



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:38 PM UTC

PDB ID : 3CCM / pdb_00003ccm
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2611U
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.55 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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

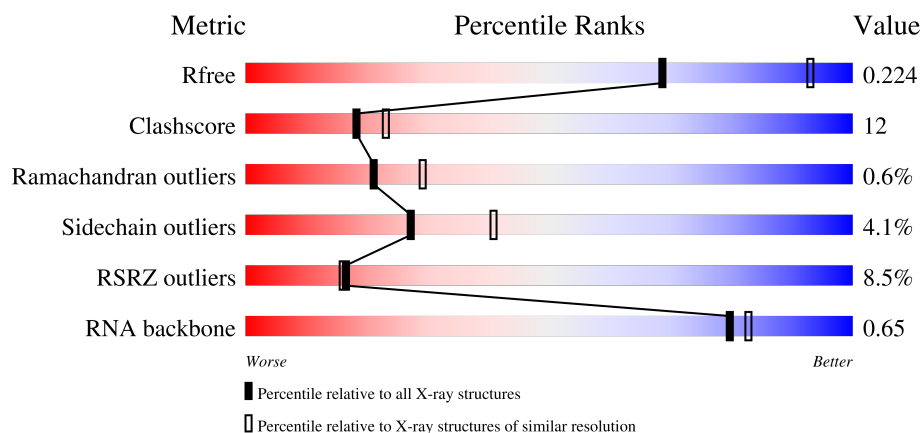
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	8% 74% 19% 6%
2	B	338	6% 65% 30%
3	C	246	4% 70% 26%
4	D	177	53% 51% 24% 21%

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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
35	NA	0	8518	-	-	-	X
35	NA	0	8562	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99119 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 protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

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

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

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

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59017	26348	10870	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
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	0	87	Total	Mg	0	0
			87	87		
32	9	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	J	3	Total Cl 3 3	0	0
33	L	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	0	10	Total Cl 10 10	0	0

- Molecule 34 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	3	Total Sr 3 3	0	0
34	B	1	Total Sr 1 1	0	0
34	F	1	Total Sr 1 1	0	0
34	R	1	Total Sr 1 1	0	0
34	S	1	Total Sr 1 1	0	0
34	1	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	0	94	Total Sr 94 94	0	0
34	9	3	Total Sr 3 3	0	0

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	T	1	Total Na 1 1	0	0
35	0	66	Total Na 66 66	0	0
35	9	2	Total Na 2 2	0	0

- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Cd 1 1	0	0
36	U	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	3	1	Total Cd 1 1	0	0

- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	117	Total O 117 117	0	0
38	B	139	Total O 139 139	0	0
38	C	165	Total O 165 165	0	0
38	D	48	Total O 48 48	0	0
38	E	49	Total O 49 49	0	0
38	F	25	Total O 25 25	0	0
38	G	18	Total O 18 18	0	0
38	H	71	Total O 71 71	0	0
38	I	8	Total O 8 8	0	0
38	J	55	Total O 55 55	0	0
38	K	55	Total O 55 55	0	0
38	L	79	Total O 79 79	0	0
38	M	138	Total O 138 138	0	0
38	N	58	Total O 58 58	0	0
38	O	40	Total O 40 40	0	0
38	P	61	Total O 61 61	0	0
38	Q	49	Total O 49 49	0	0
38	R	78	Total O 78 78	0	0
38	S	32	Total O 32 32	0	0
38	T	36	Total O 36 36	0	0
38	U	28	Total O 28 28	0	0
38	V	13	Total O 13 13	0	0

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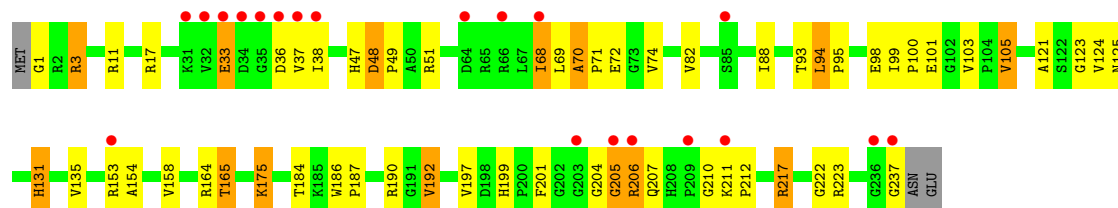
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	W	68	Total 68	O 68	0	0
38	X	24	Total 24	O 24	0	0
38	Y	97	Total 97	O 97	0	0
38	Z	29	Total 29	O 29	0	0
38	1	51	Total 51	O 51	0	0
38	2	37	Total 37	O 37	0	0
38	3	72	Total 72	O 72	0	0
38	0	5938	Total 5938	O 5938	0	0
38	9	145	Total 145	O 145	0	0

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.

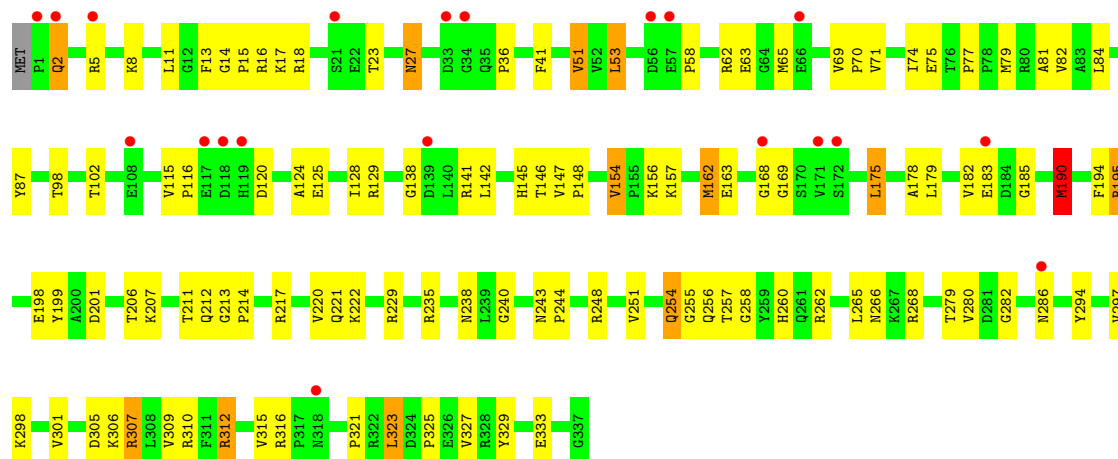
• Molecule 1: 50S ribosomal protein L2P

Chain A: 



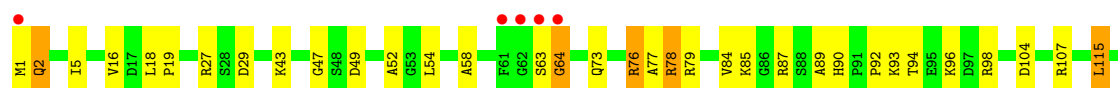
• Molecule 2: 50S ribosomal protein L3P

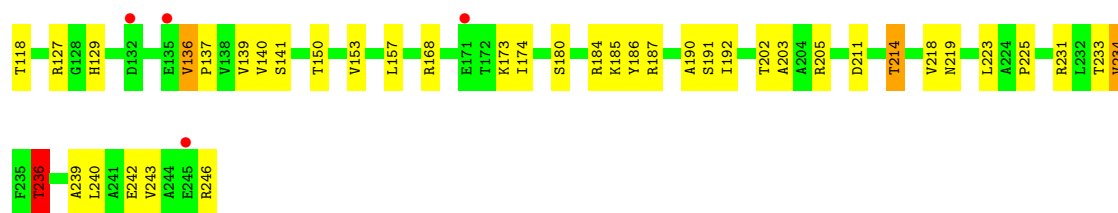
Chain B: 



• Molecule 3: 50S ribosomal protein L4P

Chain C: 

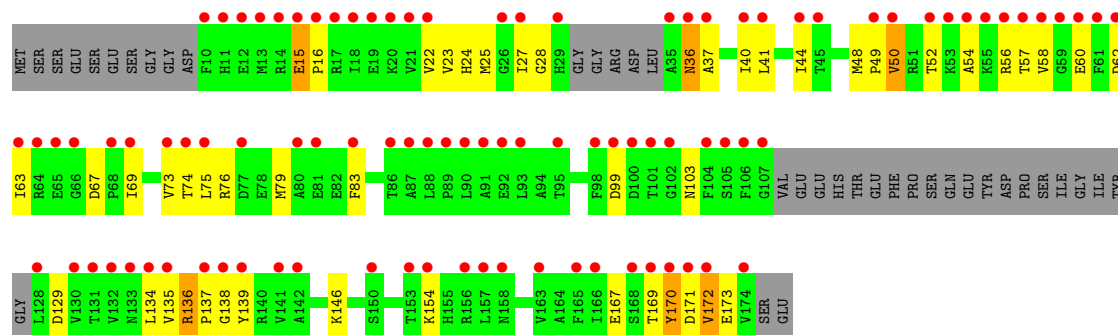




- Molecule 4: 50S ribosomal protein L5P



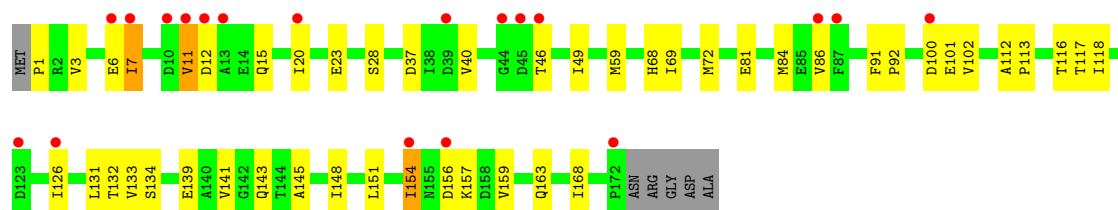
Chain D:



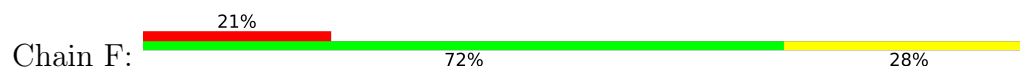
- Molecule 5: 50S ribosomal protein L6P



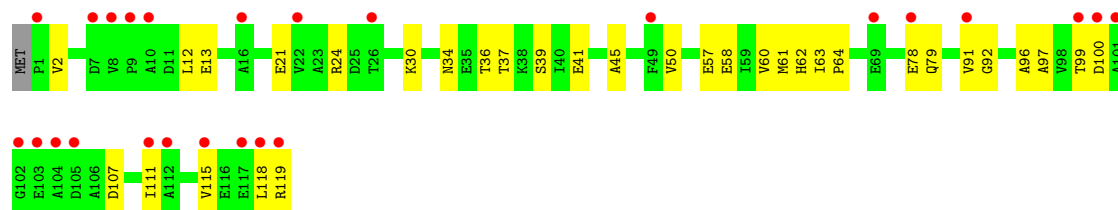
Chain E:



- Molecule 6: 50S ribosomal protein L7Ae



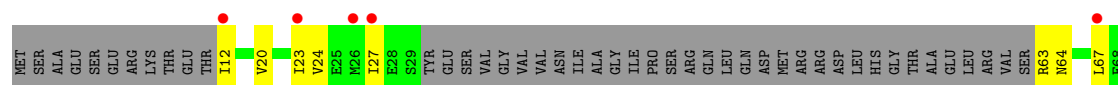
Chain F:



- Molecule 7: 50S ribosomal protein L10E

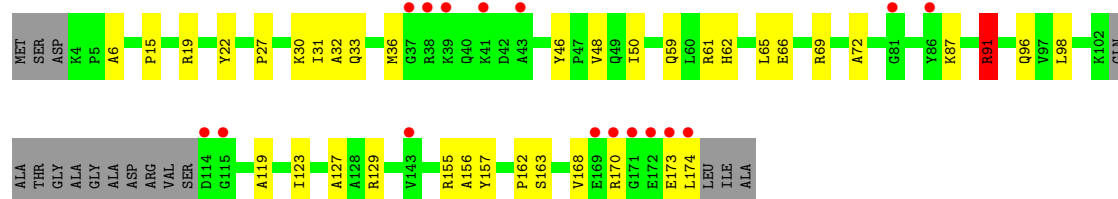


Chain G:

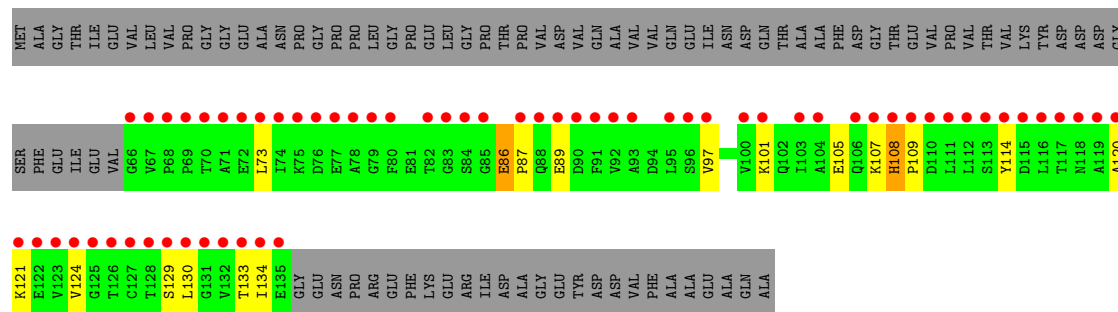
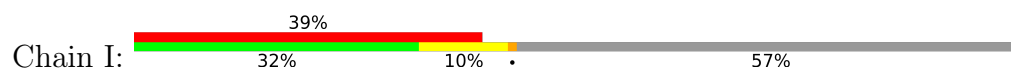




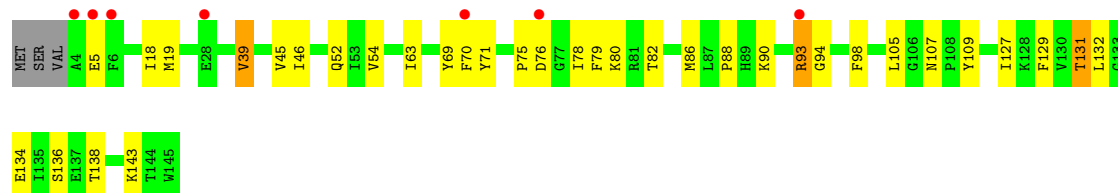
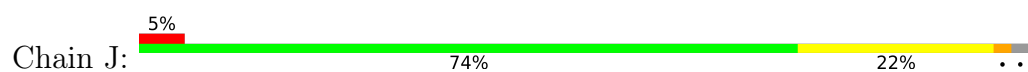
- Molecule 8: 50S ribosomal protein L10e



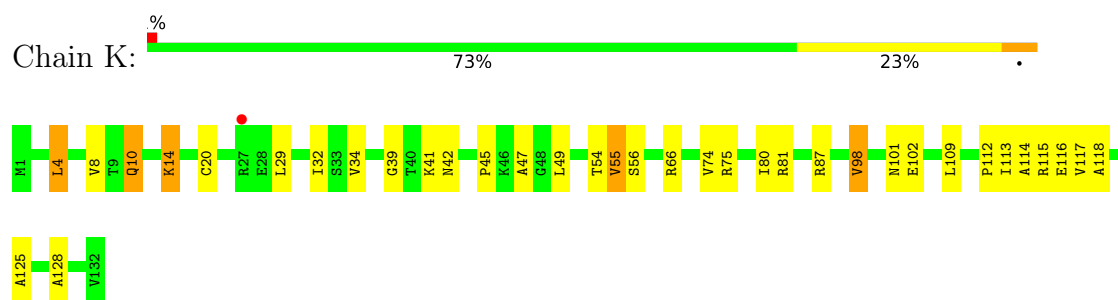
- Molecule 9: 50S ribosomal protein L11P



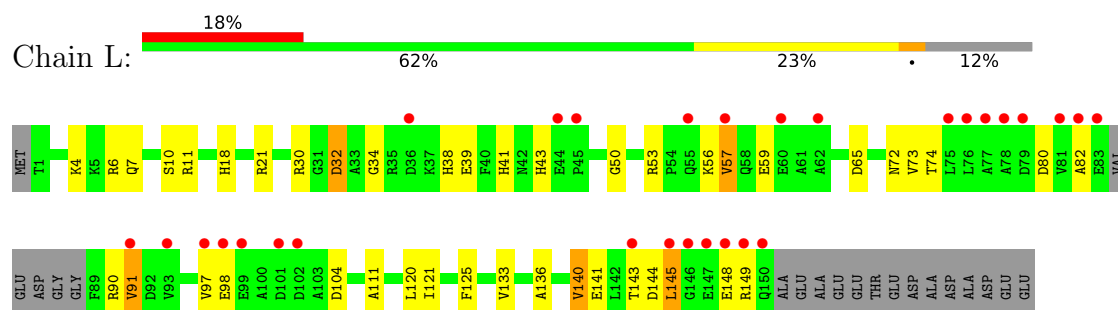
- Molecule 10: 50S ribosomal protein L13P



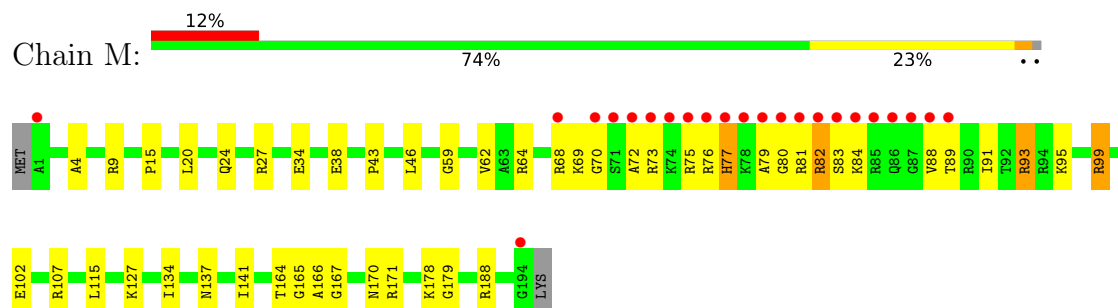
- Molecule 11: 50S ribosomal protein L14P



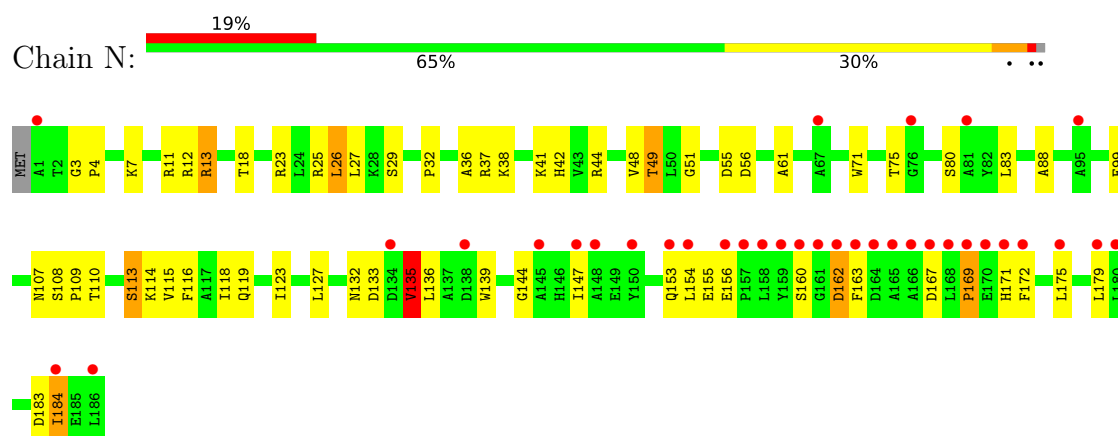
- Molecule 12: 50S ribosomal protein L15P



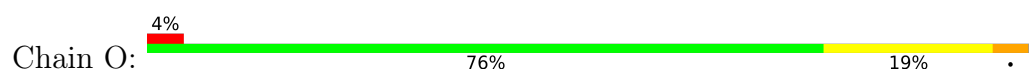
- Molecule 13: 50S ribosomal protein L15e

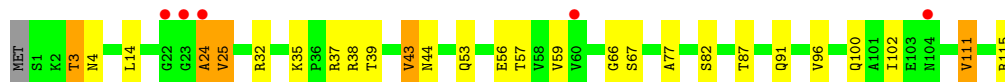


- Molecule 14: 50S ribosomal protein L18P

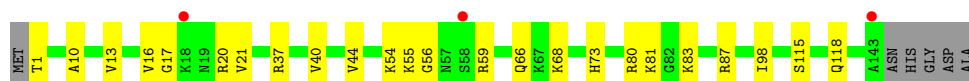
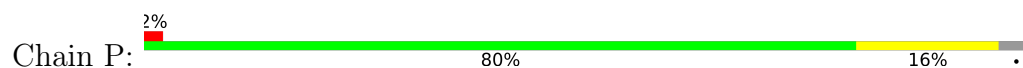


- Molecule 15: 50S ribosomal protein L18e

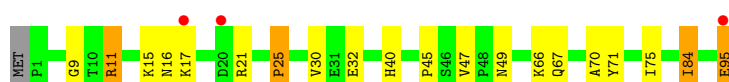
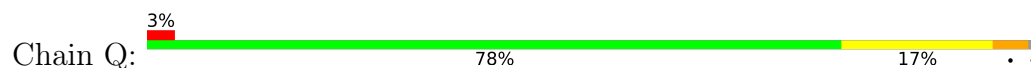




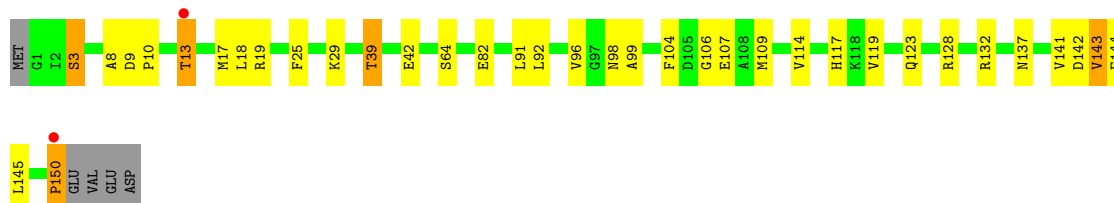
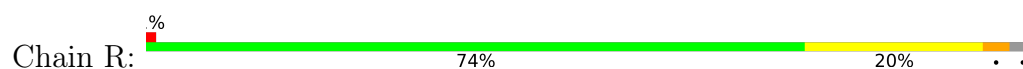
- Molecule 16: 50S ribosomal protein L19e



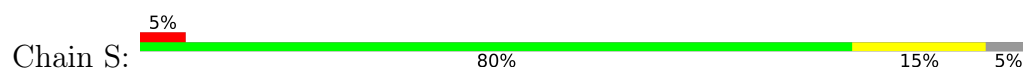
- Molecule 17: 50S ribosomal protein L21e



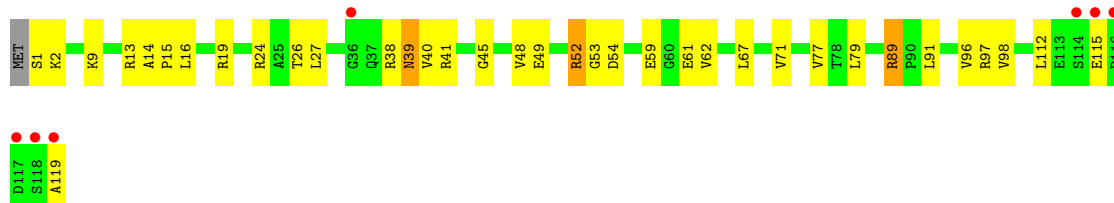
- Molecule 18: 50S ribosomal protein L22P



- Molecule 19: 50S ribosomal protein L23P



- Molecule 20: 50S ribosomal protein L24P



- Molecule 21: 50S ribosomal protein L24e



• Molecule 22: 50S ribosomal protein L29P



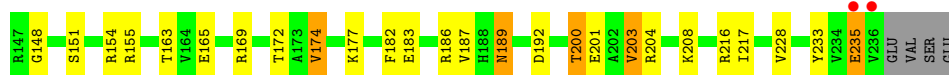
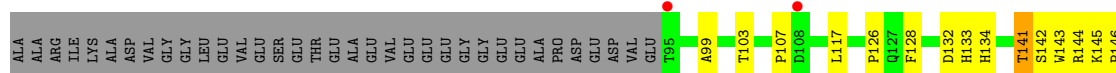
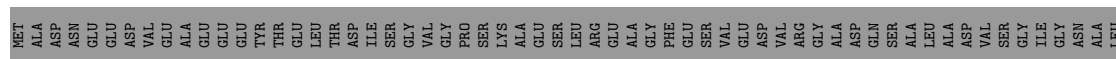
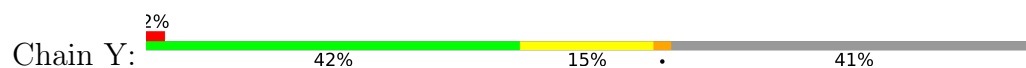
• Molecule 23: 50S ribosomal protein L30P



• Molecule 24: 50S ribosomal protein L31e

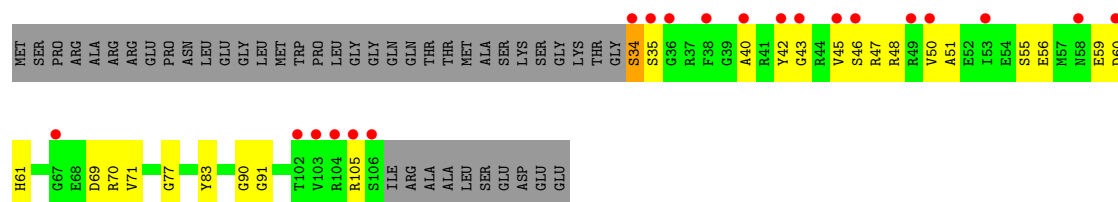


• Molecule 25: 50S ribosomal protein L32e



• Molecule 26: 50S ribosomal protein L37Ae

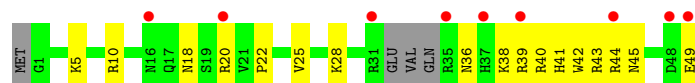




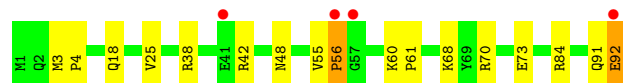
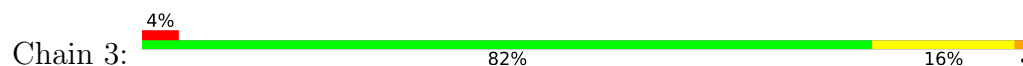
• Molecule 27: 50S ribosomal protein L37e



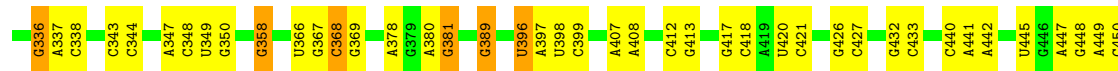
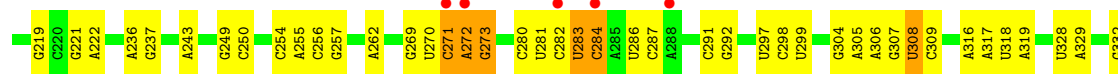
• Molecule 28: 50S ribosomal protein L39e



