Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 11:58 AM EDT

PDB ID	:	1YIJ
Title	:	Crystal Structure Of Telithromycin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors	:	Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2005-01-12
Resolution	:	2.60 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

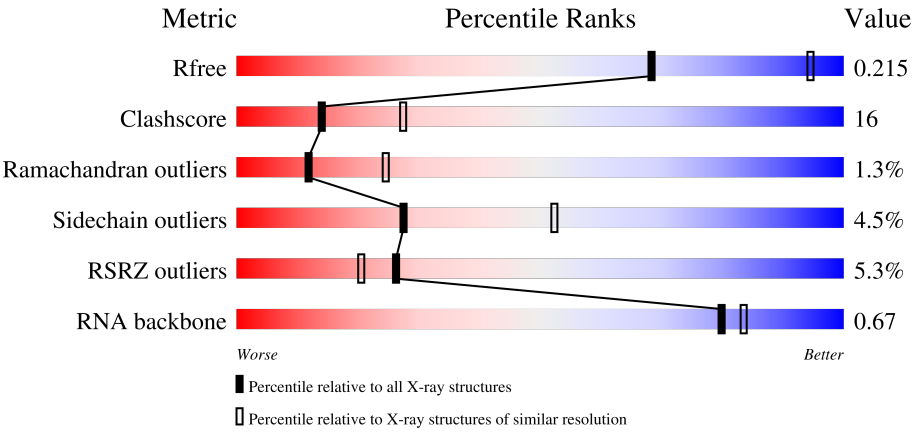
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)
RNA backbone	3102	1040 (2.90-2.30)

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 >=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 <=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	2922	2% 61% 27% 5% 6%
2	9	122	4% 53% 36% 9%
3	A	240	5% 60% 33% 5%
4	B	338	% 50% 45% 5%

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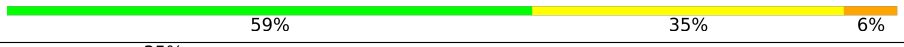
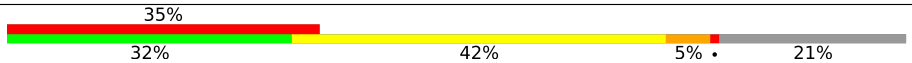
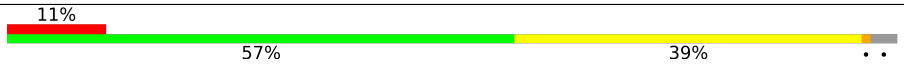
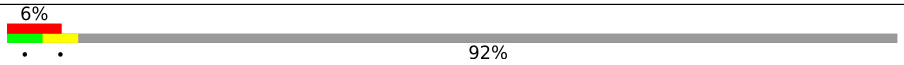
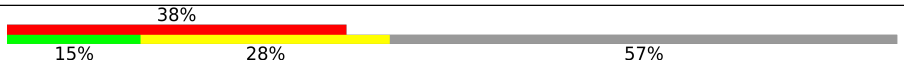
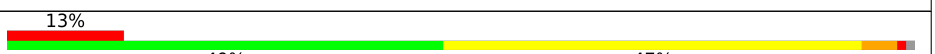
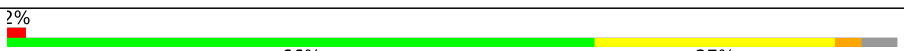
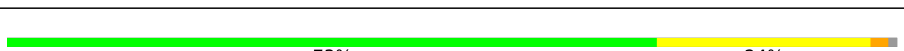
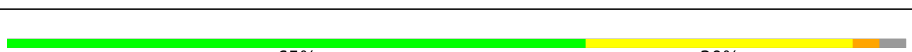
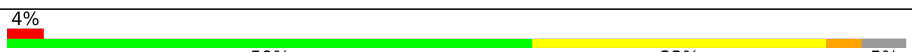
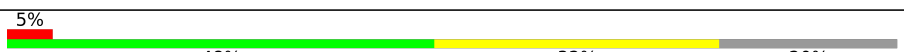
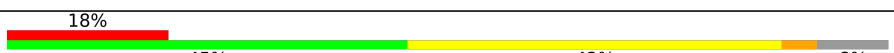
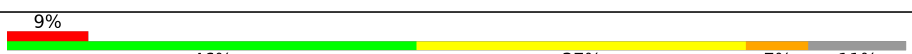
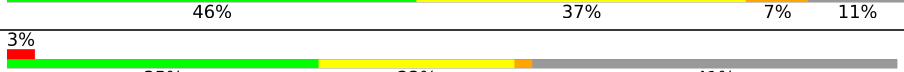
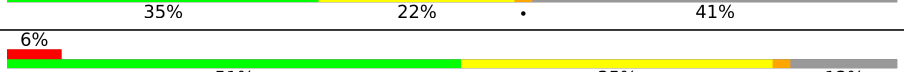
Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	

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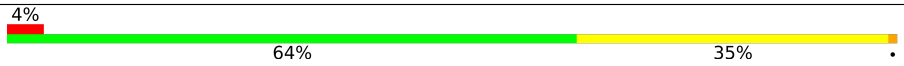
Mol	Chain	Length	Quality of chain
30	2	50	
31	3	92	

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
34	NA	0	8571	-	-	-	X
34	NA	R	8586	-	-	-	X

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 99097 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
			Total	C	N	O	P			
1	0	2754	59020	26349	10873	19053	2745	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 55229667
0	2099	A	G	engineered mutation	GB 55229667
0	2587	OMU	U	modified residue	GB 55229667
0	2588	OMG	G	modified residue	GB 55229667
0	2619	UR3	U	modified residue	GB 55229667
0	2621	PSU	U	modified residue	GB 55229667

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	9	122	2599	1160	471	847	121	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	237	1753	1072	352	324	5	0	0	0

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

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

- Molecule 5 is a protein called 50S ribosomal protein L4E.

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
			1094	685	195	210	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
			1357	840	224	289	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
			890	551	141	197	1			

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 21 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 24 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 27 is a protein called 50S ribosomal protein L32E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
27	Y	142	Total	C	N	O	0	0	0
			1130	686	228	216			

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	106	Total	Mg	0	0
			106	106		
32	9	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	B	2	Total	Mg	0	0
			2	2		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	3	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	2	Total	K	0	0
			2	2		

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	72	Total	Na	0	0
			72	72		
34	9	2	Total	Na	0	0
			2	2		
34	A	1	Total	Na	0	0
			1	1		
34	C	1	Total	Na	0	0
			1	1		

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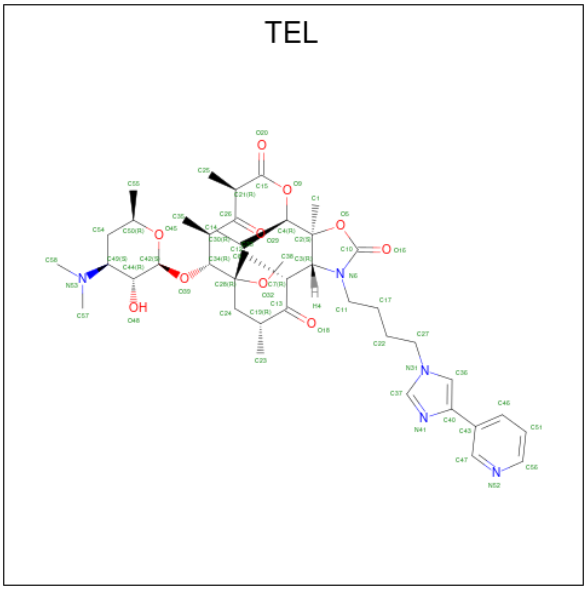
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	H	1	Total Na 1 1	0	0
34	J	1	Total Na 1 1	0	0
34	L	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	R	3	Total Na 3 3	0	0
34	S	1	Total Na 1 1	0	0
34	T	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	9	Total Cl 9 9	0	0
35	A	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	J	3	Total Cl 3 3	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	2	Total Cl 2 2	0	0
35	3	1	Total Cl 1 1	0	0

- Molecule 36 is TELITHROMYCIN (three-letter code: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	1	Total C N O 58 43 5 10	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5881	Total O 5881 5881	0	0
38	9	140	Total O 140 140	0	0
38	A	120	Total O 120 120	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	B	153	Total O 153 153	0	0
38	C	174	Total O 174 174	0	0
38	D	46	Total O 46 46	0	0
38	E	41	Total O 41 41	0	0
38	F	27	Total O 27 27	0	0
38	G	18	Total O 18 18	0	0
38	H	71	Total O 71 71	0	0
38	I	9	Total O 9 9	0	0
38	J	54	Total O 54 54	0	0
38	K	65	Total O 65 65	0	0
38	L	83	Total O 83 83	0	0
38	M	130	Total O 130 130	0	0
38	N	62	Total O 62 62	0	0
38	O	41	Total O 41 41	0	0
38	P	62	Total O 62 62	0	0
38	Q	46	Total O 46 46	0	0
38	R	81	Total O 81 81	0	0
38	S	38	Total O 38 38	0	0
38	T	37	Total O 37 37	0	0
38	U	25	Total O 25 25	0	0
38	V	14	Total O 14 14	0	0

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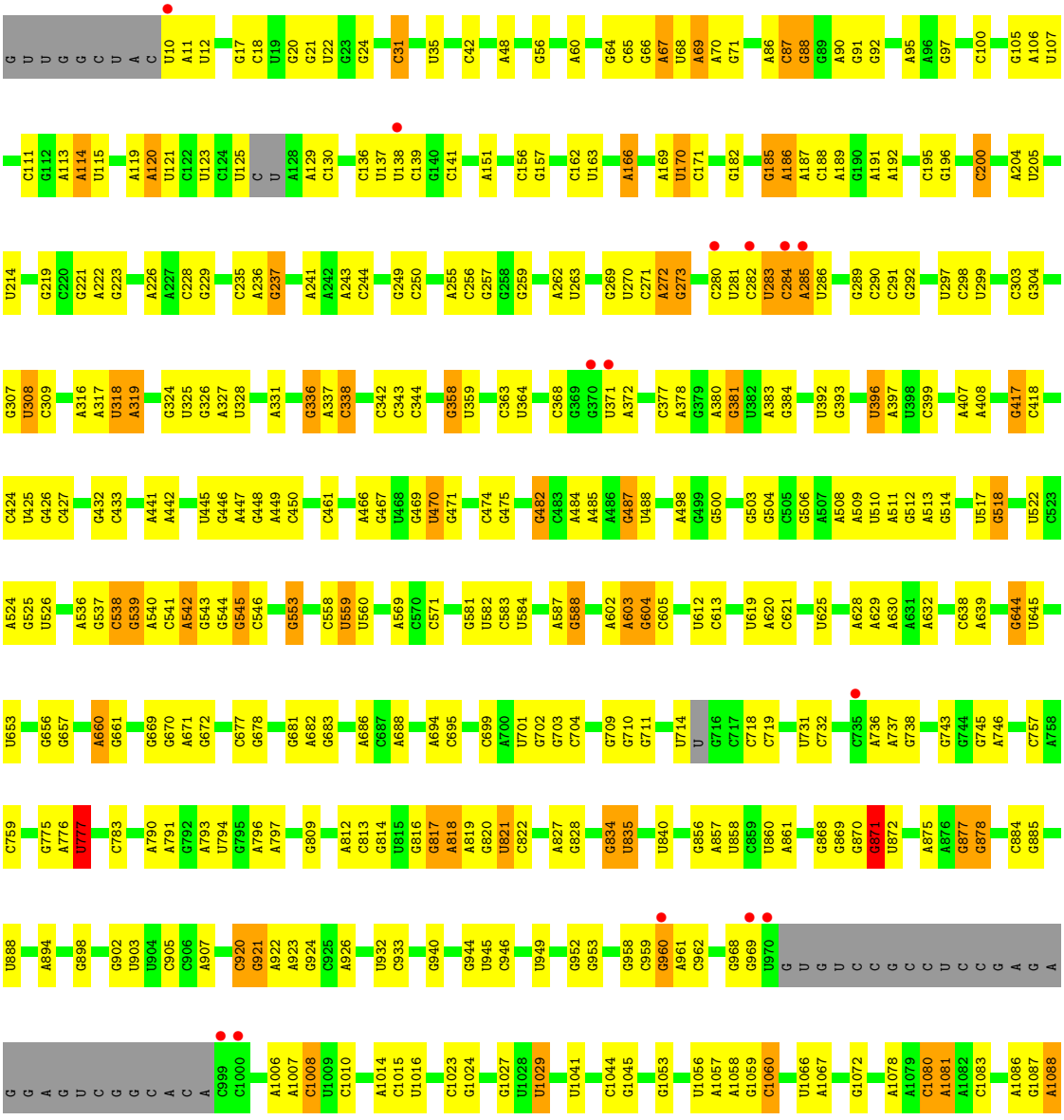
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	W	71	Total O 71 71	0	0
38	X	25	Total O 25 25	0	0
38	Y	96	Total O 96 96	0	0
38	Z	30	Total O 30 30	0	0
38	1	57	Total O 57 57	0	0
38	2	42	Total O 42 42	0	0
38	3	73	Total O 73 73	0	0

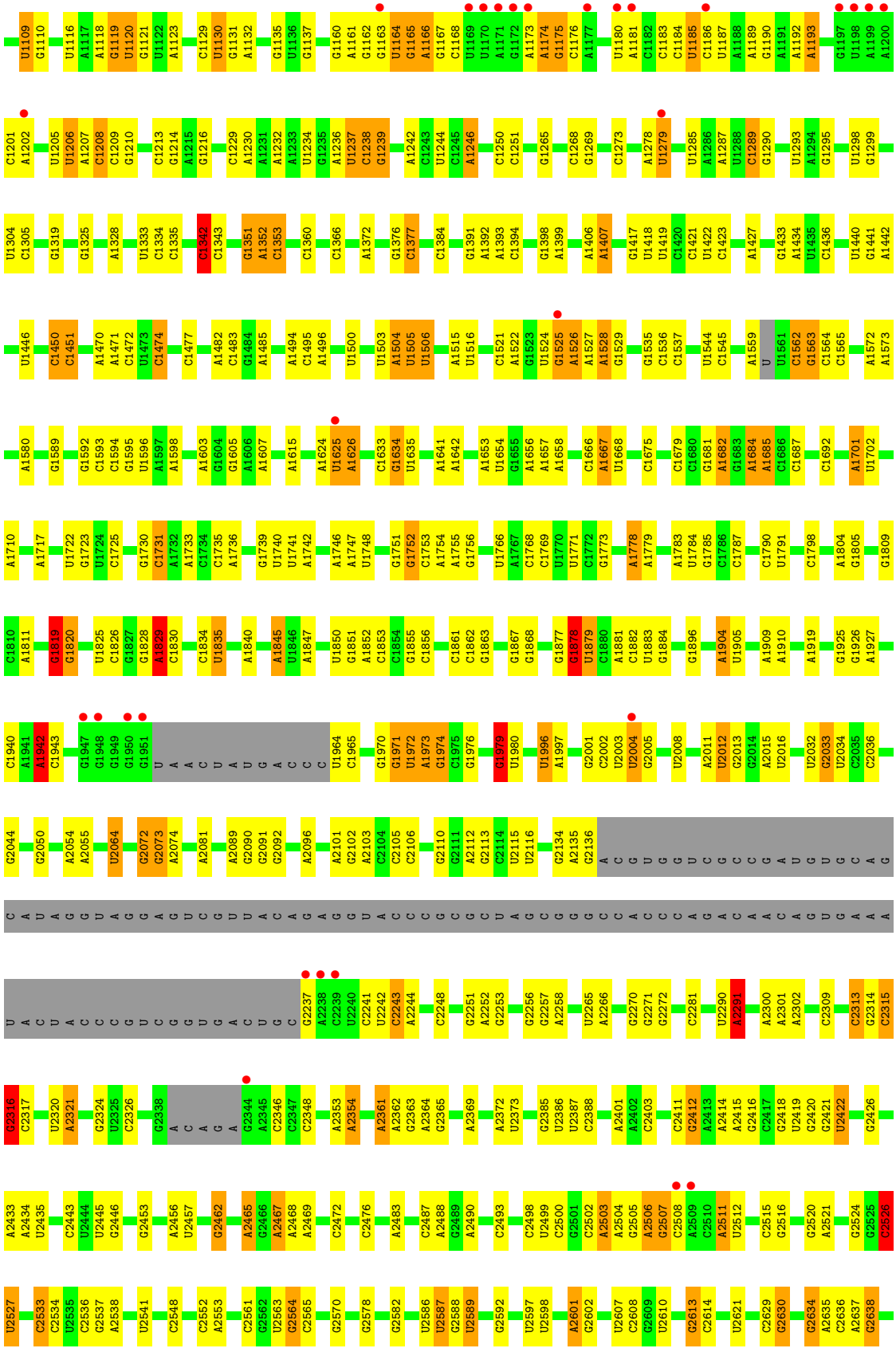
3 Residue-property plots (i)

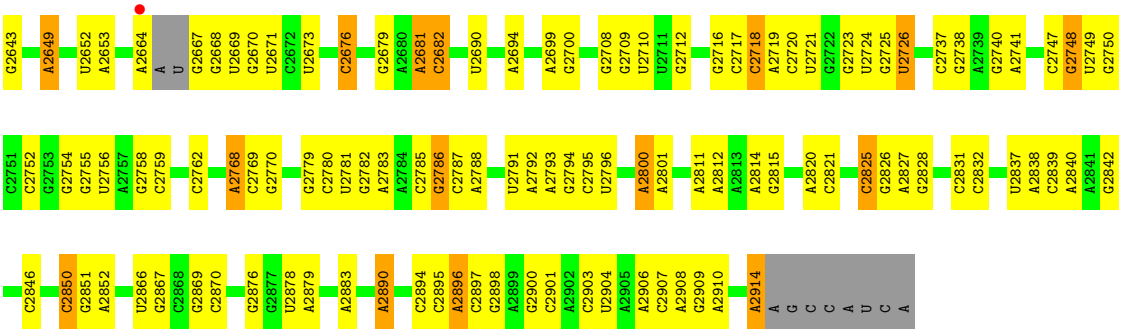
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

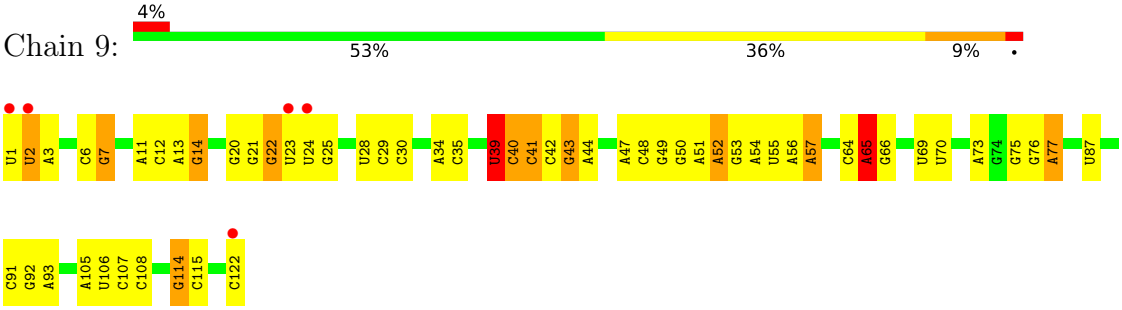
Chain 0:



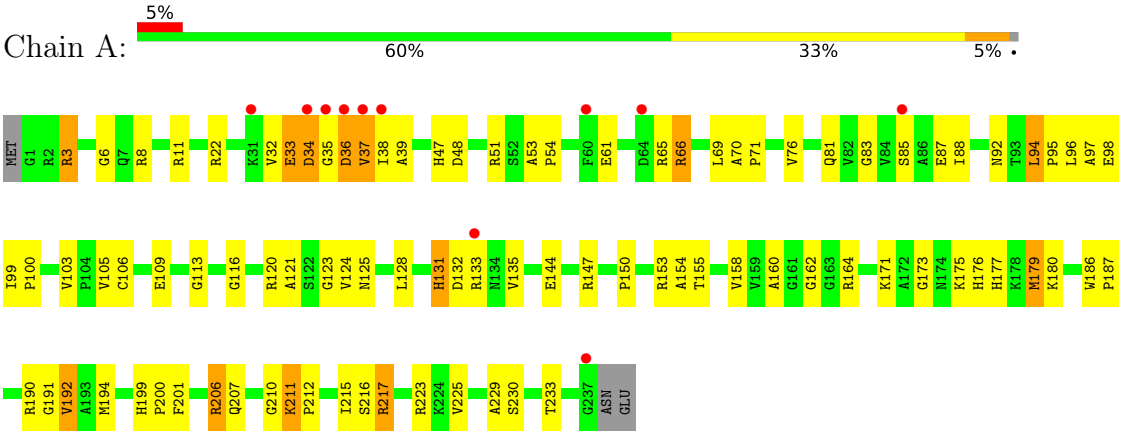




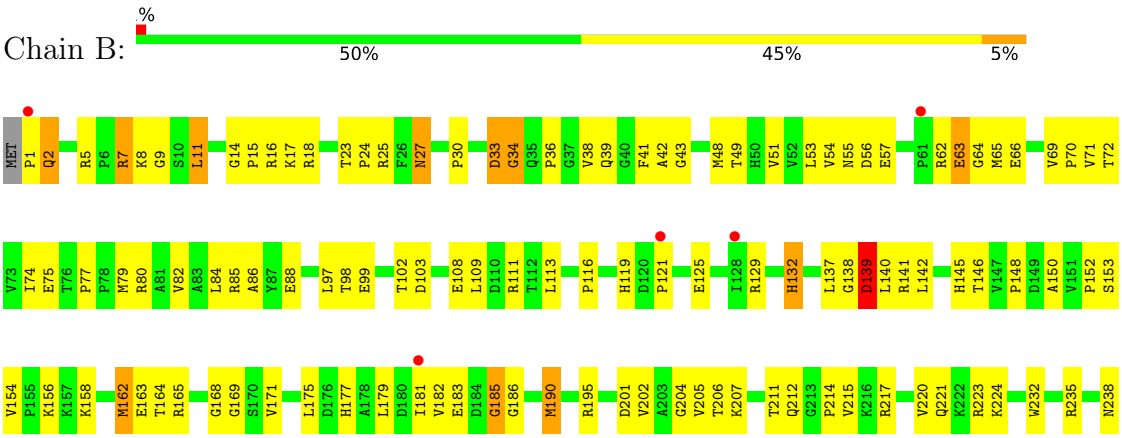
• Molecule 2: 5S Ribosomal RNA

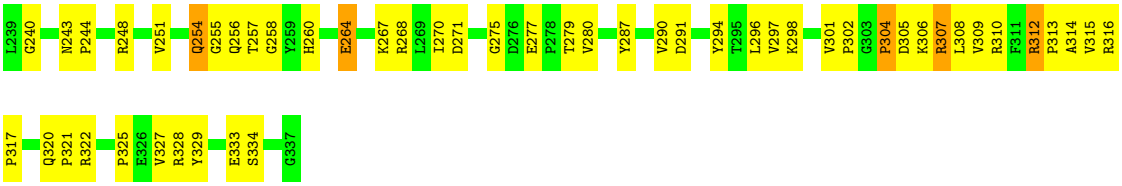


• Molecule 3: 50S ribosomal protein L2P

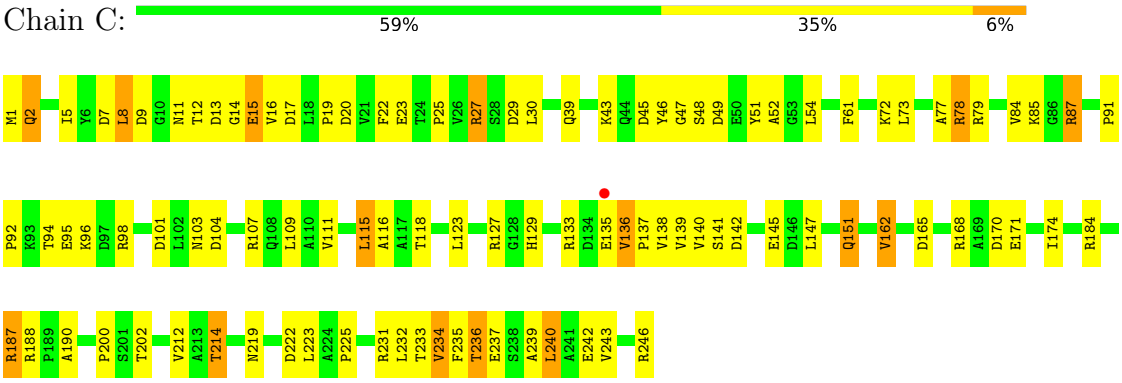


• Molecule 4: 50S ribosomal protein L3P

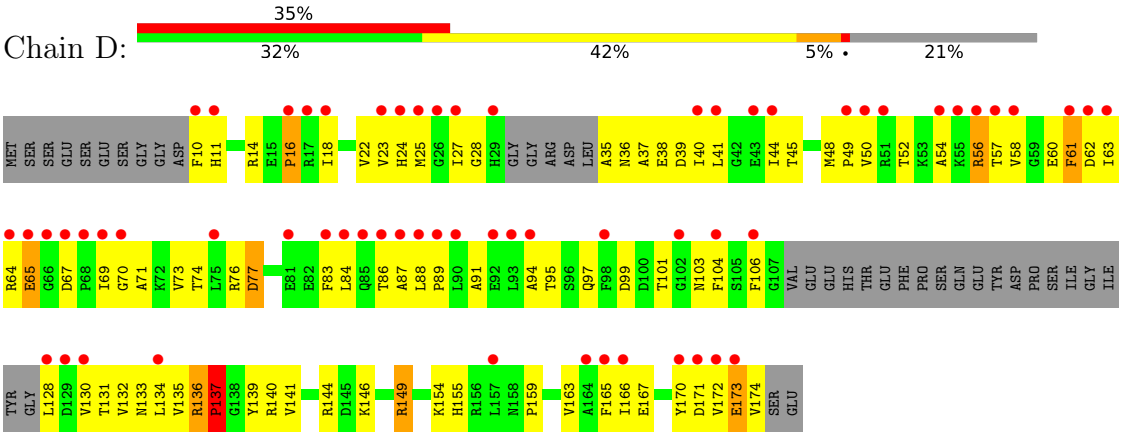




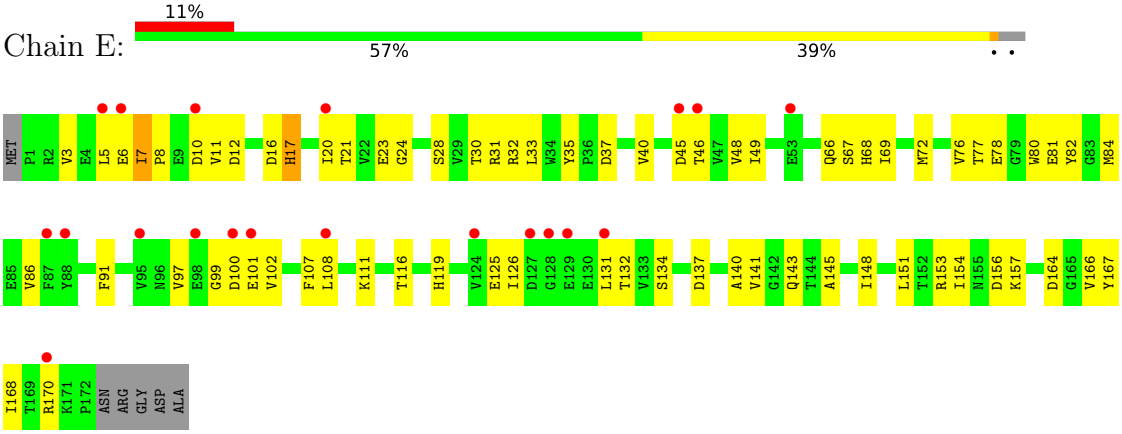
• Molecule 5: 50S ribosomal protein L4E



• Molecule 6: 50S ribosomal protein L5P

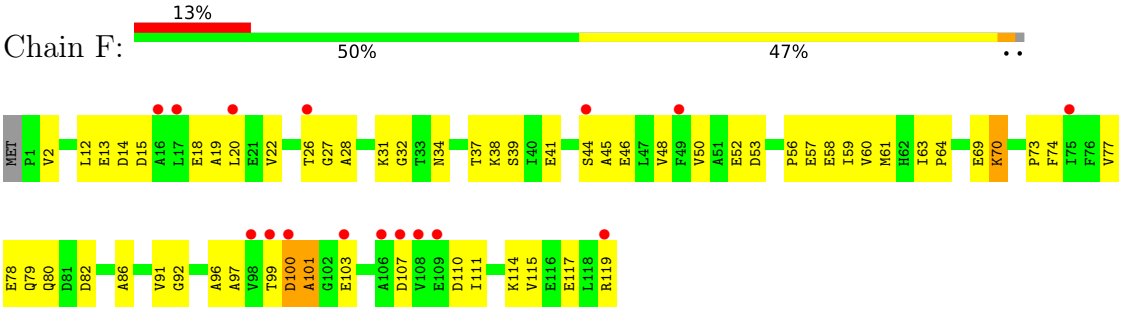


• Molecule 7: 50S ribosomal protein L6P



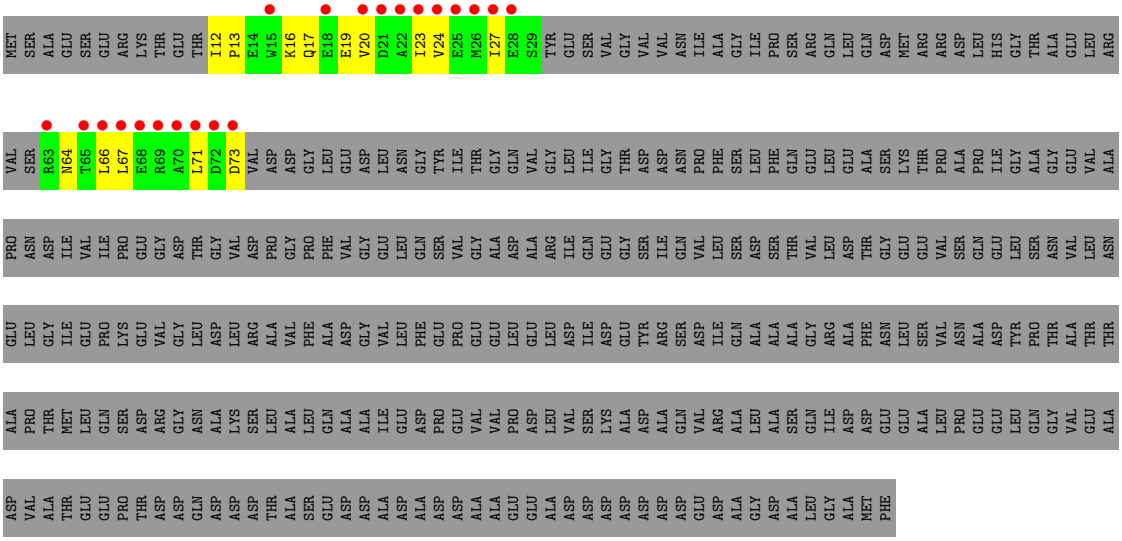
• Molecule 8: 50S ribosomal protein L7AE

Chain F:



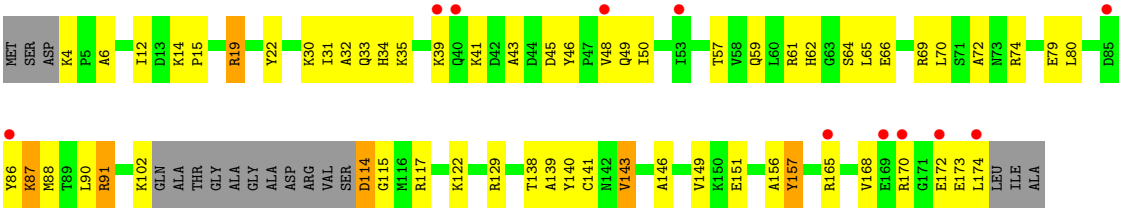
• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G:



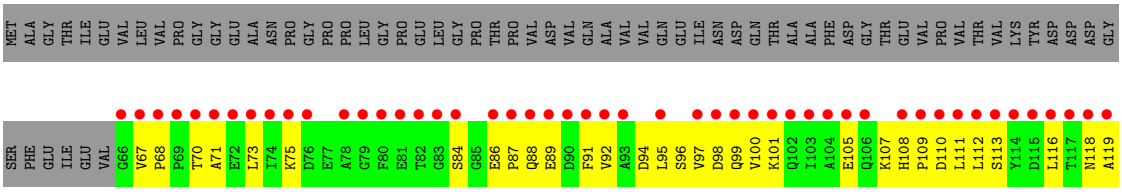
• Molecule 10: 50S RIBOSOMAL PROTEIN L10E

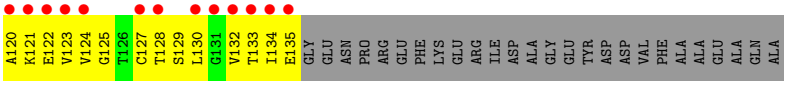
Chain H:



• Molecule 11: 50S RIBOSOMAL PROTEIN L11P

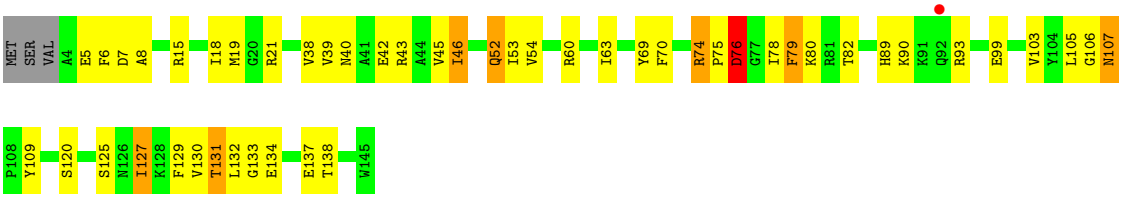
Chain I:





• Molecule 12: 50S ribosomal protein L13P

Chain J:

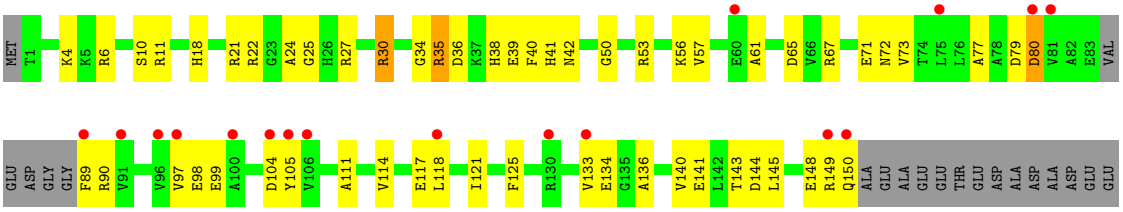


• Molecule 13: 50S ribosomal protein L14P

Chain K:

