108:LYS:HG3	1.86	0.58
4:B:175:LEU:O	4:B:175:LEU:HD23	2.04	0.58
4:B:212:GLN:OE1	4:B:216:LYS:HD3	2.03	0.58
5:C:78:ARG:HG2	5:C:78:ARG:HH11	1.68	0.58
8:F:2:VAL:HG22	8:F:57:GLU:OE1	2.03	0.58
13:K:59:GLU:HA	13:K:104:ASP:OD2	2.03	0.58
19:Q:39:THR:HB	19:Q:42:GLU:HG3	1.84	0.58
1:0:1132:A:N6	1:0:1229:C:H2'	2.19	0.58
11:I:74:ARG:O	11:I:78:ILE:HG12	2.03	0.58
15:M:184:ILE:CG2	15:M:185:GLU:H	2.12	0.58
1:0:2878:U:H2'	1:0:2879:A:O4'	2.03	0.58
3:A:107:ASN:OD1	3:A:120:ARG:HD2	2.04	0.58
6:D:27:ILE:H	6:D:27:ILE:HD12	1.69	0.58
6:D:136:ARG:NH1	6:D:157:LEU:HA	2.18	0.58
13:K:90:ARG:NH2	13:K:121:ILE:HD11	2.18	0.58
14:L:87:MET:CG	30:2:46:ILE:HG21	2.34	0.58
1:0:775:G:OP1	28:Z:16:HIS:HE1	1.87	0.58
1:0:432:G:O2'	1:0:433:C:H5'	2.04	0.58
1:0:681:G:N3	1:0:681:G:H5'	2.19	0.58
10:H:127:GLY:O	10:H:128:ALA:HB3	2.03	0.58
1:0:344:C:H2'	1:0:345:G:O4'	2.04	0.58
1:0:1289:C:O2'	1:0:1290:G:H5'	2.04	0.58
1:0:2364:A:H5''	18:P:15:LYS:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:102:VAL:HG21	7:E:148:ILE:HG12	1.86	0.58
27:Y:28:ASP:O	27:Y:31:ILE:HG22	2.04	0.58
1:O:1799:G:H21	17:O:88:GLN:HE22	1.52	0.57
1:O:2027:U:O2'	1:O:2028:U:H5'	2.04	0.57
25:W:78:GLU:HG2	25:W:79:GLU:N	2.18	0.57
4:B:305:ASP:O	4:B:306:LYS:HB2	2.05	0.57
7:E:15:GLN:HE21	7:E:20:ILE:CG1	2.14	0.57
12:J:109:LEU:HD13	12:J:113:ILE:HD11	1.86	0.57
1:O:2720:C:O2	12:J:87:ARG:NH2	2.36	0.57
3:A:9:ARG:HG2	3:A:16:PHE:CD2	2.39	0.57
24:V:52:VAL:HG22	24:V:53:ALA:H	1.67	0.57
1:O:1593:C:P	17:O:117:SER:HB3	2.44	0.57
1:O:2694:A:H4'	7:E:91:PHE:CE1	2.38	0.57
2:9:3006:C:OP1	15:M:37:ARG:HD2	2.05	0.57
5:C:153:VAL:O	5:C:157:LEU:HG	2.05	0.57
1:O:588:G:O6	24:V:154:ARG:NH1	2.38	0.57
1:O:1234:U:N3	4:B:244:PRO:HB3	2.19	0.57
8:F:46:GLU:OE1	8:F:100:ASP:HA	2.04	0.57
12:J:98:VAL:HG13	12:J:102:GLU:HA	1.85	0.57
14:L:172:GLY:C	14:L:183:VAL:HG11	2.24	0.57
1:O:1183:C:N4	1:O:1184:C:H41	2.02	0.57
2:9:3039:U:H3'	2:9:3040:C:C5'	2.34	0.57
3:A:170:VAL:HG22	27:Y:22:ILE:HG23	1.87	0.57
13:K:143:THR:HG22	13:K:144:ASP:H	1.69	0.57
28:Z:25:LYS:HD2	29:1:49:GLU:N	2.11	0.57
1:O:2064:U:H5'	1:O:2652:U:H4'	1.87	0.57
1:O:2507:G:H2'	1:O:2510:C:H42	1.70	0.57
36:O:8163:EMK:C14	36:O:8163:EMK:H12	2.35	0.57
4:B:125:GLU:HG3	4:B:179:LEU:HD11	1.87	0.57
13:K:65:ASP:CG	13:K:111:ALA:HB3	2.25	0.57
24:V:39:ASP:HA	24:V:42:ARG:NH1	2.19	0.57
1:O:1667:A:H8	1:O:1667:A:H5'	1.69	0.57
3:A:232:ARG:NH2	3:A:236:GLY:O	2.37	0.57
7:E:8:PRO:HB2	7:E:11:VAL:HG23	1.86	0.57
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.34	0.57
10:H:3:GLY:HA2	10:H:57:ARG:HH12	1.70	0.57
1:O:1361:C:H2'	1:O:1362:U:C6	2.40	0.57
1:O:1641:A:C2'	1:O:1642:A:H5'	2.35	0.57
14:L:165:SER:HB2	14:L:169:ARG:NH2	2.20	0.57
1:O:1183:C:H41	1:O:1192:A:H5'	1.70	0.56
1:O:2829:G:O2'	1:O:2830:U:H5'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:143:ARG:HH12	15:M:169:PRO:HB2	1.70	0.56
18:P:66:LYS:HB2	18:P:70:ALA:O	2.04	0.56
19:Q:82:GLU:O	19:Q:86:LYS:HG3	2.05	0.56
1:O:1441:G:O2'	1:O:1442:A:H5'	2.05	0.56
1:O:2503:A:OP1	10:H:147:ARG:NH2	2.39	0.56
10:H:151:MET:O	10:H:151:MET:HE3	2.05	0.56
11:I:75:PRO:HG2	11:I:105:LEU:CD2	2.35	0.56
24:V:19:ASP:O	24:V:23:MET:HG3	2.05	0.56
1:O:74:A:H2'	1:O:75:U:C6	2.40	0.56
1:O:1377:C:H5'	1:O:1377:C:C6	2.40	0.56
1:O:1511:U:O2'	1:O:1512:G:H5'	2.05	0.56
1:O:2073:G:OP2	1:O:2490:A:H5'	2.06	0.56
7:E:154:ILE:HD11	7:E:157:LYS:HE2	1.86	0.56
8:F:34:ASN:HA	14:L:4:ALA:HB2	1.87	0.56
8:F:58:GLU:HG3	8:F:61:MET:HE1	1.86	0.56
11:I:19:MET:CE	11:I:132:LEU:HD11	2.35	0.56
14:L:144:ASP:O	14:L:148:SER:HB3	2.05	0.56
19:Q:114:VAL:HA	19:Q:144:GLU:O	2.06	0.56
24:V:81:ASP:OD1	24:V:92:ASP:HB2	2.05	0.56
24:V:130:HIS:O	24:V:136:GLY:HA3	2.05	0.56
26:X:186:ARG:HG2	26:X:186:ARG:NH1	2.19	0.56
1:O:1173:A:H2'	1:O:1177:A:H62	1.70	0.56
1:O:1632:A:H2'	1:O:1633:C:H5'	1.85	0.56
1:O:2548:C:OP2	4:B:5:ARG:NH2	2.39	0.56
5:C:136:VAL:HG22	5:C:137:PRO:HA	1.88	0.56
23:U:20:LEU:HD22	23:U:60:GLN:HE22	1.71	0.56
1:O:1278:A:H4'	1:O:1279:U:C4	2.40	0.56
11:I:107:ASN:HD22	11:I:109:TYR:H	1.52	0.56
21:S:24:ARG:HH21	21:S:39:ASN:ND2	2.02	0.56
2:9:3018:U:H2'	2:9:3019:G:H8	1.71	0.56
2:9:3029:C:C2'	2:9:3030:C:H5'	2.36	0.56
5:C:227:GLY:O	5:C:229:PRO:HD3	2.05	0.56
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.35	0.56
1:O:1007:A:H2'	10:H:19:TYR:CZ	2.41	0.56
1:O:1134:G:H4'	10:H:151:MET:SD	2.46	0.56
1:O:1925:G:O2'	1:O:1926:G:H5'	2.06	0.56
1:O:2316:G:H5'	1:O:2317:C:O4'	2.05	0.56
1:O:2827:A:H2'	1:O:2828:G:O4'	2.06	0.56
4:B:102:THR:CG2	4:B:182:VAL:HG12	2.36	0.56
5:C:129:HIS:HD2	5:C:165:ASP:OD2	1.88	0.56
12:J:81:ARG:HD3	12:J:87:ARG:NH2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:40:VAL:O	17:O:44:VAL:HG23	2.06	0.56
24:V:29:VAL:O	24:V:30:ASN:HB2	2.05	0.56
1:O:121:U:OP2	29:1:10:ARG:NH2	2.33	0.56
1:O:1733:A:H4'	4:B:212:GLN:HA	1.87	0.56
1:O:2252:A:H2'	1:O:2253:G:O4'	2.05	0.56
1:O:2812:A:C2	1:O:2814:A:N6	2.73	0.56
3:A:162:GLY:HA3	27:Y:73:THR:HG21	1.87	0.56
13:K:40:PHE:CD1	13:K:40:PHE:C	2.79	0.56
1:O:1167:G:H2'	1:O:1168:C:O4'	2.06	0.56
1:O:1342:C:O2'	1:O:1343:C:H5'	2.06	0.56
1:O:1066:U:H2'	1:O:1067:A:C8	2.40	0.56
1:O:2256:G:O2'	1:O:2257:G:H5'	2.05	0.56
3:A:51:ARG:NH1	3:A:120:ARG:O	2.39	0.56
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.41	0.56
6:D:136:ARG:HH12	6:D:157:LEU:HA	1.69	0.56
1:O:2676:C:H4'	11:I:70:PHE:CD1	2.41	0.55
5:C:104:ASP:O	5:C:108:GLN:HG3	2.06	0.55
8:F:117:GLU:C	8:F:119:ARG:H	2.09	0.55
1:O:289:G:N1	1:O:363:A:H2	2.01	0.55
1:O:292:G:H2'	1:O:358:G:N2	2.20	0.55
4:B:254:GLN:HG2	4:B:255:GLY:N	2.20	0.55
13:K:63:THR:HG22	13:K:107:LYS:HB3	1.88	0.55
14:L:63:VAL:HG21	14:L:109:PHE:CZ	2.41	0.55
23:U:55:ARG:O	23:U:59:ILE:HG12	2.06	0.55
1:O:137:U:H2'	1:O:139:C:C5	2.41	0.55
1:O:155:C:OP2	14:L:188:ARG:HD3	2.07	0.55
1:O:1132:A:H2'	1:O:1133:A:C8	2.41	0.55
1:O:1909:A:H2'	1:O:1910:A:C8	2.42	0.55
5:C:57:PRO:HG2	5:C:73:LEU:HD13	1.87	0.55
6:D:99:ASP:N	6:D:103:ASN:O	2.37	0.55
10:H:31:PHE:HE2	10:H:87:LYS:O	1.90	0.55
14:L:138:HIS:ND1	14:L:139:PRO:O	2.40	0.55
24:V:4:LEU:HD13	24:V:52:VAL:CG2	2.33	0.55
1:O:951:A:O2'	1:O:952:G:H5'	2.06	0.55
4:B:193:ILE:N	4:B:193:ILE:HD12	2.21	0.55
6:D:57:THR:HG23	6:D:63:ILE:HA	1.88	0.55
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.36	0.55
14:L:72:SER:OG	14:L:93:ARG:CZ	2.55	0.55
1:O:2356:A:H2'	1:O:2357:G:O4'	2.06	0.55
10:H:14:TYR:N	10:H:91:HIS:CE1	2.67	0.55
1:O:119:A:H2'	1:O:120:A:H5''	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2676:C:H4'	11:I:70:PHE:CE1	2.41	0.55
4:B:80:ARG:HB2	4:B:145:HIS:CE1	2.41	0.55
7:E:81:GLU:OE1	7:E:170:ARG:NH2	2.40	0.55
14:L:67:ILE:HG21	14:L:97:ILE:HG23	1.89	0.55
1:0:1187:U:HO2'	1:0:1189:A:H2	1.53	0.55
1:0:2032:U:O2'	1:0:2033:G:H5''	2.06	0.55
1:0:2253:G:H2'	1:0:2254:G:H8	1.72	0.55
1:0:2531:U:O2'	1:0:2532:A:H5'	2.06	0.55
4:B:255:GLY:O	4:B:257:THR:HG22	2.07	0.55
6:D:27:ILE:HD12	6:D:27:ILE:N	2.22	0.55
13:K:10:SER:O	13:K:11:ARG:HB3	2.06	0.55
14:L:138:HIS:O	14:L:141:ILE:HB	2.07	0.55
15:M:110:THR:HB	15:M:113:SER:HG	1.72	0.55
22:T:17:THR:CG2	22:T:18:GLY:N	2.69	0.55
1:0:1768:C:H2'	1:0:1769:C:O4'	2.07	0.55
1:0:2372:A:H2'	1:0:2373:U:H6	1.72	0.55
4:B:53:LEU:HD21	4:B:270:ILE:HD12	1.88	0.55
4:B:106:HIS:CE1	4:B:147:VAL:HG13	2.42	0.55
14:L:38:VAL:O	14:L:63:VAL:HG13	2.06	0.55
24:V:125:HIS:HD2	24:V:127:GLY:H	1.54	0.55
1:0:1003:U:O2'	10:H:90:PHE:HE1	1.90	0.55
1:0:1166:A:H1'	1:0:1192:A:C2	2.42	0.55
1:0:1874:U:OP1	3:A:51:ARG:HD2	2.06	0.55
2:9:3076:G:C3'	2:9:3077:A:H5''	2.29	0.55
3:A:33:GLU:O	3:A:34:ASP:HB2	2.07	0.55
6:D:134:LEU:CD1	6:D:166:ILE:HD11	2.36	0.55
1:0:65:C:O2'	1:0:66:G:H5'	2.07	0.55
1:0:243:A:H61	1:0:269:G:H1'	1.72	0.55
1:0:613:C:H2'	1:0:614:U:H6	1.72	0.55
10:H:31:PHE:HA	10:H:85:ILE:CG2	2.38	0.55
21:S:41:ARG:O	21:S:43:ASN:ND2	2.40	0.55
1:0:2592:G:H2'	1:0:2593:C:C6	2.42	0.54
5:C:197:SER:HB2	5:C:242:GLU:OE2	2.06	0.54
6:D:35:ALA:C	6:D:37:ALA:H	2.10	0.54
1:0:1133:A:H3'	1:0:1134:G:C8	2.42	0.54
1:0:2478:U:O2'	1:0:2479:A:H5'	2.08	0.54
11:I:49:ARG:O	11:I:53:ILE:HG13	2.06	0.54
1:0:1886:A:O2'	27:Y:20:LEU:HB2	2.06	0.54
1:0:2415:A:H2'	1:0:2416:G:H5'	1.89	0.54
2:9:3092:G:H2'	2:9:3093:A:C8	2.42	0.54
6:D:64:ARG:NE	6:D:67:ASP:HB3	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:19:MET:HE3	11:I:132:LEU:HD21	1.90	0.54
25:W:37:LEU:CD1	25:W:85:VAL:HG11	2.31	0.54
1:0:31:C:H4'	21:S:9:LYS:HD2	1.87	0.54
1:0:952:G:N3	1:0:2302:A:H2'	2.23	0.54
1:0:1595:G:O2'	1:0:1596:U:H5'	2.07	0.54
3:A:199:HIS:HD2	3:A:201:PHE:N	1.96	0.54
6:D:10:PHE:CD1	6:D:11:HIS:N	2.74	0.54
15:M:152:GLU:C	15:M:154:LEU:H	2.11	0.54
25:W:71:ARG:HB3	25:W:88:GLU:OE1	2.07	0.54
1:0:165:A:H5''	13:K:33:ALA:HB2	1.90	0.54
1:0:736:A:H2'	1:0:737:A:O4'	2.06	0.54
1:0:1943:C:O4'	3:A:212:PRO:HA	2.08	0.54
1:0:2870:C:H2'	1:0:2871:G:H8	1.72	0.54
4:B:258:GLY:H	4:B:260:HIS:CE1	2.25	0.54
13:K:73:VAL:HG21	13:K:116:HIS:NE2	2.23	0.54
15:M:59:ALA:O	15:M:60:SER:HB3	2.08	0.54
21:S:78:THR:HG22	21:S:88:PRO:HA	1.88	0.54
22:T:35:LYS:HE2	22:T:51:TRP:CZ2	2.43	0.54
24:V:68:THR:HG23	24:V:69:ARG:HG2	1.89	0.54
24:V:125:HIS:CD2	24:V:127:GLY:H	2.25	0.54
1:0:523:C:H2'	1:0:524:A:C8	2.43	0.54
1:0:646:G:H2'	1:0:647:U:H6	1.73	0.54
1:0:861:A:C4'	1:0:1697:G:H4'	2.36	0.54
1:0:2498:C:O2'	1:0:2499:U:H5'	2.07	0.54
14:L:98:GLN:O	14:L:102:GLU:HG3	2.07	0.54
16:N:32:ARG:O	16:N:32:ARG:HD3	2.07	0.54
1:0:111:C:O2'	1:0:112:G:H5'	2.08	0.54
1:0:236:A:H8	1:0:236:A:OP1	1.91	0.54
1:0:2401:A:H2'	1:0:2402:A:C8	2.43	0.54
10:H:26:LYS:HE3	10:H:28:ILE:HB	1.89	0.54
14:L:37:VAL:HG21	14:L:108:LYS:HG3	1.90	0.54
24:V:64:THR:O	24:V:68:THR:HG22	2.08	0.54
25:W:15:ARG:HH11	25:W:15:ARG:CB	2.19	0.54
3:A:220:PRO:HD2	3:A:223:ARG:HD2	1.90	0.54
10:H:70:ARG:O	10:H:73:GLN:HB2	2.08	0.54
14:L:106:ASN:HD22	14:L:114:VAL:HG23	1.71	0.54
1:0:56:G:H5''	23:U:50:ARG:NH1	2.23	0.54
10:H:117:LYS:O	10:H:119:VAL:HG13	2.08	0.54
30:2:42:ARG:HG3	30:2:42:ARG:HH11	1.73	0.54
1:0:1333:U:H2'	1:0:1334:C:C6	2.42	0.53
1:0:2038:A:O2'	1:0:2039:A:H5'	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.41	0.53
5:C:149:LYS:HB2	5:C:152:GLU:HG3	1.91	0.53
10:H:47:GLU:OE1	10:H:133:ILE:HD12	2.07	0.53
14:L:37:VAL:CB	14:L:108:LYS:HG3	2.38	0.53
24:V:35:VAL:HG23	24:V:41:TYR:CD2	2.43	0.53
26:X:96:GLU:O	26:X:235:GLU:HA	2.08	0.53
1:O:2112:A:H2'	1:O:2113:G:C8	2.42	0.53
1:O:2353:A:H4'	1:O:2354:A:O5'	2.07	0.53
1:O:2807:U:P	4:B:27:ASN:HD21	2.31	0.53
6:D:18:ILE:HG12	6:D:134:LEU:CD2	2.39	0.53
7:E:119:HIS:HE1	7:E:147:ASP:OD2	1.92	0.53
10:H:30:GLN:H	10:H:65:ARG:HH11	1.55	0.53
23:U:44:GLY:O	23:U:48:GLU:HG2	2.08	0.53
1:O:289:G:C2	1:O:363:A:H2	2.26	0.53
1:O:821:U:H2'	1:O:822:C:H6	1.74	0.53
1:O:1119:G:OP2	11:I:49:ARG:HD3	2.08	0.53
1:O:2456:A:H2'	1:O:2457:U:C6	2.43	0.53
1:O:2597:U:H2'	1:O:2598:U:H5'	1.89	0.53
1:O:2682:C:OP2	4:B:316:ARG:NH2	2.40	0.53
14:L:61:ILE:HD12	14:L:61:ILE:N	2.23	0.53
20:R:8:PRO:HD2	23:U:32:ALA:HA	1.90	0.53
23:U:1:THR:HG23	23:U:3:LEU:H	1.72	0.53
24:V:139:GLY:O	24:V:141:HIS:HD2	1.92	0.53
1:O:2511:A:O2'	1:O:2512:U:H5'	2.09	0.53
6:D:68:PRO:C	6:D:69:ILE:HD12	2.28	0.53
1:O:638:C:H2'	1:O:639:A:C8	2.44	0.53
1:O:776:A:OP1	28:Z:28:HIS:HE1	1.92	0.53
1:O:1632:A:C2'	1:O:1633:C:H5'	2.39	0.53
4:B:41:PHE:HA	4:B:79:MET:HE2	1.90	0.53
13:K:53:ARG:HH22	13:K:57:VAL:HG12	1.74	0.53
14:L:120:VAL:CG1	14:L:130:GLU:HG3	2.38	0.53
15:M:22:GLN:CA	15:M:25:ARG:HH21	2.21	0.53
25:W:41:PHE:CZ	25:W:74:ALA:HB3	2.44	0.53
1:O:1042:U:O2'	1:O:1043:C:H5'	2.09	0.53
5:C:162:VAL:HG12	5:C:192:ILE:CD1	2.36	0.53
11:I:74:ARG:NH1	11:I:144:THR:HG21	2.23	0.53
29:1:48:ASP:O	29:1:49:GLU:HB2	2.08	0.53
1:O:771:G:H2'	1:O:772:G:C8	2.44	0.53
1:O:1573:A:H2'	1:O:1574:C:O4'	2.09	0.53
1:O:2265:U:H2'	1:O:2266:A:H8	1.74	0.53
6:D:64:ARG:CD	6:D:67:ASP:HB3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:141:ILE:C	17:O:143:ALA:H	2.10	0.53
29:1:36:ASN:N	29:1:39:ARG:HH21	2.03	0.53
1:0:123:U:O2'	1:0:124:C:H5'	2.08	0.53
1:0:136:C:H2'	1:0:137:U:O4'	2.07	0.53
9:G:16:LYS:O	9:G:20:VAL:HG23	2.09	0.53
10:H:56:ILE:CG2	10:H:61:LEU:HD13	2.37	0.53
1:0:797:A:C4'	27:Y:10:ARG:N	2.71	0.53
1:0:1462:C:H2'	1:0:1463:A:H8	1.72	0.53
24:V:4:LEU:HD22	24:V:54:PHE:HB3	1.91	0.53
1:0:277:U:O2'	1:0:278:A:H5'	2.10	0.53
1:0:2591:C:H2'	1:0:2592:G:O4'	2.09	0.53
4:B:38:VAL:HG22	4:B:142:LEU:HD12	1.91	0.53
5:C:35:VAL:HG23	5:C:220:THR:HG22	1.90	0.53
5:C:84:VAL:O	5:C:85:LYS:HB2	2.09	0.53
10:H:13:ALA:CA	10:H:91:HIS:HE1	2.16	0.53
1:0:695:C:H2'	1:0:696:C:C6	2.45	0.52
1:0:1298:U:H2'	1:0:1299:G:H8	1.73	0.52
1:0:1423:C:O2'	1:0:1424:A:H5'	2.09	0.52
1:0:2274:A:H1'	14:L:86:MET:SD	2.49	0.52
7:E:32:ARG:O	7:E:33:LEU:HD23	2.09	0.52
8:F:108:LEU:HD12	8:F:108:LEU:C	2.29	0.52
13:K:38:HIS:HD2	13:K:39:GLU:HG3	1.73	0.52
22:T:17:THR:HG22	22:T:18:GLY:N	2.24	0.52
24:V:88:THR:HG23	24:V:110:GLN:HE21	1.74	0.52
1:0:2838:A:H2'	1:0:2839:C:C6	2.44	0.52
4:B:320:GLN:HE21	4:B:321:PRO:CD	2.22	0.52
10:H:166:ASN:HD22	10:H:166:ASN:N	2.06	0.52
12:J:55:VAL:HG12	12:J:56:SER:N	2.24	0.52
20:R:44:GLN:OE1	20:R:44:GLN:HA	2.09	0.52
20:R:51:GLN:NE2	20:R:53:ASN:HD21	1.90	0.52
1:0:475:G:C5'	5:C:73:LEU:HD23	2.38	0.52
1:0:790:A:H1'	1:0:1710:A:H2'	1.90	0.52
1:0:2089:A:O2'	1:0:2090:G:H5'	2.09	0.52
10:H:157:ILE:HG22	10:H:158:ASN:N	2.24	0.52
1:0:1198:U:H1'	1:0:1201:C:H5	1.74	0.52
1:0:1505:U:O2	1:0:1505:U:H2'	2.10	0.52
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.91	0.52
5:C:49:ASP:HB3	5:C:52:ALA:HB2	1.91	0.52
1:0:876:A:H2'	1:0:876:A:N3	2.25	0.52
1:0:1166:A:H61	1:0:1180:U:H3	1.57	0.52
1:0:1178:G:H2'	1:0:1179:C:C6	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2837:U:H1'	4:B:307:ARG:HH12	1.74	0.52
2:9:3050:G:H5''	15:M:159:TYR:HE1	1.73	0.52
10:H:45:GLN:HB3	10:H:163:PRO:HD3	1.91	0.52
13:K:83:GLU:CD	13:K:83:GLU:H	2.13	0.52
17:O:134:VAL:O	17:O:138:GLU:HG3	2.10	0.52
1:O:447:A:OP1	21:S:2:LYS:HG2	2.09	0.52
1:O:559:U:H2'	1:O:560:C:O4'	2.09	0.52
1:O:1080:C:H4'	1:O:1081:A:OP1	2.10	0.52
1:O:1634:G:H2'	1:O:1635:U:C6	2.44	0.52
1:O:2769:C:C2'	1:O:2770:G:H5'	2.39	0.52
1:O:2900:G:H2'	1:O:2901:C:O4'	2.09	0.52
7:E:11:VAL:HG12	7:E:12:ASP:N	2.25	0.52
8:F:28:ALA:CB	8:F:99:THR:HG23	2.39	0.52
25:W:24:LYS:HA	25:W:63:ARG:HG2	1.91	0.52
29:1:36:ASN:H	29:1:39:ARG:NH2	2.03	0.52
1:O:449:A:N7	5:C:43:LYS:HG2	2.24	0.52
1:O:2406:U:O2'	1:O:2407:G:H5'	2.09	0.52
1:O:2594:C:O2'	1:O:2595:U:H5'	2.10	0.52
5:C:7:ASP:OD2	5:C:9:ASP:HB2	2.09	0.52
7:E:84:MET:HG2	7:E:168:ILE:HA	1.91	0.52
7:E:101:GLU:HB3	7:E:117:THR:HA	1.91	0.52
10:H:45:GLN:HB3	10:H:163:PRO:CD	2.39	0.52
11:I:42:GLU:HG2	11:I:43:ARG:HG3	1.92	0.52
11:I:130:VAL:HG12	11:I:131:THR:N	2.24	0.52
15:M:72:GLU:O	15:M:72:GLU:HG2	2.10	0.52
1:O:799:C:O2'	1:O:800:G:H5'	2.10	0.52
1:O:1835:U:C5	1:O:1840:A:N7	2.73	0.52
2:9:3072:C:H2'	2:9:3073:G:H8	1.75	0.52
4:B:175:LEU:HD23	4:B:175:LEU:C	2.30	0.52
4:B:320:GLN:HE21	4:B:321:PRO:HD3	1.75	0.52
6:D:11:HIS:O	6:D:12:GLU:HB3	2.10	0.52
10:H:3:GLY:HA2	10:H:57:ARG:NH1	2.25	0.52
10:H:72:VAL:O	10:H:72:VAL:HG13	2.08	0.52
11:I:6:PHE:HB3	11:I:109:TYR:OH	2.09	0.52
15:M:143:ARG:NH1	15:M:169:PRO:HB2	2.24	0.52
25:W:76:ARG:O	25:W:77:PHE:HB3	2.10	0.52
25:W:78:GLU:CG	25:W:79:GLU:H	2.22	0.52
29:1:23:ALA:HA	29:1:26:MET:HE2	1.92	0.52
1:O:858:U:H2'	1:O:859:C:H6	1.74	0.52
1:O:1370:G:OP1	19:Q:64:SER:HB3	2.09	0.52
1:O:2456:A:H2'	1:O:2457:U:H6	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2506:A:O2'	1:0:2507:G:O5'	2.27	0.52
3:A:30:ARG:HG2	3:A:31:LYS:N	2.25	0.52
3:A:93:THR:C	3:A:94:LEU:HD23	2.30	0.52
6:D:95:THR:HG21	6:D:174:VAL:HG22	1.92	0.52
19:Q:39:THR:HG22	19:Q:42:GLU:N	2.15	0.52
29:1:23:ALA:HA	29:1:26:MET:HE3	1.89	0.52
1:0:1133:A:H3'	1:0:1134:G:H8	1.75	0.52
1:0:2361:A:H2'	1:0:2362:A:C8	2.45	0.52
1:0:2363:G:O2'	18:P:11:ARG:HG3	2.10	0.52
1:0:2533:C:H5'	1:0:2533:C:C6	2.38	0.52
1:0:2717:C:O2'	1:0:2718:C:H5'	2.09	0.52
1:0:2894:C:O2'	1:0:2895:C:H5'	2.10	0.52
1:0:2908:A:O2'	1:0:2909:G:H5'	2.10	0.52
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.44	0.52
6:D:101:THR:O	6:D:101:THR:HG22	2.10	0.52
6:D:128:LEU:C	6:D:128:LEU:HD23	2.31	0.52
13:K:125:PHE:CZ	13:K:140:VAL:HG13	2.45	0.52
24:V:3:ALA:O	24:V:54:PHE:HA	2.10	0.52
1:0:611:U:H2'	1:0:612:U:C6	2.45	0.51
1:0:685:C:O2	1:0:748:C:H4'	2.10	0.51
1:0:820:G:H5'	1:0:821:U:H5'	1.92	0.51
14:L:24:MET:SD	14:L:27:ARG:NH1	2.83	0.51
21:S:24:ARG:HH21	21:S:39:ASN:HD22	1.56	0.51
28:Z:5:THR:HB	28:Z:6:PRO:HD3	1.92	0.51
1:0:1116:U:H3	1:0:1246:A:H62	1.58	0.51
1:0:1641:A:H2'	1:0:1642:A:C5'	2.40	0.51
2:9:3057:A:C8	6:D:141:VAL:HG21	2.45	0.51
6:D:94:ALA:HB3	6:D:174:VAL:CA	2.40	0.51
8:F:91:VAL:CG1	8:F:92:GLY:N	2.73	0.51
25:W:30:MET:CE	25:W:58:ALA:HB3	2.40	0.51
1:0:204:A:C2'	1:0:205:U:H5'	2.40	0.51
1:0:706:G:HO2'	1:0:707:C:H6	1.57	0.51
1:0:1218:U:H2'	1:0:1219:U:H6	1.75	0.51
1:0:1755:A:H2'	1:0:1756:G:O4'	2.10	0.51
1:0:2237:G:O2'	1:0:2238:A:C8	2.63	0.51
10:H:46:VAL:O	10:H:146:TRP:HH2	1.92	0.51
17:O:71:LYS:HG3	17:O:71:LYS:O	2.09	0.51
23:U:12:THR:HG23	23:U:13:PRO:HD2	1.92	0.51
23:U:39:ALA:O	23:U:41:GLU:N	2.43	0.51
25:W:27:ASP:OD2	25:W:27:ASP:N	2.40	0.51
30:2:3:MET:O	30:2:90:PHE:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:216:A:O2'	1:0:217:C:H5'	2.10	0.51
1:0:667:C:H2'	1:0:668:C:H6	1.75	0.51
1:0:1803:C:H2'	1:0:1804:A:C8	2.46	0.51
3:A:84:VAL:HG13	3:A:98:GLU:HG3	1.92	0.51
4:B:62:ARG:HA	4:B:65:MET:HE3	1.93	0.51
8:F:36:THR:HG23	8:F:97:ALA:HB2	1.92	0.51
8:F:57:GLU:HB2	14:L:23:LEU:HD11	1.93	0.51
24:V:5:VAL:O	24:V:52:VAL:HG23	2.10	0.51
26:X:235:GLU:CD	26:X:235:GLU:N	2.56	0.51
6:D:58:VAL:CG1	6:D:60:GLU:HG2	2.40	0.51
13:K:57:VAL:HG12	13:K:57:VAL:O	2.10	0.51
15:M:138:ASP:CG	15:M:138:ASP:O	2.48	0.51
20:R:44:GLN:HE21	23:U:28:LEU:CD2	2.24	0.51
23:U:56:ILE:HG22	23:U:60:GLN:NE2	2.24	0.51
1:0:797:A:H4'	27:Y:10:ARG:N	2.25	0.51
1:0:870:G:OP2	3:A:3:ARG:HD3	2.10	0.51
3:A:170:VAL:HG22	27:Y:22:ILE:CG2	2.41	0.51
5:C:35:VAL:CG2	5:C:220:THR:HG22	2.40	0.51
10:H:45:GLN:HB3	10:H:163:PRO:CG	2.40	0.51
20:R:57:THR:CG2	20:R:58:MET:N	2.74	0.51
1:0:1878:G:O2'	1:0:1879:U:OP2	2.27	0.51
1:0:2563:U:H2'	1:0:2565:C:O5'	2.11	0.51
4:B:8:LYS:HG3	4:B:220:VAL:HG12	1.93	0.51
8:F:102:GLY:C	8:F:104:ALA:H	2.12	0.51
10:H:53:PRO:HA	10:H:125:VAL:O	2.10	0.51
12:J:28:GLU:OE2	12:J:58:THR:HG21	2.11	0.51
1:0:1505:U:O2	1:0:1505:U:C2'	2.59	0.51
1:0:1878:G:O2'	1:0:1879:U:P	2.68	0.51
1:0:2890:A:H1'	22:T:56:ARG:NH2	2.25	0.51
18:P:94:GLN:O	18:P:95:GLU:HB2	2.10	0.51
24:V:6:GLN:HB2	24:V:26:ILE:CD1	2.38	0.51
26:X:151:SER:HB3	26:X:154:ARG:HB2	1.92	0.51
1:0:682:A:H2'	1:0:683:G:O4'	2.10	0.51
1:0:1667:A:H5'	1:0:1667:A:C8	2.46	0.51
1:0:2081:A:H4'	11:I:69:TYR:CE1	2.46	0.51
8:F:28:ALA:HB3	8:F:99:THR:O	2.11	0.51
9:G:64:ASN:HD22	9:G:64:ASN:N	2.08	0.51
10:H:46:VAL:CG1	10:H:146:TRP:HZ3	2.24	0.51
11:I:14:ALA:HB1	11:I:44:ALA:HB2	1.92	0.51
17:O:10:ALA:HA	17:O:13:VAL:HG12	1.93	0.51
2:9:3023:U:C3'	2:9:3024:U:C5'	2.81	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:55:TRP:HB2	27:Y:64:ILE:HG13	1.92	0.51
1:0:951:A:C2'	1:0:952:G:H5'	2.41	0.50
4:B:145:HIS:HD2	4:B:146:THR:O	1.93	0.50
6:D:94:ALA:O	6:D:95:THR:O	2.29	0.50
10:H:97:LYS:HD3	10:H:117:LYS:HD3	1.93	0.50
12:J:115:ARG:HG3	12:J:116:GLU:N	2.26	0.50
19:Q:111:ILE:HG23	19:Q:145:LEU:HD11	1.93	0.50
24:V:22:GLU:HG2	24:V:27:HIS:CD2	2.46	0.50
1:0:407:A:O2'	1:0:408:A:H5'	2.11	0.50
1:0:1279:U:O2	1:0:1279:U:H2'	2.09	0.50
1:0:1470:A:OP1	14:L:93:ARG:HD2	2.11	0.50
1:0:2871:G:H2'	1:0:2872:U:C6	2.47	0.50
1:0:2896:A:OP1	25:W:15:ARG:NH1	2.44	0.50
3:A:179:MET:HG2	3:A:186:TRP:CG	2.46	0.50
5:C:172:THR:HG22	5:C:188:ARG:CZ	2.41	0.50
13:K:73:VAL:HG23	13:K:74:THR:N	2.23	0.50
13:K:73:VAL:HG21	13:K:116:HIS:CD2	2.47	0.50
14:L:35:PRO:HB2	14:L:38:VAL:HG23	1.91	0.50
24:V:6:GLN:HG2	24:V:29:VAL:HA	1.92	0.50
1:0:907:A:H2'	1:0:908:A:H8	1.75	0.50
1:0:1616:A:H2'	1:0:1618:G:C8	2.46	0.50
1:0:2908:A:H2'	1:0:2909:G:C5'	2.42	0.50
1:0:2908:A:H2'	1:0:2909:G:H5'	1.93	0.50
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.40	0.50
5:C:127:ARG:HH22	5:C:225:PRO:HB2	1.76	0.50
1:0:164:G:H4'	13:K:30:ARG:HD2	1.92	0.50
1:0:625:U:H5''	1:0:1044:C:N4	2.26	0.50
1:0:858:U:H2'	1:0:859:C:C6	2.45	0.50
1:0:1700:C:H5''	1:0:1701:A:OP2	2.12	0.50
1:0:1787:C:OP1	17:O:68:LYS:HE2	2.12	0.50
10:H:48:LEU:HD13	10:H:146:TRP:HB3	1.92	0.50
11:I:93:ARG:HB3	11:I:93:ARG:HH11	1.76	0.50
15:M:154:LEU:O	15:M:155:GLU:CB	2.58	0.50
1:0:766:A:O2'	1:0:767:A:H5''	2.11	0.50
4:B:26:PHE:CE1	4:B:310:ARG:HB3	2.46	0.50
4:B:214:PRO:C	4:B:220:VAL:HG22	2.32	0.50
5:C:172:THR:HG22	5:C:188:ARG:NH1	2.26	0.50
10:H:112:ARG:O	10:H:113:ALA:C	2.49	0.50
14:L:107:ARG:O	14:L:110:PRO:HD3	2.12	0.50
15:M:163:PHE:H	15:M:163:PHE:HD2	1.59	0.50
16:N:25:VAL:HG11	16:N:111:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:57:THR:HB	16:N:111:VAL:HG23	1.94	0.50
20:R:73:ASP:HB3	20:R:76:GLU:OE1	2.11	0.50
24:V:56:GLU:O	24:V:143:THR:HG23	2.12	0.50
1:O:263:U:O4'	8:F:59:ILE:HD13	2.12	0.50
1:O:1064:U:H2'	1:O:1065:G:C8	2.47	0.50
1:O:1165:G:H21	1:O:1173:A:H5''	1.76	0.50
1:O:1242:A:OP2	11:I:60:ARG:NH2	2.42	0.50
1:O:1298:U:H2'	1:O:1299:G:C8	2.46	0.50
1:O:2090:G:H2'	1:O:2091:G:C8	2.47	0.50
36:O:8163:EMK:C20	36:O:8163:EMK:N9	2.73	0.50
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.93	0.50
6:D:165:PHE:CD2	6:D:166:ILE:HD12	2.47	0.50
10:H:86:ARG:NH1	10:H:133:ILE:CG1	2.59	0.50
17:O:98:ILE:HD12	17:O:102:ARG:NE	2.26	0.50
1:O:1250:C:O2'	1:O:1251:C:H5'	2.12	0.50
1:O:1677:U:OP2	29:1:8:LYS:NZ	2.44	0.50
14:L:173:LEU:HD23	14:L:183:VAL:HG12	1.94	0.50
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.94	0.50
4:B:307:ARG:HH11	4:B:307:ARG:CG	2.24	0.50
5:C:233:THR:HG22	5:C:234:VAL:N	2.26	0.50
10:H:57:ARG:HG3	10:H:57:ARG:NH1	2.27	0.50
16:N:87:THR:O	16:N:91:GLN:HG3	2.11	0.50
17:O:13:VAL:HG21	17:O:41:ARG:HG2	1.93	0.50
27:Y:30:GLU:HA	27:Y:33:HIS:HB3	1.94	0.50
4:B:84:LEU:HD13	4:B:84:LEU:O	2.12	0.50
6:D:146:LYS:HZ3	15:M:107:ASN:HD21	1.58	0.50
18:P:30:VAL:O	18:P:30:VAL:HG12	2.11	0.50
20:R:51:GLN:HE21	20:R:53:ASN:ND2	1.91	0.50
28:Z:19:CYS:HB2	28:Z:27:TYR:HB2	1.94	0.50
1:O:731:U:H2'	1:O:732:C:C6	2.47	0.49
1:O:1456:C:H2'	1:O:1457:U:C6	2.46	0.49
1:O:1762:C:H2'	1:O:1763:C:H6	1.77	0.49
1:O:2039:A:H2'	1:O:2040:C:C6	2.47	0.49
1:O:2717:C:OP1	4:B:207:LYS:HG3	2.12	0.49
2:9:3011:A:P	18:P:19:ARG:HH21	2.34	0.49
6:D:58:VAL:HG12	6:D:60:GLU:HG2	1.94	0.49
8:F:61:MET:HB3	14:L:19:GLN:OE1	2.11	0.49
10:H:51:GLU:HB2	10:H:156:THR:O	2.11	0.49
17:O:55:LYS:HG2	17:O:56:GLY:N	2.27	0.49
25:W:47:ALA:HB1	25:W:82:GLU:CB	2.42	0.49
1:O:398:U:H2'	1:O:399:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1739:G:H1'	1:0:2726:U:O4	2.11	0.49
7:E:1:PRO:HG3	7:E:59:MET:SD	2.53	0.49
8:F:28:ALA:HB3	8:F:99:THR:HG23	1.93	0.49
10:H:130:HIS:H	10:H:130:HIS:CD2	2.30	0.49
14:L:164:THR:CG2	14:L:165:SER:N	2.75	0.49
27:Y:46:LYS:HD3	27:Y:59:HIS:HB2	1.94	0.49
1:0:1751:G:C2'	1:0:1752:G:H5''	2.43	0.49
1:0:1964:U:H2'	1:0:1965:C:C6	2.47	0.49
5:C:140:VAL:HG12	5:C:141:SER:N	2.27	0.49
1:0:20:G:H21	19:Q:117:HIS:HD2	1.59	0.49
1:0:56:G:H5''	23:U:50:ARG:HH12	1.76	0.49
1:0:565:A:H2'	1:0:566:A:C8	2.47	0.49
1:0:794:U:H3	1:0:819:A:H61	1.60	0.49
1:0:945:U:H2'	1:0:946:C:C6	2.47	0.49
1:0:969:G:H1	1:0:999:C:N4	2.09	0.49
1:0:1684:A:H1'	29:1:43:ARG:HH22	1.77	0.49
3:A:173:GLY:O	3:A:176:HIS:HB3	2.11	0.49
4:B:51:VAL:HG22	4:B:330:VAL:HG22	1.93	0.49
4:B:238:ASN:HD22	4:B:240:GLY:H	1.59	0.49
10:H:56:ILE:HG22	10:H:61:LEU:HD22	1.95	0.49
15:M:139:TRP:CE3	15:M:139:TRP:HA	2.47	0.49
1:0:282:C:HO2'	1:0:283:U:H4'	1.72	0.49
1:0:524:A:H5''	19:Q:29:LYS:HE2	1.95	0.49
4:B:62:ARG:HG2	4:B:62:ARG:HH11	1.77	0.49
4:B:312:ARG:HH11	4:B:315:VAL:HG13	1.76	0.49
6:D:62:ASP:O	6:D:64:ARG:N	2.46	0.49
15:M:1:ALA:HA	15:M:6:TYR:CD2	2.47	0.49
20:R:17:ASP:HB3	20:R:23:LYS:HB2	1.93	0.49
23:U:29:ASN:O	23:U:33:VAL:HG23	2.13	0.49
24:V:52:VAL:CG2	24:V:53:ALA:N	2.74	0.49
29:1:22:PRO:HB2	29:1:25:VAL:HG23	1.95	0.49
1:0:372:A:H2'	1:0:373:G:C8	2.48	0.49
1:0:820:G:C5	3:A:171:LYS:HB2	2.48	0.49
1:0:1102:C:HO2'	11:I:24:SER:HG	1.61	0.49
1:0:2082:G:O2'	1:0:2083:A:H5'	2.12	0.49
36:0:8163:EMK:C14	36:0:8163:EMK:C24	2.83	0.49
2:9:3096:C:H2'	2:9:3097:U:C6	2.47	0.49
6:D:93:LEU:HD12	6:D:97:GLN:NE2	2.27	0.49
10:H:14:TYR:H	10:H:91:HIS:HE1	1.56	0.49
10:H:148:ARG:O	10:H:151:MET:HB2	2.13	0.49
13:K:125:PHE:CE1	13:K:140:VAL:HG13	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:47:ARG:HG3	16:N:47:ARG:NH1	2.27	0.49
17:O:27:ARG:O	17:O:31:ILE:HG13	2.12	0.49
20:R:42:GLU:HG2	20:R:49:VAL:HG23	1.94	0.49