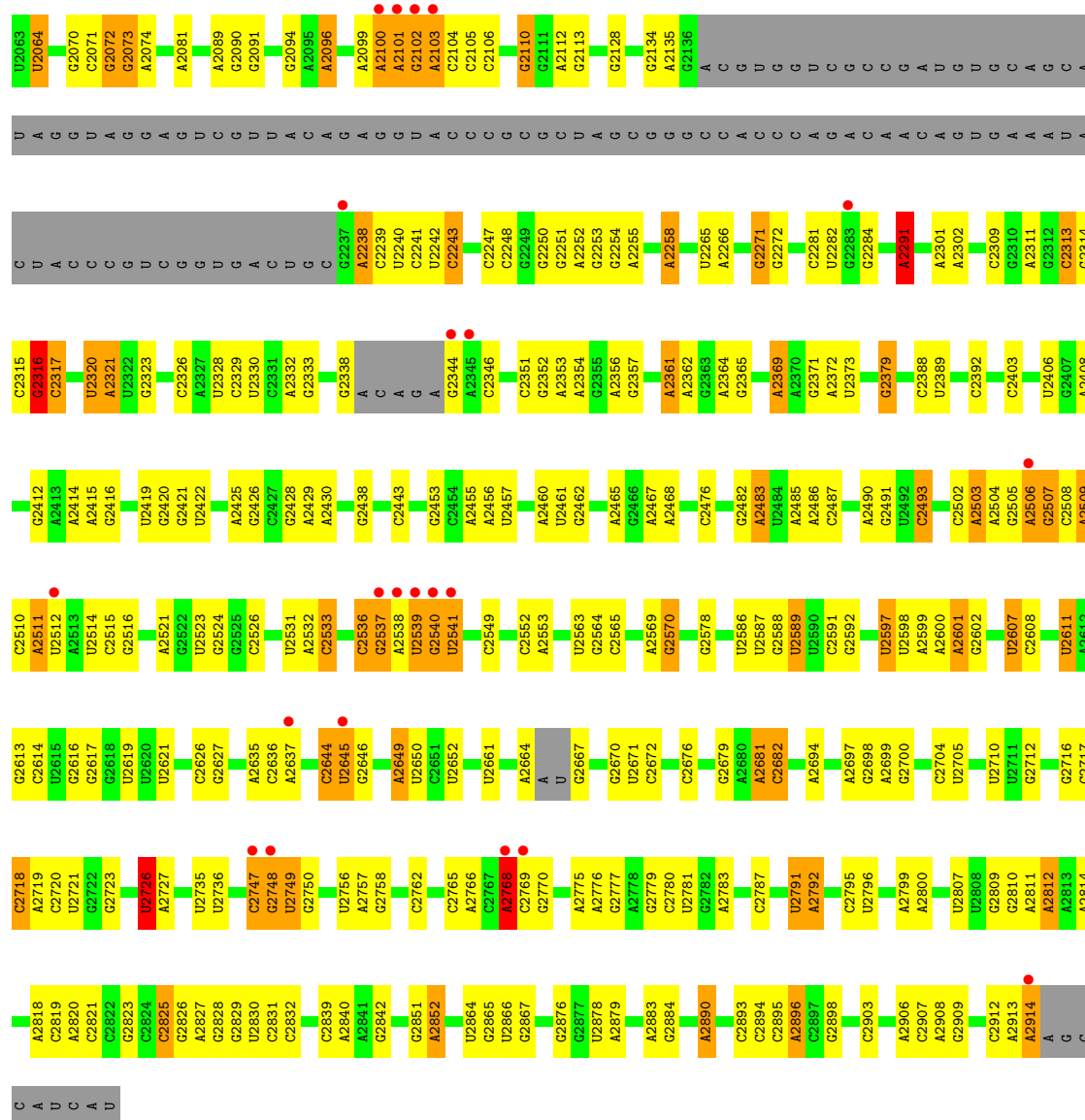
• Molecule 29: 50S ribosomal protein L44E



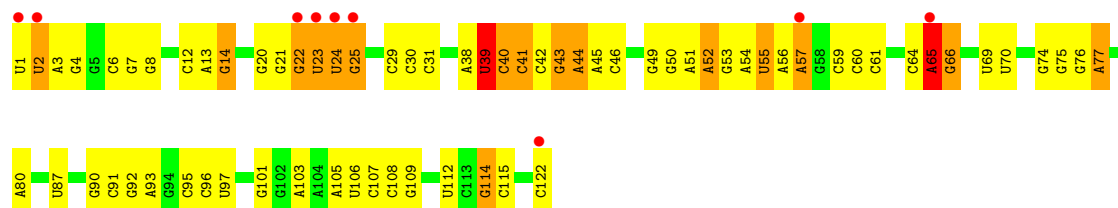
• Molecule 30: 23S RIBOSOMAL RNA







• Molecule 31: 5S RIBOSOMAL RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.53Å 298.18Å 573.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.55 49.70 – 2.55	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.70-2.55) 94.5 (49.70-2.55)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.240 0.189 , 0.224	Depositor DCC
R_{free} test set	6547 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99119	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	A	0.43	0/1786	0.96	7/2408 (0.3%)
2	B	0.44	1/2690 (0.0%)	1.01	15/3652 (0.4%)
3	C	0.45	0/1885	0.99	10/2552 (0.4%)
4	D	0.38	0/1111	0.95	8/1498 (0.5%)
5	E	0.38	0/1382	0.87	5/1880 (0.3%)
6	F	0.40	0/901	0.91	2/1224 (0.2%)
7	G	0.35	0/241	0.80	0/324
8	H	0.38	0/1302	0.93	6/1743 (0.3%)
9	I	0.40	0/526	0.91	2/716 (0.3%)
10	J	0.42	0/1136	0.89	2/1530 (0.1%)
11	K	0.40	0/1004	0.96	3/1351 (0.2%)
12	L	0.40	0/1130	0.93	4/1509 (0.3%)
13	M	0.44	0/1582	0.88	3/2116 (0.1%)
14	N	0.37	0/1474	1.04	13/1999 (0.7%)
15	O	0.42	0/874	0.95	6/1181 (0.5%)
16	P	0.40	0/1147	0.84	0/1528
17	Q	0.41	0/749	1.06	6/1005 (0.6%)
18	R	1.28	7/1172 (0.6%)	1.39	11/1578 (0.7%)
19	S	0.38	0/648	0.87	1/875 (0.1%)
20	T	0.38	0/958	0.95	2/1289 (0.2%)
21	U	0.37	0/417	0.80	1/562 (0.2%)
22	V	0.38	0/502	0.94	2/675 (0.3%)
23	W	0.44	0/1219	0.94	2/1655 (0.1%)
24	X	0.44	0/664	0.96	4/895 (0.4%)
25	Y	0.43	0/1146	0.95	2/1536 (0.1%)
26	Z	0.38	0/584	0.99	2/781 (0.3%)
27	1	0.46	0/438	0.86	1/578 (0.2%)
28	2	0.43	0/401	0.79	0/529
29	3	0.41	0/771	0.85	2/1024 (0.2%)
30	0	0.37	0/65953	0.61	26/102860 (0.0%)
31	9	0.36	0/2904	0.59	2/4526 (0.0%)
All	All	0.41	8/98697 (0.0%)	0.72	150/147579 (0.1%)

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
18	R	1	0
30	0	0	46
31	9	0	3
All	All	1	49

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	26.63	2.82	1.49
18	R	150	PRO	CA-C	-18.15	1.14	1.52
18	R	150	PRO	CG-CD	13.66	1.97	1.50
18	R	150	PRO	N-CA	13.28	1.67	1.47
18	R	150	PRO	C-O	11.79	1.47	1.23
18	R	150	PRO	N-CD	10.84	1.62	1.47
18	R	150	PRO	CA-CB	7.96	1.69	1.53
2	B	190	MET	SD-CE	-6.03	1.64	1.79

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-28.38	56.17	110.10
18	R	150	PRO	N-CA-C	-20.39	61.12	112.10
18	R	150	PRO	N-CA-CB	12.19	116.40	103.00
18	R	150	PRO	CA-N-CD	11.97	128.76	112.00
4	D	170	TYR	N-CA-C	9.94	125.35	113.23
14	N	163	PHE	N-CA-C	-9.77	98.88	112.45
30	0	1942	A	C5'-C4'-C3'	8.78	129.17	116.00
5	E	156	ASP	N-CA-C	8.40	120.44	111.28
13	M	89	THR	N-CA-C	8.34	120.15	111.14
30	0	1352	A	C2'-C3'-O3'	8.09	121.64	109.50
18	R	141	VAL	N-CA-C	8.06	119.39	108.11
17	Q	17	LYS	N-CA-C	-8.05	99.95	109.93
2	B	175	LEU	N-CA-C	-7.55	103.13	111.36
1	A	222	GLY	N-CA-C	-7.54	105.52	113.58
3	C	205	ARG	N-CA-C	7.29	120.16	111.33
15	O	24	ALA	N-CA-C	-7.26	106.34	114.62
30	0	1592	G	N9-C1'-C2'	7.17	122.76	112.00
1	A	70	ALA	N-CA-C	7.10	118.59	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	143	TRP	N-CA-C	6.96	120.47	110.10
2	B	157	LYS	N-CA-C	-6.91	105.40	114.31
4	D	15	GLU	CA-C-N	6.89	128.45	119.84
4	D	15	GLU	C-N-CA	6.89	128.45	119.84
26	Z	45	VAL	N-CA-C	6.82	117.52	110.36
24	X	22	ASN	N-CA-C	6.70	119.44	111.33
31	9	39	U	N1-C1'-C2'	6.68	122.03	112.00
2	B	323	LEU	N-CA-C	6.67	119.42	110.35
30	0	1819	G	C5'-C4'-C3'	6.64	125.96	116.00
30	0	920	C	C2'-C3'-O3'	-6.63	103.76	113.70
30	0	871	G	C5'-C4'-O4'	-6.59	99.91	109.80
24	X	12	ILE	N-CA-C	6.53	114.35	107.76
2	B	120	ASP	CA-C-N	6.52	126.45	119.28
2	B	120	ASP	C-N-CA	6.52	126.45	119.28
14	N	169	PRO	N-CA-C	-6.40	105.86	113.86
29	3	55	VAL	CA-C-N	6.40	127.84	119.84
29	3	55	VAL	C-N-CA	6.40	127.84	119.84
30	0	921	G	N9-C1'-C2'	6.36	121.54	112.00
14	N	13	ARG	N-CA-C	-6.13	103.92	112.45
24	X	77	PHE	N-CA-C	6.11	115.91	107.73
3	C	192	ILE	N-CA-C	6.10	117.51	109.21
19	S	27	ALA	N-CA-C	-6.09	98.81	108.73
30	0	834	G	C2'-C3'-O3'	-6.07	104.60	113.70
30	0	1737	A	C5'-C4'-C3'	-6.06	106.91	116.00
18	R	150	PRO	CA-C-O	-6.06	100.83	119.00
18	R	150	PRO	CA-CB-CG	-6.05	93.00	104.50
11	K	8	VAL	N-CA-C	6.00	117.12	108.48
30	0	2536	C	N1-C1'-C2'	5.99	120.98	112.00
5	E	11	VAL	N-CA-C	5.96	118.54	109.12
20	T	52	ARG	N-CA-C	5.95	123.47	110.80
15	O	82	SER	N-CA-C	-5.92	102.56	110.55
3	C	191	SER	N-CA-C	5.92	113.63	108.78
2	B	222	LYS	N-CA-C	-5.91	101.25	110.42
18	R	137	ASN	N-CA-C	5.91	119.58	110.42
30	0	1504	A	N9-C1'-C2'	5.91	120.87	112.00
30	0	1452	G	C5'-C4'-C3'	-5.90	107.15	116.00
15	O	43	VAL	N-CA-C	5.88	116.40	108.17
12	L	7	GLN	N-CA-C	5.86	118.62	111.82
1	A	135	VAL	N-CA-C	5.83	116.26	108.27
15	O	66	GLY	N-CA-C	5.77	125.07	115.66
30	0	206	G	C5'-C4'-C3'	-5.77	107.34	116.00
14	N	42	HIS	N-CA-C	5.76	117.99	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	35	VAL	N-CA-C	5.75	114.46	107.61
30	0	2726	U	N1-C1'-C2'	5.74	120.61	112.00
17	Q	84	ILE	N-CA-C	5.74	116.20	108.17
4	D	171	ASP	N-CA-C	5.71	116.83	108.14
14	N	51	GLY	CA-C-N	5.71	125.56	119.28
14	N	51	GLY	C-N-CA	5.71	125.56	119.28
8	H	119	ALA	N-CA-C	5.68	119.82	113.01
3	C	219	ASN	N-CA-C	5.67	118.12	109.95
2	B	213	GLY	CA-C-N	5.65	125.77	119.32
2	B	213	GLY	C-N-CA	5.65	125.77	119.32
22	V	42	ASN	CA-C-N	5.65	126.90	119.84
22	V	42	ASN	C-N-CA	5.65	126.90	119.84
20	T	16	LEU	N-CA-C	5.65	117.89	111.11
3	C	90	HIS	CA-C-N	5.64	126.19	120.38
3	C	90	HIS	C-N-CA	5.64	126.19	120.38
30	0	1819	G	C4'-C3'-C2'	-5.63	96.97	102.60
1	A	48	ASP	CA-C-N	5.61	125.45	119.28
1	A	48	ASP	C-N-CA	5.61	125.45	119.28
30	0	2316	G	C5'-C4'-C3'	-5.61	106.78	115.20
30	0	2301	A	N9-C1'-C2'	5.60	120.40	112.00
5	E	7	ILE	CA-C-N	5.58	125.53	119.78
5	E	7	ILE	C-N-CA	5.58	125.53	119.78
2	B	23	THR	CA-C-N	5.58	125.52	119.78
2	B	23	THR	C-N-CA	5.58	125.52	119.78
3	C	89	ALA	N-CA-C	5.58	117.05	110.97
30	0	1942	A	C4'-C3'-C2'	-5.52	97.08	102.60
3	C	64	GLY	N-CA-C	5.51	120.24	113.79
9	I	86	GLU	CA-C-N	5.51	125.41	119.85
9	I	86	GLU	C-N-CA	5.51	125.41	119.85
24	X	25	ARG	N-CA-C	5.50	117.27	111.28
30	0	1615	A	C5'-C4'-C3'	5.46	124.19	116.00
2	B	266	ASN	N-CA-C	5.44	118.84	111.17
30	0	2291	A	N9-C1'-C2'	5.42	120.12	112.00
25	Y	183	GLU	N-CA-C	-5.40	100.89	109.96
6	F	79	GLN	N-CA-C	5.39	118.19	109.40
13	M	70	GLY	N-CA-C	5.39	121.35	112.84
18	R	123	GLN	N-CA-C	5.38	118.69	110.20
8	H	162	PRO	N-CA-C	5.38	119.14	111.13
14	N	135	VAL	N-CA-C	-5.37	107.58	113.43
17	Q	25	PRO	CA-C-N	5.31	125.12	119.28
17	Q	25	PRO	C-N-CA	5.31	125.12	119.28
27	1	54	ALA	N-CA-C	5.30	117.48	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2313	C	C5'-C4'-C3'	5.30	123.96	116.00
21	U	50	GLU	N-CA-C	5.30	117.74	111.33
2	B	147	VAL	CA-C-N	5.29	125.61	119.47
2	B	147	VAL	C-N-CA	5.29	125.61	119.47
31	9	65	A	N9-C1'-C2'	5.29	119.94	112.00
4	D	136	ARG	CA-C-N	5.29	126.45	119.84
4	D	136	ARG	C-N-CA	5.29	126.45	119.84
13	M	77	HIS	N-CA-C	5.29	117.84	109.96
8	H	91	ARG	N-CA-C	5.26	119.55	113.18
12	L	57	VAL	N-CA-C	-5.25	107.86	112.90
14	N	133	ASP	N-CA-C	5.25	117.00	111.28
12	L	91	VAL	N-CA-C	5.24	115.81	108.17
10	J	71	TYR	CA-C-N	5.23	125.17	119.78
10	J	71	TYR	C-N-CA	5.23	125.17	119.78
4	D	67	ASP	CA-C-N	5.23	125.53	119.93
4	D	67	ASP	C-N-CA	5.23	125.53	119.93
17	Q	47	VAL	CA-C-N	5.23	126.38	119.84
17	Q	47	VAL	C-N-CA	5.23	126.38	119.84
8	H	163	SER	N-CA-C	-5.21	103.52	110.55
30	0	129	A	C2'-C3'-O3'	5.16	121.44	113.70
26	Z	48	ARG	N-CA-C	-5.16	104.61	112.04
14	N	3	GLY	CA-C-N	5.15	124.77	119.05
14	N	3	GLY	C-N-CA	5.15	124.77	119.05
1	A	68	ILE	N-CA-C	5.15	115.89	108.48
14	N	113	SER	N-CA-C	5.12	116.70	110.41
30	0	1700	C	C2'-C3'-O3'	-5.11	106.04	113.70
2	B	154	VAL	CA-C-N	5.09	124.70	119.05
2	B	154	VAL	C-N-CA	5.09	124.70	119.05
14	N	75	THR	N-CA-C	5.09	119.44	112.88
18	R	13	THR	N-CA-C	5.08	116.79	109.07
30	0	1942	A	C5'-C4'-O4'	5.07	117.41	109.80
14	N	153	GLN	N-CA-C	-5.07	102.84	110.70
6	F	62	HIS	N-CA-C	5.06	117.69	111.82
1	A	123	GLY	N-CA-C	5.06	122.27	115.59
5	E	37	ASP	N-CA-C	5.06	118.71	112.24
12	L	145	LEU	N-CA-C	-5.05	105.85	111.36
23	W	142	ASP	N-CA-C	-5.05	103.86	110.53
11	K	54	THR	N-CA-C	-5.04	101.49	109.96
3	C	18	LEU	N-CA-C	-5.04	101.97	109.42
15	O	4	ASN	CA-C-N	5.03	124.81	119.28
15	O	4	ASN	C-N-CA	5.03	124.81	119.28
18	R	3	SER	N-CA-C	-5.03	101.56	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	389	G	C5'-C4'-C3'	-5.02	108.48	116.00
3	C	236	THR	N-CA-C	-5.01	101.52	109.59
30	0	1504	A	C1'-O4'-C4'	-5.01	104.89	109.90
8	H	46	TYR	CA-C-N	5.00	124.69	119.64
8	H	46	TYR	C-N-CA	5.00	124.69	119.64
11	K	14	LYS	N-CA-C	-5.00	102.24	109.59

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1122	U	Sidechain
30	0	1237	U	Sidechain
30	0	1340	G	Sidechain
30	0	1342	C	Sidechain
30	0	1417	G	Sidechain
30	0	1488	U	Sidechain
30	0	1714	C	Sidechain
30	0	1744	G	Sidechain
30	0	1777	G	Sidechain
30	0	1819	G	Sidechain
30	0	182	G	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1979	G	Sidechain
30	0	2036	C	Sidechain
30	0	2316	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2552	C	Sidechain
30	0	2597	U	Sidechain
30	0	2599	A	Sidechain
30	0	26	U	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2607	U	Sidechain
30	0	270	U	Sidechain
30	0	2768	A	Sidechain
30	0	2842	G	Sidechain
30	0	332	G	Sidechain
30	0	396	U	Sidechain
30	0	460	A	Sidechain
30	0	462	A	Sidechain
30	0	469	G	Sidechain
30	0	470	U	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	664	U	Sidechain
30	0	795	G	Sidechain
30	0	817	G	Sidechain
30	0	867	A	Sidechain
30	0	868	G	Sidechain
31	9	39	U	Sidechain
31	9	87	U	Sidechain
31	9	90	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	52	0
2	B	2625	0	2533	89	0
3	C	1860	0	1813	57	0
4	D	1094	0	1085	40	0
5	E	1357	0	1266	37	0
6	F	890	0	843	24	0
7	G	240	0	231	6	0
8	H	1282	0	1292	32	0
9	I	519	0	500	19	0
10	J	1120	0	1098	38	0
11	K	994	0	1027	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	1118	0	1076	36	0
13	M	1558	0	1572	48	0
14	N	1445	0	1401	50	0
15	O	865	0	873	24	0
16	P	1136	0	1123	23	0
17	Q	735	0	729	16	0
18	R	1149	0	1122	33	0
19	S	641	0	605	9	0
20	T	950	0	924	25	0
21	U	410	0	364	14	0
22	V	499	0	511	15	0
23	W	1196	0	1137	54	0
24	X	654	0	653	16	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	15	0
27	1	431	0	426	23	0
28	2	396	0	413	19	0
29	3	755	0	728	13	0
30	0	59017	0	29811	1046	0
31	9	2599	0	1325	79	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	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	10	0	0	1	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	94	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	A	3	0	0	0	0
34	B	1	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5938	0	0	160	0
38	1	51	0	0	1	0
38	2	37	0	0	1	0
38	3	72	0	0	4	0
38	9	145	0	0	9	0
38	A	117	0	0	8	0
38	B	139	0	0	16	0
38	C	165	0	0	10	0
38	D	48	0	0	5	0
38	E	49	0	0	1	0
38	F	25	0	0	1	0
38	G	18	0	0	1	0
38	H	71	0	0	5	0
38	I	8	0	0	0	0
38	J	55	0	0	1	0
38	K	55	0	0	1	0
38	L	79	0	0	8	0
38	M	138	0	0	3	0
38	N	58	0	0	6	0
38	O	40	0	0	0	0
38	P	61	0	0	1	0
38	Q	49	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	R	78	0	0	2	0
38	S	32	0	0	3	0
38	T	36	0	0	3	0
38	U	28	0	0	2	0
38	V	13	0	0	2	0
38	W	68	0	0	5	0
38	X	24	0	0	3	0
38	Y	97	0	0	8	0
38	Z	29	0	0	3	0
All	All	99119	0	59911	1813	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 12.