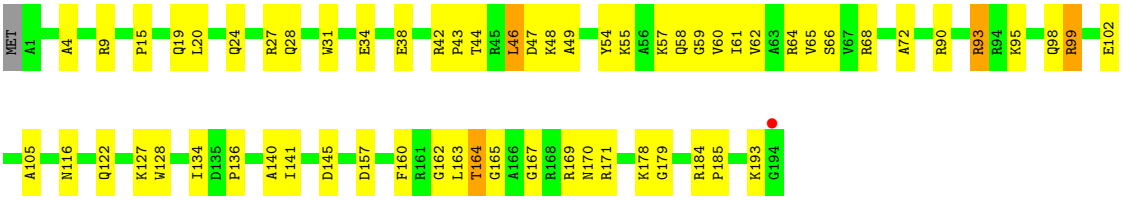
• Molecule 14: 50S ribosomal protein L15P

Chain L:



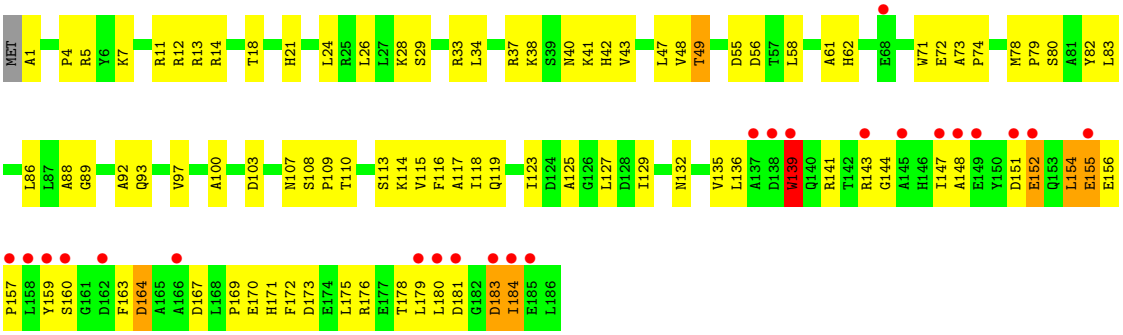
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



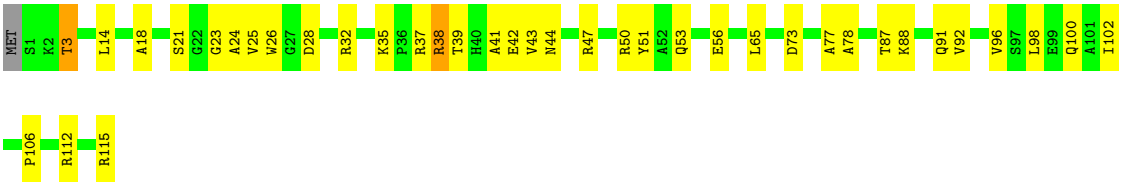
• Molecule 16: 50S ribosomal protein L18P

Chain N:



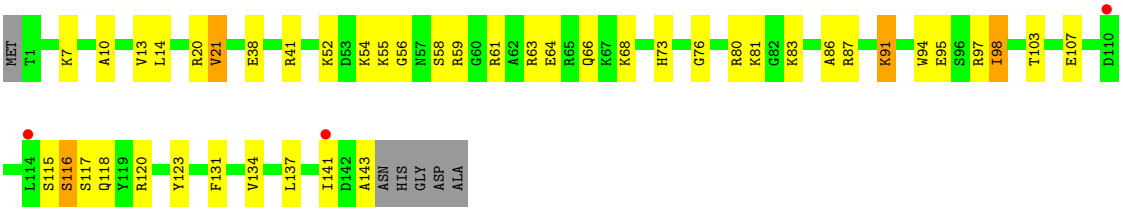
• Molecule 17: 50S ribosomal protein L18e

Chain O:



• Molecule 18: 50S ribosomal protein L19E

Chain P:

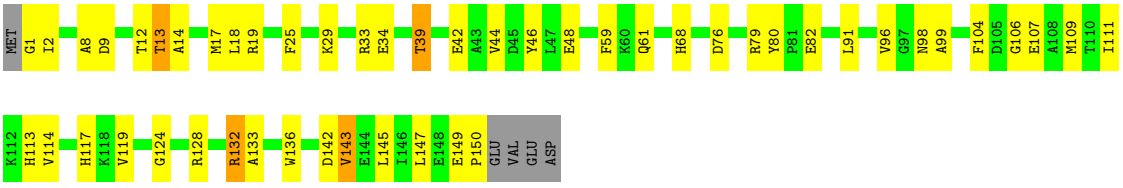


• Molecule 19: 50S ribosomal protein L21e

Chain Q:

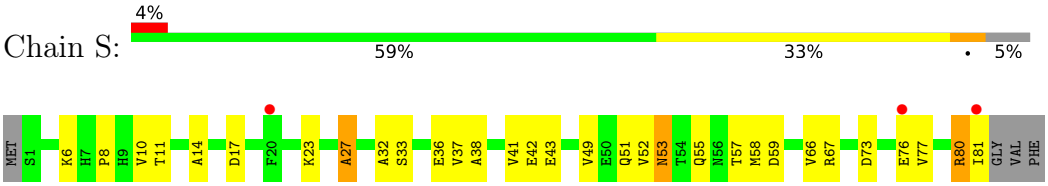
• Molecule 20: 50S ribosomal protein L22P

Chain R:



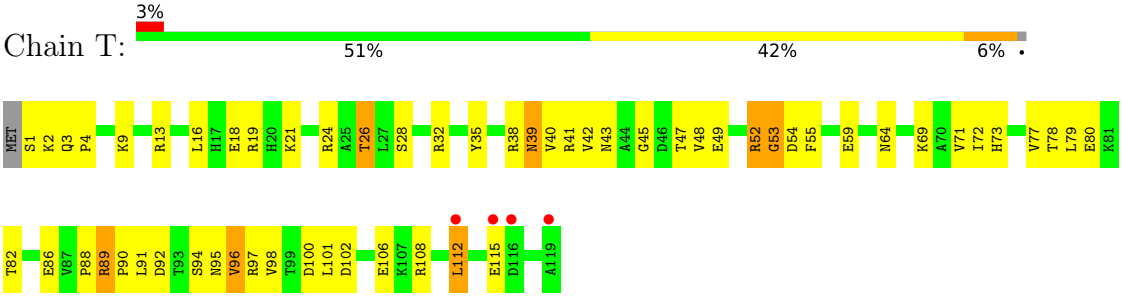
• Molecule 21: 50S ribosomal protein L23P

Chain S:



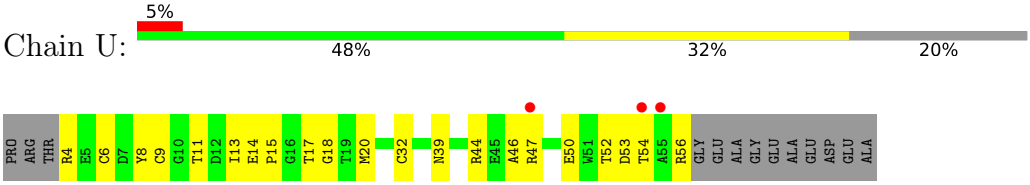
• Molecule 22: 50S ribosomal protein L24P

Chain T:



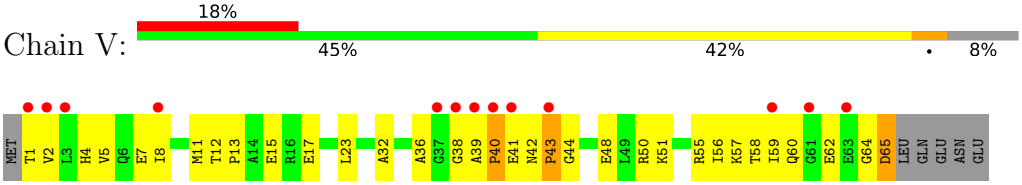
• Molecule 23: 50S ribosomal protein L24E

Chain U:



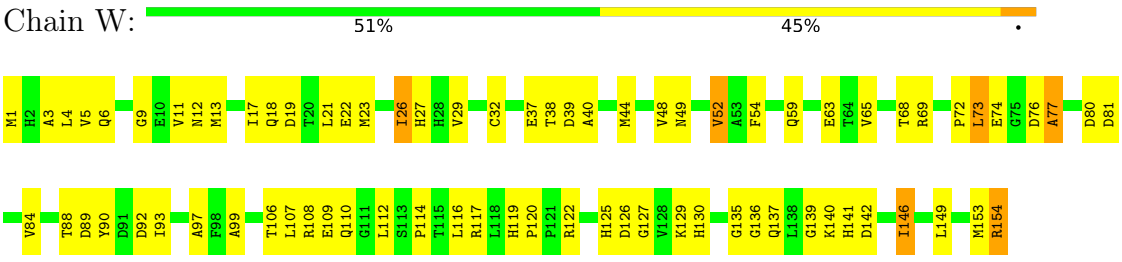
• Molecule 24: 50S ribosomal protein L29P

Chain V:



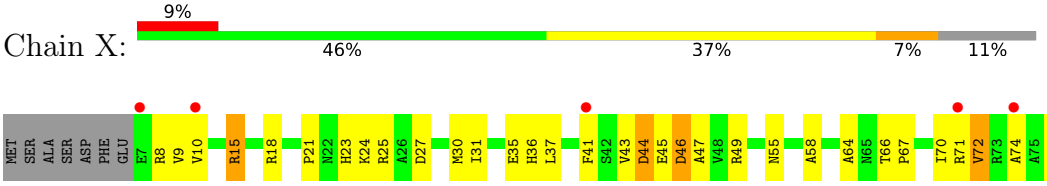
• Molecule 25: 50S ribosomal protein L30P

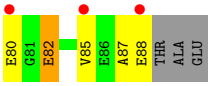
Chain W:



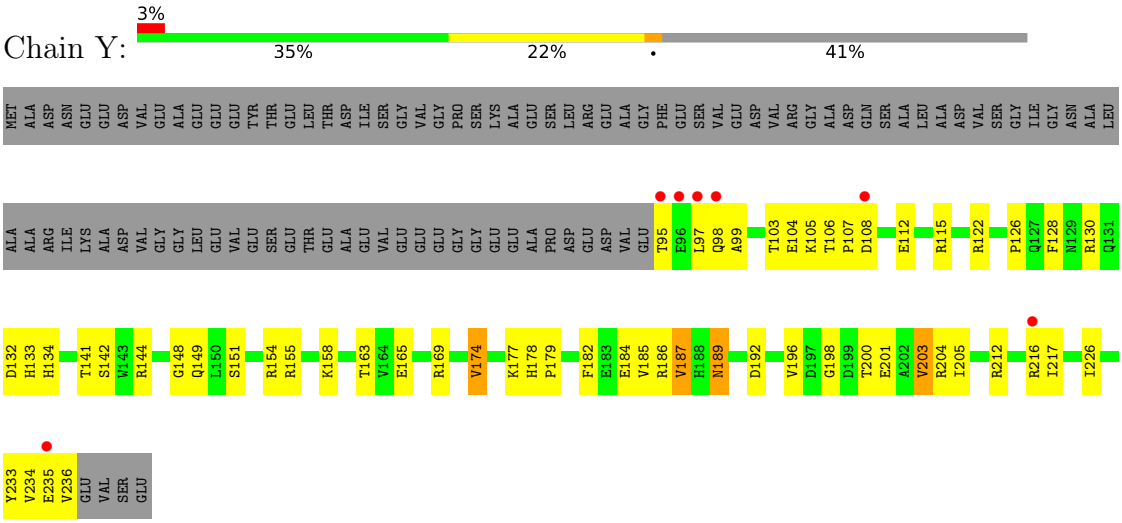
• Molecule 26: 50S ribosomal protein L31e

Chain X:

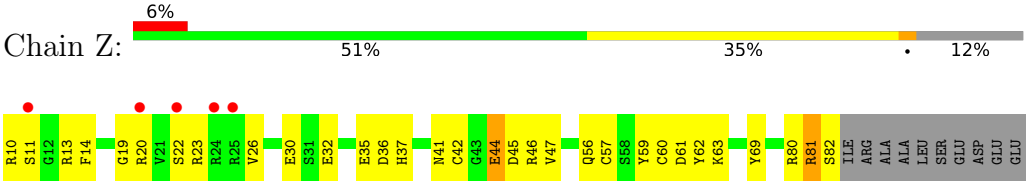




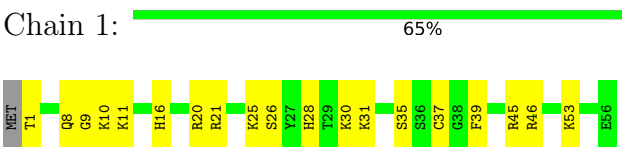
• Molecule 27: 50S ribosomal protein L32E



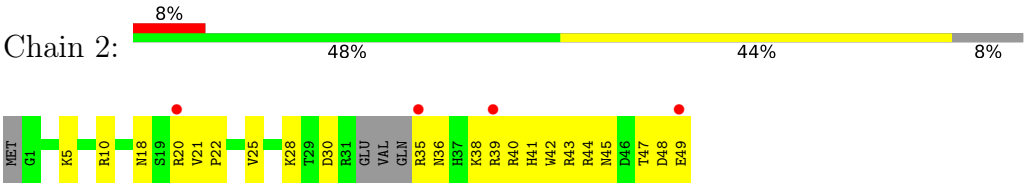
• Molecule 28: 50S ribosomal protein L37Ae



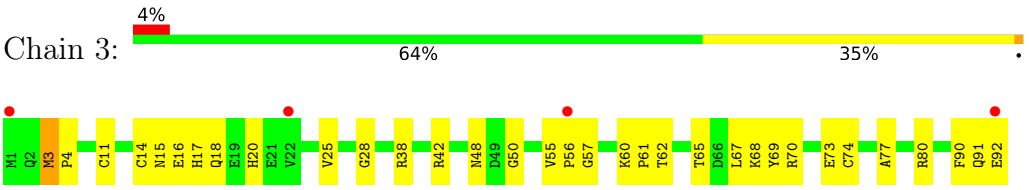
• Molecule 29: 50S ribosomal protein L37e



• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	212.22Å 300.19Å 574.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.60 49.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.6 (29.96-2.60) 93.7 (49.84-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.182 , 0.220 0.177 , 0.215	Depositor DCC
R_{free} test set	5105 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	99097	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CD, CL, 1MA, UR3, PSU, MG, K, OMG, TEL, OMU, NA

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	0.35	0/65957	0.69	18/102867 (0.0%)
2	9	0.33	0/2904	0.69	2/4526 (0.0%)
3	A	0.31	0/1786	0.64	0/2408
4	B	0.32	0/2690	0.64	0/3652
5	C	0.37	0/1884	0.64	0/2551
6	D	0.30	0/1111	0.53	0/1498
7	E	0.31	0/1382	0.56	0/1880
8	F	0.31	0/901	0.55	0/1224
9	G	0.27	0/241	0.46	0/324
10	H	0.33	0/1302	0.65	0/1743
11	I	0.30	0/526	0.53	0/716
12	J	0.35	0/1136	0.61	0/1530
13	K	0.34	0/1001	0.67	0/1347
14	L	0.32	0/1130	0.63	0/1509
15	M	0.34	0/1582	0.61	0/2117
16	N	0.29	0/1474	0.61	0/1999
17	O	0.32	0/874	0.57	0/1181
18	P	0.33	0/1147	0.53	0/1528
19	Q	0.35	0/749	0.69	0/1005
20	R	0.34	0/1172	0.64	0/1578
21	S	0.33	0/648	0.58	1/875 (0.1%)
22	T	0.30	0/958	0.62	1/1289 (0.1%)
23	U	0.32	0/417	0.55	0/562
24	V	0.28	0/502	0.54	0/675
25	W	0.34	0/1219	0.62	0/1655
26	X	0.34	0/664	0.57	0/895
27	Y	0.35	0/1146	0.63	0/1536
28	Z	0.32	0/589	0.62	0/787
29	1	0.39	0/438	0.63	0/578
30	2	0.33	0/401	0.53	0/529
31	3	0.36	0/771	0.57	0/1024
All	All	0.34	0/98702	0.67	22/147588 (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	46
2	9	0	3
All	All	0	49

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1563	G	C2'-C3'-O3'	9.32	130.00	109.50
1	0	1942	A	C5'-C4'-C3'	7.76	128.42	116.00
1	0	871	G	C5'-C4'-O4'	-7.10	100.58	109.10
2	9	39	U	N1-C1'-C2'	6.67	122.67	114.00
1	0	1504	A	C1'-O4'-C4'	-6.47	104.72	109.90
1	0	2313	C	C5'-C4'-O4'	5.96	116.25	109.10
1	0	2291	A	N9-C1'-C2'	5.92	121.70	114.00
1	0	1878	G	N9-C1'-C2'	-5.82	105.59	112.00
1	0	2467	A	C1'-O4'-C4'	-5.74	105.31	109.90
1	0	1120	U	C5'-C4'-C3'	-5.71	106.86	116.00
1	0	1819	G	C5'-C4'-C3'	5.53	124.84	116.00
1	0	777	U	O4'-C1'-N1	5.52	112.62	108.20
2	9	65	A	N9-C1'-C2'	5.43	121.06	114.00
1	0	2316	G	C5'-C4'-C3'	-5.40	107.35	116.00
1	0	2526	C	N1-C1'-C2'	5.28	120.86	114.00
1	0	1971	G	N9-C1'-C2'	5.25	120.83	114.00
1	0	1979	G	N9-C1'-C2'	5.21	120.77	114.00
21	S	27	ALA	N-CA-C	-5.18	97.02	111.00
22	T	52	ARG	N-CA-C	5.12	124.82	111.00
1	0	1829	A	N9-C1'-C2'	-5.04	106.46	112.00
1	0	2726	U	N1-C1'-C2'	5.03	120.54	114.00
1	0	2313	C	C5'-C4'-C3'	5.03	124.04	116.00