27:Y:10:ARG:HG3	27:Y:11:THR:N	2.26	0.49
1:O:154:C:H2'	1:O:155:C:C6	2.48	0.49
1:O:1015:C:H2'	1:O:1016:U:H6	1.77	0.49
5:C:45:ASP:OD2	5:C:98:ARG:HD2	2.13	0.49
7:E:23:GLU:HG2	7:E:28:SER:CB	2.41	0.49
1:O:841:A:OP2	19:Q:128:ARG:HD2	2.12	0.49
1:O:1183:C:C4	1:O:1184:C:N4	2.77	0.49
1:O:2032:U:H2'	1:O:2033:G:C5'	2.42	0.49
4:B:268:ARG:HG2	4:B:268:ARG:HH11	1.78	0.49
14:L:38:VAL:C	14:L:63:VAL:HG13	2.32	0.49
26:X:187:VAL:HG22	26:X:192:ASP:CB	2.41	0.49
1:O:159:G:H5''	14:L:74:ARG:NH2	2.28	0.49
1:O:316:A:N3	1:O:336:G:O2'	2.44	0.49
1:O:797:A:O4'	27:Y:10:ARG:N	2.46	0.49
1:O:2389:U:H4'	18:P:53:HIS:CD2	2.48	0.49
1:O:2856:A:OP1	25:W:15:ARG:NH2	2.46	0.49
7:E:1:PRO:HD2	7:E:53:GLU:O	2.13	0.49
10:H:45:GLN:H	10:H:163:PRO:CD	2.26	0.49
10:H:130:HIS:CG	10:H:133:ILE:HD11	2.48	0.49
14:L:164:THR:HG22	14:L:166:ALA:N	2.28	0.49
23:U:13:PRO:O	23:U:17:GLU:HG3	2.12	0.49
24:V:88:THR:CG2	24:V:89:ASP:N	2.75	0.49
28:Z:28:HIS:O	28:Z:32:LYS:N	2.39	0.49
1:O:371:U:H2'	1:O:372:A:H8	1.77	0.49
1:O:1039:G:H2'	1:O:1040:A:O4'	2.13	0.49
1:O:1894:C:N4	1:O:1939:U:H2'	2.28	0.49
1:O:2506:A:O2'	1:O:2507:G:P	2.71	0.49
1:O:2870:C:H2'	1:O:2871:G:C8	2.48	0.49
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.94	0.49
5:C:88:SER:OG	5:C:91:PRO:HB3	2.13	0.49
13:K:67:ARG:HB2	13:K:112:GLY:HA3	1.94	0.49
14:L:31:TRP:O	14:L:34:GLU:HB2	2.12	0.49
20:R:33:SER:OG	20:R:36:GLU:HG3	2.12	0.49
22:T:45:GLU:HB2	22:T:48:ASN:HD22	1.78	0.49
1:O:95:A:H5''	1:O:97:G:O4'	2.13	0.48
1:O:1419:U:H2'	1:O:1685:A:C2	2.48	0.48
1:O:1528:A:H2'	1:O:1529:G:O4'	2.13	0.48
1:O:1791:U:H2'	1:O:1792:C:H6	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2346:C:H6	1:0:2346:C:O5'	1.95	0.48
1:0:2504:A:H4'	10:H:70:ARG:HD3	1.95	0.48
1:0:2820:A:OP1	4:B:98:THR:HG22	2.13	0.48
2:9:3061:C:H2'	2:9:3062:A:H8	1.77	0.48
6:D:54:ALA:HB2	6:D:69:ILE:HG12	1.94	0.48
26:X:178:HIS:CG	26:X:179:PRO:HD2	2.47	0.48
1:0:154:C:H2'	1:0:155:C:H6	1.77	0.48
1:0:466:A:H2'	1:0:467:G:O4'	2.13	0.48
1:0:1838:U:O2'	1:0:2644:C:H5'	2.13	0.48
36:0:8163:EMK:H12	36:0:8163:EMK:H23B	1.94	0.48
5:C:211:ASP:HB2	5:C:231:ARG:HH22	1.78	0.48
6:D:94:ALA:HB3	6:D:174:VAL:HA	1.95	0.48
9:G:23:ILE:O	9:G:27:ILE:HG13	2.13	0.48
17:O:98:ILE:O	17:O:98:ILE:HD13	2.14	0.48
1:0:175:G:H2'	14:L:192:ALA:HB3	1.96	0.48
1:0:1819:G:OP1	1:0:1819:G:H4'	2.13	0.48
1:0:2883:A:H2'	1:0:2884:G:O4'	2.14	0.48
5:C:211:ASP:HB2	5:C:231:ARG:NH2	2.28	0.48
19:Q:39:THR:CG2	19:Q:42:GLU:HG3	2.43	0.48
20:R:2:TRP:CZ2	20:R:31:ARG:HB2	2.48	0.48
24:V:90:TYR:N	24:V:90:TYR:CD1	2.81	0.48
30:2:69:TYR:HB2	30:2:78:HIS:CE1	2.48	0.48
1:0:1515:A:H2'	1:0:1516:C:C6	2.48	0.48
1:0:2266:A:H2'	1:0:2267:G:C8	2.48	0.48
2:9:3008:G:O6	15:M:11:ARG:NH1	2.47	0.48
28:Z:28:HIS:CE1	28:Z:31:LYS:HE2	2.48	0.48
1:0:24:G:N2	1:0:518:G:H1'	2.28	0.48
1:0:280:C:H2'	1:0:281:U:O4'	2.14	0.48
1:0:1762:C:H2'	1:0:1763:C:C6	2.49	0.48
1:0:1926:G:H2'	1:0:1927:A:H8	1.74	0.48
1:0:2768:A:C8	4:B:316:ARG:HB2	2.47	0.48
1:0:2828:G:O2'	1:0:2829:G:H5'	2.13	0.48
21:S:43:ASN:HD22	21:S:43:ASN:N	2.11	0.48
26:X:99:ALA:HB2	26:X:233:TYR:CE2	2.47	0.48
1:0:684:G:H2'	1:0:685:C:C6	2.48	0.48
1:0:869:G:OP2	14:L:79:LYS:HE3	2.13	0.48
1:0:1791:U:H2'	1:0:1792:C:C6	2.48	0.48
1:0:1803:C:H2'	1:0:1804:A:H8	1.78	0.48
3:A:39:ALA:HB3	3:A:61:GLU:OE2	2.13	0.48
6:D:172:VAL:HG12	6:D:173:GLU:N	2.27	0.48
8:F:26:THR:HG22	8:F:102:GLY:HA3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:8:ARG:HG2	17:O:8:ARG:HH11	1.78	0.48
18:P:77:ASP:HB3	18:P:82:LYS:HE3	1.95	0.48
27:Y:31:ILE:HG23	27:Y:32:LYS:N	2.28	0.48
1:O:271:C:C2	1:O:273:G:O4'	2.67	0.48
1:O:757:C:OP1	13:K:27:ARG:HD2	2.13	0.48
1:O:812:A:H2'	1:O:813:C:C6	2.48	0.48
1:O:1333:U:H2'	1:O:1334:C:H6	1.79	0.48
1:O:1398:G:H2'	1:O:1399:A:C8	2.49	0.48
1:O:1451:C:C5'	1:O:1505:U:H3	2.07	0.48
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.95	0.48
8:F:48:VAL:HG23	8:F:74:PHE:HB3	1.92	0.48
11:I:39:VAL:HG11	11:I:107:ASN:CB	2.43	0.48
11:I:54:VAL:O	11:I:58:GLU:HG3	2.12	0.48
14:L:120:VAL:HG11	14:L:130:GLU:HG3	1.95	0.48
21:S:47:THR:HB	21:S:100:ASP:HB3	1.94	0.48
1:O:470:U:O2'	28:Z:16:HIS:CD2	2.64	0.48
1:O:960:G:N3	1:O:960:G:C2'	2.77	0.48
3:A:88:ILE:HD13	3:A:100:PRO:CD	2.39	0.48
9:G:71:LEU:C	9:G:73:ASP:H	2.17	0.48
10:H:29:ALA:HB3	10:H:65:ARG:NH1	2.24	0.48
10:H:132:PHE:O	10:H:133:ILE:HD13	2.14	0.48
15:M:180:LEU:O	15:M:181:ASP:HB3	2.13	0.48
1:O:120:A:H2'	1:O:120:A:N3	2.28	0.48
1:O:1181:A:C2'	1:O:1182:C:H5'	2.44	0.48
1:O:1576:G:H2'	1:O:1577:U:C6	2.49	0.48
1:O:2072:G:C6	1:O:2533:C:H1'	2.49	0.48
1:O:2549:C:H1'	4:B:248:ARG:NH2	2.29	0.48
1:O:2737:C:OP2	17:O:61:ARG:NH2	2.39	0.48
1:O:2780:C:H1'	7:E:143:GLN:NE2	2.27	0.48
2:9:3013:A:H3'	2:9:3014:G:H5'	1.96	0.48
2:9:3057:A:H8	6:D:141:VAL:HG21	1.79	0.48
8:F:20:LEU:HD13	8:F:49:PHE:CE1	2.49	0.48
10:H:71:TYR:C	10:H:73:GLN:N	2.67	0.48
13:K:55:GLN:HA	13:K:58:GLN:NE2	2.29	0.48
14:L:67:ILE:CG2	14:L:97:ILE:HG23	2.44	0.48
20:R:44:GLN:HE21	23:U:28:LEU:HD22	1.78	0.48
1:O:138:U:OP2	1:O:139:C:H5	1.96	0.48
1:O:656:G:OP2	16:N:37:ARG:HD2	2.13	0.48
1:O:1008:C:H5''	10:H:16:ARG:HH12	1.79	0.48
2:9:3013:A:O2'	2:9:3014:G:H5''	2.14	0.48
2:9:3020:G:O2'	2:9:3021:G:H5'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:312:ARG:HD3	4:B:315:VAL:CG1	2.44	0.48
8:F:60:VAL:O	8:F:61:MET:C	2.53	0.48
12:J:99:ASP:OD1	12:J:101:ASN:N	2.45	0.48
14:L:114:VAL:HG21	14:L:159:THR:HG21	1.94	0.48
14:L:139:PRO:C	14:L:141:ILE:N	2.63	0.48
16:N:29:VAL:O	16:N:33:LEU:HG	2.13	0.48
20:R:77:VAL:O	20:R:80:ARG:HG2	2.14	0.48
27:Y:38:LYS:HG3	27:Y:45:LYS:HB3	1.94	0.48
1:0:161:A:H2'	1:0:162:C:C6	2.48	0.47
1:0:758:A:H2'	1:0:759:C:O4'	2.14	0.47
1:0:1205:U:H2'	1:0:1206:U:O4'	2.13	0.47
1:0:1307:A:H2'	1:0:1308:A:C8	2.48	0.47
1:0:2685:C:H2'	1:0:2686:C:C6	2.50	0.47
4:B:53:LEU:CD1	4:B:327:VAL:HG22	2.44	0.47
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.78	0.47
14:L:139:PRO:O	14:L:140:ALA:CB	2.57	0.47
24:V:151:GLU:O	24:V:154:ARG:HB3	2.14	0.47
1:0:338:C:H4'	5:C:174:ILE:CD1	2.44	0.47
1:0:2507:G:H2'	1:0:2510:C:N4	2.28	0.47
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.14	0.47
27:Y:25:ARG:O	27:Y:29:VAL:HG23	2.14	0.47
1:0:2281:C:C2'	1:0:2282:U:H5'	2.44	0.47
1:0:2866:U:H2'	22:T:50:GLU:OE1	2.14	0.47
2:9:3114:G:H2'	2:9:3115:C:C6	2.50	0.47
5:C:78:ARG:HG2	5:C:78:ARG:NH1	2.29	0.47
6:D:51:ARG:HH11	6:D:68:PRO:CG	2.26	0.47
11:I:39:VAL:HG11	11:I:107:ASN:HB2	1.96	0.47
16:N:25:VAL:O	16:N:29:VAL:HG23	2.15	0.47
1:0:88:G:N7	29:1:28:LYS:HD2	2.29	0.47
1:0:523:C:H2'	1:0:524:A:H8	1.79	0.47
1:0:558:C:C2'	1:0:559:U:C5'	2.88	0.47
1:0:1268:C:O2'	26:X:169:ARG:HB2	2.14	0.47
1:0:1501:A:OP2	17:O:37:ARG:HD2	2.14	0.47
1:0:1714:C:O2'	1:0:1715:C:H5'	2.14	0.47
1:0:2415:A:O2'	15:M:29:SER:HB3	2.14	0.47
2:9:3092:G:H2'	2:9:3093:A:H8	1.80	0.47
4:B:145:HIS:HD2	4:B:159:PRO:HB3	1.78	0.47
4:B:304:PRO:HD2	4:B:307:ARG:HD2	1.95	0.47
6:D:39:ASP:O	6:D:43:GLU:HG3	2.14	0.47
24:V:65:VAL:HA	24:V:68:THR:HG22	1.97	0.47
27:Y:47:LEU:HD23	27:Y:57:CYS:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:371:U:H2'	1:0:372:A:C8	2.49	0.47
1:0:475:G:H5'	5:C:74:ASP:OD2	2.14	0.47
1:0:1116:U:O2'	1:0:1118:A:C2	2.51	0.47
1:0:2783:A:H2'	1:0:2784:A:C8	2.50	0.47
1:0:2791:U:H1'	1:0:2792:A:H5''	1.96	0.47
3:A:179:MET:HG2	3:A:186:TRP:CB	2.45	0.47
10:H:68:ALA:HB2	10:H:149:ALA:HB2	1.95	0.47
14:L:99:ARG:HD2	14:L:167:GLY:CA	2.40	0.47
21:S:21:LYS:HA	21:S:24:ARG:HG3	1.96	0.47
1:0:177:A:H2'	1:0:178:U:O4'	2.13	0.47
1:0:522:U:O2'	1:0:1366:C:H5'	2.14	0.47
1:0:1182:C:O2'	1:0:1192:A:H8	1.98	0.47
1:0:1213:C:O2'	1:0:1214:G:H5'	2.15	0.47
1:0:1849:G:H1'	1:0:2011:A:N1	2.30	0.47
1:0:2044:G:OP1	25:W:23:HIS:HE1	1.96	0.47
1:0:2114:C:O2'	1:0:2115:U:H5'	2.14	0.47
4:B:307:ARG:HG3	4:B:307:ARG:NH1	2.29	0.47
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.44	0.47
15:M:49:THR:HG22	15:M:50:LEU:N	2.29	0.47
1:0:222:A:H2'	1:0:223:G:O4'	2.14	0.47
1:0:255:A:H2'	1:0:256:C:C6	2.50	0.47
1:0:602:A:O2'	1:0:605:C:H4'	2.14	0.47
1:0:926:A:H5'	13:K:39:GLU:OE2	2.15	0.47
1:0:1165:G:O3'	1:0:1174:A:H4'	2.14	0.47
1:0:1181:A:N1	1:0:1192:A:O2'	2.48	0.47
1:0:1187:U:H1'	1:0:1189:A:H2	1.79	0.47
1:0:1422:U:H2'	1:0:1423:C:C6	2.50	0.47
1:0:1666:C:C2'	1:0:1667:A:C5'	2.79	0.47
2:9:3014:G:H1'	15:M:1:ALA:HB2	1.96	0.47
3:A:66:ARG:HH11	3:A:66:ARG:HB2	1.80	0.47
3:A:76:VAL:HG23	27:Y:63:LYS:HB3	1.97	0.47
4:B:43:GLY:O	4:B:308:LEU:HD12	2.14	0.47
4:B:97:LEU:O	4:B:98:THR:HG23	2.14	0.47
4:B:201:ASP:OD2	4:B:312:ARG:NH1	2.48	0.47
6:D:25:MET:CE	6:D:41:LEU:HG	2.43	0.47
6:D:140:ARG:HH11	6:D:140:ARG:HG3	1.79	0.47
6:D:162:ALA:O	6:D:166:ILE:HD13	2.14	0.47
7:E:10:ASP:OD1	7:E:10:ASP:O	2.33	0.47
7:E:16:ASP:O	7:E:17:HIS:HB2	2.13	0.47
8:F:57:GLU:O	8:F:61:MET:HG3	2.15	0.47
10:H:136:VAL:CG2	10:H:137:ASN:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:48:ARG:NH1	14:L:52:LEU:HD21	2.29	0.47
17:O:89:ASN:HB3	17:O:92:GLU:HB2	1.97	0.47
19:Q:113:HIS:HE1	19:Q:144:GLU:CD	2.18	0.47
21:S:98:VAL:HG11	21:S:101:LEU:CD2	2.45	0.47
22:T:33:SER:O	22:T:37:GLU:HG3	2.15	0.47
24:V:11:VAL:O	24:V:12:ASN:HB2	2.14	0.47
25:W:54:ILE:HD12	25:W:85:VAL:HG23	1.95	0.47
29:1:48:ASP:O	29:1:49:GLU:CB	2.62	0.47
1:O:451:C:O2'	1:O:452:G:H5'	2.14	0.47
1:O:778:C:C2	1:O:881:C:H5'	2.48	0.47
1:O:2524:G:H21	1:O:2526:C:H5	1.60	0.47
1:O:2657:G:OP1	4:B:17:LYS:HB2	2.14	0.47
5:C:194:PHE:CD2	5:C:234:VAL:HG11	2.49	0.47
16:N:98:LEU:O	16:N:102:ILE:HG13	2.15	0.47
1:O:1760:G:H5'	1:O:1818:C:O2'	2.14	0.47
4:B:5:ARG:HD2	4:B:8:LYS:NZ	2.29	0.47
5:C:61:PHE:CD1	5:C:65:ARG:HD2	2.50	0.47
6:D:19:GLU:O	6:D:133:ASN:HB3	2.15	0.47
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.44	0.47
11:I:19:MET:HE3	11:I:132:LEU:CG	2.44	0.47
12:J:74:VAL:HG12	12:J:75:ARG:HG3	1.97	0.47
13:K:41:HIS:CD2	13:K:41:HIS:H	2.31	0.47
21:S:42:VAL:C	21:S:43:ASN:HD22	2.18	0.47
22:T:31:PHE:CG	22:T:37:GLU:HG2	2.49	0.47
24:V:52:VAL:CG2	24:V:53:ALA:H	2.27	0.47
1:O:79:G:H22	1:O:97:G:H1'	1.80	0.47
1:O:105:G:O2'	1:O:106:A:H5'	2.14	0.47
1:O:474:C:O2'	5:C:73:LEU:HD21	2.15	0.47
1:O:474:C:O3'	5:C:73:LEU:HD21	2.15	0.47
1:O:949:U:C4'	18:P:95:GLU:HA	2.38	0.47
1:O:1512:G:O2'	1:O:1513:C:H5'	2.15	0.47
1:O:2133:U:H4'	1:O:2134:G:H5'	1.95	0.47
1:O:2488:A:O2'	1:O:2489:G:H5'	2.15	0.47
2:9:3092:G:H22	10:H:52:LYS:NZ	2.12	0.47
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.96	0.47
7:E:8:PRO:HB2	7:E:11:VAL:CG2	2.45	0.47
11:I:74:ARG:NH2	11:I:76:ASP:OD2	2.47	0.47
19:Q:113:HIS:HE1	19:Q:144:GLU:OE1	1.97	0.47
23:U:43:PRO:O	23:U:46:ILE:HG22	2.14	0.47
26:X:184:GLU:OE2	26:X:204:ARG:HD2	2.15	0.47
1:O:20:G:O3'	19:Q:3:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:431:G:OP1	14:L:48:ARG:NH1	2.48	0.46
1:0:1565:C:H2'	1:0:1566:C:H6	1.80	0.46
36:0:8163:EMK:C23	36:0:8163:EMK:H12	2.45	0.46
6:D:167:GLU:C	6:D:169:THR:H	2.18	0.46
9:G:67:LEU:O	9:G:71:LEU:HG	2.15	0.46
10:H:84:ARG:NH2	10:H:135:TRP:HH2	2.14	0.46
12:J:62:PRO:HG3	12:J:65:ARG:NH2	2.30	0.46
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.46	0.46
4:B:14:GLY:CA	4:B:15:PRO:C	2.84	0.46
8:F:1:PRO:H3	8:F:4:VAL:HG23	1.80	0.46
14:L:19:GLN:O	14:L:22:GLU:HB3	2.15	0.46
14:L:52:LEU:HD13	14:L:116:ASN:HB3	1.97	0.46
1:0:503:G:H2'	1:0:504:G:H8	1.80	0.46
1:0:703:G:O2'	1:0:704:C:H5'	2.15	0.46
1:0:2104:C:O2	1:0:2485:A:N1	2.48	0.46
1:0:2721:U:C4'	12:J:87:ARG:HG3	2.45	0.46
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.15	0.46
2:9:3050:G:H5''	15:M:159:TYR:CE1	2.50	0.46
4:B:162:MET:HE1	4:B:308:LEU:HD21	1.97	0.46
13:K:128:GLY:O	13:K:132:LYS:HG3	2.16	0.46
19:Q:104:PHE:HB3	19:Q:109:MET:CE	2.45	0.46
27:Y:57:CYS:SG	27:Y:60:CYS:SG	3.02	0.46
1:0:162:C:H2'	1:0:163:U:H5'	1.98	0.46
1:0:612:U:H2'	1:0:613:C:C6	2.51	0.46
1:0:622:G:P	26:X:148:GLY:HA3	2.55	0.46
1:0:1321:A:H2'	1:0:1322:G:C8	2.51	0.46
1:0:2750:G:H2'	1:0:2751:C:C6	2.50	0.46
36:0:8163:EMK:H30	36:0:8163:EMK:H5	1.96	0.46
3:A:192:VAL:HA	3:A:201:PHE:O	2.14	0.46
4:B:268:ARG:NH2	4:B:325:PRO:HG3	2.30	0.46
6:D:35:ALA:C	6:D:37:ALA:N	2.68	0.46
6:D:57:THR:CG2	6:D:63:ILE:HA	2.46	0.46
13:K:124:ASP:OD1	13:K:149:ARG:NH2	2.48	0.46
16:N:21:SER:OG	16:N:106:PRO:HB2	2.15	0.46
26:X:130:ARG:HB2	26:X:142:SER:O	2.16	0.46
1:0:26:U:H2'	1:0:27:U:C6	2.51	0.46
1:0:70:A:H4'	1:0:71:G:O5'	2.16	0.46
1:0:473:A:OP1	28:Z:51:GLN:NE2	2.49	0.46
1:0:1335:C:H2'	1:0:1336:U:C6	2.50	0.46
5:C:136:VAL:HA	5:C:137:PRO:C	2.35	0.46
8:F:40:ILE:HD11	8:F:48:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:15:THR:HG22	10:H:91:HIS:HA	1.97	0.46
10:H:131:ILE:HG23	10:H:132:PHE:HD1	1.79	0.46
11:I:19:MET:HE3	11:I:132:LEU:HD11	1.95	0.46
20:R:51:GLN:HB3	20:R:67:ARG:NH1	2.30	0.46
21:S:26:THR:HG23	21:S:97:ARG:HG3	1.97	0.46
1:0:138:U:H5'	1:0:139:C:OP2	2.15	0.46
1:0:561:G:O2'	1:0:562:A:H5'	2.15	0.46
1:0:601:G:O2'	1:0:602:A:H5'	2.15	0.46
1:0:848:C:H2'	1:0:849:C:C6	2.50	0.46
1:0:1119:G:N2	1:0:1246:A:N1	2.63	0.46
1:0:2379:G:N7	1:0:2408:A:N1	2.64	0.46
1:0:2472:C:O2'	1:0:2634:G:H4'	2.16	0.46
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.78	0.46
10:H:49:VAL:C	10:H:157:ILE:HG23	2.35	0.46
15:M:67:ALA:HA	15:M:71:TRP:HB3	1.97	0.46
19:Q:4:TYR:CE1	19:Q:15:LYS:HD3	2.51	0.46
1:0:492:C:O2'	1:0:493:U:H5'	2.16	0.46
1:0:1029:U:O2'	1:0:1273:C:OP1	2.30	0.46
1:0:1198:U:H1'	1:0:1201:C:C5	2.51	0.46
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.79	0.46
1:0:1942:A:O2'	1:0:1943:C:H5'	2.15	0.46
1:0:2032:U:H2'	1:0:2033:G:H5'	1.97	0.46
1:0:2670:G:O2'	1:0:2671:U:H5'	2.16	0.46
5:C:162:VAL:HG13	5:C:232:LEU:HD21	1.98	0.46
6:D:159:PRO:O	6:D:163:VAL:HG23	2.15	0.46
7:E:7:ILE:HD11	7:E:11:VAL:O	2.15	0.46
19:Q:106:GLY:HA2	19:Q:109:MET:CE	2.44	0.46
25:W:72:VAL:CG2	25:W:85:VAL:HB	2.45	0.46
1:0:380:A:OP2	14:L:9:ARG:HD2	2.16	0.46
1:0:638:C:H2'	1:0:639:A:H8	1.81	0.46
1:0:702:G:O2'	1:0:703:G:H5'	2.15	0.46
1:0:1160:G:HO2'	1:0:1190:G:H8	1.63	0.46
1:0:1845:A:OP2	3:A:190:ARG:NH1	2.49	0.46
1:0:2389:U:H4'	18:P:53:HIS:HD2	1.81	0.46
1:0:2510:C:H42	1:0:2564:G:H22	1.63	0.46
1:0:2672:C:O2'	1:0:2673:U:H5'	2.16	0.46
4:B:62:ARG:HA	4:B:65:MET:HE1	1.98	0.46
5:C:142:ASP:OD1	5:C:237:GLU:HB3	2.15	0.46
8:F:79:GLN:HB2	8:F:82:ASP:OD2	2.16	0.46
10:H:75:SER:C	10:H:79:ALA:HB2	2.37	0.46
10:H:166:ASN:N	10:H:166:ASN:ND2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:15:ARG:CZ	11:I:43:ARG:NH1	2.79	0.46
14:L:37:VAL:HG13	14:L:63:VAL:CG1	2.43	0.46
19:Q:39:THR:HB	19:Q:42:GLU:CG	2.46	0.46
21:S:28:SER:O	21:S:32:ARG:HG3	2.16	0.46
1:O:17:G:O2'	1:O:18:C:H5'	2.16	0.46
1:O:372:A:H2'	1:O:373:G:H8	1.81	0.46
1:O:1304:U:H2'	1:O:1305:C:C6	2.51	0.46
1:O:1353:C:N3	13:K:5:LYS:NZ	2.63	0.46
1:O:1527:A:H1'	1:O:1528:A:C8	2.51	0.46
1:O:2121:G:O2'	1:O:2122:C:H5'	2.16	0.46
1:O:2429:A:H2'	1:O:2430:A:C8	2.51	0.46
1:O:2704:C:O2	7:E:110:GLU:HB3	2.16	0.46
3:A:64:ASP:OD2	3:A:64:ASP:N	2.49	0.46
3:A:190:ARG:HH11	3:A:190:ARG:HG3	1.81	0.46
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.98	0.46
14:L:114:VAL:CG2	14:L:159:THR:HG21	2.46	0.46
14:L:155:HIS:CE1	14:L:158:ARG:HH21	2.34	0.46
15:M:69:TYR:CD1	15:M:69:TYR:N	2.83	0.46
1:O:862:U:O2'	1:O:863:G:H5'	2.16	0.46
1:O:932:U:H2'	1:O:933:C:C6	2.51	0.46
5:C:145:GLU:OE1	5:C:198:ASP:HB2	2.15	0.46
6:D:166:ILE:HD12	6:D:166:ILE:N	2.30	0.46
18:P:21:ARG:HG2	18:P:22:GLY:N	2.31	0.46
28:Z:25:LYS:O	28:Z:25:LYS:HG2	2.16	0.46
1:O:263:U:C2	8:F:59:ILE:CD1	2.99	0.45
1:O:286:U:H2'	1:O:287:C:C6	2.52	0.45
1:O:1636:G:O2'	1:O:1637:A:H5'	2.16	0.45
1:O:2011:A:H4'	1:O:2012:U:O5'	2.16	0.45
5:C:193:LEU:HD12	5:C:211:ASP:O	2.15	0.45
10:H:53:PRO:O	10:H:54:VAL:HG13	2.16	0.45
10:H:55:GLN:HE21	10:H:124:ARG:HG2	1.81	0.45
14:L:102:GLU:CD	14:L:164:THR:HG21	2.34	0.45
15:M:69:TYR:HE2	15:M:183:ASP:OD2	1.99	0.45
15:M:78:MET:HB2	15:M:79:PRO:HD3	1.98	0.45
20:R:10:VAL:HG11	23:U:36:ALA:HA	1.98	0.45
27:Y:20:LEU:O	27:Y:24:VAL:HG23	2.16	0.45
1:O:279:C:H42	1:O:370:G:H1	1.64	0.45
1:O:1008:C:H2'	1:O:1009:U:C6	2.51	0.45
1:O:1182:C:H4'	1:O:1192:A:N7	2.31	0.45
1:O:1318:A:H4'	1:O:1343:C:H4'	1.99	0.45
1:O:2681:A:H4'	1:O:2682:C:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:195:ARG:HD2	4:B:324:ASP:OD1	2.16	0.45
6:D:48:MET:HA	6:D:49:PRO:HD3	1.81	0.45
6:D:93:LEU:HD12	6:D:97:GLN:HE22	1.80	0.45
11:I:19:MET:CE	11:I:132:LEU:HD21	2.46	0.45
11:I:88:PRO:HG2	11:I:94:GLY:HA3	1.98	0.45
13:K:38:HIS:CD2	13:K:39:GLU:HG3	2.51	0.45
19:Q:95:ALA:HB2	19:Q:145:LEU:HD23	1.98	0.45
23:U:39:ALA:N	23:U:40:PRO:HD2	2.30	0.45
27:Y:31:ILE:CG2	27:Y:32:LYS:N	2.79	0.45
29:1:40:ARG:HG3	29:1:45:ASN:CB	2.46	0.45
1:0:249:G:O2'	1:0:250:C:H5'	2.16	0.45
1:0:631:A:C6	1:0:2074:A:H5'	2.52	0.45
1:0:1002:G:C2'	1:0:1003:U:H5''	2.40	0.45
1:0:1131:G:C6	1:0:1230:A:C4	3.04	0.45
1:0:1220:U:H2'	1:0:1221:G:H8	1.81	0.45
1:0:1463:A:H8	1:0:1463:A:O5'	1.98	0.45
1:0:2003:U:H4'	1:0:2004:U:C5	2.37	0.45
1:0:2112:A:H2'	1:0:2113:G:H8	1.80	0.45
1:0:2329:C:O2'	1:0:2330:U:H5'	2.15	0.45
3:A:36:ASP:HA	3:A:83:GLY:HA3	1.97	0.45
6:D:62:ASP:C	6:D:64:ARG:N	2.69	0.45
6:D:88:LEU:N	6:D:89:PRO:CD	2.80	0.45
6:D:92:GLU:O	6:D:93:LEU:O	2.35	0.45
9:G:24:VAL:O	9:G:28:GLU:HG3	2.16	0.45
12:J:81:ARG:HD3	12:J:87:ARG:CZ	2.47	0.45
25:W:34:ARG:NH1	25:W:48:VAL:O	2.48	0.45
1:0:883:U:H2'	1:0:883:U:O2	2.17	0.45
1:0:1471:A:H2'	1:0:1472:C:C6	2.51	0.45
1:0:1596:U:H2'	1:0:1598:A:OP2	2.17	0.45
1:0:2274:A:O2'	1:0:2275:G:H5'	2.16	0.45
1:0:2690:U:O2'	7:E:111:LYS:HD2	2.16	0.45
4:B:162:MET:HE2	4:B:310:ARG:CD	2.33	0.45
15:M:7:LYS:HE2	15:M:8:VAL:O	2.16	0.45
17:O:18:LYS:O	17:O:21:VAL:HG13	2.15	0.45
17:O:37:ARG:HG2	17:O:37:ARG:HH11	1.82	0.45
21:S:24:ARG:NH2	21:S:39:ASN:HD22	2.15	0.45
1:0:295:C:O2'	1:0:296:G:H5'	2.17	0.45
1:0:329:A:OP2	5:C:206:ASN:HB2	2.16	0.45
1:0:368:C:H2'	1:0:369:G:O4'	2.16	0.45
1:0:876:A:N3	1:0:876:A:C2'	2.80	0.45
1:0:1225:C:H2'	1:0:1226:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:34:VAL:HG22	12:J:47:ALA:HB2	1.97	0.45
20:R:37:VAL:O	20:R:41:VAL:HG23	2.16	0.45
23:U:13:PRO:HA	23:U:16:ARG:NH1	2.31	0.45
25:W:25:ARG:HD3	25:W:64:ALA:O	2.17	0.45
28:Z:21:ARG:HD2	28:Z:37:CYS:SG	2.56	0.45
1:0:1006:A:N1	1:0:2311:A:H1'	2.31	0.45
1:0:1041:U:H4'	1:0:1295:G:H5'	1.98	0.45
1:0:1249:U:H2'	1:0:1250:C:C6	2.51	0.45
1:0:1794:G:N2	1:0:1796:A:H3'	2.32	0.45
1:0:1943:C:H4'	3:A:211:LYS:O	2.17	0.45
1:0:2839:C:H2'	1:0:2840:A:H5''	1.98	0.45
4:B:157:LYS:O	4:B:159:PRO:HD3	2.17	0.45
7:E:108:LEU:HD13	7:E:164:ASP:HB2	1.98	0.45
10:H:31:PHE:HD2	10:H:85:ILE:O	2.00	0.45
10:H:45:GLN:NE2	10:H:135:TRP:HE1	2.15	0.45
10:H:75:SER:O	10:H:79:ALA:HB2	2.17	0.45
10:H:84:ARG:CZ	10:H:135:TRP:CH2	2.99	0.45
12:J:90:PHE:N	12:J:90:PHE:CD1	2.85	0.45
14:L:47:ASP:CG	14:L:48:ARG:N	2.69	0.45
14:L:138:HIS:C	14:L:139:PRO:O	2.55	0.45
19:Q:104:PHE:CB	19:Q:109:MET:HE1	2.47	0.45
22:T:6:CYS:HB2	22:T:32:CYS:HB3	1.99	0.45
22:T:9:CYS:CB	22:T:52:THR:HG22	2.47	0.45
24:V:90:TYR:CE2	24:V:99:ALA:HB2	2.52	0.45
1:0:835:U:P	4:B:229:ARG:HH12	2.39	0.45
1:0:999:C:H2'	1:0:1000:C:O4'	2.16	0.45
1:0:2125:G:H2'	1:0:2126:C:C6	2.51	0.45
1:0:2362:A:H2'	1:0:2363:G:C8	2.52	0.45
1:0:2517:A:O2'	1:0:2518:C:H5'	2.16	0.45
8:F:58:GLU:HA	8:F:61:MET:CE	2.44	0.45
13:K:66:VAL:HG23	13:K:67:ARG:N	2.31	0.45
14:L:83:SER:HA	14:L:86:MET:HE2	1.98	0.45
15:M:182:GLY:O	15:M:183:ASP:O	2.35	0.45
1:0:544:G:C3'	1:0:545:G:H5''	2.46	0.45
1:0:836:G:OP1	4:B:230:GLN:CD	2.55	0.45
1:0:1142:C:O2'	1:0:1143:G:H5'	2.17	0.45
1:0:1155:G:H2'	1:0:1156:C:C6	2.52	0.45
1:0:1829:A:H61	27:Y:18:TYR:H	1.63	0.45
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.82	0.45
4:B:102:THR:HG23	4:B:182:VAL:HG12	1.98	0.45
6:D:63:ILE:HD12	6:D:63:ILE:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:46:GLU:O	8:F:73:PRO:HD2	2.16	0.45
12:J:55:VAL:CG1	12:J:56:SER:N	2.79	0.45
12:J:65:ARG:O	12:J:66:ARG:HB2	2.17	0.45
13:K:145:LEU:O	13:K:145:LEU:HD23	2.17	0.45
14:L:12:TRP:HH2	14:L:24:MET:HE1	1.81	0.45
1:0:1160:G:H5'	1:0:1161:A:C4'	2.46	0.45
1:0:1328:A:OP1	26:X:169:ARG:HD2	2.17	0.45
1:0:1415:G:H5'	28:Z:12:ASN:O	2.17	0.45
1:0:1930:A:H2'	1:0:1931:A:C8	2.52	0.45
1:0:2831:C:O3'	19:Q:71:LYS:HE2	2.16	0.45
4:B:145:HIS:CD2	4:B:146:THR:O	2.69	0.45
4:B:294:TYR:CD1	4:B:294:TYR:C	2.90	0.45
11:I:107:ASN:ND2	11:I:107:ASN:C	2.66	0.45
15:M:151:ASP:OD1	15:M:166:ALA:HA	2.16	0.45
21:S:19:ARG:HD3	21:S:67:LEU:O	2.17	0.45
26:X:126:PRO:HD2	26:X:128:PHE:CE1	2.52	0.45
1:0:226:A:H1'	1:0:393:G:C5	2.52	0.45
1:0:293:A:O2'	1:0:294:C:H5'	2.17	0.45
1:0:407:A:H2'	1:0:408:A:C8	2.52	0.45
1:0:667:C:H2'	1:0:668:C:C6	2.52	0.45
1:0:1334:C:O2'	1:0:1335:C:H5'	2.16	0.45
1:0:1927:A:O2'	1:0:1928:C:H5'	2.17	0.45
1:0:1945:G:O2'	1:0:1946:C:H5'	2.17	0.45
1:0:2281:C:H2'	1:0:2282:U:H5'	2.00	0.45
1:0:2388:C:H5'	18:P:83:THR:O	2.16	0.45
1:0:2909:G:H2'	1:0:2910:A:H8	1.82	0.45
2:9:3014:G:C2'	2:9:3015:C:H5'	2.47	0.45
2:9:3014:G:H2'	2:9:3015:C:H5'	1.99	0.45
5:C:19:PRO:HG2	5:C:22:PHE:CE1	2.51	0.45
5:C:115:LEU:O	5:C:118:THR:HB	2.15	0.45
6:D:51:ARG:HD3	6:D:68:PRO:HB3	1.99	0.45
11:I:142:ASN:O	11:I:144:THR:N	2.50	0.45
14:L:107:ARG:NH1	14:L:107:ARG:CG	2.73	0.45
17:O:55:LYS:CG	17:O:56:GLY:N	2.80	0.45
18:P:50:GLY:HA3	18:P:87:THR:OG1	2.17	0.45
20:R:38:ALA:O	20:R:42:GLU:HG3	2.17	0.45
21:S:112:LEU:CD2	21:S:119:ALA:HB3	2.46	0.45
1:0:79:G:N2	1:0:97:G:H1'	2.32	0.44
1:0:793:A:H5''	17:O:83:LYS:HG2	2.00	0.44
1:0:830:G:O2'	1:0:831:U:H5'	2.17	0.44
1:0:895:A:H2'	1:0:896:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1210:G:O2'	1:0:1211:G:H5'	2.17	0.44
1:0:1400:C:O2'	1:0:1401:G:H5'	2.17	0.44
1:0:1419:U:H5'	1:0:1420:C:OP2	2.17	0.44
1:0:1486:A:C5	29:1:2:LYS:HG3	2.51	0.44
1:0:2754:G:H2'	1:0:2755:G:O4'	2.17	0.44
1:0:2781:U:C2'	1:0:2782:G:H5'	2.47	0.44
2:9:3107:C:O2'	2:9:3108:C:H5'	2.18	0.44
4:B:138:GLY:O	4:B:139:ASP:O	2.35	0.44
6:D:103:ASN:HD21	6:D:133:ASN:HD22	1.64	0.44
7:E:68:HIS:O	7:E:72:MET:HG3	2.16	0.44
14:L:167:GLY:O	14:L:171:ARG:HG3	2.17	0.44
16:N:32:ARG:HH21	16:N:35:LYS:HZ2	1.63	0.44
23:U:64:GLY:O	23:U:65:ASP:CB	2.65	0.44
27:Y:32:LYS:HA	27:Y:35:LYS:HE3	1.99	0.44
1:0:258:G:O2'	1:0:259:G:H5'	2.18	0.44
1:0:843:A:C2	1:0:846:A:C8	3.05	0.44
1:0:907:A:H2'	1:0:908:A:C8	2.51	0.44
1:0:1060:C:H6	1:0:1060:C:H5'	1.82	0.44
1:0:1163:G:N1	1:0:1184:C:C4	2.86	0.44
1:0:1761:U:H2'	1:0:1762:C:C6	2.52	0.44
1:0:1847:A:OP1	3:A:175:LYS:HG3	2.17	0.44
1:0:2123:A:H5'	14:L:89:ASN:HD21	1.83	0.44
1:0:2735:U:H2'	1:0:2736:U:C6	2.52	0.44
5:C:118:THR:HG22	5:C:137:PRO:HB3	1.99	0.44
7:E:5:LEU:HD21	7:E:66:GLN:CG	2.45	0.44
10:H:45:GLN:NE2	10:H:135:TRP:NE1	2.65	0.44
10:H:55:GLN:HE21	10:H:124:ARG:CG	2.31	0.44
14:L:138:HIS:HD1	14:L:139:PRO:N	2.16	0.44
19:Q:96:VAL:HG13	19:Q:106:GLY:HA3	1.99	0.44
22:T:4:ARG:HG2	22:T:5:GLU:N	2.33	0.44
24:V:31:HIS:HB3	24:V:115:THR:HG21	1.98	0.44
1:0:750:A:O3'	5:C:101:ASP:HB2	2.17	0.44
1:0:1181:A:H2'	1:0:1182:C:H5'	1.99	0.44
1:0:1211:G:O2'	1:0:1212:C:H5'	2.18	0.44
1:0:1426:C:C5	1:0:1435:U:H5''	2.52	0.44
1:0:1942:A:H5''	3:A:233:THR:OG1	2.18	0.44
1:0:2269:C:C2'	1:0:2270:G:H5'	2.47	0.44
3:A:125:ASN:CB	3:A:158:VAL:HG12	2.47	0.44
3:A:128:LEU:HD12	3:A:129:LEU:H	1.82	0.44
7:E:66:GLN:O	7:E:70:GLU:HG3	2.17	0.44
10:H:84:ARG:NH2	10:H:135:TRP:CH2	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:74:ARG:HD3	14:L:91:ILE:HD12	1.98	0.44
1:0:958:G:O2'	1:0:959:C:H5'	2.17	0.44
1:0:1268:C:O2'	1:0:1269:G:H5'	2.17	0.44
1:0:1386:G:O2'	1:0:1387:G:H5'	2.17	0.44
1:0:2032:U:C2'	1:0:2033:G:H5''	2.47	0.44
3:A:128:LEU:HD12	3:A:129:LEU:N	2.32	0.44
5:C:127:ARG:HG2	5:C:127:ARG:HH11	1.82	0.44
8:F:36:THR:O	8:F:39:SER:HB3	2.17	0.44
8:F:81:ASP:HA	8:F:92:GLY:HA2	2.00	0.44
1:0:259:G:O2'	1:0:260:C:H5'	2.17	0.44
1:0:1015:C:H2'	1:0:1016:U:C6	2.52	0.44
1:0:1481:G:H2'	1:0:1482:A:O4'	2.18	0.44
1:0:1869:A:H2'	1:0:1870:C:O4'	2.18	0.44
2:9:3069:U:OP1	15:M:4:PRO:HG3	2.17	0.44
3:A:192:VAL:HG23	3:A:201:PHE:HB3	1.99	0.44
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.36	0.44
12:J:28:GLU:HG2	12:J:58:THR:HB	2.00	0.44
1:0:309:C:OP1	21:S:97:ARG:NH2	2.50	0.44
1:0:1181:A:O2'	1:0:1182:C:H5'	2.17	0.44
1:0:1384:C:H5'	25:W:30:MET:HG2	2.00	0.44
1:0:2592:G:H2'	1:0:2593:C:H6	1.82	0.44
1:0:2697:A:H2'	1:0:2698:G:O4'	2.17	0.44
1:0:2821:C:H2'	1:0:2822:C:H6	1.82	0.44
1:0:2898:G:O3'	4:B:288:GLY:HA2	2.17	0.44
2:9:3036:C:N4	2:9:3048:C:H1'	2.33	0.44
2:9:3052:A:O2'	2:9:3053:G:H5'	2.17	0.44
7:E:158:ASP:O	7:E:162:PHE:HD1	2.01	0.44
14:L:57:LYS:HB3	14:L:60:ILE:HD12	1.99	0.44
17:O:27:ARG:HH21	17:O:30:ASP:CG	2.21	0.44
24:V:88:THR:HG22	24:V:89:ASP:H	1.83	0.44
1:0:326:G:O2'	1:0:327:A:H5'	2.17	0.44