All (1813) 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.97	1.41
30:0:2537:G:H5''	30:0:2538:A:H5''	1.17	1.14
30:0:871:G:C8	30:0:871:G:H5'	1.83	1.14
30:0:1205:U:H2'	30:0:1206:U:H5''	1.27	1.12
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.12
30:0:1160:G:H5'	30:0:1161:A:H5'	1.13	1.11
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.30	1.11
15:O:3:THR:HG22	30:0:656:G:H5'	1.26	1.10
14:N:37:ARG:NH1	31:9:6:C:H5''	1.67	1.09
30:0:2102:G:H21	30:0:2103:A:H2'	0.97	1.09
30:0:1160:G:C5'	30:0:1161:A:H5'	1.84	1.07
30:0:871:G:H5'	30:0:871:G:H8	1.12	1.07
30:0:1165:G:H1'	30:0:1174:A:H1'	1.34	1.07
30:0:1189:A:H3'	38:0:7701:HOH:O	1.56	1.04
9:I:130:LEU:HD21	30:0:1167:G:H4'	1.40	1.04
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.41	1.02
10:J:82:THR:HG23	30:0:1242:A:H5'	1.37	1.02
30:0:542:A:H5'	30:0:542:A:H8	1.24	1.02
31:9:56:A:H2'	31:9:57:A:H5''	1.42	1.01
30:0:1160:G:H5'	30:0:1161:A:C5'	1.91	1.01
30:0:1166:A:H61	30:0:1180:U:H3	1.04	1.01
3:C:236:THR:HG22	3:C:239:ALA:H	1.22	1.01
30:0:2748:G:OP1	30:0:2749:U:H5''	1.58	1.00
31:9:76:G:H3'	31:9:77:A:H5''	1.41	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:171:ARG:HD3	30:0:156:C:H5''	1.39	0.98
30:0:2100:A:H5'	38:0:7413:HOH:O	1.63	0.98
30:0:870:G:H2'	30:0:871:G:H5''	1.42	0.98
22:V:1:THR:HB	30:0:93:C:H5''	1.43	0.97
30:0:282:C:O2'	30:0:283:U:H5'	1.64	0.96
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.11	0.96
30:0:1372:A:H3'	38:0:7215:HOH:O	1.65	0.95
30:0:1625:U:H4'	38:0:4678:HOH:O	1.67	0.95
30:0:2102:G:H1'	30:0:2103:A:C8	2.02	0.95
30:0:2541:U:C6	30:0:2541:U:H5'	2.00	0.95
30:0:2102:G:N2	30:0:2103:A:H2'	1.82	0.95
30:0:2588:OMG:H5''	38:0:7509:HOH:O	1.64	0.94
16:P:115:SER:H	16:P:118:GLN:HE21	1.09	0.94
30:0:2717:C:C2'	30:0:2718:C:H5''	1.98	0.94
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.48	0.93
11:K:10:GLN:HE21	11:K:10:GLN:H	1.05	0.93
30:0:2710:U:H1'	38:0:7642:HOH:O	1.66	0.93
30:0:2491:G:H1'	38:0:6895:HOH:O	1.68	0.93
38:B:9058:HOH:O	30:0:2672:C:H1'	1.67	0.92
30:0:1116:U:H3	30:0:1246:A:H62	1.16	0.92
30:0:1205:U:C2'	30:0:1206:U:H5''	1.99	0.92
30:0:2896:A:H5''	38:0:6127:HOH:O	1.70	0.92
30:0:2103:A:H62	30:0:2538:A:H8	1.16	0.91
30:0:2851:G:C2'	30:0:2852:A:H5'	2.01	0.91
30:0:1878:G:H1'	38:0:6149:HOH:O	1.71	0.91
30:0:1290:G:H3'	38:0:5188:HOH:O	1.70	0.90
30:0:1701:A:H4'	30:0:1702:U:H5''	1.54	0.90
30:0:2748:G:H5'	38:0:7565:HOH:O	1.71	0.90
30:0:2406:U:H1'	38:0:6728:HOH:O	1.71	0.90
30:0:2506:A:O2'	30:0:2507:G:H8	1.55	0.90
30:0:2851:G:H2'	30:0:2852:A:H5'	1.54	0.89
30:0:1118:A:H8	30:0:1118:A:H3'	1.36	0.88
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.55	0.88
30:0:1184:C:H1'	38:0:7491:HOH:O	1.73	0.88
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.88
30:0:2812:A:H2	30:0:2814:A:H62	1.06	0.88
30:0:2541:U:H5'	30:0:2541:U:H6	1.34	0.88
30:0:2717:C:H2'	30:0:2718:C:H5''	1.54	0.88
30:0:1300:G:H1'	38:0:4694:HOH:O	1.72	0.88
6:F:58:GLU:HA	6:F:61:MET:HE2	1.55	0.87
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.52	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2637:A:H5'	38:0:9280:HOH:O	1.73	0.87
28:2:41:HIS:H	28:2:45:ASN:HD22	1.22	0.87
30:0:871:G:H8	30:0:871:G:C5'	1.88	0.87
1:A:211:LYS:HG2	1:A:212:PRO:HD2	1.55	0.87
30:0:1118:A:H3'	30:0:1118:A:C8	2.09	0.86
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.40	0.86
30:0:2537:G:C5'	30:0:2538:A:H5''	2.03	0.86
2:B:238:ASN:HD22	2:B:240:GLY:H	1.19	0.85
30:0:256:C:H5''	38:0:5505:HOH:O	1.77	0.85
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.19	0.85
30:0:506:G:H22	30:0:509:A:C5'	1.89	0.85
30:0:545:G:H5'	30:0:545:G:H8	1.41	0.85
30:0:1119:G:N2	30:0:1246:A:C2	2.43	0.85
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.41	0.85
30:0:2004:U:H2'	30:0:2004:U:O2	1.76	0.85
30:0:1426:C:H2'	38:0:9601:HOH:O	1.76	0.84
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.59	0.84
30:0:1183:C:N4	30:0:1184:C:H41	1.75	0.84
30:0:2586:U:H3	30:0:2592:G:H22	1.24	0.84
8:H:30:LYS:H	8:H:62:HIS:HD2	1.26	0.84
15:O:3:THR:CG2	30:0:656:G:H5'	2.08	0.84
31:9:23:U:O2'	31:9:24:U:H4'	1.78	0.84
15:O:57:THR:HB	15:O:111:VAL:HG23	1.60	0.83
30:0:1632:A:H2'	30:0:1633:C:H5'	1.60	0.83
30:0:559:U:H6	30:0:559:U:H5'	1.42	0.83
30:0:1750:C:H4'	38:0:7509:HOH:O	1.76	0.83
30:0:2505:G:O2'	30:0:2506:A:H5'	1.79	0.83
30:0:1165:G:O3'	30:0:1174:A:H4'	1.78	0.82
30:0:2783:A:H3'	38:0:5253:HOH:O	1.78	0.82
30:0:960:G:H3'	30:0:960:G:N3	1.94	0.82
30:0:1615:A:H5'	38:0:4198:HOH:O	1.76	0.82
30:0:1666:C:O2'	30:0:1667:A:H5''	1.78	0.82
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.13	0.82
11:K:39:GLY:HA2	38:0:5242:HOH:O	1.79	0.82
2:B:62:ARG:HA	2:B:65:MET:HE3	1.60	0.82
14:N:113:SER:HB2	38:N:8854:HOH:O	1.78	0.82
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.15	0.82
30:0:1116:U:HO2'	30:0:1118:A:H2	0.82	0.82
30:0:544:G:H2'	30:0:545:G:H5''	1.62	0.81
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.62	0.81
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:1:THR:HG23	22:V:2:VAL:H	1.43	0.81
23:W:149:LEU:HG	23:W:153:MET:HE2	1.60	0.81
30:0:558:C:C2'	30:0:559:U:H5''	2.10	0.81
30:0:558:C:O2'	30:0:559:U:H5''	1.81	0.81
30:0:2506:A:HO2'	30:0:2507:G:H8	0.82	0.81
30:0:1667:A:H8	30:0:1667:A:H5'	1.45	0.81
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.95	0.81
30:0:1183:C:H2'	38:0:6274:HOH:O	1.79	0.81
30:0:2005:G:H3'	30:0:2005:G:OP2	1.81	0.81
30:0:1632:A:C2'	30:0:1633:C:H5'	2.10	0.81
30:0:69:A:H5'	30:0:69:A:C8	2.16	0.81
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.16	0.80
2:B:190:MET:HE2	2:B:194:PHE:HD1	1.46	0.80
30:0:870:G:C2'	30:0:871:G:H5''	2.09	0.80
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.62	0.80
4:D:172:VAL:HG12	4:D:173:GLU:H	1.47	0.80
30:0:272:A:H3'	38:0:7553:HOH:O	1.81	0.80
30:0:282:C:H1'	30:0:368:C:N4	1.97	0.80
31:9:56:A:C2'	31:9:57:A:H5''	2.12	0.80
30:0:1474:C:H6	30:0:1474:C:H5'	1.47	0.79
30:0:1189:A:H1'	30:0:1209:C:O4'	1.82	0.79
27:1:25:LYS:HD2	28:2:49:GLU:H	1.48	0.79
30:0:558:C:H2'	30:0:559:U:C5'	2.13	0.79
30:0:1973:A:H5'	30:0:1973:A:H8	1.46	0.79
2:B:206:THR:HG21	30:0:2716:G:H5''	1.65	0.79
30:0:2100:A:H1'	38:0:5670:HOH:O	1.83	0.79
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.64	0.79
1:A:199:HIS:HD2	1:A:201:PHE:H	1.28	0.79
30:0:1634:G:H3'	38:0:3910:HOH:O	1.82	0.78
31:9:29:C:H2'	31:9:30:C:H5'	1.65	0.78
2:B:211:THR:HG23	30:0:2840:A:OP1	1.82	0.78
30:0:1118:A:H62	30:0:1244:U:H3	1.31	0.78
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.12	0.78
30:0:381:G:H5''	38:0:4335:HOH:O	1.82	0.78
30:0:1279:U:O2	30:0:1279:U:H2'	1.83	0.78
30:0:2524:G:N2	30:0:2526:C:H41	1.82	0.78
31:9:39:U:H1'	31:9:44:A:H61	1.46	0.78
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.14	0.78
30:0:1377:C:H5'	30:0:1377:C:H6	1.48	0.77
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.67	0.77
30:0:69:A:H5'	30:0:69:A:H8	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:SER:OG	30:0:2101:A:H2'	1.85	0.77
23:W:21:LEU:HD22	23:W:26:ILE:HD13	1.67	0.77
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.67	0.77
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.66	0.77
30:0:877:G:H5'	30:0:878:G:OP1	1.84	0.77
30:0:2852:A:H5''	38:0:5255:HOH:O	1.85	0.77
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.50	0.76
28:2:20:ARG:HG3	28:2:39:ARG:HH21	1.49	0.76
30:0:1175:G:H1'	30:0:1193:A:H2'	1.65	0.76
30:0:2765:C:H4'	38:0:5545:HOH:O	1.85	0.76
30:0:1730:G:H5''	30:0:1731:C:H6	1.51	0.76
30:0:2769:C:O2'	30:0:2770:G:H5'	1.86	0.76
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.51	0.76
30:0:1700:C:H5''	30:0:1701:A:OP2	1.86	0.76
30:0:2537:G:H5''	30:0:2538:A:C5'	2.10	0.75
30:0:1603:A:H5'	30:0:1605:G:O4'	1.86	0.75
30:0:2769:C:C2'	30:0:2770:G:H5'	2.17	0.75
31:9:39:U:H1'	31:9:44:A:N6	2.01	0.75
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.69	0.75
30:0:1165:G:H21	30:0:1173:A:H5''	1.52	0.75
30:0:2502:C:C2'	30:0:2503:A:H5'	2.17	0.75
30:0:506:G:H22	30:0:509:A:H5''	1.50	0.75
6:F:91:VAL:HG12	6:F:92:GLY:H	1.51	0.75
21:U:14:GLU:O	21:U:17:THR:HB	1.87	0.75
30:0:1116:U:O2'	30:0:1118:A:H2	1.66	0.75
1:A:48:ASP:HB3	38:A:9069:HOH:O	1.87	0.74
30:0:2524:G:H21	30:0:2526:C:H41	1.31	0.74
30:0:1206:U:H5'	30:0:1206:U:H6	1.52	0.74
31:9:2:U:H4'	38:9:9099:HOH:O	1.88	0.74
14:N:144:GLY:O	14:N:147:ILE:HG22	1.87	0.74
23:W:88:THR:HB	38:W:6679:HOH:O	1.88	0.74
4:D:154:LYS:H	4:D:154:LYS:HD2	1.53	0.74
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.68	0.74
18:R:128:ARG:NH2	30:0:2054:A:N3	2.36	0.74
30:0:1552:G:N2	30:0:1634:G:H1'	2.03	0.74
30:0:1666:C:H2'	30:0:1667:A:H5'	1.69	0.74
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.68	0.74
30:0:541:C:C2'	30:0:542:A:H5''	2.17	0.74
30:0:1701:A:H4'	30:0:1702:U:C5'	2.17	0.74
30:0:541:C:H2'	30:0:542:A:C5'	2.18	0.74
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:39:THR:HG22	18:R:42:GLU:H	1.53	0.73
30:0:396:U:H1'	38:0:7649:HOH:O	1.87	0.73
30:0:871:G:C8	30:0:871:G:C5'	2.64	0.73
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.69	0.73
30:0:1209:C:H2'	30:0:1210:G:H8	1.53	0.73
30:0:2438:G:H5'	38:0:6199:HOH:O	1.87	0.73
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.71	0.73
4:D:58:VAL:HB	4:D:62:ASP:HB3	1.69	0.73
13:M:171:ARG:CD	30:0:156:C:H5''	2.17	0.73
30:0:558:C:H2'	30:0:559:U:H5'	1.71	0.73
31:9:14:G:H5'	31:9:14:G:H8	1.53	0.73
30:0:542:A:H5'	30:0:542:A:C8	2.15	0.73
30:0:1201:C:H5''	38:0:6263:HOH:O	1.87	0.73
29:3:48:ASN:HD21	30:0:2468:A:H61	1.37	0.73
30:0:1165:G:C1'	30:0:1174:A:H1'	2.17	0.73
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.71	0.72
30:0:1166:A:N6	30:0:1180:U:H3	1.85	0.72
30:0:2502:C:H2'	30:0:2503:A:H5'	1.71	0.72
30:0:2769:C:H2'	30:0:2770:G:O4'	1.88	0.72
30:0:1476:A:O2'	30:0:1477:C:H5'	1.89	0.72
30:0:2812:A:C2	30:0:2814:A:N6	2.54	0.72
30:0:119:A:H2'	30:0:120:A:H5''	1.71	0.72
30:0:1119:G:H22	30:0:1246:A:H2	1.37	0.72
30:0:1165:G:H1'	30:0:1174:A:C1'	2.15	0.72
30:0:1730:G:H5''	30:0:1731:C:C6	2.23	0.72
30:0:544:G:C2'	30:0:545:G:H5''	2.19	0.72
30:0:2718:C:H6	30:0:2718:C:H5'	1.54	0.72
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.37	0.72
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.02	0.71
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.72	0.71
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.71	0.71
30:0:138:U:H5''	30:0:139:C:OP2	1.90	0.71
30:0:2908:A:H2'	30:0:2909:G:O4'	1.90	0.71
30:0:2635:A:O2'	30:0:2636:C:H5'	1.91	0.71
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.73	0.71
25:Y:235:GLU:CD	25:Y:235:GLU:H	1.96	0.71
3:C:139:VAL:HG13	38:C:8641:HOH:O	1.89	0.71
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.21	0.71
30:0:506:G:H22	30:0:509:A:H5'	1.55	0.71
30:0:848:C:H5'	38:0:7298:HOH:O	1.91	0.71
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2747:C:O3'	30:0:2748:G:H4'	1.90	0.71
30:0:1878:G:O2'	30:0:1879:U:C6	2.44	0.71
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.90	0.70
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.72	0.70
30:0:2106:C:H5'	30:0:2284:G:H21	1.55	0.70
30:0:2487:C:H5	38:0:4903:HOH:O	1.74	0.70
30:0:2507:G:H2'	30:0:2510:C:H42	1.57	0.70
30:0:272:A:H5'	30:0:273:G:OP2	1.91	0.70
30:0:2578:G:H5'	30:0:2578:G:H8	1.56	0.70
30:0:282:C:C2'	30:0:283:U:H5'	2.21	0.70
18:R:29:LYS:HD3	30:0:524:A:H5''	1.73	0.70
30:0:1058:A:H2'	30:0:1060:C:H5''	1.73	0.70
30:0:1730:G:H5'	30:0:1731:C:C5	2.27	0.70
30:0:462:A:H2'	38:0:4898:HOH:O	1.91	0.70
30:0:1724:U:H5''	38:0:3745:HOH:O	1.92	0.70
4:D:48:MET:HE2	31:9:41:C:H5'	1.74	0.69
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.74	0.69
30:0:1278:A:O2'	30:0:1279:U:H3'	1.92	0.69
31:9:49:G:H5''	38:9:9086:HOH:O	1.91	0.69
30:0:280:C:H2'	30:0:281:U:O4'	1.90	0.69
30:0:1165:G:H21	30:0:1173:A:C5'	2.04	0.69
30:0:1380:U:O4	30:0:2748:G:H1'	1.92	0.69
30:0:1299:G:H5'	38:0:4092:HOH:O	1.92	0.69
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.69
30:0:1666:C:C2'	30:0:1667:A:H5''	2.22	0.69
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.41	0.69
18:R:39:THR:HG23	18:R:107:GLU:O	1.92	0.69
30:0:1666:C:H2'	30:0:1667:A:C5'	2.22	0.69
30:0:2748:G:H5'	30:0:2748:G:C8	2.28	0.69
23:W:44:MET:HE2	30:0:944:G:H21	1.57	0.69
30:0:681:G:N3	30:0:681:G:H5'	2.08	0.69
30:0:2064:U:H5'	30:0:2652:U:H4'	1.75	0.69
30:0:2421:G:H4'	38:0:4795:HOH:O	1.92	0.69
30:0:2541:U:H3'	38:0:9415:HOH:O	1.93	0.69
30:0:2717:C:O2'	30:0:2718:C:H5''	1.91	0.69
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.74	0.69
9:I:108:HIS:H	9:I:109:PRO:HD2	1.56	0.69
30:0:282:C:H1'	30:0:368:C:H42	1.58	0.69
30:0:292:G:H2'	30:0:358:G:N2	2.08	0.69
1:A:199:HIS:CD2	1:A:201:PHE:H	2.09	0.69
2:B:238:ASN:HD22	2:B:240:GLY:N	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2533:C:H5'	30:0:2533:C:H6	1.57	0.69
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.07	0.68
30:0:1505:U:H1'	38:0:7611:HOH:O	1.92	0.68
3:C:1:MET:HG2	3:C:2:GLN:H	1.59	0.68
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.90	0.68
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.75	0.68
30:0:2524:G:H21	30:0:2526:C:N4	1.90	0.68
31:9:13:A:O2'	31:9:14:G:H5''	1.92	0.68
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.94	0.68
30:0:2102:G:H2'	38:0:7788:HOH:O	1.93	0.68
30:0:558:C:C2'	30:0:559:U:C5'	2.72	0.68
8:H:168:VAL:HG13	38:H:214:HOH:O	1.93	0.68
14:N:7:LYS:HE3	17:Q:21:ARG:O	1.92	0.68
28:2:28:LYS:O	30:0:87:C:H2'	1.93	0.68
30:0:2896:A:N3	30:0:2896:A:H2'	2.08	0.68
30:0:1118:A:C8	30:0:1118:A:C3'	2.73	0.67
30:0:2420:G:O2'	30:0:2421:G:H5'	1.94	0.67
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.76	0.67
30:0:2291:A:C8	30:0:2309:C:H5'	2.29	0.67
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.75	0.67
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.59	0.67
1:A:51:ARG:HB2	38:A:9069:HOH:O	1.94	0.67
14:N:160:SER:HB3	31:9:51:A:H5'	1.77	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.27	0.67
6:F:96:ALA:HA	38:F:3111:HOH:O	1.94	0.67
30:0:1377:C:H5'	30:0:1377:C:C6	2.29	0.67
30:0:2661:U:H3	30:0:2812:A:H62	1.42	0.67
30:0:2505:G:C2'	30:0:2506:A:H5'	2.25	0.67
30:0:2878:U:H2'	30:0:2879:A:O4'	1.94	0.67
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.29	0.67
12:L:18:HIS:HD2	30:0:902:G:N7	1.93	0.67
12:L:136:ALA:HB3	38:L:8867:HOH:O	1.95	0.67
14:N:160:SER:CB	31:9:51:A:H5'	2.25	0.67
28:2:49:GLU:HB2	38:2:131:HOH:O	1.93	0.67
30:0:1641:A:H2'	30:0:1642:A:H5'	1.77	0.67
30:0:1878:G:HO2'	30:0:1879:U:H6	1.39	0.67
10:J:131:THR:HG22	10:J:134:GLU:H	1.61	0.66
14:N:37:ARG:NH1	31:9:6:C:C5'	2.53	0.66
18:R:150:PRO:CG	18:R:150:PRO:O	2.42	0.66
25:Y:200:THR:HG22	25:Y:201:GLU:HG3	1.77	0.66
30:0:182:G:H5'	38:0:5177:HOH:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1603:A:H5''	30:0:1605:G:H5'	1.77	0.66
30:0:2004:U:O2	30:0:2004:U:C2'	2.43	0.66
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.77	0.66
2:B:162:MET:HE3	2:B:310:ARG:HD3	1.77	0.66
27:1:16:HIS:HD2	30:0:470:U:O2'	1.78	0.66
30:0:541:C:H2'	30:0:542:A:H5''	1.78	0.66
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.78	0.66
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.33	0.66
30:0:1730:G:C5'	30:0:1731:C:C6	2.79	0.66
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.77	0.65
23:W:26:ILE:HB	38:W:5420:HOH:O	1.96	0.65
30:0:2426:G:H1'	38:0:6120:HOH:O	1.95	0.65
30:0:256:C:H2'	30:0:257:G:O4'	1.96	0.65
2:B:211:THR:HG21	38:0:7480:HOH:O	1.96	0.65
30:0:545:G:H5'	30:0:545:G:C8	2.30	0.65
30:0:1119:G:N2	30:0:1246:A:H2	1.94	0.65
30:0:1187:U:H5''	38:0:6214:HOH:O	1.96	0.65
30:0:299:U:H5'	38:0:7361:HOH:O	1.96	0.65
30:0:567:U:H5''	38:0:6432:HOH:O	1.96	0.65
30:0:2032:U:H2'	30:0:2033:G:C5'	2.26	0.65
10:J:19:MET:HE1	10:J:78:ILE:HG22	1.79	0.65
24:X:61:ARG:HH11	24:X:65:ASN:HB3	1.62	0.65
30:0:2524:G:H21	30:0:2526:C:H5	1.44	0.65
2:B:51:VAL:CG1	2:B:53:LEU:HD13	2.26	0.65
12:L:140:VAL:HB	38:L:8851:HOH:O	1.96	0.65
15:O:32:ARG:HH21	15:O:35:LYS:NZ	1.94	0.65
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.89	0.65
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.80	0.64
30:0:125:U:H2'	38:0:3780:HOH:O	1.97	0.64
31:9:24:U:H3'	31:9:25:G:H5'	1.79	0.64
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.78	0.64
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.97	0.64
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.79	0.64
3:C:174:ILE:CD1	30:0:338:C:H4'	2.28	0.64
17:Q:25:PRO:HB2	38:9:9078:HOH:O	1.98	0.64
30:0:1166:A:H1'	30:0:1192:A:C2	2.31	0.64
30:0:1166:A:H1'	30:0:1192:A:N3	2.13	0.64
30:0:1187:U:H1'	30:0:1189:A:H2	1.62	0.64
30:0:196:G:H2'	38:0:6681:HOH:O	1.98	0.64
30:0:271:C:H41	30:0:378:A:H2	1.46	0.64
30:0:1451:C:H5'	30:0:1505:U:C5	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:76:ASP:HA	38:J:5907:HOH:O	1.97	0.64
30:0:1187:U:HO2'	30:0:1188:A:H8	1.44	0.64
30:0:2539:U:H3'	38:0:9174:HOH:O	1.96	0.64
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.78	0.64
20:T:9:LYS:HD3	38:0:3770:HOH:O	1.97	0.64
24:X:61:ARG:NH1	24:X:65:ASN:HB3	2.12	0.64
27:1:10:LYS:HG3	38:1:2979:HOH:O	1.98	0.64
8:H:59:GLN:HE22	8:H:96:GLN:HG2	1.62	0.64
30:0:541:C:H2'	30:0:542:A:H5'	1.78	0.64
30:0:380:A:H2'	38:0:7253:HOH:O	1.97	0.63
3:C:2:GLN:HB3	38:C:8580:HOH:O	1.97	0.63
18:R:98:ASN:HD21	30:0:500:G:H21	1.46	0.63
23:W:80:ASP:O	23:W:84:VAL:HG23	1.97	0.63
31:9:54:A:H2	38:9:9062:HOH:O	1.80	0.63
6:F:91:VAL:HG12	6:F:92:GLY:N	2.13	0.63
2:B:179:LEU:O	2:B:183:GLU:HG2	1.99	0.63
27:1:20:ARG:HG2	30:0:111:C:O2'	1.98	0.63
30:0:1187:U:O2'	30:0:1188:A:H8	1.80	0.63
30:0:1666:C:C2'	30:0:1667:A:C5'	2.77	0.63
30:0:283:U:H5	30:0:284:C:N3	1.97	0.63
30:0:1919:A:H4'	38:0:4866:HOH:O	1.98	0.63
18:R:117:HIS:HD2	30:0:20:G:H21	1.46	0.63
24:X:25:ARG:HD2	38:X:5356:HOH:O	1.98	0.63
30:0:1207:A:H8	30:0:1207:A:OP2	1.81	0.63
30:0:1878:G:O2'	30:0:1879:U:H6	1.82	0.63
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.99	0.63
16:P:115:SER:H	16:P:118:GLN:NE2	1.90	0.63
30:0:2670:G:O2'	30:0:2671:U:H5'	1.99	0.63
30:0:2908:A:C2'	30:0:2909:G:H5'	2.29	0.63
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.81	0.62
30:0:441:A:H1'	30:0:442:A:N7	2.13	0.62
30:0:1835:U:C5	30:0:1840:A:N7	2.62	0.62
31:9:1:U:H5''	31:9:3:A:OP1	1.99	0.62
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.81	0.62
30:0:1681:G:H5''	30:0:1682:A:H5'	1.80	0.62
1:A:211:LYS:O	30:0:1943:C:H4'	1.99	0.62
25:Y:169:ARG:HD2	30:0:1328:A:OP1	2.00	0.62
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.29	0.62
30:0:2537:G:H3'	38:0:3125:HOH:O	1.98	0.62
7:G:12:ILE:HG23	38:0:5483:HOH:O	1.98	0.62
30:0:42:C:H1'	38:0:4687:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1359:U:C6	30:0:2537:G:N2	2.67	0.62
30:0:2112:A:H2'	30:0:2113:G:C8	2.33	0.62
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.82	0.62
2:B:214:PRO:HD2	38:B:8953:HOH:O	2.00	0.62
11:K:10:GLN:HE21	11:K:10:GLN:N	1.88	0.62
22:V:5:VAL:HG23	38:V:2271:HOH:O	1.99	0.62
4:D:57:THR:HG23	4:D:63:ILE:HA	1.80	0.62
15:O:3:THR:HG22	30:0:656:G:C5'	2.16	0.62
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.35	0.62
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.30	0.62
23:W:65:VAL:HA	23:W:68:THR:HG22	1.81	0.62
30:0:1205:U:H2'	30:0:1206:U:C5'	2.18	0.62
1:A:125:ASN:HB3	1:A:158:VAL:HG12	1.81	0.62
23:W:125:HIS:HD2	23:W:127:GLY:H	1.48	0.62
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.81	0.61
30:0:1167:G:H2'	30:0:1168:C:O4'	1.99	0.61
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.40	0.61
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.82	0.61
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.82	0.61
3:C:236:THR:HG22	3:C:239:ALA:N	2.05	0.61
18:R:99:ALA:CB	18:R:109:MET:HE1	2.23	0.61
30:0:1183:C:H5	30:0:1192:A:OP1	1.83	0.61
10:J:19:MET:HE2	10:J:79:PHE:HA	1.82	0.61
31:9:92:G:H2'	31:9:93:A:C8	2.35	0.61
4:D:103:ASN:ND2	4:D:134:LEU:H	1.98	0.61
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.98	0.61
30:0:2607:U:H4'	38:0:9446:HOH:O	1.99	0.61
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.31	0.61
30:0:1200:A:H3'	38:0:5785:HOH:O	2.00	0.61
30:0:2748:G:H8	38:0:7565:HOH:O	1.84	0.61
12:L:6:ARG:HD3	30:0:1299:G:O6	2.00	0.61
30:0:1973:A:H5'	30:0:1973:A:C8	2.33	0.61
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.65	0.61
5:E:68:HIS:O	5:E:72:MET:HG3	2.00	0.61
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.81	0.61
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.81	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.30	0.61
3:C:140:VAL:HB	38:C:8644:HOH:O	2.00	0.60
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.00	0.60
30:0:558:C:H2'	30:0:559:U:H5''	1.77	0.60
30:0:1187:U:O2'	30:0:1188:A:C8	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:95:GLU:HA	30:0:949:U:H4'	1.82	0.60
1:A:3:ARG:HD3	30:0:870:G:OP2	2.01	0.60
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.15	0.60
30:0:204:A:C2'	30:0:205:U:H5'	2.31	0.60
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.60
14:N:80:SER:HB2	38:N:8834:HOH:O	2.01	0.60
31:9:54:A:O2'	31:9:55:U:H5'	2.01	0.60
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.83	0.60
13:M:164:THR:HG22	13:M:166:ALA:H	1.66	0.60
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.83	0.60
30:0:1189:A:H1'	30:0:1209:C:C1'	2.31	0.60
30:0:1679:C:H5'	38:0:9330:HOH:O	2.02	0.60
2:B:254:GLN:HG2	2:B:255:GLY:N	2.16	0.60
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.67	0.60
13:M:83:SER:HB3	38:0:4395:HOH:O	2.01	0.60
23:W:21:LEU:CD2	23:W:48:VAL:HG11	2.29	0.60
4:D:25:MET:SD	4:D:40:ILE:HD11	2.42	0.60
13:M:82:ARG:HD2	38:0:9124:HOH:O	2.01	0.60
25:Y:141:THR:HG23	38:Y:8888:HOH:O	2.00	0.60
30:0:254:C:O2	30:0:254:C:H2'	2.01	0.60
30:0:1342:C:C2'	30:0:1343:C:H5'	2.32	0.60
12:L:104:ASP:HB2	38:L:8857:HOH:O	2.00	0.60
30:0:1189:A:O2'	30:0:1208:C:H2'	2.02	0.60
2:B:145:HIS:HD2	2:B:146:THR:O	1.85	0.60
30:0:1476:A:N7	38:0:5190:HOH:O	2.32	0.60
30:0:1528:A:H2'	30:0:1529:G:O4'	2.02	0.60
30:0:1667:A:H5'	30:0:1667:A:C8	2.33	0.60
30:0:1766:U:O2	30:0:1778:A:H5'	2.02	0.60
15:O:32:ARG:O	15:O:32:ARG:HD3	2.02	0.59
23:W:125:HIS:CD2	23:W:127:GLY:H	2.20	0.59
30:0:2769:C:H2'	30:0:2770:G:C5'	2.32	0.59
14:N:179:LEU:HA	14:N:184:ILE:HD12	1.84	0.59
30:0:1632:A:C3'	30:0:1633:C:H5'	2.33	0.59
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.84	0.59
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.84	0.59
14:N:11:ARG:HD3	31:9:114:G:O6	2.02	0.59
30:0:2825:C:H4'	30:0:2826:G:O5'	2.02	0.59
12:L:30:ARG:HD3	30:0:164:G:H4'	1.85	0.59
38:Z:8718:HOH:O	30:0:819:A:H5''	2.01	0.59
30:0:1116:U:O2'	30:0:1118:A:C2	2.47	0.59
30:0:1342:C:O2'	30:0:1343:C:H5'	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2073:G:OP2	30:0:2490:A:H5'	2.03	0.59
16:P:81:LYS:HG2	38:0:9547:HOH:O	2.02	0.59
20:T:112:LEU:HD23	20:T:119:ALA:HB3	1.84	0.59
30:0:2626:C:H2'	30:0:2627:G:C8	2.38	0.59
11:K:32:ILE:HD11	11:K:56:SER:HB2	1.84	0.59
17:Q:45:PRO:O	30:0:2365:G:H4'	2.03	0.59
28:2:10:ARG:NH2	30:0:121:U:OP2	2.32	0.59
30:0:2239:C:H2'	30:0:2240:U:H6	1.67	0.59
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.85	0.59
3:C:214:THR:HB	38:0:9688:HOH:O	2.02	0.59
4:D:57:THR:HA	38:D:5728:HOH:O	2.01	0.59
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.84	0.59
30:0:407:A:H3'	38:0:4474:HOH:O	2.03	0.59
30:0:1278:A:H4'	30:0:1279:U:C4	2.37	0.59
20:T:26:THR:HA	20:T:39:ASN:HB3	1.85	0.59
30:0:291:C:H2'	30:0:292:G:O4'	2.03	0.59
30:0:960:G:N3	30:0:960:G:C3'	2.66	0.59
30:0:1862:C:H1'	38:0:7245:HOH:O	2.01	0.59
3:C:174:ILE:HD11	30:0:338:C:H4'	1.85	0.59
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.85	0.59
30:0:834:G:H4'	30:0:835:U:OP2	2.03	0.59
30:0:2239:C:H2'	30:0:2240:U:C6	2.38	0.59
10:J:93:ARG:HB3	10:J:93:ARG:HH11	1.68	0.59
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.68	0.59
30:0:603:A:H4'	30:0:604:G:O5'	2.03	0.59
30:0:1182:C:H1'	30:0:1192:A:C8	2.38	0.59
30:0:1819:G:H2'	30:0:1820:G:H4'	1.85	0.59
30:0:2372:A:H2'	30:0:2373:U:C6	2.38	0.59
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.84	0.58
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.84	0.58
30:0:1218:U:H2'	30:0:1219:U:C6	2.38	0.58
30:0:2102:G:H21	30:0:2103:A:C2'	1.91	0.58
30:0:2894:C:O2'	30:0:2895:C:H5'	2.02	0.58
30:0:396:U:O2'	30:0:418:C:H4'	2.03	0.58
30:0:1118:A:H8	30:0:1119:G:H5''	1.68	0.58
30:0:2089:A:O2'	30:0:2090:G:H5'	2.03	0.58
30:0:1165:G:N2	30:0:1173:A:C5'	2.67	0.58
2:B:16:ARG:NH1	38:B:9042:HOH:O	2.35	0.58
30:0:200:C:H2'	38:0:3459:HOH:O	2.03	0.58
30:0:2453:G:H5''	38:0:4736:HOH:O	2.04	0.58
3:C:202:THR:HG22	30:0:328:U:O4'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.85	0.58
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.19	0.58
12:L:39:GLU:OE2	30:0:926:A:H5'	2.02	0.58
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.01	0.58
14:N:162:ASP:HA	38:N:8831:HOH:O	2.03	0.58
20:T:1:SER:HB2	30:0:447:A:P	2.44	0.58
30:0:541:C:C2'	30:0:542:A:C5'	2.80	0.58
30:0:999:C:C2'	30:0:1000:C:H5'	2.34	0.58
2:B:298:LYS:HG2	38:0:5545:HOH:O	2.04	0.58
30:0:1595:G:O2'	30:0:1596:U:H5'	2.04	0.58
30:0:2541:U:C6	30:0:2541:U:C5'	2.82	0.58
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.19	0.57
2:B:17:LYS:O	2:B:260:HIS:HD2	1.87	0.57
30:0:12:U:H2'	30:0:13:G:H5'	1.86	0.57
30:0:1730:G:C5'	30:0:1731:C:C5	2.86	0.57
4:D:103:ASN:HD22	4:D:134:LEU:H	1.50	0.57
22:V:55:ARG:O	22:V:59:ILE:HG12	2.05	0.57
30:0:130:C:H5'	38:0:5234:HOH:O	2.02	0.57
30:0:2102:G:H1'	30:0:2103:A:H8	1.65	0.57
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.39	0.57
16:P:55:LYS:HG2	16:P:56:GLY:N	2.19	0.57
20:T:1:SER:HB2	30:0:447:A:OP2	2.05	0.57
23:W:44:MET:CE	30:0:944:G:H21	2.16	0.57
28:2:36:ASN:HB3	28:2:39:ARG:HG3	1.86	0.57
30:0:951:A:C2'	30:0:952:G:H5'	2.34	0.57
30:0:1667:A:H2'	30:0:1668:U:H6	1.70	0.57
30:0:2032:U:H2'	30:0:2033:G:H5'	1.86	0.57
19:S:57:THR:HG22	19:S:58:MET:N	2.20	0.57
30:0:2320:U:H4'	30:0:2321:A:O4'	2.05	0.57
2:B:162:MET:CE	2:B:310:ARG:HD3	2.33	0.57
15:O:32:ARG:NE	15:O:35:LYS:HD2	2.16	0.57
22:V:1:THR:CB	30:0:93:C:H5''	2.28	0.57
30:0:1044:C:H3'	30:0:1045:G:H5''	1.86	0.57
30:0:1355:A:H2'	38:0:4139:HOH:O	2.05	0.57
31:9:2:U:OP2	31:9:3:A:H5'	2.05	0.57
11:K:29:LEU:HB3	11:K:55:VAL:HG21	1.85	0.57
30:0:59:A:H5'	38:0:4347:HOH:O	2.05	0.57
30:0:2717:C:H2'	30:0:2718:C:C5'	2.30	0.57
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.39	0.57
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.87	0.57
30:0:1878:G:H4'	38:0:4133:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:58:VAL:HG12	4:D:60:GLU:HG2	1.87	0.57
10:J:63:ILE:HD11	30:0:1236:A:C8	2.40	0.57
30:0:1201:C:H2'	30:0:1202:A:H5'	1.86	0.57
30:0:2541:U:H6	30:0:2541:U:C5'	2.11	0.57
30:0:2827:A:H2'	30:0:2828:G:O4'	2.05	0.57
31:9:24:U:H3'	31:9:25:G:C5'	2.35	0.57
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.40	0.56
3:C:236:THR:HG21	38:C:8570:HOH:O	2.04	0.56
30:0:1174:A:C5	30:0:1201:C:H4'	2.39	0.56
26:Z:34:SER:HB3	30:0:797:A:H4'	1.86	0.56
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.41	0.56
5:E:15:GLN:HG3	5:E:20:ILE:HG12	1.88	0.56
21:U:49:LEU:HG	38:U:3805:HOH:O	2.05	0.56
24:X:30:MET:HG2	30:0:1384:C:H5'	1.85	0.56
30:0:1165:G:N2	30:0:1173:A:H5''	2.17	0.56
30:0:2316:G:H4'	38:0:6120:HOH:O	2.05	0.56
30:0:2361:A:H2'	30:0:2362:A:C8	2.40	0.56
30:0:2866:U:H4'	30:0:2867:G:H5'	1.87	0.56
30:0:2912:C:H3'	38:0:6403:HOH:O	2.03	0.56
29:3:61:PRO:HG2	38:0:7581:HOH:O	2.04	0.56
29:3:73:GLU:HB3	38:3:9055:HOH:O	2.04	0.56
30:0:1474:C:H5'	30:0:1474:C:C6	2.34	0.56
30:0:1838:U:O2'	30:0:2644:C:H5'	2.05	0.56
18:R:9:ASP:O	18:R:13:THR:HG22	2.06	0.56
38:Z:8706:HOH:O	30:0:1886:A:H4'	2.05	0.56
29:3:70:ARG:HG2	38:3:9067:HOH:O	2.05	0.56
30:0:432:G:O2'	30:0:433:C:H5'	2.06	0.56
30:0:2697:A:H2'	30:0:2698:G:O4'	2.06	0.56
30:0:2851:G:O2'	30:0:2852:A:H5'	2.04	0.56
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.21	0.56
30:0:1921:A:C6	30:0:1922:A:C2	2.93	0.56
30:0:2032:U:O2'	30:0:2033:G:H5''	2.05	0.56
30:0:2712:G:H5'	38:0:5242:HOH:O	2.03	0.56
31:9:1:U:O3'	31:9:3:A:H5''	2.05	0.56
30:0:349:U:O2'	30:0:350:G:H5'	2.06	0.56
30:0:1527:A:H1'	30:0:1528:A:C8	2.41	0.56
30:0:1667:A:H2'	30:0:1668:U:C6	2.41	0.56
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.70	0.56
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.87	0.56
14:N:4:PRO:HG3	31:9:69:U:OP1	2.06	0.56