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1342	C	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	0	1351	G	Sidechain
1	0	1376	G	Sidechain
1	0	1417	G	Sidechain
1	0	1653	A	Sidechain
1	0	1809	G	Sidechain
1	0	1829	A	Sidechain
1	0	1835	U	Sidechain
1	0	1845	A	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1972	U	Sidechain
1	0	22	U	Sidechain
1	0	221	G	Sidechain
1	0	2315	C	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2526	C	Sidechain
1	0	2552	C	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2643	G	Sidechain
1	0	2673	U	Sidechain
1	0	270	U	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	48	A	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	817	G	Sidechain
1	0	818	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	888	U	Sidechain
1	0	903	U	Sidechain
2	9	39	U	Sidechain
2	9	65	A	Sidechain
2	9	87	U	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59020	0	29810	819	0
2	9	2599	0	1325	62	0
3	A	1753	0	1766	126	0
4	B	2625	0	2533	173	0
5	C	1859	0	1816	118	0
6	D	1094	0	1085	81	0
7	E	1357	0	1266	63	0
8	F	890	0	843	53	0
9	G	240	0	231	15	0
10	H	1282	0	1292	71	0
11	I	519	0	500	60	0
12	J	1120	0	1098	62	0
13	K	992	0	1031	56	0
14	L	1118	0	1076	55	0
15	M	1558	0	1566	63	0
16	N	1445	0	1401	117	0
17	O	865	0	873	33	0
18	P	1136	0	1123	44	0
19	Q	735	0	729	25	0
20	R	1149	0	1122	59	0
21	S	641	0	605	26	0
22	T	950	0	923	60	0
23	U	410	0	364	22	0
24	V	499	0	511	38	0
25	W	1196	0	1137	93	0
26	X	654	0	653	44	0
27	Y	1130	0	1133	60	0
28	Z	578	0	540	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	1	431	0	426	29	0
30	2	396	0	413	29	0
31	3	755	0	728	29	0
32	0	106	0	0	0	0
32	2	1	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	72	0	0	0	0
34	9	2	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	3	0	0	0	0
34	S	1	0	0	0	0
34	T	1	0	0	0	0
35	0	9	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	2	0	0	0	0
36	0	58	0	65	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	0	5881	0	0	140	0
38	1	57	0	0	4	0
38	2	42	0	0	3	0
38	3	73	0	0	7	0
38	9	140	0	0	8	0
38	A	120	0	0	22	0
38	B	153	0	0	25	0
38	C	174	0	0	23	0
38	D	46	0	0	14	0
38	E	41	0	0	8	0
38	F	27	0	0	6	0
38	G	18	0	0	2	0
38	H	71	0	0	17	0
38	I	9	0	0	3	0
38	J	54	0	0	3	0
38	K	65	0	0	15	0
38	L	83	0	0	21	0
38	M	130	0	0	9	0
38	N	62	0	0	14	0
38	O	41	0	0	9	0
38	P	62	0	0	5	0
38	Q	46	0	0	5	0
38	R	81	0	0	9	0
38	S	38	0	0	4	0
38	T	37	0	0	7	0
38	U	25	0	0	2	0
38	V	14	0	0	3	0
38	W	71	0	0	9	0
38	X	25	0	0	7	0
38	Y	96	0	0	13	0
38	Z	30	0	0	1	0
All	All	99097	0	59984	2362	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (2362) 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)
4:B:162:MET:HE1	4:B:308:LEU:HD21	1.31	1.06
5:C:236:THR:HG22	5:C:239:ALA:H	1.15	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:154:LYS:H	6:D:154:LYS:HD2	1.14	1.06
2:9:6:C:H5"	16:N:37:ARG:NH1	1.71	1.05
2:9:6:C:H5"	16:N:37:ARG:HH12	1.15	1.05
1:0:1242:A:H5'	12:J:82:THR:HG23	1.40	1.03
1:0:156:C:H5"	15:M:171:ARG:HD3	1.40	1.03
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.41	1.01
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.43	1.00
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.39	1.00
30:2:41:HIS:H	30:2:45:ASN:HD22	1.04	1.00
18:P:115:SER:H	18:P:118:GLN:HE21	1.02	1.00
1:0:1160:G:H5'	1:0:1161:A:H5'	1.40	0.99
11:I:127:CYS:HB3	11:I:132:VAL:HB	1.45	0.99
2:9:76:G:H3'	2:9:77:A:H5"	1.41	0.99
2:9:56:A:H2'	2:9:57:A:H5"	1.42	0.98
13:K:10:GLN:NE2	13:K:10:GLN:H	1.60	0.98
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.45	0.98
4:B:238:ASN:HD22	4:B:240:GLY:H	1.13	0.97
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.48	0.96
15:M:164:THR:HG22	15:M:167:GLY:H	1.26	0.96
10:H:59:GLN:HE21	10:H:129:ARG:HE	1.13	0.96
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.31	0.95
1:0:871:G:C8	1:0:871:G:H5'	1.99	0.95
5:C:78:ARG:HH11	5:C:78:ARG:HG3	1.30	0.95
1:0:1187:U:HO2'	1:0:1189:A:H2	1.06	0.95
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.49	0.95
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.82	0.94
1:0:1751:G:H2'	1:0:1752:G:H5"	1.49	0.94
1:0:871:G:H5'	1:0:871:G:H8	1.31	0.93
13:K:10:GLN:HE21	13:K:10:GLN:N	1.65	0.93
1:0:21:G:H5'	20:R:2:ILE:HA	1.51	0.92
12:J:76:ASP:HA	38:J:5907:HOH:O	1.66	0.92
1:0:870:G:H2'	1:0:871:G:H5"	1.49	0.92
10:H:49:GLN:HE21	10:H:140:TYR:HE2	1.09	0.92
1:0:1559:A:H1'	38:0:5848:HOH:O	1.67	0.92
1:0:2717:C:H2'	1:0:2718:C:H5"	1.52	0.91
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.33	0.91
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.86	0.90
16:N:144:GLY:O	16:N:147:ILE:HG22	1.71	0.90
13:K:39:GLY:HA2	38:K:4183:HOH:O	1.71	0.90
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.52	0.90
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.86	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:C2'	1:0:2718:C:H5"	2.03	0.89
1:0:545:G:H5'	1:0:545:G:H8	1.38	0.89
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.36	0.89
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.56	0.88
25:W:88:THR:HB	38:W:6679:HOH:O	1.72	0.88
1:0:1474:C:H6	1:0:1474:C:H5'	1.39	0.88
6:D:25:MET:HE2	6:D:41:LEU:HG	1.56	0.87
6:D:25:MET:HE1	6:D:37:ALA:HB1	1.57	0.87
1:0:381:G:H5"	38:0:4314:HOH:O	1.72	0.86
1:0:200:C:H2'	38:0:3440:HOH:O	1.74	0.86
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.56	0.86
17:O:42:GLU:HB2	38:O:2176:HOH:O	1.75	0.86
6:D:57:THR:HG23	6:D:63:ILE:HA	1.57	0.86
5:C:236:THR:HG22	5:C:239:ALA:N	1.90	0.86
10:H:174:LEU:HA	38:H:8573:HOH:O	1.75	0.86
1:0:2291:A:C8	1:0:2309:C:H5'	2.11	0.86
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.57	0.86
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.06	0.86
1:0:282:C:H1'	1:0:368:C:N4	1.91	0.85
1:0:1593:C:H5'	18:P:116:SER:O	1.75	0.85
3:A:35:GLY:O	3:A:36:ASP:HB3	1.75	0.85
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.23	0.85
4:B:179:LEU:O	4:B:183:GLU:HG2	1.74	0.84
12:J:93:ARG:HB3	12:J:93:ARG:HH11	1.42	0.84
1:0:2506:A:HO2'	1:0:2507:G:H8	0.88	0.84
5:C:1:MET:HG2	5:C:2:GLN:H	1.42	0.84
4:B:321:PRO:HA	38:B:8961:HOH:O	1.78	0.83
10:H:32:ALA:HB3	10:H:69:ARG:HH12	1.41	0.83
25:W:88:THR:HG22	25:W:89:ASP:H	1.43	0.83
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.58	0.83
1:0:1184:C:H1'	38:0:7430:HOH:O	1.78	0.83
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.58	0.83
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.58	0.83
3:A:36:ASP:OD2	3:A:85:SER:HB2	1.78	0.83
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.78	0.83
1:0:236:A:H4'	1:0:237:G:H5'	1.61	0.83
1:0:1667:A:H8	1:0:1667:A:H5'	1.43	0.82
12:J:131:THR:HG22	12:J:134:GLU:H	1.44	0.82
1:0:1160:G:C5'	1:0:1161:A:H5'	2.08	0.82
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.44	0.82
5:C:242:GLU:HG3	38:C:8587:HOH:O	1.76	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1835:U:H5	1:0:1840:A:N7	1.76	0.82
1:0:2586:U:H3	1:0:2592:G:H22	1.25	0.82
1:0:1701:A:H4'	1:0:1702:U:H5"	1.62	0.81
6:D:28:GLY:HA2	6:D:69:ILE:HG23	1.61	0.81
10:H:168:VAL:HG13	38:H:8562:HOH:O	1.79	0.81
1:0:2716:G:H5"	4:B:206:THR:HG21	1.63	0.81
13:K:10:GLN:H	13:K:10:GLN:HE21	0.84	0.81
1:0:1450:C:H4'	1:0:1451:C:OP2	1.79	0.81
1:0:2890:A:H1'	23:U:56:ARG:NH2	1.95	0.81
21:S:57:THR:HG22	21:S:59:ASP:H	1.45	0.81
24:V:1:THR:HG23	24:V:2:VAL:H	1.46	0.81
1:0:542:A:H5'	1:0:542:A:H8	1.45	0.81
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.46	0.81
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.61	0.81
10:H:30:LYS:H	10:H:62:HIS:HD2	1.24	0.81
16:N:113:SER:HB2	38:N:8856:HOH:O	1.80	0.80
18:P:64:GLU:HG2	38:P:168:HOH:O	1.82	0.80
1:0:2364:A:H5"	19:Q:15:LYS:HD3	1.63	0.80
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.61	0.80
1:0:506:G:H22	1:0:509:A:C5'	1.94	0.80
1:0:2812:A:H2	1:0:2814:A:H62	1.28	0.80
1:0:1116:U:HO2'	1:0:1118:A:H2	0.83	0.80
1:0:1116:U:O2'	1:0:1118:A:H2	1.64	0.80
1:0:1701:A:H5'	38:0:6257:HOH:O	1.81	0.80
25:W:13:MET:HE1	25:W:18:GLN:HA	1.64	0.80
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.62	0.80
1:0:56:G:H5"	24:V:50:ARG:HH12	1.47	0.80
1:0:2533:C:H5'	1:0:2533:C:H6	1.47	0.79
28:Z:10:ARG:HA	38:Z:8715:HOH:O	1.80	0.79
13:K:98:VAL:HG11	13:K:102:GLU:HA	1.65	0.79
1:0:1160:G:H5'	1:0:1161:A:C5'	2.13	0.79
1:0:2756:U:H3	1:0:2896:A:H2	1.30	0.79
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.65	0.79
1:0:1162:G:H1'	11:I:112:LEU:HD11	1.63	0.79
7:E:97:VAL:HG12	38:E:4191:HOH:O	1.81	0.79
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.64	0.79
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.47	0.79
1:0:962:C:H1'	16:N:5:ARG:NH1	1.98	0.79
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.12	0.79
6:D:99:ASP:HA	38:D:5675:HOH:O	1.83	0.78
10:H:59:GLN:NE2	10:H:129:ARG:HE	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:97:VAL:HG12	11:I:101:LYS:HE3	1.64	0.78
4:B:98:THR:HG22	4:B:99:GLU:H	1.48	0.78
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.81	0.78
1:0:182:G:H5'	38:0:5140:HOH:O	1.81	0.78
12:J:74:ARG:HH11	12:J:74:ARG:CB	1.97	0.78
10:H:170:ARG:HD2	38:H:8541:HOH:O	1.83	0.78
1:0:214:U:H5'	38:0:6118:HOH:O	1.83	0.78
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.64	0.78
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.13	0.78
1:0:2506:A:O2'	1:0:2507:G:H8	1.66	0.78
1:0:871:G:H8	1:0:871:G:C5'	1.97	0.78
1:0:1183:C:H2'	38:0:6218:HOH:O	1.84	0.78
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.66	0.78
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.65	0.77
24:V:42:ASN:HB3	38:V:7247:HOH:O	1.84	0.77
18:P:115:SER:OG	18:P:118:GLN:HG3	1.83	0.77
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.64	0.77
1:0:2840:A:OP1	4:B:211:THR:HG23	1.85	0.77
5:C:139:VAL:HG13	38:C:8655:HOH:O	1.84	0.77
7:E:6:GLU:HA	7:E:46:THR:HG22	1.67	0.77
14:L:143:THR:HG22	14:L:145:LEU:H	1.49	0.77
1:0:506:G:H22	1:0:509:A:H5'	1.49	0.76
2:9:14:G:H5'	2:9:14:G:H8	1.50	0.76
5:C:236:THR:H	5:C:239:ALA:HB3	1.49	0.76
15:M:164:THR:HG22	15:M:167:GLY:N	1.99	0.76
1:0:870:G:C2'	1:0:871:G:H5"	2.15	0.76
16:N:164:ASP:CG	16:N:167:ASP:HA	2.05	0.76
38:0:5440:HOH:O	9:G:12:ILE:HA	1.85	0.76
3:A:192:VAL:HG12	38:A:8890:HOH:O	1.84	0.76
1:0:10:U:H3'	38:0:3330:HOH:O	1.85	0.76
25:W:13:MET:CE	25:W:18:GLN:HA	2.16	0.76
8:F:91:VAL:HG12	8:F:92:GLY:N	2.01	0.76
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.50	0.76
22:T:101:LEU:HD13	22:T:112:LEU:HD11	1.66	0.76
1:0:877:G:H5'	1:0:878:G:OP1	1.86	0.75
1:0:2054:A:N3	20:R:128:ARG:NH2	2.34	0.75
16:N:80:SER:HB2	38:N:8834:HOH:O	1.85	0.75
2:9:56:A:C2'	2:9:57:A:H5"	2.15	0.75
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.85	0.75
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.50	0.75
1:0:559:U:H6	1:0:559:U:H5'	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:115:SER:N	18:P:118:GLN:HE21	1.82	0.75
24:V:56:ILE:O	24:V:60:GLN:HG3	1.86	0.75
1:0:2426:G:H1'	38:0:6069:HOH:O	1.87	0.74
1:0:544:G:H2'	1:0:545:G:H5"	1.69	0.74
20:R:39:THR:HG23	20:R:107:GLU:O	1.87	0.74
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.68	0.74
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.70	0.74
25:W:108:ARG:HH21	25:W:114:PRO:HG2	1.52	0.74
1:0:1206:U:H5'	1:0:1206:U:H6	1.53	0.74
2:9:75:G:H1	2:9:106:U:H3	1.35	0.74
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.18	0.74
1:0:1603:A:H5'	1:0:1605:G:O4'	1.87	0.74
3:A:11:ARG:HA	38:A:8913:HOH:O	1.86	0.74
1:0:1118:A:C8	1:0:1118:A:H3'	2.23	0.73
1:0:1118:A:H3'	1:0:1118:A:H8	1.52	0.73
5:C:140:VAL:HB	38:C:8658:HOH:O	1.87	0.73
5:C:2:GLN:HB3	38:C:8589:HOH:O	1.89	0.73
1:0:1979:G:H2'	38:0:3291:HOH:O	1.87	0.73
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.88	0.73
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.70	0.73
14:L:133:VAL:HA	38:L:8872:HOH:O	1.86	0.73
1:0:21:G:C5'	20:R:2:ILE:HA	2.18	0.73
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.71	0.73
38:0:7421:HOH:O	5:C:188:ARG:HD2	1.89	0.73
1:0:2637:A:H5'	38:0:9266:HOH:O	1.87	0.73
2:9:6:C:C5'	16:N:37:ARG:NH1	2.52	0.73
24:V:12:THR:HG22	24:V:15:GLU:CG	2.18	0.73
1:0:450:C:OP1	5:C:184:ARG:NH2	2.22	0.72
3:A:223:ARG:HG3	38:A:8899:HOH:O	1.88	0.72
4:B:162:MET:HG3	4:B:310:ARG:HD3	1.71	0.72
5:C:236:THR:HA	38:C:8658:HOH:O	1.89	0.72
8:F:96:ALA:HA	38:F:3111:HOH:O	1.88	0.72
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.69	0.72
27:Y:141:THR:HG23	38:Y:8888:HOH:O	1.89	0.72
1:0:2908:A:H2'	1:0:2909:G:O4'	1.90	0.72
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.04	0.72
16:N:164:ASP:OD1	16:N:167:ASP:HA	1.89	0.72
30:2:39:ARG:HG2	38:2:3143:HOH:O	1.89	0.72
38:0:6845:HOH:O	15:M:178:LYS:HB2	1.90	0.72
10:H:114:ASP:HB2	38:H:8548:HOH:O	1.90	0.72
1:0:1116:U:H3	1:0:1246:A:H62	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1474:C:H5'	1:0:1474:C:C6	2.25	0.71
1:0:1819:G:H2'	1:0:1820:G:H4'	1.72	0.71
1:0:2768:A:H2'	1:0:2769:C:O4'	1.89	0.71
4:B:320:GLN:NE2	4:B:321:PRO:HD2	2.06	0.71
1:0:1878:G:H1'	38:0:6098:HOH:O	1.90	0.71
1:0:2850:C:H6	1:0:2850:C:H5'	1.55	0.71
20:R:39:THR:HG22	20:R:42:GLU:H	1.55	0.71
1:0:56:G:H5"	24:V:50:ARG:NH1	2.05	0.71
1:0:272:A:H3'	38:0:7493:HOH:O	1.89	0.71
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.72	0.71
6:D:146:LYS:NZ	16:N:107:ASN:HD21	1.88	0.71
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.56	0.71
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.91	0.71
1:0:396:U:H1'	38:0:7587:HOH:O	1.89	0.71
21:S:57:THR:HG22	21:S:59:ASP:N	2.04	0.71
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.19	0.71
1:0:1189:A:H1'	1:0:1209:C:C1'	2.19	0.71
1:0:1751:G:C2'	1:0:1752:G:H5"	2.21	0.71
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.73	0.71
1:0:1189:A:H1'	1:0:1209:C:O4'	1.90	0.70
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.72	0.70
4:B:62:ARG:HA	4:B:65:MET:HE3	1.71	0.70
5:C:145:GLU:HG3	38:C:8579:HOH:O	1.90	0.70
11:I:73:LEU:HD12	11:I:107:LYS:HZ2	1.57	0.70
1:0:1666:C:H2'	1:0:1667:A:H5'	1.73	0.70
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.72	0.70
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.72	0.70
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.22	0.70
1:0:1165:G:H4'	1:0:1174:A:O2'	1.92	0.70
1:0:2783:A:H3'	38:0:5214:HOH:O	1.91	0.70
29:1:10:LYS:HG3	38:1:8733:HOH:O	1.92	0.70
2:9:69:U:OP1	16:N:4:PRO:HG3	1.92	0.69
4:B:41:PHE:HB3	4:B:190:MET:HE3	1.74	0.69
1:0:796:A:HO2'	28:Z:10:ARG:N	1.88	0.69
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.74	0.69
11:I:87:PRO:O	11:I:89:GLU:HG3	1.92	0.69
12:J:45:VAL:HG23	12:J:130:VAL:O	1.91	0.69
30:2:41:HIS:HD2	30:2:44:ARG:H	1.38	0.69
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.73	0.69
1:0:545:G:H5'	1:0:545:G:C8	2.26	0.69
1:0:2533:C:H5'	1:0:2533:C:C6	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.08	0.69
16:N:151:ASP:O	16:N:154:LEU:HB2	1.93	0.69
20:R:17:MET:HE1	20:R:19:ARG:NH2	2.08	0.69
12:J:52:GLN:HG3	12:J:53:ILE:N	2.06	0.69
6:D:99:ASP:HB3	6:D:103:ASN:H	1.57	0.69
13:K:65:ARG:HD3	38:K:5358:HOH:O	1.93	0.69
1:0:657:G:OP1	5:C:27:ARG:NH2	2.26	0.68
3:A:66:ARG:HH11	3:A:66:ARG:HB2	1.58	0.68
1:0:2508:C:H2'	38:0:6725:HOH:O	1.93	0.68
3:A:191:GLY:HA2	3:A:194:MET:CE	2.23	0.68
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.58	0.68
4:B:185:GLY:HA2	38:B:8934:HOH:O	1.92	0.68
1:0:380:A:H2'	38:0:7194:HOH:O	1.94	0.68
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.07	0.68
1:0:1299:G:O6	14:L:6:ARG:HD3	1.94	0.68
5:C:151:GLN:HA	5:C:151:GLN:HE21	1.58	0.68
7:E:154:ILE:HD11	7:E:157:LYS:HE2	1.75	0.68
1:0:814:G:H4'	38:0:3129:HOH:O	1.94	0.68
14:L:143:THR:HG21	38:L:8837:HOH:O	1.92	0.68
1:0:653:U:H5"	38:O:7674:HOH:O	1.93	0.68
4:B:66:GLU:OE1	4:B:328:ARG:HD2	1.94	0.68
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.03	0.68
21:S:43:GLU:HB3	38:S:8546:HOH:O	1.94	0.68
1:0:2896:A:H5"	38:0:6076:HOH:O	1.94	0.68
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.76	0.68
27:Y:144:ARG:NH1	38:Y:8873:HOH:O	2.27	0.67
1:0:1119:G:N2	1:0:1246:A:C2	2.62	0.67
8:F:2:VAL:HG22	8:F:57:GLU:OE1	1.94	0.67
3:A:191:GLY:HA2	3:A:194:MET:HE3	1.77	0.67
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.94	0.67
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.35	0.67
1:0:2768:A:H5"	38:0:4419:HOH:O	1.95	0.67
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.76	0.67
7:E:100:ASP:HB2	38:E:2789:HOH:O	1.93	0.67
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.09	0.67
1:0:553:G:P	27:Y:204:ARG:HH22	2.18	0.67
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.77	0.67
1:0:1819:G:H5'	38:0:4704:HOH:O	1.93	0.67
5:C:236:THR:CG2	5:C:239:ALA:H	2.01	0.67
1:0:541:C:C2'	1:0:542:A:H5"	2.25	0.67
16:N:132:ASN:O	16:N:135:VAL:HG12	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:541:C:H2'	1:0:542:A:H5"	1.75	0.67
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.94	0.67
1:0:2320:U:H4'	1:0:2321:A:O4'	1.94	0.67
1:0:2414:A:H2'	1:0:2415:A:C8	2.29	0.67
1:0:2649:A:H5'	1:0:2649:A:H8	1.59	0.67
2:9:114:G:O6	16:N:11:ARG:HD3	1.95	0.67
13:K:63:GLU:HG2	38:K:6344:HOH:O	1.95	0.67
1:0:31:C:H4'	38:T:7242:HOH:O	1.94	0.67
1:0:281:U:H2'	1:0:282:C:O4'	1.94	0.67
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.77	0.66
8:F:58:GLU:CD	15:M:27:ARG:HH22	1.97	0.66
20:R:14:ALA:HB3	20:R:147:LEU:HB2	1.75	0.66
25:W:38:THR:HG22	25:W:39:ASP:H	1.59	0.66
1:0:2827:A:H2'	1:0:2828:G:O4'	1.96	0.66
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.76	0.66
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.61	0.66
5:C:16:VAL:HG12	5:C:17:ASP:H	1.60	0.66
6:D:50:VAL:O	6:D:71:ALA:HA	1.96	0.66
6:D:154:LYS:H	6:D:154:LYS:CD	1.95	0.66
14:L:148:GLU:HA	38:L:8871:HOH:O	1.96	0.66
1:0:544:G:C2'	1:0:545:G:H5"	2.25	0.66
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.28	0.66
6:D:163:VAL:HA	38:D:6326:HOH:O	1.95	0.66
1:0:1234:U:N3	4:B:244:PRO:HB3	2.10	0.66
1:0:1666:C:O2'	1:0:1667:A:H5"	1.96	0.66
10:H:62:HIS:HA	10:H:65:LEU:HD23	1.76	0.66
20:R:39:THR:HB	20:R:42:GLU:HG3	1.76	0.66
27:Y:112:GLU:CD	27:Y:115:ARG:HH12	1.98	0.66
1:0:541:C:H2'	1:0:542:A:C5'	2.25	0.66
3:A:164:ARG:CZ	38:A:8885:HOH:O	2.43	0.66
4:B:275:GLY:O	4:B:291:ASP:HA	1.95	0.66
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.78	0.66
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.77	0.66
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.78	0.66
2:9:92:G:H2'	2:9:93:A:C8	2.31	0.66
10:H:12:ILE:HD12	10:H:57:THR:HG22	1.76	0.66
25:W:88:THR:HG22	25:W:89:ASP:N	2.09	0.66
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.76	0.66
1:0:1372:A:H3'	38:0:7158:HOH:O	1.96	0.66
5:C:236:THR:HG21	38:C:8579:HOH:O	1.95	0.66
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:797:A:C4'	28:Z:10:ARG:N	2.59	0.65
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.24	0.65
1:0:188:C:H5"	15:M:163:LEU:HD21	1.77	0.65
15:M:64:ARG:HD2	38:M:8883:HOH:O	1.95	0.65
18:P:103:THR:O	18:P:107:GLU:HG3	1.95	0.65
18:P:115:SER:H	18:P:118:GLN:NE2	1.85	0.65
1:0:1205:U:H2'	1:0:1206:U:H5"	1.78	0.65
1:0:871:G:C8	1:0:871:G:C5'	2.73	0.65
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.26	0.65
38:0:5514:HOH:O	15:M:58:GLN:HG3	1.96	0.65
11:I:124:VAL:HG13	11:I:134:ILE:HD11	1.77	0.65
1:0:1130:U:H5'	38:0:7631:HOH:O	1.95	0.65
7:E:68:HIS:O	7:E:72:MET:HG3	1.97	0.65
18:P:91:LYS:O	18:P:95:GLU:HG3	1.97	0.65
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.32	0.65
3:A:51:ARG:HB2	38:A:8904:HOH:O	1.97	0.65
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.79	0.65
6:D:136:ARG:HD2	6:D:155:HIS:O	1.97	0.65
38:0:6743:HOH:O	16:N:4:PRO:HD2	1.95	0.65
10:H:165:ARG:HD3	38:H:8585:HOH:O	1.97	0.65
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.62	0.65
31:3:17:HIS:O	31:3:18:GLN:HG3	1.97	0.65
11:I:101:LYS:O	11:I:105:GLU:HG3	1.97	0.65
14:L:79:ASP:HB3	38:L:8858:HOH:O	1.96	0.65
1:0:603:A:H5"	1:0:604:G:OP1	1.97	0.65
1:0:1165:G:H1'	1:0:1174:A:H1'	1.79	0.65
1:0:2502:C:C2'	1:0:2503:A:H5'	2.27	0.65
7:E:132:THR:HB	38:E:2227:HOH:O	1.96	0.65
10:H:12:ILE:O	10:H:12:ILE:HG22	1.95	0.65
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.43	0.65
1:0:2851:G:O2'	1:0:2852:A:H5'	1.96	0.64
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.26	0.64
3:A:164:ARG:NE	38:A:8885:HOH:O	2.30	0.64
8:F:31:LYS:HE3	38:F:2623:HOH:O	1.96	0.64
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.78	0.64
2:9:54:A:O2'	2:9:55:U:H5'	1.97	0.64
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.79	0.64
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.80	0.64
1:0:338:C:H4'	5:C:174:ILE:CD1	2.27	0.64
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.63	0.64
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1641:A:H2'	1:0:1642:A:H5'	1.79	0.64
27:Y:187:VAL:HG12	27:Y:205:ILE:HA	1.79	0.64
1:0:447:A:OP1	22:T:2:LYS:HG2	1.98	0.64
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.98	0.64
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.10	0.64
1:0:1377:C:H5'	1:0:1377:C:H6	1.63	0.64
31:3:70:ARG:HB3	38:3:8872:HOH:O	1.96	0.64
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.80	0.64
20:R:33:ARG:NH1	38:R:8841:HOH:O	2.27	0.64
24:V:64:GLY:O	24:V:65:ASP:HB2	1.97	0.64
26:X:25:ARG:HD2	38:X:3861:HOH:O	1.98	0.64
1:0:2846:C:OP1	4:B:158:LYS:HD3	1.98	0.63
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.79	0.63
8:F:91:VAL:HG12	8:F:92:GLY:H	1.63	0.63
16:N:154:LEU:O	16:N:155:GLU:HB3	1.98	0.63
20:R:99:ALA:HB1	20:R:109:MET:CE	2.26	0.63
4:B:27:ASN:HD22	4:B:27:ASN:H	1.46	0.63
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.27	0.63
26:X:31:ILE:O	26:X:35:GLU:HG3	1.98	0.63
1:0:818:A:O2'	28:Z:13:ARG:HD3	1.97	0.63
1:0:1351:G:OP1	5:C:96:LYS:NZ	2.29	0.63
23:U:17:THR:HG22	23:U:18:GLY:N	2.13	0.63
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.79	0.63
1:0:1527:A:H1'	1:0:1528:A:C8	2.34	0.63
6:D:166:ILE:HB	38:D:6326:HOH:O	1.98	0.63
1:0:1862:C:H1'	38:A:8913:HOH:O	1.99	0.63
11:I:100:VAL:HG11	11:I:124:VAL:CG2	2.29	0.63
20:R:29:LYS:HD3	38:R:8830:HOH:O	1.97	0.63
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.29	0.63
1:0:1835:U:C5	1:0:1840:A:N7	2.64	0.63
1:0:2679:G:H2'	1:0:2681:A:OP2	1.98	0.63
2:9:14:G:H5'	2:9:14:G:C8	2.32	0.63
3:A:121:ALA:O	3:A:124:VAL:HG22	1.98	0.63
17:O:87:THR:O	17:O:91:GLN:HG3	1.98	0.63
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.79	0.63
26:X:71:ARG:HD3	38:X:2171:HOH:O	1.98	0.63
31:3:62:THR:HB	38:3:8850:HOH:O	1.97	0.63
1:0:1667:A:H5'	1:0:1667:A:C8	2.31	0.63
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.62	0.63
3:A:39:ALA:HB3	3:A:61:GLU:OE2	1.98	0.63
28:Z:42:CYS:SG	28:Z:44:GLU:HB2	2.38	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:56:ASP:HB3	4:B:322:ARG:HH21	1.63	0.63
5:C:115:LEU:O	5:C:118:THR:HB	1.98	0.63
8:F:46:GLU:OE1	8:F:100:ASP:HA	1.98	0.63
16:N:169:PRO:O	16:N:172:PHE:HB3	1.99	0.63
24:V:39:ALA:N	24:V:40:PRO:HD2	2.13	0.63
1:0:111:C:O2'	29:1:20:ARG:HG2	1.99	0.62
2:9:29:C:H2'	2:9:30:C:H5'	1.81	0.62
4:B:102:THR:HG23	4:B:182:VAL:HG12	1.81	0.62
23:U:52:THR:CG2	23:U:54:THR:HB	2.29	0.62
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.81	0.62
1:0:399:C:H5'	15:M:179:GLY:O	1.99	0.62
1:0:902:G:N7	14:L:18:HIS:HD2	1.97	0.62
1:0:1834:C:H2'	1:0:1840:A:N6	2.14	0.62
2:9:28:U:H5"	16:N:40:ASN:ND2	2.14	0.62
9:G:16:LYS:O	9:G:20:VAL:HG23	1.98	0.62
14:L:77:ALA:HB3	38:L:8829:HOH:O	1.99	0.62
1:0:536:A:H3'	38:0:5036:HOH:O	1.99	0.62
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.81	0.62
1:0:558:C:C2'	1:0:559:U:H5"	2.30	0.62
4:B:238:ASN:HD22	4:B:240:GLY:N	1.91	0.62
12:J:99:GLU:HA	38:J:7377:HOH:O	1.99	0.62
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.34	0.62
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.30	0.62
1:0:1164:U:H3	1:0:1192:A:H2	1.47	0.62
5:C:246:ARG:NH2	38:C:8630:HOH:O	2.33	0.62
11:I:120:ALA:O	11:I:124:VAL:HG23	1.98	0.62
1:0:447:A:P	22:T:1:SER:HB2	2.40	0.62
11:I:73:LEU:HD12	11:I:107:LYS:NZ	2.14	0.62
11:I:94:ASP:OD1	11:I:133:THR:HB	1.99	0.62
12:J:93:ARG:HB3	12:J:93:ARG:NH1	2.15	0.62
14:L:143:THR:HG22	14:L:144:ASP:N	2.15	0.62
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.81	0.62
1:0:470:U:O2'	29:1:16:HIS:HD2	1.82	0.62
1:0:870:G:OP2	3:A:3:ARG:HD3	2.00	0.62
1:0:1080:C:H4'	1:0:1081:A:OP1	1.99	0.62
1:0:2570:G:H5"	38:0:4901:HOH:O	1.99	0.62
10:H:30:LYS:H	10:H:62:HIS:CD2	2.13	0.62
15:M:60:VAL:C	15:M:61:ILE:HD12	2.20	0.62
1:0:1189:A:H1'	1:0:1209:C:H1'	1.80	0.62
2:9:2:U:OP2	2:9:3:A:H5'	2.00	0.62
1:0:1878:G:O2'	1:0:1879:U:C6	2.51	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2502:C:H2'	1:0:2503:A:H5'	1.82	0.62
38:0:4222:HOH:O	30:2:38:LYS:HE3	1.99	0.62
14:L:36:ASP:HB2	38:L:8835:HOH:O	1.99	0.62
7:E:11:VAL:HG12	7:E:12:ASP:N	2.14	0.61
10:H:66:GLU:HA	38:H:8582:HOH:O	2.00	0.61
14:L:145:LEU:O	14:L:148:GLU:HG3	2.00	0.61
1:0:2505:G:O2'	1:0:2506:A:H5'	2.00	0.61
10:H:6:ALA:HA	10:H:61:ARG:NH1	2.15	0.61
27:Y:174:VAL:HG13	27:Y:177:LYS:HD2	1.82	0.61
1:0:542:A:H5'	1:0:542:A:C8	2.33	0.61
1:0:2649:A:H5'	1:0:2649:A:C8	2.36	0.61
14:L:114:VAL:HG11	38:L:8872:HOH:O	1.99	0.61
31:3:48:ASN:ND2	31:3:50:GLY:H	1.97	0.61
1:0:926:A:O2'	14:L:41:HIS:HD2	1.83	0.61
1:0:1681:G:H5"	1:0:1682:A:H5'	1.80	0.61
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.34	0.61
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.30	0.61
22:T:9:LYS:HD2	38:T:7242:HOH:O	1.99	0.61
38:0:9545:HOH:O	25:W:119:HIS:HE1	1.84	0.61
2:9:49:G:H5"	38:9:8666:HOH:O	2.00	0.61
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.82	0.61
27:Y:144:ARG:CZ	38:Y:8912:HOH:O	2.48	0.61
1:0:20:G:H21	20:R:117:HIS:HD2	1.48	0.61
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.81	0.61
2:9:39:U:H1'	2:9:44:A:H61	1.64	0.61
13:K:55:VAL:HG12	13:K:56:SER:N	2.16	0.61
16:N:154:LEU:HD11	16:N:157:PRO:HA	1.82	0.61
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.30	0.61
27:Y:133:HIS:HD2	38:Y:8880:HOH:O	1.82	0.61
1:0:558:C:O2'	1:0:559:U:H5"	2.01	0.61
1:0:2420:G:O2'	1:0:2421:G:H5'	2.01	0.61
4:B:71:VAL:HG11	4:B:296:LEU:HB3	1.81	0.61
5:C:219:ASN:O	5:C:222:ASP:HB2	2.00	0.61
6:D:154:LYS:HD2	6:D:154:LYS:N	2.00	0.61
8:F:27:GLY:HA3	8:F:101:ALA:O	2.01	0.61
14:L:149:ARG:O	14:L:150:GLN:HB2	2.01	0.61
18:P:115:SER:O	18:P:117:SER:N	2.31	0.61
24:V:4:HIS:HB3	38:V:6622:HOH:O	1.99	0.61
1:0:272:A:H5'	1:0:273:G:OP2	2.00	0.61
1:0:317:A:H5"	22:T:52:ARG:HD2	1.83	0.61
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2635:A:O2'	1:0:2636:C:H5'	2.02	0.60
6:D:146:LYS:NZ	16:N:107:ASN:ND2	2.49	0.60
12:J:19:MET:CE	12:J:132:LEU:HD11	2.30	0.60
1:0:1187:U:H2'	38:0:6867:HOH:O	2.02	0.60
1:0:2630:G:O6	3:A:206:ARG:NH2	2.35	0.60
15:M:99:ARG:HE	15:M:170:ASN:HD22	1.49	0.60
25:W:38:THR:HG22	25:W:39:ASP:N	2.17	0.60
4:B:56:ASP:OD1	4:B:322:ARG:HB3	2.01	0.60
12:J:107:ASN:ND2	12:J:109:TYR:H	2.00	0.60
14:L:136:ALA:HB3	38:L:8872:HOH:O	2.00	0.60
21:S:81:ILE:HG12	38:S:8539:HOH:O	2.01	0.60
1:0:1086:A:C6	25:W:11:VAL:HG11	2.35	0.60
1:0:1130:U:H2'	1:0:1131:G:O4'	2.02	0.60
1:0:1132:A:N6	1:0:1229:C:H2'	2.16	0.60
3:A:88:ILE:O	3:A:88:ILE:HG22	2.00	0.60
25:W:6:GLN:HG2	25:W:29:VAL:HA	1.82	0.60
30:2:41:HIS:N	30:2:45:ASN:HD22	1.87	0.60
5:C:246:ARG:NE	38:C:8630:HOH:O	2.35	0.60
18:P:143:ALA:HA	38:P:187:HOH:O	2.00	0.60
1:0:1701:A:H4'	1:0:1702:U:C5'	2.31	0.60
1:0:2717:C:O2'	1:0:2718:C:H5"	2.01	0.60
1:0:2779:G:H21	7:E:143:GLN:NE2	2.00	0.60
7:E:69:ILE:HA	7:E:72:MET:CE	2.31	0.60
14:L:61:ALA:HA	38:L:8863:HOH:O	2.01	0.60
38:0:3230:HOH:O	11:I:87:PRO:HD3	2.02	0.60
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.30	0.60
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.16	0.60
17:O:32:ARG:O	17:O:32:ARG:HD3	2.00	0.60
1:0:2265:U:H2'	1:0:2266:A:C8	2.37	0.60
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.16	0.60
4:B:258:GLY:H	4:B:260:HIS:CE1	2.20	0.60
9:G:23:ILE:O	9:G:27:ILE:HG13	2.01	0.60
21:S:52:VAL:C	21:S:53:ASN:HD22	2.05	0.60
1:0:2578:G:H5'	1:0:2578:G:H8	1.66	0.60
2:9:39:U:H1'	2:9:44:A:N6	2.17	0.60
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.36	0.60
1:0:1120:U:H5"	1:0:1120:U:C6	2.37	0.59
5:C:72:LYS:HD2	38:C:8631:HOH:O	2.02	0.59
9:G:64:ASN:HD22	9:G:64:ASN:N	1.99	0.59
30:2:35:ARG:HG2	38:2:6391:HOH:O	2.01	0.59
4:B:85:ARG:NH1	38:B:8935:HOH:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:38:THR:HG22	38:W:3580:HOH:O	2.02	0.59