1:0:1482:A:O2'	1:0:1483:C:H5'	2.18	0.44
2:9:3049:G:C2'	2:9:3050:G:H5'	2.48	0.44
4:B:101:TRP:HB2	4:B:119:HIS:CD2	2.53	0.44
5:C:55:ARG:NH2	28:Z:56:GLU:OE2	2.45	0.44
5:C:88:SER:O	5:C:91:PRO:HD3	2.18	0.44
13:K:144:ASP:HA	13:K:147:GLU:HG3	1.98	0.44
14:L:37:VAL:HG22	14:L:65:VAL:HG22	2.00	0.44
19:Q:34:GLU:HG2	19:Q:46:TYR:OH	2.17	0.44
1:0:445:U:O2'	1:0:446:G:H5'	2.17	0.44
1:0:1741:U:O2'	1:0:2723:G:H4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2015:A:H2'	1:0:2016:U:O4'	2.18	0.44
1:0:2276:U:H2'	1:0:2277:U:C6	2.53	0.44
1:0:2462:G:N7	30:2:60:LYS:NZ	2.66	0.44
2:9:3065:A:H61	2:9:3112:U:H2'	1.81	0.44
16:N:14:LEU:CD2	16:N:102:ILE:HD11	2.48	0.44
24:V:139:GLY:O	24:V:141:HIS:CD2	2.69	0.44
26:X:99:ALA:HB2	26:X:233:TYR:CZ	2.53	0.44
28:Z:25:LYS:CD	29:1:49:GLU:H	2.17	0.44
1:0:23:G:H1'	1:0:520:A:N6	2.33	0.44
1:0:161:A:H2'	1:0:162:C:H6	1.82	0.44
1:0:420:U:H2'	1:0:421:C:C6	2.52	0.44
1:0:920:C:OP1	13:K:37:LYS:NZ	2.51	0.44
1:0:1166:A:H1'	1:0:1192:A:H2	1.81	0.44
1:0:2568:A:H2'	1:0:2569:A:O4'	2.18	0.44
1:0:2712:G:O2'	1:0:2713:G:H5'	2.18	0.44
1:0:2906:A:H5'	1:0:2907:C:O4'	2.17	0.44
4:B:79:MET:O	4:B:187:GLU:HA	2.17	0.44
6:D:166:ILE:O	6:D:169:THR:N	2.51	0.44
8:F:20:LEU:HD12	8:F:98:VAL:HG22	2.00	0.44
1:0:396:U:O2'	1:0:397:A:P	2.76	0.43
1:0:1204:C:H2'	1:0:1205:U:C4'	2.48	0.43
1:0:1946:C:H2'	1:0:1971:G:C8	2.53	0.43
1:0:2300:A:H4'	1:0:2301:A:O5'	2.18	0.43
1:0:2432:C:O2'	1:0:2433:A:H5'	2.18	0.43
1:0:2504:A:H2'	1:0:2505:G:O4'	2.18	0.43
36:0:8163:EMK:C13	36:0:8163:EMK:H15	2.48	0.43
2:9:3002:U:P	2:9:3003:A:H5'	2.58	0.43
5:C:77:ALA:O	5:C:78:ARG:HG2	2.18	0.43
5:C:140:VAL:CG1	5:C:141:SER:N	2.81	0.43
10:H:55:GLN:HE22	10:H:91:HIS:CD2	2.36	0.43
10:H:85:ILE:O	10:H:85:ILE:HG23	2.18	0.43
11:I:80:LYS:HE2	11:I:98:PHE:CE1	2.52	0.43
14:L:37:VAL:CG1	14:L:108:LYS:HG3	2.46	0.43
17:O:8:ARG:HG2	17:O:8:ARG:NH1	2.31	0.43
25:W:78:GLU:CG	25:W:79:GLU:N	2.81	0.43
1:0:241:A:C2	1:0:378:A:H4'	2.53	0.43
1:0:731:U:O2'	1:0:732:C:H5'	2.18	0.43
1:0:2314:G:C2'	1:0:2315:C:H5'	2.48	0.43
2:9:3041:C:H5''	6:D:48:MET:CE	2.48	0.43
3:A:88:ILE:O	3:A:88:ILE:HG22	2.18	0.43
3:A:94:LEU:HD23	3:A:94:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:41:LYS:O	12:J:42:ASN:HB2	2.18	0.43
14:L:114:VAL:HB	14:L:159:THR:HG23	1.98	0.43
16:N:77:ALA:HA	16:N:96:VAL:O	2.18	0.43
25:W:28:LYS:HA	25:W:28:LYS:HE3	2.00	0.43
30:2:3:MET:HG3	30:2:4:PRO:HD2	2.00	0.43
1:0:287:C:H2'	1:0:288:A:C8	2.53	0.43
1:0:327:A:H2'	5:C:150:THR:OG1	2.18	0.43
1:0:527:U:H2'	1:0:528:G:H8	1.83	0.43
1:0:1158:G:O2'	1:0:1159:G:H5'	2.18	0.43
1:0:2105:C:H2'	1:0:2106:C:C6	2.53	0.43
1:0:2646:G:C8	36:0:8163:EMK:H17A	2.54	0.43
1:0:2781:U:O2'	1:0:2782:G:H5'	2.18	0.43
4:B:41:PHE:CE1	4:B:79:MET:HG3	2.53	0.43
4:B:108:GLU:HB3	4:B:111:ARG:HD2	1.99	0.43
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.19	0.43
5:C:233:THR:HG22	5:C:234:VAL:H	1.83	0.43
6:D:27:ILE:H	6:D:27:ILE:CD1	2.31	0.43
7:E:102:VAL:HG22	7:E:116:THR:HG23	1.99	0.43
11:I:52:GLN:HG3	11:I:53:ILE:N	2.34	0.43
23:U:20:LEU:HD11	23:U:53:ILE:HG23	2.00	0.43
24:V:88:THR:HG22	24:V:90:TYR:CD1	2.34	0.43
1:0:196:G:H1'	1:0:198:A:N7	2.34	0.43
1:0:327:A:H4'	1:0:329:A:C8	2.54	0.43
1:0:506:G:H22	1:0:509:A:H5''	1.83	0.43
1:0:677:C:O2'	1:0:678:G:H5'	2.18	0.43
1:0:690:G:H4'	1:0:741:C:O2	2.18	0.43
1:0:1739:G:O2'	1:0:1740:U:H5'	2.18	0.43
1:0:2793:A:H2'	1:0:2794:G:H5'	2.00	0.43
2:9:3044:A:O4'	6:D:76:ARG:NE	2.52	0.43
3:A:164:ARG:HB2	27:Y:68:CYS:SG	2.58	0.43
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.49	0.43
10:H:48:LEU:CG	10:H:157:ILE:HG21	2.44	0.43
14:L:23:LEU:O	14:L:26:HIS:HB2	2.18	0.43
24:V:48:VAL:HG12	24:V:52:VAL:CG1	2.48	0.43
29:1:25:VAL:O	29:1:29:THR:HG23	2.17	0.43
1:0:90:A:H2'	1:0:91:G:O4'	2.18	0.43
1:0:661:G:C5	1:0:686:A:C2	3.06	0.43
1:0:1167:G:H2'	1:0:1168:C:C6	2.54	0.43
1:0:1204:C:H2'	1:0:1205:U:H5''	2.00	0.43
1:0:1295:G:H5''	13:K:14:GLY:O	2.19	0.43
1:0:1524:U:OP1	1:0:1524:U:H4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1525:G:H5'	1:0:1526:A:OP2	2.19	0.43
1:0:1538:C:O2'	1:0:1539:U:H5'	2.18	0.43
1:0:1840:A:H4'	1:0:1841:C:O5'	2.18	0.43
1:0:2091:G:O3'	4:B:235:ARG:HD3	2.17	0.43
1:0:2256:G:C2'	1:0:2257:G:H5'	2.48	0.43
1:0:2266:A:OP2	14:L:90:ARG:NH2	2.51	0.43
5:C:57:PRO:HG2	5:C:73:LEU:CD1	2.48	0.43
5:C:193:LEU:HA	5:C:211:ASP:O	2.18	0.43
5:C:218:VAL:O	5:C:246:ARG:NH2	2.52	0.43
8:F:102:GLY:C	8:F:104:ALA:N	2.71	0.43
19:Q:17:MET:HE1	19:Q:19:ARG:NH2	2.33	0.43
21:S:48:VAL:O	21:S:59:GLU:HG3	2.18	0.43
21:S:48:VAL:HG22	21:S:96:VAL:HG22	2.01	0.43
1:0:291:C:H2'	1:0:292:G:O4'	2.19	0.43
1:0:366:U:H2'	1:0:367:G:O4'	2.18	0.43
1:0:1154:A:H2'	1:0:1155:G:C8	2.54	0.43
1:0:1171:A:H2'	1:0:1172:G:O4'	2.19	0.43
1:0:1257:C:O2'	1:0:1258:G:H5'	2.19	0.43
5:C:27:ARG:HG2	5:C:30:LEU:HG	1.99	0.43
6:D:67:ASP:O	6:D:69:ILE:HD13	2.19	0.43
15:M:90:LEU:HD13	15:M:186:LEU:HD21	2.00	0.43
22:T:39:ASN:ND2	22:T:44:ARG:HH11	2.16	0.43
29:1:40:ARG:HG3	29:1:45:ASN:HB2	2.00	0.43
30:2:11:CYS:HB2	30:2:20:HIS:HE1	1.82	0.43
1:0:185:G:C4'	1:0:186:A:H4'	2.49	0.43
1:0:790:A:H2'	1:0:791:A:O4'	2.19	0.43
1:0:861:A:H2'	1:0:862:U:C6	2.54	0.43
1:0:1211:G:H2'	1:0:1212:C:C6	2.53	0.43
1:0:1535:G:H2'	1:0:1536:C:C6	2.53	0.43
1:0:1603:A:H5''	1:0:1604:G:H3'	2.00	0.43
1:0:2758:G:H2'	1:0:2759:C:C6	2.53	0.43
2:9:3059:C:H2'	2:9:3060:C:C6	2.54	0.43
7:E:105:GLU:HG2	7:E:113:PRO:HB3	2.00	0.43
10:H:57:ARG:HB3	10:H:59:ASN:ND2	2.30	0.43
15:M:33:ARG:O	15:M:47:LEU:HA	2.18	0.43
15:M:37:ARG:NH2	15:M:103:ASP:OD1	2.52	0.43
21:S:48:VAL:HG21	21:S:96:VAL:CG1	2.48	0.43
25:W:21:PRO:HG2	25:W:24:LYS:HD2	2.00	0.43
1:0:301:G:O2'	1:0:302:A:H5'	2.19	0.43
1:0:945:U:H2'	1:0:946:C:H6	1.84	0.43
1:0:1072:G:OP2	26:X:154:ARG:NH2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1119:G:H8	11:I:52:GLN:NE2	2.17	0.43
1:0:1306:U:OP1	5:C:184:ARG:HD2	2.19	0.43
1:0:1909:A:N1	1:0:2128:G:H1'	2.34	0.43
1:0:1985:U:C2	1:0:1996:U:O4'	2.72	0.43
1:0:2587:U:H2'	1:0:2589:U:H5''	2.00	0.43
6:D:51:ARG:NH1	6:D:68:PRO:HG2	2.33	0.43
13:K:68:GLU:O	13:K:72:ASN:ND2	2.50	0.43
13:K:134:GLU:O	13:K:137:GLY:N	2.48	0.43
14:L:37:VAL:HG21	14:L:108:LYS:CG	2.48	0.43
27:Y:41:VAL:HG12	27:Y:42:CYS:N	2.33	0.43
1:0:111:C:C2'	1:0:112:G:H5'	2.49	0.43
1:0:751:U:H5''	5:C:100:LEU:HD22	2.01	0.43
1:0:963:C:H2'	1:0:964:G:C8	2.54	0.43
1:0:1267:C:O2'	1:0:1268:C:H5'	2.19	0.43
1:0:1367:A:C2'	1:0:1368:U:H5'	2.49	0.43
1:0:1594:C:C5	17:O:120:ARG:NH1	2.87	0.43
1:0:2039:A:OP2	4:B:234:ARG:NH2	2.51	0.43
1:0:2348:C:H2'	1:0:2349:G:H8	1.84	0.43
1:0:2385:G:H2'	1:0:2386:U:C6	2.54	0.43
1:0:2415:A:C2'	1:0:2416:G:H5'	2.48	0.43
1:0:2425:A:H5'	1:0:2426:G:OP2	2.19	0.43
1:0:2580:G:N3	1:0:2600:A:H2	2.16	0.43
1:0:2716:G:C5'	4:B:206:THR:HG21	2.44	0.43
6:D:10:PHE:CG	6:D:11:HIS:N	2.87	0.43
14:L:115:LEU:HB2	14:L:134:ILE:HG12	2.00	0.43
1:0:17:G:H2'	1:0:18:C:C6	2.54	0.43
1:0:797:A:H5'	27:Y:10:ARG:HG2	2.01	0.43
1:0:1056:U:H2'	1:0:1057:A:O4'	2.18	0.43
1:0:1134:G:C8	1:0:1134:G:O5'	2.71	0.43
1:0:2443:C:H5'	13:K:57:VAL:HG21	2.00	0.43
1:0:2502:C:H2'	1:0:2503:A:C5'	2.47	0.43
36:0:8163:EMK:C7	36:0:8163:EMK:H9	2.44	0.43
4:B:51:VAL:HG12	4:B:53:LEU:HD13	1.97	0.43
5:C:20:ASP:O	5:C:23:GLU:HB2	2.19	0.43
5:C:27:ARG:N	5:C:113:SER:OG	2.51	0.43
8:F:39:SER:OG	8:F:45:ALA:HB2	2.19	0.43
11:I:63:ILE:HG22	11:I:64:GLY:N	2.33	0.43
14:L:23:LEU:HD22	14:L:27:ARG:CZ	2.49	0.43
15:M:23:ARG:NH2	15:M:55:ASP:OD2	2.52	0.43
23:U:16:ARG:NH1	23:U:65:ASP:O	2.52	0.43
24:V:89:ASP:HB2	24:V:90:TYR:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:660:A:H4'	1:0:661:G:O5'	2.19	0.42
1:0:1211:G:H2'	1:0:1212:C:H6	1.83	0.42
1:0:1689:A:H8	1:0:1689:A:OP2	2.02	0.42
1:0:1734:C:OP1	4:B:234:ARG:HD3	2.19	0.42
2:9:3072:C:H2'	2:9:3073:G:C8	2.54	0.42
4:B:274:GLU:HA	4:B:292:GLY:O	2.19	0.42
7:E:69:ILE:HG12	7:E:72:MET:HE3	2.00	0.42
7:E:75:GLY:O	7:E:79:GLY:HA2	2.19	0.42
12:J:34:VAL:HG21	12:J:46:LYS:O	2.19	0.42
14:L:74:ARG:HG3	14:L:74:ARG:NH1	2.34	0.42
15:M:26:LEU:HD12	15:M:26:LEU:HA	1.87	0.42
16:N:49:GLU:OE1	16:N:70:LEU:HA	2.19	0.42
20:R:57:THR:HG22	20:R:59:ASP:H	1.84	0.42
24:V:31:HIS:HB3	24:V:115:THR:CG2	2.49	0.42
1:0:245:C:H2'	1:0:246:G:H5'	2.00	0.42
1:0:483:C:C4	1:0:484:A:C6	3.07	0.42
1:0:654:A:OP2	16:N:38:ARG:HD3	2.19	0.42
1:0:1244:U:H4'	1:0:1246:A:O4'	2.19	0.42
1:0:2499:U:H2'	1:0:2500:C:H6	1.84	0.42
1:0:2550:U:O2'	1:0:2551:C:H5'	2.19	0.42
4:B:214:PRO:HB2	4:B:220:VAL:HG21	2.01	0.42
12:J:30:LYS:O	12:J:55:VAL:HG13	2.18	0.42
17:O:142:ASP:O	17:O:143:ALA:O	2.37	0.42
22:T:41:ASP:C	22:T:43:GLY:H	2.21	0.42
1:0:204:A:H2'	1:0:205:U:H5'	2.00	0.42
1:0:527:U:H2'	1:0:528:G:C8	2.54	0.42
1:0:592:G:H5''	1:0:593:A:OP1	2.18	0.42
1:0:1020:A:H2'	1:0:1021:G:C8	2.54	0.42
1:0:1102:C:H2'	1:0:1103:C:C6	2.54	0.42
1:0:1964:U:H2'	1:0:1965:C:H6	1.84	0.42
1:0:2779:G:H21	7:E:143:GLN:NE2	2.17	0.42
3:A:32:VAL:O	3:A:33:GLU:C	2.56	0.42
3:A:135:VAL:HA	3:A:150:PRO:HD3	2.01	0.42
5:C:194:PHE:HA	5:C:234:VAL:HG13	2.02	0.42
6:D:24:HIS:HB2	6:D:72:LYS:HB3	1.99	0.42
7:E:7:ILE:HA	7:E:8:PRO:HD3	1.91	0.42
13:K:107:LYS:HE3	13:K:124:ASP:OD2	2.19	0.42
14:L:187:LEU:HD23	14:L:194:ALA:HB3	2.00	0.42
15:M:22:GLN:O	15:M:26:LEU:HB2	2.19	0.42
15:M:61:ALA:HB3	15:M:88:ALA:HB2	2.01	0.42
18:P:92:ARG:HA	18:P:92:ARG:HD2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:20:G:H21	19:Q:117:HIS:CD2	2.35	0.42
1:0:25:A:O2'	1:0:640:G:H5'	2.20	0.42
1:0:1096:U:O2'	1:0:1097:A:H5'	2.18	0.42
1:0:2699:A:H2'	1:0:2700:G:O4'	2.19	0.42
6:D:25:MET:HG3	6:D:41:LEU:CD1	2.48	0.42
10:H:150:LYS:HB2	10:H:157:ILE:HD12	2.01	0.42
14:L:164:THR:HG22	14:L:166:ALA:H	1.83	0.42
15:M:37:ARG:NH2	15:M:105:GLY:N	2.67	0.42
15:M:114:LYS:O	15:M:118:ILE:HG13	2.19	0.42
22:T:20:MET:HE2	22:T:28:THR:HG21	2.01	0.42
24:V:88:THR:C	24:V:90:TYR:H	2.22	0.42
27:Y:31:ILE:O	27:Y:35:LYS:HG3	2.20	0.42
30:2:91:GLN:O	30:2:92:GLU:HB2	2.20	0.42
1:0:189:A:OP1	14:L:171:ARG:NH2	2.52	0.42
1:0:210:U:O2'	1:0:211:U:H5'	2.20	0.42
1:0:304:G:H1'	1:0:347:A:N6	2.33	0.42
1:0:383:A:H2'	1:0:384:G:O4'	2.19	0.42
1:0:710:G:O2'	1:0:711:G:H5'	2.19	0.42
1:0:941:G:C5	1:0:942:U:C4	3.07	0.42
1:0:1170:U:H2'	1:0:1172:G:OP2	2.19	0.42
1:0:1503:U:H2'	1:0:1504:A:O4'	2.19	0.42
4:B:316:ARG:N	4:B:317:PRO:HD3	2.34	0.42
6:D:59:GLY:C	6:D:61:PHE:H	2.21	0.42
14:L:49:ALA:C	14:L:54:TYR:HB3	2.40	0.42
15:M:22:GLN:HA	15:M:25:ARG:HE	1.83	0.42
16:N:24:ALA:O	16:N:28:ASP:HB2	2.20	0.42
20:R:5:ILE:HD11	20:R:41:VAL:HG22	2.00	0.42
21:S:51:LEU:O	21:S:52:ARG:HG2	2.20	0.42
27:Y:39:CYS:O	27:Y:42:CYS:O	2.37	0.42
27:Y:42:CYS:SG	27:Y:44:PHE:N	2.81	0.42
27:Y:56:MET:HA	27:Y:62:TYR:O	2.18	0.42
1:0:370:G:O2'	1:0:371:U:H5'	2.18	0.42
1:0:1169:U:H2'	1:0:1170:U:O4'	2.20	0.42
1:0:1310:U:OP2	5:C:168:ARG:NH1	2.53	0.42
1:0:1342:C:C2'	1:0:1343:C:H5'	2.49	0.42
1:0:1345:A:H2'	1:0:1346:U:C6	2.54	0.42
1:0:2685:C:H2'	1:0:2686:C:H6	1.85	0.42
1:0:2782:G:O6	1:0:2790:C:H5''	2.20	0.42
2:9:3026:C:O2'	2:9:3027:C:H5'	2.20	0.42
2:9:3095:C:O2'	2:9:3096:C:H5'	2.20	0.42
6:D:44:ILE:HG12	6:D:83:PHE:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:137:ASP:O	7:E:141:VAL:HG23	2.19	0.42
15:M:97:VAL:HG12	15:M:127:LEU:HD11	2.01	0.42
19:Q:104:PHE:HB3	19:Q:109:MET:HE1	2.01	0.42
28:Z:34:CYS:HB3	28:Z:39:PHE:H	1.84	0.42
1:0:352:A:H2'	1:0:353:G:C8	2.55	0.42
1:0:401:C:H2'	1:0:402:U:C6	2.55	0.42
1:0:1808:C:O2'	1:0:1809:G:H5'	2.19	0.42
1:0:2133:U:H4'	1:0:2134:G:C5'	2.49	0.42
1:0:2714:U:H2'	1:0:2715:G:C8	2.54	0.42
1:0:2780:C:H2'	1:0:2781:U:C6	2.55	0.42
10:H:114:PRO:O	10:H:115:PHE:C	2.58	0.42
15:M:164:ASP:CG	15:M:167:ASP:HA	2.39	0.42
17:O:28:GLN:O	17:O:32:ALA:N	2.46	0.42
25:W:76:ARG:HH11	25:W:76:ARG:HG3	1.84	0.42
1:0:23:G:C6	1:0:24:G:N1	2.88	0.42
1:0:316:A:H5'	21:S:54:ASP:OD2	2.19	0.42
3:A:55:VAL:CG2	3:A:68:ILE:O	2.68	0.42
5:C:165:ASP:O	5:C:168:ARG:HB3	2.19	0.42
11:I:15:ARG:NH1	11:I:43:ARG:NH1	2.67	0.42
13:K:117:GLU:HG3	13:K:117:GLU:O	2.20	0.42
14:L:48:ARG:HH11	14:L:52:LEU:HD21	1.83	0.42
19:Q:119:VAL:O	19:Q:119:VAL:CG1	2.68	0.42
27:Y:33:HIS:HA	27:Y:69:TYR:O	2.20	0.42
1:0:14:C:H2'	1:0:15:C:C6	2.54	0.42
1:0:213:G:O2'	1:0:214:U:OP2	2.38	0.42
1:0:696:C:O2'	1:0:697:G:H5'	2.19	0.42
1:0:920:C:H4'	1:0:921:G:C2	2.55	0.42
1:0:1183:C:N4	1:0:1184:C:N4	2.67	0.42
1:0:1184:C:HO2'	1:0:1185:U:H6	1.66	0.42
1:0:1594:C:OP2	17:O:120:ARG:HD2	2.20	0.42
1:0:2289:G:H21	1:0:2291:A:H2	1.63	0.42
29:1:41:HIS:HD2	29:1:44:ARG:H	1.67	0.42
1:0:901:G:OP2	13:K:18:HIS:HE1	2.03	0.42
1:0:1204:C:H2'	1:0:1205:U:O4'	2.20	0.42
1:0:1434:A:O2'	1:0:1435:U:H2'	2.20	0.42
1:0:2893:C:O2'	1:0:2894:C:H5'	2.19	0.42
3:A:66:ARG:HH11	3:A:66:ARG:CB	2.33	0.42
4:B:305:ASP:O	4:B:306:LYS:CB	2.66	0.42
19:Q:18:LEU:HB2	19:Q:143:VAL:HG13	1.99	0.42
1:0:47:G:N3	1:0:114:A:C2	2.88	0.41
1:0:349:U:O2'	1:0:350:C:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:710:G:H5'	16:N:25:VAL:HG22	2.02	0.41
1:0:2634:G:OP2	3:A:204:GLY:N	2.30	0.41
1:0:2635:A:HO2'	1:0:2636:C:H5'	1.83	0.41
2:9:3006:C:H5''	15:M:37:ARG:HH11	1.82	0.41
2:9:3071:C:O2'	2:9:3072:C:H5'	2.20	0.41
3:A:197:VAL:HG22	3:A:197:VAL:O	2.20	0.41
4:B:320:GLN:NE2	4:B:321:PRO:HD3	2.34	0.41
10:H:86:ARG:H	10:H:86:ARG:HG2	1.70	0.41
15:M:154:LEU:O	15:M:155:GLU:HB3	2.19	0.41
19:Q:39:THR:CB	19:Q:42:GLU:HG3	2.50	0.41
19:Q:124:GLY:HA3	19:Q:136:TRP:O	2.19	0.41
26:X:151:SER:HB3	26:X:154:ARG:CB	2.50	0.41
1:0:12:U:C2'	1:0:13:G:H5'	2.50	0.41
1:0:251:C:H2'	1:0:252:C:C6	2.55	0.41
1:0:262:A:C6	8:F:89:LEU:HD21	2.55	0.41
1:0:274:G:H2'	1:0:275:G:H8	1.85	0.41
1:0:644:G:O2'	13:K:4:LYS:HE3	2.20	0.41
1:0:926:A:C4'	13:K:39:GLU:HG2	2.50	0.41
1:0:1369:A:H5''	19:Q:64:SER:OG	2.20	0.41
1:0:1514:C:H2'	1:0:1515:A:C8	2.55	0.41
1:0:1520:G:H2'	1:0:1521:C:C6	2.55	0.41
1:0:1816:C:H2'	1:0:1817:U:O4'	2.20	0.41
1:0:1826:C:O2'	1:0:1827:G:H5'	2.20	0.41
1:0:2065:C:H2'	1:0:2066:C:C6	2.55	0.41
1:0:2115:U:H2'	1:0:2116:U:C6	2.54	0.41
1:0:2125:G:H2'	1:0:2126:C:H6	1.85	0.41
1:0:2269:C:H2'	1:0:2270:G:H5'	2.01	0.41
1:0:2330:U:H4'	1:0:2331:C:OP1	2.19	0.41
1:0:2445:U:H2'	1:0:2446:G:C8	2.56	0.41
1:0:2614:C:O2'	1:0:2615:U:H5'	2.20	0.41
10:H:127:GLY:O	10:H:128:ALA:CB	2.68	0.41
10:H:151:MET:HE3	10:H:151:MET:CA	2.50	0.41
13:K:35:ARG:C	13:K:35:ARG:HD3	2.40	0.41
24:V:80:ASP:O	24:V:84:VAL:HG23	2.21	0.41
1:0:834:G:H3'	1:0:835:U:H4'	2.02	0.41
1:0:861:A:H4'	1:0:1697:G:C4'	2.45	0.41
1:0:1141:U:O2'	1:0:1142:C:H5'	2.20	0.41
1:0:1287:A:O4'	24:V:117:ARG:HD3	2.19	0.41
8:F:13:GLU:OE1	8:F:77:VAL:HG13	2.20	0.41
11:I:54:VAL:HG11	11:I:138:THR:HG21	2.02	0.41
11:I:88:PRO:O	11:I:94:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:105:ASN:HD21	16:N:109:SER:N	2.17	0.41
19:Q:126:LYS:HA	19:Q:127:PRO:HD3	1.94	0.41
19:Q:149:GLU:HA	19:Q:150:PRO:HD3	1.94	0.41
24:V:4:LEU:CD2	24:V:54:PHE:HB3	2.49	0.41
27:Y:29:VAL:O	27:Y:33:HIS:CB	2.63	0.41
1:O:282:C:C2'	1:O:283:U:H4'	2.50	0.41
1:O:353:G:O2'	1:O:354:A:H5'	2.20	0.41
1:O:764:C:H2'	1:O:765:G:O4'	2.19	0.41
1:O:1367:A:H2'	1:O:1368:U:H5'	2.01	0.41
1:O:1514:C:O2'	1:O:1515:A:H5'	2.20	0.41
1:O:1586:G:O2'	1:O:1587:U:H5'	2.20	0.41
1:O:1790:C:H5	17:O:71:LYS:HE3	1.85	0.41
1:O:1913:C:H2'	1:O:1914:C:C6	2.55	0.41
1:O:2819:C:H2'	1:O:2820:A:C8	2.55	0.41
36:O:8163:EMK:H9	36:O:8163:EMK:O72	2.19	0.41
4:B:238:ASN:HD22	4:B:240:GLY:N	2.18	0.41
6:D:146:LYS:HG2	15:M:106:LEU:HB2	2.03	0.41
10:H:136:VAL:CG2	10:H:137:ASN:H	2.31	0.41
14:L:115:LEU:O	14:L:116:ASN:HB2	2.18	0.41
19:Q:17:MET:CE	19:Q:19:ARG:NH2	2.83	0.41
19:Q:114:VAL:HG13	19:Q:114:VAL:O	2.20	0.41
21:S:1:SER:O	21:S:7:GLN:NE2	2.43	0.41
22:T:9:CYS:HB2	22:T:52:THR:HG22	2.01	0.41
22:T:20:MET:CG	22:T:28:THR:HG23	2.50	0.41
25:W:47:ALA:O	25:W:82:GLU:HB2	2.19	0.41
27:Y:30:GLU:HA	27:Y:33:HIS:CB	2.50	0.41
1:O:97:G:C6	21:S:107:LYS:HE3	2.56	0.41
1:O:117:A:H2'	1:O:118:G:O4'	2.20	0.41
1:O:121:U:O4	28:Z:18:LYS:HD3	2.19	0.41
1:O:155:C:O2'	1:O:156:C:H5'	2.20	0.41
1:O:283:U:C5	1:O:284:C:N3	2.89	0.41
1:O:1202:A:H2'	1:O:1203:G:O4'	2.21	0.41
1:O:1594:C:O2'	1:O:1595:G:H5'	2.19	0.41
1:O:1697:G:O2'	1:O:1698:U:H5'	2.21	0.41
1:O:2241:C:O2'	1:O:2242:U:H5'	2.20	0.41
4:B:24:PRO:HG3	4:B:204:GLY:HA2	2.02	0.41
5:C:138:VAL:O	5:C:234:VAL:HA	2.20	0.41
10:H:14:TYR:N	10:H:91:HIS:HE1	2.15	0.41
10:H:26:LYS:HD3	10:H:89:PRO:CG	2.50	0.41
11:I:63:ILE:CG2	11:I:64:GLY:N	2.83	0.41
15:M:24:LEU:O	15:M:28:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:48:VAL:HG21	21:S:96:VAL:HG13	2.03	0.41
27:Y:62:TYR:CE2	27:Y:64:ILE:CG2	3.02	0.41
1:O:664:U:O4	1:O:681:G:H5''	2.21	0.41
1:O:1924:A:O2'	30:2:29:ARG:NH1	2.54	0.41
1:O:2316:G:OP1	1:O:2317:C:H1'	2.20	0.41
1:O:2575:C:H2'	1:O:2576:A:O4'	2.20	0.41
7:E:95:VAL:O	7:E:126:ILE:HD13	2.21	0.41
11:I:80:LYS:HE2	11:I:98:PHE:CZ	2.56	0.41
13:K:53:ARG:NH2	13:K:57:VAL:CG1	2.82	0.41
14:L:16:LYS:C	14:L:21:ALA:HB2	2.41	0.41
22:T:20:MET:HE2	22:T:30:HIS:CE1	2.56	0.41
24:V:21:LEU:HD23	24:V:21:LEU:HA	1.81	0.41
1:O:1067:A:O2'	24:V:12:ASN:HA	2.20	0.41
1:O:1791:U:O2'	1:O:1792:C:H5'	2.21	0.41
1:O:1928:C:H2'	1:O:1929:G:O4'	2.21	0.41
3:A:1:GLY:HA2	3:A:197:VAL:HG23	2.02	0.41
5:C:35:VAL:HG23	5:C:220:THR:CG2	2.51	0.41
7:E:112:ALA:HA	7:E:113:PRO:HD3	1.94	0.41
8:F:12:LEU:O	8:F:12:LEU:HD23	2.20	0.41
10:H:113:ALA:N	10:H:114:PRO:HD3	2.35	0.41
19:Q:39:THR:O	19:Q:40:ALA:C	2.58	0.41
21:S:40:VAL:HG22	21:S:41:ARG:N	2.35	0.41
21:S:73:HIS:HE1	21:S:90:PRO:HG3	1.86	0.41
24:V:39:ASP:HA	24:V:42:ARG:HH12	1.84	0.41
1:O:1421:C:O2'	1:O:1422:U:H5'	2.20	0.41
2:9:3048:C:H4'	15:M:141:ARG:HH21	1.86	0.41
2:9:3049:G:H2'	2:9:3050:G:O4'	2.21	0.41
3:A:65:ARG:C	3:A:66:ARG:HG3	2.41	0.41
7:E:154:ILE:HG23	7:E:154:ILE:O	2.21	0.41
16:N:73:ASP:HA	16:N:92:VAL:O	2.21	0.41
19:Q:35:ILE:HA	19:Q:38:LYS:HD2	2.02	0.41
23:U:8:ILE:HG21	23:U:59:ILE:HG13	2.03	0.41
24:V:26:ILE:O	24:V:26:ILE:HG13	2.20	0.41
1:O:490:C:O2'	1:O:491:C:H5'	2.21	0.41
1:O:510:U:H6	1:O:510:U:O5'	2.04	0.41
1:O:870:G:OP2	3:A:3:ARG:NH1	2.50	0.41
1:O:911:G:H5'	1:O:932:U:OP1	2.21	0.41
1:O:1139:U:H2'	1:O:1140:C:C6	2.55	0.41
1:O:1293:U:O2'	1:O:1294:A:H5'	2.21	0.41
1:O:1396:C:H1'	17:O:1:THR:O	2.21	0.41
1:O:1565:C:O4'	1:O:2738:G:H1'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2237:G:O2'	1:0:2238:A:H8	2.03	0.41
1:0:2578:G:H5'	1:0:2578:G:C8	2.45	0.41
1:0:2777:G:O2'	1:0:2778:A:H5'	2.20	0.41
1:0:2909:G:H2'	1:0:2910:A:C8	2.56	0.41
2:9:3064:C:H2'	2:9:3065:A:H5'	2.02	0.41
7:E:93:MET:HB2	7:E:93:MET:HE2	1.89	0.41
10:H:139:ASP:H	10:H:140:PRO:HD3	1.76	0.41
13:K:143:THR:CG2	13:K:144:ASP:N	2.80	0.41
14:L:37:VAL:CG2	14:L:108:LYS:HG3	2.50	0.41
14:L:183:VAL:HG12	14:L:184:ARG:N	2.35	0.41
19:Q:111:ILE:HG23	19:Q:145:LEU:CD1	2.50	0.41
20:R:11:THR:H	20:R:14:ALA:HB3	1.85	0.41
21:S:26:THR:HA	21:S:39:ASN:HB3	2.01	0.41
24:V:65:VAL:HG12	24:V:116:LEU:HD13	2.02	0.41
24:V:69:ARG:HD2	24:V:117:ARG:O	2.21	0.41
24:V:110:GLN:NE2	24:V:110:GLN:HA	2.36	0.41
26:X:106:THR:CG2	26:X:107:PRO:HD2	2.48	0.41
30:2:6:ARG:HG2	30:2:6:ARG:HH11	1.85	0.41
1:0:424:C:H2'	1:0:425:U:C6	2.55	0.41
1:0:449:A:C8	5:C:43:LYS:HG2	2.56	0.41
1:0:1603:A:H5''	1:0:1605:G:H5'	2.02	0.41
1:0:2016:U:H2'	1:0:2017:U:C6	2.56	0.41
1:0:2416:G:H2'	1:0:2417:C:C6	2.56	0.41
1:0:2661:U:C2	1:0:2812:A:N6	2.89	0.41
1:0:2866:U:H4'	1:0:2867:G:H5'	2.01	0.41
6:D:58:VAL:HG12	6:D:59:GLY:N	2.36	0.41
7:E:84:MET:HB2	7:E:131:LEU:HB2	2.03	0.41
11:I:132:LEU:HD23	11:I:132:LEU:HA	1.84	0.41
15:M:86:LEU:HD12	15:M:125:ALA:HB2	2.03	0.41
19:Q:119:VAL:O	19:Q:119:VAL:HG12	2.20	0.41
27:Y:39:CYS:HA	27:Y:47:LEU:HD11	2.03	0.41
1:0:157:G:H4'	14:L:95:LYS:HG3	2.02	0.40
1:0:192:A:C4'	14:L:176:GLN:HE22	2.34	0.40
1:0:419:A:H1'	1:0:1921:A:C2	2.56	0.40
1:0:757:C:H2'	1:0:758:A:C8	2.55	0.40
1:0:820:G:O2'	1:0:856:G:H4'	2.21	0.40
1:0:840:U:H2'	19:Q:128:ARG:NH1	2.36	0.40
1:0:862:U:H2'	1:0:863:G:H8	1.86	0.40
1:0:1104:C:H4'	11:I:88:PRO:HD3	2.03	0.40
1:0:1165:G:H4'	1:0:1174:A:O2'	2.21	0.40
1:0:1398:G:H5'	17:O:23:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1477:C:H4'	1:0:1868:G:H5''	2.03	0.40
1:0:2310:G:OP2	10:H:114:PRO:HD2	2.22	0.40
1:0:2317:C:OP2	30:2:62:THR:HB	2.21	0.40
1:0:2428:G:N7	30:2:60:LYS:HE2	2.36	0.40
2:9:3093:A:N1	10:H:52:LYS:HD2	2.36	0.40
3:A:28:GLU:HA	3:A:115:GLY:O	2.21	0.40
10:H:1:LYS:HA	10:H:2:PRO:HD3	1.92	0.40
10:H:45:GLN:O	10:H:163:PRO:HD3	2.21	0.40
10:H:158:ASN:C	10:H:158:ASN:OD1	2.60	0.40
11:I:15:ARG:CZ	11:I:43:ARG:HH11	2.34	0.40
15:M:22:GLN:CB	15:M:25:ARG:HH21	2.34	0.40
20:R:73:ASP:OD1	20:R:76:GLU:HG3	2.21	0.40
22:T:9:CYS:SG	22:T:11:THR:HG23	2.61	0.40
23:U:45:ARG:C	23:U:47:LYS:N	2.74	0.40
1:0:110:C:H2'	1:0:111:C:H6	1.86	0.40
1:0:272:A:H5'	1:0:273:G:OP2	2.21	0.40
1:0:1145:G:H2'	1:0:1146:C:O4'	2.22	0.40
1:0:1204:C:C2'	1:0:1205:U:H5''	2.51	0.40
1:0:1825:U:O2'	1:0:1826:C:H5'	2.21	0.40
1:0:2083:A:H61	11:I:90:LYS:HD3	1.87	0.40
4:B:1:PRO:O	4:B:2:GLN:O	2.38	0.40
8:F:34:ASN:ND2	8:F:38:LYS:HE2	2.35	0.40
14:L:20:ILE:HA	14:L:23:LEU:HB2	2.03	0.40
23:U:39:ALA:O	23:U:41:GLU:HG3	2.22	0.40
1:0:62:C:C4	1:0:63:U:C4	3.09	0.40
1:0:74:A:C4	1:0:104:G:N2	2.90	0.40
1:0:120:A:H5'	28:Z:20:ARG:HH21	1.86	0.40
1:0:137:U:OP1	1:0:259:G:O2'	2.40	0.40
1:0:191:A:C4	1:0:237:G:N7	2.90	0.40
1:0:327:A:H4'	1:0:329:A:N7	2.37	0.40
1:0:653:C:H2'	1:0:654:A:C8	2.56	0.40
1:0:737:A:H8	1:0:737:A:O5'	2.04	0.40
1:0:1362:U:H1'	5:C:84:VAL:HG21	2.04	0.40
1:0:2326:U:H2'	1:0:2327:A:C8	2.57	0.40
1:0:2908:A:H2'	1:0:2909:G:C4'	2.52	0.40
2:9:3024:U:O2'	2:9:3025:G:C4'	2.68	0.40
3:A:36:ASP:OD1	3:A:37:VAL:N	2.54	0.40
6:D:140:ARG:HG3	6:D:140:ARG:NH1	2.37	0.40
8:F:24:ARG:HB2	8:F:29:VAL:HG21	2.04	0.40
10:H:129:ASN:N	10:H:129:ASN:HD22	2.17	0.40
14:L:119:SER:HA	14:L:129:HIS:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:47:VAL:HA	18:P:48:PRO:HD3	1.88	0.40
22:T:11:THR:HG22	22:T:53:ASP:OD2	2.21	0.40
1:O:1593:C:OP1	17:O:117:SER:HB3	2.20	0.40
1:O:1827:G:H2'	1:O:1828:G:C8	2.56	0.40
1:O:2084:C:H2'	1:O:2085:A:C8	2.56	0.40
1:O:2438:G:H2'	1:O:2439:C:O4'	2.21	0.40
1:O:2719:A:C2	4:B:70:PRO:HB3	2.56	0.40
4:B:109:LEU:CG	4:B:113:LEU:HD11	2.49	0.40
4:B:233:ARG:HH11	4:B:233:ARG:HG2	1.85	0.40
4:B:279:THR:HG22	4:B:280:VAL:H	1.85	0.40
13:K:134:GLU:C	13:K:136:ALA:N	2.75	0.40
1:O:283:U:H5	1:O:284:C:N3	2.19	0.40
1:O:678:G:OP2	5:C:107:ARG:NH2	2.55	0.40
1:O:695:C:H2'	1:O:696:C:H6	1.83	0.40
1:O:816:G:H5'	1:O:1598:A:H4'	2.03	0.40
1:O:836:G:OP1	4:B:230:GLN:NE2	2.55	0.40
1:O:1076:G:C2	1:O:1084:C:C2	3.10	0.40
1:O:1134:G:H8	1:O:1134:G:O5'	2.05	0.40
1:O:1883:U:OP2	3:A:190:ARG:NE	2.46	0.40
1:O:2756:U:O2	1:O:2896:A:H2	2.04	0.40
5:C:1:MET:CG	5:C:2:GLN:H	2.24	0.40
6:D:23:VAL:O	6:D:23:VAL:HG23	2.21	0.40
11:I:19:MET:HE1	11:I:78:ILE:HG22	2.02	0.40
13:K:65:ASP:OD1	13:K:109:LEU:HB2	2.22	0.40
17:O:37:ARG:O	17:O:41:ARG:HG3	2.21	0.40
20:R:57:THR:HG22	20:R:58:MET:H	1.84	0.40
23:U:1:THR:HG23	23:U:2:VAL:N	2.37	0.40
29:1:14:LEU:HD13	29:1:47:THR:CG2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
3	A	235/237 (99%)	209 (89%)	21 (9%)	5 (2%)	5	15
4	B	335/337 (99%)	309 (92%)	20 (6%)	6 (2%)	7	18
5	C	244/246 (99%)	229 (94%)	13 (5%)	2 (1%)	16	38
6	D	134/165 (81%)	103 (77%)	20 (15%)	11 (8%)	1	1
7	E	170/172 (99%)	160 (94%)	9 (5%)	1 (1%)	22	45
8	F	117/119 (98%)	101 (86%)	14 (12%)	2 (2%)	7	20
9	G	25/62 (40%)	23 (92%)	1 (4%)	1 (4%)	2	5
10	H	152/167 (91%)	134 (88%)	13 (9%)	5 (3%)	3	7
11	I	140/142 (99%)	130 (93%)	7 (5%)	3 (2%)	5	15
12	J	130/132 (98%)	122 (94%)	7 (5%)	1 (1%)	16	38
13	K	141/150 (94%)	117 (83%)	22 (16%)	2 (1%)	9	24
14	L	192/194 (99%)	174 (91%)	16 (8%)	2 (1%)	13	33
15	M	184/186 (99%)	159 (86%)	17 (9%)	8 (4%)	2	4
16	N	113/115 (98%)	107 (95%)	5 (4%)	1 (1%)	14	35
17	O	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
18	P	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	12	30
19	Q	148/150 (99%)	138 (93%)	9 (6%)	1 (1%)	19	42
20	R	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
21	S	117/119 (98%)	111 (95%)	4 (3%)	2 (2%)	7	20
22	T	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
23	U	63/65 (97%)	58 (92%)	1 (2%)	4 (6%)	1	2
24	V	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	19	42
25	W	80/82 (98%)	71 (89%)	5 (6%)	4 (5%)	1	3
26	X	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
27	Y	71/73 (97%)	63 (89%)	5 (7%)	3 (4%)	2	5
28	Z	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
29	1	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
30	2	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	12	30
All	All	3633/3777 (96%)	3317 (91%)	249 (7%)	67 (2%)	7	18