30:0:1819:G:H5'	38:0:4724:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2524:G:N2	30:0:2526:C:H5	2.04	0.56
5:E:3:VAL:CG2	5:E:49:ILE:HB	2.35	0.56
10:J:82:THR:HG23	30:0:1242:A:C5'	2.25	0.56
24:X:22:ASN:ND2	30:0:2726:U:O2'	2.39	0.56
30:0:204:A:H2'	30:0:205:U:H5'	1.86	0.56
30:0:1166:A:P	30:0:1174:A:H4'	2.46	0.56
3:C:115:LEU:O	3:C:118:THR:HB	2.06	0.56
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.88	0.56
18:R:150:PRO:CG	18:R:150:PRO:CB	2.82	0.56
30:0:602:A:O2'	30:0:605:C:H4'	2.05	0.56
3:C:214:THR:HG23	38:C:8628:HOH:O	2.05	0.55
30:0:2100:A:C8	30:0:2538:A:C2	2.94	0.55
1:A:211:LYS:CG	1:A:212:PRO:HD2	2.32	0.55
30:0:2645:U:O2'	30:0:2646:G:P	2.65	0.55
31:9:76:G:C3'	31:9:77:A:H5''	2.27	0.55
30:0:1477:C:H5'	30:0:1868:G:H5'	1.87	0.55
30:0:2101:A:O4'	30:0:2537:G:H1'	2.05	0.55
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.06	0.55
13:M:69:LYS:O	13:M:73:ARG:NH2	2.39	0.55
30:0:1279:U:O2	30:0:1279:U:C2'	2.53	0.55
30:0:1477:C:H5'	30:0:1868:G:C5'	2.36	0.55
30:0:1044:C:H5	38:0:6631:HOH:O	1.90	0.55
31:9:7:G:H5'	38:9:9096:HOH:O	2.06	0.55
31:9:52:A:O2'	31:9:53:G:H5'	2.06	0.55
5:E:143:GLN:NE2	30:0:2779:G:H21	2.05	0.55
13:M:76:ARG:HG3	13:M:88:VAL:HG21	1.89	0.55
6:F:118:LEU:O	6:F:119:ARG:HB3	2.07	0.55
12:L:143:THR:HG22	12:L:144:ASP:N	2.22	0.55
14:N:110:THR:HB	14:N:113:SER:OG	2.07	0.55
26:Z:51:ALA:HA	38:Z:8715:HOH:O	2.05	0.55
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.87	0.55
30:0:271:C:C2	30:0:273:G:O4'	2.60	0.55
30:0:1972:U:H2'	30:0:1973:A:C5'	2.36	0.55
30:0:2415:A:H2'	30:0:2416:G:H5'	1.87	0.55
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.89	0.55
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.71	0.55
9:I:101:LYS:O	9:I:105:GLU:HG3	2.07	0.55
30:0:1191:A:H2	30:0:1206:U:H3	1.55	0.55
30:0:1406:A:H4'	30:0:1407:A:H5''	1.87	0.55
31:9:3:A:H2'	38:9:9042:HOH:O	2.05	0.55
3:C:79:ARG:O	3:C:87:ARG:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:129:SER:HB3	30:0:1192:A:H61	1.72	0.55
10:J:70:PHE:HD1	30:0:2676:C:H4'	1.71	0.55
13:M:9:ARG:HD2	30:0:380:A:OP2	2.07	0.55
14:N:37:ARG:NH1	31:9:6:C:OP1	2.37	0.55
30:0:999:C:O2'	30:0:1000:C:H5'	2.07	0.55
30:0:1946:C:H2'	30:0:1971:G:C8	2.41	0.55
3:C:184:ARG:NH2	30:0:450:C:OP1	2.34	0.55
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.71	0.55
30:0:2718:C:H5'	30:0:2718:C:C6	2.40	0.55
30:0:2908:A:H2'	30:0:2909:G:C4'	2.37	0.55
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.70	0.54
25:Y:133:HIS:HD2	38:Y:8882:HOH:O	1.90	0.54
26:Z:40:ALA:HA	30:0:1773:G:C8	2.41	0.54
27:1:16:HIS:HE1	30:0:775:G:OP1	1.90	0.54
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.90	0.54
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.35	0.54
11:K:81:ARG:HD3	11:K:87:ARG:CZ	2.37	0.54
30:0:271:C:H4'	30:0:272:A:OP1	2.08	0.54
30:0:2323:G:H5''	38:0:4795:HOH:O	2.05	0.54
31:9:42:C:H5'	31:9:43:G:OP2	2.07	0.54
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.36	0.54
2:B:297:VAL:HB	38:B:9030:HOH:O	2.08	0.54
15:O:37:ARG:HD2	30:0:656:G:OP2	2.08	0.54
30:0:1118:A:C8	30:0:1119:G:H5''	2.42	0.54
30:0:1730:G:H5'	30:0:1731:C:H5	1.70	0.54
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.88	0.54
30:0:2769:C:H2'	30:0:2770:G:H5'	1.89	0.54
30:0:249:G:O2'	30:0:250:C:H5'	2.08	0.54
30:0:482:G:H4'	30:0:508:A:N1	2.22	0.54
30:0:541:C:O2'	30:0:542:A:H5''	2.07	0.54
30:0:952:G:N3	30:0:2302:A:H2'	2.22	0.54
30:0:1183:C:H42	30:0:1184:C:H41	1.51	0.54
30:0:1350:U:H4'	38:0:5141:HOH:O	2.06	0.54
30:0:2681:A:H4'	30:0:2682:C:H5'	1.90	0.54
31:9:52:A:H2'	31:9:53:G:O4'	2.06	0.54
23:W:21:LEU:O	23:W:26:ILE:HG23	2.08	0.54
30:0:2032:U:C2'	30:0:2033:G:H5''	2.38	0.54
14:N:37:ARG:NE	38:N:8832:HOH:O	2.36	0.54
15:O:24:ALA:HB3	30:0:710:G:OP1	2.07	0.54
20:T:49:GLU:HB3	20:T:59:GLU:HG2	1.90	0.54
23:W:48:VAL:O	23:W:48:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1175:G:H1'	30:0:1193:A:C2'	2.34	0.54
3:C:43:LYS:HG2	30:0:449:A:N7	2.23	0.54
13:M:80:GLY:O	13:M:81:ARG:HD2	2.08	0.54
23:W:130:HIS:O	23:W:136:GLY:HA3	2.08	0.54
30:0:1206:U:H2'	30:0:1207:A:O4'	2.06	0.54
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.38	0.54
30:0:1878:G:C1'	38:0:6149:HOH:O	2.40	0.54
1:A:17:ARG:HD2	38:A:9013:HOH:O	2.08	0.53
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.89	0.53
4:D:135:VAL:HG22	4:D:136:ARG:H	1.73	0.53
8:H:30:LYS:N	8:H:62:HIS:HD2	2.02	0.53
13:M:59:GLY:HA3	13:M:141:ILE:HD12	1.89	0.53
22:V:64:GLY:O	22:V:65:ASP:HB2	2.06	0.53
23:W:38:THR:HB	38:W:5390:HOH:O	2.08	0.53
27:1:17:THR:HG21	30:0:120:A:C6	2.43	0.53
15:O:39:THR:O	15:O:115:ARG:NH2	2.41	0.53
25:Y:186:ARG:HG2	25:Y:186:ARG:HH11	1.72	0.53
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.08	0.53
30:0:2102:G:N3	30:0:2103:A:C8	2.75	0.53
2:B:125:GLU:O	2:B:129:ARG:HG3	2.08	0.53
4:D:169:THR:HG22	4:D:170:TYR:HD1	1.72	0.53
27:1:9:GLY:HA2	30:0:1687:C:O2	2.09	0.53
30:0:2104:C:O2	30:0:2485:A:N1	2.41	0.53
30:0:2506:A:O2'	30:0:2507:G:C8	2.42	0.53
30:0:2506:A:N6	30:0:2511:A:O2'	2.40	0.53
4:D:25:MET:HE1	4:D:37:ALA:HB1	1.89	0.53
30:0:368:C:H2'	30:0:369:G:H5'	1.91	0.53
30:0:2766:A:H5'	38:0:9572:HOH:O	2.06	0.53
31:9:39:U:C2'	31:9:40:C:OP1	2.56	0.53
38:B:9058:HOH:O	30:0:2818:A:H2	1.92	0.53
3:C:64:GLY:O	30:0:2100:A:H4'	2.08	0.53
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.90	0.53
14:N:29:SER:HB3	30:0:2415:A:O2'	2.08	0.53
30:0:307:G:H3'	38:0:6710:HOH:O	2.06	0.53
8:H:66:GLU:HA	38:H:234:HOH:O	2.09	0.53
20:T:19:ARG:HD3	20:T:67:LEU:O	2.09	0.53
23:W:38:THR:HG22	23:W:39:ASP:N	2.23	0.53
30:0:821:U:H2'	30:0:822:C:H6	1.73	0.53
30:0:1741:U:O2'	30:0:2723:G:H4'	2.09	0.53
13:M:178:LYS:HB2	38:0:6901:HOH:O	2.08	0.53
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2591:C:H2'	30:0:2592:G:O4'	2.09	0.53
30:0:2795:C:O2'	30:0:2796:U:H5'	2.09	0.53
1:A:210:GLY:N	38:A:9052:HOH:O	2.40	0.53
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.23	0.53
24:X:23:HIS:CD2	24:X:24:LYS:HG3	2.44	0.53
30:0:151:A:H2'	30:0:152:A:O4'	2.09	0.53
30:0:347:A:H2'	30:0:348:C:O4'	2.08	0.53
30:0:407:A:H5'	38:0:6054:HOH:O	2.09	0.53
30:0:2112:A:H2'	30:0:2113:G:H8	1.72	0.53
30:0:2505:G:H2'	30:0:2506:A:H5'	1.91	0.53
30:0:2735:U:H2'	30:0:2736:U:C6	2.44	0.53
12:L:41:HIS:HD2	30:0:926:A:O2'	1.91	0.52
28:2:20:ARG:HG3	28:2:39:ARG:NH2	2.23	0.52
30:0:644:G:H5'	30:0:644:G:N3	2.24	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.91	0.52
30:0:2379:G:N7	30:0:2408:A:N1	2.57	0.52
12:L:133:VAL:HA	38:L:8867:HOH:O	2.10	0.52
23:W:119:HIS:HE1	38:0:9563:HOH:O	1.91	0.52
25:Y:204:ARG:HH22	30:0:553:G:P	2.32	0.52
30:0:2515:C:C2'	30:0:2516:G:H5'	2.39	0.52
30:0:2563:U:H2'	30:0:2565:C:O5'	2.09	0.52
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.08	0.52
11:K:41:LYS:HE3	38:0:6239:HOH:O	2.08	0.52
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.91	0.52
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.52
30:0:559:U:H6	30:0:559:U:C5'	2.19	0.52
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.07	0.52
30:0:136:C:H2'	30:0:137:U:O4'	2.10	0.52
30:0:485:A:N3	30:0:487:G:H5''	2.24	0.52
30:0:920:C:H4'	30:0:921:G:C2	2.45	0.52
1:A:192:VAL:HB	38:0:5683:HOH:O	2.09	0.52
2:B:53:LEU:HD11	2:B:327:VAL:HG22	1.92	0.52
4:D:50:VAL:HG13	31:9:41:C:O4'	2.10	0.52
7:G:64:ASN:HD22	7:G:64:ASN:N	2.08	0.52
14:N:4:PRO:HD2	38:0:6797:HOH:O	2.09	0.52
30:0:958:G:O2'	30:0:959:C:H5'	2.10	0.52
30:0:2346:C:H6	30:0:2346:C:O5'	1.92	0.52
2:B:229:ARG:HD2	38:0:9115:HOH:O	2.09	0.52
10:J:52:GLN:NE2	30:0:1119:G:H8	2.07	0.52
11:K:29:LEU:HB3	11:K:55:VAL:CG2	2.40	0.52
12:L:41:HIS:CD2	30:0:926:A:O2'	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:132:ASN:O	14:N:135:VAL:HG12	2.10	0.52
30:0:137:U:H2'	30:0:139:C:C5	2.44	0.52
30:0:2820:A:H2'	30:0:2821:C:C6	2.44	0.52
31:9:92:G:H2'	31:9:93:A:H8	1.74	0.52
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.24	0.52
13:M:82:ARG:HB3	38:0:7854:HOH:O	2.09	0.52
14:N:11:ARG:NH1	31:9:8:G:O6	2.42	0.52
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.39	0.52
20:T:38:ARG:HH21	30:0:306:A:P	2.33	0.52
30:0:1878:G:O2'	30:0:1879:U:P	2.68	0.52
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.92	0.52
2:B:53:LEU:HD12	2:B:327:VAL:HA	1.90	0.52
2:B:268:ARG:NH2	2:B:325:PRO:HG3	2.23	0.52
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.90	0.52
30:0:95:A:H5''	30:0:97:G:O4'	2.10	0.52
30:0:1160:G:H5'	30:0:1161:A:C4'	2.40	0.52
30:0:2070:G:H2'	30:0:2072:G:OP1	2.10	0.52
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.73	0.52
29:3:84:ARG:NE	38:3:9045:HOH:O	2.43	0.52
30:0:1724:U:H4'	38:0:4582:HOH:O	2.09	0.52
30:0:1778:A:H2'	30:0:1779:A:H5'	1.92	0.52
30:0:2072:G:C6	30:0:2533:C:H1'	2.45	0.52
2:B:27:ASN:HD21	30:0:2807:U:P	2.32	0.52
2:B:178:ALA:O	2:B:182:VAL:HG23	2.10	0.52
26:Z:42:TYR:HA	30:0:1829:A:N6	2.25	0.52
30:0:255:A:H2'	30:0:256:C:C6	2.45	0.52
30:0:544:G:H2'	30:0:545:G:C5'	2.37	0.52
30:0:790:A:H1'	30:0:1710:A:H2'	1.92	0.52
30:0:2531:U:O2'	30:0:2532:A:H5'	2.10	0.52
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.55	0.51
23:W:151:GLU:O	23:W:154:ARG:HB2	2.10	0.51
30:0:1164:U:O2	30:0:1166:A:H4'	2.09	0.51
30:0:2252:A:C5	30:0:2253:G:H1'	2.43	0.51
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.46	0.51
13:M:69:LYS:HG3	13:M:127:LYS:HG3	1.91	0.51
25:Y:144:ARG:NE	38:Y:8913:HOH:O	2.43	0.51
27:1:25:LYS:HD2	28:2:49:GLU:N	2.21	0.51
29:3:91:GLN:O	29:3:92:GLU:HB2	2.10	0.51
30:0:343:C:O2'	30:0:344:C:H5'	2.09	0.51
30:0:389:G:H5''	38:0:6487:HOH:O	2.10	0.51
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.10	0.51
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.74	0.51
4:D:49:PRO:HB3	4:D:73:VAL:HG22	1.93	0.51
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.76	0.51
13:M:164:THR:HG22	13:M:165:GLY:N	2.24	0.51
21:U:37:GLU:HB3	38:U:408:HOH:O	2.09	0.51
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.45	0.51
30:0:564:G:H1'	38:0:6341:HOH:O	2.10	0.51
30:0:1209:C:H2'	30:0:1210:G:C8	2.41	0.51
30:0:2883:A:H2'	30:0:2884:G:O4'	2.10	0.51
31:9:20:G:O2'	31:9:21:G:H5'	2.10	0.51
30:0:542:A:H2'	30:0:543:G:O4'	2.11	0.51
30:0:661:G:C5	30:0:686:A:C2	2.99	0.51
1:A:206:ARG:H	1:A:206:ARG:HD3	1.75	0.51
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.17	0.51
3:C:87:ARG:NH2	30:0:894:A:N1	2.58	0.51
9:I:114:TYR:CE1	30:0:1186:C:H5''	2.45	0.51
24:X:43:VAL:HG12	24:X:44:ASP:N	2.25	0.51
25:Y:174:VAL:HG22	25:Y:177:LYS:HD2	1.92	0.51
30:0:856:G:C8	38:0:5452:HOH:O	2.54	0.51
30:0:1506:U:H6	30:0:1506:U:H5'	1.75	0.51
30:0:1909:A:N1	30:0:2128:G:H1'	2.25	0.51
12:L:90:ARG:NH2	12:L:121:ILE:HD11	2.25	0.51
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.58	0.51
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.73	0.51
30:0:2251:G:H2'	30:0:2252:A:C8	2.46	0.51
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.92	0.51
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.08	0.51
30:0:1067:A:H5'	38:0:4364:HOH:O	2.10	0.51
30:0:2510:C:H5'	30:0:2511:A:OP2	2.11	0.51
30:0:2908:A:H2'	30:0:2909:G:H5'	1.92	0.51
30:0:282:C:O2'	30:0:283:U:C5'	2.48	0.51
30:0:1947:G:N2	30:0:1966:U:C2	2.79	0.51
30:0:2414:A:H2'	30:0:2415:A:C8	2.46	0.51
2:B:294:TYR:HE2	38:B:9074:HOH:O	1.94	0.51
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.11	0.51
23:W:139:GLY:O	23:W:141:HIS:HD2	1.93	0.51
26:Z:35:SER:CB	26:Z:47:ARG:HB2	2.39	0.51
28:2:18:ASN:ND2	28:2:40:ARG:H	2.08	0.51
30:0:1218:U:H2'	30:0:1219:U:H6	1.75	0.51
3:C:153:VAL:O	3:C:157:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:31:ILE:HG23	38:H:234:HOH:O	2.11	0.51
16:P:1:THR:O	30:0:1396:C:H1'	2.10	0.51
22:V:39:ALA:N	22:V:40:PRO:HD2	2.26	0.51
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.46	0.51
30:0:101:C:H2'	30:0:102:A:C8	2.46	0.51
30:0:1182:C:H4'	30:0:1192:A:N7	2.26	0.51
31:9:108:C:H2'	31:9:109:G:C8	2.46	0.51
1:A:223:ARG:NH1	38:A:8987:HOH:O	2.44	0.50
10:J:39:VAL:HG21	10:J:107:ASN:ND2	2.25	0.50
30:0:440:C:H2'	30:0:441:A:C8	2.46	0.50
30:0:1196:C:H2'	30:0:1197:G:H5'	1.93	0.50
30:0:1739:G:H1'	30:0:2726:U:O4	2.11	0.50
3:C:93:LYS:O	3:C:98:ARG:NH2	2.44	0.50
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.76	0.50
30:0:1745:G:H22	30:0:2033:G:H5'	1.76	0.50
30:0:2515:C:H2'	30:0:2516:G:H5'	1.93	0.50
11:K:10:GLN:H	11:K:10:GLN:NE2	1.90	0.50
30:0:407:A:H2'	30:0:408:A:C8	2.47	0.50
30:0:441:A:H8	30:0:441:A:O5'	1.94	0.50
30:0:1948:G:H2'	30:0:1949:G:O4'	2.11	0.50
30:0:2908:A:H2'	30:0:2909:G:C5'	2.40	0.50
31:9:51:A:H8	31:9:51:A:OP2	1.94	0.50
5:E:145:ALA:HB1	5:E:168:ILE:CD1	2.41	0.50
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.12	0.50
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.98	0.50
30:0:522:U:O2'	30:0:1366:C:H5'	2.12	0.50
30:0:1060:C:H6	30:0:1060:C:H5'	1.76	0.50
30:0:2769:C:C2'	30:0:2770:G:C5'	2.87	0.50
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.12	0.50
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.69	0.50
14:N:160:SER:HB2	31:9:51:A:H5'	1.92	0.50
23:W:119:HIS:HD2	23:W:120:PRO:O	1.95	0.50
30:0:532:A:H3'	38:0:9472:HOH:O	2.11	0.50
30:0:1149:U:H5''	30:0:1151:G:O4'	2.11	0.50
30:0:2032:U:H2'	30:0:2033:G:H5''	1.91	0.50
30:0:2265:U:H2'	30:0:2266:A:C8	2.47	0.50
31:9:49:G:H2'	31:9:50:G:O4'	2.12	0.50
8:H:48:VAL:HA	8:H:170:ARG:O	2.12	0.50
16:P:73:HIS:HE1	30:0:1789:G:O6	1.95	0.50
30:0:612:U:H2'	30:0:613:C:C6	2.47	0.50
30:0:830:G:O2'	30:0:831:U:H5'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1314:U:H5''	30:0:1316:G:O4'	2.11	0.50
30:0:2756:U:O2	30:0:2896:A:H2	1.95	0.50
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.10	0.50
24:X:78:GLU:HB3	38:X:5564:HOH:O	2.12	0.50
25:Y:144:ARG:NH1	38:Y:8875:HOH:O	2.44	0.50
30:0:497:A:H5''	38:0:3610:HOH:O	2.11	0.50
30:0:585:C:H5''	38:0:4886:HOH:O	2.10	0.50
30:0:920:C:H5''	30:0:921:G:O5'	2.11	0.50
30:0:2252:A:H2'	30:0:2253:G:O4'	2.12	0.50
30:0:2587:OMU:HM23	30:0:2589:U:C6	2.47	0.50
31:9:49:G:O2'	31:9:50:G:H5'	2.12	0.50
2:B:321:PRO:HA	38:B:9081:HOH:O	2.11	0.50
5:E:20:ILE:HD11	5:E:40:VAL:CG1	2.41	0.50
12:L:145:LEU:O	12:L:148:GLU:HG3	2.12	0.50
27:1:1:THR:HA	38:0:9363:HOH:O	2.11	0.50
30:0:1131:G:C6	30:0:1230:A:C4	2.99	0.50
30:0:1193:A:C2	30:0:1194:A:N6	2.80	0.50
30:0:2649:A:H5'	30:0:2649:A:C8	2.47	0.50
30:0:2649:A:H5'	30:0:2649:A:H8	1.77	0.50
5:E:81:GLU:HG2	5:E:134:SER:CB	2.42	0.50
8:H:48:VAL:HG13	38:H:214:HOH:O	2.11	0.50
13:M:188:ARG:HD3	30:0:155:C:OP2	2.11	0.50
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.47	0.50
30:0:282:C:C2'	30:0:283:U:C5'	2.89	0.50
30:0:861:A:H4'	30:0:1697:G:H4'	1.94	0.50
13:M:75:ARG:HH11	30:0:1864:C:H5	1.58	0.49
30:0:69:A:H8	30:0:69:A:C5'	2.23	0.49
30:0:834:G:H3'	30:0:835:U:H4'	1.94	0.49
30:0:1422:U:H2'	30:0:1423:C:C6	2.47	0.49
10:J:19:MET:CE	10:J:132:LEU:HD11	2.35	0.49
12:L:143:THR:HG22	12:L:144:ASP:H	1.75	0.49
30:0:2032:U:C2'	30:0:2033:G:C5'	2.89	0.49
1:A:121:ALA:O	1:A:124:VAL:HG22	2.11	0.49
9:I:120:ALA:O	9:I:124:VAL:HG23	2.11	0.49
18:R:29:LYS:NZ	38:R:8943:HOH:O	2.46	0.49
25:Y:165:GLU:HB3	38:0:6729:HOH:O	2.12	0.49
30:0:603:A:H5''	30:0:604:G:OP1	2.11	0.49
30:0:1168:C:H5	38:0:7521:HOH:O	1.94	0.49
31:9:64:C:C2'	31:9:65:A:H5'	2.42	0.49
24:X:30:MET:HE1	24:X:58:ALA:CB	2.40	0.49
30:0:1044:C:H5''	38:0:9029:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1159:G:H1	30:0:1208:C:H42	1.58	0.49
30:0:1207:A:C8	30:0:1208:C:C5	3.00	0.49
31:9:105:A:H2'	31:9:106:U:H5'	1.94	0.49
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.45	0.49
2:B:280:VAL:HG13	2:B:333:GLU:O	2.12	0.49
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.94	0.49
11:K:66:ARG:HH22	30:0:1994:A:P	2.35	0.49
12:L:41:HIS:HE1	38:0:9778:HOH:O	1.95	0.49
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.37	0.49
28:2:42:TRP:HB3	30:0:1418:U:OP1	2.12	0.49
30:0:912:A:C4	30:0:1294:A:C2	3.01	0.49
30:0:1834:C:H2'	30:0:1840:A:N6	2.27	0.49
3:C:1:MET:HG2	3:C:2:GLN:N	2.25	0.49
25:Y:146:PRO:O	25:Y:154:ARG:HG3	2.13	0.49
27:1:28:HIS:HE1	30:0:776:A:OP1	1.95	0.49
28:2:41:HIS:HD2	28:2:44:ARG:H	1.60	0.49
30:0:1163:G:N2	30:0:1184:C:C4	2.81	0.49
2:B:36:PRO:HG3	2:B:169:GLY:H	1.76	0.49
3:C:77:ALA:O	3:C:78:ARG:HD3	2.12	0.49
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.43	0.49
13:M:59:GLY:HA3	13:M:141:ILE:CD1	2.42	0.49
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.12	0.49
30:0:1865:A:C2	38:0:3075:HOH:O	2.55	0.49
1:A:175:LYS:HG3	30:0:1847:A:OP1	2.13	0.49
5:E:101:GLU:HB3	5:E:117:THR:HA	1.94	0.49
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.48	0.49
14:N:41:LYS:HD3	38:9:9059:HOH:O	2.12	0.49
30:0:1562:C:N4	38:0:5891:HOH:O	2.45	0.49
30:0:1761:U:H2'	30:0:1762:C:C6	2.47	0.49
30:0:1909:A:H2'	30:0:1910:A:C8	2.47	0.49
2:B:87:TYR:HD1	38:B:9004:HOH:O	1.95	0.49
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.94	0.49
15:O:59:VAL:HG23	15:O:111:VAL:HG22	1.94	0.49
30:0:304:G:H1'	30:0:347:A:N6	2.27	0.49
30:0:426:G:H2'	30:0:427:C:O4'	2.12	0.49
30:0:1414:A:H2'	30:0:1415:G:O4'	2.12	0.49
30:0:2587:OMU:O5'	30:0:2587:OMU:H6	2.12	0.49
2:B:256:GLN:HG2	38:B:9080:HOH:O	2.11	0.49
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.95	0.49
11:K:66:ARG:HD2	30:0:1992:U:OP2	2.13	0.49
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:117:HIS:CD2	30:0:20:G:H21	2.30	0.49
27:1:20:ARG:HH21	30:0:120:A:H5'	1.77	0.49
29:3:60:LYS:HE2	30:0:2428:G:N7	2.27	0.49
30:0:1196:C:C2'	30:0:1197:G:H5'	2.42	0.49
30:0:1755:A:H2'	30:0:1756:G:O4'	2.13	0.49
2:B:41:PHE:HB3	2:B:190:MET:CE	2.43	0.48
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.04	0.48
12:L:6:ARG:NH2	38:L:8843:HOH:O	2.45	0.48
14:N:169:PRO:O	14:N:172:PHE:HB3	2.13	0.48
20:T:54:ASP:OD2	30:0:316:A:H5'	2.13	0.48
23:W:4:LEU:O	23:W:32:CYS:HA	2.13	0.48
27:1:28:HIS:CD2	27:1:31:LYS:H	2.31	0.48
30:0:696:C:O2'	30:0:697:G:H5'	2.13	0.48
30:0:1166:A:C6	30:0:1181:A:C2	3.01	0.48
30:0:1321:A:H2'	30:0:1322:G:C8	2.48	0.48
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.95	0.48
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.95	0.48
2:B:75:GLU:C	2:B:77:PRO:HD3	2.38	0.48
2:B:248:ARG:NH2	30:0:2549:C:H1'	2.28	0.48
2:B:258:GLY:H	2:B:260:HIS:CE1	2.30	0.48
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.94	0.48
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.13	0.48
30:0:2512:U:H4'	30:0:2514:U:O4	2.13	0.48
30:0:2637:A:C5'	38:0:4944:HOH:O	2.61	0.48
3:C:173:LYS:HE3	30:0:1311:G:O6	2.13	0.48
4:D:25:MET:HE2	4:D:41:LEU:HG	1.95	0.48
10:J:88:PRO:O	10:J:94:GLY:HA3	2.13	0.48
11:K:49:LEU:CD2	11:K:80:ILE:HD13	2.43	0.48
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.45	0.48
13:M:107:ARG:NH2	30:0:181:G:H4'	2.27	0.48
30:0:221:G:H5''	38:0:5772:HOH:O	2.13	0.48
30:0:635:A:H2'	30:0:636:G:H5''	1.95	0.48
30:0:820:G:O2'	30:0:856:G:H4'	2.13	0.48
14:N:147:ILE:HD12	38:9:9086:HOH:O	2.13	0.48
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.94	0.48
26:Z:55:SER:O	26:Z:59:GLU:HG3	2.14	0.48
30:0:120:A:H2'	30:0:120:A:N3	2.28	0.48
30:0:625:U:H5''	30:0:1044:C:N4	2.28	0.48
30:0:1185:U:H2'	30:0:1186:C:C6	2.48	0.48
10:J:52:GLN:HE22	30:0:1119:G:H8	1.62	0.48
10:J:75:PRO:HD3	10:J:136:SER:OG	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:50:GLY:C	30:0:2453:G:H4'	2.38	0.48
6:F:91:VAL:HG11	30:0:262:A:OP2	2.14	0.48
18:R:17:MET:HE1	18:R:19:ARG:NH2	2.28	0.48
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.43	0.48
30:0:856:G:H2'	38:0:5452:HOH:O	2.13	0.48
30:0:1205:U:C3'	30:0:1206:U:H5''	2.43	0.48
30:0:1205:U:H5	38:0:4455:HOH:O	1.97	0.48
30:0:1353:C:H6	30:0:1353:C:H5'	1.78	0.48
30:0:2134:G:C6	30:0:2258:A:C8	3.02	0.48
30:0:2506:A:H1'	38:0:3761:HOH:O	2.13	0.48
2:B:254:GLN:HG3	38:B:8960:HOH:O	2.13	0.48
2:B:305:ASP:O	2:B:306:LYS:HB2	2.14	0.48
30:0:316:A:N3	30:0:336:G:O2'	2.42	0.48
30:0:447:A:O2'	30:0:448:G:H5'	2.14	0.48
30:0:627:G:H2'	30:0:2071:C:C4	2.48	0.48
30:0:1298:U:H2'	30:0:1299:G:C8	2.48	0.48
30:0:1790:C:H2'	30:0:1791:U:C6	2.49	0.48
30:0:1972:U:C2'	30:0:1973:A:H5''	2.44	0.48
1:A:36:ASP:O	1:A:38:ILE:N	2.38	0.48
3:C:233:THR:HG22	3:C:234:VAL:N	2.28	0.48
4:D:25:MET:HE1	4:D:37:ALA:O	2.14	0.48
30:0:10:U:H3'	30:0:10:U:H6	1.79	0.48
30:0:152:A:O2'	30:0:153:C:H5'	2.13	0.48
30:0:1117:A:C2	30:0:1244:U:C2	3.01	0.48
30:0:1559:A:H4'	38:0:5891:HOH:O	2.13	0.48
30:0:1632:A:H2'	30:0:1633:C:C5'	2.38	0.48
30:0:1838:U:H1'	30:0:2644:C:H5'	1.96	0.48
30:0:1902:G:H2'	30:0:1903:U:O4'	2.14	0.48
30:0:2101:A:H1'	30:0:2537:G:O4'	2.14	0.48
6:F:111:ILE:O	6:F:115:VAL:HG23	2.14	0.48
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.48
25:Y:145:LYS:HE2	38:Y:8907:HOH:O	2.14	0.48
30:0:697:G:H4'	30:0:730:G:O3'	2.14	0.48
30:0:1081:A:H5''	38:0:3162:HOH:O	2.14	0.48
30:0:1194:A:C2	30:0:1206:U:H1'	2.48	0.48
30:0:1535:G:H2'	30:0:1536:C:C6	2.49	0.48
30:0:1555:G:H4'	30:0:1630:A:H2	1.79	0.48
30:0:2809:G:H2'	30:0:2810:G:O4'	2.14	0.48
1:A:33:GLU:H	1:A:33:GLU:CD	2.22	0.47
2:B:102:THR:HG21	2:B:182:VAL:O	2.14	0.47
3:C:246:ARG:NE	38:C:8616:HOH:O	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:30:ARG:HD2	38:0:9024:HOH:O	2.14	0.47
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.28	0.47
13:M:64:ARG:HD2	38:M:8887:HOH:O	2.15	0.47
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.43	0.47
23:W:41:TYR:HA	23:W:44:MET:HE3	1.95	0.47
23:W:154:ARG:NH1	30:0:588:G:O6	2.47	0.47
28:2:5:LYS:HD2	30:0:1675:C:H5''	1.96	0.47
30:0:821:U:H2'	30:0:822:C:C6	2.49	0.47
30:0:960:G:N3	30:0:960:G:C2'	2.76	0.47
30:0:1181:A:N1	30:0:1192:A:O2'	2.41	0.47
30:0:1333:U:H2'	30:0:1334:C:C6	2.49	0.47
30:0:2238:A:C2	30:0:2239:C:C6	3.02	0.47
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.14	0.47
12:L:73:VAL:HG23	12:L:74:THR:H	1.79	0.47
14:N:155:GLU:O	14:N:156:GLU:HG3	2.14	0.47
19:S:76:GLU:HB3	38:S:7263:HOH:O	2.13	0.47
30:0:23:G:C6	30:0:24:G:N1	2.83	0.47
1:A:237:GLY:HA3	30:0:1939:U:H5''	1.95	0.47
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.30	0.47
14:N:114:LYS:O	14:N:118:ILE:HG13	2.14	0.47
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.96	0.47
30:0:999:C:H2'	30:0:1000:C:H5'	1.95	0.47
3:C:242:GLU:HB2	38:C:8578:HOH:O	2.14	0.47
15:O:25:VAL:HG13	30:0:710:G:H5'	1.97	0.47
25:Y:155:ARG:NH1	38:Y:8857:HOH:O	2.47	0.47
25:Y:216:ARG:HD2	38:Y:8869:HOH:O	2.12	0.47
27:1:28:HIS:HD2	27:1:30:LYS:H	1.61	0.47
30:0:1132:A:N6	30:0:1229:C:H2'	2.30	0.47
30:0:1182:C:C1'	30:0:1192:A:C8	2.97	0.47
30:0:1656:A:H2'	30:0:1657:A:O4'	2.15	0.47
30:0:2001:G:O2'	30:0:2002:C:H5'	2.14	0.47
30:0:2102:G:H3'	38:0:3643:HOH:O	2.14	0.47
31:9:50:G:H2'	31:9:51:A:C8	2.48	0.47
7:G:23:ILE:O	7:G:27:ILE:HG13	2.14	0.47
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.96	0.47
17:Q:75:ILE:HD13	17:Q:84:ILE:HD11	1.95	0.47
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.48	0.47
30:0:1406:A:H4'	30:0:1407:A:C5'	2.45	0.47
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.97	0.47
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.80	0.47
3:C:127:ARG:HD3	3:C:129:HIS:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:THR:HG21	30:0:2346:C:O2'	2.14	0.47
17:Q:32:GLU:HA	17:Q:71:TYR:OH	2.15	0.47
20:T:79:LEU:HG	20:T:89:ARG:HB2	1.96	0.47
23:W:11:VAL:HG11	30:0:1086:A:C6	2.49	0.47
26:Z:46:SER:O	26:Z:50:VAL:HG23	2.14	0.47
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.45	0.47
30:0:538:C:H5''	30:0:539:G:C8	2.48	0.47
30:0:1165:G:N2	30:0:1173:A:H5'	2.30	0.47
30:0:1178:G:C6	30:0:1179:C:N4	2.83	0.47
30:0:1477:C:H2'	30:0:1478:U:C6	2.50	0.47
30:0:1925:G:O2'	30:0:1926:G:H5'	2.15	0.47
30:0:2502:C:H2'	30:0:2503:A:C5'	2.42	0.47
30:0:2616:G:N3	30:0:2616:G:H2'	2.28	0.47
31:9:65:A:N6	31:9:112:U:C6	2.82	0.47
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.45	0.47
10:J:39:VAL:HG22	10:J:107:ASN:HA	1.95	0.47
12:L:91:VAL:HG13	12:L:120:LEU:HD23	1.96	0.47
25:Y:148:GLY:HA3	30:0:622:G:P	2.55	0.47
28:2:38:LYS:HE3	38:0:4243:HOH:O	2.15	0.47
30:0:10:U:O4	30:0:532:A:OP2	2.32	0.47
30:0:561:G:O2'	30:0:562:A:H5'	2.15	0.47
30:0:999:C:H2'	30:0:1000:C:C5'	2.45	0.47
30:0:1181:A:H2'	30:0:1182:C:H5'	1.95	0.47
30:0:1193:A:H2	30:0:1194:A:N6	2.13	0.47
30:0:2456:A:H2'	30:0:2457:U:C6	2.50	0.47
30:0:2541:U:H5''	38:0:5423:HOH:O	2.14	0.47
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.40	0.47
10:J:107:ASN:HD22	10:J:109:TYR:H	1.63	0.47
30:0:280:C:O2'	30:0:281:U:H5'	2.15	0.47
30:0:1014:A:H5''	31:9:101:G:O2'	2.15	0.47
30:0:1252:A:H2'	30:0:1253:C:O4'	2.15	0.47
30:0:1985:U:C2	30:0:1996:U:O4'	2.68	0.47
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.15	0.47
9:I:114:TYR:HE1	30:0:1186:C:H5''	1.78	0.47
10:J:52:GLN:NE2	30:0:1119:G:H2'	2.30	0.47
30:0:1496:A:H2'	30:0:1497:G:O4'	2.15	0.47
30:0:2828:G:O2'	30:0:2829:G:H5'	2.14	0.47
31:9:95:C:O2'	31:9:96:C:H5'	2.15	0.47
1:A:36:ASP:C	1:A:38:ILE:H	2.21	0.46
5:E:84:MET:HE1	5:E:148:ILE:CD1	2.44	0.46
7:G:20:VAL:O	7:G:24:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:49:GLU:CB	20:T:59:GLU:HG2	2.46	0.46
27:1:25:LYS:CD	28:2:49:GLU:H	2.24	0.46
30:0:64:G:H2'	30:0:65:C:O4'	2.15	0.46
30:0:1163:G:N1	30:0:1184:C:N4	2.63	0.46
2:B:258:GLY:HA2	38:0:4025:HOH:O	2.15	0.46
8:H:30:LYS:H	8:H:62:HIS:CD2	2.17	0.46
10:J:45:VAL:CG2	10:J:129:PHE:HD1	2.29	0.46
14:N:37:ARG:HH11	31:9:6:C:P	2.37	0.46
16:P:16:VAL:HG12	16:P:17:GLY:N	2.30	0.46
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.28	0.46
30:0:1120:U:H5''	30:0:1120:U:C6	2.51	0.46
30:0:1160:G:H5''	30:0:1161:A:H5'	1.87	0.46
30:0:1735:C:O2'	30:0:1736:A:H5'	2.14	0.46
30:0:2247:C:H2'	30:0:2248:C:H6	1.81	0.46
31:9:60:C:O2'	31:9:61:C:H5'	2.15	0.46
2:B:282:GLY:O	30:0:2898:G:H1'	2.15	0.46
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.96	0.46
5:E:126:ILE:HB	5:E:131:LEU:HD23	1.97	0.46
10:J:45:VAL:CG2	10:J:129:PHE:CD1	2.98	0.46
13:M:77:HIS:HD2	13:M:79:ALA:O	1.98	0.46
30:0:1592:G:O2'	30:0:1593:C:O5'	2.34	0.46
13:M:68:ARG:NH2	13:M:73:ARG:HD3	2.30	0.46
16:P:40:VAL:O	16:P:44:VAL:HG23	2.16	0.46
30:0:690:G:H4'	30:0:741:C:O2	2.16	0.46
30:0:1120:U:H5'	30:0:1121:G:OP2	2.16	0.46
30:0:1164:U:C2	30:0:1166:A:H4'	2.50	0.46
30:0:1192:A:H3'	30:0:1193:A:H5'	1.98	0.46
30:0:1518:A:H2'	30:0:1519:U:C6	2.50	0.46
30:0:1942:A:H3'	38:0:7372:HOH:O	2.15	0.46
30:0:2241:C:O2'	30:0:2242:U:H5'	2.15	0.46
30:0:2372:A:H2'	30:0:2373:U:H6	1.80	0.46
30:0:2515:C:H2'	30:0:2516:G:C5'	2.46	0.46
1:A:71:PRO:HD2	1:A:74:VAL:HG21	1.98	0.46
1:A:211:LYS:HB3	38:0:7455:HOH:O	2.15	0.46
2:B:307:ARG:HD2	38:B:9077:HOH:O	2.15	0.46
6:F:37:THR:O	6:F:41:GLU:HG3	2.15	0.46
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.97	0.46
27:1:48:TYR:HE2	38:0:9317:HOH:O	1.99	0.46
30:0:255:A:C5	30:0:256:C:C4	3.03	0.46
30:0:703:G:O2'	30:0:704:C:H5'	2.16	0.46
30:0:2004:U:H5''	30:0:2005:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ASN:HA	2:B:244:PRO:C	2.39	0.46
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.45	0.46
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.97	0.46
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.84	0.46
30:0:1203:G:O2'	30:0:1204:C:H5'	2.16	0.46
30:0:2103:A:N6	30:0:2538:A:H8	1.97	0.46
30:0:2356:A:H5'	38:0:5662:HOH:O	2.15	0.46
30:0:2507:G:H2'	30:0:2510:C:N4	2.27	0.46
1:A:11:ARG:HD3	38:0:9224:HOH:O	2.15	0.46
2:B:148:PRO:HD2	38:B:9005:HOH:O	2.15	0.46
6:F:107:ASP:O	6:F:111:ILE:HG13	2.16	0.46
38:Q:2875:HOH:O	30:0:2392:C:H4'	2.15	0.46
30:0:816:G:C6	30:0:817:G:N1	2.84	0.46
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.98	0.46
10:J:80:LYS:HE2	10:J:98:PHE:CE1	2.51	0.46
12:L:32:ASP:HB3	30:0:222:A:H5''	1.97	0.46
18:R:3:SER:HB2	30:0:20:G:O3'	2.16	0.46
21:U:33:SER:O	21:U:37:GLU:HG3	2.15	0.46
30:0:1211:G:H2'	30:0:1212:C:H6	1.81	0.46
30:0:1819:G:H2'	30:0:1820:G:C4'	2.45	0.46
30:0:2072:G:H3'	30:0:2073:G:C5'	2.46	0.46
30:0:2351:C:H2'	30:0:2352:G:O4'	2.16	0.46
30:0:2587:OMU:CM2	30:0:2589:U:C6	2.99	0.46
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.98	0.46
1:A:105:VAL:HG11	1:A:154:ALA:CB	2.46	0.46
13:M:75:ARG:NH1	30:0:1864:C:H5	2.14	0.46
17:Q:67:GLN:NE2	30:0:2403:C:O2	2.47	0.46
30:0:1014:A:H2'	30:0:1015:C:H5'	1.97	0.46
30:0:1484:G:H3'	38:0:7841:HOH:O	2.16	0.46
30:0:1524:U:OP1	30:0:1524:U:H4'	2.16	0.46
30:0:1615:A:H4'	38:0:5912:HOH:O	2.16	0.46
30:0:1641:A:C2'	30:0:1642:A:H5'	2.45	0.46
30:0:1851:G:O2'	30:0:1852:A:H5'	2.16	0.46
30:0:1996:U:O2'	30:0:1997:A:H5'	2.16	0.46
31:9:22:G:H5'	31:9:23:U:OP1	2.16	0.46
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.78	0.46
10:J:107:ASN:HD22	10:J:107:ASN:C	2.24	0.46
12:L:97:VAL:HG12	12:L:98:GLU:O	2.16	0.46