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.83	0.59
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.84	0.59
1:0:2252:A:C5	1:0:2253:G:H1'	2.38	0.59
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.17	0.59
1:0:125:U:H2'	38:0:3759:HOH:O	2.01	0.59
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.85	0.59
16:N:47:LEU:HD13	16:N:97:VAL:HG11	1.85	0.59
1:0:944:G:H21	25:W:44:MET:CE	2.16	0.59
1:0:962:C:H1'	16:N:5:ARG:HH12	1.64	0.59
1:0:1058:A:H2'	1:0:1060:C:H5"	1.83	0.59
1:0:2737:C:OP2	18:P:61:ARG:NH2	2.35	0.59
38:9:8666:HOH:O	16:N:147:ILE:HB	2.02	0.59
8:F:69:GLU:O	8:F:70:LYS:HG2	2.03	0.59
22:T:26:THR:HA	22:T:39:ASN:HB3	1.83	0.59
24:V:38:GLY:C	24:V:40:PRO:HD2	2.23	0.59
27:Y:144:ARG:NH2	38:Y:8912:HOH:O	2.36	0.59
1:0:2504:A:H4'	10:H:74:ARG:HH11	1.68	0.59
10:H:61:ARG:HH11	10:H:61:ARG:HG3	1.68	0.59
10:H:102:LYS:HD3	10:H:122:LYS:HD3	1.82	0.59
29:1:1:THR:HA	38:1:8712:HOH:O	2.02	0.59
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.42	0.59
1:0:558:C:H2'	1:0:559:U:C5'	2.32	0.59
1:0:797:A:H4'	28:Z:10:ARG:N	2.18	0.59
1:0:1634:G:H3'	38:0:3887:HOH:O	2.02	0.59
10:H:12:ILE:HG23	10:H:129:ARG:CZ	2.32	0.59
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.00	0.59
1:0:584:U:H3'	38:0:6072:HOH:O	2.03	0.59
1:0:1205:U:H2'	1:0:1206:U:C5'	2.31	0.59
3:A:153:ARG:HB2	3:A:153:ARG:HH11	1.68	0.59
8:F:58:GLU:OE1	15:M:27:ARG:NH2	2.33	0.59
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.03	0.59
18:P:134:VAL:O	18:P:137:LEU:HB3	2.03	0.59
27:Y:216:ARG:HD2	38:Y:8866:HOH:O	2.01	0.59
4:B:48:MET:HG2	4:B:72:THR:HA	1.85	0.59
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.38	0.59
1:0:1183:C:N4	1:0:1184:C:H41	2.01	0.59
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.68	0.59
5:C:142:ASP:OD1	5:C:237:GLU:HB3	2.03	0.59
20:R:9:ASP:O	20:R:13:THR:HB	2.02	0.59
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:65:VAL:HA	25:W:68:THR:HG22	1.85	0.59
4:B:254:GLN:HG2	4:B:255:GLY:N	2.18	0.58
15:M:145:ASP:HB2	38:M:8867:HOH:O	2.02	0.58
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.32	0.58
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.02	0.58
1:0:1278:A:H4'	1:0:1279:U:C4	2.38	0.58
21:S:33:SER:OG	21:S:36:GLU:HG3	2.03	0.58
1:0:2717:C:H2'	1:0:2718:C:C5'	2.29	0.58
1:0:2769:C:C2'	1:0:2770:G:H5'	2.34	0.58
4:B:16:ARG:NH1	38:B:8918:HOH:O	2.35	0.58
1:0:121:U:OP2	30:2:10:ARG:NH2	2.33	0.58
4:B:119:HIS:O	4:B:121:PRO:HD3	2.03	0.58
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.85	0.58
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.85	0.58
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.37	0.58
4:B:103:ASP:HB2	38:B:8894:HOH:O	2.04	0.58
14:L:42:ASN:HB2	38:L:8874:HOH:O	2.03	0.58
1:0:328:U:O4'	5:C:202:THR:HG22	2.03	0.58
1:0:960:G:H4'	38:0:7395:HOH:O	2.02	0.58
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.68	0.58
3:A:94:LEU:HD23	3:A:94:LEU:N	2.18	0.58
11:I:113:SER:HB2	11:I:118:ASN:HB2	1.86	0.58
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.04	0.58
1:0:396:U:O2'	1:0:418:C:H4'	2.03	0.58
1:0:417:G:P	38:0:7384:HOH:O	2.62	0.58
5:C:200:PRO:HB3	5:C:212:VAL:HG23	1.85	0.58
18:P:61:ARG:HH11	18:P:61:ARG:HB2	1.69	0.58
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.85	0.58
26:X:30:MET:HE1	26:X:55:ASN:HA	1.86	0.58
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.04	0.58
3:A:65:ARG:C	3:A:66:ARG:HG3	2.24	0.58
8:F:37:THR:O	8:F:41:GLU:HG3	2.03	0.58
21:S:37:VAL:O	21:S:41:VAL:HG23	2.04	0.58
24:V:39:ALA:C	24:V:41:GLU:H	2.07	0.58
1:0:1441:G:O2'	1:0:1442:A:H5'	2.03	0.58
1:0:2004:U:H4'	38:0:5290:HOH:O	2.03	0.58
4:B:62:ARG:HA	4:B:65:MET:CE	2.33	0.58
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.84	0.58
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.86	0.58
1:0:2755:G:H1'	38:0:4674:HOH:O	2.03	0.58
1:0:2769:C:O2'	1:0:2770:G:H5'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:41:LYS:HE2	10:H:45:ASP:HB3	1.86	0.58
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.19	0.58
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.84	0.58
1:0:645:U:OP2	14:L:4:LYS:HE2	2.03	0.57
7:E:32:ARG:O	7:E:33:LEU:HD23	2.04	0.57
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.85	0.57
16:N:151:ASP:OD1	16:N:154:LEU:HD13	2.04	0.57
1:0:1741:U:H5'	1:0:1742:A:OP1	2.04	0.57
1:0:2064:U:H5'	1:0:2652:U:H4'	1.85	0.57
5:C:168:ARG:NH2	5:C:190:ALA:O	2.37	0.57
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.66	0.57
1:0:656:G:H5'	17:O:3:THR:HG22	1.86	0.57
6:D:65:GLU:HA	38:D:6752:HOH:O	2.05	0.57
11:I:97:VAL:CG1	11:I:101:LYS:HE3	2.32	0.57
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.02	0.57
1:0:65:C:O2'	1:0:66:G:H5'	2.04	0.57
1:0:2587:OMU:H2'	1:0:2589:U:H5"	1.86	0.57
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.86	0.57
1:0:1972:U:H2'	1:0:1973:A:H5'	1.87	0.57
2:9:73:A:H61	2:9:108:C:H42	1.52	0.57
4:B:248:ARG:O	4:B:251:VAL:HG13	2.05	0.57
5:C:27:ARG:HG3	5:C:29:ASP:OD1	2.04	0.57
18:P:20:ARG:HH12	18:P:54:LYS:HD3	1.69	0.57
19:Q:94:GLN:O	19:Q:95:GLU:HB2	2.04	0.57
1:0:2748:G:H2'	38:0:7503:HOH:O	2.04	0.57
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.69	0.57
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.34	0.57
3:A:199:HIS:HD2	3:A:201:PHE:H	1.53	0.57
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.04	0.57
4:B:310:ARG:HD2	38:B:8952:HOH:O	2.05	0.57
10:H:12:ILE:HG23	10:H:129:ARG:NE	2.19	0.57
25:W:149:LEU:HG	25:W:153:MET:HE2	1.87	0.57
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.85	0.57
31:3:65:THR:HG23	31:3:67:LEU:HG	1.86	0.57
1:0:2036:C:O4'	13:K:44:LEU:HG	2.05	0.57
1:0:2878:U:H2'	1:0:2879:A:O4'	2.05	0.57
3:A:66:ARG:HH11	3:A:66:ARG:CB	2.16	0.57
6:D:135:VAL:HG22	6:D:136:ARG:N	2.19	0.57
8:F:58:GLU:HA	8:F:61:MET:HG3	1.85	0.57
16:N:37:ARG:NE	38:N:8832:HOH:O	2.38	0.57
21:S:33:SER:O	21:S:37:VAL:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:107:LEU:O	25:W:112:LEU:HB2	2.04	0.57
1:0:447:A:OP2	22:T:1:SER:HB2	2.05	0.57
1:0:656:G:H5'	17:O:3:THR:CG2	2.35	0.57
4:B:145:HIS:HD2	4:B:146:THR:O	1.88	0.57
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.35	0.57
11:I:118:ASN:HA	11:I:121:LYS:HD2	1.86	0.57
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.05	0.57
1:0:2710:U:H1'	38:0:7580:HOH:O	2.04	0.57
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.70	0.57
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.05	0.57
15:M:164:THR:HG23	15:M:165:GLY:N	2.19	0.57
1:0:1209:C:H2'	1:0:1210:G:H8	1.70	0.57
1:0:2769:C:H2'	1:0:2770:G:O4'	2.04	0.57
25:W:125:HIS:HE1	38:W:3071:HOH:O	1.87	0.57
1:0:407:A:H5'	38:0:6004:HOH:O	2.04	0.56
2:9:28:U:H5"	16:N:40:ASN:HD21	1.69	0.56
2:9:64:C:H2'	2:9:65:A:H5'	1.87	0.56
13:K:14:LYS:CB	13:K:45:PRO:HG2	2.34	0.56
14:L:133:VAL:HB	38:L:8857:HOH:O	2.05	0.56
25:W:126:ASP:HB3	25:W:135:GLY:O	2.05	0.56
1:0:2681:A:H4'	1:0:2682:C:H5'	1.87	0.56
4:B:98:THR:HG22	4:B:99:GLU:N	2.17	0.56
7:E:24:GLY:HA3	7:E:76:VAL:HB	1.87	0.56
11:I:100:VAL:HG11	11:I:124:VAL:HG22	1.86	0.56
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.53	0.56
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.86	0.56
26:X:78:GLU:HG2	26:X:79:GLU:H	1.70	0.56
1:0:282:C:O2'	1:0:283:U:H5'	2.05	0.56
1:0:506:G:H22	1:0:509:A:H5"	1.66	0.56
1:0:625:U:H5"	1:0:1044:C:N4	2.19	0.56
1:0:1181:A:H5'	11:I:89:GLU:OE2	2.05	0.56
1:0:1477:C:H5'	1:0:1868:G:C5'	2.36	0.56
3:A:65:ARG:O	3:A:66:ARG:HG3	2.05	0.56
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.38	0.56
3:A:199:HIS:CD2	3:A:201:PHE:H	2.23	0.56
4:B:62:ARG:HG2	4:B:65:MET:HE3	1.87	0.56
4:B:84:LEU:HD23	4:B:142:LEU:HD23	1.86	0.56
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.40	0.56
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.87	0.56
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.05	0.56
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:189:ASN:C	27:Y:189:ASN:HD22	2.07	0.56
1:0:1603:A:H5"	1:0:1605:G:H5'	1.88	0.56
3:A:33:GLU:O	3:A:34:ASP:HB2	2.05	0.56
8:F:61:MET:HB3	15:M:19:GLN:OE1	2.04	0.56
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.39	0.56
2:9:44:A:O4'	6:D:76:ARG:NE	2.39	0.56
5:C:246:ARG:HB3	5:C:246:ARG:NH1	2.21	0.56
6:D:159:PRO:O	6:D:163:VAL:HG23	2.06	0.56
11:I:95:LEU:HD23	11:I:99:GLN:OE1	2.05	0.56
1:0:1682:A:H5"	38:0:9447:HOH:O	2.04	0.56
1:0:2563:U:H2'	1:0:2565:C:O5'	2.05	0.56
1:0:1168:C:H4'	38:I:5128:HOH:O	2.04	0.56
1:0:1679:C:H5'	38:0:9318:HOH:O	2.06	0.56
1:0:2256:G:H2'	1:0:2257:G:H5'	1.88	0.56
1:0:2488:A:H61	1:0:2534:C:H42	1.54	0.56
2:9:13:A:O2'	2:9:14:G:H5"	2.06	0.56
4:B:140:LEU:HD23	38:B:8878:HOH:O	2.05	0.56
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.88	0.56
10:H:50:ILE:HG12	10:H:168:VAL:HG22	1.88	0.56
16:N:151:ASP:HB3	38:N:8826:HOH:O	2.05	0.56
1:0:1589:G:N2	1:0:1605:G:H1'	2.20	0.56
1:0:2256:G:C2'	1:0:2257:G:H5'	2.36	0.56
5:C:2:GLN:HB3	38:C:8538:HOH:O	2.06	0.56
11:I:96:SER:H	11:I:99:GLN:NE2	2.03	0.56
11:I:108:HIS:HE1	11:I:116:LEU:HD22	1.70	0.56
25:W:84:VAL:HG12	38:W:6679:HOH:O	2.05	0.56
1:0:777:U:O2'	29:1:11:LYS:HG2	2.06	0.56
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.40	0.56
4:B:294:TYR:HE2	38:B:8954:HOH:O	1.88	0.56
38:C:8563:HOH:O	17:O:3:THR:HG21	2.05	0.56
7:E:137:ASP:O	7:E:141:VAL:HG23	2.05	0.56
21:S:42:GLU:HG2	21:S:49:VAL:HG23	1.87	0.56
1:0:949:U:H4'	19:Q:95:GLU:HA	1.88	0.56
1:0:1120:U:H5"	1:0:1120:U:H6	1.71	0.56
1:0:1778:A:H2'	1:0:1779:A:H5'	1.87	0.56
11:I:71:ALA:O	11:I:75:LYS:HG3	2.05	0.56
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.86	0.56
26:X:30:MET:CE	26:X:58:ALA:HB3	2.36	0.56
26:X:43:VAL:HG11	26:X:82:GLU:HA	1.88	0.56
27:Y:165:GLU:HB3	38:Y:8893:HOH:O	2.05	0.56
1:0:285:A:C2	1:0:368:C:H4'	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:588:G:O6	25:W:154:ARG:NH1	2.38	0.55
1:0:1053:G:OP1	10:H:15:PRO:HG3	2.05	0.55
1:0:1289:C:O2'	1:0:1290:G:H5'	2.05	0.55
6:D:25:MET:CE	6:D:37:ALA:HB1	2.32	0.55
10:H:41:LYS:HE2	10:H:45:ASP:CB	2.35	0.55
10:H:49:GLN:HG3	10:H:140:TYR:CE2	2.41	0.55
1:0:1060:C:H6	1:0:1060:C:H5'	1.72	0.55
1:0:2300:A:H4'	1:0:2301:A:O5'	2.07	0.55
4:B:102:THR:HG21	4:B:182:VAL:O	2.07	0.55
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.86	0.55
8:F:91:VAL:CG1	8:F:92:GLY:N	2.68	0.55
11:I:95:LEU:HD22	11:I:99:GLN:HB3	1.88	0.55
11:I:129:SER:O	11:I:130:LEU:HD23	2.06	0.55
20:R:132:ARG:CZ	38:R:8880:HOH:O	2.54	0.55
27:Y:144:ARG:NE	38:Y:8912:HOH:O	2.38	0.55
5:C:111:VAL:HB	38:C:8525:HOH:O	2.06	0.55
6:D:39:ASP:HB2	38:D:5583:HOH:O	2.06	0.55
7:E:107:PHE:CE2	7:E:108:LEU:HD13	2.41	0.55
8:F:46:GLU:O	8:F:73:PRO:HD2	2.05	0.55
10:H:143:VAL:HG22	10:H:173:GLU:OE1	2.05	0.55
15:M:46:LEU:HG	38:M:8921:HOH:O	2.06	0.55
23:U:9:CYS:HA	23:U:52:THR:HG23	1.87	0.55
1:0:447:A:O2'	1:0:448:G:H5'	2.07	0.55
1:0:1741:U:O2'	1:0:2723:G:H4'	2.07	0.55
6:D:149:ARG:NH1	38:D:3066:HOH:O	2.36	0.55
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.36	0.55
24:V:39:ALA:N	24:V:40:PRO:CD	2.70	0.55
1:0:1118:A:C8	1:0:1118:A:C3'	2.86	0.55
1:0:2415:A:O2'	16:N:29:SER:HB3	2.07	0.55
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.87	0.55
9:G:12:ILE:N	9:G:13:PRO:HD3	2.22	0.55
19:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.06	0.55
22:T:16:LEU:HA	22:T:19:ARG:HG3	1.87	0.55
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.87	0.55
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.19	0.55
1:0:88:G:H8	1:0:88:G:H5'	1.71	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.89	0.55
16:N:47:LEU:HD12	16:N:92:ALA:HB1	1.88	0.55
1:0:1187:U:O2'	1:0:1189:A:H2	1.82	0.55
2:9:49:G:O2'	2:9:50:G:H5'	2.06	0.55
2:9:76:G:C3'	2:9:77:A:H5"	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:194:MET:CE	3:A:199:HIS:HB2	2.37	0.55
3:A:211:LYS:NZ	38:A:8918:HOH:O	2.38	0.55
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.36	0.55
6:D:58:VAL:CG1	6:D:60:GLU:HG2	2.37	0.55
10:H:12:ILE:HD12	10:H:57:THR:CG2	2.36	0.55
18:P:7:LYS:HD3	18:P:21:VAL:CG2	2.36	0.55
1:0:1014:A:H2'	1:0:1015:C:H5'	1.89	0.55
1:0:1086:A:N6	25:W:11:VAL:HG11	2.21	0.55
1:0:1377:C:H5'	1:0:1377:C:C6	2.42	0.55
38:0:6994:HOH:O	3:A:211:LYS:HG2	2.05	0.55
6:D:101:THR:O	6:D:101:THR:HG22	2.07	0.55
11:I:133:THR:HG22	11:I:134:ILE:N	2.22	0.55
21:S:23:LYS:HE2	38:S:8533:HOH:O	2.06	0.55
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.03	0.55
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.88	0.55
26:X:43:VAL:HG12	26:X:44:ASP:N	2.21	0.55
27:Y:155:ARG:NH1	38:Y:8854:HOH:O	2.39	0.55
1:0:31:C:H2'	38:0:7647:HOH:O	2.06	0.55
1:0:136:C:H2'	1:0:137:U:O4'	2.07	0.55
1:0:1926:G:H2'	1:0:1927:A:C8	2.42	0.55
12:J:107:ASN:C	12:J:107:ASN:HD22	2.10	0.55
16:N:37:ARG:CZ	38:N:8832:HOH:O	2.54	0.55
21:S:77:VAL:O	21:S:80:ARG:HG2	2.07	0.55
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.88	0.55
1:0:280:C:H2'	1:0:281:U:O4'	2.07	0.54
4:B:75:GLU:C	4:B:77:PRO:HD3	2.26	0.54
11:I:70:THR:OG1	11:I:107:LYS:HE2	2.08	0.54
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.89	0.54
26:X:10:VAL:HG11	26:X:36:HIS:HE1	1.71	0.54
1:0:2243:C:H5"	38:0:3744:HOH:O	2.07	0.54
1:0:2748:G:H5'	38:0:7503:HOH:O	2.06	0.54
2:9:6:C:OP1	16:N:37:ARG:NH1	2.40	0.54
3:A:128:LEU:HD21	3:A:131:HIS:HE1	1.73	0.54
16:N:100:ALA:O	16:N:129:ILE:HG23	2.07	0.54
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.88	0.54
3:A:6:GLY:HA3	38:A:8863:HOH:O	2.06	0.54
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.89	0.54
11:I:88:GLN:NE2	11:I:128:THR:HG21	2.22	0.54
1:0:119:A:H2'	1:0:120:A:H5"	1.90	0.54
1:0:2712:G:H5'	38:K:4183:HOH:O	2.07	0.54
4:B:297:VAL:HB	38:B:8907:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.07	0.54
1:0:2256:G:H2'	1:0:2257:G:C5'	2.38	0.54
1:0:2670:G:O2'	1:0:2671:U:H5'	2.07	0.54
3:A:48:ASP:HB3	38:A:8904:HOH:O	2.08	0.54
5:C:39:GLN:O	5:C:43:LYS:HD3	2.07	0.54
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.89	0.54
7:E:84:MET:HE1	7:E:148:ILE:HD12	1.89	0.54
1:0:602:A:O2'	1:0:605:C:H4'	2.07	0.54
1:0:776:A:OP1	29:1:28:HIS:HE1	1.91	0.54
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.19	0.54
5:C:246:ARG:NH1	38:C:8575:HOH:O	2.40	0.54
11:I:108:HIS:N	11:I:109:PRO:HD2	2.23	0.54
14:L:104:ASP:HB3	38:L:8863:HOH:O	2.07	0.54
25:W:129:LYS:HG2	38:W:1990:HOH:O	2.07	0.54
1:0:1733:A:H4'	4:B:212:GLN:HA	1.88	0.54
1:0:2248:C:H3'	38:0:5423:HOH:O	2.08	0.54
7:E:69:ILE:HA	7:E:72:MET:HE3	1.90	0.54
13:K:27:ARG:HD2	38:K:4747:HOH:O	2.06	0.54
25:W:139:GLY:O	25:W:141:HIS:HD2	1.91	0.54
1:0:1766:U:O2	1:0:1778:A:H5'	2.07	0.54
7:E:166:VAL:HG12	38:E:3134:HOH:O	2.07	0.54
16:N:119:GLN:O	16:N:123:ILE:HG13	2.08	0.54
27:Y:174:VAL:CG1	27:Y:177:LYS:HD2	2.38	0.54
1:0:1173:A:H2	38:0:6254:HOH:O	1.90	0.54
4:B:305:ASP:O	4:B:306:LYS:HB2	2.08	0.54
16:N:152:GLU:C	16:N:154:LEU:H	2.09	0.54
16:N:176:ARG:O	16:N:180:LEU:HD13	2.08	0.54
1:0:263:U:O4'	8:F:59:ILE:HD13	2.08	0.54
1:0:485:A:N3	1:0:487:G:H5"	2.23	0.54
1:0:1299:G:N7	14:L:6:ARG:NH1	2.56	0.54
4:B:280:VAL:CG1	4:B:334:SER:HA	2.37	0.54
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.37	0.54
21:S:17:ASP:HB3	21:S:23:LYS:HB2	1.90	0.54
1:0:2487:C:H5	38:0:4875:HOH:O	1.91	0.53
1:0:2768:A:H3'	38:0:4419:HOH:O	2.08	0.53
3:A:179:MET:HG2	3:A:186:TRP:CG	2.44	0.53
6:D:25:MET:SD	6:D:40:ILE:HD11	2.48	0.53
14:L:21:ARG:N	38:L:8830:HOH:O	2.40	0.53
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.89	0.53
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.89	0.53
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1477:C:H5'	1:0:1868:G:H5"	1.89	0.53
1:0:1589:G:H4'	38:0:6828:HOH:O	2.08	0.53
3:A:194:MET:HE1	3:A:199:HIS:HB2	1.90	0.53
5:C:1:MET:HG2	5:C:2:GLN:N	2.17	0.53
5:C:16:VAL:HG12	5:C:17:ASP:N	2.22	0.53
15:M:169:ARG:HD2	38:M:8890:HOH:O	2.08	0.53
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.23	0.53
20:R:132:ARG:HG2	20:R:133:ALA:N	2.22	0.53
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.90	0.53
4:B:148:PRO:HD2	38:B:8879:HOH:O	2.08	0.53
4:B:223:ARG:HG3	4:B:232:TRP:O	2.08	0.53
16:N:49:THR:HB	16:N:58:LEU:HD11	1.90	0.53
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.90	0.53
23:U:52:THR:HG22	23:U:54:THR:N	2.24	0.53
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.90	0.53
1:0:638:C:H2'	1:0:639:A:C8	2.44	0.53
1:0:2270:G:C4'	3:A:223:ARG:HH12	2.20	0.53
3:A:8:ARG:HG2	38:A:8847:HOH:O	2.08	0.53
3:A:212:PRO:HB2	38:A:8855:HOH:O	2.07	0.53
13:K:115:ARG:HG3	13:K:116:GLU:N	2.22	0.53
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.89	0.53
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.56	0.53
1:0:681:G:N3	1:0:681:G:H5'	2.24	0.53
1:0:702:G:O2'	1:0:703:G:H5'	2.09	0.53
1:0:1926:G:H2'	1:0:1927:A:H8	1.74	0.53
11:I:88:GLN:HA	11:I:91:PHE:CE2	2.43	0.53
12:J:52:GLN:HG3	12:J:53:ILE:H	1.72	0.53
14:L:67:ARG:O	14:L:71:GLU:HG3	2.08	0.53
16:N:33:ARG:NH1	16:N:103:ASP:OD2	2.35	0.53
20:R:12:THR:HG22	20:R:149:GLU:OE1	2.08	0.53
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.74	0.53
1:0:2361:A:H5"	38:0:9001:HOH:O	2.09	0.53
2:9:91:C:H2'	2:9:92:G:O4'	2.09	0.53
5:C:77:ALA:O	5:C:78:ARG:HG3	2.08	0.53
6:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.55	0.53
1:0:1166:A:H1'	1:0:1192:A:C2	2.42	0.53
1:0:2524:G:H21	1:0:2526:C:N4	2.05	0.53
3:A:53:ALA:HB3	38:A:8904:HOH:O	2.08	0.53
11:I:70:THR:HA	11:I:107:LYS:NZ	2.24	0.53
20:R:39:THR:HB	20:R:42:GLU:CG	2.39	0.53
24:V:5:VAL:HG23	38:V:2271:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1189:A:H3'	38:0:7639:HOH:O	2.08	0.53
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.44	0.53
1:0:2601:A:N1	13:K:38:SER:HB2	2.24	0.53
2:9:114:G:H2'	2:9:115:C:C6	2.44	0.53
4:B:41:PHE:CD2	4:B:190:MET:HE3	2.44	0.53
4:B:238:ASN:ND2	4:B:240:GLY:H	1.95	0.53
22:T:9:LYS:HB2	38:T:7242:HOH:O	2.08	0.53
25:W:26:ILE:O	25:W:26:ILE:HG13	2.09	0.53
30:2:41:HIS:H	30:2:45:ASN:ND2	1.89	0.53
1:0:377:C:H5	38:0:3304:HOH:O	1.91	0.53
1:0:1279:U:O2	1:0:1279:U:H2'	2.07	0.53
5:C:233:THR:HG22	5:C:234:VAL:N	2.24	0.53
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.91	0.53
27:Y:95:THR:N	27:Y:236:VAL:O	2.42	0.53
1:0:1201:C:H2'	1:0:1202:A:H5'	1.90	0.53
1:0:1687:C:O2	29:1:9:GLY:HA2	2.09	0.53
1:0:2629:C:N4	3:A:206:ARG:HH21	2.07	0.53
9:G:20:VAL:O	9:G:24:VAL:HG23	2.09	0.53
10:H:79:GLU:O	10:H:80:LEU:HD23	2.09	0.53
11:I:133:THR:HG22	11:I:134:ILE:H	1.72	0.53
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.56	0.53
1:0:338:C:H4'	5:C:174:ILE:HD11	1.91	0.52
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.09	0.52
1:0:1878:G:O2'	1:0:1879:U:P	2.67	0.52
1:0:2521:A:OP2	10:H:6:ALA:HB3	2.08	0.52
3:A:88:ILE:HD13	3:A:100:PRO:CD	2.34	0.52
4:B:304:PRO:HD2	4:B:307:ARG:HD2	1.91	0.52
13:K:87:ARG:NH1	38:K:4066:HOH:O	2.43	0.52
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.44	0.52
1:0:644:G:H5'	1:0:644:G:N3	2.23	0.52
1:0:894:A:C2	5:C:87:ARG:NH2	2.77	0.52
1:0:2411:C:H4'	38:0:4942:HOH:O	2.09	0.52
38:0:9690:HOH:O	4:B:254:GLN:HG3	2.08	0.52
2:9:14:G:O2'	16:N:1:ALA:HB2	2.09	0.52
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.90	0.52
4:B:80:ARG:HA	4:B:186:GLY:O	2.10	0.52
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.91	0.52
16:N:37:ARG:NH2	38:N:8832:HOH:O	2.41	0.52
24:V:13:PRO:O	24:V:17:GLU:HG3	2.08	0.52
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.44	0.52
1:0:856:G:H2'	38:0:5409:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2840:A:H3'	38:0:7606:HOH:O	2.08	0.52
5:C:19:PRO:HG2	5:C:22:PHE:CE1	2.44	0.52
5:C:25:PRO:HG2	38:C:8526:HOH:O	2.08	0.52
1:0:256:C:H2'	1:0:257:G:O4'	2.10	0.52
1:0:517:U:H1'	38:0:7536:HOH:O	2.09	0.52
1:0:714:U:H3'	38:0:6912:HOH:O	2.10	0.52
1:0:1008:C:H5"	10:H:19:ARG:HH12	1.74	0.52
1:0:2073:G:OP2	1:0:2490:A:H5'	2.09	0.52
1:0:2468:A:H61	31:3:48:ASN:HD21	1.55	0.52
1:0:2831:C:H2'	1:0:2832:C:H5'	1.92	0.52
4:B:5:ARG:NH1	4:B:8:LYS:HE2	2.25	0.52
4:B:132:HIS:NE2	4:B:171:VAL:HG23	2.25	0.52
4:B:139:ASP:CB	4:B:165:ARG:HE	2.21	0.52
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.56	0.52
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.90	0.52
16:N:163:PHE:O	16:N:164:ASP:O	2.27	0.52
30:2:48:ASP:O	30:2:49:GLU:HB2	2.10	0.52
1:0:2064:U:H5'	1:0:2652:U:O3'	2.10	0.52
4:B:82:VAL:O	4:B:82:VAL:HG12	2.09	0.52
7:E:125:GLU:HB2	7:E:132:THR:CG2	2.39	0.52
9:G:12:ILE:HG22	9:G:17:GLN:NE2	2.24	0.52
23:U:47:ARG:HG2	38:U:4381:HOH:O	2.09	0.52
24:V:55:ARG:O	24:V:59:ILE:HG12	2.09	0.52
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.40	0.52
1:0:407:A:H2'	1:0:408:A:C8	2.45	0.52
1:0:1342:C:C2'	1:0:1343:C:H5'	2.40	0.52
2:9:48:C:H4'	16:N:141:ARG:HH21	1.74	0.52
3:A:109:GLU:HG2	3:A:116:GLY:N	2.25	0.52
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.92	0.52
11:I:134:ILE:HG22	11:I:135:GLU:N	2.24	0.52
24:V:7:GLU:O	24:V:11:MET:HG3	2.09	0.52
27:Y:187:VAL:HG22	27:Y:192:ASP:HB2	1.90	0.52
27:Y:212:ARG:HD2	38:Y:8901:HOH:O	2.10	0.52
1:0:474:C:O3'	5:C:73:LEU:CD2	2.57	0.52
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.92	0.52
1:0:656:G:OP2	17:O:37:ARG:HD2	2.08	0.52
1:0:1118:A:H62	1:0:1244:U:H3	1.56	0.52
1:0:1730:G:H5'	1:0:1731:C:C5	2.45	0.52
1:0:2365:G:H4'	19:Q:45:PRO:O	2.10	0.52
4:B:132:HIS:HB2	4:B:137:LEU:HD22	1.92	0.52
8:F:91:VAL:CG1	8:F:92:GLY:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:69:LYS:O	22:T:71:VAL:HG23	2.10	0.52
26:X:43:VAL:HG12	26:X:44:ASP:H	1.72	0.52
1:0:960:G:N3	1:0:960:G:H2'	2.24	0.52
1:0:2266:A:OP2	15:M:90:ARG:NH2	2.43	0.52
4:B:41:PHE:HA	4:B:79:MET:HE2	1.90	0.52
4:B:102:THR:CG2	4:B:182:VAL:HG12	2.39	0.52
5:C:162:VAL:HG22	5:C:232:LEU:HD21	1.92	0.52
8:F:19:ALA:O	8:F:22:VAL:HG22	2.10	0.52
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.92	0.52
25:W:39:ASP:HB2	38:W:3580:HOH:O	2.09	0.52
1:0:524:A:H5'	20:R:29:LYS:HE2	1.92	0.52
1:0:1333:U:H2'	1:0:1334:C:C6	2.45	0.52
38:0:9981:HOH:O	14:L:22:ARG:HG2	2.09	0.52
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.92	0.52
12:J:103:VAL:HG12	38:J:5907:HOH:O	2.09	0.52
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.10	0.52
29:1:25:LYS:O	29:1:25:LYS:HG2	2.10	0.52
1:0:500:G:H21	20:R:98:ASN:HD21	1.56	0.52
1:0:2316:G:H4'	38:0:6069:HOH:O	2.10	0.52
1:0:2909:G:H2'	1:0:2910:A:H8	1.75	0.52
3:A:105:VAL:HG13	3:A:155:THR:O	2.10	0.52
5:C:140:VAL:HG12	5:C:141:SER:N	2.25	0.52
6:D:35:ALA:N	38:D:5576:HOH:O	2.43	0.52
7:E:10:ASP:HA	38:E:3707:HOH:O	2.09	0.52
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.75	0.52
16:N:34:LEU:HA	16:N:47:LEU:HD23	1.91	0.52
17:O:18:ALA:HA	17:O:23:GLY:O	2.10	0.52
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.44	0.52
25:W:90:TYR:CE2	25:W:99:ALA:HB2	2.44	0.52
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.45	0.52
1:0:794:U:H3	1:0:819:A:H61	1.58	0.51
1:0:2256:G:O2'	1:0:2257:G:H5'	2.10	0.51
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.91	0.51
6:D:104:PHE:CE2	6:D:132:VAL:HB	2.45	0.51
1:0:90:A:H2'	1:0:91:G:O4'	2.09	0.51
1:0:1250:C:O2'	1:0:1251:C:H5'	2.10	0.51
1:0:1596:U:H2'	1:0:1598:A:OP2	2.10	0.51
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.24	0.51
11:I:87:PRO:C	11:I:89:GLU:H	2.12	0.51
19:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.09	0.51
1:0:166:A:N7	14:L:25:GLY:HA2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1625:U:H4'	38:0:4659:HOH:O	2.11	0.51
1:0:1787:C:H4'	1:0:2883:A:O4'	2.10	0.51
1:0:2638:G:H5'	38:0:4916:HOH:O	2.10	0.51
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.40	0.51
4:B:7:ARG:HD3	4:B:9:GLY:O	2.11	0.51
4:B:62:ARG:NH2	4:B:66:GLU:O	2.43	0.51
4:B:171:VAL:O	4:B:175:LEU:HB2	2.11	0.51
6:D:58:VAL:HB	6:D:62:ASP:HB3	1.91	0.51
12:J:39:VAL:HG13	12:J:106:GLY:O	2.10	0.51
13:K:30:LYS:O	13:K:55:VAL:HG13	2.10	0.51
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.40	0.51
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.09	0.51
1:0:316:A:H5'	22:T:54:ASP:OD2	2.09	0.51
1:0:338:C:H5"	38:0:3794:HOH:O	2.11	0.51
1:0:1183:C:H42	1:0:1184:C:H41	1.58	0.51
1:0:2629:C:H41	3:A:206:ARG:HH21	1.57	0.51
3:A:132:ASP:OD1	3:A:133:ARG:N	2.43	0.51
18:P:115:SER:C	18:P:117:SER:H	2.11	0.51
23:U:14:GLU:O	23:U:17:THR:HB	2.09	0.51
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.10	0.51
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.10	0.51
2:9:35:C:H5"	38:9:8655:HOH:O	2.11	0.51
5:C:118:THR:O	5:C:136:VAL:HG13	2.10	0.51
13:K:75:ARG:HG2	13:K:90:PHE:CD2	2.45	0.51
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.93	0.51
1:0:259:G:H21	15:M:58:GLN:NE2	2.09	0.51
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.11	0.51
2:9:55:U:H4'	2:9:56:A:C8	2.45	0.51
3:A:36:ASP:HA	3:A:83:GLY:HA3	1.93	0.51
4:B:221:GLN:HE22	13:K:42:ASN:HD22	1.56	0.51
4:B:329:TYR:CE2	23:U:15:PRO:HG2	2.46	0.51
7:E:23:GLU:HG2	7:E:28:SER:CB	2.41	0.51
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.92	0.51
17:O:21:SER:OG	17:O:106:PRO:HB2	2.10	0.51
1:0:1667:A:H2'	1:0:1668:U:C6	2.45	0.51
1:0:1884:G:O6	3:A:190:ARG:HD2	2.11	0.51
1:0:2241:C:O2'	1:0:2242:U:H5'	2.11	0.51
1:0:2526:C:O2'	1:0:2527:U:H5'	2.11	0.51
2:9:55:U:H4'	2:9:56:A:H8	1.75	0.51
4:B:43:GLY:O	4:B:308:LEU:HD12	2.10	0.51
6:D:23:VAL:HG12	6:D:130:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:139:GLY:O	25:W:141:HIS:CD2	2.64	0.51
1:0:1717:A:H5"	18:P:54:LYS:HB2	1.93	0.51
1:0:2237:G:H1'	38:0:4841:HOH:O	2.10	0.51
1:0:2690:U:O2'	7:E:111:LYS:HE3	2.11	0.51
3:A:37:VAL:HG13	38:A:8908:HOH:O	2.11	0.51
5:C:127:ARG:HG2	5:C:127:ARG:NH1	2.26	0.51
6:D:76:ARG:O	6:D:77:ASP:HB2	2.10	0.51
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.93	0.51
25:W:80:ASP:O	25:W:84:VAL:HG23	2.09	0.51
28:Z:80:ARG:O	28:Z:81:ARG:O	2.29	0.51
30:2:41:HIS:CD2	30:2:44:ARG:H	2.26	0.51
31:3:56:PRO:N	38:3:8849:HOH:O	2.43	0.51
1:0:292:G:H2'	1:0:358:G:N2	2.26	0.51
1:0:1176:C:H1'	38:0:3923:HOH:O	2.11	0.51
1:0:2506:A:H1'	38:0:3740:HOH:O	2.09	0.51
4:B:150:ALA:O	4:B:152:PRO:HD3	2.11	0.51
4:B:280:VAL:HG13	4:B:333:GLU:O	2.11	0.51
5:C:127:ARG:HG2	5:C:127:ARG:HH11	1.76	0.51
6:D:56:ARG:N	38:D:6752:HOH:O	2.44	0.51
7:E:80:TRP:O	7:E:134:SER:HA	2.10	0.51
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.41	0.51
22:T:47:THR:HB	22:T:100:ASP:HB3	1.92	0.51
22:T:71:VAL:HG12	22:T:72:ILE:N	2.26	0.51
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.45	0.51
25:W:149:LEU:HG	25:W:153:MET:CE	2.40	0.51
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.41	0.51
29:1:45:ARG:NH2	38:1:8730:HOH:O	2.22	0.51
1:0:1163:G:N2	38:0:4717:HOH:O	2.43	0.51
1:0:1213:C:O2'	1:0:1214:G:H5'	2.11	0.51
1:0:1925:G:O2'	1:0:1926:G:H5'	2.11	0.51
1:0:2362:A:H2'	1:0:2363:G:C8	2.46	0.51
6:D:23:VAL:HG23	6:D:23:VAL:O	2.09	0.51
7:E:20:ILE:HD11	7:E:40:VAL:CG1	2.40	0.51
7:E:37:ASP:OD1	12:J:125:SER:HB3	2.11	0.51
21:S:32:ALA:HA	21:S:36:GLU:OE1	2.11	0.51
22:T:18:GLU:O	22:T:21:LYS:HG2	2.11	0.51
24:V:44:GLY:O	24:V:48:GLU:HG2	2.10	0.51
1:0:318:U:O2'	1:0:338:C:H2'	2.10	0.50
1:0:2506:A:O2'	1:0:2507:G:O5'	2.29	0.50
2:9:6:C:C5'	16:N:37:ARG:HH12	2.05	0.50
2:9:30:C:OP1	6:D:137:PRO:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.41	0.50
17:O:73:ASP:HA	17:O:92:VAL:O	2.11	0.50
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.94	0.50
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.10	0.50
2:9:20:G:O2'	2:9:21:G:H5'	2.12	0.50
2:9:42:C:H5'	2:9:43:G:OP2	2.12	0.50
3:A:210:GLY:HA3	38:A:8884:HOH:O	2.10	0.50
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.29	0.50
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.40	0.50
1:0:1007:A:H2'	10:H:22:TYR:CZ	2.47	0.50
1:0:1116:U:O2'	1:0:1118:A:C2	2.49	0.50
1:0:1162:G:H1'	11:I:112:LEU:CD1	2.36	0.50
5:C:22:PHE:HA	5:C:116:ALA:HA	1.92	0.50
6:D:38:GLU:HB3	6:D:49:PRO:HG3	1.94	0.50
22:T:38:ARG:NH1	38:T:6217:HOH:O	2.44	0.50
23:U:6:CYS:HA	23:U:13:ILE:HD11	1.93	0.50
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.93	0.50
1:0:371:U:H2'	1:0:372:A:C8	2.46	0.50
1:0:660:A:H4'	1:0:661:G:O5'	2.12	0.50
1:0:821:U:H2'	1:0:822:C:H6	1.76	0.50
1:0:1422:U:H2'	1:0:1423:C:C6	2.47	0.50
1:0:1535:G:H2'	1:0:1536:C:C6	2.47	0.50
1:0:2244:A:H1'	38:M:8868:HOH:O	2.12	0.50
38:0:4058:HOH:O	4:B:27:ASN:HB2	2.11	0.50
38:0:6437:HOH:O	4:B:27:ASN:HB3	2.11	0.50
38:0:9072:HOH:O	4:B:214:PRO:HD2	2.11	0.50
3:A:105:VAL:HG12	3:A:106:CYS:N	2.25	0.50
5:C:95:GLU:HG3	38:C:8678:HOH:O	2.11	0.50
6:D:28:GLY:CA	6:D:69:ILE:HG23	2.37	0.50
13:K:34:VAL:HB	38:K:7169:HOH:O	2.11	0.50