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	139	ASP
6	D	63	ILE
6	D	93	LEU
6	D	95	THR
6	D	173	GLU
10	H	163	PRO
13	K	80	ASP
15	M	154	LEU
15	M	183	ASP
25	W	66	THR
4	B	2	GLN
6	D	11	HIS
6	D	27	ILE
6	D	56	ARG
6	D	171	ASP
11	I	5	GLU
11	I	143	LYS
13	K	73	VAL
21	S	53	GLY
3	A	34	ASP
4	B	169	GLY
4	B	185	GLY
5	C	8	LEU
6	D	97	GLN
8	F	101	ALA
10	H	72	VAL
10	H	79	ALA
10	H	138	PRO
14	L	35	PRO
14	L	116	ASN
15	M	113	SER
15	M	155	GLU
15	M	181	ASP
16	N	24	ALA
23	U	40	PRO
24	V	49	ASN
25	W	87	ALA
30	2	56	PRO
3	A	229	ALA
5	C	79	ARG
6	D	16	PRO
8	F	61	MET
11	I	65	ASN

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Mol	Chain	Res	Type
15	M	60	SER
23	U	39	ALA
23	U	43	PRO
25	W	77	PHE
27	Y	20	LEU
3	A	132	ASP
4	B	287	TYR
7	E	17	HIS
15	M	68	GLU
19	Q	81	PRO
21	S	116	ASP
27	Y	67	GLY
4	B	184	ASP
6	D	20	LYS
9	G	72	ASP
12	J	21	ALA
18	P	18	PRO
25	W	81	GLY
10	H	43	PRO
23	U	38	GLY
27	Y	41	VAL
3	A	123	GLY
3	A	88	ILE
15	M	184	ILE