13:M:79:ALA:HB3	13:M:81:ARG:NH1	2.31	0.46
13:M:82:ARG:HA	38:M:8836:HOH:O	2.16	0.46
30:0:407:A:H8	38:0:4474:HOH:O	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:830:G:H2'	30:0:831:U:C6	2.51	0.46
30:0:2839:C:H2'	30:0:2840:A:H5''	1.98	0.46
2:B:316:ARG:HB2	30:0:2768:A:C8	2.51	0.45
3:C:180:SER:HB2	38:C:8638:HOH:O	2.15	0.45
4:D:36:ASN:HB3	38:D:7502:HOH:O	2.15	0.45
4:D:76:ARG:CZ	31:9:44:A:H1'	2.46	0.45
30:0:666:A:H2'	30:0:667:C:O4'	2.16	0.45
30:0:2282:U:H4'	30:0:2309:C:C5	2.51	0.45
30:0:2421:G:H2'	38:0:4096:HOH:O	2.16	0.45
2:B:13:PHE:HB2	2:B:16:ARG:NH1	2.31	0.45
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.98	0.45
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.98	0.45
15:O:96:VAL:HG13	15:O:100:GLN:HB2	1.98	0.45
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.16	0.45
30:0:664:U:O4	30:0:681:G:H5''	2.16	0.45
30:0:2506:A:H2'	30:0:2506:A:O5'	2.16	0.45
30:0:2748:G:C8	30:0:2748:G:C5'	2.98	0.45
4:D:37:ALA:HA	38:D:5583:HOH:O	2.16	0.45
4:D:167:GLU:C	4:D:169:THR:H	2.24	0.45
5:E:1:PRO:HG2	5:E:59:MET:SD	2.57	0.45
5:E:126:ILE:HB	5:E:131:LEU:CD2	2.46	0.45
10:J:86:MET:HE2	30:0:1241:G:N3	2.31	0.45
11:K:114:ALA:HB3	11:K:117:VAL:HG23	1.97	0.45
15:O:32:ARG:HH21	15:O:35:LYS:HZ3	1.62	0.45
19:S:67:ARG:HD3	38:S:3430:HOH:O	2.17	0.45
29:3:42:ARG:NH1	30:0:396:U:H5'	2.31	0.45
30:0:560:U:C2	30:0:561:G:C8	3.04	0.45
30:0:1008:C:H2'	30:0:1009:U:C6	2.51	0.45
30:0:1185:U:H5'	38:0:7491:HOH:O	2.15	0.45
30:0:1948:G:H2'	30:0:1949:G:H8	1.80	0.45
30:0:2314:G:C2'	30:0:2315:C:H5'	2.47	0.45
30:0:2906:A:H5'	30:0:2907:C:O4'	2.17	0.45
3:C:150:THR:HA	3:C:203:ALA:O	2.17	0.45
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.15	0.45
9:I:129:SER:HB3	30:0:1192:A:N6	2.31	0.45
24:X:22:ASN:O	24:X:64:ALA:HA	2.17	0.45
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.51	0.45
27:1:28:HIS:HD2	27:1:31:LYS:H	1.64	0.45
30:0:24:G:N2	30:0:518:G:H1'	2.31	0.45
30:0:1021:G:O2'	30:0:1022:A:H5'	2.17	0.45
30:0:1335:C:H2'	30:0:1336:U:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1739:G:O2'	30:0:1740:U:H5'	2.16	0.45
30:0:2679:G:H2'	30:0:2681:A:OP2	2.17	0.45
31:9:59:C:H2'	31:9:60:C:C6	2.52	0.45
1:A:125:ASN:CB	1:A:158:VAL:HG12	2.44	0.45
30:0:806:A:H2'	30:0:807:A:O4'	2.16	0.45
30:0:1119:G:C5	30:0:1243:C:C4	3.04	0.45
30:0:1163:G:H2'	30:0:1164:U:C5	2.51	0.45
30:0:1236:A:H2'	30:0:1237:U:O4'	2.16	0.45
31:9:29:C:H2'	31:9:30:C:C5'	2.43	0.45
31:9:76:G:H3'	31:9:77:A:C5'	2.30	0.45
2:B:212:GLN:HA	30:0:1733:A:H4'	1.98	0.45
9:I:87:PRO:C	9:I:89:GLU:H	2.23	0.45
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.98	0.45
30:0:2502:C:O2'	30:0:2503:A:H5'	2.17	0.45
30:0:2831:C:H2'	30:0:2832:C:H5'	1.99	0.45
1:A:186:TRP:CG	1:A:187:PRO:HA	2.52	0.45
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.98	0.45
14:N:108:SER:HA	14:N:109:PRO:HD3	1.76	0.45
20:T:52:ARG:O	30:0:317:A:OP1	2.33	0.45
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.52	0.45
23:W:3:ALA:O	23:W:54:PHE:HA	2.16	0.45
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.52	0.45
30:0:95:A:O5'	30:0:97:G:H5'	2.17	0.45
30:0:407:A:O2'	30:0:408:A:H5'	2.17	0.45
30:0:969:G:H1	30:0:999:C:N4	2.15	0.45
30:0:1182:C:H1'	30:0:1192:A:H8	1.82	0.45
30:0:2238:A:O2'	30:0:2239:C:H5'	2.17	0.45
30:0:2493:C:O2	30:0:2493:C:H2'	2.16	0.45
30:0:2508:C:H2'	30:0:2509:A:O5'	2.17	0.45
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.97	0.45
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.37	0.45
9:I:108:HIS:N	9:I:109:PRO:HD2	2.29	0.45
13:M:164:THR:CG2	13:M:165:GLY:N	2.80	0.45
21:U:52:THR:HG22	21:U:55:ALA:H	1.81	0.45
30:0:1391:G:H2'	30:0:1392:A:H5'	1.99	0.45
30:0:1419:U:H2'	30:0:1685:A:C2	2.51	0.45
1:A:165:THR:HG22	38:A:9083:HOH:O	2.17	0.45
3:C:218:VAL:N	38:C:8616:HOH:O	2.48	0.45
3:C:236:THR:HA	38:C:8644:HOH:O	2.16	0.45
5:E:6:GLU:HA	5:E:46:THR:HG22	1.99	0.45
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:52:THR:CG2	21:U:54:THR:HB	2.47	0.45
30:0:1714:C:O2'	30:0:1715:C:H5'	2.17	0.45
30:0:2429:A:H2'	30:0:2430:A:C8	2.52	0.45
4:D:23:VAL:HG11	4:D:83:PHE:CZ	2.52	0.45
17:Q:49:ASN:HB2	38:Q:5227:HOH:O	2.17	0.45
30:0:195:C:H5''	38:0:5427:HOH:O	2.17	0.45
30:0:1759:A:N3	30:0:1818:C:H2'	2.32	0.45
30:0:2096:A:N7	30:0:2539:U:C4	2.84	0.45
30:0:2102:G:H1'	30:0:2103:A:N7	2.29	0.45
30:0:2509:A:OP2	30:0:2510:C:H5	2.00	0.45
2:B:235:ARG:HD3	30:0:2091:G:O3'	2.16	0.44
16:P:68:LYS:HE2	30:0:1787:C:OP1	2.17	0.44
30:0:368:C:C2'	30:0:369:G:H5'	2.46	0.44
30:0:1198:U:C6	30:0:1200:A:OP2	2.70	0.44
30:0:1588:G:C5	30:0:1589:G:C6	3.05	0.44
30:0:2775:A:C6	30:0:2799:A:C8	3.04	0.44
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.99	0.44
4:D:173:GLU:HA	38:D:6326:HOH:O	2.17	0.44
8:H:33:GLN:H	8:H:69:ARG:NH1	2.15	0.44
14:N:37:ARG:HD2	31:9:6:C:OP1	2.16	0.44
18:R:104:PHE:HB3	18:R:109:MET:HE2	1.99	0.44
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.99	0.44
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.17	0.44
30:0:638:C:H2'	30:0:639:A:C8	2.52	0.44
30:0:2038:A:O2'	30:0:2039:A:H5'	2.16	0.44
30:0:2072:G:P	38:0:3107:HOH:O	2.76	0.44
30:0:2425:A:H5'	30:0:2426:G:OP2	2.18	0.44
30:0:2819:C:H2'	30:0:2820:A:C8	2.53	0.44
31:9:105:A:C2'	31:9:106:U:H5'	2.46	0.44
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.98	0.44
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.99	0.44
30:0:286:U:H2'	30:0:287:C:C6	2.52	0.44
30:0:699:C:H2'	30:0:744:G:O4'	2.16	0.44
30:0:1334:C:O2'	30:0:1335:C:H5'	2.17	0.44
30:0:1592:G:O2'	30:0:1593:C:O4'	2.27	0.44
30:0:2064:U:H5'	30:0:2652:U:O3'	2.17	0.44
30:0:2506:A:O2'	30:0:2507:G:P	2.75	0.44
11:K:20:CYS:HB2	11:K:29:LEU:HG	2.00	0.44
14:N:171:HIS:CE1	38:N:8860:HOH:O	2.70	0.44
20:T:52:ARG:HD2	30:0:317:A:H5''	1.98	0.44
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:319:A:H4'	30:0:338:C:C4	2.53	0.44
30:0:557:C:C2	30:0:601:G:N2	2.85	0.44
30:0:750:A:H2'	30:0:751:U:C6	2.53	0.44
30:0:876:A:H2'	30:0:876:A:N3	2.33	0.44
30:0:2896:A:N3	30:0:2896:A:C2'	2.78	0.44
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.17	0.44
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.16	0.44
20:T:77:VAL:HG11	20:T:91:LEU:HD11	1.98	0.44
23:W:115:THR:HG23	38:W:5420:HOH:O	2.16	0.44
25:Y:144:ARG:NH2	38:Y:8913:HOH:O	2.51	0.44
30:0:2090:G:H2'	30:0:2091:G:C8	2.53	0.44
31:9:74:G:C6	31:9:75:G:N7	2.85	0.44
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.17	0.44
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.17	0.44
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.47	0.44
20:T:2:LYS:HG2	30:0:447:A:OP1	2.17	0.44
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.33	0.44
30:0:1182:C:O2'	30:0:1192:A:H8	1.99	0.44
30:0:1588:G:C6	30:0:1589:G:N1	2.86	0.44
30:0:1790:C:H2'	30:0:1791:U:H6	1.83	0.44
30:0:1819:G:H2'	30:0:1820:G:C5'	2.48	0.44
30:0:2505:G:H2'	30:0:2506:A:C5'	2.48	0.44
31:9:65:A:C2'	31:9:66:G:OP2	2.65	0.44
4:D:135:VAL:HG22	4:D:136:ARG:N	2.32	0.44
14:N:71:TRP:HB2	38:N:8837:HOH:O	2.17	0.44
23:W:88:THR:HG22	23:W:89:ASP:N	2.32	0.44
30:0:366:U:H2'	30:0:367:G:O4'	2.17	0.44
30:0:1183:C:H41	30:0:1192:A:P	2.41	0.44
30:0:1471:A:H5'	38:0:3202:HOH:O	2.17	0.44
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.17	0.44
14:N:119:GLN:O	14:N:123:ILE:HG13	2.18	0.44
22:V:12:THR:HG22	22:V:15:GLU:CG	2.48	0.44
23:W:52:VAL:HG13	23:W:53:ALA:N	2.32	0.44
25:Y:151:SER:HB3	25:Y:154:ARG:HB2	1.99	0.44
30:0:496:G:H3'	38:0:7689:HOH:O	2.18	0.44
30:0:1121:G:H4'	38:0:5565:HOH:O	2.17	0.44
30:0:1367:A:H2'	30:0:1368:U:O4'	2.18	0.44
30:0:1603:A:C5'	30:0:1605:G:O4'	2.59	0.44
33:0:8813:CL:CL	38:0:4694:HOH:O	2.58	0.44
31:9:1:U:O3'	31:9:3:A:C5'	2.66	0.44
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.44
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.01	0.44
27:1:17:THR:HG21	30:0:120:A:C5	2.52	0.44
30:0:101:C:H2'	30:0:102:A:H8	1.83	0.44
30:0:816:G:H5'	30:0:1598:A:H4'	2.00	0.44
30:0:1304:U:H2'	30:0:1305:C:C6	2.53	0.44
30:0:1883:U:H5'	30:0:2012:U:OP2	2.18	0.44
30:0:1996:U:H6	30:0:2586:U:O2	2.00	0.44
30:0:2611:U:O2'	30:0:2614:C:OP2	2.32	0.44
3:C:49:ASP:HB3	3:C:52:ALA:HB2	1.99	0.43
11:K:75:ARG:HD3	11:K:112:PRO:O	2.18	0.43
13:M:95:LYS:HG2	13:M:99:ARG:HB3	2.00	0.43
14:N:116:PHE:HB3	14:N:136:LEU:HD23	2.00	0.43
19:S:8:PRO:HD2	22:V:32:ALA:HA	2.00	0.43
20:T:97:ARG:NH2	30:0:308:U:H5'	2.32	0.43
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.99	0.43
30:0:59:A:C5'	38:0:4347:HOH:O	2.64	0.43
30:0:1210:G:O2'	30:0:1211:G:H5'	2.17	0.43
30:0:1211:G:O2'	30:0:1212:C:H5'	2.18	0.43
30:0:2105:C:H2'	30:0:2106:C:C6	2.53	0.43
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.83	0.43
12:L:21:ARG:N	38:L:8826:HOH:O	2.51	0.43
14:N:36:ALA:HB1	14:N:118:ILE:HD12	2.01	0.43
30:0:177:A:H2'	30:0:178:U:O4'	2.18	0.43
30:0:445:U:H1'	38:0:7361:HOH:O	2.18	0.43
30:0:523:C:H2'	30:0:524:A:C8	2.53	0.43
30:0:1257:C:H2'	30:0:1258:G:O4'	2.19	0.43
30:0:2369:A:C8	30:0:2371:G:C6	3.06	0.43
30:0:2617:G:N3	30:0:2617:G:H2'	2.32	0.43
30:0:2756:U:N3	30:0:2896:A:C2	2.76	0.43
8:H:59:GLN:NE2	8:H:96:GLN:HG2	2.30	0.43
10:J:132:LEU:HD23	10:J:132:LEU:HA	1.80	0.43
20:T:62:VAL:N	38:T:3851:HOH:O	2.52	0.43
30:0:776:A:H1'	30:0:779:U:O4	2.19	0.43
30:0:951:A:H2'	30:0:952:G:H5'	1.99	0.43
30:0:1736:A:H1'	38:0:7607:HOH:O	2.18	0.43
31:9:39:U:HO2'	31:9:42:C:H5	1.59	0.43
2:B:82:VAL:O	2:B:82:VAL:HG12	2.18	0.43
3:C:118:THR:CG2	3:C:137:PRO:HB3	2.48	0.43
5:E:159:VAL:O	5:E:163:GLN:HG2	2.18	0.43
11:K:74:VAL:HG13	11:K:113:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:208:LYS:O	30:0:1313:A:H5'	2.18	0.43
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.83	0.43
30:0:305:A:C5	30:0:329:A:C2	3.06	0.43
30:0:542:A:C5'	30:0:542:A:C8	2.96	0.43
30:0:566:A:N1	30:0:1093:G:O2'	2.45	0.43
30:0:1849:G:H1'	30:0:2011:A:N1	2.34	0.43
30:0:2099:A:N6	30:0:2100:A:N6	2.66	0.43
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.31	0.43
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.48	0.43
23:W:108:ARG:NH2	23:W:114:PRO:HG2	2.31	0.43
29:3:3:MET:CG	29:3:4:PRO:HD2	2.49	0.43
30:0:38:G:N2	38:0:7361:HOH:O	2.50	0.43
30:0:887:G:H2'	30:0:888:U:C6	2.53	0.43
30:0:960:G:C2'	30:0:961:A:OP2	2.66	0.43
30:0:1015:C:H2'	30:0:1016:U:H6	1.84	0.43
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.43
30:0:1787:C:H4'	30:0:2883:A:O4'	2.19	0.43
30:0:1940:C:H4'	38:0:7372:HOH:O	2.17	0.43
30:0:2004:U:H2'	30:0:2005:G:OP1	2.18	0.43
31:9:96:C:H2'	31:9:97:U:C6	2.54	0.43
3:C:104:ASP:HA	3:C:107:ARG:NH1	2.34	0.43
3:C:104:ASP:HA	3:C:107:ARG:HH12	1.83	0.43
21:U:20:MET:CG	21:U:28:THR:HG23	2.48	0.43
30:0:39:G:H2'	30:0:40:C:O4'	2.19	0.43
30:0:708:A:H2'	30:0:709:G:O4'	2.18	0.43
30:0:1183:C:H42	30:0:1184:C:N4	2.16	0.43
30:0:1377:C:H6	30:0:1377:C:C5'	2.24	0.43
30:0:1871:U:O4'	30:0:1873:G:C8	2.72	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.97	0.43
30:0:2329:C:O2'	30:0:2330:U:H5'	2.17	0.43
1:A:82:VAL:HG13	1:A:93:THR:HB	2.00	0.43
2:B:286:ASN:O	2:B:306:LYS:HE3	2.18	0.43
22:V:43:PRO:O	22:V:46:ILE:HG22	2.18	0.43
24:X:80:GLU:HB3	38:X:5564:HOH:O	2.18	0.43
30:0:31:C:H4'	38:0:7452:HOH:O	2.19	0.43
30:0:1179:C:H2'	30:0:1180:U:H6	1.83	0.43
30:0:1682:A:H2'	38:0:9811:HOH:O	2.19	0.43
30:0:2004:U:H4'	38:0:5331:HOH:O	2.19	0.43
30:0:2460:A:C2	30:0:2461:U:C2	3.06	0.43
31:9:12:C:H5'	31:9:70:U:O4'	2.18	0.43
1:A:164:ARG:NE	38:A:9053:HOH:O	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:LEU:HD23	3:C:79:ARG:HG3	2.01	0.43
5:E:69:ILE:HA	5:E:72:MET:HE3	2.00	0.43
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.01	0.43
12:L:59:GLU:HB3	38:L:8857:HOH:O	2.17	0.43
12:L:72:ASN:HB2	38:L:8876:HOH:O	2.19	0.43
14:N:26:LEU:HD13	30:0:2415:A:N3	2.33	0.43
30:0:767:A:H2	30:0:2110:G:N3	2.16	0.43
30:0:1280:A:H3'	30:0:1280:A:P	2.58	0.43
30:0:1588:G:C6	30:0:1589:G:C6	3.06	0.43
30:0:2252:A:H2'	30:0:2253:G:H5'	1.99	0.43
30:0:2321:A:C5	30:0:2323:G:C8	3.06	0.43
30:0:2569:A:H2'	30:0:2570:G:O4'	2.19	0.43
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.54	0.43
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.54	0.43
3:C:140:VAL:HG12	3:C:141:SER:N	2.33	0.43
5:E:11:VAL:HG12	5:E:12:ASP:N	2.33	0.43
9:I:86:GLU:CG	30:0:1180:U:H4'	2.43	0.43
15:O:25:VAL:HG12	30:0:709:G:O2'	2.19	0.43
15:O:96:VAL:CG1	15:O:100:GLN:HB2	2.49	0.43
30:0:883:U:O2	30:0:883:U:H3'	2.19	0.43
30:0:2704:C:H2'	30:0:2705:U:O4'	2.19	0.43
30:0:2791:U:H1'	30:0:2792:A:H5''	2.00	0.43
31:9:45:A:C5	31:9:46:C:C4	3.06	0.43
31:9:114:G:H2'	31:9:115:C:C6	2.54	0.43
2:B:58:PRO:HA	2:B:63:GLU:CD	2.44	0.43
2:B:333:GLU:HB2	21:U:14:GLU:OE2	2.18	0.43
12:L:121:ILE:HG12	12:L:141:GLU:HB2	2.01	0.43
17:Q:9:GLY:HA2	38:0:7028:HOH:O	2.19	0.43
30:0:398:U:H2'	30:0:399:C:C6	2.54	0.43
30:0:1482:A:O2'	30:0:1483:C:H5'	2.19	0.43
30:0:2456:A:H2'	30:0:2457:U:H6	1.84	0.43
30:0:2523:U:O2'	30:0:2524:G:H5'	2.19	0.43
30:0:2787:C:H5	38:0:4644:HOH:O	2.02	0.43
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.48	0.42
2:B:198:GLU:HA	38:B:9081:HOH:O	2.18	0.42
8:H:91:ARG:H	8:H:91:ARG:HG2	1.69	0.42
9:I:133:THR:HG22	9:I:134:ILE:N	2.34	0.42
11:K:115:ARG:HG3	11:K:116:GLU:N	2.34	0.42
13:M:24:GLN:NE2	13:M:24:GLN:HA	2.34	0.42
18:R:18:LEU:HB2	18:R:143:VAL:HG13	2.01	0.42
18:R:96:VAL:HG13	18:R:106:GLY:HA3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:38:THR:HG22	23:W:39:ASP:H	1.83	0.42
30:0:523:C:H2'	30:0:524:A:H8	1.83	0.42
30:0:1188:A:H62	30:0:1189:A:N6	2.17	0.42
30:0:1503:U:H2'	30:0:1504:A:O4'	2.19	0.42
30:0:2344:G:H2'	30:0:2344:G:N3	2.34	0.42
30:0:2505:G:C2'	30:0:2506:A:C5'	2.94	0.42
30:0:2893:C:O2'	30:0:2894:C:H5'	2.19	0.42
1:A:153:ARG:HB2	1:A:153:ARG:HH11	1.84	0.42
2:B:16:ARG:NH2	38:B:8982:HOH:O	2.49	0.42
28:2:40:ARG:HG3	28:2:45:ASN:HB2	2.00	0.42
30:0:69:A:C8	30:0:69:A:C5'	2.96	0.42
30:0:951:A:O2'	30:0:952:G:H5'	2.20	0.42
30:0:1213:C:O2'	30:0:1214:G:H5'	2.19	0.42
30:0:1249:U:H2'	30:0:1250:C:C6	2.54	0.42
30:0:1279:U:C5'	30:0:1280:A:OP2	2.68	0.42
30:0:1659:A:H2'	30:0:1660:G:O4'	2.18	0.42
30:0:1934:A:C8	30:0:1935:C:C5	3.07	0.42
30:0:2316:G:OP1	30:0:2317:C:H1'	2.19	0.42
30:0:2588:OMG:HM23	30:0:2617:G:C2	2.54	0.42
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.01	0.42
4:D:172:VAL:HG12	4:D:173:GLU:N	2.23	0.42
14:N:37:ARG:HH11	31:9:6:C:H5''	1.71	0.42
14:N:115:VAL:HG13	38:9:9105:HOH:O	2.19	0.42
22:V:1:THR:HG23	22:V:2:VAL:N	2.24	0.42
30:0:660:A:H4'	30:0:661:G:O5'	2.20	0.42
30:0:1163:G:H2'	30:0:1164:U:H5	1.84	0.42
30:0:1522:A:H2'	30:0:1523:G:H5'	2.01	0.42
30:0:2486:A:H3'	38:0:4903:HOH:O	2.18	0.42
30:0:2536:C:HO2'	30:0:2537:G:P	2.42	0.42
4:D:99:ASP:HB3	4:D:103:ASN:H	1.84	0.42
5:E:145:ALA:HB1	5:E:168:ILE:HD11	2.02	0.42
13:M:179:GLY:O	30:0:399:C:H5'	2.19	0.42
16:P:13:VAL:HG11	16:P:40:VAL:HG12	2.00	0.42
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.54	0.42
30:0:128:A:C8	30:0:128:A:H3'	2.55	0.42
30:0:2254:G:O2'	30:0:2255:A:H5'	2.19	0.42
30:0:2540:G:N2	38:0:9380:HOH:O	2.52	0.42
30:0:2829:G:O2'	30:0:2830:U:H5'	2.20	0.42
2:B:41:PHE:HB3	2:B:190:MET:HE1	2.00	0.42
2:B:124:ALA:O	2:B:128:ILE:HG13	2.19	0.42
3:C:236:THR:H	3:C:239:ALA:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:101:GLU:HA	5:E:118:ILE:HG13	2.01	0.42
15:O:44:ASN:OD1	15:O:67:SER:HB2	2.20	0.42
16:P:115:SER:OG	16:P:118:GLN:HG3	2.20	0.42
23:W:88:THR:HG22	23:W:90:TYR:CD1	2.51	0.42
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.20	0.42
30:0:867:A:H2	30:0:880:C:O2	2.03	0.42
30:0:1099:G:H2'	30:0:1100:G:O4'	2.20	0.42
30:0:1183:C:C6	30:0:1192:A:N7	2.87	0.42
30:0:1552:G:N2	30:0:1634:G:C1'	2.80	0.42
30:0:1701:A:H4'	30:0:1702:U:O5'	2.20	0.42
30:0:2637:A:H5''	38:0:4944:HOH:O	2.18	0.42
2:B:244:PRO:HB3	30:0:1234:U:N3	2.35	0.42
3:C:168:ARG:NH2	3:C:190:ALA:O	2.53	0.42
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.45	0.42
8:H:32:ALA:C	8:H:33:GLN:HG3	2.44	0.42
26:Z:56:GLU:O	26:Z:61:HIS:HE1	2.03	0.42
30:0:807:A:N1	30:0:808:A:C2	2.88	0.42
30:0:1342:C:H2'	30:0:1343:C:H5'	2.02	0.42
30:0:1842:A:C4	30:0:1979:G:C6	3.06	0.42
30:0:1972:U:H2'	30:0:1973:A:H5''	1.99	0.42
30:0:2645:U:C6	30:0:2645:U:OP2	2.72	0.42
3:C:87:ARG:NH2	30:0:894:A:C2	2.88	0.42
7:G:63:ARG:N	38:G:2569:HOH:O	2.52	0.42
17:Q:11:ARG:HB2	38:0:7028:HOH:O	2.20	0.42
18:R:92:LEU:HD23	18:R:145:LEU:HD21	2.02	0.42
19:S:33:SER:O	19:S:37:VAL:HG23	2.19	0.42
23:W:44:MET:HE2	30:0:944:G:N2	2.31	0.42
30:0:138:U:OP2	30:0:139:C:H5	2.02	0.42
30:0:812:A:H2'	30:0:813:C:C6	2.54	0.42
30:0:1042:U:O2'	30:0:1043:C:H5'	2.19	0.42
30:0:1380:U:C4	30:0:2748:G:H1'	2.54	0.42
30:0:1520:G:H2'	30:0:1521:C:C6	2.54	0.42
38:A:9042:HOH:O	30:0:2271:G:H5'	2.20	0.42
6:F:91:VAL:CG1	6:F:92:GLY:N	2.83	0.42
8:H:61:ARG:NH1	8:H:61:ARG:HG3	2.34	0.42
13:M:84:LYS:HG3	30:0:171:C:OP2	2.20	0.42
18:R:18:LEU:HD12	18:R:143:VAL:HG11	2.01	0.42
25:Y:107:PRO:HD3	25:Y:182:PHE:CE1	2.55	0.42
30:0:451:C:O2'	30:0:452:G:H5'	2.19	0.42
30:0:1066:U:H2'	30:0:1067:A:C8	2.54	0.42
30:0:1167:G:N2	30:0:1180:U:C2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1201:C:C2'	30:0:1202:A:H5'	2.49	0.42
30:0:1367:A:H2'	30:0:1368:U:H5'	2.02	0.42
30:0:2356:A:H2'	30:0:2357:G:O4'	2.19	0.42
30:0:2419:U:H5''	30:0:2420:G:H5'	2.02	0.42
30:0:2504:A:H2'	30:0:2505:G:O4'	2.20	0.42
31:9:108:C:H2'	31:9:109:G:H8	1.82	0.42
13:M:68:ARG:O	13:M:68:ARG:HD3	2.19	0.42
19:S:43:GLU:HB3	38:S:7106:HOH:O	2.18	0.42
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	2.02	0.42
30:0:90:A:H2'	30:0:91:G:O4'	2.19	0.42
30:0:629:A:H2'	30:0:630:A:O4'	2.20	0.42
30:0:1335:C:H2'	30:0:1336:U:H6	1.85	0.42
30:0:1626:A:H2'	30:0:1627:G:O4'	2.20	0.42
30:0:1926:G:H2'	30:0:1927:A:C8	2.54	0.42
30:0:2699:A:H2'	30:0:2700:G:O4'	2.19	0.42
31:9:38:A:H2	31:9:43:G:H5''	1.84	0.42
31:9:80:A:C2	31:9:103:A:C4	3.08	0.42
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.31	0.42
8:H:36:MET:SD	8:H:69:ARG:HD2	2.60	0.42
14:N:13:ARG:HA	14:N:13:ARG:HD2	1.89	0.42
15:O:32:ARG:HH21	15:O:35:LYS:HZ2	1.68	0.42
15:O:87:THR:O	15:O:91:GLN:HG3	2.19	0.42
16:P:37:ARG:HD2	30:0:1501:A:OP2	2.20	0.42
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.42
30:0:734:U:O2'	30:0:737:A:N6	2.53	0.42
30:0:1055:G:N7	38:0:4091:HOH:O	2.51	0.42
30:0:1103:C:C2	30:0:1241:G:N2	2.88	0.42
30:0:1181:A:C2'	30:0:1182:C:H5'	2.49	0.42
30:0:1189:A:H1'	30:0:1209:C:H1'	2.02	0.42
30:0:2326:C:H4'	30:0:2412:G:C4'	2.50	0.42
30:0:2757:A:H2'	30:0:2758:G:O4'	2.20	0.42
31:9:107:C:O2'	31:9:108:C:H5'	2.20	0.42
5:E:84:MET:HG2	5:E:168:ILE:HD13	2.02	0.41
9:I:86:GLU:HA	9:I:87:PRO:HD2	1.94	0.41
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.55	0.41
30:0:506:G:N2	30:0:509:A:H5''	2.27	0.41
30:0:1183:C:N3	30:0:1184:C:C5	2.88	0.41
30:0:1298:U:H2'	30:0:1299:G:H8	1.85	0.41
30:0:1309:U:O2'	30:0:1310:U:H5'	2.20	0.41
30:0:2099:A:N6	30:0:2100:A:H61	2.17	0.41
30:0:2281:C:C2'	30:0:2282:U:H5'	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2776:A:H2'	30:0:2777:G:O4'	2.19	0.41
31:9:49:G:C2'	31:9:50:G:H5'	2.50	0.41
3:C:76:ARG:HH22	30:0:1363:G:P	2.42	0.41
10:J:88:PRO:HD3	30:0:1104:C:H4'	2.01	0.41
11:K:101:ASN:O	11:K:102:GLU:HB2	2.20	0.41
16:P:16:VAL:CG1	16:P:17:GLY:N	2.83	0.41
30:0:607:G:H2'	30:0:608:A:O4'	2.21	0.41
30:0:1006:A:N1	30:0:2311:A:H1'	2.35	0.41
30:0:1183:C:C5	30:0:1192:A:C8	3.08	0.41
30:0:1367:A:C2'	30:0:1368:U:H5'	2.51	0.41
30:0:1641:A:C8	30:0:1702:U:O4	2.73	0.41
30:0:2011:A:H4'	30:0:2012:U:O5'	2.20	0.41
31:9:40:C:H2'	31:9:41:C:OP1	2.20	0.41
11:K:81:ARG:HB2	11:K:87:ARG:HH11	1.84	0.41
12:L:10:SER:O	12:L:11:ARG:HB3	2.19	0.41
12:L:56:LYS:HE3	30:0:2443:C:H1'	2.02	0.41
21:U:17:THR:CG2	21:U:18:GLY:N	2.83	0.41
30:0:537:G:O4'	30:0:538:C:C5	2.73	0.41
30:0:876:A:N3	30:0:876:A:C2'	2.83	0.41
30:0:1878:G:O2'	30:0:1879:U:OP2	2.38	0.41
30:0:1980:U:O2'	30:0:1981:A:H5'	2.20	0.41
30:0:2089:A:C2'	30:0:2090:G:H5'	2.50	0.41
31:9:31:C:C2	31:9:50:G:N2	2.89	0.41
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.55	0.41
6:F:99:THR:HG23	6:F:99:THR:O	2.20	0.41
23:W:23:MET:HE2	30:0:943:A:C5	2.54	0.41
25:Y:117:LEU:HB2	25:Y:174:VAL:HG21	2.01	0.41
25:Y:174:VAL:CG2	25:Y:177:LYS:HD2	2.50	0.41
29:3:73:GLU:HB2	38:3:9023:HOH:O	2.20	0.41
30:0:254:C:O2	30:0:254:C:C2'	2.64	0.41
30:0:581:G:O2'	30:0:582:U:H5'	2.21	0.41
30:0:696:C:C2'	30:0:697:G:H5'	2.51	0.41
30:0:1116:U:H3	30:0:1246:A:N6	1.98	0.41
30:0:1552:G:C6	30:0:1553:C:C4	3.08	0.41
30:0:1657:A:H2'	30:0:1658:A:C8	2.55	0.41
3:C:19:PRO:HD2	3:C:240:LEU:HD11	2.03	0.41
5:E:143:GLN:OE1	30:0:2796:U:H1'	2.21	0.41
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.55	0.41
8:H:174:LEU:HD21	30:0:1220:U:H4'	2.03	0.41
14:N:44:ARG:NH1	31:9:4:G:H21	2.18	0.41
22:V:7:GLU:O	22:V:11:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:80:A:H4'	30:0:81:G:O5'	2.21	0.41
30:0:236:A:H8	30:0:236:A:OP1	2.03	0.41
30:0:969:G:H1	30:0:999:C:H42	1.67	0.41
30:0:1406:A:H5'	30:0:1407:A:C8	2.56	0.41
30:0:1948:G:H2'	30:0:1949:G:C8	2.55	0.41
30:0:1971:G:H5'	38:0:7098:HOH:O	2.20	0.41
30:0:2667:G:H1'	30:0:2914:A:N3	2.36	0.41
31:9:64:C:H2'	31:9:65:A:H5'	2.01	0.41
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.87	0.41
2:B:254:GLN:NE2	38:B:9014:HOH:O	2.52	0.41
3:C:5:ILE:HD11	3:C:16:VAL:HG13	2.03	0.41
13:M:79:ALA:HB1	30:0:770:C:OP1	2.21	0.41
17:Q:30:VAL:HG12	17:Q:30:VAL:O	2.20	0.41
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.20	0.41
20:T:40:VAL:HG22	20:T:41:ARG:N	2.35	0.41
21:U:6:CYS:HB2	21:U:32:CYS:HB3	2.03	0.41
23:W:146:ILE:HD13	23:W:146:ILE:HA	1.83	0.41
30:0:204:A:O2'	30:0:205:U:H5'	2.20	0.41
30:0:484:A:N1	30:0:506:G:H4'	2.35	0.41
30:0:559:U:H5'	30:0:559:U:C6	2.34	0.41
30:0:612:U:H2'	30:0:613:C:H6	1.86	0.41
30:0:1116:U:C2	30:0:1246:A:N6	2.88	0.41
30:0:1211:G:H2'	30:0:1212:C:C6	2.56	0.41
30:0:2094:G:O6	30:0:2649:A:H2	2.04	0.41
30:0:2823:G:H4'	30:0:2827:A:O4'	2.20	0.41
30:0:2864:U:O2'	30:0:2865:G:H5'	2.20	0.41
1:A:211:LYS:CB	38:0:7455:HOH:O	2.69	0.41
4:D:138:GLY:N	38:D:7597:HOH:O	2.53	0.41
13:M:68:ARG:HG3	13:M:73:ARG:HE	1.84	0.41
13:M:137:ASN:ND2	30:0:145:A:H4'	2.36	0.41
14:N:32:PRO:HD2	14:N:99:GLU:O	2.21	0.41
17:Q:75:ILE:CD1	17:Q:84:ILE:HD11	2.51	0.41
18:R:114:VAL:HA	18:R:144:GLU:O	2.21	0.41
20:T:27:LEU:HD23	20:T:98:VAL:HB	2.02	0.41
30:0:69:A:C8	30:0:69:A:C3'	3.04	0.41
30:0:466:A:H2'	30:0:467:G:O4'	2.20	0.41
30:0:503:G:H2'	30:0:504:G:H8	1.84	0.41
30:0:1131:G:H4'	31:9:91:C:O4'	2.20	0.41
30:0:1523:G:C6	30:0:1524:U:O4	2.74	0.41
30:0:2506:A:O5'	30:0:2506:A:C2'	2.68	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2644:C:O2'	30:0:2645:U:O5'	2.37	0.41
5:E:133:VAL:HG12	5:E:141:VAL:HG13	2.02	0.41
12:L:4:LYS:HE2	30:0:645:U:OP2	2.20	0.41
16:P:55:LYS:CG	16:P:56:GLY:N	2.84	0.41
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.89	0.41
30:0:1046:G:N3	30:0:1082:A:H2	2.19	0.41
30:0:2388:C:H2'	30:0:2389:U:O4'	2.21	0.41
30:0:2597:U:H2'	30:0:2598:U:H5'	2.02	0.41
30:0:2826:G:C5	30:0:2913:A:C6	3.08	0.41
2:B:81:ALA:HB1	2:B:142:LEU:HD13	2.03	0.41
2:B:87:TYR:O	2:B:138:GLY:N	2.47	0.41
3:C:118:THR:O	3:C:136:VAL:HG13	2.20	0.41
4:D:154:LYS:HD2	4:D:154:LYS:N	2.30	0.41
6:F:21:GLU:O	6:F:24:ARG:HG2	2.21	0.41
8:H:50:ILE:HG21	38:H:231:HOH:O	2.21	0.41
8:H:98:LEU:HD11	8:H:127:ALA:HB2	2.02	0.41
13:M:91:ILE:HG23	38:M:8953:HOH:O	2.20	0.41
13:M:102:GLU:OE1	13:M:164:THR:HG21	2.20	0.41
14:N:23:ARG:O	14:N:27:LEU:HG	2.21	0.41
18:R:64:SER:OG	30:0:1369:A:H4'	2.21	0.41
30:0:243:A:H61	30:0:269:G:H1'	1.86	0.41
30:0:757:C:H2'	30:0:758:A:C8	2.56	0.41
30:0:1076:G:C2	30:0:1084:C:C2	3.09	0.41
30:0:1165:G:H3'	30:0:1166:A:C5'	2.50	0.41
30:0:1206:U:H6	30:0:1206:U:C5'	2.28	0.41
30:0:1441:G:O2'	30:0:1442:A:H5'	2.21	0.41
30:0:1592:G:H2'	30:0:1593:C:C6	2.56	0.41
30:0:2061:C:C2'	30:0:2062:A:H5'	2.51	0.41
30:0:2453:G:H5'	38:0:4702:HOH:O	2.21	0.41
30:0:2455:A:H2'	30:0:2456:A:O4'	2.20	0.41
30:0:2526:C:H5''	38:0:7627:HOH:O	2.20	0.41
30:0:2644:C:HO2'	30:0:2645:U:P	2.44	0.41
7:G:67:LEU:O	7:G:71:LEU:HG	2.21	0.41
15:O:25:VAL:HG13	30:0:709:G:O3'	2.20	0.41
19:S:57:THR:HG22	19:S:58:MET:H	1.84	0.41
22:V:1:THR:CG2	22:V:2:VAL:H	2.21	0.41
30:0:1484:G:H2'	38:0:9110:HOH:O	2.20	0.41
30:0:1768:C:H2'	30:0:1769:C:O4'	2.21	0.41
30:0:1816:C:H2'	30:0:1817:U:O4'	2.21	0.41
30:0:2588:OMG:HM23	30:0:2617:G:N2	2.36	0.41
30:0:2645:U:H6	30:0:2645:U:H2'	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:185:LYS:HD3	3:C:186:TYR:CE1	2.56	0.40
4:D:40:ILE:HG13	4:D:41:LEU:N	2.36	0.40
5:E:143:GLN:HE22	30:0:2779:G:H21	1.67	0.40
11:K:118:ALA:HA	11:K:125:ALA:HB2	2.03	0.40
15:O:53:GLN:HG2	15:O:56:GLU:OE1	2.21	0.40
18:R:9:ASP:HA	18:R:10:PRO:HD2	1.94	0.40
18:R:132:ARG:NH2	38:R:8983:HOH:O	2.54	0.40
30:0:12:U:C2'	30:0:13:G:H5'	2.49	0.40
30:0:304:G:H1'	30:0:347:A:H61	1.86	0.40
30:0:336:G:H5''	38:0:3737:HOH:O	2.21	0.40
30:0:553:G:O4'	30:0:1325:G:H5'	2.21	0.40
30:0:1400:C:H1'	38:0:4150:HOH:O	2.20	0.40
30:0:2748:G:P	30:0:2749:U:H5''	2.59	0.40
30:0:2831:C:C2'	30:0:2832:C:H5'	2.51	0.40
1:A:212:PRO:HA	30:0:1943:C:O4'	2.21	0.40
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.89	0.40
6:F:58:GLU:HG3	6:F:61:MET:HE2	2.04	0.40
12:L:6:ARG:NH1	30:0:1299:G:N7	2.69	0.40
12:L:65:ASP:CG	12:L:111:ALA:HB3	2.46	0.40
15:O:77:ALA:HA	15:O:96:VAL:O	2.20	0.40
20:T:2:LYS:HE2	38:0:7433:HOH:O	2.21	0.40
27:1:32:LYS:NZ	30:0:120:A:OP1	2.53	0.40
29:3:38:ARG:HB3	29:3:42:ARG:HH12	1.85	0.40
30:0:669:G:O2'	30:0:670:G:H5'	2.21	0.40
30:0:787:G:O2'	30:0:788:A:H5'	2.20	0.40
30:0:1573:A:H2'	30:0:1574:C:O4'	2.21	0.40
30:0:2102:G:C2	30:0:2103:A:C4	3.10	0.40
30:0:2332:A:H5'	30:0:2333:G:OP2	2.20	0.40
2:B:14:GLY:HA2	2:B:15:PRO:C	2.47	0.40
2:B:16:ARG:NE	38:B:8982:HOH:O	2.46	0.40
5:E:84:MET:HE1	5:E:148:ILE:HD13	2.04	0.40
6:F:30:LYS:HD3	6:F:30:LYS:HA	1.88	0.40
25:Y:186:ARG:HG2	25:Y:186:ARG:NH1	2.35	0.40
30:0:1339:G:C6	30:0:1340:G:N1	2.89	0.40
30:0:1624:A:H4'	30:0:1625:U:H5'	2.03	0.40
30:0:2250:G:H2'	30:0:2251:G:O4'	2.20	0.40
30:0:2328:U:C4	30:0:2329:C:C5	3.09	0.40
30:0:2712:G:P	38:0:5242:HOH:O	2.80	0.40
30:0:2819:C:H2'	30:0:2820:A:H8	1.87	0.40
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.51	0.40
3:C:84:VAL:O	3:C:85:LYS:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.92	0.40
6:F:57:GLU:O	6:F:61:MET:HG3	2.21	0.40
10:J:90:LYS:HB2	33:J:8802:CL:CL	2.57	0.40
16:P:115:SER:HB2	38:P:4299:HOH:O	2.21	0.40
23:W:23:MET:O	30:0:1025:C:H5'	2.21	0.40
30:0:297:U:H2'	30:0:298:C:C6	2.55	0.40
30:0:412:C:H2'	30:0:413:G:O4'	2.21	0.40
30:0:482:G:O4'	30:0:511:A:C2	2.74	0.40
30:0:907:A:H4'	30:0:1328:A:C2	2.57	0.40
30:0:1398:G:H2'	30:0:1399:A:C8	2.56	0.40
30:0:1476:A:H1'	30:0:1867:G:O2'	2.21	0.40
30:0:1524:U:H3'	38:0:5355:HOH:O	2.21	0.40
30:0:2135:A:O4'	30:0:2243:C:N4	2.55	0.40
30:0:2482:G:H4'	30:0:2483:A:C5'	2.52	0.40
30:0:2578:G:H5'	30:0:2578:G:C8	2.44	0.40
1:A:1:GLY:HA2	1:A:197:VAL:HG23	2.04	0.40
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.88	0.40
1:A:204:GLY:O	1:A:205:GLY:C	2.65	0.40
16:P:83:LYS:HG2	30:0:793:A:H5''	2.03	0.40
23:W:73:LEU:HD12	23:W:73:LEU:HA	1.87	0.40
30:0:420:U:H2'	30:0:421:C:C6	2.57	0.40
30:0:483:C:C4	30:0:484:A:C6	3.10	0.40
30:0:968:G:C2	30:0:1001:U:O2	2.75	0.40
30:0:1345:A:H2'	30:0:1346:U:C6	2.55	0.40
30:0:1511:U:O2'	30:0:1512:G:H5'	2.21	0.40
30:0:1589:G:N2	30:0:1605:G:H1'	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
1	A	235/240 (98%)	209 (89%)	24 (10%)	2 (1%)	14	20
2	B	335/338 (99%)	315 (94%)	18 (5%)	2 (1%)	21	29
3	C	244/246 (99%)	233 (96%)	11 (4%)	0	100	100
4	D	134/177 (76%)	111 (83%)	20 (15%)	3 (2%)	5	5
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	14	20
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	149 (96%)	7 (4%)	0	100	100
9	I	68/162 (42%)	55 (81%)	12 (18%)	1 (2%)	8	10
10	J	140/145 (97%)	133 (95%)	5 (4%)	2 (1%)	9	11
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	5	5
13	M	192/196 (98%)	183 (95%)	9 (5%)	0	100	100
14	N	184/187 (98%)	171 (93%)	8 (4%)	5 (3%)	4	3
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	77 (98%)	2 (2%)	0	100	100
20	T	117/120 (98%)	113 (97%)	3 (3%)	1 (1%)	14	20
21	U	51/67 (76%)	49 (96%)	2 (4%)	0	100	100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100	100
23	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
24	X	80/92 (87%)	76 (95%)	2 (2%)	2 (2%)	4	4
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	63 (89%)	7 (10%)	1 (1%)	9	11
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	11	15
All	All	3705/4472 (83%)	3486 (94%)	195 (5%)	24 (1%)	21	29