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.94	0.50
29:1:25:LYS:HD2	30:2:49:GLU:H	1.76	0.50
30:2:40:ARG:HD2	30:2:47:THR:HG22	1.92	0.50
1:0:1589:G:H22	1:0:1605:G:H1'	1.76	0.50
1:0:1675:C:H5"	30:2:5:LYS:HD2	1.93	0.50
2:9:34:A:H2'	2:9:35:C:O4'	2.11	0.50
4:B:138:GLY:O	4:B:139:ASP:O	2.29	0.50
17:O:39:THR:O	17:O:115:ARG:NH2	2.45	0.50
22:T:48:VAL:HG11	22:T:96:VAL:CG1	2.42	0.50
1:0:282:C:H1'	1:0:368:C:H42	1.74	0.50
1:0:371:U:H2'	1:0:372:A:H8	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:522:U:O2'	1:0:1366:C:H5'	2.12	0.50
1:0:703:G:O2'	1:0:704:C:H5'	2.12	0.50
1:0:1942:A:H3'	38:0:7311:HOH:O	2.12	0.50
4:B:162:MET:CE	4:B:310:ARG:HD3	2.42	0.50
11:I:130:LEU:HA	38:I:7210:HOH:O	2.12	0.50
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.93	0.50
22:T:40:VAL:HG22	22:T:41:ARG:N	2.27	0.50
22:T:48:VAL:HG22	22:T:98:VAL:HA	1.94	0.50
23:U:52:THR:HG21	23:U:54:THR:HB	1.94	0.50
1:0:1205:U:C2'	1:0:1206:U:H5"	2.42	0.50
1:0:2500:C:H1'	38:0:4657:HOH:O	2.12	0.50
10:H:43:ALA:HB1	10:H:140:TYR:CE2	2.47	0.50
14:L:143:THR:CG2	14:L:144:ASP:N	2.74	0.50
20:R:17:MET:HE3	20:R:19:ARG:CZ	2.42	0.50
24:V:64:GLY:O	24:V:65:ASP:CB	2.58	0.50
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.25	0.50
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.59	0.50
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.95	0.50
1:0:1165:G:O3'	1:0:1174:A:H4'	2.12	0.50
2:9:49:G:H2'	2:9:50:G:O4'	2.12	0.50
2:9:64:C:C2'	2:9:65:A:H5'	2.42	0.50
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.42	0.50
15:M:95:LYS:HG2	15:M:99:ARG:HB3	1.93	0.50
16:N:38:LYS:HD2	16:N:114:LYS:HE3	1.94	0.50
16:N:176:ARG:HE	16:N:180:LEU:HD21	1.77	0.50
18:P:55:LYS:HG2	18:P:56:GLY:N	2.27	0.50
1:0:816:G:H5'	1:0:1598:A:H4'	1.93	0.50
1:0:1878:G:O2'	1:0:1879:U:H6	1.93	0.50
1:0:2756:U:N3	1:0:2896:A:H2	2.04	0.50
10:H:151:GLU:OE1	10:H:151:GLU:HA	2.12	0.50
15:M:57:LYS:HE2	15:M:140:ALA:O	2.12	0.50
15:M:99:ARG:HE	15:M:170:ASN:ND2	2.09	0.50
16:N:115:VAL:HG23	38:N:8856:HOH:O	2.12	0.50
1:0:67:A:H5"	1:0:69:A:C8	2.47	0.49
1:0:542:A:H2'	1:0:543:G:O4'	2.12	0.49
1:0:1434:A:H2'	1:0:1436:C:C5	2.47	0.49
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.94	0.49
11:I:124:VAL:O	11:I:124:VAL:HG12	2.11	0.49
16:N:49:THR:HB	16:N:58:LEU:CD1	2.42	0.49
1:0:1496:A:H5'	1:0:1572:A:H1'	1.94	0.49
38:0:6258:HOH:O	27:Y:158:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:6836:HOH:O	3:A:211:LYS:HD3	2.12	0.49
4:B:320:GLN:HE21	4:B:321:PRO:CD	2.16	0.49
5:C:46:TYR:CE2	5:C:98:ARG:NH1	2.80	0.49
5:C:214:THR:HG23	38:C:8644:HOH:O	2.11	0.49
6:D:35:ALA:HB3	38:D:3279:HOH:O	2.12	0.49
11:I:96:SER:H	11:I:99:GLN:CD	2.16	0.49
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.27	0.49
20:R:29:LYS:HD3	38:R:8838:HOH:O	2.12	0.49
1:0:1087:G:H4'	1:0:1088:A:OP1	2.12	0.49
4:B:7:ARG:NH1	4:B:11:LEU:HD21	2.27	0.49
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.46	0.49
4:B:204:GLY:HA3	38:B:8957:HOH:O	2.12	0.49
7:E:166:VAL:HB	38:E:6341:HOH:O	2.12	0.49
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.42	0.49
22:T:24:ARG:HH21	22:T:39:ASN:ND2	2.11	0.49
24:V:1:THR:HG23	24:V:2:VAL:N	2.21	0.49
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.47	0.49
1:0:120:A:H2'	1:0:120:A:N3	2.27	0.49
1:0:1503:U:H2'	1:0:1504:A:O4'	2.12	0.49
1:0:2837:U:H1'	4:B:307:ARG:HH12	1.77	0.49
3:A:217:ARG:HG2	3:A:229:ALA:HB2	1.94	0.49
5:C:138:VAL:O	5:C:234:VAL:HA	2.13	0.49
7:E:16:ASP:O	7:E:17:HIS:HB2	2.12	0.49
8:F:101:ALA:HA	38:F:5413:HOH:O	2.12	0.49
10:H:70:LEU:O	10:H:74:ARG:HB2	2.11	0.49
25:W:130:HIS:O	25:W:136:GLY:HA3	2.13	0.49
26:X:25:ARG:NH1	38:X:3861:HOH:O	2.44	0.49
1:0:920:C:H5'	1:0:921:G:C4	2.47	0.49
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.94	0.49
5:C:7:ASP:OD2	5:C:9:ASP:HB2	2.13	0.49
8:F:14:ASP:O	8:F:18:GLU:HG3	2.12	0.49
25:W:19:ASP:O	25:W:23:MET:HG3	2.12	0.49
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.27	0.49
1:0:558:C:C2'	1:0:559:U:C5'	2.90	0.49
1:0:1185:U:OP1	11:I:121:LYS:HD3	2.12	0.49
1:0:1973:A:H5'	1:0:1973:A:H8	1.76	0.49
8:F:110:ASP:O	8:F:114:LYS:HG3	2.13	0.49
1:0:2724:U:H2'	1:0:2725:G:O4'	2.12	0.49
4:B:307:ARG:HH11	4:B:307:ARG:HB2	1.78	0.49
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.46	0.49
16:N:183:ASP:O	16:N:184:ILE:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:57:THR:CG2	21:S:58:MET:N	2.76	0.49
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.46	0.49
1:0:541:C:H2'	1:0:542:A:H5'	1.94	0.49
1:0:583:C:H2'	1:0:584:U:H6	1.78	0.49
1:0:1342:C:O2'	1:0:1343:C:H5'	2.13	0.49
1:0:1634:G:H2'	1:0:1635:U:C6	2.47	0.49
1:0:1730:G:H5"	1:0:1731:C:H6	1.77	0.49
7:E:69:ILE:HA	7:E:72:MET:HE2	1.94	0.49
7:E:154:ILE:HG23	7:E:154:ILE:O	2.13	0.49
10:H:172:GLU:C	10:H:174:LEU:H	2.16	0.49
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.22	0.49
22:T:78:THR:OG1	22:T:86:GLU:HG2	2.12	0.49
31:3:73:GLU:HB3	38:3:8860:HOH:O	2.12	0.49
1:0:1185:U:H2'	1:0:1186:C:C6	2.47	0.49
1:0:2718:C:H6	1:0:2718:C:H5'	1.78	0.49
1:0:2897:C:H2'	1:0:2898:G:H8	1.75	0.49
2:9:50:G:H5"	16:N:159:TYR:HE1	1.77	0.49
5:C:14:GLY:O	5:C:15:GLU:HB3	2.13	0.49
1:0:952:G:H4'	38:0:4023:HOH:O	2.12	0.49
1:0:1118:A:H8	1:0:1119:G:H5"	1.76	0.49
1:0:1751:G:H2'	1:0:1752:G:C5'	2.33	0.49
38:0:7111:HOH:O	29:1:1:THR:HB	2.12	0.49
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.48	0.49
12:J:39:VAL:HG11	12:J:107:ASN:HB2	1.93	0.49
12:J:42:GLU:O	12:J:131:THR:HG23	2.12	0.49
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.32	0.49
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.59	0.49
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.95	0.49
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.13	0.49
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.47	0.49
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.95	0.49
1:0:1702:U:H5'	38:0:3422:HOH:O	2.13	0.48
38:0:9529:HOH:O	18:P:81:LYS:HG2	2.12	0.48
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.43	0.48
6:D:64:ARG:HG2	6:D:67:ASP:HB3	1.95	0.48
6:D:95:THR:OG1	6:D:174:VAL:HG22	2.13	0.48
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.46	0.48
17:O:47:ARG:HB2	38:O:6739:HOH:O	2.12	0.48
25:W:4:LEU:O	25:W:32:CYS:HA	2.12	0.48
29:1:21:ARG:HD2	29:1:39:PHE:HB2	1.95	0.48
1:0:1525:G:H5'	1:0:1526:A:OP2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1641:A:C2'	1:0:1642:A:H5'	2.43	0.48
1:0:2421:G:H3'	1:0:2422:U:H5"	1.95	0.48
1:0:2821:C:H4'	4:B:116:PRO:HB3	1.94	0.48
13:K:55:VAL:CG1	13:K:56:SER:N	2.76	0.48
18:P:63:ARG:NH2	38:P:189:HOH:O	2.46	0.48
22:T:71:VAL:HG13	22:T:91:LEU:O	2.13	0.48
25:W:88:THR:CG2	25:W:89:ASP:H	2.22	0.48
1:0:1180:U:H1'	38:0:3230:HOH:O	2.13	0.48
1:0:1701:A:H5"	1:0:1702:U:H3'	1.94	0.48
4:B:54:VAL:HB	38:B:8914:HOH:O	2.12	0.48
4:B:268:ARG:NE	38:B:8909:HOH:O	2.38	0.48
7:E:23:GLU:HG2	7:E:28:SER:HB3	1.96	0.48
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.43	0.48
17:O:26:TRP:HB2	38:O:3062:HOH:O	2.12	0.48
25:W:76:ASP:O	25:W:77:ALA:C	2.51	0.48
1:0:775:G:OP1	29:1:16:HIS:HE1	1.97	0.48
1:0:1285:U:H4'	25:W:74:GLU:OE1	2.14	0.48
17:O:44:ASN:OD1	17:O:65:LEU:HB2	2.13	0.48
22:T:106:GLU:HG3	38:T:4913:HOH:O	2.12	0.48
1:0:907:A:H4'	1:0:1328:A:C2	2.48	0.48
1:0:1972:U:H2'	1:0:1973:A:C5'	2.44	0.48
5:C:61:PHE:HB3	38:C:8652:HOH:O	2.14	0.48
7:E:11:VAL:HG12	7:E:12:ASP:H	1.75	0.48
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.95	0.48
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.94	0.48
25:W:13:MET:CE	25:W:18:GLN:CA	2.89	0.48
1:0:1506:U:H6	1:0:1506:U:H5'	1.77	0.48
1:0:2301:A:H5"	1:0:2302:A:H5'	1.95	0.48
1:0:2720:C:O2	13:K:87:ARG:NH2	2.47	0.48
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.93	0.48
6:D:58:VAL:HG12	6:D:60:GLU:HG2	1.95	0.48
7:E:7:ILE:HG22	7:E:45:ASP:O	2.13	0.48
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.43	0.48
10:H:69:ARG:HB3	38:H:8582:HOH:O	2.13	0.48
11:I:134:ILE:C	11:I:135:GLU:HG3	2.33	0.48
15:M:184:ARG:HG3	15:M:185:PRO:HA	1.96	0.48
18:P:7:LYS:HD3	18:P:21:VAL:HG21	1.94	0.48
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.95	0.48
23:U:17:THR:CG2	23:U:18:GLY:N	2.77	0.48
26:X:25:ARG:HD3	26:X:64:ALA:O	2.13	0.48
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:24:G:N2	1:0:518:G:H1'	2.28	0.48
1:0:2668:G:H2'	1:0:2669:U:C6	2.48	0.48
38:0:5926:HOH:O	18:P:87:ARG:HG2	2.12	0.48
3:A:97:ALA:HB2	3:A:150:PRO:HB2	1.96	0.48
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.95	0.48
8:F:111:ILE:O	8:F:115:VAL:HG23	2.13	0.48
9:G:64:ASN:N	9:G:64:ASN:ND2	2.61	0.48
9:G:67:LEU:O	9:G:71:LEU:HG	2.13	0.48
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.96	0.48
6:D:91:ALA:HB2	6:D:106:PHE:CD2	2.48	0.48
11:I:96:SER:OG	11:I:99:GLN:HG3	2.13	0.48
30:2:36:ASN:HB3	30:2:39:ARG:HE	1.79	0.48
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.49	0.48
1:0:317:A:OP1	22:T:52:ARG:O	2.31	0.48
1:0:790:A:H2'	1:0:791:A:O4'	2.14	0.48
1:0:1265:G:H1'	38:0:7121:HOH:O	2.14	0.48
1:0:1852:A:H4'	3:A:230:SER:HB2	1.96	0.48
1:0:2894:C:O2'	1:0:2895:C:H5'	2.13	0.48
7:E:101:GLU:HB2	7:E:116:THR:O	2.13	0.48
8:F:56:PRO:HG2	15:M:43:PRO:O	2.14	0.48
12:J:133:GLY:O	12:J:137:GLU:HG3	2.14	0.48
25:W:125:HIS:CD2	25:W:127:GLY:H	2.32	0.48
1:0:482:G:H4'	1:0:508:A:N1	2.29	0.48
1:0:524:A:C5'	20:R:29:LYS:HE2	2.43	0.48
1:0:558:C:H2'	1:0:559:U:H5"	1.95	0.48
1:0:559:U:H5'	1:0:559:U:C6	2.40	0.48
1:0:1730:G:C5'	1:0:1731:C:C6	2.96	0.48
1:0:1811:A:C2	1:0:2752:C:H1'	2.49	0.48
3:A:164:ARG:HA	28:Z:69:TYR:CE1	2.48	0.48
5:C:236:THR:O	5:C:237:GLU:C	2.51	0.48
7:E:8:PRO:HB2	7:E:11:VAL:HG23	1.95	0.48
7:E:132:THR:HG23	7:E:132:THR:O	2.14	0.48
8:F:99:THR:HA	38:F:3461:HOH:O	2.13	0.48
10:H:31:ILE:HA	10:H:66:GLU:OE1	2.14	0.48
10:H:157:TYR:CD1	10:H:157:TYR:C	2.86	0.48
11:I:118:ASN:HA	11:I:121:LYS:CD	2.44	0.48
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.38	0.48
16:N:86:LEU:HD21	16:N:180:LEU:HD11	1.95	0.48
25:W:13:MET:CE	25:W:17:ILE:HG22	2.44	0.48
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.65	0.48
1:0:1595:G:O2'	1:0:1596:U:H5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:217:ARG:HH11	3:A:217:ARG:CG	2.27	0.47
4:B:79:MET:HE1	38:B:8927:HOH:O	2.13	0.47
5:C:104:ASP:HA	5:C:107:ARG:HH12	1.78	0.47
7:E:145:ALA:HB1	7:E:168:ILE:HD11	1.96	0.47
8:F:26:THR:HG21	8:F:103:GLU:HB2	1.95	0.47
10:H:6:ALA:HA	10:H:61:ARG:HH12	1.78	0.47
10:H:157:TYR:C	10:H:157:TYR:HD1	2.18	0.47
15:M:66:SER:HB3	15:M:128:TRP:NE1	2.29	0.47
21:S:53:ASN:HD22	21:S:53:ASN:N	2.11	0.47
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.75	0.47
1:0:226:A:H1'	1:0:393:G:C5	2.49	0.47
1:0:392:U:C5'	15:M:193:LYS:HB3	2.44	0.47
1:0:488:U:H2'	38:0:3999:HOH:O	2.13	0.47
1:0:711:G:H1'	38:0:7062:HOH:O	2.13	0.47
1:0:2896:A:OP1	26:X:15:ARG:NH1	2.47	0.47
5:C:27:ARG:HG2	5:C:30:LEU:HG	1.96	0.47
8:F:117:GLU:C	8:F:119:ARG:H	2.17	0.47
19:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.15	0.47
26:X:70:ILE:HG23	26:X:70:ILE:O	2.14	0.47
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.49	0.47
1:0:87:C:C2	30:2:30:ASP:OD2	2.67	0.47
1:0:694:A:H2'	1:0:695:C:H5'	1.96	0.47
1:0:1167:G:H2'	1:0:1168:C:O4'	2.14	0.47
4:B:162:MET:CE	4:B:308:LEU:HD21	2.22	0.47
6:D:10:PHE:CD1	6:D:11:HIS:N	2.82	0.47
6:D:64:ARG:CD	6:D:67:ASP:HB3	2.44	0.47
7:E:35:TYR:HA	12:J:127:ILE:HD12	1.95	0.47
18:P:59:ARG:NH2	18:P:66:GLN:HE22	2.11	0.47
25:W:38:THR:HB	38:W:5390:HOH:O	2.13	0.47
25:W:122:ARG:HG3	25:W:122:ARG:HH11	1.78	0.47
1:0:1825:U:O2'	1:0:1826:C:H5'	2.14	0.47
1:0:1940:C:H4'	38:0:7311:HOH:O	2.14	0.47
1:0:2815:G:N7	12:J:80:LYS:NZ	2.59	0.47
4:B:207:LYS:HG2	4:B:304:PRO:HB3	1.95	0.47
6:D:10:PHE:CG	6:D:11:HIS:N	2.82	0.47
13:K:66:ARG:HG2	13:K:66:ARG:HH11	1.80	0.47
13:K:98:VAL:CG1	13:K:99:ASP:N	2.78	0.47
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.95	0.47
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.28	0.47
27:Y:112:GLU:OE1	27:Y:115:ARG:NH1	2.48	0.47
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:21:G:H4'	20:R:2:ILE:HG22	1.95	0.47
1:0:42:C:H1'	38:0:4668:HOH:O	2.13	0.47
1:0:661:G:C5	1:0:686:A:C2	3.03	0.47
1:0:2699:A:H2'	1:0:2700:G:O4'	2.15	0.47
1:0:2900:G:H2'	1:0:2901:C:O4'	2.14	0.47
3:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.95	0.47
3:A:186:TRP:CG	3:A:187:PRO:HA	2.50	0.47
5:C:12:THR:HB	38:C:8648:HOH:O	2.14	0.47
5:C:162:VAL:CG2	5:C:232:LEU:HD21	2.45	0.47
7:E:77:THR:OG1	7:E:78:GLU:N	2.47	0.47
20:R:17:MET:CE	20:R:19:ARG:NH2	2.77	0.47
30:2:49:GLU:HB2	38:2:719:HOH:O	2.14	0.47
1:0:308:U:C4	1:0:342:C:H1'	2.49	0.47
1:0:383:A:H2'	1:0:384:G:O4'	2.15	0.47
1:0:2533:C:H6	1:0:2533:C:C5'	2.22	0.47
3:A:215:ILE:HG13	3:A:216:SER:N	2.30	0.47
4:B:84:LEU:HD23	4:B:142:LEU:CD2	2.45	0.47
9:G:12:ILE:HG13	38:G:692:HOH:O	2.13	0.47
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.78	0.47
25:W:69:ARG:NH2	38:W:4276:HOH:O	2.41	0.47
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.96	0.47
1:0:64:G:H2'	1:0:65:C:O4'	2.15	0.47
1:0:138:U:H5"	1:0:139:C:OP2	2.14	0.47
1:0:204:A:C2'	1:0:205:U:H5'	2.44	0.47
1:0:319:A:H4'	1:0:338:C:C4	2.50	0.47
1:0:793:A:H5"	18:P:83:LYS:HG2	1.97	0.47
1:0:968:G:H1'	10:H:35:LYS:HD2	1.96	0.47
1:0:1304:U:H2'	1:0:1305:C:C6	2.50	0.47
1:0:1790:C:H2'	1:0:1791:U:H6	1.79	0.47
1:0:1973:A:H2'	1:0:1974:G:O4'	2.15	0.47
1:0:2251:G:H2'	1:0:2252:A:C8	2.48	0.47
1:0:2520:G:H5'	10:H:64:SER:OG	2.14	0.47
1:0:2769:C:H2'	1:0:2770:G:C5'	2.44	0.47
4:B:86:ALA:HA	38:B:8878:HOH:O	2.15	0.47
4:B:139:ASP:HB2	4:B:165:ARG:NE	2.26	0.47
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.34	0.47
5:C:8:LEU:HD13	5:C:147:LEU:HD21	1.97	0.47
5:C:54:LEU:HD23	5:C:79:ARG:HG3	1.96	0.47
5:C:72:LYS:HG2	5:C:77:ALA:HA	1.96	0.47
6:D:146:LYS:HZ1	16:N:107:ASN:ND2	2.12	0.47
7:E:84:MET:HG2	7:E:168:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:46:GLU:N	38:F:3461:HOH:O	2.47	0.47
10:H:61:ARG:HG3	38:H:8555:HOH:O	2.14	0.47
10:H:69:ARG:HD3	38:H:8582:HOH:O	2.15	0.47
13:K:99:ASP:OD1	13:K:101:ASN:N	2.46	0.47
14:L:30:ARG:NH2	38:L:8821:HOH:O	2.42	0.47
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.15	0.47
20:R:114:VAL:HG13	20:R:114:VAL:O	2.14	0.47
24:V:58:THR:O	24:V:62:GLU:HG3	2.14	0.47
25:W:3:ALA:O	25:W:54:PHE:HA	2.14	0.47
25:W:13:MET:HE2	25:W:18:GLN:N	2.30	0.47
26:X:41:PHE:O	26:X:43:VAL:HG23	2.14	0.47
1:0:189:A:OP1	15:M:171:ARG:NH2	2.47	0.47
1:0:812:A:H2'	1:0:813:C:O4'	2.14	0.47
1:0:834:G:H4'	1:0:835:U:OP2	2.15	0.47
1:0:1174:A:C5	1:0:1201:C:H4'	2.49	0.47
1:0:1624:A:H5'	1:0:1626:A:O4'	2.15	0.47
1:0:1850:U:H2'	1:0:1851:G:H8	1.78	0.47
1:0:1909:A:H2'	1:0:1910:A:C8	2.50	0.47
2:9:29:C:C2'	2:9:30:C:H5'	2.45	0.47
4:B:320:GLN:NE2	4:B:321:PRO:CD	2.76	0.47
5:C:45:ASP:OD2	5:C:98:ARG:HD2	2.15	0.47
11:I:108:HIS:N	11:I:109:PRO:CD	2.78	0.47
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.45	0.47
17:O:78:ALA:C	17:O:98:LEU:HD13	2.35	0.47
1:0:1500:U:P	18:P:41:ARG:HH22	2.38	0.47
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.15	0.47
1:0:2346:C:H6	1:0:2346:C:O5'	1.98	0.47
1:0:2419:U:H5"	1:0:2420:G:H5'	1.97	0.47
2:9:12:C:H5'	2:9:70:U:O4'	2.15	0.47
3:A:113:GLY:HA2	3:A:153:ARG:NH2	2.30	0.47
6:D:54:ALA:CB	6:D:69:ILE:HD12	2.45	0.47
8:F:34:ASN:O	8:F:38:LYS:HG3	2.15	0.47
22:T:48:VAL:CG1	22:T:96:VAL:HG13	2.44	0.47
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.45	0.47
1:0:343:C:O2'	1:0:344:C:H5'	2.15	0.47
1:0:1471:A:H2'	1:0:1472:C:C6	2.50	0.47
1:0:1847:A:OP1	3:A:175:LYS:HG3	2.15	0.47
1:0:2090:G:H2'	1:0:2091:G:C8	2.49	0.47
38:0:4099:HOH:O	4:B:158:LYS:HB2	2.15	0.47
38:9:8666:HOH:O	16:N:147:ILE:HD12	2.15	0.47
3:A:36:ASP:O	3:A:38:ILE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:125:ASN:ND2	38:A:8831:HOH:O	2.48	0.47
4:B:175:LEU:O	4:B:175:LEU:HD23	2.15	0.47
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.44	0.47
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.45	0.47
12:J:6:PHE:HB3	12:J:109:TYR:OH	2.15	0.47
12:J:45:VAL:HG22	12:J:46:ILE:N	2.29	0.47
20:R:17:MET:CE	20:R:19:ARG:CZ	2.92	0.47
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.45	0.47
31:3:74:CYS:N	38:3:8860:HOH:O	2.48	0.47
2:9:22:G:H5'	38:9:8721:HOH:O	2.15	0.46
3:A:65:ARG:HG2	3:A:65:ARG:HH11	1.80	0.46
4:B:205:VAL:O	4:B:307:ARG:NE	2.47	0.46
15:M:28:GLN:HA	15:M:31:TRP:HB2	1.97	0.46
16:N:179:LEU:HA	16:N:184:ILE:HD12	1.97	0.46
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.80	0.46
1:0:105:G:O2'	1:0:106:A:H5'	2.15	0.46
1:0:1015:C:H2'	1:0:1016:U:C6	2.50	0.46
1:0:1236:A:H2'	1:0:1237:U:O4'	2.15	0.46
1:0:2001:G:O2'	1:0:2002:C:H5'	2.15	0.46
4:B:137:LEU:HD21	4:B:140:LEU:HD21	1.96	0.46
4:B:312:ARG:HG2	4:B:313:PRO:N	2.30	0.46
6:D:18:ILE:HD13	6:D:84:LEU:CD1	2.44	0.46
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.97	0.46
38:K:7438:HOH:O	23:U:20:MET:HE1	2.15	0.46
16:N:154:LEU:O	16:N:155:GLU:CB	2.62	0.46
26:X:76:ARG:O	26:X:77:PHE:HB3	2.15	0.46
1:0:69:A:C8	1:0:69:A:H5'	2.49	0.46
1:0:316:A:N3	1:0:336:G:O2'	2.44	0.46
1:0:432:G:O2'	1:0:433:C:H5'	2.15	0.46
1:0:737:A:H2'	1:0:738:G:O4'	2.16	0.46
1:0:1384:C:H5'	26:X:30:MET:HG2	1.97	0.46
1:0:2421:G:H3'	1:0:2422:U:C5'	2.45	0.46
1:0:2825:C:H4'	1:0:2826:G:O5'	2.15	0.46
1:0:2852:A:H5"	38:0:5216:HOH:O	2.15	0.46
2:9:47:A:C2	2:9:48:C:C2	3.03	0.46
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.98	0.46
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.51	0.46
11:I:67:VAL:CG1	11:I:68:PRO:HD2	2.45	0.46
14:L:97:VAL:HG12	14:L:98:GLU:O	2.14	0.46
15:M:162:GLY:HA2	38:M:8819:HOH:O	2.14	0.46
1:0:289:G:O2'	1:0:290:C:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:581:G:O2'	1:0:582:U:H5'	2.14	0.46
1:0:816:G:C6	1:0:817:G:N1	2.84	0.46
1:0:922:A:N7	1:0:2281:C:H5'	2.31	0.46
1:0:1446:U:H2'	21:S:55:GLN:NE2	2.29	0.46
3:A:211:LYS:HB2	38:A:8917:HOH:O	2.14	0.46
4:B:248:ARG:NH2	38:B:8824:HOH:O	2.47	0.46
7:E:21:THR:HG23	7:E:30:THR:OG1	2.16	0.46
14:L:134:GLU:HG3	38:L:8857:HOH:O	2.14	0.46
1:0:68:U:O2'	1:0:69:A:H5"	2.16	0.46
1:0:820:G:C6	3:A:171:LYS:HB2	2.50	0.46
1:0:1167:G:H4'	11:I:130:LEU:HD22	1.97	0.46
1:0:1942:A:O2'	1:0:1943:C:H5'	2.16	0.46
1:0:2115:U:H2'	1:0:2116:U:C6	2.50	0.46
3:A:95:PRO:HA	3:A:153:ARG:HA	1.98	0.46
5:C:200:PRO:HB3	5:C:212:VAL:CG2	2.45	0.46
6:D:35:ALA:C	6:D:37:ALA:H	2.16	0.46
10:H:4:LYS:HA	38:H:8569:HOH:O	2.15	0.46
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.79	0.46
29:1:37:CYS:SG	29:1:39:PHE:HB2	2.55	0.46
1:0:926:A:O2'	14:L:41:HIS:CD2	2.65	0.46
1:0:1236:A:C8	12:J:63:ILE:HD11	2.50	0.46
1:0:1289:C:H3'	38:0:6380:HOH:O	2.15	0.46
1:0:1495:C:H1'	1:0:1573:A:H1'	1.98	0.46
1:0:1834:C:H2'	1:0:1840:A:H62	1.80	0.46
5:C:78:ARG:NH1	5:C:78:ARG:CG	2.75	0.46
5:C:129:HIS:HD2	5:C:165:ASP:OD2	1.99	0.46
11:I:94:ASP:O	11:I:95:LEU:HG	2.15	0.46
16:N:58:LEU:N	16:N:58:LEU:HD12	2.30	0.46
16:N:154:LEU:C	16:N:156:GLU:H	2.18	0.46
21:S:11:THR:H	21:S:14:ALA:HB3	1.80	0.46
27:Y:187:VAL:HB	27:Y:203:VAL:HG22	1.98	0.46
1:0:204:A:H2'	1:0:205:U:H5'	1.96	0.46
1:0:484:A:N1	1:0:506:G:H4'	2.31	0.46
1:0:1184:C:O2'	1:0:1185:U:OP2	2.30	0.46
1:0:1768:C:H2'	1:0:1769:C:O4'	2.15	0.46
16:N:89:GLY:O	16:N:92:ALA:HB3	2.15	0.46
17:O:50:ARG:HD2	17:O:51:TYR:CE1	2.50	0.46
31:3:16:GLU:HG3	31:3:18:GLN:HE21	1.79	0.46
1:0:92:G:H4'	24:V:44:GLY:HA3	1.98	0.46
1:0:396:U:OP2	31:3:38:ARG:HD2	2.15	0.46
1:0:1168:C:H5	38:0:7461:HOH:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1391:G:H2'	1:0:1392:A:H5'	1.97	0.46
1:0:1666:C:C2'	1:0:1667:A:C5'	2.94	0.46
6:D:128:LEU:C	6:D:128:LEU:HD23	2.36	0.46
16:N:181:ASP:O	16:N:184:ILE:HG22	2.16	0.46
18:P:61:ARG:HB2	18:P:61:ARG:NH1	2.31	0.46
1:0:285:A:H2'	1:0:286:U:O4'	2.15	0.46
1:0:2072:G:C6	1:0:2533:C:H1'	2.51	0.46
1:0:2265:U:H2'	1:0:2266:A:H8	1.79	0.46
1:0:2781:U:C2'	1:0:2782:G:H5'	2.46	0.46
3:A:33:GLU:OE1	3:A:33:GLU:N	2.41	0.46
4:B:307:ARG:HH11	4:B:307:ARG:CG	2.29	0.46
14:L:35:ARG:O	14:L:40:PHE:HA	2.16	0.46
16:N:93:GLN:HG2	38:N:8854:HOH:O	2.15	0.46
20:R:29:LYS:NZ	38:R:8838:HOH:O	2.48	0.46
24:V:12:THR:HB	24:V:15:GLU:OE2	2.15	0.46
24:V:12:THR:H	24:V:15:GLU:HB2	1.80	0.46
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.16	0.46
1:0:820:G:C5	3:A:171:LYS:HB2	2.51	0.46
1:0:1044:C:H5	38:0:6576:HOH:O	1.99	0.46
1:0:1804:A:H2'	1:0:1805:G:C8	2.51	0.46
1:0:1855:G:H8	3:A:144:GLU:OE2	1.99	0.46
1:0:2346:C:O2'	6:D:52:THR:HG21	2.15	0.46
4:B:310:ARG:NH2	38:B:8854:HOH:O	2.47	0.46
5:C:7:ASP:O	5:C:9:ASP:N	2.49	0.46
5:C:51:TYR:CE2	29:1:53:LYS:HB3	2.51	0.46
6:D:67:ASP:O	6:D:69:ILE:HG13	2.16	0.46
10:H:30:LYS:N	10:H:62:HIS:HD2	2.03	0.46
15:M:9:ARG:HG3	38:M:8846:HOH:O	2.16	0.46
16:N:13:ARG:O	16:N:13:ARG:NH1	2.49	0.46
18:P:94:TRP:CZ2	18:P:98:ILE:HG13	2.51	0.46
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.16	0.46
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.16	0.46
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.97	0.46
1:0:757:C:OP1	14:L:27:ARG:HD2	2.15	0.45
1:0:1666:C:C2'	1:0:1667:A:H5'	2.43	0.45
1:0:2324:G:H4'	1:0:2418:G:O2'	2.16	0.45
5:C:7:ASP:OD1	5:C:11:ASN:O	2.34	0.45
8:F:57:GLU:O	8:F:61:MET:HG3	2.16	0.45
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.97	0.45
10:H:41:LYS:HD3	10:H:46:TYR:OH	2.16	0.45
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:16:ASN:HB2	38:Q:6597:HOH:O	2.14	0.45
19:Q:75:ILE:HB	38:Q:6286:HOH:O	2.15	0.45
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.98	0.45
24:V:4:HIS:HB2	24:V:7:GLU:HG3	1.98	0.45
1:0:827:A:H2'	1:0:828:G:O4'	2.16	0.45
1:0:1189:A:O2'	1:0:1208:C:H2'	2.16	0.45
38:0:9890:HOH:O	12:J:18:ILE:HG23	2.15	0.45
3:A:131:HIS:O	3:A:132:ASP:HB2	2.15	0.45
5:C:246:ARG:CZ	38:C:8630:HOH:O	2.62	0.45
11:I:134:ILE:O	11:I:135:GLU:HG3	2.16	0.45
12:J:131:THR:HB	12:J:134:GLU:OE1	2.16	0.45
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.99	0.45
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.81	0.45
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.16	0.45
26:X:18:ARG:NH1	38:X:4132:HOH:O	2.41	0.45
1:0:284:C:H4'	1:0:285:A:O5'	2.17	0.45
1:0:945:U:H2'	1:0:946:C:C6	2.52	0.45
1:0:1119:G:H8	12:J:52:GLN:HE22	1.64	0.45
1:0:1594:C:O2'	1:0:1607:A:H4'	2.16	0.45
1:0:1819:G:H2'	1:0:1820:G:C4'	2.44	0.45
1:0:2511:A:H2'	1:0:2512:U:O4'	2.17	0.45
1:0:2740:G:H2'	1:0:2741:A:O4'	2.16	0.45
38:0:3979:HOH:O	22:T:82:THR:HA	2.16	0.45
6:D:86:THR:C	6:D:89:PRO:HD2	2.36	0.45
16:N:47:LEU:HD12	16:N:92:ALA:CB	2.46	0.45
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.47	0.45
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.97	0.45
1:0:282:C:H2'	1:0:283:U:O4'	2.17	0.45
1:0:407:A:H8	38:0:4452:HOH:O	2.00	0.45
1:0:952:G:N3	1:0:2302:A:H2'	2.31	0.45
1:0:1135:G:H5'	38:0:5911:HOH:O	2.16	0.45
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.46	0.45
1:0:2314:G:C2'	1:0:2315:C:H5'	2.46	0.45
1:0:2456:A:H2'	1:0:2457:U:C6	2.51	0.45
3:A:211:LYS:CB	3:A:212:PRO:CD	2.94	0.45
5:C:7:ASP:C	5:C:9:ASP:H	2.20	0.45
12:J:130:VAL:HG12	12:J:131:THR:N	2.30	0.45
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.31	0.45
16:N:147:ILE:HG23	16:N:148:ALA:N	2.31	0.45
23:U:6:CYS:C	23:U:8:TYR:H	2.19	0.45
1:0:228:C:H2'	1:0:229:G:H5'	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2372:A:H2'	1:0:2373:U:C6	2.52	0.45
1:0:2769:C:H2'	1:0:2770:G:H5'	1.99	0.45
5:C:98:ARG:NH1	38:C:8561:HOH:O	2.49	0.45
14:L:73:VAL:HG11	14:L:118:LEU:HD21	1.98	0.45
14:L:117:GLU:HG3	38:L:8861:HOH:O	2.16	0.45
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.46	0.45
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.81	0.45
22:T:35:TYR:CD2	22:T:112:LEU:HD22	2.51	0.45
24:V:1:THR:O	24:V:4:HIS:CE1	2.69	0.45
1:0:11:A:H5'	1:0:12:U:OP2	2.16	0.45
1:0:185:G:O3'	1:0:186:A:H4'	2.16	0.45
1:0:1209:C:H2'	1:0:1210:G:C8	2.50	0.45
1:0:2850:C:H5'	1:0:2850:C:C6	2.43	0.45
38:0:7418:HOH:O	4:B:211:THR:HG21	2.16	0.45
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.81	0.45
5:C:127:ARG:HH21	5:C:225:PRO:HG2	1.74	0.45
5:C:133:ARG:NE	5:C:135:GLU:O	2.49	0.45
6:D:140:ARG:O	6:D:144:ARG:HG2	2.17	0.45
13:K:125:ALA:C	13:K:127:ALA:H	2.20	0.45
14:L:89:PHE:N	38:L:8870:HOH:O	2.49	0.45
16:N:110:THR:HB	16:N:113:SER:OG	2.16	0.45
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.52	0.45
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.46	0.45
21:S:81:ILE:HG23	38:S:8539:HOH:O	2.16	0.45
1:0:426:G:H2'	1:0:427:C:O4'	2.17	0.45
1:0:1785:G:OP1	18:P:76:GLY:HA3	2.16	0.45
1:0:2445:U:H2'	1:0:2446:G:C8	2.52	0.45
3:A:135:VAL:HG11	3:A:147:ARG:NH1	2.31	0.45
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.43	0.45
5:C:13:ASP:OD1	5:C:13:ASP:O	2.34	0.45
22:T:28:SER:O	22:T:32:ARG:HG3	2.16	0.45
1:0:1450:C:O2'	1:0:1494:A:H5'	2.17	0.45
1:0:2846:C:H4'	4:B:156:LYS:HB3	1.98	0.45
38:0:3839:HOH:O	10:H:14:LYS:HE2	2.16	0.45
38:0:9211:HOH:O	3:A:11:ARG:HD3	2.17	0.45
4:B:1:PRO:O	4:B:2:GLN:HB2	2.16	0.45
5:C:107:ARG:O	5:C:111:VAL:HG23	2.17	0.45
10:H:91:ARG:NH1	10:H:138:THR:OG1	2.43	0.45
12:J:19:MET:HE2	12:J:79:PHE:HA	1.99	0.45
15:M:164:THR:HB	38:M:8819:HOH:O	2.17	0.45
1:0:1393:A:H2'	1:0:1394:C:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1996:U:O2'	1:0:1997:A:H5'	2.17	0.45
1:0:2050:G:H5"	20:R:80:TYR:O	2.16	0.45
1:0:2433:A:H2'	1:0:2434:A:C8	2.51	0.45
3:A:36:ASP:CG	3:A:85:SER:HB2	2.37	0.45
3:A:66:ARG:CB	3:A:66:ARG:NH1	2.79	0.45
4:B:108:GLU:HB3	4:B:111:ARG:HD2	1.99	0.45
5:C:133:ARG:NE	5:C:138:VAL:HG22	2.32	0.45
6:D:36:ASN:C	38:D:7500:HOH:O	2.55	0.45
6:D:52:THR:N	6:D:70:GLY:O	2.50	0.45
10:H:88:MET:HA	10:H:139:ALA:HA	1.98	0.45
10:H:168:VAL:CG1	38:H:8562:HOH:O	2.52	0.45
15:M:61:ILE:CG2	15:M:62:VAL:N	2.79	0.45
20:R:44:VAL:O	20:R:48:GLU:HG3	2.17	0.45
1:0:1056:U:H2'	1:0:1057:A:O4'	2.17	0.45
1:0:1521:C:H2'	1:0:1522:A:H8	1.81	0.45
1:0:2866:U:C4	23:U:50:GLU:HB3	2.52	0.45
2:9:107:C:H5	38:9:8636:HOH:O	2.00	0.45
7:E:20:ILE:HD12	7:E:33:LEU:HD12	1.99	0.45
8:F:58:GLU:HA	8:F:61:MET:HE2	1.99	0.45
10:H:34:HIS:HD2	10:H:90:LEU:O	1.99	0.45
11:I:88:GLN:HA	11:I:91:PHE:HE2	1.81	0.45
16:N:170:GLU:HA	16:N:173:ASP:OD2	2.16	0.45
20:R:119:VAL:HG12	20:R:119:VAL:O	2.15	0.45
25:W:119:HIS:HD2	25:W:120:PRO:O	1.99	0.45
1:0:960:G:N3	1:0:960:G:C2'	2.79	0.44
1:0:1160:G:O2'	1:0:1190:G:H1'	2.17	0.44
1:0:1206:U:H2'	1:0:1207:A:O4'	2.17	0.44
1:0:1427:A:H61	1:0:1440:U:C1'	2.30	0.44
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.50	0.44
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.16	0.44
1:0:2906:A:H5'	1:0:2907:C:O4'	2.18	0.44
4:B:51:VAL:HG13	4:B:53:LEU:HD13	1.98	0.44
5:C:109:LEU:HD12	5:C:109:LEU:O	2.17	0.44
10:H:149:VAL:HG22	38:H:8579:HOH:O	2.17	0.44
14:L:104:ASP:HB2	38:L:8875:HOH:O	2.17	0.44
18:P:38:GLU:HA	18:P:41:ARG:HH11	1.82	0.44
23:U:52:THR:HG22	23:U:54:THR:HB	1.97	0.44
1:0:86:A:H1'	30:2:28:LYS:HE2	2.00	0.44
1:0:449:A:N7	5:C:43:LYS:HG2	2.32	0.44
1:0:821:U:H2'	1:0:822:C:C6	2.53	0.44
1:0:1023:C:H2'	1:0:1024:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1352:A:N1	5:C:48:SER:HB3	2.31	0.44
3:A:211:LYS:CB	3:A:212:PRO:HD2	2.32	0.44
4:B:72:THR:HB	38:B:8907:HOH:O	2.16	0.44
5:C:87:ARG:NH2	38:C:8508:HOH:O	2.50	0.44
5:C:118:THR:CG2	5:C:137:PRO:HB3	2.48	0.44
6:D:170:TYR:CD1	6:D:170:TYR:N	2.85	0.44
18:P:83:LYS:O	18:P:86:ALA:HB3	2.18	0.44
25:W:5:VAL:HG11	25:W:153:MET:CE	2.47	0.44
31:3:20:HIS:HA	31:3:70:ARG:O	2.17	0.44
1:0:396:U:C1'	38:0:7587:HOH:O	2.58	0.44
1:0:466:A:H2'	1:0:467:G:O4'	2.18	0.44
1:0:682:A:H2'	1:0:683:G:O4'	2.17	0.44
1:0:1641:A:H2'	1:0:1642:A:C5'	2.46	0.44
1:0:1684:A:O2'	1:0:1685:A:H5"	2.17	0.44
1:0:2112:A:H2'	1:0:2113:G:C8	2.53	0.44
7:E:7:ILE:HD11	7:E:11:VAL:C	2.38	0.44
10:H:48:VAL:HA	10:H:170:ARG:O	2.18	0.44
15:M:99:ARG:NH1	38:M:8857:HOH:O	2.49	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.84	0.44
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.99	0.44
17:O:32:ARG:HG2	38:O:3240:HOH:O	2.17	0.44
18:P:58:SER:HB3	38:P:180:HOH:O	2.17	0.44
22:T:48:VAL:HG11	22:T:96:VAL:HG13	1.97	0.44
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.17	0.44
1:0:1180:U:H4'	11:I:86:GLU:HG2	2.00	0.44
4:B:7:ARG:HH11	4:B:7:ARG:CG	2.29	0.44
4:B:279:THR:OG1	4:B:290:VAL:HB	2.18	0.44
6:D:172:VAL:HG12	6:D:173:GLU:N	2.32	0.44
12:J:19:MET:CE	12:J:132:LEU:HD21	2.48	0.44
17:O:41:ALA:HA	38:O:5104:HOH:O	2.17	0.44
17:O:88:LYS:HB3	38:O:7061:HOH:O	2.17	0.44
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.48	0.44