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	
3	A	179/179 (100%)	168 (94%)	11 (6%)	15	36
4	B	282/282 (100%)	264 (94%)	18 (6%)	14	34
5	C	193/193 (100%)	179 (93%)	14 (7%)	11	29
6	D	117/138 (85%)	113 (97%)	4 (3%)	32	61
7	E	152/152 (100%)	148 (97%)	4 (3%)	41	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	F	92/92 (100%)	88 (96%)	4 (4%)	25	52
9	G	27/55 (49%)	27 (100%)	0	100	100
10	H	122/122 (100%)	113 (93%)	9 (7%)	11	28
11	I	118/118 (100%)	110 (93%)	8 (7%)	13	32
12	J	106/106 (100%)	104 (98%)	2 (2%)	52	79
13	K	113/116 (97%)	106 (94%)	7 (6%)	15	36
14	L	166/166 (100%)	158 (95%)	8 (5%)	21	48
15	M	149/149 (100%)	142 (95%)	7 (5%)	22	49
16	N	93/93 (100%)	89 (96%)	4 (4%)	25	52
17	O	113/113 (100%)	112 (99%)	1 (1%)	75	90
18	P	79/79 (100%)	77 (98%)	2 (2%)	42	72
19	Q	117/117 (100%)	114 (97%)	3 (3%)	41	70
20	R	71/71 (100%)	70 (99%)	1 (1%)	62	84
21	S	105/105 (100%)	98 (93%)	7 (7%)	13	33
22	T	44/44 (100%)	44 (100%)	0	100	100
23	U	51/51 (100%)	50 (98%)	1 (2%)	50	78
24	V	130/130 (100%)	126 (97%)	4 (3%)	35	64
25	W	66/66 (100%)	61 (92%)	5 (8%)	11	27
26	X	120/120 (100%)	115 (96%)	5 (4%)	25	53
27	Y	56/56 (100%)	55 (98%)	1 (2%)	54	80
28	Z	46/46 (100%)	46 (100%)	0	100	100
29	1	42/44 (96%)	41 (98%)	1 (2%)	44	73
30	2	79/79 (100%)	78 (99%)	1 (1%)	65	85
All	All	3028/3082 (98%)	2896 (96%)	132 (4%)	24	51