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
10	J	5	GLU
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
1	A	205	GLY
12	L	149	ARG
14	N	167	ASP
12	L	80	ASP
26	Z	105	ARG
2	B	2	GLN
2	B	185	GLY
4	D	56	ARG
20	T	45	GLY
24	X	87	ALA
4	D	137	PRO
10	J	143	LYS
12	L	82	ALA
14	N	162	ASP
4	D	27	ILE
6	F	100	ASP
24	X	70	ILE
29	3	56	PRO
9	I	108	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	166 (93%)	13 (7%)	13	18
2	B	282/283 (100%)	262 (93%)	20 (7%)	13	19
3	C	193/193 (100%)	180 (93%)	13 (7%)	15	21
4	D	117/148 (79%)	113 (97%)	4 (3%)	32	48
5	E	152/156 (97%)	147 (97%)	5 (3%)	33	50
6	F	93/94 (99%)	92 (99%)	1 (1%)	65	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	129 (96%)	5 (4%)	30	45
9	I	58/130 (45%)	58 (100%)	0	100	100
10	J	118/121 (98%)	114 (97%)	4 (3%)	32	48
11	K	106/106 (100%)	102 (96%)	4 (4%)	29	44
12	L	113/127 (89%)	110 (97%)	3 (3%)	39	58
13	M	158/160 (99%)	153 (97%)	5 (3%)	34	51
14	N	149/150 (99%)	145 (97%)	4 (3%)	39	58
15	O	93/94 (99%)	88 (95%)	5 (5%)	20	30
16	P	113/117 (97%)	111 (98%)	2 (2%)	51	70
17	Q	79/80 (99%)	76 (96%)	3 (4%)	29	44
18	R	117/122 (96%)	114 (97%)	3 (3%)	40	59
19	S	71/74 (96%)	70 (99%)	1 (1%)	59	75
20	T	105/106 (99%)	99 (94%)	6 (6%)	18	28
21	U	44/53 (83%)	43 (98%)	1 (2%)	44	62
22	V	51/57 (90%)	50 (98%)	1 (2%)	48	67
23	W	130/130 (100%)	124 (95%)	6 (5%)	24	36
24	X	66/74 (89%)	62 (94%)	4 (6%)	17	25
25	Y	120/196 (61%)	111 (92%)	9 (8%)	12	17
26	Z	60/94 (64%)	59 (98%)	1 (2%)	53	72
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	42 (100%)	0	100	100
29	3	79/79 (100%)	76 (96%)	3 (4%)	29	44
All	All	3095/3646 (85%)	2969 (96%)	126 (4%)	27	41