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.17	0.44
26:X:45:GLU:HG3	38:X:6178:HOH:O	2.17	0.44
27:Y:130:ARG:HB2	27:Y:142:SER:O	2.16	0.44
27:Y:185:VAL:HG12	38:Y:8867:HOH:O	2.17	0.44
1:0:243:A:H61	1:0:269:G:H1'	1.82	0.44
1:0:569:A:H5"	1:0:587:A:N1	2.33	0.44
1:0:932:U:H2'	1:0:933:C:C6	2.53	0.44
1:0:1131:G:C6	1:0:1230:A:C4	3.06	0.44
1:0:1185:U:H5'	38:0:7430:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:28:ALA:CB	8:F:99:THR:HG23	2.47	0.44
8:F:48:VAL:HG23	8:F:74:PHE:HB2	1.99	0.44
14:L:6:ARG:NH2	38:L:8848:HOH:O	2.51	0.44
31:3:14:CYS:HB3	31:3:16:GLU:HG2	1.99	0.44
1:0:249:G:H2'	1:0:250:C:C6	2.52	0.44
1:0:290:C:O2'	1:0:291:C:H5'	2.17	0.44
1:0:324:G:O2'	1:0:325:U:H5'	2.18	0.44
1:0:671:A:O2'	1:0:672:G:H2'	2.18	0.44
1:0:1537:C:H1'	38:0:6560:HOH:O	2.18	0.44
1:0:2089:A:O2'	1:0:2090:G:H5'	2.17	0.44
1:0:2793:A:H2'	1:0:2794:G:H5'	2.00	0.44
38:0:4717:HOH:O	11:I:125:GLY:C	2.56	0.44
4:B:202:VAL:HG11	4:B:301:VAL:HG13	1.99	0.44
5:C:49:ASP:HB3	5:C:52:ALA:HB2	1.99	0.44
5:C:246:ARG:HB3	5:C:246:ARG:HH11	1.82	0.44
16:N:178:THR:O	16:N:181:ASP:HB3	2.17	0.44
20:R:124:GLY:HA3	20:R:136:TRP:O	2.18	0.44
25:W:90:TYR:CD1	25:W:90:TYR:N	2.85	0.44
1:0:380:A:OP2	15:M:9:ARG:HD2	2.18	0.44
1:0:539:G:H2'	1:0:540:A:C8	2.53	0.44
1:0:958:G:H2'	1:0:959:C:C6	2.53	0.44
1:0:1298:U:H2'	1:0:1299:G:C8	2.52	0.44
1:0:1790:C:H2'	1:0:1791:U:C6	2.52	0.44
2:9:39:U:H3'	2:9:40:C:H5"	1.99	0.44
5:C:107:ARG:NH1	5:C:107:ARG:HB3	2.32	0.44
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.48	0.44
11:I:67:VAL:HG13	11:I:68:PRO:HD2	2.00	0.44
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.17	0.44
1:0:2717:C:H5'	4:B:302:PRO:HA	1.99	0.44
2:9:41:C:H4'	6:D:48:MET:HB2	2.00	0.44
2:9:56:A:O2'	6:D:14:ARG:HD3	2.18	0.44
2:9:92:G:C6	2:9:93:A:C6	3.06	0.44
3:A:88:ILE:CD1	3:A:100:PRO:HD3	2.39	0.44
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.46	0.44
3:A:164:ARG:HA	28:Z:69:TYR:HE1	1.83	0.44
11:I:70:THR:HA	11:I:107:LYS:HZ1	1.82	0.44
12:J:19:MET:HE3	12:J:132:LEU:CD1	2.46	0.44
15:M:157:ASP:HB3	15:M:160:PHE:HD1	1.83	0.44
16:N:116:PHE:HB3	16:N:136:LEU:HD23	1.99	0.44
16:N:171:HIS:CE1	38:N:8862:HOH:O	2.71	0.44
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:32:ARG:CZ	22:T:38:ARG:NH1	2.81	0.44
25:W:59:GLN:NE2	25:W:97:ALA:HB3	2.33	0.44
26:X:43:VAL:HG12	26:X:47:ALA:HB3	1.99	0.44
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.48	0.44
1:0:645:U:OP2	14:L:4:LYS:CE	2.66	0.44
1:0:920:C:H4'	1:0:921:G:C2	2.52	0.44
1:0:1175:G:H1'	1:0:1193:A:H2'	1.99	0.44
1:0:1730:G:C5'	1:0:1731:C:H6	2.30	0.44
1:0:2561:C:OP1	7:E:153:ARG:NH2	2.50	0.44
38:0:5503:HOH:O	4:B:298:LYS:HD3	2.18	0.44
5:C:84:VAL:O	5:C:85:LYS:HB2	2.17	0.44
8:F:32:GLY:N	38:F:3111:HOH:O	2.51	0.44
17:O:35:LYS:HD3	38:O:3360:HOH:O	2.18	0.44
22:T:89:ARG:HG3	22:T:89:ARG:O	2.16	0.44
24:V:51:LYS:O	24:V:55:ARG:HG3	2.18	0.44
26:X:43:VAL:HG22	26:X:76:ARG:NH1	2.32	0.44
1:0:512:G:O3'	1:0:513:A:H8	2.01	0.43
1:0:2597:U:H2'	1:0:2598:U:H5'	1.99	0.43
1:0:2851:G:C2'	1:0:2852:A:H5'	2.48	0.43
2:9:57:A:H8	6:D:141:VAL:HG21	1.83	0.43
3:A:199:HIS:HD2	3:A:201:PHE:HB2	1.83	0.43
3:A:217:ARG:HH11	3:A:217:ARG:HG3	1.82	0.43
5:C:170:ASP:O	5:C:171:GLU:HG3	2.17	0.43
8:F:99:THR:HG23	8:F:99:THR:O	2.18	0.43
9:G:12:ILE:N	38:G:4714:HOH:O	2.51	0.43
10:H:61:ARG:NH1	10:H:61:ARG:HG3	2.33	0.43
11:I:87:PRO:C	11:I:89:GLU:N	2.71	0.43
14:L:121:ILE:HA	14:L:141:GLU:O	2.18	0.43
16:N:34:LEU:HD13	16:N:47:LEU:HD21	1.98	0.43
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.33	0.43
17:O:43:VAL:HG13	17:O:47:ARG:HD2	2.00	0.43
26:X:30:MET:CE	26:X:55:ASN:HA	2.48	0.43
1:0:1173:A:H4'	1:0:1174:A:C8	2.53	0.43
1:0:1477:C:C5'	1:0:1868:G:H5"	2.48	0.43
1:0:1528:A:H2'	1:0:1529:G:O4'	2.19	0.43
1:0:2785:C:H4'	1:0:2786:G:OP2	2.18	0.43
4:B:55:ASN:HB3	4:B:64:GLY:H	1.83	0.43
4:B:57:GLU:O	4:B:63:GLU:HB2	2.18	0.43
5:C:236:THR:HG22	5:C:239:ALA:CB	2.48	0.43
6:D:10:PHE:N	38:D:7345:HOH:O	2.51	0.43
10:H:65:LEU:H	10:H:65:LEU:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:66:GLU:O	10:H:70:LEU:HB2	2.18	0.43
16:N:11:ARG:NH2	38:N:8819:HOH:O	2.50	0.43
16:N:82:TYR:C	16:N:82:TYR:CD2	2.91	0.43
22:T:98:VAL:HG11	22:T:101:LEU:CD2	2.48	0.43
27:Y:184:GLU:OE2	27:Y:204:ARG:HD2	2.18	0.43
1:0:1735:C:O2'	1:0:1736:A:H5'	2.17	0.43
1:0:2044:G:OP1	26:X:23:HIS:HE1	2.01	0.43
1:0:2435:U:OP1	31:3:28:GLY:HA3	2.17	0.43
1:0:2453:G:H4'	14:L:50:GLY:C	2.38	0.43
2:9:28:U:H2'	2:9:29:C:C6	2.53	0.43
4:B:36:PRO:HG3	4:B:169:GLY:H	1.83	0.43
4:B:41:PHE:HB3	4:B:190:MET:CE	2.45	0.43
4:B:140:LEU:HA	38:B:8878:HOH:O	2.17	0.43
11:I:129:SER:N	38:I:7330:HOH:O	2.51	0.43
14:L:34:GLY:HA3	14:L:38:HIS:CE1	2.53	0.43
31:3:3:MET:O	31:3:90:PHE:HA	2.18	0.43
1:0:21:G:H5"	20:R:1:GLY:O	2.19	0.43
1:0:475:G:H5'	5:C:73:LEU:HD23	2.00	0.43
1:0:920:C:H5"	1:0:921:G:O5'	2.19	0.43
1:0:1123:A:C2	1:0:1129:C:H4'	2.53	0.43
1:0:1333:U:H2'	1:0:1334:C:H6	1.83	0.43
1:0:1419:U:H2'	1:0:1685:A:C2	2.53	0.43
1:0:2348:C:H1'	6:D:131:THR:HG21	1.99	0.43
1:0:2768:A:O2'	1:0:2769:C:H5'	2.17	0.43
1:0:2820:A:H2'	1:0:2821:C:C6	2.53	0.43
3:A:35:GLY:O	3:A:36:ASP:CB	2.54	0.43
4:B:156:LYS:HE3	38:B:8931:HOH:O	2.19	0.43
5:C:236:THR:O	5:C:239:ALA:N	2.51	0.43
8:F:34:ASN:HA	15:M:4:ALA:HB2	2.00	0.43
15:M:65:VAL:HG21	15:M:105:ALA:HB2	2.00	0.43
28:Z:81:ARG:O	28:Z:82:SER:C	2.56	0.43
1:0:544:G:H2'	1:0:545:G:C5'	2.44	0.43
1:0:669:G:O2'	1:0:670:G:H5'	2.18	0.43
1:0:2036:C:C1'	13:K:44:LEU:HG	2.48	0.43
1:0:2401:A:H5'	38:0:9484:HOH:O	2.17	0.43
1:0:2564:G:OP2	1:0:2565:C:H5"	2.18	0.43
1:0:2787:C:H2'	1:0:2788:A:O4'	2.18	0.43
1:0:2795:C:O2'	1:0:2796:U:H5'	2.17	0.43
38:0:7323:HOH:O	3:A:177:HIS:HE1	2.01	0.43
4:B:14:GLY:HA2	4:B:15:PRO:C	2.38	0.43
4:B:17:LYS:O	4:B:260:HIS:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:48:VAL:HG12	8:F:97:ALA:CB	2.48	0.43
8:F:56:PRO:CG	15:M:44:THR:HA	2.48	0.43
11:I:119:ALA:O	11:I:123:VAL:HG23	2.18	0.43
12:J:107:ASN:HD22	12:J:109:TYR:H	1.65	0.43
15:M:15:PRO:HA	15:M:20:LEU:HD23	2.00	0.43
19:Q:21:ARG:HG2	19:Q:22:GLY:H	1.83	0.43
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.19	0.43
22:T:48:VAL:CG1	22:T:49:GLU:N	2.80	0.43
25:W:13:MET:HE2	25:W:18:GLN:CA	2.48	0.43
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.53	0.43
1:0:1494:A:O2'	1:0:1505:U:O2	2.37	0.43
1:0:2092:G:H2'	1:0:2613:G:OP1	2.19	0.43
1:0:2385:G:H2'	1:0:2386:U:C6	2.54	0.43
1:0:2758:G:H2'	1:0:2759:C:C6	2.54	0.43
1:0:2897:C:O2'	1:0:2898:G:H5'	2.19	0.43
38:0:4721:HOH:O	16:N:21:HIS:HD2	2.00	0.43
2:9:52:A:H2'	2:9:53:G:O4'	2.18	0.43
4:B:69:VAL:HA	4:B:70:PRO:HD3	1.85	0.43
4:B:109:LEU:HG	4:B:113:LEU:HD12	2.01	0.43
6:D:94:ALA:HA	6:D:174:VAL:O	2.19	0.43
12:J:39:VAL:CG1	12:J:107:ASN:HB2	2.48	0.43
14:L:57:VAL:HG12	14:L:57:VAL:O	2.19	0.43
22:T:41:ARG:NH1	22:T:42:VAL:O	2.52	0.43
24:V:8:ILE:HG21	24:V:59:ILE:HG13	2.01	0.43
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.54	0.43
29:1:28:HIS:HD2	29:1:31:LYS:H	1.66	0.43
1:0:87:C:H2'	30:2:28:LYS:O	2.18	0.43
1:0:106:A:H2'	1:0:107:U:O4'	2.18	0.43
1:0:255:A:H2'	1:0:256:C:O4'	2.18	0.43
1:0:503:G:H2'	1:0:504:G:H8	1.84	0.43
1:0:612:U:H2'	1:0:613:C:C6	2.54	0.43
1:0:1029:U:O2'	1:0:1273:C:OP1	2.33	0.43
1:0:1406:A:H4'	1:0:1407:A:H5"	2.00	0.43
38:0:9322:HOH:O	25:W:9:GLY:HA3	2.19	0.43
3:A:32:VAL:O	3:A:33:GLU:C	2.57	0.43
3:A:105:VAL:CG1	3:A:106:CYS:N	2.81	0.43
4:B:268:ARG:NH2	4:B:325:PRO:HG3	2.33	0.43
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.67	0.43
18:P:97:ARG:HD2	38:P:162:HOH:O	2.18	0.43
29:1:46:ARG:HA	38:1:8727:HOH:O	2.19	0.43
1:0:470:U:O2'	29:1:16:HIS:CD2	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1201:C:H5”	38:0:6207:HOH:O	2.19	0.43
1:0:1268:C:O2’	1:0:1269:G:H5’	2.18	0.43
1:0:1829:A:H2’	1:0:1830:C:H5’	2.01	0.43
1:0:1853:C:O2’	3:A:217:ARG:NH2	2.51	0.43
1:0:2291:A:N9	1:0:2309:C:H5’	2.34	0.43
1:0:2353:A:H4’	1:0:2354:A:O5’	2.18	0.43
1:0:2403:C:OP1	19:Q:49:ASN:HB3	2.19	0.43
1:0:2434:A:O3’	31:3:28:GLY:HA3	2.19	0.43
1:0:2694:A:C4’	7:E:91:PHE:HE1	2.30	0.43
2:9:3:A:H2	2:9:21:G:N3	2.17	0.43
4:B:24:PRO:HG2	4:B:204:GLY:HA2	1.99	0.43
4:B:24:PRO:O	4:B:25:ARG:HD3	2.19	0.43
6:D:16:PRO:HB2	6:D:165:PHE:CD1	2.53	0.43
6:D:16:PRO:HB2	6:D:165:PHE:CG	2.54	0.43
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.18	0.43
12:J:90:LYS:HB2	35:J:8802:CL:CL	2.56	0.43
13:K:63:GLU:CG	38:K:6344:HOH:O	2.62	0.43
16:N:154:LEU:HD12	16:N:156:GLU:O	2.19	0.43
17:O:77:ALA:HA	17:O:96:VAL:O	2.18	0.43
24:V:42:ASN:N	24:V:43:PRO:HD3	2.33	0.43
25:W:40:ALA:HB3	38:W:5390:HOH:O	2.18	0.43
26:X:78:GLU:HG2	26:X:79:GLU:N	2.33	0.43
1:0:1494:A:H1’	1:0:1495:C:C6	2.54	0.43
1:0:1882:C:O2’	1:0:2012:U:OP2	2.34	0.43
38:0:9108:HOH:O	5:C:103:ASN:HB3	2.19	0.43
3:A:179:MET:HA	3:A:179:MET:CE	2.48	0.43
4:B:217:ARG:CD	4:B:257:THR:HG22	2.48	0.43
10:H:86:TYR:CD1	10:H:86:TYR:C	2.92	0.43
12:J:54:VAL:HG11	12:J:138:THR:HG21	2.01	0.43
12:J:107:ASN:ND2	12:J:107:ASN:C	2.72	0.43
15:M:61:ILE:HD12	15:M:61:ILE:N	2.34	0.43
16:N:21:HIS:HB3	38:N:8860:HOH:O	2.19	0.43
25:W:26:ILE:O	25:W:26:ILE:CG1	2.65	0.43
1:0:157:G:H4’	15:M:95:LYS:HE3	2.01	0.43
1:0:638:C:H2’	1:0:639:A:H8	1.83	0.43
1:0:1015:C:H2’	1:0:1016:U:H6	1.83	0.43
1:0:1109:U:O4	12:J:21:ARG:HA	2.18	0.43
1:0:2719:A:C2	4:B:70:PRO:HG3	2.53	0.43
1:0:2866:U:H4’	1:0:2867:G:H5’	2.00	0.43
38:0:7033:HOH:O	20:R:33:ARG:HD3	2.18	0.43
4:B:138:GLY:O	4:B:139:ASP:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:153:SER:HB2	4:B:287:TYR:CZ	2.54	0.43
4:B:321:PRO:HG3	38:B:8901:HOH:O	2.18	0.43
10:H:141:CYS:HB2	38:H:8546:HOH:O	2.18	0.43
21:S:52:VAL:HG22	21:S:66:VAL:HG13	2.01	0.43
30:2:20:ARG:CG	30:2:21:VAL:N	2.82	0.43
1:0:137:U:OP1	1:0:259:G:O2'	2.37	0.42
1:0:244:C:OP2	8:F:38:LYS:HE3	2.20	0.42
1:0:731:U:H2'	1:0:732:C:C6	2.54	0.42
1:0:1118:A:C8	1:0:1119:G:H5"	2.53	0.42
1:0:1287:A:O4'	25:W:117:ARG:HD3	2.19	0.42
1:0:1739:G:O2'	1:0:1740:U:H5'	2.18	0.42
1:0:1881:A:OP1	3:A:199:HIS:HE1	2.02	0.42
2:9:7:G:H5'	38:9:8674:HOH:O	2.18	0.42
3:A:153:ARG:HH11	3:A:153:ARG:CB	2.32	0.42
3:A:190:ARG:NH2	38:A:8890:HOH:O	2.52	0.42
5:C:107:ARG:HB3	5:C:107:ARG:CZ	2.49	0.42
5:C:170:ASP:C	5:C:171:GLU:HG3	2.39	0.42
11:I:134:ILE:HG22	11:I:135:GLU:H	1.84	0.42
12:J:42:GLU:HG2	12:J:43:ARG:HG3	1.99	0.42
15:M:59:GLY:C	15:M:141:ILE:HD11	2.39	0.42
20:R:33:ARG:NH2	38:R:8830:HOH:O	2.43	0.42
25:W:73:LEU:HA	25:W:73:LEU:HD12	1.73	0.42
27:Y:108:ASP:OD1	27:Y:108:ASP:N	2.52	0.42
31:3:15:ASN:ND2	38:3:8847:HOH:O	2.52	0.42
1:0:86:A:C2	30:2:25:VAL:HG13	2.53	0.42
1:0:525:G:H2'	1:0:526:U:O4'	2.19	0.42
1:0:559:U:H2'	1:0:560:U:O4'	2.19	0.42
1:0:583:C:H2'	1:0:584:U:C6	2.54	0.42
1:0:1421:C:O2'	1:0:1422:U:H5'	2.18	0.42
1:0:1702:U:H1'	38:0:5756:HOH:O	2.19	0.42
1:0:2421:G:H1'	38:0:6987:HOH:O	2.18	0.42
1:0:2582:G:O3'	13:K:41:LYS:HA	2.19	0.42
1:0:2781:U:O2'	1:0:2782:G:H5'	2.19	0.42
3:A:36:ASP:HB2	3:A:83:GLY:HA3	2.01	0.42
5:C:187:ARG:NH2	38:C:8570:HOH:O	2.37	0.42
8:F:15:ASP:O	8:F:18:GLU:HB2	2.19	0.42
16:N:73:ALA:N	38:N:8862:HOH:O	2.52	0.42
20:R:19:ARG:HA	20:R:142:ASP:OD1	2.18	0.42
20:R:29:LYS:CD	38:R:8838:HOH:O	2.67	0.42
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.49	0.42
27:Y:115:ARG:NE	38:Y:8852:HOH:O	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	2.02	0.42
28:Z:13:ARG:NH1	28:Z:14:PHE:CZ	2.87	0.42
29:1:53:LYS:HA	29:1:53:LYS:HD3	1.87	0.42
30:2:40:ARG:HA	30:2:45:ASN:ND2	2.34	0.42
1:0:629:A:H2'	1:0:630:A:O4'	2.20	0.42
1:0:1066:U:H2'	1:0:1067:A:C8	2.54	0.42
1:0:1442:A:H1'	38:0:6981:HOH:O	2.18	0.42
1:0:1896:G:H1'	38:0:4253:HOH:O	2.18	0.42
1:0:1904:A:H2'	1:0:1905:U:O4'	2.19	0.42
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.42
7:E:99:GLY:N	38:E:4191:HOH:O	2.51	0.42
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.34	0.42
14:L:104:ASP:O	14:L:105:TYR:HB3	2.19	0.42
25:W:125:HIS:HD2	25:W:127:GLY:H	1.65	0.42
1:0:17:G:H2'	1:0:18:C:C6	2.55	0.42
1:0:326:G:O2'	1:0:327:A:H5'	2.19	0.42
1:0:719:C:O2'	17:O:112:ARG:NH2	2.52	0.42
1:0:783:C:OP1	3:A:180:LYS:HE3	2.19	0.42
1:0:1615:A:H5'	38:0:4178:HOH:O	2.19	0.42
1:0:1882:C:H2'	1:0:1883:U:C6	2.54	0.42
2:9:51:A:H5'	16:N:160:SER:HB3	2.01	0.42
5:C:79:ARG:O	5:C:87:ARG:HG2	2.19	0.42
7:E:156:ASP:OD1	7:E:156:ASP:N	2.50	0.42
13:K:18:ILE:HG22	13:K:93:ASN:HB2	2.01	0.42
16:N:34:LEU:HD22	16:N:129:ILE:HD13	2.00	0.42
16:N:37:ARG:HA	16:N:37:ARG:HD3	1.83	0.42
19:Q:93:ARG:HG3	19:Q:93:ARG:NH1	2.34	0.42
27:Y:97:LEU:O	27:Y:98:GLN:HG2	2.19	0.42
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.19	0.42
1:0:262:A:OP2	8:F:91:VAL:HG11	2.20	0.42
1:0:359:U:H3'	38:0:5748:HOH:O	2.20	0.42
1:0:797:A:H5'	28:Z:10:ARG:N	2.35	0.42
1:0:1293:U:O2'	27:Y:149:GLN:NE2	2.52	0.42
1:0:1515:A:H2'	1:0:1516:U:C6	2.55	0.42
1:0:2105:C:H2'	1:0:2106:C:C6	2.55	0.42
1:0:2781:U:H2'	1:0:2782:G:H5'	2.02	0.42
2:9:56:A:C3'	2:9:57:A:H5"	2.48	0.42
3:A:87:GLU:HB3	38:A:8920:HOH:O	2.20	0.42
3:A:109:GLU:HG2	3:A:116:GLY:H	1.85	0.42
4:B:141:ARG:HG2	4:B:165:ARG:HA	2.02	0.42
4:B:162:MET:HG3	4:B:310:ARG:CD	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:224:LYS:HA	4:B:224:LYS:HD3	1.93	0.42
5:C:46:TYR:CE1	5:C:92:PRO:HB3	2.54	0.42
7:E:31:ARG:NH1	38:E:5919:HOH:O	2.52	0.42
7:E:40:VAL:HA	7:E:48:VAL:O	2.18	0.42
8:F:52:GLU:HG3	8:F:77:VAL:O	2.20	0.42
10:H:72:ALA:HB2	10:H:156:ALA:HB2	2.00	0.42
15:M:49:ALA:C	15:M:54:TYR:HB3	2.39	0.42
15:M:59:GLY:HA3	15:M:141:ILE:HD12	2.02	0.42
29:1:8:GLN:NE2	29:1:11:LYS:NZ	2.59	0.42
1:0:1120:U:H5'	1:0:1121:G:OP2	2.19	0.42
1:0:2002:C:H2'	1:0:2003:U:H5'	2.01	0.42
1:0:2363:G:O2'	19:Q:11:ARG:HG3	2.20	0.42
1:0:2419:U:H5"	1:0:2420:G:C5'	2.49	0.42
3:A:190:ARG:CZ	38:A:8890:HOH:O	2.67	0.42
9:G:19:GLU:HG2	9:G:66:LEU:HD13	2.02	0.42
10:H:87:LYS:HB2	10:H:87:LYS:NZ	2.34	0.42
20:R:68:HIS:CG	20:R:76:ASP:HB2	2.55	0.42
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.40	0.42
1:0:222:A:H2'	1:0:223:G:O4'	2.19	0.42
1:0:299:U:H5'	38:0:7301:HOH:O	2.20	0.42
1:0:545:G:H2'	1:0:546:C:O4'	2.20	0.42
1:0:699:C:C2	1:0:743:G:N2	2.88	0.42
1:0:820:G:O2'	1:0:856:G:H4'	2.20	0.42
1:0:940:G:C5	1:0:1027:G:C2	3.08	0.42
1:0:2613:G:O2'	1:0:2614:C:H5'	2.20	0.42
1:0:2869:G:H2'	1:0:2870:C:C6	2.55	0.42
3:A:125:ASN:HB3	3:A:158:VAL:HG12	2.01	0.42
4:B:177:HIS:O	4:B:181:ILE:HG13	2.20	0.42
10:H:114:ASP:N	38:H:8581:HOH:O	2.52	0.42
20:R:59:PHE:CZ	20:R:79:ARG:HB2	2.55	0.42
25:W:11:VAL:O	25:W:12:ASN:HB2	2.20	0.42
1:0:1850:U:H2'	1:0:1851:G:C8	2.54	0.42
1:0:1964:U:O2	1:0:1964:U:H2'	2.19	0.42
1:0:2135:A:O2'	1:0:2136:G:H5'	2.20	0.42
1:0:2754:G:C2'	1:0:2755:G:H5'	2.50	0.42
6:D:10:PHE:N	38:D:1492:HOH:O	2.52	0.42
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.89	0.42
20:R:113:HIS:O	20:R:145:LEU:HD12	2.19	0.42
26:X:76:ARG:NH1	26:X:76:ARG:CG	2.83	0.42
27:Y:105:LYS:HE2	27:Y:198:GLY:O	2.20	0.42
30:2:41:HIS:CD2	30:2:43:ARG:H	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:35:U:H5'	5:C:47:GLY:O	2.20	0.42
1:0:123:U:H5'	38:0:6627:HOH:O	2.19	0.42
1:0:677:C:O2'	1:0:678:G:H5'	2.19	0.42
1:0:1406:A:H4'	1:0:1407:A:C5'	2.49	0.42
1:0:1482:A:O2'	1:0:1483:C:H5'	2.20	0.42
1:0:1976:G:H1'	1:0:2005:G:N2	2.35	0.42
1:0:2472:C:O2'	1:0:2634:G:H4'	2.19	0.42
1:0:2610:U:H4'	38:0:9471:HOH:O	2.19	0.42
38:0:9943:HOH:O	26:X:23:HIS:HD2	2.03	0.42
6:D:128:LEU:N	38:D:6007:HOH:O	2.52	0.42
25:W:4:LEU:CD2	25:W:54:PHE:HB3	2.41	0.42
1:0:235:C:O2'	1:0:236:A:H2'	2.19	0.42
1:0:553:G:O4'	1:0:1325:G:H5'	2.19	0.42
1:0:968:G:O2'	1:0:969:G:H5'	2.20	0.42
1:0:1319:G:H1'	38:0:4683:HOH:O	2.20	0.42
1:0:1845:A:O3'	3:A:187:PRO:HB2	2.20	0.42
1:0:2498:C:O2'	1:0:2499:U:H5'	2.19	0.42
38:0:9758:HOH:O	14:L:41:HIS:HE1	2.02	0.42
2:9:1:U:H4'	2:9:3:A:OP1	2.20	0.42
4:B:41:PHE:CB	4:B:190:MET:HE3	2.48	0.42
4:B:270:ILE:O	4:B:271:ASP:HB2	2.20	0.42
5:C:19:PRO:CD	5:C:240:LEU:HD22	2.50	0.42
6:D:167:GLU:HA	6:D:171:ASP:OD1	2.20	0.42
8:F:107:ASP:O	8:F:111:ILE:HG13	2.20	0.42
16:N:72:GLU:O	16:N:72:GLU:HG2	2.19	0.42
21:S:6:LYS:HB2	21:S:27:ALA:O	2.19	0.42
25:W:63:GLU:HG2	25:W:93:ILE:HG22	2.01	0.42
1:0:542:A:H1'	38:0:4669:HOH:O	2.19	0.41
1:0:711:G:C2	1:0:718:C:C2	3.08	0.41
1:0:1181:A:N1	1:0:1192:A:O2'	2.53	0.41
1:0:2326:C:H4'	1:0:2412:G:H4'	2.02	0.41
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.19	0.41
1:0:2708:G:H2'	1:0:2709:G:O4'	2.20	0.41
38:0:7516:HOH:O	31:3:60:LYS:HG3	2.19	0.41
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.50	0.41
4:B:243:ASN:HA	4:B:244:PRO:C	2.40	0.41
7:E:145:ALA:HB1	7:E:168:ILE:CD1	2.49	0.41
8:F:48:VAL:HG12	8:F:97:ALA:HB2	2.01	0.41
11:I:111:LEU:HD22	11:I:122:GLU:OE1	2.20	0.41
13:K:75:ARG:NE	38:K:4172:HOH:O	2.53	0.41
16:N:72:GLU:H	16:N:171:HIS:CE1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:61:GLN:CD	38:R:8838:HOH:O	2.58	0.41
25:W:48:VAL:CG1	25:W:48:VAL:O	2.67	0.41
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.42	0.41
1:0:710:G:OP1	17:O:24:ALA:HB3	2.20	0.41
1:0:1123:A:C6	1:0:1238:C:H5'	2.55	0.41
1:0:1353:C:P	38:0:4671:HOH:O	2.78	0.41
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.19	0.41
1:0:1657:A:H2'	1:0:1658:A:C8	2.55	0.41
1:0:1753:C:H4'	38:0:5978:HOH:O	2.19	0.41
1:0:2134:G:N2	1:0:2242:U:C2	2.89	0.41
38:9:8640:HOH:O	16:N:41:LYS:HD3	2.20	0.41
4:B:53:LEU:HD21	4:B:270:ILE:HD12	2.01	0.41
4:B:74:ILE:HG13	38:B:8907:HOH:O	2.19	0.41
11:I:98:ASP:HA	11:I:101:LYS:HB2	2.01	0.41
16:N:21:HIS:HB2	38:N:8831:HOH:O	2.19	0.41
16:N:154:LEU:HG	16:N:155:GLU:N	2.35	0.41
20:R:106:GLY:HA2	20:R:109:MET:CE	2.48	0.41
22:T:80:GLU:HG3	38:T:6653:HOH:O	2.20	0.41
26:X:25:ARG:HG2	38:X:5356:HOH:O	2.20	0.41
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.56	0.41
1:0:100:C:H4'	22:T:16:LEU:HB2	2.01	0.41
1:0:1167:G:H4'	11:I:130:LEU:CD2	2.50	0.41
1:0:1603:A:C5'	1:0:1605:G:H5'	2.51	0.41
1:0:1754:A:H2'	1:0:1755:A:O4'	2.20	0.41
38:0:9787:HOH:O	13:K:39:GLY:HA3	2.20	0.41
3:A:153:ARG:HD3	38:A:8826:HOH:O	2.20	0.41
10:H:122:LYS:HB2	10:H:122:LYS:HE3	1.88	0.41
19:Q:21:ARG:HG2	19:Q:22:GLY:N	2.36	0.41
22:T:55:PHE:CD2	22:T:77:VAL:HG13	2.56	0.41
1:0:69:A:H5'	1:0:69:A:H8	1.85	0.41
1:0:303:C:H2'	1:0:304:G:O4'	2.21	0.41
1:0:944:G:H21	25:W:44:MET:HE2	1.84	0.41
1:0:1418:U:OP1	30:2:42:TRP:HB3	2.21	0.41
1:0:1427:A:H61	1:0:1440:U:H1'	1.86	0.41
1:0:1755:A:H2'	1:0:1756:G:O4'	2.19	0.41
1:0:2005:G:H3'	1:0:2005:G:OP2	2.21	0.41
1:0:2515:C:H2'	1:0:2516:G:O4'	2.20	0.41
1:0:2667:G:H1'	1:0:2914:A:N3	2.36	0.41
3:A:54:PRO:HG2	3:A:160:ALA:HB3	2.01	0.41
3:A:192:VAL:O	3:A:207:GLN:HG2	2.21	0.41
10:H:115:GLY:N	38:H:8590:HOH:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	2.01	0.41
20:R:25:PHE:CE2	20:R:29:LYS:HE3	2.55	0.41
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.51	0.41
27:Y:122:ARG:NH2	38:Y:8834:HOH:O	2.53	0.41
1:0:441:A:H1'	1:0:442:A:N7	2.36	0.41
2:9:11:A:O2'	2:9:12:C:H3'	2.20	0.41
3:A:37:VAL:HG22	38:A:8893:HOH:O	2.19	0.41
3:A:65:ARG:HG2	3:A:65:ARG:NH1	2.34	0.41
3:A:135:VAL:HG21	3:A:147:ARG:NH1	2.36	0.41
4:B:27:ASN:HD22	4:B:27:ASN:N	2.15	0.41
4:B:38:VAL:HG22	4:B:142:LEU:HD12	2.03	0.41
5:C:118:THR:HG22	5:C:137:PRO:HB3	2.01	0.41
10:H:146:ALA:O	10:H:149:VAL:HG12	2.20	0.41
12:J:6:PHE:O	12:J:8:ALA:N	2.53	0.41
14:L:10:SER:O	14:L:11:ARG:HB3	2.20	0.41
22:T:45:GLY:HA3	22:T:102:ASP:HB2	2.01	0.41
24:V:42:ASN:O	24:V:44:GLY:N	2.53	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.41
1:0:170:U:H2'	1:0:171:C:H5'	2.01	0.41
1:0:541:C:C2'	1:0:542:A:C5'	2.91	0.41
1:0:571:C:O5'	1:0:571:C:H6	2.03	0.41
1:0:1377:C:H1'	38:0:9034:HOH:O	2.20	0.41
1:0:1771:U:O2'	1:0:1773:G:N7	2.50	0.41
1:0:2443:C:H1'	14:L:56:LYS:HE3	2.02	0.41
8:F:20:LEU:HD23	8:F:86:ALA:HB3	2.02	0.41
13:K:49:LEU:HD11	13:K:114:ALA:HB2	2.03	0.41
18:P:13:VAL:HG13	18:P:14:LEU:N	2.35	0.41
21:S:51:GLN:HB3	21:S:67:ARG:NH1	2.36	0.41
1:0:745:G:H5"	1:0:746:A:OP1	2.21	0.41
1:0:1185:U:H2'	1:0:1186:C:H6	1.84	0.41
1:0:1748:U:H4'	38:0:7484:HOH:O	2.20	0.41
1:0:1828:G:H2'	1:0:1829:A:H5'	2.01	0.41
1:0:2064:U:H4'	1:0:2653:A:OP1	2.20	0.41
38:0:5391:HOH:O	14:L:34:GLY:HA2	2.20	0.41
3:A:173:GLY:O	3:A:176:HIS:HB3	2.21	0.41
4:B:62:ARG:CA	4:B:65:MET:HE3	2.46	0.41
5:C:20:ASP:O	5:C:23:GLU:HB2	2.21	0.41
10:H:39:LYS:HA	10:H:87:LYS:NZ	2.35	0.41
11:I:70:THR:HG1	11:I:107:LYS:HE2	1.86	0.41
18:P:120:ARG:NH2	18:P:123:TYR:CD2	2.89	0.41
18:P:141:ILE:C	18:P:143:ALA:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:149:GLU:HA	20:R:150:PRO:HD3	1.89	0.41
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.35	0.41
1:0:1544:U:H2'	1:0:1545:C:H6	1.86	0.41
1:0:2821:C:H4'	4:B:116:PRO:CB	2.51	0.41
4:B:260:HIS:HE1	38:B:8886:HOH:O	2.03	0.41
4:B:315:VAL:HG23	4:B:316:ARG:HG2	2.03	0.41
8:F:79:GLN:HG3	8:F:82:ASP:OD2	2.20	0.41
10:H:39:LYS:HD3	38:H:8580:HOH:O	2.20	0.41
10:H:48:VAL:HG21	10:H:143:VAL:HA	2.02	0.41
14:L:24:ALA:HB2	14:L:30:ARG:HD2	2.03	0.41
15:M:134:ILE:O	15:M:136:PRO:HD3	2.21	0.41
15:M:184:ARG:HB2	15:M:184:ARG:CZ	2.51	0.41
1:0:56:G:C5'	24:V:50:ARG:HH12	2.25	0.41
1:0:187:A:H3'	1:0:188:C:H6	1.86	0.41
1:0:297:U:H2'	1:0:298:C:H6	1.85	0.41
1:0:307:G:H3'	1:0:342:C:OP2	2.20	0.41
1:0:424:C:H2'	1:0:425:U:C6	2.56	0.41
1:0:835:U:H3'	38:0:9366:HOH:O	2.19	0.41
1:0:921:G:H4'	1:0:924:G:C6	2.56	0.41
1:0:926:A:H5'	14:L:39:GLU:OE2	2.21	0.41
1:0:1041:U:H4'	1:0:1295:G:H5'	2.03	0.41
1:0:1163:G:H5'	11:I:110:ASP:O	2.20	0.41
1:0:1180:U:H2'	1:0:1181:A:C8	2.56	0.41
1:0:1398:G:O2'	1:0:1399:A:H5'	2.21	0.41
1:0:2387:U:H2'	1:0:2388:C:C6	2.55	0.41
1:0:2415:A:H2'	1:0:2416:G:H5'	2.02	0.41
4:B:23:THR:HA	4:B:24:PRO:HD3	1.89	0.41
4:B:25:ARG:HA	4:B:310:ARG:HH21	1.86	0.41
5:C:19:PRO:HD2	5:C:240:LEU:HD22	2.02	0.41
5:C:85:LYS:HA	5:C:85:LYS:HD2	1.90	0.41
5:C:104:ASP:HA	5:C:107:ARG:NH1	2.35	0.41
6:D:23:VAL:HG11	6:D:83:PHE:CZ	2.55	0.41
6:D:49:PRO:HA	6:D:73:VAL:HG22	2.02	0.41
7:E:11:VAL:CG1	7:E:12:ASP:N	2.81	0.41
7:E:23:GLU:HG2	7:E:28:SER:HB2	2.02	0.41
7:E:82:TYR:HA	7:E:170:ARG:O	2.21	0.41
11:I:84:SER:HB3	11:I:92:VAL:CG2	2.50	0.41
13:K:90:PHE:CD1	13:K:90:PHE:N	2.89	0.41
13:K:98:VAL:HG12	13:K:99:ASP:O	2.21	0.41
14:L:72:ASN:HB2	38:L:8882:HOH:O	2.21	0.41
15:M:47:ASP:CG	15:M:48:LYS:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:54:TYR:CG	15:M:55:LYS:N	2.88	0.41
18:P:115:SER:C	18:P:117:SER:N	2.75	0.41
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.56	0.41
19:Q:64:GLU:OE1	19:Q:64:GLU:HA	2.21	0.41
20:R:104:PHE:CB	20:R:109:MET:HE1	2.50	0.41
22:T:73:HIS:CD2	22:T:88:PRO:CG	3.03	0.41
22:T:79:LEU:HG	22:T:89:ARG:HB2	2.02	0.41
25:W:1:MET:N	25:W:37:GLU:HG3	2.36	0.41
30:2:10:ARG:HD2	30:2:49:GLU:OE2	2.21	0.41
1:0:95:A:H5"	1:0:97:G:O4'	2.21	0.41
1:0:790:A:H1'	1:0:1710:A:H2'	2.03	0.41
1:0:860:U:H2'	1:0:861:A:C8	2.56	0.41
1:0:1119:G:H8	12:J:52:GLN:NE2	2.18	0.41
1:0:1565:C:O4'	1:0:2738:G:H1'	2.21	0.41
1:0:1783:A:O2'	1:0:1784:U:H5'	2.20	0.41
1:0:2055:A:H4'	20:R:132:ARG:NH2	2.36	0.41
1:0:2453:G:H5"	38:L:8841:HOH:O	2.21	0.41
1:0:2800:A:H5'	1:0:2801:A:OP2	2.21	0.41
4:B:254:GLN:NE2	38:B:8890:HOH:O	2.54	0.41
5:C:165:ASP:O	5:C:168:ARG:HB3	2.21	0.41
16:N:139:TRP:CZ2	16:N:176:ARG:NH1	2.89	0.41
19:Q:28:ARG:HD2	19:Q:92:ARG:NH1	2.36	0.41
21:S:38:ALA:O	21:S:42:GLU:HG3	2.22	0.41
23:U:6:CYS:HB2	23:U:32:CYS:HB3	2.02	0.41
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	2.20	0.41
31:3:91:GLN:O	31:3:92:GLU:HB2	2.21	0.41
1:0:553:G:P	27:Y:204:ARG:NH2	2.91	0.40
1:0:1238:C:H5"	1:0:1239:G:OP2	2.22	0.40
1:0:1334:C:H2'	1:0:1335:C:H6	1.86	0.40
1:0:1562:C:O2	1:0:1562:C:H2'	2.19	0.40
1:0:1943:C:O4'	3:A:212:PRO:HA	2.20	0.40
1:0:2290:U:H2'	38:0:7103:HOH:O	2.21	0.40
1:0:2838:A:H2'	1:0:2839:C:O4'	2.22	0.40
4:B:42:ALA:HB1	4:B:308:LEU:HD11	2.02	0.40
4:B:141:ARG:HB3	4:B:164:THR:O	2.21	0.40
7:E:119:HIS:O	7:E:140:ALA:HB1	2.20	0.40
16:N:24:LEU:O	16:N:28:LYS:HG3	2.22	0.40
16:N:71:TRP:HE3	16:N:175:LEU:HD22	1.86	0.40
16:N:110:THR:HG22	38:N:8850:HOH:O	2.20	0.40
16:N:163:PHE:O	16:N:164:ASP:OD1	2.38	0.40
20:R:132:ARG:NH2	38:R:8880:HOH:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:57:THR:C	21:S:59:ASP:H	2.23	0.40
31:3:70:ARG:CB	38:3:8872:HOH:O	2.63	0.40
1:0:241:A:C2	1:0:378:A:H4'	2.56	0.40
1:0:445:U:H2'	1:0:446:G:H8	1.85	0.40
1:0:1942:A:H5'	3:A:233:THR:HB	2.02	0.40
1:0:2754:G:O2'	1:0:2755:G:H5'	2.20	0.40
1:0:2909:G:H2'	1:0:2910:A:C8	2.55	0.40
4:B:77:PRO:HG3	38:B:8874:HOH:O	2.21	0.40
4:B:215:VAL:HA	4:B:220:VAL:HG22	2.02	0.40
5:C:140:VAL:CG1	5:C:141:SER:N	2.84	0.40
6:D:41:LEU:CA	6:D:44:ILE:HG22	2.49	0.40
9:G:71:LEU:C	9:G:73:ASP:N	2.75	0.40
10:H:117:ARG:HB3	38:H:8590:HOH:O	2.21	0.40
12:J:74:ARG:O	12:J:78:ILE:HG12	2.21	0.40
13:K:87:ARG:NH2	38:K:4854:HOH:O	2.54	0.40
20:R:96:VAL:HG13	20:R:106:GLY:HA3	2.03	0.40
22:T:43:ASN:ND2	22:T:108:ARG:CZ	2.84	0.40
25:W:13:MET:CE	25:W:21:LEU:HD12	2.51	0.40
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.37	0.40
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.21	0.40
1:0:113:A:OP2	1:0:114:A:H2'	2.21	0.40
1:0:318:U:O2'	1:0:319:A:OP1	2.32	0.40
1:0:363:C:O2'	1:0:364:U:H5'	2.21	0.40
1:0:506:G:N2	1:0:509:A:H5'	2.27	0.40
1:0:2032:U:H2'	1:0:2033:G:C5'	2.51	0.40
38:0:9890:HOH:O	12:J:46:ILE:HA	2.20	0.40
2:9:11:A:P	19:Q:19:ARG:HH21	2.43	0.40
3:A:123:GLY:HA3	3:A:162:GLY:HA2	2.04	0.40
5:C:123:LEU:HD23	5:C:123:LEU:HA	1.94	0.40
9:G:12:ILE:N	9:G:13:PRO:CD	2.84	0.40
10:H:41:LYS:HE2	10:H:45:ASP:HB2	2.03	0.40
13:K:87:ARG:NE	38:K:4854:HOH:O	2.53	0.40
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.20	0.40
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.91	0.40
29:1:26:SER:HB3	29:1:35:SER:OG	2.22	0.40
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.56	0.40
1:0:195:C:H2'	1:0:196:G:H5'	2.04	0.40
1:0:736:A:H2'	1:0:737:A:O4'	2.21	0.40
1:0:1746:A:O4'	1:0:1747:A:C2	2.74	0.40
38:0:9362:HOH:O	3:A:22:ARG:NH2	2.53	0.40
2:9:105:A:H2'	2:9:106:U:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:88:GLU:O	4:B:88:GLU:HG3	2.21	0.40
5:C:129:HIS:CE1	5:C:232:LEU:H	2.39	0.40
6:D:65:GLU:HG3	38:D:6752:HOH:O	2.21	0.40
12:J:38:VAL:HB	12:J:103:VAL:HG13	2.03	0.40
13:K:75:ARG:NH1	38:K:5638:HOH:O	2.54	0.40
16:N:79:PRO:O	16:N:83:LEU:HG	2.22	0.40
16:N:114:LYS:O	16:N:117:ALA:HB3	2.21	0.40
22:T:32:ARG:CZ	22:T:38:ARG:HH12	2.34	0.40
23:U:4:ARG:N	38:U:5334:HOH:O	2.53	0.40
24:V:23:LEU:HD12	24:V:56:ILE:HD12	2.03	0.40
24:V:39:ALA:C	24:V:41:GLU:N	2.75	0.40
1:0:249:G:O2'	1:0:250:C:H5'	2.22	0.40
1:0:709:G:O2'	17:O:25:VAL:CG1	2.69	0.40
1:0:1433:G:O2'	1:0:1434:A:H5'	2.22	0.40
1:0:1965:C:O5'	1:0:1965:C:H6	2.04	0.40
1:0:2462:G:N7	31:3:60:LYS:NZ	2.68	0.40
4:B:33:ASP:O	4:B:34:GLY:O	2.40	0.40
4:B:125:GLU:O	4:B:129:ARG:HG3	2.21	0.40
6:D:173:GLU:O	6:D:174:VAL:C	2.60	0.40
7:E:84:MET:HA	7:E:167:TYR:O	2.21	0.40
15:M:98:GLN:O	15:M:102:GLU:HG3	2.20	0.40
26:X:44:ASP:HB3	26:X:46:ASP:OD2	2.22	0.40
27:Y:196:VAL:CG1	27:Y:226:ILE:HD13	2.52	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	235/240 (98%)	205 (87%)	27 (12%)	3 (1%)	12	24
4	B	335/338 (99%)	302 (90%)	29 (9%)	4 (1%)	13	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	C	244/246 (99%)	225 (92%)	17 (7%)	2 (1%)	19 39
6	D	134/177 (76%)	103 (77%)	22 (16%)	9 (7%)	1 1
7	E	170/178 (96%)	159 (94%)	10 (6%)	1 (1%)	25 47
8	F	117/120 (98%)	103 (88%)	10 (8%)	4 (3%)	3 5
9	G	25/348 (7%)	23 (92%)	2 (8%)	0	100 100
10	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	12 24
11	I	68/162 (42%)	53 (78%)	15 (22%)	0	100 100
12	J	140/145 (97%)	128 (91%)	8 (6%)	4 (3%)	4 7
13	K	130/132 (98%)	119 (92%)	11 (8%)	0	100 100
14	L	141/165 (86%)	122 (86%)	18 (13%)	1 (1%)	22 43
15	M	192/195 (98%)	177 (92%)	15 (8%)	0	100 100
16	N	184/187 (98%)	169 (92%)	9 (5%)	6 (3%)	4 6
17	O	113/116 (97%)	109 (96%)	4 (4%)	0	100 100
18	P	141/149 (95%)	136 (96%)	4 (3%)	1 (1%)	22 43
19	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100 100
20	R	148/155 (96%)	137 (93%)	11 (7%)	0	100 100
21	S	79/85 (93%)	72 (91%)	7 (9%)	0	100 100
22	T	117/120 (98%)	110 (94%)	6 (5%)	1 (1%)	17 35
23	U	51/66 (77%)	47 (92%)	4 (8%)	0	100 100
24	V	63/71 (89%)	57 (90%)	4 (6%)	2 (3%)	4 6
25	W	152/154 (99%)	148 (97%)	2 (1%)	2 (1%)	12 24
26	X	80/92 (87%)	70 (88%)	9 (11%)	1 (1%)	12 24
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100 100
28	Z	71/83 (86%)	60 (84%)	8 (11%)	3 (4%)	3 3
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
30	2	42/50 (84%)	39 (93%)	3 (7%)	0	100 100
31	3	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	14 30
All	All	3705/4437 (84%)	3379 (91%)	279 (8%)	47 (1%)	12 24