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	33	GLU
3	A	34	ASP
3	A	62	ASP
3	A	64	ASP
3	A	69	LEU

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Mol	Chain	Res	Type
3	A	94	LEU
3	A	131	HIS
3	A	153	ARG
3	A	179	MET
3	A	192	VAL
4	B	11	LEU
4	B	27	ASN
4	B	51	VAL
4	B	53	LEU
4	B	71	VAL
4	B	97	LEU
4	B	112	THR
4	B	162	MET
4	B	190	MET
4	B	234	ARG
4	B	251	VAL
4	B	254	GLN
4	B	257	THR
4	B	264	GLU
4	B	268	ARG
4	B	274	GLU
4	B	279	THR
4	B	307	ARG
5	C	2	GLN
5	C	27	ARG
5	C	76	ARG
5	C	78	ARG
5	C	94	THR
5	C	101	ASP
5	C	115	LEU
5	C	136	VAL
5	C	187	ARG
5	C	211	ASP
5	C	223	LEU
5	C	236	THR
5	C	240	LEU
5	C	243	VAL
6	D	24	HIS
6	D	61	PHE
6	D	62	ASP
6	D	133	ASN
7	E	7	ILE

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Mol	Chain	Res	Type
7	E	10	ASP
7	E	86	VAL
7	E	116	THR
8	F	24	ARG
8	F	46	GLU
8	F	64	PRO
8	F	99	THR
10	H	18	GLU
10	H	61	LEU
10	H	72	VAL
10	H	73	GLN
10	H	85	ILE
10	H	130	HIS
10	H	138	PRO
10	H	158	ASN
10	H	163	PRO
11	I	46	ILE
11	I	52	GLN
11	I	76	ASP
11	I	79	PHE
11	I	93	ARG
11	I	107	ASN
11	I	127	ILE
11	I	131	THR
12	J	10	GLN
12	J	84	ASP
13	K	32	ASP
13	K	35	ARG
13	K	40	PHE
13	K	43	HIS
13	K	80	ASP
13	K	83	GLU
13	K	102	ASP
14	L	23	LEU
14	L	46	LEU
14	L	68	ARG
14	L	87	MET
14	L	93	ARG
14	L	99	ARG
14	L	116	ASN
14	L	158	ARG
15	M	23	ARG

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Mol	Chain	Res	Type
15	M	56	ASP
15	M	65	ASP
15	M	138	ASP
15	M	152	GLU
15	M	163	PHE
15	M	175	LEU
16	N	31	GLU
16	N	38	ARG
16	N	103	GLU
16	N	111	VAL
17	O	98	ILE
18	P	16	ASN
18	P	42	LYS
19	Q	13	THR
19	Q	39	THR
19	Q	123	GLN
20	R	80	ARG
21	S	9	LYS
21	S	39	ASN
21	S	43	ASN
21	S	48	VAL
21	S	89	ARG
21	S	96	VAL
21	S	115	GLU
23	U	22	ASP
24	V	4	LEU
24	V	78	ASP
24	V	142	ASP
24	V	146	ILE
25	W	15	ARG
25	W	27	ASP
25	W	49	ARG
25	W	79	GLU
25	W	82	GLU
26	X	141	THR
26	X	163	THR
26	X	187	VAL
26	X	189	ASN
26	X	235	GLU
27	Y	42	CYS
29	1	18	ASN
30	2	18	GLN



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	HIS
3	A	199	HIS
4	B	27	ASN
4	B	106	HIS
4	B	145	HIS
4	B	238	ASN
4	B	256	GLN
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	129	HIS
5	C	163	HIS
6	D	29	HIS
6	D	47	GLN
6	D	103	ASN
6	D	133	ASN
7	E	15	GLN
7	E	94	GLN
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
9	G	64	ASN
10	H	8	ASN
10	H	55	GLN
10	H	58	HIS
10	H	69	ASN
10	H	74	ASN
10	H	80	ASN
10	H	91	HIS
10	H	129	ASN
10	H	137	ASN
10	H	166	ASN
11	I	25	GLN
11	I	52	GLN
11	I	107	ASN
12	J	10	GLN
13	K	18	HIS
13	K	41	HIS
13	K	42	ASN

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Mol	Chain	Res	Type
14	L	58	GLN
14	L	89	ASN
14	L	176	GLN
15	M	93	GLN
15	M	107	ASN
17	O	50	GLN
17	O	66	GLN
17	O	73	HIS
17	O	88	GLN
17	O	101	GLN
17	O	118	GLN
18	P	40	HIS
19	Q	61	GLN
19	Q	94	ASN
19	Q	98	ASN
19	Q	113	HIS
19	Q	117	HIS
20	R	9	HIS
20	R	21	GLN
20	R	44	GLN
20	R	53	ASN
21	S	11	GLN
21	S	39	ASN
21	S	43	ASN
21	S	73	HIS
22	T	39	ASN
22	T	48	ASN
23	U	60	GLN
24	V	12	ASN
24	V	27	HIS
24	V	59	GLN
24	V	87	HIS
24	V	110	GLN
24	V	119	HIS
24	V	125	HIS
24	V	141	HIS
25	W	22	ASN
25	W	23	HIS
25	W	36	HIS
26	X	119	GLN
26	X	134	HIS
26	X	149	GLN

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Mol	Chain	Res	Type
26	X	189	ASN
27	Y	33	HIS
27	Y	70	GLN
28	Z	8	GLN
28	Z	16	HIS
28	Z	28	HIS
29	1	18	ASN
29	1	41	HIS
29	1	45	ASN
30	2	15	ASN
30	2	30	GLN
30	2	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2902 (94%)	233 (8%)	22 (0%)
2	9	121/122 (99%)	14 (11%)	2 (1%)
All	All	2866/3024 (94%)	247 (8%)	24 (0%)

All (247) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	130	C
1	0	131	A
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	186	A
1	0	191	A
1	0	192	A

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Mol	Chain	Res	Type
1	0	198	A
1	0	200	U
1	0	204	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	368	C
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	632	A
1	0	660	A
1	0	688	A
1	0	701	U
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U

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Mol	Chain	Res	Type
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1003	U
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1131	G
1	0	1137	G
1	0	1164	U
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1205	U

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Mol	Chain	Res	Type
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1287	A
1	0	1289	C
1	0	1331	A
1	0	1342	C
1	0	1351	G
1	0	1353	C
1	0	1357	A
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1488	U
1	0	1505	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1562	C
1	0	1564	C
1	0	1592	G
1	0	1603	A
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G

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Mol	Chain	Res	Type
1	0	1774	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1996	U
1	0	2004	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2034	U
1	0	2063	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A

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Mol	Chain	Res	Type
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2526	C
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2540	G
1	0	2553	A
1	0	2564	G
1	0	2570	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2638	G
1	0	2648	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2727	A
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C

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Mol	Chain	Res	Type
1	0	2835	C
1	0	2876	G
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3026	C
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3057	A
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	129	A
1	0	169	A
1	0	338	C
1	0	604	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	877	G
1	0	1080	C
1	0	1232	A
1	0	1237	U
1	0	1352	A
1	0	1684	A
1	0	1752	G
1	0	1856	C
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C

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Mol	Chain	Res	Type
1	0	2536	C
1	0	2726	U
1	0	2791	U
2	9	3024	U
2	9	3055	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 204 ligands modelled in this entry, 203 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	EMK	0	8163	-	75,78,78	6.25	57 (76%)	107,118,118	3.35	41 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	EMK	0	8163	-	-	29/93/133/133	0/5/5/5