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	33	GLU
1	A	68	ILE
1	A	69	LEU
1	A	94	LEU
1	A	105	VAL

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Mol	Chain	Res	Type
1	A	131	HIS
1	A	165	THR
1	A	175	LYS
1	A	184	THR
1	A	192	VAL
1	A	206	ARG
1	A	217	ARG
2	B	2	GLN
2	B	5	ARG
2	B	11	LEU
2	B	27	ASN
2	B	51	VAL
2	B	53	LEU
2	B	71	VAL
2	B	84	LEU
2	B	98	THR
2	B	162	MET
2	B	175	LEU
2	B	190	MET
2	B	195	ARG
2	B	251	VAL
2	B	254	GLN
2	B	265	LEU
2	B	279	THR
2	B	301	VAL
2	B	307	ARG
2	B	312	ARG
3	C	2	GLN
3	C	76	ARG
3	C	78	ARG
3	C	94	THR
3	C	115	LEU
3	C	136	VAL
3	C	187	ARG
3	C	211	ASP
3	C	214	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	243	VAL
4	D	24	HIS
4	D	36	ASN

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Mol	Chain	Res	Type
4	D	50	VAL
4	D	172	VAL
5	E	7	ILE
5	E	86	VAL
5	E	102	VAL
5	E	132	THR
5	E	154	ILE
6	F	12	LEU
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	173	GLU
10	J	39	VAL
10	J	46	ILE
10	J	93	ARG
10	J	131	THR
11	K	4	LEU
11	K	10	GLN
11	K	55	VAL
11	K	98	VAL
12	L	32	ASP
12	L	43	HIS
12	L	140	VAL
13	M	46	LEU
13	M	82	ARG
13	M	93	ARG
13	M	99	ARG
13	M	115	LEU
14	N	26	LEU
14	N	49	THR
14	N	127	LEU
14	N	135	VAL
15	O	3	THR
15	O	25	VAL
15	O	38	ARG
15	O	43	VAL
15	O	111	VAL
16	P	21	VAL
16	P	98	ILE
17	Q	11	ARG
17	Q	16	ASN

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Mol	Chain	Res	Type
17	Q	95	GLU
18	R	39	THR
18	R	82	GLU
18	R	143	VAL
19	S	10	VAL
20	T	39	ASN
20	T	48	VAL
20	T	71	VAL
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
21	U	17	THR
22	V	65	ASP
23	W	26	ILE
23	W	52	VAL
23	W	76	ASP
23	W	78	ASP
23	W	142	ASP
23	W	146	ILE
24	X	72	VAL
24	X	79	GLU
24	X	80	GLU
24	X	82	GLU
25	Y	103	THR
25	Y	141	THR
25	Y	163	THR
25	Y	172	THR
25	Y	174	VAL
25	Y	189	ASN
25	Y	200	THR
25	Y	203	VAL
25	Y	235	GLU
26	Z	34	SER
29	3	18	GLN
29	3	56	PRO
29	3	92	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	131	HIS

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Mol	Chain	Res	Type
1	A	188	ASN
1	A	199	HIS
1	A	218	ASN
2	B	27	ASN
2	B	145	HIS
2	B	230	GLN
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	103	ASN
4	D	133	ASN
4	D	158	ASN
5	E	106	ASN
5	E	143	GLN
6	F	55	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	73	ASN
8	H	75	HIS
9	I	99	GLN
10	J	25	GLN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	42	ASN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
13	M	24	GLN
13	M	58	GLN
13	M	77	HIS
13	M	137	ASN
13	M	170	ASN

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Mol	Chain	Res	Type
14	N	21	HIS
14	N	22	GLN
14	N	107	ASN
14	N	140	GLN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
18	R	22	GLN
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
18	R	122	GLN
18	R	140	GLN
19	S	44	GLN
19	S	53	ASN
19	S	55	GLN
20	T	37	GLN
20	T	39	ASN
21	U	39	ASN
22	V	60	GLN
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	22	ASN
24	X	23	HIS
25	Y	119	GLN
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	153	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	18	ASN

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Mol	Chain	Res	Type
28	2	37	HIS
28	2	41	HIS
28	2	45	ASN
29	3	18	GLN
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	251 (9%)	28 (1%)
31	9	121/122 (99%)	17 (14%)	3 (2%)
All	All	2866/3045 (94%)	268 (9%)	31 (1%)

All (268) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	131	A
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	185	G
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	200	C
30	0	219	G
30	0	237	G

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Mol	Chain	Res	Type
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	368	C
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	645	U
30	0	660	A
30	0	688	A
30	0	701	U
30	0	702	G
30	0	759	C
30	0	777	U
30	0	809	G

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Mol	Chain	Res	Type
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G
30	0	1088	A
30	0	1100	G
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1151	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A

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Mol	Chain	Res	Type
30	0	1193	A
30	0	1206	U
30	0	1207	A
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1280	A
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1357	A
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1562	C
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1633	C
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1686	C
30	0	1692	C
30	0	1693	A
30	0	1701	A
30	0	1722	U

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Mol	Chain	Res	Type
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1943	C
30	0	1971	G
30	0	1973	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2100	A
30	0	2101	A
30	0	2102	G
30	0	2103	A
30	0	2110	G
30	0	2238	A
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G

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Mol	Chain	Res	Type
30	0	2291	A
30	0	2317	C
30	0	2320	U
30	0	2321	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2467	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2539	U
30	0	2540	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2611	U
30	0	2613	G
30	0	2644	C
30	0	2645	U
30	0	2649	A
30	0	2650	U
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2718	C
30	0	2719	A
30	0	2726	U
30	0	2727	A
30	0	2747	C

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Mol	Chain	Res	Type
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	39	U
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	603	A
30	0	644	G
30	0	699	C

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Mol	Chain	Res	Type
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1506	U
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1856	C
30	0	1942	A
30	0	1979	G
30	0	2313	C
30	0	2467	A
30	0	2541	U
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2748	G
30	0	2791	U
31	9	43	G
31	9	55	U
31	9	65	A

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

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	$\# Z > 2$
30	OMG	0	2588	30	23,26,27	0.28	0	32,38,41	0.33	0
30	1MA	0	628	30,35	21,25,26	0.72	1 (4%)	30,37,40	0.74	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PSU	0	2621	30	18,21,22	1.49	2 (11%)	21,30,33	1.38	3 (14%)
30	OMU	0	2587	30	19,22,23	0.33	0	25,31,34	0.45	0
30	UR3	0	2619	30	19,22,23	0.36	0	26,32,35	0.71	1 (3%)

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
30	OMG	0	2588	30	-	0/9/27/28	0/3/3/3
30	1MA	0	628	30,35	-	2/7/25/26	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	4.99	1.43	1.36
30	0	628	1MA	C6-N6	2.45	1.33	1.28
30	0	2621	PSU	C6-C5	2.15	1.37	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C6-C5-C4	4.00	120.87	118.17
30	0	2619	UR3	C4-N3-C2	2.83	126.86	124.58
30	0	2621	PSU	C6-N1-C2	-2.83	120.06	122.69
30	0	628	1MA	N1-C2-N3	2.79	129.31	126.00
30	0	2621	PSU	O2-C2-N1	2.74	125.61	122.79

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8
30	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2588	OMG	3	0
30	0	2587	OMU	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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	A	237/240 (98%)	0.40	20 (8%) 17 16	20, 40, 77, 100	0
2	B	337/338 (99%)	0.45	20 (5%) 28 27	21, 44, 73, 83	0
3	C	246/246 (100%)	0.16	9 (3%) 45 46	17, 36, 60, 73	0
4	D	140/177 (79%)	2.77	94 (67%) 0 0	48, 89, 116, 126	0
5	E	172/178 (96%)	0.97	19 (11%) 10 10	34, 59, 79, 85	0
6	F	119/120 (99%)	1.15	25 (21%) 2 2	34, 61, 91, 105	0
7	G	29/348 (8%)	1.96	10 (34%) 1 0	70, 87, 96, 98	0
8	H	160/177 (90%)	0.69	16 (10%) 12 12	32, 50, 85, 91	0
9	I	70/162 (43%)	4.06	63 (90%) 0 0	124, 138, 156, 156	0
10	J	142/145 (97%)	0.34	7 (4%) 35 34	27, 41, 63, 89	0
11	K	132/132 (100%)	0.14	1 (0%) 82 84	23, 39, 63, 72	0
12	L	145/165 (87%)	0.99	29 (20%) 3 2	18, 55, 103, 118	0
13	M	194/196 (98%)	0.35	23 (11%) 9 8	23, 34, 54, 59	0
14	N	186/187 (99%)	1.16	35 (18%) 3 2	34, 52, 104, 112	0
15	O	115/116 (99%)	0.49	5 (4%) 40 40	31, 45, 61, 69	0
16	P	143/149 (95%)	0.39	3 (2%) 63 64	28, 43, 56, 68	0
17	Q	95/96 (98%)	0.11	3 (3%) 50 51	29, 37, 55, 66	0
18	R	150/155 (96%)	-0.06	2 (1%) 75 75	23, 36, 57, 71	0
19	S	81/85 (95%)	0.39	4 (4%) 35 34	33, 48, 70, 81	0
20	T	119/120 (99%)	0.62	7 (5%) 28 27	29, 46, 74, 101	0
21	U	53/67 (79%)	0.43	2 (3%) 44 45	33, 46, 65, 74	0
22	V	65/71 (91%)	1.47	15 (23%) 2 1	41, 63, 106, 113	0
23	W	154/154 (100%)	0.21	2 (1%) 75 75	26, 42, 59, 71	0
24	X	82/92 (89%)	0.75	10 (12%) 8 7	34, 49, 77, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.09	4 (2%) 55 56	19, 34, 58, 80	0
26	Z	73/116 (62%)	1.35	20 (27%) 1 1	36, 55, 72, 89	0
27	1	56/57 (98%)	-0.38	0 100 100	18, 24, 34, 41	0
28	2	46/50 (92%)	0.95	9 (19%) 3 2	25, 49, 74, 86	0
29	3	92/92 (100%)	0.36	4 (4%) 40 40	27, 45, 60, 74	0
30	0	2749/2923 (94%)	-0.49	92 (3%) 49 50	14, 35, 77, 154	0
31	9	122/122 (100%)	0.22	9 (7%) 20 19	29, 54, 76, 138	0
All	All	6646/7517 (88%)	0.18	562 (8%) 16 16	14, 41, 89, 156	0

All (562) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	10.7
22	V	39	ALA	9.8
14	N	166	ALA	9.2
9	I	113	SER	9.2
4	D	10	PHE	8.9
9	I	128	THR	8.9
4	D	63	ILE	8.4
4	D	57	THR	7.6
30	0	2101	A	7.6
28	2	49	GLU	7.3
4	D	174	VAL	7.1
9	I	120	ALA	7.0
30	0	2537	G	6.9
14	N	168	LEU	6.9
9	I	132	VAL	6.8
13	M	70	GLY	6.8
9	I	127	CYS	6.8
9	I	112	LEU	6.8
31	9	1	U	6.8
30	0	2539	U	6.7
30	0	2102	G	6.6
9	I	74	ILE	6.5
22	V	2	VAL	6.3
4	D	90	LEU	6.2
30	0	2103	A	6.2
30	0	2540	G	6.2
1	A	37	VAL	6.2
8	H	174	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
22	V	40	PRO	6.2
5	E	45	ASP	6.2
9	I	134	ILE	6.1
9	I	111	LEU	6.0
26	Z	106	SER	6.0
13	M	71	SER	5.9
4	D	61	PHE	5.9
9	I	104	ALA	5.9
4	D	107	GLY	5.9
20	T	117	ASP	5.8
13	M	74	LYS	5.8
24	X	88	GLU	5.7
4	D	135	VAL	5.7
9	I	100	VAL	5.7
9	I	116	LEU	5.7
20	T	119	ALA	5.7
9	I	71	ALA	5.6
9	I	124	VAL	5.6
9	I	117	THR	5.6
13	M	80	GLY	5.5
9	I	73	LEU	5.5
7	G	12	ILE	5.4
10	J	4	ALA	5.4
8	H	171	GLY	5.4
9	I	80	PHE	5.4
13	M	75	ARG	5.4
9	I	70	THR	5.3
5	E	6	GLU	5.3
30	0	2538	A	5.3
4	D	59	GLY	5.3
9	I	118	ASN	5.2
26	Z	46	SER	5.2
30	0	2645	U	5.2
9	I	103	ILE	5.2
14	N	154	LEU	5.1
26	Z	35	SER	5.1
2	B	1	PRO	5.0
13	M	79	ALA	5.0
4	D	62	ASP	5.0
14	N	161	GLY	5.0
30	0	10	U	5.0
14	N	165	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
12	L	75	LEU	4.9
4	D	44	ILE	4.9
10	J	70	PHE	4.9
4	D	172	VAL	4.9
14	N	167	ASP	4.8
9	I	88	GLN	4.8
31	9	2	U	4.8
4	D	35	ALA	4.8
9	I	122	GLU	4.8
9	I	67	VAL	4.8
14	N	164	ASP	4.8
4	D	157	LEU	4.8
30	0	2100	A	4.8
12	L	78	ALA	4.8
13	M	78	LYS	4.8
4	D	55	LYS	4.7
9	I	133	THR	4.7
5	E	10	ASP	4.6
30	0	2769	C	4.6
9	I	121	LYS	4.6
4	D	40	ILE	4.6
4	D	54	ALA	4.6
4	D	171	ASP	4.6
24	X	87	ALA	4.6
30	0	1161	A	4.5
9	I	114	TYR	4.5
9	I	84	SER	4.5
12	L	82	ALA	4.5
9	I	119	ALA	4.5
12	L	149	ARG	4.5
3	C	62	GLY	4.4
9	I	66	GLY	4.4
4	D	18	ILE	4.4
14	N	163	PHE	4.4
31	9	24	U	4.4
30	0	1162	G	4.4
9	I	97	VAL	4.4
9	I	123	VAL	4.4
4	D	134	LEU	4.4
4	D	74	THR	4.3
26	Z	34	SER	4.3
1	A	36	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
13	M	77	HIS	4.3
30	O	2748	G	4.3
22	V	43	PRO	4.3
1	A	31	LYS	4.3
4	D	36	ASN	4.2
14	N	160	SER	4.2
9	I	85	GLY	4.2
30	O	514	G	4.2
14	N	169	PRO	4.2
9	I	83	GLY	4.2
9	I	72	GLU	4.2
7	G	26	MET	4.2
5	E	154	ILE	4.2
13	M	89	THR	4.2
9	I	130	LEU	4.2
14	N	147	ILE	4.1
7	G	71	LEU	4.1
13	M	86	GLN	4.1
24	X	83	ALA	4.1
30	O	138	U	4.0
26	Z	45	VAL	4.0
9	I	91	PHE	4.0
30	O	2237	G	4.0
24	X	85	VAL	4.0
28	2	35	ARG	4.0
6	F	101	ALA	3.9
13	M	88	VAL	3.9
8	H	114	ASP	3.9
4	D	11	HIS	3.9
20	T	114	SER	3.9
20	T	118	SER	3.9
14	N	162	ASP	3.9
4	D	105	SER	3.9
30	O	2637	A	3.9
12	L	77	ALA	3.9
12	L	145	LEU	3.9
30	O	1175	G	3.8
4	D	106	PHE	3.8
30	O	1172	G	3.8
8	H	115	GLY	3.8
12	L	57	VAL	3.8
14	N	1	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
30	0	2345	A	3.8
13	M	76	ARG	3.8
9	I	108	HIS	3.8
4	D	66	GLY	3.8
30	0	1160	G	3.8
4	D	73	VAL	3.7
4	D	170	TYR	3.7
4	D	101	THR	3.7
9	I	82	THR	3.7
4	D	58	VAL	3.7
6	F	102	GLY	3.7
4	D	150	SER	3.7
30	0	1176	C	3.7
16	P	143	ALA	3.7
14	N	158	LEU	3.7
9	I	101	LYS	3.7
30	0	999	C	3.6
1	A	35	GLY	3.6
30	0	1177	A	3.6
31	9	23	U	3.6
4	D	130	VAL	3.6
3	C	63	SER	3.6
30	0	272	A	3.6
9	I	95	LEU	3.6
30	0	271	C	3.6
30	0	2747	C	3.6
4	D	86	THR	3.6
3	C	64	GLY	3.6
13	M	72	ALA	3.6
13	M	87	GLY	3.6
30	0	1173	A	3.5
12	L	148	GLU	3.5
6	F	118	LEU	3.5
25	Y	235	GLU	3.5
1	A	203	GLY	3.5
18	R	150	PRO	3.5
5	E	100	ASP	3.5
30	0	1524	U	3.5
4	D	37	ALA	3.4
12	L	150	GLN	3.4
5	E	11	VAL	3.4
30	0	1951	G	3.4

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Mol	Chain	Res	Type	RSRZ
4	D	88	LEU	3.4
13	M	81	ARG	3.4
29	3	41	GLU	3.4
22	V	36	ALA	3.4
4	D	17	ARG	3.4
30	0	1964	U	3.4
12	L	55	GLN	3.4
16	P	18	LYS	3.4
4	D	89	PRO	3.4
9	I	107	LYS	3.3
4	D	169	THR	3.3
2	B	168	GLY	3.3
7	G	73	ASP	3.3
15	O	23	GLY	3.3
9	I	109	PRO	3.3
26	Z	43	GLY	3.3
4	D	154	LYS	3.3
30	0	1199	A	3.3
9	I	110	ASP	3.3
25	Y	236	VAL	3.3
4	D	53	LYS	3.3
2	B	57	GLU	3.2
12	L	98	GLU	3.2
26	Z	36	GLY	3.2
4	D	69	ILE	3.2
4	D	142	ALA	3.2
8	H	43	ALA	3.2
2	B	2	GLN	3.2
26	Z	38	PHE	3.2
4	D	93	LEU	3.2
26	Z	42	TYR	3.2
4	D	60	GLU	3.2
1	A	38	ILE	3.2
5	E	7	ILE	3.2
19	S	81	ILE	3.2
20	T	116	ASP	3.2
4	D	128	LEU	3.2
24	X	65	ASN	3.2
26	Z	58	ASN	3.2
1	A	237	GLY	3.2
13	M	73	ARG	3.2
13	M	83	SER	3.2

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Mol	Chain	Res	Type	RSRZ
4	D	29	HIS	3.2
12	L	83	GLU	3.2
14	N	159	TYR	3.2
25	Y	95	THR	3.2
14	N	145	ALA	3.1
2	B	118	ASP	3.1
4	D	75	LEU	3.1
4	D	132	VAL	3.1
2	B	33	ASP	3.1
4	D	52	THR	3.1
5	E	20	ILE	3.1
9	I	69	PRO	3.1
4	D	56	ARG	3.1
6	F	99	THR	3.1
17	Q	17	LYS	3.1
30	0	1171	A	3.1
12	L	146	GLY	3.1
7	G	23	ILE	3.1
9	I	129	SER	3.0
13	M	68	ARG	3.0
1	A	32	VAL	3.0
28	2	37	HIS	3.0
1	A	34	ASP	3.0
30	0	2344	G	3.0
12	L	97	VAL	3.0
12	L	147	GLU	3.0
30	0	1188	A	3.0
12	L	79	ASP	3.0
30	0	1929	G	3.0
24	X	84	ILE	3.0
4	D	153	THR	3.0
4	D	91	ALA	3.0
30	0	1192	A	3.0
4	D	133	ASN	3.0
13	M	194	GLY	3.0
1	A	206	ARG	2.9
4	D	104	PHE	2.9
1	A	236	GLY	2.9
5	E	156	ASP	2.9
22	V	65	ASP	2.9
30	0	960	G	2.9
30	0	1190	G	2.9