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	34	ASP

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Mol	Chain	Res	Type
4	B	139	ASP
5	C	8	LEU
6	D	137	PRO
8	F	101	ALA
16	N	154	LEU
16	N	164	ASP
16	N	184	ILE
28	Z	81	ARG
4	B	34	GLY
6	D	173	GLU
10	H	19	ARG
10	H	143	VAL
12	J	5	GLU
16	N	183	ASP
18	P	116	SER
22	T	53	GLY
25	W	49	ASN
28	Z	41	ASN
3	A	37	VAL
4	B	185	GLY
6	D	56	ARG
6	D	65	GLU
8	F	44	SER
16	N	139	TRP
24	V	43	PRO
28	Z	20	ARG
5	C	15	GLU
6	D	61	PHE
12	J	76	ASP
12	J	89	HIS
14	L	80	ASP
16	N	155	GLU
25	W	77	ALA
26	X	87	ALA
4	B	2	GLN
6	D	27	ILE
6	D	77	ASP
6	D	97	GLN
7	E	17	HIS
8	F	100	ASP
12	J	7	ASP
3	A	211	LYS

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Mol	Chain	Res	Type
6	D	16	PRO
8	F	70	LYS
31	3	57	GLY
24	V	40	PRO

5.3.2 Protein sidechains (i)

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	179/182 (98%)	167 (93%)	12 (7%)	16	33
4	B	282/283 (100%)	264 (94%)	18 (6%)	17	35
5	C	193/193 (100%)	176 (91%)	17 (9%)	10	19
6	D	117/148 (79%)	111 (95%)	6 (5%)	24	46
7	E	152/156 (97%)	147 (97%)	5 (3%)	38	64
8	F	93/94 (99%)	92 (99%)	1 (1%)	73	88
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	134/145 (92%)	129 (96%)	5 (4%)	34	60
11	I	58/130 (45%)	58 (100%)	0	100	100
12	J	118/121 (98%)	109 (92%)	9 (8%)	13	26
13	K	106/106 (100%)	103 (97%)	3 (3%)	43	69
14	L	113/127 (89%)	109 (96%)	4 (4%)	36	62
15	M	158/159 (99%)	152 (96%)	6 (4%)	33	59
16	N	149/150 (99%)	145 (97%)	4 (3%)	44	71
17	O	93/94 (99%)	90 (97%)	3 (3%)	39	65
18	P	113/117 (97%)	108 (96%)	5 (4%)	28	53
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	59
20	R	117/122 (96%)	112 (96%)	5 (4%)	29	54
21	S	71/74 (96%)	69 (97%)	2 (3%)	43	69
22	T	105/106 (99%)	99 (94%)	6 (6%)	20	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	U	44/52 (85%)	44 (100%)	0	100 100
24	V	51/57 (90%)	50 (98%)	1 (2%)	55 78
25	W	130/130 (100%)	124 (95%)	6 (5%)	27 51
26	X	66/74 (89%)	58 (88%)	8 (12%)	5 9
27	Y	120/196 (61%)	115 (96%)	5 (4%)	30 55
28	Z	60/68 (88%)	59 (98%)	1 (2%)	60 81
29	1	46/47 (98%)	46 (100%)	0	100 100
30	2	42/46 (91%)	41 (98%)	1 (2%)	49 74
31	3	79/79 (100%)	77 (98%)	2 (2%)	47 73
All	All	3095/3619 (86%)	2957 (96%)	138 (4%)	27 52

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	33	GLU
3	A	36	ASP
3	A	66	ARG
3	A	69	LEU
3	A	94	LEU
3	A	120	ARG
3	A	131	HIS
3	A	179	MET
3	A	192	VAL
3	A	206	ARG
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	33	ASP
4	B	49	THR
4	B	63	GLU
4	B	97	LEU
4	B	132	HIS
4	B	139	ASP
4	B	162	MET
4	B	190	MET
4	B	195	ARG
4	B	254	GLN

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Mol	Chain	Res	Type
4	B	264	GLU
4	B	277	GLU
4	B	304	PRO
4	B	307	ARG
4	B	312	ARG
5	C	2	GLN
5	C	27	ARG
5	C	78	ARG
5	C	87	ARG
5	C	91	PRO
5	C	94	THR
5	C	101	ASP
5	C	115	LEU
5	C	136	VAL
5	C	151	GLN
5	C	162	VAL
5	C	187	ARG
5	C	214	THR
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	240	LEU
6	D	24	HIS
6	D	61	PHE
6	D	133	ASN
6	D	136	ARG
6	D	137	PRO
6	D	149	ARG
7	E	7	ILE
7	E	67	SER
7	E	86	VAL
7	E	102	VAL
7	E	164	ASP
8	F	12	LEU
10	H	33	GLN
10	H	87	LYS
10	H	91	ARG
10	H	114	ASP
10	H	157	TYR
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG

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Mol	Chain	Res	Type
12	J	76	ASP
12	J	79	PHE
12	J	107	ASN
12	J	120	SER
12	J	127	ILE
12	J	131	THR
13	K	7	ASP
13	K	10	GLN
13	K	84	ASP
14	L	30	ARG
14	L	35	ARG
14	L	80	ASP
14	L	99	GLU
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
15	M	164	THR
16	N	26	LEU
16	N	49	THR
16	N	139	TRP
16	N	152	GLU
17	O	3	THR
17	O	28	ASP
17	O	38	ARG
18	P	21	VAL
18	P	52	LYS
18	P	73	HIS
18	P	91	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	30	VAL
19	Q	57	ASP
20	R	13	THR
20	R	39	THR
20	R	82	GLU
20	R	132	ARG
20	R	143	VAL
21	S	53	ASN
21	S	80	ARG
22	T	26	THR

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Mol	Chain	Res	Type
22	T	39	ASN
22	T	89	ARG
22	T	96	VAL
22	T	112	LEU
22	T	115	GLU
24	V	65	ASP
25	W	26	ILE
25	W	52	VAL
25	W	73	LEU
25	W	142	ASP
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	27	ASP
26	X	44	ASP
26	X	46	ASP
26	X	49	ARG
26	X	72	VAL
26	X	79	GLU
26	X	82	GLU
27	Y	163	THR
27	Y	174	VAL
27	Y	187	VAL
27	Y	189	ASN
27	Y	203	VAL
28	Z	44	GLU
30	2	18	ASN
31	3	3	MET
31	3	42	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	47	HIS
3	A	92	ASN
3	A	199	HIS
4	B	27	ASN
4	B	106	HIS
4	B	145	HIS
4	B	221	GLN
4	B	238	ASN
4	B	256	GLN

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Mol	Chain	Res	Type
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	151	GLN
6	D	97	GLN
6	D	103	ASN
6	D	133	ASN
7	E	143	GLN
9	G	17	GLN
9	G	64	ASN
10	H	34	HIS
10	H	59	GLN
10	H	62	HIS
10	H	73	ASN
11	I	88	GLN
11	I	108	HIS
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	116	HIS
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	137	ASN
15	M	170	ASN
15	M	190	ASN
16	N	40	ASN
16	N	107	ASN
18	P	50	GLN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS

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Mol	Chain	Res	Type
20	R	117	HIS
20	R	123	GLN
21	S	9	HIS
21	S	53	ASN
22	T	39	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	4	HIS
24	V	60	GLN
25	W	12	ASN
25	W	27	HIS
25	W	28	HIS
25	W	87	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
26	X	36	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	37	HIS
30	2	41	HIS
30	2	45	ASN
31	3	15	ASN
31	3	30	GLN
31	3	48	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	236 (8%)	32 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2866/3044 (94%)	252 (8%)	33 (1%)

All (252) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	170	U
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	C
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	284	C
1	0	285	A
1	0	308	U
1	0	309	C
1	0	319	A
1	0	331	A
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G

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Mol	Chain	Res	Type
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C

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Mol	Chain	Res	Type
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	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	1083	C
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1451	C

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Mol	Chain	Res	Type
1	0	1474	C
1	0	1485	A
1	0	1505	U
1	0	1506	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	1580	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
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	1731	C
1	0	1752	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	1879	U
1	0	1904	A
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1979	G

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Mol	Chain	Res	Type
1	0	1980	U
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	2033	G
1	0	2034	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	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
1	0	2369	A
1	0	2422	U
1	0	2462	G
1	0	2465	A
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A

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Mol	Chain	Res	Type
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2638	G
1	0	2649	A
1	0	2664	A
1	0	2676	C
1	0	2681	A
1	0	2682	C
1	0	2726	U
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	2825	C
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	2	U
2	9	7	G
2	9	14	G
2	9	22	G
2	9	23	U
2	9	24	U
2	9	25	G
2	9	40	C
2	9	41	C
2	9	43	G
2	9	52	A

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Mol	Chain	Res	Type
2	9	57	A
2	9	66	G
2	9	77	A
2	9	114	G
2	9	122	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	129	A
1	0	169	A
1	0	318	U
1	0	338	C
1	0	603	A
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1165	G
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1563	G
1	0	1692	C
1	0	1856	C
1	0	1878	G
1	0	1942	A
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2538	A
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2791	U
2	9	65	A

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	UR3	0	2619	1	14,22,23	0.81	0	15,32,35	0.61	0
1	OMG	0	2588	1	18,26,27	1.09	2 (11%)	20,38,41	2.59	4 (20%)
1	1MA	0	628	1	15,25,26	0.71	0	15,37,40	1.41	1 (6%)
1	OMU	0	2587	1	14,22,23	0.99	1 (7%)	14,31,34	1.15	1 (7%)
1	PSU	0	2621	1	17,21,22	1.54	3 (17%)	20,30,33	5.48	4 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.64	1.48	1.52
1	0	2588	OMG	C6-N1	3.53	1.39	1.33
1	0	2621	PSU	C4-N3	3.00	1.38	1.33
1	0	2621	PSU	C2-N1	2.64	1.43	1.38
1	0	2587	OMU	C4-N3	2.63	1.37	1.33
1	0	2588	OMG	C8-N7	-2.14	1.30	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	2621	PSU	N1-C2-N3	-17.47	114.54	128.43
1	0	2621	PSU	C4-N3-C2	14.45	127.34	115.14
1	0	2588	OMG	C5-C6-N1	-8.62	111.64	123.43
1	0	2621	PSU	C5-C4-N3	-8.19	114.80	125.36
1	0	2588	OMG	C6-N1-C2	5.80	125.15	115.93
1	0	628	1MA	C2-N3-C4	-4.69	110.72	116.58
1	0	2587	OMU	C5-C4-N3	-3.89	114.75	123.31
1	0	2588	OMG	C2-N3-C4	-3.11	111.81	115.36
1	0	2621	PSU	C6-N1-C2	2.86	120.07	115.36
1	0	2588	OMG	N3-C2-N1	-2.41	124.01	127.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 232 ligands modelled in this entry, 231 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	TEL	0	9000	-	59,62,62	1.68	14 (23%)	77,92,92	1.38	11 (14%)

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	TEL	0	9000	-	-	2/73/108/108	0/4/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	9000	TEL	C7-C3	4.57	1.60	1.54
36	0	9000	TEL	C47-C43	4.18	1.46	1.39
36	0	9000	TEL	C46-C43	3.90	1.47	1.39
36	0	9000	TEL	C7-C13	3.22	1.57	1.52
36	0	9000	TEL	C51-C46	3.02	1.45	1.38
36	0	9000	TEL	C30-C34	2.96	1.58	1.54
36	0	9000	TEL	C47-N52	2.89	1.40	1.34
36	0	9000	TEL	O9-C4	2.66	1.51	1.46
36	0	9000	TEL	C51-C56	2.65	1.45	1.37
36	0	9000	TEL	C56-N52	2.64	1.41	1.33
36	0	9000	TEL	C36-N31	2.26	1.41	1.38
36	0	9000	TEL	C24-C28	2.17	1.55	1.52
36	0	9000	TEL	C12-C7	2.08	1.57	1.53
36	0	9000	TEL	O32-C28	2.04	1.48	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	0	9000	TEL	C17-C11-N6	-4.97	105.64	113.31
36	0	9000	TEL	C40-C36-N31	-4.16	103.56	107.91
36	0	9000	TEL	C2-O5-C10	3.14	111.77	109.29
36	0	9000	TEL	O9-C4-C2	2.81	111.82	105.48
36	0	9000	TEL	O16-C10-N6	2.58	131.41	128.01
36	0	9000	TEL	C35-C30-C26	-2.33	104.02	108.08
36	0	9000	TEL	C1-C2-C3	2.33	119.49	116.69
36	0	9000	TEL	C36-N31-C37	2.25	110.36	108.22
36	0	9000	TEL	O5-C10-O16	-2.18	119.95	122.46
36	0	9000	TEL	C28-C24-C19	2.16	119.77	116.11
36	0	9000	TEL	C54-C49-C44	-2.12	106.91	109.97

There are no chirality outliers.

All (2) torsion outliers are listed below:

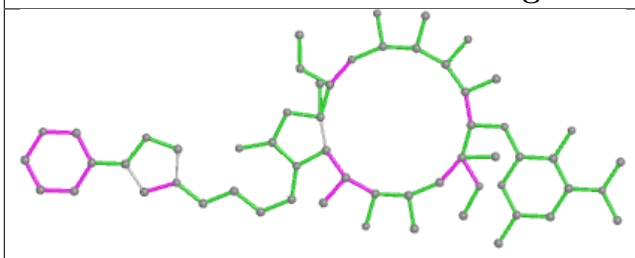
Mol	Chain	Res	Type	Atoms
36	0	9000	TEL	O18-C13-C19-C23
36	0	9000	TEL	C7-C13-C19-C23

There are no ring outliers.

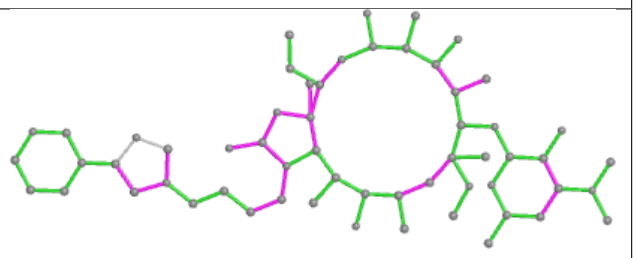
No monomer is involved in short contacts.

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 then 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.