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	8163	EMK	C12-N9	14.19	1.71	1.49
36	0	8163	EMK	C20-C12	12.97	1.76	1.52
36	0	8163	EMK	O42-C5	-12.59	1.13	1.44
36	0	8163	EMK	C14-C15	11.41	1.75	1.55
36	0	8163	EMK	O74-C14	11.29	1.63	1.44
36	0	8163	EMK	O72-C6	10.41	1.61	1.44
36	0	8163	EMK	O77-C28	10.29	1.63	1.42
36	0	8163	EMK	O76-C26	9.95	1.63	1.44
36	0	8163	EMK	C18-C6	9.87	1.68	1.52
36	0	8163	EMK	C14-C13	9.80	1.78	1.55
36	0	8163	EMK	C23-C14	9.49	1.68	1.52
36	0	8163	EMK	O78-C10	9.27	1.66	1.42
36	0	8163	EMK	C6-C5	9.14	1.73	1.55
36	0	8163	EMK	O70-C1	9.06	1.44	1.21
36	0	8163	EMK	C43-N46	8.99	1.60	1.48
36	0	8163	EMK	C21-C10	8.92	1.70	1.51
36	0	8163	EMK	O75-C1	8.40	1.53	1.34
36	0	8163	EMK	C87-C86	7.60	1.51	1.39
36	0	8163	EMK	C38-N9	7.34	1.62	1.46
36	0	8163	EMK	O71-C10	7.31	1.61	1.41
36	0	8163	EMK	C17-C4	7.19	1.68	1.53
36	0	8163	EMK	O75-C15	6.84	1.57	1.46
36	0	8163	EMK	C21-C26	6.54	1.66	1.52
36	0	8163	EMK	C45-C43	6.43	1.67	1.53
36	0	8163	EMK	C30-C28	6.35	1.67	1.53
36	0	8163	EMK	O94-S1	6.30	1.59	1.44
36	0	8163	EMK	C88-C87	6.24	1.48	1.38
36	0	8163	EMK	C91-C86	6.17	1.48	1.39
36	0	8163	EMK	C34-C26	5.90	1.64	1.52
36	0	8163	EMK	C91-C90	5.89	1.48	1.38
36	0	8163	EMK	C7-C6	5.56	1.63	1.54
36	0	8163	EMK	O95-S1	5.42	1.57	1.44
36	0	8163	EMK	C9-C8	5.28	1.75	1.52
36	0	8163	EMK	O71-C3	5.20	1.57	1.43
36	0	8163	EMK	C16-C2	5.16	1.64	1.53
36	0	8163	EMK	O78-C30	5.08	1.56	1.44
36	0	8163	EMK	C88-C89	5.04	1.46	1.38
36	0	8163	EMK	C90-C89	5.03	1.46	1.38
36	0	8163	EMK	C93-C95	4.97	1.43	1.36
36	0	8163	EMK	C2-C1	4.97	1.62	1.51
36	0	8163	EMK	C2-C3	4.92	1.66	1.54
36	0	8163	EMK	C45-C47	4.91	1.60	1.52
36	0	8163	EMK	C89-S1	4.89	1.82	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	8163	EMK	C86-C85	4.20	1.58	1.51
36	0	8163	EMK	C24-C15	3.92	1.65	1.53
36	0	8163	EMK	O41-C39	3.67	1.51	1.41
36	0	8163	EMK	C85-C83	3.40	1.58	1.54
36	0	8163	EMK	C92-S1	3.40	1.87	1.75
36	0	8163	EMK	O96-C85	3.28	1.48	1.42
36	0	8163	EMK	C40-C43	3.09	1.59	1.53
36	0	8163	EMK	C4-C5	3.07	1.62	1.54
36	0	8163	EMK	C26-C28	2.82	1.59	1.53
36	0	8163	EMK	C95-N83	2.66	1.37	1.34
36	0	8163	EMK	O76-C35	2.49	1.51	1.43
36	0	8163	EMK	O73-C13	2.17	1.47	1.42
36	0	8163	EMK	N82-N81	2.10	1.38	1.34
36	0	8163	EMK	C39-C40	2.01	1.58	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	0	8163	EMK	C7-C8-C9	-14.43	91.72	112.10
36	0	8163	EMK	C39-O42-C5	13.40	139.06	116.26
36	0	8163	EMK	C92-S1-C89	9.33	114.82	104.55
36	0	8163	EMK	C81-N46-C43	-8.11	96.03	112.52
36	0	8163	EMK	C6-C7-C8	-6.16	100.28	117.11
36	0	8163	EMK	O73-C13-C14	-6.11	95.36	106.57
36	0	8163	EMK	O74-C14-C15	5.97	116.37	107.24
36	0	8163	EMK	O71-C3-C4	5.64	114.88	108.23
36	0	8163	EMK	C15-O75-C1	-5.59	108.43	118.20
36	0	8163	EMK	O72-C6-C7	5.33	121.65	108.34
36	0	8163	EMK	C3-C2-C1	-5.14	99.53	109.93
36	0	8163	EMK	C20-C12-N9	-4.99	103.70	113.76
36	0	8163	EMK	C25-C24-C15	4.94	125.04	113.11
36	0	8163	EMK	O42-C5-C6	4.93	112.28	106.40
36	0	8163	EMK	C6-C5-C4	-4.84	106.87	113.89
36	0	8163	EMK	C50-N46-C81	4.82	117.56	110.51
36	0	8163	EMK	C39-C40-C43	-4.05	102.66	109.15
36	0	8163	EMK	O75-C1-O70	-3.96	116.79	123.95
36	0	8163	EMK	O75-C15-C14	3.95	113.51	107.28
36	0	8163	EMK	O95-S1-C92	-3.84	102.84	108.47
36	0	8163	EMK	O75-C1-C2	3.68	119.40	111.53
36	0	8163	EMK	C10-O71-C3	3.66	122.01	114.72
36	0	8163	EMK	O72-C6-C18	-3.62	100.12	108.48
36	0	8163	EMK	C8-C9-N9	3.54	120.99	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	0	8163	EMK	C15-C14-C13	-3.49	101.52	108.21
36	0	8163	EMK	C45-C43-C40	-3.29	105.29	110.02
36	0	8163	EMK	C23-C14-C15	3.13	115.50	111.26
36	0	8163	EMK	C26-C21-C10	-3.13	109.70	114.99
36	0	8163	EMK	O76-C26-C28	3.09	108.34	103.86
36	0	8163	EMK	C81-C82-C94	-2.93	105.35	113.05
36	0	8163	EMK	C23-C14-C13	-2.87	108.17	113.14
36	0	8163	EMK	C38-N9-C9	-2.82	106.06	110.26
36	0	8163	EMK	C14-C13-C12	-2.67	109.60	115.81
36	0	8163	EMK	C50-N46-C43	2.66	119.71	113.96
36	0	8163	EMK	O95-S1-C89	-2.60	106.21	108.23
36	0	8163	EMK	O71-C3-C2	-2.38	107.15	111.16
36	0	8163	EMK	C45-C43-N46	-2.33	108.88	115.54
36	0	8163	EMK	C35-O76-C26	2.25	122.09	117.51
36	0	8163	EMK	O73-C13-C12	2.20	117.40	112.03
36	0	8163	EMK	C87-C86-C85	2.07	123.83	120.71
36	0	8163	EMK	O76-C26-C34	-2.05	105.47	110.77

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	0	8163	EMK	O70-C1-C2-C3
36	0	8163	EMK	O75-C1-C2-C3
36	0	8163	EMK	C8-C9-N9-C12
36	0	8163	EMK	C13-C12-N9-C9
36	0	8163	EMK	N9-C12-C13-C14
36	0	8163	EMK	N9-C12-C13-O73
36	0	8163	EMK	C20-C12-C13-C14
36	0	8163	EMK	C20-C12-C13-O73
36	0	8163	EMK	C13-C14-C15-C24
36	0	8163	EMK	C13-C14-C15-O75
36	0	8163	EMK	C23-C14-C15-C24
36	0	8163	EMK	C23-C14-C15-O75
36	0	8163	EMK	O74-C14-C15-C24
36	0	8163	EMK	O74-C14-C15-O75
36	0	8163	EMK	C14-C15-O75-C1
36	0	8163	EMK	C82-C81-N46-C50
36	0	8163	EMK	C82-C94-C95-N83
36	0	8163	EMK	C14-C15-C24-C25
36	0	8163	EMK	C2-C1-O75-C15
36	0	8163	EMK	C24-C15-O75-C1

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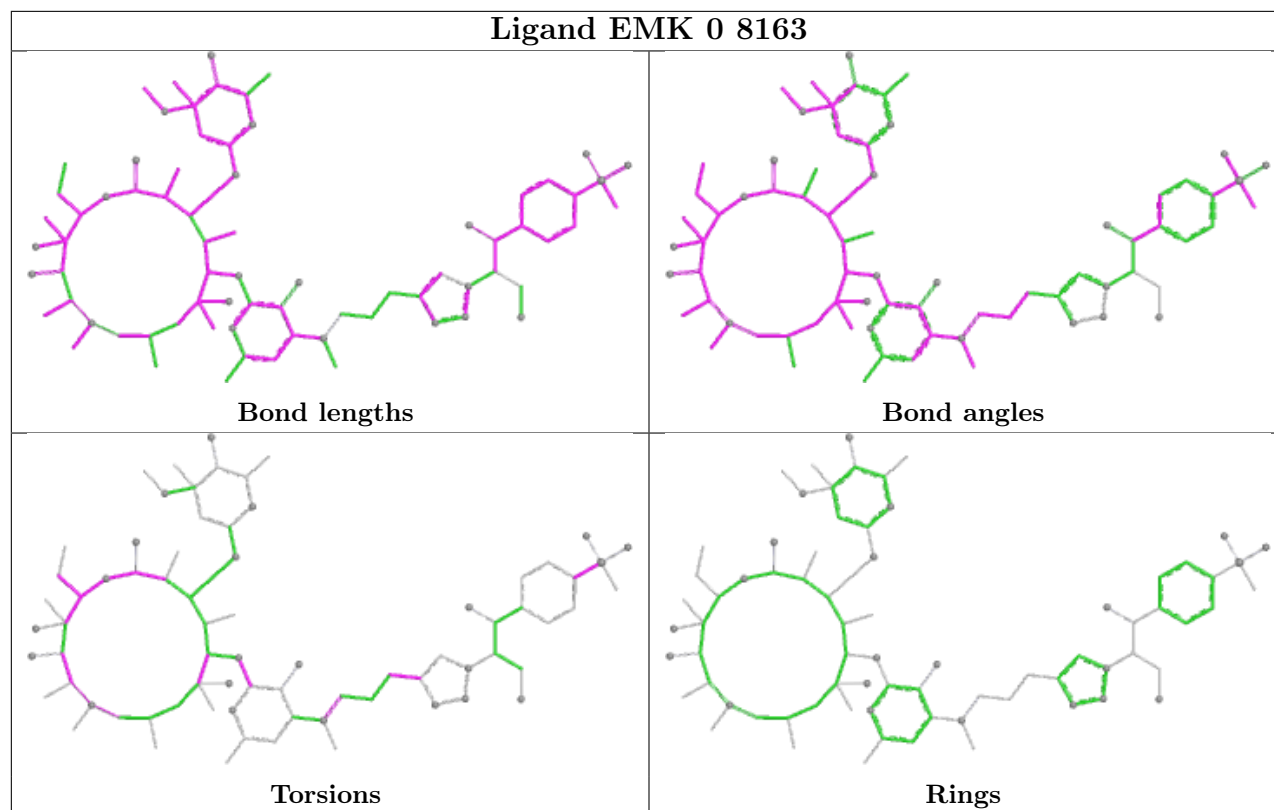
Mol	Chain	Res	Type	Atoms
36	0	8163	EMK	C4-C5-C6-O72
36	0	8163	EMK	C20-C12-N9-C9
36	0	8163	EMK	O41-C39-O42-C5
36	0	8163	EMK	O75-C15-C24-C25
36	0	8163	EMK	O42-C5-C6-C7
36	0	8163	EMK	C40-C39-O42-C5
36	0	8163	EMK	C4-C5-C6-C18
36	0	8163	EMK	O70-C1-O75-C15
36	0	8163	EMK	C90-C89-S1-O95

There are no ring outliers.

1 monomer is involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	0	8163	EMK	30	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2754/2902 (94%)	-0.06	147 (5%) 33 31	18, 37, 79, 130	0
2	9	122/122 (100%)	0.66	8 (6%) 26 24	30, 54, 76, 135	0
3	A	237/237 (100%)	0.41	15 (6%) 27 25	21, 41, 70, 88	0
4	B	337/337 (100%)	0.40	17 (5%) 35 33	21, 42, 67, 79	0
5	C	246/246 (100%)	0.15	4 (1%) 70 70	20, 37, 59, 70	0
6	D	140/165 (84%)	2.46	67 (47%) 0 1	49, 82, 103, 111	0
7	E	172/172 (100%)	0.71	9 (5%) 34 31	37, 55, 72, 78	0
8	F	119/119 (100%)	1.10	17 (14%) 7 7	39, 60, 86, 91	0
9	G	29/62 (46%)	2.32	14 (48%) 0 1	65, 81, 86, 91	0
10	H	156/167 (93%)	0.95	26 (16%) 5 5	28, 47, 72, 78	0
11	I	142/142 (100%)	0.35	6 (4%) 41 39	29, 40, 56, 75	0
12	J	132/132 (100%)	0.14	5 (3%) 44 42	26, 38, 60, 71	0
13	K	145/150 (96%)	1.05	28 (19%) 4 4	21, 52, 89, 104	0
14	L	194/194 (100%)	0.40	14 (7%) 23 21	27, 37, 51, 58	0
15	M	186/186 (100%)	1.14	35 (18%) 4 4	34, 52, 93, 104	0
16	N	115/115 (100%)	0.53	6 (5%) 34 31	33, 45, 60, 65	0
17	O	143/143 (100%)	0.32	4 (2%) 55 53	29, 42, 54, 64	0
18	P	95/95 (100%)	0.32	5 (5%) 33 31	29, 38, 53, 66	0
19	Q	150/150 (100%)	-0.08	1 (0%) 84 83	24, 35, 52, 60	0
20	R	81/81 (100%)	0.57	4 (4%) 36 34	35, 49, 69, 77	0
21	S	119/119 (100%)	0.55	10 (8%) 18 17	33, 44, 66, 91	0
22	T	53/53 (100%)	0.36	1 (1%) 66 65	34, 42, 60, 70	0
23	U	65/65 (100%)	1.43	15 (23%) 2 3	44, 64, 98, 105	0
24	V	154/154 (100%)	0.22	3 (1%) 66 65	28, 39, 56, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	82/82 (100%)	0.81	12 (14%) 7 6	34, 46, 69, 87	0
26	X	142/142 (100%)	0.06	5 (3%) 47 45	22, 34, 55, 73	0
27	Y	73/73 (100%)	1.49	21 (28%) 1 2	39, 52, 64, 74	0
28	Z	56/56 (100%)	-0.20	1 (1%) 67 67	20, 27, 32, 42	0
29	1	46/48 (95%)	0.83	8 (17%) 5 5	27, 45, 63, 80	0
30	2	92/92 (100%)	0.18	1 (1%) 77 77	25, 44, 55, 66	0
All	All	6577/6801 (96%)	0.32	509 (7%) 21 19	18, 41, 80, 135	0

All (509) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	1	THR	12.6
2	9	3001	U	9.5
6	D	63	ILE	8.4
6	D	10	PHE	8.1
23	U	40	PRO	8.0
1	0	2748	G	7.9
25	W	88	GLU	7.6
15	M	165	ALA	7.5
29	1	35	ARG	7.3
15	M	166	ALA	7.3
3	A	37	VAL	7.1
9	G	12	ILE	7.0
11	I	4	ALA	7.0
6	D	172	VAL	6.9
2	9	3025	G	6.7
23	U	2	VAL	6.5
15	M	168	LEU	6.4
21	S	117	ASP	6.4
2	9	3024	U	6.3
6	D	35	ALA	6.3
27	Y	11	THR	6.3
1	0	1199	A	6.1
1	0	10	U	6.1
4	B	1	PRO	6.1
1	0	1173	A	6.0
1	0	514	G	6.0
2	9	3002	U	6.0
1	0	960	G	6.0
6	D	19	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
15	M	154	LEU	6.0
15	M	162	ASP	5.9
1	0	2637	A	5.8
6	D	107	GLY	5.8
1	0	1200	A	5.8
23	U	39	ALA	5.8
1	0	2237	G	5.7
15	M	184	ILE	5.7
6	D	59	GLY	5.7
29	1	49	GLU	5.6
1	0	736	A	5.6
15	M	160	SER	5.5
6	D	135	VAL	5.4
1	0	1195	G	5.3
7	E	87	PHE	5.3
1	0	2345	A	5.3
1	0	1175	G	5.2
14	L	165	SER	5.2
1	0	1161	A	5.2
1	0	1197	G	5.2
13	K	148	GLU	5.2
1	0	735	C	5.1
6	D	18	ILE	5.0
6	D	66	GLY	5.0
13	K	149	ARG	5.0
1	0	1929	G	5.0
20	R	81	ILE	5.0
1	0	1561	U	4.9
1	0	1951	G	4.9
10	H	164	ALA	4.9
13	K	78	ALA	4.9
14	L	87	MET	4.9
25	W	87	ALA	4.9
6	D	134	LEU	4.8
1	0	2747	C	4.8
6	D	61	PHE	4.8
6	D	171	ASP	4.8
15	M	163	PHE	4.8
1	0	1176	C	4.8
6	D	93	LEU	4.8
1	0	1172	G	4.7
6	D	170	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	0	1965	C	4.7
1	0	272	A	4.7
9	G	71	LEU	4.7
6	D	55	LYS	4.7
1	0	1157	C	4.6
6	D	44	ILE	4.6
6	D	53	LYS	4.6
1	0	128	A	4.5
14	L	89	ASN	4.5
1	0	1203	G	4.5
6	D	174	VAL	4.5
7	E	45	ASP	4.5
1	0	1174	A	4.5
1	0	1202	A	4.4
13	K	146	GLY	4.4
13	K	99	GLU	4.4
1	0	1165	G	4.4
27	Y	78	ALA	4.4
7	E	154	ILE	4.4
26	X	235	GLU	4.4
21	S	118	SER	4.4
1	0	1201	C	4.3
1	0	2911	C	4.3
6	D	54	ALA	4.3
3	A	236	GLY	4.3
1	0	284	C	4.3
7	E	10	ASP	4.3
6	D	37	ALA	4.3
15	M	169	PRO	4.3
1	0	2508	C	4.3
1	0	2769	C	4.3
1	0	1950	G	4.3
1	0	1169	U	4.3
13	K	150	GLN	4.3
1	0	497	A	4.3
13	K	77	ALA	4.2
14	L	79	LYS	4.2
10	H	40	PRO	4.2
8	F	100	ASP	4.2
15	M	186	LEU	4.2
15	M	182	GLY	4.2
1	0	1196	C	4.2

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Mol	Chain	Res	Type	RSRZ
1	0	1966	U	4.2
27	Y	10	ARG	4.1
1	0	1967	U	4.1
13	K	75	LEU	4.1
2	9	3023	U	4.1
1	0	1699	C	4.1
1	0	734	U	4.1
1	0	1948	G	4.1
1	0	1171	A	4.1
27	Y	80	MET	4.1
10	H	78	ALA	4.0
3	A	211	LYS	4.0
1	0	1204	C	4.0
15	M	164	ASP	4.0
15	M	167	ASP	4.0
23	U	43	PRO	4.0
14	L	152	ARG	4.0
13	K	147	GLU	4.0
1	0	1947	G	4.0
14	L	35	PRO	4.0
6	D	90	LEU	4.0
1	0	970	U	4.0
8	F	101	ALA	3.9
6	D	101	THR	3.9
6	D	36	ASN	3.9
6	D	11	HIS	3.9
1	0	2004	U	3.9
8	F	107	VAL	3.9
18	P	20	ASP	3.9
9	G	26	MET	3.9
11	I	70	PHE	3.9
14	L	16	LYS	3.9
1	0	2511	A	3.9
6	D	138	GLY	3.9
10	H	140	PRO	3.9
27	Y	19	GLY	3.9
25	W	85	VAL	3.8
10	H	165	GLY	3.8
1	0	1184	C	3.8
13	K	98	GLU	3.8
10	H	138	PRO	3.8
11	I	92	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
13	K	60	GLU	3.7
6	D	153	THR	3.7
30	2	56	PRO	3.7
8	F	103	ALA	3.7
1	0	1162	G	3.7
1	0	2344	G	3.7
1	0	1964	U	3.7
1	0	1205	U	3.7
25	W	83	ALA	3.7
8	F	106	THR	3.6
5	C	61	PHE	3.6
27	Y	44	PHE	3.6
21	S	119	ALA	3.6
1	0	1170	U	3.6
1	0	1198	U	3.6
1	0	1701	A	3.6
1	0	2913	A	3.6
15	M	21	HIS	3.6
1	0	1206	U	3.6
13	K	82	ALA	3.6
6	D	62	ASP	3.6
21	S	116	ASP	3.6
27	Y	47	LEU	3.5
1	0	271	C	3.5
18	P	17	LYS	3.5
1	0	2909	G	3.5
1	0	1177	A	3.5
1	0	1207	A	3.5
15	M	161	GLY	3.5
8	F	78	GLU	3.5
18	P	18	PRO	3.5
9	G	21	ASP	3.4
13	K	73	VAL	3.4
1	0	2512	U	3.4
10	H	77	ALA	3.4
10	H	167	ALA	3.4
8	F	8	VAL	3.4
6	D	150	SER	3.4
9	G	29	SER	3.4
6	D	29	HIS	3.4
6	D	17	ARG	3.4
27	Y	82	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
10	H	126	HIS	3.4
9	G	73	ASP	3.3
1	0	282	C	3.3
2	9	3122	C	3.3
4	B	21	SER	3.3
16	N	23	GLY	3.3
15	M	185	GLU	3.3
27	Y	22	ILE	3.3
10	H	136	VAL	3.3
12	J	119	GLN	3.3
1	0	737	A	3.2
6	D	22	VAL	3.2
13	K	76	LEU	3.2
25	W	46	ASP	3.2
6	D	64	ARG	3.2
4	B	183	GLU	3.2
1	0	1160	G	3.2
1	0	2664	A	3.2
15	M	183	ASP	3.2
1	0	999	C	3.2
8	F	105	ALA	3.2
10	H	38	ALA	3.2
29	1	20	ARG	3.2
29	1	44	ARG	3.2
21	S	36	GLY	3.2
1	0	1194	A	3.2
1	0	1625	U	3.2
6	D	154	LYS	3.2
1	0	1156	C	3.2
1	0	1186	C	3.2
6	D	91	ALA	3.2
27	Y	41	VAL	3.2
1	0	1190	G	3.1
6	D	40	ILE	3.1
15	M	179	LEU	3.1
14	L	174	ARG	3.1
6	D	102	GLY	3.1
6	D	86	THR	3.1
10	H	85	ILE	3.1
6	D	65	GLU	3.1
1	0	1524	U	3.1
1	0	2914	A	3.1

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Mol	Chain	Res	Type	RSRZ
10	H	41	THR	3.1
14	L	140	ALA	3.1
16	N	24	ALA	3.1
13	K	55	GLN	3.1
3	A	35	GLY	3.1
1	0	1163	G	3.0
15	M	95	ALA	3.0
6	D	13	MET	3.0
1	0	1168	C	3.0
1	0	1182	C	3.0
21	S	53	GLY	3.0
3	A	36	ASP	3.0
10	H	109	ASP	3.0
1	0	2506	A	3.0
10	H	146	TRP	3.0
7	E	156	ASP	3.0
1	0	283	U	3.0
4	B	108	GLU	3.0
13	K	44	GLU	3.0
15	M	158	LEU	3.0
1	0	2850	C	3.0
13	K	96	VAL	3.0
11	I	96	GLU	2.9
20	R	12	GLU	2.9
1	0	2419	U	2.9
9	G	14	GLU	2.9
1	0	2768	A	2.9
6	D	20	LYS	2.9
13	K	62	ALA	2.9
28	Z	47	ASP	2.9
23	U	38	GLY	2.9
15	M	152	GLU	2.9
1	0	1279	U	2.9
6	D	169	THR	2.9
6	D	69	ILE	2.9
26	X	216	ARG	2.9
1	0	1634	G	2.9
13	K	100	ALA	2.9
6	D	133	ASN	2.9
1	0	1192	A	2.9
1	0	1193	A	2.9
9	G	24	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
6	D	81	GLU	2.8
25	W	79	GLU	2.8
25	W	80	GLU	2.8
1	0	1191	A	2.8
6	D	68	PRO	2.8
1	0	969	G	2.8
6	D	12	GLU	2.8
27	Y	16	PRO	2.8
15	M	175	LEU	2.8
23	U	65	ASP	2.8
25	W	69	LYS	2.8
7	E	6	GLU	2.8
20	R	76	GLU	2.8
23	U	41	GLU	2.8
1	0	138	U	2.8
1	0	2749	U	2.8
21	S	114	SER	2.8
1	0	280	C	2.8
1	0	2825	C	2.8
23	U	44	GLY	2.8
3	A	85	ASP	2.8
4	B	118	ASP	2.8
23	U	42	ASN	2.7
24	V	86	GLU	2.7
1	0	1185	U	2.7
1	0	1178	G	2.7
15	M	68	GLU	2.7
6	D	52	THR	2.7
12	J	118	ALA	2.7
25	W	71	ARG	2.7
12	J	100	GLU	2.7
1	0	273	G	2.7
1	0	716	G	2.7
6	D	58	VAL	2.7
6	D	157	LEU	2.7
9	G	23	ILE	2.7
3	A	33	GLU	2.7
15	M	138	ASP	2.7
16	N	31	GLU	2.7
24	V	76	ASP	2.7
3	A	31	LYS	2.7
1	0	87	C	2.7