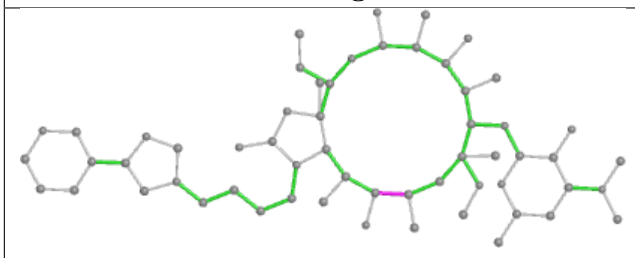
Ligand TEL 0 9000



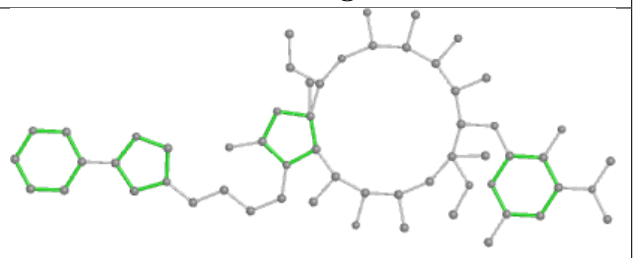
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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^2)	Q<0.9
1	0	2749/2922 (94%)	-0.49	44 (1%) 72 68	21, 45, 89, 149	0
2	9	122/122 (100%)	-0.39	5 (4%) 37 30	37, 61, 87, 150	0
3	A	237/240 (98%)	0.22	11 (4%) 32 26	27, 50, 86, 107	0
4	B	337/338 (99%)	0.03	5 (1%) 73 70	26, 54, 78, 90	0
5	C	246/246 (100%)	-0.17	1 (0%) 92 91	22, 43, 68, 78	0
6	D	140/177 (79%)	2.05	62 (44%) 0 0	52, 98, 120, 129	0
7	E	172/178 (96%)	0.74	20 (11%) 4 3	42, 67, 86, 90	0
8	F	119/120 (99%)	0.78	16 (13%) 3 2	46, 71, 93, 108	0
9	G	29/348 (8%)	2.53	21 (72%) 0 0	71, 88, 98, 99	0
10	H	160/177 (90%)	0.42	11 (6%) 16 12	40, 59, 92, 96	0
11	I	70/162 (43%)	4.49	62 (88%) 0 0	106, 119, 137, 138	0
12	J	142/145 (97%)	-0.06	1 (0%) 87 86	32, 48, 69, 89	0
13	K	132/132 (100%)	-0.11	0 100 100	31, 51, 71, 82	0
14	L	145/165 (87%)	0.55	17 (11%) 4 3	23, 63, 106, 119	0
15	M	194/195 (99%)	-0.19	1 (0%) 91 89	30, 40, 57, 64	0
16	N	186/187 (99%)	0.60	24 (12%) 3 2	36, 62, 106, 114	0
17	O	115/116 (99%)	-0.06	0 100 100	35, 52, 70, 73	0
18	P	143/149 (95%)	0.10	3 (2%) 63 58	35, 53, 69, 78	0
19	Q	95/96 (98%)	-0.09	0 100 100	35, 41, 59, 72	0
20	R	150/155 (96%)	-0.25	0 100 100	29, 42, 63, 72	0
21	S	81/85 (95%)	0.08	3 (3%) 41 34	40, 58, 77, 85	0
22	T	119/120 (99%)	0.32	4 (3%) 45 38	35, 55, 79, 96	0
23	U	53/66 (80%)	0.24	3 (5%) 23 18	40, 55, 73, 82	0
24	V	65/71 (91%)	1.45	13 (20%) 1 0	52, 72, 111, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	W	154/154 (100%)	-0.27	0 100 100	34, 44, 61, 74	0
26	X	82/92 (89%)	0.40	8 (9%) 7 5	42, 57, 79, 96	0
27	Y	142/241 (58%)	-0.03	7 (4%) 29 23	24, 43, 66, 84	0
28	Z	73/83 (87%)	0.30	5 (6%) 17 12	49, 65, 81, 94	0
29	1	56/57 (98%)	-0.53	0 100 100	24, 31, 36, 44	0
30	2	46/50 (92%)	0.18	4 (8%) 10 7	29, 54, 82, 98	0
31	3	92/92 (100%)	0.23	4 (4%) 35 28	33, 53, 67, 80	0
All	All	6646/7481 (88%)	-0.02	355 (5%) 26 20	21, 50, 96, 150	0

All (355) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	63	ILE	11.5
11	I	128	THR	11.5
11	I	66	GLY	9.8
24	V	1	THR	9.3
11	I	104	ALA	9.2
11	I	132	VAL	9.1
24	V	39	ALA	8.4
11	I	91	PHE	8.2
11	I	108	HIS	7.9
11	I	74	ILE	7.8
11	I	88	GLN	7.8
11	I	112	LEU	7.1
11	I	71	ALA	7.0
6	D	69	ILE	6.9
6	D	10	PHE	6.6
6	D	18	ILE	6.5
11	I	113	SER	6.4
11	I	72	GLU	6.4
6	D	64	ARG	6.4
2	9	1	U	6.2
11	I	97	VAL	6.1
11	I	100	VAL	6.1
11	I	70	THR	6.1
11	I	80	PHE	6.1
6	D	88	LEU	6.0
24	V	40	PRO	6.0
6	D	61	PHE	6.0
11	I	111	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
1	0	1198	U	5.8
11	I	83	GLY	5.7
11	I	92	VAL	5.7
9	G	27	ILE	5.4
9	G	23	ILE	5.3
3	A	37	VAL	5.3
11	I	79	GLY	5.2
24	V	43	PRO	5.2
26	X	88	GLU	5.2
11	I	86	GLU	5.2
6	D	93	LEU	5.1
11	I	98	ASP	5.1
7	E	45	ASP	5.0
3	A	35	GLY	5.0
6	D	85	GLN	4.8
2	9	24	U	4.8
6	D	170	TYR	4.8
11	I	99	GLN	4.8
16	N	166	ALA	4.8
6	D	90	LEU	4.7
11	I	124	VAL	4.7
1	0	1173	A	4.7
11	I	105	GLU	4.7
1	0	1171	A	4.6
11	I	118	ASN	4.6
11	I	106	GLN	4.6
1	0	1177	A	4.6
11	I	121	LYS	4.6
1	0	1951	G	4.6
11	I	117	THR	4.6
10	H	174	LEU	4.6
8	F	119	ARG	4.5
11	I	109	PRO	4.5
6	D	58	VAL	4.5
1	0	2237	G	4.5
11	I	116	LEU	4.5
6	D	57	THR	4.5
11	I	76	ASP	4.4
1	0	970	U	4.4
2	9	23	U	4.4
14	L	80	ASP	4.3
3	A	237	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
14	L	106	VAL	4.3
30	2	35	ARG	4.3
1	0	1172	G	4.3
6	D	75	LEU	4.3
11	I	101	LYS	4.3
6	D	56	ARG	4.2
11	I	102	GLN	4.2
10	H	40	GLN	4.2
11	I	67	VAL	4.2
11	I	127	CYS	4.2
1	0	282	C	4.2
1	0	2238	A	4.2
9	G	71	LEU	4.2
6	D	166	ILE	4.2
6	D	87	ALA	4.2
6	D	62	ASP	4.2
6	D	165	PHE	4.1
9	G	24	VAL	4.1
11	I	81	GLU	4.1
11	I	73	LEU	4.1
6	D	89	PRO	4.1
11	I	87	PRO	4.1
24	V	38	GLY	4.0
8	F	17	LEU	4.0
11	I	130	LEU	3.9
16	N	138	ASP	3.9
11	I	119	ALA	3.9
3	A	36	ASP	3.9
6	D	27	ILE	3.9
6	D	17	ARG	3.8
6	D	86	THR	3.8
11	I	68	PRO	3.8
6	D	171	ASP	3.7
1	0	10	U	3.7
6	D	128	LEU	3.7
11	I	78	ALA	3.6
11	I	120	ALA	3.6
1	0	1169	U	3.6
1	0	1170	U	3.6
6	D	172	VAL	3.6
6	D	106	PHE	3.6
16	N	147	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	0	1199	A	3.6
6	D	92	GLU	3.6
11	I	131	GLY	3.6
27	Y	235	GLU	3.5
8	F	106	ALA	3.5
6	D	44	ILE	3.5
23	U	47	ARG	3.5
22	T	115	GLU	3.5
1	0	1202	A	3.5
26	X	85	VAL	3.5
11	I	93	ALA	3.5
28	Z	20	ARG	3.5
11	I	134	ILE	3.4
14	L	60	GLU	3.4
14	L	105	TYR	3.4
7	E	170	ARG	3.4
16	N	149	GLU	3.4
11	I	110	ASP	3.4
11	I	69	PRO	3.4
6	D	84	LEU	3.4
6	D	66	GLY	3.4
8	F	44	SER	3.4
1	0	735	C	3.4
6	D	98	PHE	3.3
26	X	80	GLU	3.3
1	0	960	G	3.3
9	G	69	ARG	3.3
8	F	16	ALA	3.3
9	G	70	ALA	3.3
11	I	75	LYS	3.3
6	D	134	LEU	3.3
6	D	11	HIS	3.2
22	T	112	LEU	3.2
1	0	1200	A	3.2
1	0	284	C	3.2
3	A	133	ARG	3.2
11	I	84	SER	3.2
11	I	90	ASP	3.1
7	E	100	ASP	3.1
3	A	38	ILE	3.1
6	D	68	PRO	3.1
11	I	103	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
22	T	119	ALA	3.1
1	0	2004	U	3.1
9	G	21	ASP	3.1
16	N	152	GLU	3.1
11	I	82	THR	3.0
6	D	130	VAL	3.0
6	D	102	GLY	3.0
10	H	48	VAL	3.0
26	X	10	VAL	3.0
11	I	135	GLU	3.0
26	X	74	ALA	3.0
23	U	55	ALA	3.0
6	D	65	GLU	3.0
30	2	49	GLU	3.0
21	S	81	ILE	3.0
6	D	23	VAL	3.0
9	G	63	ARG	2.9
11	I	133	THR	2.9
6	D	40	ILE	2.9
11	I	123	VAL	2.9
16	N	162	ASP	2.9
6	D	104	PHE	2.9
14	L	91	VAL	2.9
16	N	160	SER	2.8
8	F	49	PHE	2.8
14	L	75	LEU	2.8
3	A	34	ASP	2.8
8	F	107	ASP	2.8
1	0	1279	U	2.8
8	F	99	THR	2.8
1	0	1950	G	2.8
4	B	1	PRO	2.8
1	0	2508	C	2.8
14	L	149	ARG	2.8
7	E	6	GLU	2.7
24	V	37	GLY	2.7
14	L	133	VAL	2.7
1	0	999	C	2.7
6	D	83	PHE	2.7
1	0	371	U	2.7
16	N	157	PRO	2.7
10	H	170	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	0	1525	G	2.7
6	D	16	PRO	2.7
28	Z	11	SER	2.7
24	V	2	VAL	2.7
7	E	87	PHE	2.7
2	9	2	U	2.7
11	I	115	ASP	2.7
16	N	183	ASP	2.7
14	L	81	VAL	2.7
9	G	73	ASP	2.7
1	0	1163	G	2.6
10	H	169	GLU	2.6
6	D	43	GLU	2.6
31	3	1	MET	2.6
18	P	110	ASP	2.6
18	P	141	ILE	2.6
27	Y	95	THR	2.6
16	N	180	LEU	2.6
7	E	101	GLU	2.6
7	E	108	LEU	2.6
8	F	103	GLU	2.6
9	G	68	GLU	2.6
16	N	68	GLU	2.6
31	3	92	GLU	2.6
9	G	15	TRP	2.6
10	H	53	ILE	2.6
22	T	116	ASP	2.6
9	G	65	THR	2.6
11	I	114	TYR	2.6
14	L	96	VAL	2.5
30	2	39	ARG	2.5
1	0	2509	A	2.5
24	V	8	ILE	2.5
1	0	138	U	2.5
14	L	104	ASP	2.5
16	N	139	TRP	2.5
7	E	5	LEU	2.5
1	0	1000	C	2.5
6	D	26	GLY	2.5
9	G	66	LEU	2.5
1	0	285	A	2.5
6	D	25	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	0	370	G	2.5
1	0	969	G	2.5
1	0	2239	C	2.5
2	9	122	C	2.5
16	N	145	ALA	2.5
9	G	28	GLU	2.5
7	E	128	GLY	2.5
9	G	25	GLU	2.5
14	L	97	VAL	2.5
31	3	22	VAL	2.5
28	Z	22	SER	2.5
1	0	1625	U	2.5
9	G	72	ASP	2.5
15	M	194	GLY	2.5
24	V	3	LEU	2.5
7	E	88	TYR	2.5
5	C	135	GLU	2.4
3	A	64	ASP	2.4
1	0	1180	U	2.4
16	N	179	LEU	2.4
16	N	184	ILE	2.4
8	F	109	GLU	2.4
1	0	2664	A	2.4
14	L	118	LEU	2.4
24	V	41	GLU	2.4
7	E	127	ASP	2.4
24	V	59	ILE	2.4
9	G	26	MET	2.4
1	0	1948	G	2.4
8	F	108	VAL	2.4
1	0	1186	C	2.4
26	X	71	ARG	2.4
6	D	41	LEU	2.4
11	I	95	LEU	2.4
6	D	70	GLY	2.4
26	X	7	GLU	2.4
1	0	1181	A	2.3
16	N	159	TYR	2.3
6	D	94	ALA	2.3
10	H	85	ASP	2.3
6	D	51	ARG	2.3
8	F	75	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
27	Y	216	ARG	2.3
8	F	98	VAL	2.3
1	0	2344	G	2.3
6	D	54	ALA	2.3
6	D	157	LEU	2.3
14	L	89	PHE	2.3
16	N	181	ASP	2.3
6	D	67	ASP	2.3
16	N	151	ASP	2.3
9	G	67	LEU	2.3
27	Y	98	GLN	2.3
24	V	63	GLU	2.3
26	X	41	PHE	2.3
14	L	150	GLN	2.3
27	Y	97	LEU	2.3
7	E	46	THR	2.3
16	N	155	GLU	2.3
28	Z	24	ARG	2.3
4	B	128	ILE	2.3
11	I	122	GLU	2.2
16	N	137	ALA	2.2
10	H	86	TYR	2.2
11	I	89	GLU	2.2
14	L	100	ALA	2.2
16	N	148	ALA	2.2
9	G	18	GLU	2.2
1	0	1947	G	2.2
8	F	26	THR	2.2
6	D	129	ASP	2.2
4	B	181	ILE	2.2
6	D	50	VAL	2.2
3	A	85	SER	2.1
7	E	98	GLU	2.1
10	H	172	GLU	2.1
23	U	54	THR	2.1
1	0	280	C	2.1
24	V	61	GLY	2.1
16	N	143	ARG	2.1
16	N	185	GLU	2.1
7	E	131	LEU	2.1
16	N	158	LEU	2.1
27	Y	108	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
7	E	53	GLU	2.1
21	S	76	GLU	2.1
7	E	10	ASP	2.1
6	D	24	HIS	2.1
10	H	165	ARG	2.1
7	E	124	VAL	2.1
4	B	121	PRO	2.1
6	D	49	PRO	2.1
3	A	31	LYS	2.1
10	H	39	LYS	2.1
3	A	60	PHE	2.1
30	2	20	ARG	2.1
8	F	100	ASP	2.1
27	Y	96	GLU	2.1
6	D	164	ALA	2.1
21	S	20	PHE	2.1
6	D	55	LYS	2.1
14	L	130	ARG	2.1
1	0	1197	G	2.0
7	E	20	ILE	2.0
6	D	173	GLU	2.0
9	G	22	ALA	2.0
7	E	95	VAL	2.0
31	3	56	PRO	2.0
6	D	81	GLU	2.0
12	J	92	GLN	2.0
8	F	20	LEU	2.0
6	D	29	HIS	2.0
7	E	129	GLU	2.0
9	G	20	VAL	2.0
28	Z	25	ARG	2.0
18	P	114	LEU	2.0
4	B	61	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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(Å^2)	Q<0.9
1	OMU	0	2587	21/22	0.98	0.13	30,32,34,37	0
1	OMG	0	2588	24/25	0.98	0.13	30,33,34,35	0
1	UR3	0	2619	21/22	0.98	0.13	29,35,39,43	0
1	PSU	0	2621	20/21	0.98	0.14	24,27,32,32	0
1	1MA	0	628	23/24	0.99	0.16	25,28,29,29	0

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, 95th 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(Å^2)	Q<0.9
34	NA	0	8571	1/1	0.49	0.45	62,62,62,62	0
34	NA	0	8582	1/1	0.65	0.29	88,88,88,88	0
34	NA	R	8586	1/1	0.66	0.80	90,90,90,90	0
34	NA	0	8529	1/1	0.70	0.21	66,66,66,66	0
32	MG	0	8031	1/1	0.71	0.19	35,35,35,35	0
32	MG	0	8087	1/1	0.72	0.19	61,61,61,61	0
34	NA	0	8563	1/1	0.76	0.35	58,58,58,58	0
32	MG	0	8090	1/1	0.78	0.24	61,61,61,61	0
34	NA	0	8569	1/1	0.81	0.42	59,59,59,59	0
34	NA	0	8526	1/1	0.81	0.32	51,51,51,51	0
34	NA	9	8551	1/1	0.82	0.25	36,36,36,36	0
34	NA	0	8566	1/1	0.82	0.27	59,59,59,59	0
34	NA	0	8577	1/1	0.83	0.42	64,64,64,64	0
32	MG	0	8041	1/1	0.83	0.18	52,52,52,52	0
34	NA	0	8581	1/1	0.84	0.32	59,59,59,59	0
34	NA	0	8584	1/1	0.85	0.10	53,53,53,53	0
34	NA	0	8524	1/1	0.85	0.19	56,56,56,56	0
32	MG	0	8050	1/1	0.85	0.09	72,72,72,72	0
32	MG	2	8076	1/1	0.86	0.09	56,56,56,56	0
34	NA	0	8541	1/1	0.86	0.17	46,46,46,46	0
34	NA	0	8550	1/1	0.87	0.36	48,48,48,48	0
34	NA	0	8507	1/1	0.88	0.31	51,51,51,51	0
32	MG	0	8049	1/1	0.88	0.29	68,68,68,68	0
34	NA	0	8585	1/1	0.88	0.44	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	0	8532	1/1	0.88	0.17	40,40,40,40	0
34	NA	0	8533	1/1	0.88	0.12	28,28,28,28	0
34	NA	0	8511	1/1	0.89	0.10	53,53,53,53	0
34	NA	0	8568	1/1	0.89	0.14	61,61,61,61	0
34	NA	0	8542	1/1	0.89	0.25	49,49,49,49	0
32	MG	0	8092	1/1	0.89	0.48	93,93,93,93	0
34	NA	0	8573	1/1	0.89	0.27	54,54,54,54	0
34	NA	R	8537	1/1	0.89	0.08	40,40,40,40	0
32	MG	0	8105	1/1	0.89	0.27	55,55,55,55	0
34	NA	0	8540	1/1	0.90	0.35	46,46,46,46	0
32	MG	K	8069	1/1	0.90	0.08	47,47,47,47	0
34	NA	0	8567	1/1	0.90	0.11	46,46,46,46	0
32	MG	0	8103	1/1	0.90	0.19	63,63,63,63	0
32	MG	0	8070	1/1	0.90	0.07	41,41,41,41	0
34	NA	0	8570	1/1	0.90	0.30	52,52,52,52	0
34	NA	0	8552	1/1	0.90	0.38	54,54,54,54	0
34	NA	0	8557	1/1	0.90	0.07	53,53,53,53	0
35	CL	J	8802	1/1	0.90	0.11	61,61,61,61	0
34	NA	0	8508	1/1	0.91	0.25	56,56,56,56	0
34	NA	0	8555	1/1	0.91	0.49	72,72,72,72	0
34	NA	C	8504	1/1	0.91	0.12	34,34,34,34	0
32	MG	0	8112	1/1	0.91	0.12	44,44,44,44	0
34	NA	0	8514	1/1	0.91	0.20	44,44,44,44	0
32	MG	0	8081	1/1	0.91	0.10	56,56,56,56	0
34	NA	0	8561	1/1	0.92	0.23	50,50,50,50	0
34	NA	9	8583	1/1	0.92	0.35	61,61,61,61	0
32	MG	0	8100	1/1	0.92	0.18	68,68,68,68	0
34	NA	0	8564	1/1	0.92	0.23	42,42,42,42	0
32	MG	0	8099	1/1	0.92	0.16	44,44,44,44	0
35	CL	A	8809	1/1	0.92	0.16	61,61,61,61	0
34	NA	0	8517	1/1	0.92	0.12	44,44,44,44	0
36	TEL	0	9000	58/58	0.92	0.21	53,63,75,76	0
34	NA	0	8527	1/1	0.93	0.17	39,39,39,39	0
32	MG	0	8053	1/1	0.93	0.10	48,48,48,48	0
32	MG	T	8073	1/1	0.93	0.06	60,60,60,60	0
32	MG	0	8045	1/1	0.93	0.09	62,62,62,62	0
34	NA	0	8535	1/1	0.93	0.29	44,44,44,44	0
34	NA	J	8546	1/1	0.93	0.10	49,49,49,49	0
34	NA	0	8572	1/1	0.93	0.30	67,67,67,67	0
34	NA	0	8562	1/1	0.93	0.23	63,63,63,63	0
32	MG	0	8047	1/1	0.93	0.11	72,72,72,72	0
34	NA	0	8525	1/1	0.93	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8085	1/1	0.93	0.09	38,38,38,38	0
32	MG	0	8097	1/1	0.94	0.08	34,34,34,34	0
34	NA	0	8510	1/1	0.94	0.19	40,40,40,40	0
32	MG	A	8066	1/1	0.94	0.05	63,63,63,63	0
34	NA	0	8513	1/1	0.94	0.10	62,62,62,62	0
34	NA	A	8545	1/1	0.94	0.14	53,53,53,53	0
34	NA	0	8559	1/1	0.94	0.20	57,57,57,57	0
32	MG	0	8057	1/1	0.94	0.16	48,48,48,48	0
34	NA	L	8580	1/1	0.94	0.36	48,48,48,48	0
34	NA	Q	8548	1/1	0.94	0.20	45,45,45,45	0
34	NA	0	8515	1/1	0.94	0.21	45,45,45,45	0
32	MG	0	8091	1/1	0.94	0.05	49,49,49,49	0
35	CL	0	8822	1/1	0.94	0.21	81,81,81,81	0
34	NA	0	8579	1/1	0.94	0.14	61,61,61,61	0
32	MG	0	8068	1/1	0.94	0.12	68,68,68,68	0
35	CL	N	8807	1/1	0.94	0.17	58,58,58,58	0
32	MG	0	8093	1/1	0.94	0.08	51,51,51,51	0
32	MG	0	8113	1/1	0.95	0.12	45,45,45,45	0
34	NA	0	8565	1/1	0.95	0.27	37,37,37,37	0
32	MG	0	8114	1/1	0.95	0.07	46,46,46,46	0
32	MG	9	8095	1/1	0.95	0.08	68,68,68,68	0
32	MG	0	8048	1/1	0.95	0.13	58,58,58,58	0
32	MG	0	8101	1/1	0.95	0.09	61,61,61,61	0
34	NA	0	8516	1/1	0.95	0.15	41,41,41,41	0
32	MG	0	8088	1/1	0.95	0.06	31,31,31,31	0
32	MG	0	8104	1/1	0.95	0.17	49,49,49,49	0
34	NA	R	8538	1/1	0.95	0.08	54,54,54,54	0
34	NA	0	8556	1/1	0.95	0.43	44,44,44,44	0
33	K	0	8401	1/1	0.95	0.17	72,72,72,72	0
34	NA	0	8502	1/1	0.95	0.15	50,50,50,50	0
35	CL	J	8801	1/1	0.95	0.11	64,64,64,64	0
34	NA	0	8505	1/1	0.95	0.14	33,33,33,33	0
32	MG	0	8062	1/1	0.95	0.10	56,56,56,56	0
35	CL	Y	8820	1/1	0.95	0.09	42,42,42,42	0
32	MG	0	8014	1/1	0.95	0.06	33,33,33,33	0
34	NA	0	8534	1/1	0.96	0.07	37,37,37,37	0
32	MG	0	8027	1/1	0.96	0.08	44,44,44,44	0
32	MG	0	8028	1/1	0.96	0.09	31,31,31,31	0
32	MG	0	8046	1/1	0.96	0.07	42,42,42,42	0
34	NA	S	8512	1/1	0.96	0.23	16,16,16,16	0
34	NA	T	8543	1/1	0.96	0.09	38,38,38,38	0
35	CL	0	8805	1/1	0.96	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	NA	0	8560	1/1	0.96	0.41	45,45,45,45	0
32	MG	0	8107	1/1	0.96	0.12	77,77,77,77	0
34	NA	0	8544	1/1	0.96	0.06	28,28,28,28	0
34	NA	0	8549	1/1	0.96	0.10	36,36,36,36	0
34	NA	0	8519	1/1	0.96	0.08	35,35,35,35	0
32	MG	0	8007	1/1	0.96	0.08	23,23,23,23	0
35	CL	3	8804	1/1	0.96	0.11	65,65,65,65	0
34	NA	M	8547	1/1	0.96	0.14	29,29,29,29	0
34	NA	0	8531	1/1	0.97	0.12	38,38,38,38	0
34	NA	0	8574	1/1	0.97	0.68	68,68,68,68	0
34	NA	0	8575	1/1	0.97	0.20	45,45,45,45	0
34	NA	0	8576	1/1	0.97	0.19	51,51,51,51	0
32	MG	B	8055	1/1	0.97	0.07	42,42,42,42	0
34	NA	0	8578	1/1	0.97	0.21	42,42,42,42	0
32	MG	0	8051	1/1	0.97	0.07	52,52,52,52	0
32	MG	0	8040	1/1	0.97	0.10	46,46,46,46	0
32	MG	0	8022	1/1	0.97	0.10	36,36,36,36	0
32	MG	3	8078	1/1	0.97	0.12	41,41,41,41	0
32	MG	0	8061	1/1	0.97	0.08	37,37,37,37	0
32	MG	0	8094	1/1	0.97	0.06	70,70,70,70	0
32	MG	0	8042	1/1	0.97	0.10	37,37,37,37	0
34	NA	0	8506	1/1	0.97	0.47	39,39,39,39	0
32	MG	0	8064	1/1	0.97	0.08	28,28,28,28	0
34	NA	H	8522	1/1	0.97	0.17	61,61,61,61	0
32	MG	0	8067	1/1	0.97	0.12	37,37,37,37	0
34	NA	0	8509	1/1	0.97	0.08	37,37,37,37	0
32	MG	0	8023	1/1	0.97	0.08	33,33,33,33	0
32	MG	0	8013	1/1	0.97	0.15	34,34,34,34	0
32	MG	0	8072	1/1	0.97	0.10	53,53,53,53	0
32	MG	0	8080	1/1	0.97	0.08	45,45,45,45	0
32	MG	0	8006	1/1	0.97	0.04	33,33,33,33	0
32	MG	0	8110	1/1	0.97	0.08	40,40,40,40	0
32	MG	0	8111	1/1	0.97	0.07	35,35,35,35	0
35	CL	0	8803	1/1	0.97	0.14	52,52,52,52	0
34	NA	0	8518	1/1	0.97	0.11	31,31,31,31	0
35	CL	0	8815	1/1	0.97	0.28	77,77,77,77	0
32	MG	0	8082	1/1	0.97	0.12	50,50,50,50	0
34	NA	0	8521	1/1	0.97	0.32	57,57,57,57	0
32	MG	0	8083	1/1	0.97	0.05	35,35,35,35	0
32	MG	0	8016	1/1	0.97	0.16	33,33,33,33	0
35	CL	J	8821	1/1	0.97	0.14	52,52,52,52	0
35	CL	L	8810	1/1	0.97	0.17	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8116	1/1	0.97	0.09	36,36,36,36	0
35	CL	R	8806	1/1	0.97	0.09	40,40,40,40	0
32	MG	0	8033	1/1	0.97	0.10	32,32,32,32	0
32	MG	0	8036	1/1	0.97	0.06	33,33,33,33	0
34	NA	0	8530	1/1	0.97	0.13	41,41,41,41	0
32	MG	0	8003	1/1	0.98	0.14	33,33,33,33	0
34	NA	0	8553	1/1	0.98	0.13	27,27,27,27	0
34	NA	0	8554	1/1	0.98	0.16	31,31,31,31	0
32	MG	0	8012	1/1	0.98	0.09	26,26,26,26	0
32	MG	0	8115	1/1	0.98	0.07	47,47,47,47	0
32	MG	0	8035	1/1	0.98	0.03	36,36,36,36	0
34	NA	0	8558	1/1	0.98	0.46	86,86,86,86	0
32	MG	0	8004	1/1	0.98	0.05	23,23,23,23	0
32	MG	0	8038	1/1	0.98	0.10	28,28,28,28	0
34	NA	0	8520	1/1	0.98	0.11	34,34,34,34	0
32	MG	0	8096	1/1	0.98	0.08	40,40,40,40	0
34	NA	0	8523	1/1	0.98	0.12	33,33,33,33	0
32	MG	0	8071	1/1	0.98	0.07	49,49,49,49	0
32	MG	0	8098	1/1	0.98	0.08	37,37,37,37	0
32	MG	Y	8108	1/1	0.98	0.08	31,31,31,31	0
32	MG	0	8025	1/1	0.98	0.08	36,36,36,36	0
32	MG	0	8077	1/1	0.98	0.10	23,23,23,23	0
32	MG	0	8002	1/1	0.98	0.05	31,31,31,31	0
35	CL	0	8812	1/1	0.98	0.10	48,48,48,48	0
35	CL	0	8814	1/1	0.98	0.07	44,44,44,44	0
33	K	0	8402	1/1	0.98	0.12	59,59,59,59	0
34	NA	0	8501	1/1	0.98	0.21	23,23,23,23	0
32	MG	0	8102	1/1	0.98	0.13	56,56,56,56	0
32	MG	0	8052	1/1	0.98	0.07	44,44,44,44	0
32	MG	0	8015	1/1	0.98	0.08	29,29,29,29	0
34	NA	0	8539	1/1	0.98	0.11	32,32,32,32	0
32	MG	0	8043	1/1	0.98	0.08	40,40,40,40	0
35	CL	M	8818	1/1	0.98	0.18	43,43,43,43	0
32	MG	0	8084	1/1	0.98	0.07	49,49,49,49	0
35	CL	O	8808	1/1	0.98	0.16	66,66,66,66	0
32	MG	0	8109	1/1	0.98	0.12	16,16,16,16	0
32	MG	0	8059	1/1	0.98	0.05	27,27,27,27	0
32	MG	0	8060	1/1	0.98	0.14	40,40,40,40	0
32	MG	0	8044	1/1	0.98	0.09	39,39,39,39	0
37	CD	O	8705	1/1	0.98	0.09	65,65,65,65	0
32	MG	0	8020	1/1	0.99	0.08	25,25,25,25	0
32	MG	0	8054	1/1	0.99	0.08	26,26,26,26	0

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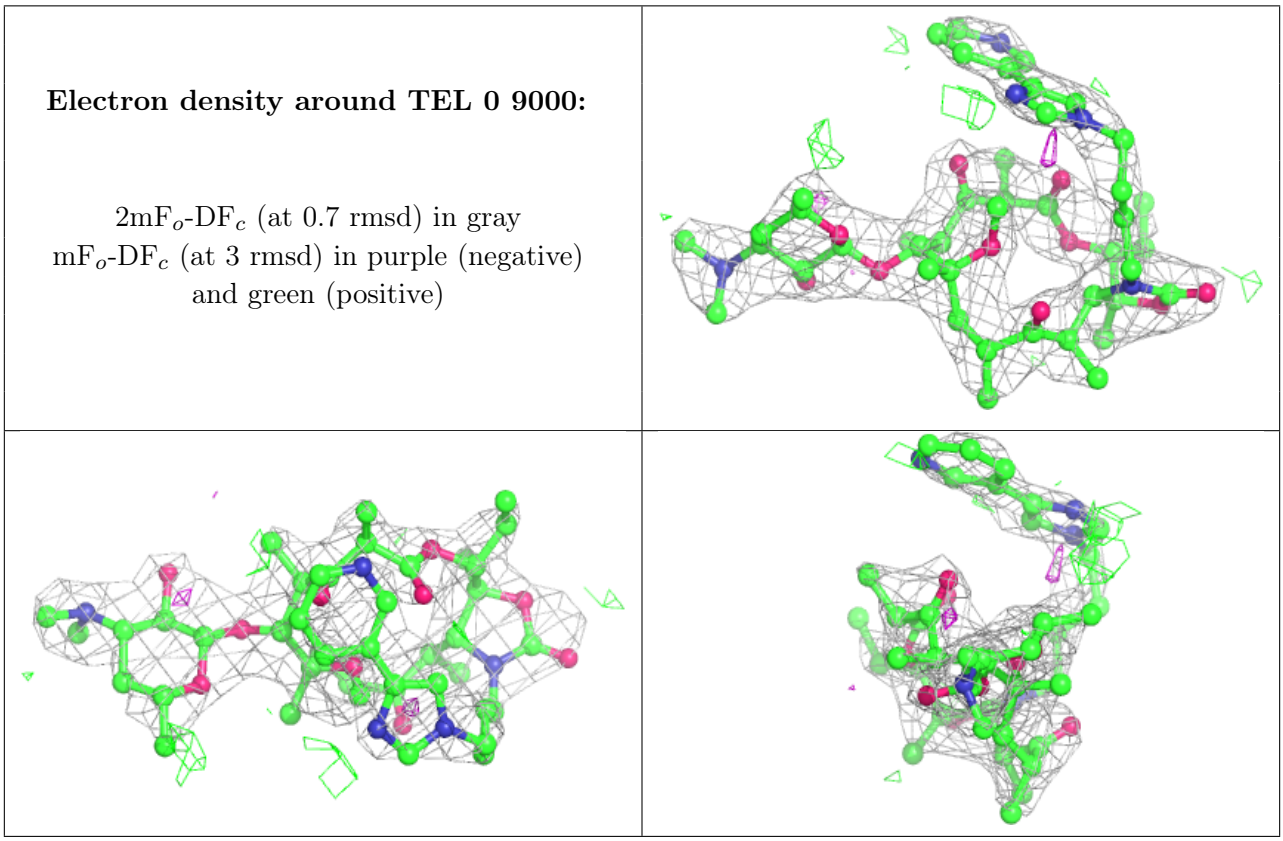
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	MG	0	8086	1/1	0.99	0.14	45,45,45,45	0
32	MG	0	8037	1/1	0.99	0.05	43,43,43,43	0
32	MG	0	8058	1/1	0.99	0.08	36,36,36,36	0
32	MG	0	8089	1/1	0.99	0.10	59,59,59,59	0
32	MG	A	8065	1/1	0.99	0.07	32,32,32,32	0
32	MG	0	8005	1/1	0.99	0.12	24,24,24,24	0
32	MG	0	8039	1/1	0.99	0.04	41,41,41,41	0
32	MG	B	8056	1/1	0.99	0.09	51,51,51,51	0
32	MG	0	8008	1/1	0.99	0.07	27,27,27,27	0
32	MG	0	8024	1/1	0.99	0.14	23,23,23,23	0
34	NA	0	8528	1/1	0.99	0.33	39,39,39,39	0
32	MG	0	8063	1/1	0.99	0.12	68,68,68,68	0
35	CL	0	8811	1/1	0.99	0.10	48,48,48,48	0
32	MG	0	8009	1/1	0.99	0.06	30,30,30,30	0
35	CL	0	8813	1/1	0.99	0.15	49,49,49,49	0
32	MG	0	8026	1/1	0.99	0.09	25,25,25,25	0
32	MG	0	8010	1/1	0.99	0.08	31,31,31,31	0
35	CL	0	8816	1/1	0.99	0.12	54,54,54,54	0
32	MG	0	8011	1/1	0.99	0.10	22,22,22,22	0
32	MG	0	8029	1/1	0.99	0.10	37,37,37,37	0
35	CL	B	8819	1/1	0.99	0.10	45,45,45,45	0
32	MG	0	8030	1/1	0.99	0.09	24,24,24,24	0
34	NA	0	8536	1/1	0.99	0.07	48,48,48,48	0
34	NA	0	8503	1/1	0.99	0.12	34,34,34,34	0
32	MG	0	8074	1/1	0.99	0.06	35,35,35,35	0
32	MG	0	8075	1/1	0.99	0.07	33,33,33,33	0
32	MG	0	8017	1/1	0.99	0.05	23,23,23,23	0
32	MG	0	8079	1/1	0.99	0.12	26,26,26,26	0
32	MG	0	8106	1/1	0.99	0.06	34,34,34,34	0
35	CL	Y	8817	1/1	0.99	0.14	58,58,58,58	0
32	MG	0	8032	1/1	0.99	0.08	32,32,32,32	0
32	MG	0	8018	1/1	0.99	0.10	38,38,38,38	0
32	MG	0	8034	1/1	0.99	0.06	28,28,28,28	0
32	MG	0	8019	1/1	0.99	0.05	31,31,31,31	0
37	CD	U	8701	1/1	0.99	0.10	61,61,61,61	0
37	CD	Z	8703	1/1	0.99	0.09	67,67,67,67	0
37	CD	3	8704	1/1	0.99	0.06	61,61,61,61	0
32	MG	0	8001	1/1	1.00	0.06	31,31,31,31	0
37	CD	1	8702	1/1	1.00	0.04	51,51,51,51	0
32	MG	0	8021	1/1	1.00	0.10	28,28,28,28	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.

Electron density around TEL 0 9000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.