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Mol	Chain	Res	Type	RSRZ
1	0	1000	C	2.7
1	0	583	G	2.7
1	0	1159	G	2.7
6	D	56	ARG	2.7
15	M	170	GLU	2.6
17	O	92	GLU	2.6
13	K	143	THR	2.6
14	L	156	ARG	2.6
27	Y	58	GLY	2.6
4	B	139	ASP	2.6
7	E	12	ASP	2.6
26	X	95	THR	2.6
11	I	5	GLU	2.6
1	0	1183	C	2.6
1	0	2912	C	2.6
1	0	1525	G	2.6
1	0	1970	G	2.6
15	M	180	LEU	2.6
1	0	1164	U	2.6
13	K	130	ARG	2.6
22	T	47	ARG	2.6
21	S	58	GLU	2.6
3	A	84	VAL	2.6
1	0	1208	C	2.6
5	C	2	GLN	2.6
1	0	1180	U	2.6
17	O	12	ASP	2.5
29	1	16	ASN	2.5
23	U	37	GLY	2.5
1	0	1181	A	2.5
1	0	2238	A	2.5
27	Y	36	LYS	2.5
1	0	714	U	2.5
1	0	1158	G	2.5
6	D	21	VAL	2.5
6	D	99	ASP	2.5
13	K	36	ASP	2.5
26	X	236	VAL	2.5
6	D	106	PHE	2.5
7	E	155	ASN	2.5
10	H	37	GLY	2.5
16	N	3	THR	2.5

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Mol	Chain	Res	Type	RSRZ
16	N	22	GLY	2.5
1	0	1179	C	2.5
6	D	105	SER	2.5
6	D	104	PHE	2.5
13	K	43	HIS	2.5
15	M	67	ALA	2.5
27	Y	50	ALA	2.5
27	Y	21	LYS	2.5
29	1	31	GLU	2.5
15	M	157	PRO	2.5
1	0	1189	A	2.5
3	A	64	ASP	2.5
10	H	59	ASN	2.5
25	W	84	ILE	2.5
8	F	99	THR	2.5
1	0	369	G	2.4
1	0	2826	G	2.4
4	B	2	GLN	2.4
4	B	230	GLN	2.4
10	H	83	PHE	2.4
16	N	80	ASP	2.4
26	X	108	ASP	2.4
1	0	1698	U	2.4
1	0	285	A	2.4
4	B	64	GLY	2.4
10	H	86	ARG	2.4
1	0	2136	G	2.4
14	L	1	ALA	2.4
3	A	38	ILE	2.4
4	B	33	ASP	2.4
10	H	35	ASN	2.4
13	K	101	ASP	2.4
20	R	3	ASP	2.4
1	0	300	C	2.4
3	A	206	ARG	2.4
1	0	2620	U	2.4
1	0	2334	C	2.4
8	F	102	GLY	2.4
6	D	145	ASP	2.4
6	D	60	GLU	2.3
6	D	88	LEU	2.3
1	0	301	G	2.3

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Mol	Chain	Res	Type	RSRZ
2	9	3022	G	2.3
14	L	26	HIS	2.3
1	0	2910	A	2.3
1	0	130	C	2.3
17	O	15	ASP	2.3
14	L	75	THR	2.3
29	1	39	ARG	2.3
6	D	49	PRO	2.3
1	0	1526	A	2.3
25	W	81	GLY	2.3
6	D	75	LEU	2.3
4	B	20	THR	2.3
15	M	40	ASN	2.3
21	S	115	GLU	2.3
5	C	162	VAL	2.3
18	P	84	ILE	2.3
8	F	28	ALA	2.3
11	I	93	ARG	2.2
3	A	34	ASP	2.2
1	0	809	G	2.2
8	F	91	VAL	2.2
13	K	81	VAL	2.2
1	0	2291	A	2.2
4	B	185	GLY	2.2
8	F	108	LEU	2.2
9	G	67	LEU	2.2
8	F	90	GLU	2.2
9	G	68	GLU	2.2
7	E	100	ASP	2.2
29	1	48	ASP	2.2
4	B	171	VAL	2.2
13	K	97	VAL	2.2
17	O	143	ALA	2.2
1	0	1167	G	2.2
1	0	1949	G	2.2
1	0	1527	A	2.2
8	F	119	ARG	2.2
10	H	161	SER	2.2
6	D	159	PRO	2.2
23	U	13	PRO	2.2
10	H	166	ASN	2.2
14	L	78	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
15	M	65	ASP	2.2
15	M	181	ASP	2.2
15	M	147	ILE	2.2
19	Q	122	GLN	2.2
13	K	83	GLU	2.2
15	M	149	GLU	2.2
1	0	1188	A	2.2
2	9	3051	A	2.2
1	0	1523	G	2.2
4	B	286	ASN	2.2
6	D	98	PHE	2.2
10	H	56	ILE	2.2
12	J	8	VAL	2.2
6	D	72	LYS	2.2
27	Y	48	LYS	2.2
25	W	10	VAL	2.1
6	D	48	MET	2.1
1	0	2770	G	2.1
10	H	158	ASN	2.1
4	B	5	ARG	2.1
1	0	288	A	2.1
3	A	1	GLY	2.1
3	A	210	GLY	2.1
6	D	26	GLY	2.1
27	Y	38	LYS	2.1
1	0	125	U	2.1
8	F	2	VAL	2.1
8	F	16	ALA	2.1
12	J	127	ALA	2.1
23	U	17	GLU	2.1
1	0	2509	A	2.1
13	K	26	HIS	2.1
27	Y	35	LYS	2.1
5	C	233	THR	2.1
27	Y	64	ILE	2.1
1	0	2831	C	2.1
1	0	200	U	2.1
24	V	148	ASP	2.1
4	B	34	GLY	2.1
15	M	2	THR	2.0
15	M	153	GLN	2.0
27	Y	20	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
4	B	191	ASN	2.0
23	U	31	ARG	2.0
23	U	45	ARG	2.0
9	G	70	ALA	2.0
27	Y	65	ALA	2.0
1	0	281	U	2.0
1	0	1488	U	2.0
1	0	31	C	2.0
1	0	368	C	2.0
1	0	1209	C	2.0
9	G	28	GLU	2.0
18	P	81	GLU	2.0
10	H	156	THR	2.0
9	G	20	VAL	2.0
10	H	73	GLN	2.0
1	0	363	A	2.0
6	D	142	ALA	2.0
21	S	5	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	K	0	8056	1/1	0.60	0.38	88,88,88,88	0
33	NA	I	201	1/1	0.64	0.37	54,54,54,54	0
31	MG	0	8012	1/1	0.65	0.51	53,53,53,53	0
33	NA	0	8063	1/1	0.66	0.46	48,48,48,48	0
31	MG	0	8035	1/1	0.66	0.69	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	0	8074	1/1	0.67	0.33	60,60,60,60	0
33	NA	0	8075	1/1	0.67	0.49	63,63,63,63	0
31	MG	B	401	1/1	0.67	0.46	66,66,66,66	0
33	NA	0	8064	1/1	0.69	0.36	61,61,61,61	0
33	NA	9	3202	1/1	0.70	0.43	93,93,93,93	0
31	MG	0	8053	1/1	0.71	0.44	52,52,52,52	0
31	MG	0	8043	1/1	0.73	0.65	63,63,63,63	0
31	MG	0	8018	1/1	0.73	0.44	47,47,47,47	0
35	SR	0	8154	1/1	0.73	0.24	147,147,147,147	0
33	NA	0	8068	1/1	0.74	0.34	42,42,42,42	0
31	MG	0	8050	1/1	0.74	0.42	78,78,78,78	0
35	SR	0	8149	1/1	0.75	0.25	200,200,200,200	0
35	SR	0	8146	1/1	0.75	0.23	156,156,156,156	0
31	MG	J	201	1/1	0.77	0.33	32,32,32,32	0
31	MG	0	8047	1/1	0.77	0.32	49,49,49,49	0
31	MG	0	8054	1/1	0.79	0.17	53,53,53,53	0
35	SR	0	8128	1/1	0.79	0.22	92,92,92,92	0
33	NA	0	8058	1/1	0.79	0.26	62,62,62,62	0
31	MG	0	8032	1/1	0.79	0.36	46,46,46,46	0
31	MG	0	8027	1/1	0.79	0.26	51,51,51,51	0
31	MG	0	8017	1/1	0.80	0.34	36,36,36,36	0
31	MG	S	201	1/1	0.80	0.47	59,59,59,59	0
31	MG	0	8038	1/1	0.80	0.48	54,54,54,54	0
35	SR	Z	103	1/1	0.80	0.28	140,140,140,140	0
35	SR	0	8081	1/1	0.81	0.20	91,91,91,91	0
31	MG	0	8041	1/1	0.81	0.34	52,52,52,52	0
33	NA	0	8073	1/1	0.81	0.20	54,54,54,54	0
35	SR	0	8148	1/1	0.82	0.26	132,132,132,132	0
33	NA	0	8057	1/1	0.82	0.34	46,46,46,46	0
33	NA	Q	201	1/1	0.82	0.37	57,57,57,57	0
35	SR	0	8162	1/1	0.82	0.16	103,103,103,103	0
33	NA	Q	202	1/1	0.82	0.37	66,66,66,66	0
33	NA	0	8070	1/1	0.83	0.33	69,69,69,69	0
33	NA	0	8062	1/1	0.83	0.26	39,39,39,39	0
35	SR	0	8155	1/1	0.83	0.26	135,135,135,135	0
33	NA	0	8065	1/1	0.83	0.21	48,48,48,48	0
31	MG	0	8033	1/1	0.83	0.30	62,62,62,62	0
31	MG	0	8051	1/1	0.84	0.35	54,54,54,54	0
31	MG	0	8036	1/1	0.84	0.20	52,52,52,52	0
31	MG	0	8005	1/1	0.84	0.28	32,32,32,32	0
35	SR	B	402	1/1	0.84	0.35	90,90,90,90	0
33	NA	0	8072	1/1	0.84	0.53	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	SR	0	8141	1/1	0.85	0.19	160,160,160,160	0
35	SR	0	8142	1/1	0.85	0.23	138,138,138,138	0
31	MG	0	8028	1/1	0.85	0.19	48,48,48,48	0
31	MG	0	8025	1/1	0.85	0.25	56,56,56,56	0
31	MG	0	8044	1/1	0.85	0.23	51,51,51,51	0
35	SR	0	8158	1/1	0.86	0.15	128,128,128,128	0
35	SR	0	8106	1/1	0.86	0.26	128,128,128,128	0
35	SR	9	3204	1/1	0.86	0.14	122,122,122,122	0
33	NA	0	8071	1/1	0.86	0.43	51,51,51,51	0
31	MG	0	8010	1/1	0.86	0.32	42,42,42,42	0
33	NA	P	101	1/1	0.87	0.19	45,45,45,45	0
31	MG	0	8014	1/1	0.87	0.49	50,50,50,50	0
35	SR	0	8151	1/1	0.87	0.12	122,122,122,122	0
31	MG	0	8026	1/1	0.87	0.28	56,56,56,56	0
31	MG	0	8016	1/1	0.87	0.30	40,40,40,40	0
31	MG	0	8021	1/1	0.87	0.27	42,42,42,42	0
31	MG	0	8037	1/1	0.87	0.27	58,58,58,58	0
31	MG	0	8029	1/1	0.87	0.28	54,54,54,54	0
35	SR	9	3205	1/1	0.87	0.19	141,141,141,141	0
35	SR	A	305	1/1	0.87	0.15	133,133,133,133	0
31	MG	0	8052	1/1	0.87	0.44	56,56,56,56	0
33	NA	L	201	1/1	0.87	0.37	62,62,62,62	0
31	MG	0	8001	1/1	0.88	0.23	27,27,27,27	0
33	NA	0	8059	1/1	0.88	0.27	39,39,39,39	0
31	MG	0	8031	1/1	0.88	0.41	50,50,50,50	0
35	SR	0	8116	1/1	0.88	0.15	117,117,117,117	0
33	NA	0	8067	1/1	0.88	0.29	57,57,57,57	0
35	SR	0	8145	1/1	0.89	0.20	126,126,126,126	0
31	MG	0	8034	1/1	0.89	0.21	60,60,60,60	0
35	SR	0	8122	1/1	0.89	0.14	113,113,113,113	0
31	MG	0	8011	1/1	0.89	0.43	40,40,40,40	0
35	SR	0	8137	1/1	0.89	0.14	151,151,151,151	0
31	MG	0	8045	1/1	0.89	0.45	75,75,75,75	0
35	SR	B	403	1/1	0.89	0.16	106,106,106,106	0
31	MG	0	8023	1/1	0.89	0.38	56,56,56,56	0
36	EMK	0	8163	74/74	0.89	0.20	40,48,59,62	0
35	SR	0	8161	1/1	0.90	0.36	137,137,137,137	0
31	MG	0	8015	1/1	0.90	0.47	39,39,39,39	0
35	SR	9	3203	1/1	0.90	0.17	110,110,110,110	0
31	MG	0	8013	1/1	0.90	0.39	34,34,34,34	0
35	SR	0	8099	1/1	0.90	0.24	94,94,94,94	0
35	SR	0	8152	1/1	0.90	0.16	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	0	8061	1/1	0.90	0.35	56,56,56,56	0
31	MG	0	8055	1/1	0.90	0.19	45,45,45,45	0
31	MG	0	8003	1/1	0.90	0.30	43,43,43,43	0
35	SR	0	8159	1/1	0.90	0.13	118,118,118,118	0
35	SR	0	8157	1/1	0.91	0.12	125,125,125,125	0
31	MG	0	8046	1/1	0.91	0.28	47,47,47,47	0
35	SR	0	8114	1/1	0.91	0.18	101,101,101,101	0
31	MG	0	8006	1/1	0.91	0.28	26,26,26,26	0
35	SR	0	8119	1/1	0.91	0.20	106,106,106,106	0
35	SR	0	8120	1/1	0.91	0.12	82,82,82,82	0
33	NA	C	301	1/1	0.91	0.20	35,35,35,35	0
35	SR	0	8150	1/1	0.91	0.13	128,128,128,128	0
33	NA	0	8069	1/1	0.91	0.12	37,37,37,37	0
35	SR	0	8130	1/1	0.91	0.13	106,106,106,106	0
35	SR	0	8153	1/1	0.91	0.15	130,130,130,130	0
35	SR	F	201	1/1	0.91	0.18	102,102,102,102	0
35	SR	0	8135	1/1	0.91	0.15	99,99,99,99	0
31	MG	9	3201	1/1	0.91	0.34	46,46,46,46	0
35	SR	0	8117	1/1	0.92	0.20	104,104,104,104	0
31	MG	0	8040	1/1	0.92	0.38	21,21,21,21	0
35	SR	0	8131	1/1	0.92	0.12	104,104,104,104	0
31	MG	0	8020	1/1	0.92	0.33	44,44,44,44	0
33	NA	0	8066	1/1	0.92	0.24	42,42,42,42	0
35	SR	0	8123	1/1	0.92	0.12	96,96,96,96	0
35	SR	0	8125	1/1	0.92	0.16	105,105,105,105	0
35	SR	0	8144	1/1	0.92	0.11	126,126,126,126	0
37	CD	Z	101	1/1	0.92	0.23	141,141,141,141	0
31	MG	0	8049	1/1	0.93	0.14	51,51,51,51	0
34	CL	Q	203	1/1	0.93	0.10	55,55,55,55	0
35	SR	0	8134	1/1	0.93	0.16	94,94,94,94	0
31	MG	0	8039	1/1	0.93	0.27	36,36,36,36	0
35	SR	0	8092	1/1	0.93	0.10	75,75,75,75	0
35	SR	0	8095	1/1	0.93	0.11	92,92,92,92	0
35	SR	0	8121	1/1	0.93	0.12	79,79,79,79	0
35	SR	0	8098	1/1	0.93	0.14	71,71,71,71	0
31	MG	0	8019	1/1	0.93	0.28	37,37,37,37	0
35	SR	0	8105	1/1	0.93	0.11	85,85,85,85	0
31	MG	0	8048	1/1	0.93	0.18	38,38,38,38	0
34	CL	L	202	1/1	0.94	0.13	51,51,51,51	0
35	SR	0	8147	1/1	0.94	0.18	105,105,105,105	0
35	SR	0	8133	1/1	0.94	0.15	102,102,102,102	0
31	MG	0	8009	1/1	0.94	0.42	35,35,35,35	0

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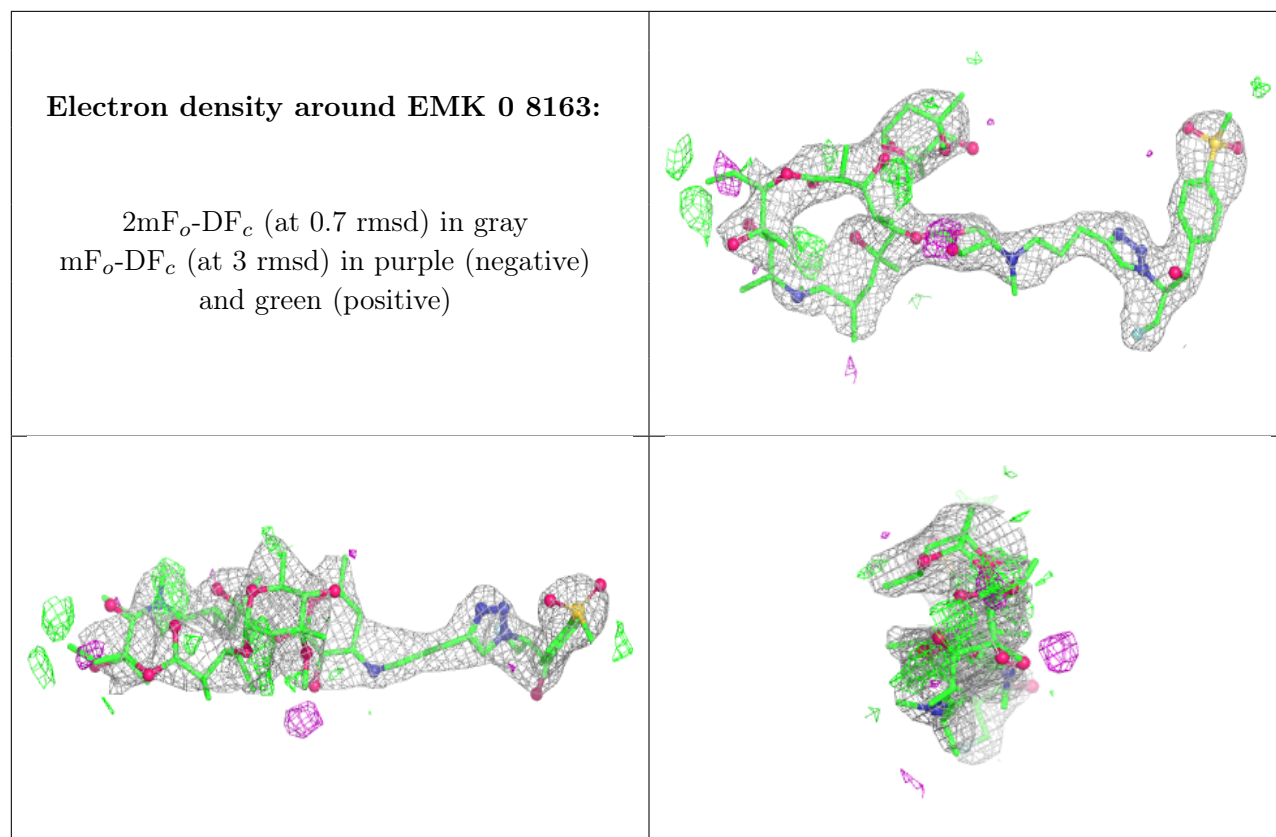
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	0	8030	1/1	0.94	0.37	49,49,49,49	0
33	NA	0	8060	1/1	0.94	0.13	46,46,46,46	0
35	SR	0	8139	1/1	0.94	0.12	101,101,101,101	0
35	SR	0	8140	1/1	0.94	0.14	108,108,108,108	0
35	SR	0	8115	1/1	0.94	0.10	101,101,101,101	0
31	MG	0	8007	1/1	0.94	0.28	28,28,28,28	0
35	SR	R	101	1/1	0.94	0.12	119,119,119,119	0
35	SR	0	8156	1/1	0.94	0.16	137,137,137,137	0
31	MG	0	8008	1/1	0.94	0.41	35,35,35,35	0
35	SR	0	8118	1/1	0.94	0.09	96,96,96,96	0
31	MG	X	301	1/1	0.95	0.16	39,39,39,39	0
34	CL	0	8080	1/1	0.95	0.09	51,51,51,51	0
35	SR	0	8109	1/1	0.95	0.11	88,88,88,88	0
35	SR	0	8113	1/1	0.95	0.11	75,75,75,75	0
35	SR	0	8094	1/1	0.95	0.12	56,56,56,56	0
34	CL	A	301	1/1	0.95	0.12	74,74,74,74	0
35	SR	0	8138	1/1	0.95	0.24	137,137,137,137	0
31	MG	0	8022	1/1	0.95	0.35	43,43,43,43	0
35	SR	0	8126	1/1	0.95	0.16	118,118,118,118	0
31	MG	0	8004	1/1	0.95	0.32	38,38,38,38	0
35	SR	0	8129	1/1	0.96	0.12	107,107,107,107	0
34	CL	0	8079	1/1	0.96	0.10	56,56,56,56	0
31	MG	0	8042	1/1	0.96	0.29	28,28,28,28	0
35	SR	0	8082	1/1	0.96	0.20	64,64,64,64	0
35	SR	0	8108	1/1	0.96	0.09	63,63,63,63	0
31	MG	0	8002	1/1	0.96	0.17	57,57,57,57	0
35	SR	A	304	1/1	0.96	0.09	95,95,95,95	0
35	SR	0	8136	1/1	0.96	0.10	80,80,80,80	0
35	SR	0	8112	1/1	0.96	0.09	75,75,75,75	0
34	CL	D	201	1/1	0.96	0.05	49,49,49,49	0
35	SR	0	8124	1/1	0.96	0.15	84,84,84,84	0
34	CL	0	8076	1/1	0.96	0.14	58,58,58,58	0
35	SR	0	8097	1/1	0.96	0.13	85,85,85,85	0
35	SR	0	8127	1/1	0.96	0.07	96,96,96,96	0
34	CL	N	201	1/1	0.96	0.16	74,74,74,74	0
35	SR	0	8087	1/1	0.97	0.12	77,77,77,77	0
35	SR	0	8088	1/1	0.97	0.09	62,62,62,62	0
35	SR	0	8089	1/1	0.97	0.11	69,69,69,69	0
35	SR	0	8160	1/1	0.97	0.06	59,59,59,59	0
35	SR	0	8091	1/1	0.97	0.10	81,81,81,81	0
35	SR	0	8110	1/1	0.97	0.13	89,89,89,89	0
35	SR	0	8111	1/1	0.97	0.07	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	CL	0	8077	1/1	0.97	0.13	55,55,55,55	0
34	CL	0	8078	1/1	0.97	0.12	63,63,63,63	0
35	SR	A	303	1/1	0.97	0.23	89,89,89,89	0
31	MG	K	201	1/1	0.97	0.34	3,3,3,3	0
35	SR	0	8096	1/1	0.97	0.10	63,63,63,63	0
35	SR	0	8132	1/1	0.97	0.10	100,100,100,100	0
34	CL	X	302	1/1	0.97	0.08	44,44,44,44	0
34	CL	I	202	1/1	0.97	0.10	58,58,58,58	0
34	CL	I	203	1/1	0.97	0.11	62,62,62,62	0
35	SR	0	8102	1/1	0.97	0.10	72,72,72,72	0
35	SR	2	103	1/1	0.97	0.07	74,74,74,74	0
35	SR	0	8103	1/1	0.97	0.10	84,84,84,84	0
37	CD	T	8701	1/1	0.97	0.17	118,118,118,118	0
35	SR	0	8104	1/1	0.97	0.13	77,77,77,77	0
35	SR	0	8101	1/1	0.98	0.14	75,75,75,75	0
35	SR	0	8090	1/1	0.98	0.15	72,72,72,72	0
35	SR	2	102	1/1	0.98	0.10	67,67,67,67	0
35	SR	0	8084	1/1	0.98	0.13	49,49,49,49	0
35	SR	A	302	1/1	0.98	0.09	86,86,86,86	0
31	MG	0	8024	1/1	0.98	0.36	20,20,20,20	0
37	CD	Y	101	1/1	0.98	0.16	112,112,112,112	0
35	SR	Q	204	1/1	0.98	0.10	70,70,70,70	0
35	SR	Z	102	1/1	0.99	0.10	56,56,56,56	0
35	SR	0	8085	1/1	0.99	0.11	50,50,50,50	0
35	SR	0	8100	1/1	0.99	0.12	68,68,68,68	0
35	SR	0	8086	1/1	0.99	0.09	46,46,46,46	0
35	SR	0	8143	1/1	0.99	0.07	63,63,63,63	0
35	SR	0	8107	1/1	0.99	0.08	62,62,62,62	0
35	SR	0	8093	1/1	0.99	0.08	57,57,57,57	0
35	SR	0	8083	1/1	0.99	0.12	46,46,46,46	0
37	CD	2	101	1/1	0.99	0.13	87,87,87,87	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.