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Mol	Chain	Res	Type	RSRZ
14	N	175	LEU	2.9
30	0	1525	G	2.9
12	L	44	GLU	2.9
4	D	138	GLY	2.9
2	B	119	HIS	2.8
6	F	8	VAL	2.8
9	I	68	PRO	2.8
12	L	143	THR	2.8
30	0	2768	A	2.8
28	2	48	ASP	2.8
4	D	92	GLU	2.8
5	E	12	ASP	2.8
6	F	117	GLU	2.8
30	0	1965	C	2.8
30	0	1189	A	2.8
19	S	21	GLN	2.8
6	F	119	ARG	2.8
14	N	134	ASP	2.8
3	C	61	PHE	2.8
14	N	150	TYR	2.8
9	I	96	SER	2.8
9	I	87	PRO	2.8
9	I	78	ALA	2.8
30	0	1164	U	2.8
1	A	211	LYS	2.8
12	L	99	GLU	2.8
30	0	128	A	2.8
30	0	1204	C	2.8
4	D	99	ASP	2.8
1	A	205	GLY	2.7
22	V	37	GLY	2.7
5	E	13	ALA	2.7
13	M	84	LYS	2.7
9	I	77	GLU	2.7
28	2	39	ARG	2.7
2	B	34	GLY	2.7
5	E	172	PRO	2.7
9	I	75	LYS	2.7
13	M	82	ARG	2.7
2	B	108	GLU	2.7
30	0	1966	U	2.7
9	I	79	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
6	F	9	PRO	2.7
9	I	92	VAL	2.7
12	L	81	VAL	2.7
12	L	76	LEU	2.7
1	A	66	ARG	2.7
11	K	27	ARG	2.7
21	U	47	ARG	2.7
4	D	65	GLU	2.7
6	F	105	ASP	2.7
4	D	166	ILE	2.7
22	V	46	ILE	2.7
30	0	1163	G	2.7
8	H	170	ARG	2.7
30	0	1170	U	2.7
30	0	1279	U	2.7
2	B	56	ASP	2.6
7	G	69	ARG	2.6
13	M	85	ARG	2.6
12	L	93	VAL	2.6
5	E	87	PHE	2.6
12	L	45	PRO	2.6
2	B	117	GLU	2.6
1	A	85	SER	2.6
30	0	1202	A	2.6
5	E	126	ILE	2.6
7	G	27	ILE	2.6
22	V	41	GLU	2.6
9	I	106	GLN	2.6
14	N	171	HIS	2.6
30	0	1182	C	2.6
4	D	26	GLY	2.6
4	D	137	PRO	2.6
30	0	1206	U	2.6
2	B	183	GLU	2.6
6	F	78	GLU	2.6
26	Z	49	ARG	2.5
12	L	101	ASP	2.5
15	O	22	GLY	2.5
26	Z	60	ASP	2.5
4	D	81	GLU	2.5
4	D	98	PHE	2.5
8	H	172	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
20	T	36	GLY	2.5
30	0	284	C	2.5
6	F	103	GLU	2.5
30	0	2541	U	2.5
2	B	318	ASN	2.5
14	N	95	ALA	2.5
9	I	126	THR	2.5
4	D	64	ARG	2.5
5	E	44	GLY	2.5
30	0	1191	A	2.5
24	X	7	GLU	2.5
4	D	165	PHE	2.5
14	N	180	LEU	2.5
1	A	33	GLU	2.5
4	D	102	GLY	2.5
9	I	89	GLU	2.5
14	N	170	GLU	2.5
29	3	57	GLY	2.5
30	0	1193	A	2.5
30	0	1184	C	2.5
28	2	16	ASN	2.5
30	0	1169	U	2.5
4	D	80	ALA	2.5
6	F	10	ALA	2.5
22	V	32	ALA	2.5
6	F	26	THR	2.5
30	0	1197	G	2.5
30	0	1948	G	2.5
1	A	68	ILE	2.4
3	C	132	ASP	2.4
4	D	77	ASP	2.4
6	F	16	ALA	2.4
30	0	1198	U	2.4
30	0	1165	G	2.4
30	0	1195	G	2.4
4	D	27	ILE	2.4
9	I	115	ASP	2.4
25	Y	108	ASP	2.4
9	I	93	ALA	2.4
30	0	510	U	2.4
9	I	135	GLU	2.4
24	X	82	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
8	H	37	GLY	2.4
14	N	138	ASP	2.4
4	D	50	VAL	2.4
15	O	24	ALA	2.4
4	D	45	THR	2.4
5	E	46	THR	2.4
12	L	60	GLU	2.4
6	F	111	ILE	2.4
9	I	90	ASP	2.4
22	V	31	ARG	2.4
4	D	13	MET	2.4
4	D	22	VAL	2.4
6	F	22	VAL	2.4
6	F	91	VAL	2.4
30	0	497	A	2.4
4	D	68	PRO	2.3
4	D	95	THR	2.3
22	V	38	GLY	2.3
1	A	153	ARG	2.3
14	N	184	ILE	2.3
2	B	139	ASP	2.3
6	F	7	ASP	2.3
3	C	245	GLU	2.3
14	N	148	ALA	2.3
19	S	12	GLU	2.3
30	0	2914	A	2.3
28	2	31	ARG	2.3
28	2	44	ARG	2.3
14	N	153	GLN	2.3
30	0	1205	U	2.3
30	0	1196	C	2.3
3	C	135	GLU	2.3
4	D	87	ALA	2.3
9	I	125	GLY	2.3
14	N	76	GLY	2.3
30	0	1187	U	2.3
7	G	72	ASP	2.3
4	D	19	GLU	2.3
8	H	169	GLU	2.3
2	B	21	SER	2.3
14	N	179	LEU	2.3
14	N	186	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	20	LYS	2.3
4	D	12	GLU	2.3
4	D	83	PHE	2.3
10	J	28	GLU	2.3
23	W	86	GLU	2.3
30	0	1186	C	2.3
2	B	171	VAL	2.3
4	D	156	ARG	2.3
14	N	81	ALA	2.2
7	G	67	LEU	2.2
8	H	39	LYS	2.2
30	0	1174	A	2.2
30	0	1178	G	2.2
4	D	49	PRO	2.2
4	D	141	VAL	2.2
4	D	163	VAL	2.2
26	Z	67	GLY	2.2
19	S	1	SER	2.2
30	0	1200	A	2.2
28	2	20	ARG	2.2
30	0	1523	G	2.2
2	B	286	ASN	2.2
4	D	158	ASN	2.2
6	F	69	GLU	2.2
30	0	288	A	2.2
14	N	157	PRO	2.2
30	0	970	U	2.2
26	Z	50	VAL	2.2
30	0	1159	G	2.2
26	Z	102	THR	2.2
4	D	41	LEU	2.2
4	D	16	PRO	2.2
6	F	1	PRO	2.2
6	F	49	PHE	2.2
4	D	21	VAL	2.1
12	L	91	VAL	2.1
30	0	883	U	2.2
30	0	1185	U	2.2
26	Z	40	ALA	2.1
4	D	131	THR	2.1
22	V	44	GLY	2.1
2	B	5	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	171	GLU	2.1
4	D	14	ARG	2.1
14	N	156	GLU	2.1
5	E	39	ASP	2.1
12	L	36	ASP	2.1
16	P	58	SER	2.1
8	H	143	VAL	2.1
26	Z	103	VAL	2.1
30	0	1561	U	2.1
7	G	70	ALA	2.1
13	M	1	ALA	2.1
30	0	1166	A	2.1
30	0	1181	A	2.1
24	X	22	ASN	2.1
5	E	123	ASP	2.1
12	L	102	ASP	2.1
30	0	282	C	2.1
31	9	122	C	2.1
6	F	115	VAL	2.1
31	9	57	A	2.1
31	9	65	A	2.1
18	R	13	THR	2.1
8	H	38	ARG	2.1
10	J	93	ARG	2.1
26	Z	104	ARG	2.1
2	B	66	GLU	2.1
10	J	5	GLU	2.1
24	X	79	GLU	2.1
1	A	64	ASP	2.1
6	F	100	ASP	2.1
8	H	41	LYS	2.1
2	B	172	SER	2.1
10	J	76	ASP	2.1
23	W	76	ASP	2.1
30	0	1167	G	2.1
30	0	1203	G	2.1
31	9	25	G	2.1
15	O	104	ASN	2.1
26	Z	105	ARG	2.1
30	0	1967	U	2.1
30	0	2512	U	2.1
8	H	81	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
9	I	131	GLY	2.1
20	T	115	GLU	2.1
9	I	76	ASP	2.1
17	Q	20	ASP	2.1
29	3	56	PRO	2.1
31	9	22	G	2.0
14	N	172	PHE	2.0
15	O	60	VAL	2.0
6	F	104	ALA	2.0
8	H	173	GLU	2.0
17	Q	95	GLU	2.0
29	3	92	GLU	2.0
4	D	100	ASP	2.0
5	E	86	VAL	2.0
10	J	6	PHE	2.0
21	U	56	ARG	2.0
22	V	45	ARG	2.0
6	F	112	ALA	2.0
12	L	62	ALA	2.0
14	N	67	ALA	2.0
30	0	2283	G	2.0
4	D	15	GLU	2.0
26	Z	53	ILE	2.0
30	0	1625	U	2.0
1	A	209	PRO	2.0
30	0	2506	A	2.0
3	C	1	MET	2.0
4	D	139	TYR	2.0
4	D	168	SER	2.0
8	H	86	TYR	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, 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($\text{\AA}^2$)	Q<0.9
30	UR3	0	2619	21/22	0.95	0.09	43,48,52,56	0
30	PSU	0	2621	20/21	0.97	0.07	29,31,42,42	0
30	OMG	0	2588	24/25	0.98	0.06	23,29,30,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	1MA	0	628	23/24	0.98	0.05	20,23,25,25	0
30	OMU	0	2587	21/22	0.98	0.06	23,27,29,29	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
34	SR	0	9006	1/1	0.48	0.20	199,199,199,199	0
32	MG	0	8010	1/1	0.65	0.19	69,69,69,69	0
32	MG	0	8038	1/1	0.67	0.13	80,80,80,80	0
32	MG	0	8037	1/1	0.67	0.39	77,77,77,77	0
37	K	0	8401	1/1	0.67	0.30	97,97,97,97	0
35	NA	0	8562	1/1	0.72	0.40	61,61,61,61	0
32	MG	0	8085	1/1	0.74	0.34	90,90,90,90	0
32	MG	0	8082	1/1	0.74	0.15	63,63,63,63	0
34	SR	0	8983	1/1	0.75	0.20	151,151,151,151	0
32	MG	0	8079	1/1	0.75	0.18	52,52,52,52	0
34	SR	0	8979	1/1	0.76	0.20	193,193,193,193	0
32	MG	0	8056	1/1	0.77	0.23	66,66,66,66	0
34	SR	0	8971	1/1	0.78	0.17	153,153,153,153	0
35	NA	0	8518	1/1	0.78	0.50	81,81,81,81	0
35	NA	0	8569	1/1	0.79	0.27	61,61,61,61	0
32	MG	B	8042	1/1	0.79	0.30	75,75,75,75	0
35	NA	0	8517	1/1	0.80	0.29	68,68,68,68	0
35	NA	0	8556	1/1	0.81	0.21	38,38,38,38	0
32	MG	0	8040	1/1	0.81	0.38	81,81,81,81	0
34	SR	0	8919	1/1	0.81	0.17	167,167,167,167	0
35	NA	0	8575	1/1	0.81	0.48	78,78,78,78	0
35	NA	0	8520	1/1	0.81	0.33	49,49,49,49	0
35	NA	0	8525	1/1	0.82	0.22	57,57,57,57	0
35	NA	0	8573	1/1	0.82	0.26	69,69,69,69	0
35	NA	0	8509	1/1	0.82	0.25	60,60,60,60	0
34	SR	0	9001	1/1	0.82	0.15	142,142,142,142	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8533	1/1	0.83	0.16	57,57,57,57	0
35	NA	0	8554	1/1	0.83	0.17	55,55,55,55	0
32	MG	0	8063	1/1	0.83	0.43	74,74,74,74	0
32	MG	0	8067	1/1	0.83	0.22	55,55,55,55	0
35	NA	0	8514	1/1	0.84	0.21	34,34,34,34	0
35	NA	0	8571	1/1	0.84	0.19	83,83,83,83	0
34	SR	0	8991	1/1	0.84	0.28	171,171,171,171	0
35	NA	0	8559	1/1	0.84	0.31	67,67,67,67	0
35	NA	0	8536	1/1	0.84	0.29	62,62,62,62	0
34	SR	0	9004	1/1	0.85	0.15	182,182,182,182	0
32	MG	0	8049	1/1	0.85	0.25	78,78,78,78	0
34	SR	0	8996	1/1	0.85	0.26	173,173,173,173	0
35	NA	0	8511	1/1	0.85	0.14	61,61,61,61	0
35	NA	9	8543	1/1	0.85	0.30	60,60,60,60	0
34	SR	0	8987	1/1	0.85	0.47	199,199,199,199	0
34	SR	0	8922	1/1	0.86	0.45	164,164,164,164	0
34	SR	0	8959	1/1	0.86	0.11	129,129,129,129	0
32	MG	0	8071	1/1	0.87	0.26	73,73,73,73	0
35	NA	0	8542	1/1	0.87	0.13	44,44,44,44	0
32	MG	0	8081	1/1	0.87	0.24	65,65,65,65	0
32	MG	0	8035	1/1	0.88	0.22	63,63,63,63	0
32	MG	0	8065	1/1	0.88	0.39	68,68,68,68	0
35	NA	0	8516	1/1	0.88	0.21	50,50,50,50	0
35	NA	0	8555	1/1	0.88	0.34	59,59,59,59	0
35	NA	0	8528	1/1	0.88	0.19	67,67,67,67	0
35	NA	0	8558	1/1	0.88	0.14	39,39,39,39	0
32	MG	0	8048	1/1	0.88	0.11	55,55,55,55	0
32	MG	0	8017	1/1	0.89	0.31	67,67,67,67	0
35	NA	0	8561	1/1	0.89	0.32	67,67,67,67	0
35	NA	0	8534	1/1	0.89	0.12	56,56,56,56	0
34	SR	0	8976	1/1	0.89	0.17	122,122,122,122	0
34	SR	9	8980	1/1	0.89	0.14	144,144,144,144	0
34	SR	9	9003	1/1	0.89	0.12	122,122,122,122	0
34	SR	0	8955	1/1	0.89	0.21	140,140,140,140	0
32	MG	0	8064	1/1	0.89	0.12	54,54,54,54	0
35	NA	9	8572	1/1	0.89	0.19	66,66,66,66	0
35	NA	0	8512	1/1	0.89	0.25	63,63,63,63	0
37	K	0	8402	1/1	0.89	0.15	77,77,77,77	0
35	NA	0	8504	1/1	0.90	0.10	34,34,34,34	0
32	MG	0	8076	1/1	0.90	0.11	52,52,52,52	0
34	SR	0	8949	1/1	0.90	0.35	184,184,184,184	0
35	NA	0	8564	1/1	0.90	0.10	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8565	1/1	0.90	0.12	39,39,39,39	0
32	MG	0	8089	1/1	0.90	0.09	48,48,48,48	0
35	NA	0	8535	1/1	0.90	0.19	55,55,55,55	0
34	SR	0	9002	1/1	0.90	0.19	141,141,141,141	0
32	MG	0	8045	1/1	0.90	0.18	40,40,40,40	0
34	SR	0	8986	1/1	0.90	0.22	136,136,136,136	0
34	SR	0	8962	1/1	0.90	0.38	165,165,165,165	0
34	SR	0	8989	1/1	0.90	0.18	149,149,149,149	0
35	NA	0	8522	1/1	0.90	0.15	52,52,52,52	0
34	SR	0	8993	1/1	0.91	0.14	154,154,154,154	0
35	NA	0	8526	1/1	0.91	0.10	43,43,43,43	0
34	SR	0	9007	1/1	0.91	0.45	178,178,178,178	0
35	NA	0	8557	1/1	0.91	0.26	63,63,63,63	0
32	MG	0	8069	1/1	0.91	0.13	75,75,75,75	0
34	SR	0	9000	1/1	0.91	0.12	125,125,125,125	0
32	MG	9	8074	1/1	0.91	0.28	42,42,42,42	0
32	MG	0	8044	1/1	0.91	0.17	62,62,62,62	0
32	MG	0	8080	1/1	0.91	0.10	54,54,54,54	0
35	NA	M	8539	1/1	0.92	0.10	34,34,34,34	0
35	NA	0	8546	1/1	0.92	0.13	51,51,51,51	0
32	MG	0	8066	1/1	0.92	0.29	67,67,67,67	0
35	NA	0	8570	1/1	0.92	0.08	35,35,35,35	0
32	MG	0	8016	1/1	0.92	0.12	75,75,75,75	0
34	SR	0	8969	1/1	0.92	0.32	115,115,115,115	0
32	MG	0	8092	1/1	0.92	0.08	53,53,53,53	0
34	SR	0	8990	1/1	0.92	0.11	132,132,132,132	0
32	MG	0	8050	1/1	0.92	0.15	63,63,63,63	0
34	SR	0	8957	1/1	0.92	0.19	149,149,149,149	0
34	SR	0	8981	1/1	0.92	0.14	115,115,115,115	0
32	MG	0	8030	1/1	0.93	0.19	51,51,51,51	0
34	SR	0	8994	1/1	0.93	0.36	173,173,173,173	0
32	MG	0	8078	1/1	0.93	0.10	52,52,52,52	0
35	NA	0	8552	1/1	0.93	0.19	51,51,51,51	0
35	NA	0	8553	1/1	0.93	0.20	61,61,61,61	0
35	NA	S	8510	1/1	0.93	0.08	32,32,32,32	0
34	SR	0	8902	1/1	0.93	0.38	112,112,112,112	0
35	NA	0	8574	1/1	0.93	0.27	47,47,47,47	0
32	MG	0	8041	1/1	0.93	0.11	52,52,52,52	0
32	MG	0	8007	1/1	0.93	0.14	53,53,53,53	0
34	SR	0	8944	1/1	0.93	0.14	117,117,117,117	0
34	SR	0	8975	1/1	0.93	0.11	114,114,114,114	0
32	MG	0	8090	1/1	0.93	0.07	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8560	1/1	0.94	0.17	67,67,67,67	0
34	SR	0	8982	1/1	0.94	0.22	116,116,116,116	0
32	MG	0	8068	1/1	0.94	0.09	50,50,50,50	0
35	NA	0	8563	1/1	0.94	0.30	64,64,64,64	0
32	MG	0	8047	1/1	0.94	0.22	66,66,66,66	0
33	CL	B	8819	1/1	0.94	0.14	57,57,57,57	0
35	NA	0	8545	1/1	0.94	0.16	40,40,40,40	0
32	MG	A	8051	1/1	0.94	0.12	51,51,51,51	0
32	MG	0	8073	1/1	0.94	0.14	72,72,72,72	0
34	SR	0	8974	1/1	0.94	0.14	119,119,119,119	0
32	MG	0	8084	1/1	0.94	0.18	59,59,59,59	0
35	NA	0	8523	1/1	0.94	0.10	48,48,48,48	0
32	MG	0	8062	1/1	0.94	0.17	46,46,46,46	0
32	MG	0	8077	1/1	0.94	0.06	34,34,34,34	0
35	NA	0	8506	1/1	0.94	0.06	44,44,44,44	0
32	MG	0	8002	1/1	0.94	0.08	33,33,33,33	0
35	NA	R	8532	1/1	0.95	0.05	32,32,32,32	0
32	MG	0	8070	1/1	0.95	0.06	50,50,50,50	0
35	NA	T	8537	1/1	0.95	0.05	26,26,26,26	0
34	SR	0	8963	1/1	0.95	0.09	135,135,135,135	0
35	NA	0	8505	1/1	0.95	0.18	37,37,37,37	0
34	SR	0	8997	1/1	0.95	0.14	115,115,115,115	0
34	SR	0	8951	1/1	0.95	0.07	99,99,99,99	0
34	SR	0	8985	1/1	0.95	0.23	98,98,98,98	0
35	NA	0	8544	1/1	0.95	0.22	53,53,53,53	0
34	SR	0	8970	1/1	0.95	0.08	73,73,73,73	0
33	CL	0	8816	1/1	0.95	0.19	49,49,49,49	0
35	NA	0	8548	1/1	0.95	0.26	41,41,41,41	0
34	SR	0	8988	1/1	0.95	0.12	110,110,110,110	0
34	SR	0	8956	1/1	0.95	0.11	111,111,111,111	0
34	SR	0	8938	1/1	0.95	0.14	102,102,102,102	0
32	MG	T	8057	1/1	0.95	0.18	32,32,32,32	0
35	NA	J	8538	1/1	0.95	0.05	47,47,47,47	0
34	SR	0	8960	1/1	0.95	0.09	100,100,100,100	0
34	SR	S	8961	1/1	0.96	0.08	98,98,98,98	0
32	MG	0	8087	1/1	0.96	0.05	33,33,33,33	0
35	NA	0	8521	1/1	0.96	0.16	70,70,70,70	0
32	MG	0	8043	1/1	0.96	0.07	51,51,51,51	0
32	MG	0	8027	1/1	0.96	0.03	36,36,36,36	0
32	MG	0	8091	1/1	0.96	0.10	50,50,50,50	0
34	SR	0	8992	1/1	0.96	0.25	108,108,108,108	0
32	MG	0	8029	1/1	0.96	0.10	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8059	1/1	0.96	0.04	31,31,31,31	0
33	CL	A	8809	1/1	0.96	0.14	51,51,51,51	0
32	MG	0	8025	1/1	0.96	0.09	40,40,40,40	0
35	NA	0	8508	1/1	0.96	0.06	36,36,36,36	0
35	NA	0	8541	1/1	0.96	0.10	33,33,33,33	0
35	NA	0	8566	1/1	0.96	0.08	37,37,37,37	0
35	NA	0	8567	1/1	0.96	0.33	59,59,59,59	0
32	MG	0	8026	1/1	0.96	0.06	44,44,44,44	0
34	SR	A	8929	1/1	0.96	0.12	78,78,78,78	0
34	SR	0	8958	1/1	0.96	0.04	57,57,57,57	0
34	SR	0	8984	1/1	0.96	0.06	75,75,75,75	0
35	NA	0	8547	1/1	0.96	0.14	49,49,49,49	0
34	SR	A	8977	1/1	0.96	0.09	88,88,88,88	0
35	NA	0	8549	1/1	0.96	0.16	73,73,73,73	0
35	NA	0	8550	1/1	0.96	0.20	37,37,37,37	0
35	NA	0	8551	1/1	0.96	0.08	40,40,40,40	0
34	SR	B	8950	1/1	0.96	0.08	83,83,83,83	0
34	SR	0	8998	1/1	0.97	0.07	99,99,99,99	0
34	SR	0	8939	1/1	0.97	0.04	62,62,62,62	0
32	MG	0	8039	1/1	0.97	0.16	42,42,42,42	0
34	SR	0	8946	1/1	0.97	0.05	75,75,75,75	0
33	CL	J	8802	1/1	0.97	0.06	49,49,49,49	0
33	CL	J	8821	1/1	0.97	0.07	52,52,52,52	0
33	CL	3	8804	1/1	0.97	0.05	48,48,48,48	0
33	CL	0	8803	1/1	0.97	0.09	38,38,38,38	0
32	MG	0	8075	1/1	0.97	0.05	37,37,37,37	0
35	NA	C	8503	1/1	0.97	0.09	19,19,19,19	0
32	MG	0	8031	1/1	0.97	0.07	39,39,39,39	0
35	NA	0	8530	1/1	0.97	0.15	41,41,41,41	0
32	MG	0	8088	1/1	0.97	0.05	25,25,25,25	0
35	NA	Q	8540	1/1	0.97	0.05	39,39,39,39	0
32	MG	0	8032	1/1	0.97	0.04	42,42,42,42	0
32	MG	0	8023	1/1	0.97	0.04	30,30,30,30	0
32	MG	0	8036	1/1	0.97	0.12	37,37,37,37	0
34	SR	0	8965	1/1	0.97	0.07	80,80,80,80	0
32	MG	0	8060	1/1	0.97	0.11	41,41,41,41	0
32	MG	Y	8086	1/1	0.97	0.04	30,30,30,30	0
35	NA	0	8507	1/1	0.97	0.07	19,19,19,19	0
34	SR	0	8926	1/1	0.97	0.10	69,69,69,69	0
34	SR	0	8995	1/1	0.97	0.09	94,94,94,94	0
34	SR	0	8972	1/1	0.97	0.21	121,121,121,121	0
36	CD	O	8705	1/1	0.97	0.07	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8015	1/1	0.97	0.09	50,50,50,50	0
35	NA	0	8513	1/1	0.97	0.07	32,32,32,32	0
35	NA	0	8527	1/1	0.98	0.05	35,35,35,35	0
32	MG	0	8083	1/1	0.98	0.03	35,35,35,35	0
35	NA	0	8529	1/1	0.98	0.07	29,29,29,29	0
32	MG	0	8014	1/1	0.98	0.09	23,23,23,23	0
33	CL	0	8811	1/1	0.98	0.05	54,54,54,54	0
33	CL	0	8812	1/1	0.98	0.06	43,43,43,43	0
33	CL	0	8813	1/1	0.98	0.05	34,34,34,34	0
32	MG	0	8053	1/1	0.98	0.17	45,45,45,45	0
33	CL	0	8822	1/1	0.98	0.21	46,46,46,46	0
34	SR	0	8964	1/1	0.98	0.05	76,76,76,76	0
34	SR	0	9008	1/1	0.98	0.03	59,59,59,59	0
34	SR	9	8968	1/1	0.98	0.07	96,96,96,96	0
32	MG	0	8001	1/1	0.98	0.03	9,9,9,9	0
34	SR	0	8966	1/1	0.98	0.05	68,68,68,68	0
34	SR	0	8967	1/1	0.98	0.06	86,86,86,86	0
32	MG	0	8072	1/1	0.98	0.04	36,36,36,36	0
32	MG	0	8008	1/1	0.98	0.10	27,27,27,27	0
34	SR	F	9005	1/1	0.98	0.07	77,77,77,77	0
32	MG	K	8054	1/1	0.98	0.03	20,20,20,20	0
34	SR	0	8973	1/1	0.98	0.05	79,79,79,79	0
34	SR	3	8999	1/1	0.98	0.05	63,63,63,63	0
35	NA	0	8501	1/1	0.98	0.05	30,30,30,30	0
35	NA	0	8502	1/1	0.98	0.26	52,52,52,52	0
32	MG	0	8018	1/1	0.98	0.11	13,13,13,13	0
34	SR	0	8910	1/1	0.98	0.13	60,60,60,60	0
34	SR	0	8915	1/1	0.98	0.04	58,58,58,58	0
32	MG	0	8020	1/1	0.98	0.10	22,22,22,22	0
32	MG	0	8093	1/1	0.98	0.06	29,29,29,29	0
34	SR	0	8925	1/1	0.98	0.06	55,55,55,55	0
32	MG	0	8022	1/1	0.98	0.04	7,7,7,7	0
34	SR	0	8928	1/1	0.98	0.04	67,67,67,67	0
34	SR	0	8931	1/1	0.98	0.04	61,61,61,61	0
34	SR	0	8933	1/1	0.98	0.04	54,54,54,54	0
35	NA	0	8515	1/1	0.98	0.06	28,28,28,28	0
35	NA	0	8568	1/1	0.98	0.17	33,33,33,33	0
32	MG	0	8033	1/1	0.98	0.05	45,45,45,45	0
32	MG	0	8034	1/1	0.98	0.04	25,25,25,25	0
34	SR	0	8941	1/1	0.98	0.03	60,60,60,60	0
35	NA	0	8519	1/1	0.98	0.11	29,29,29,29	0
32	MG	0	8013	1/1	0.98	0.04	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8024	1/1	0.98	0.06	45,45,45,45	0
33	CL	L	8810	1/1	0.98	0.10	43,43,43,43	0
33	CL	N	8807	1/1	0.98	0.08	43,43,43,43	0
35	NA	0	8524	1/1	0.98	0.07	27,27,27,27	0
34	SR	0	8953	1/1	0.98	0.06	76,76,76,76	0
33	CL	R	8806	1/1	0.98	0.07	28,28,28,28	0
34	SR	0	8942	1/1	0.99	0.03	55,55,55,55	0
34	SR	0	8943	1/1	0.99	0.03	49,49,49,49	0
32	MG	0	8021	1/1	0.99	0.06	24,24,24,24	0
34	SR	0	8945	1/1	0.99	0.03	71,71,71,71	0
35	NA	0	8531	1/1	0.99	0.04	17,17,17,17	0
34	SR	A	8930	1/1	0.99	0.04	57,57,57,57	0
34	SR	0	8947	1/1	0.99	0.06	73,73,73,73	0
34	SR	0	8948	1/1	0.99	0.03	57,57,57,57	0
32	MG	0	8012	1/1	0.99	0.06	4,4,4,4	0
32	MG	0	8005	1/1	0.99	0.03	29,29,29,29	0
33	CL	M	8818	1/1	0.99	0.04	22,22,22,22	0
34	SR	0	8954	1/1	0.99	0.05	60,60,60,60	0
34	SR	R	8912	1/1	0.99	0.03	55,55,55,55	0
32	MG	0	8052	1/1	0.99	0.03	29,29,29,29	0
34	SR	1	8952	1/1	0.99	0.02	47,47,47,47	0
33	CL	O	8808	1/1	0.99	0.07	52,52,52,52	0
32	MG	0	8003	1/1	0.99	0.04	24,24,24,24	0
34	SR	0	8904	1/1	0.99	0.07	20,20,20,20	0
34	SR	0	8906	1/1	0.99	0.04	50,50,50,50	0
34	SR	0	8907	1/1	0.99	0.08	50,50,50,50	0
34	SR	0	8908	1/1	0.99	0.03	46,46,46,46	0
33	CL	Y	8820	1/1	0.99	0.05	27,27,27,27	0
34	SR	0	8911	1/1	0.99	0.03	48,48,48,48	0
34	SR	0	8914	1/1	0.99	0.08	67,67,67,67	0
32	MG	0	8055	1/1	0.99	0.07	12,12,12,12	0
34	SR	0	8916	1/1	0.99	0.02	45,45,45,45	0
34	SR	0	8917	1/1	0.99	0.03	46,46,46,46	0
32	MG	0	8019	1/1	0.99	0.09	18,18,18,18	0
34	SR	0	8920	1/1	0.99	0.04	63,63,63,63	0
34	SR	0	8921	1/1	0.99	0.03	46,46,46,46	0
33	CL	0	8805	1/1	0.99	0.05	39,39,39,39	0
34	SR	0	8923	1/1	0.99	0.02	54,54,54,54	0
34	SR	0	8978	1/1	0.99	0.02	47,47,47,47	0
34	SR	0	8924	1/1	0.99	0.03	50,50,50,50	0
32	MG	0	8058	1/1	0.99	0.09	3,3,3,3	0
32	MG	0	8046	1/1	0.99	0.02	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	8927	1/1	0.99	0.06	58,58,58,58	0
32	MG	0	8011	1/1	0.99	0.05	26,26,26,26	0
33	CL	0	8814	1/1	0.99	0.11	35,35,35,35	0
33	CL	0	8815	1/1	0.99	0.06	38,38,38,38	0
34	SR	0	8934	1/1	0.99	0.03	52,52,52,52	0
34	SR	0	8935	1/1	0.99	0.02	54,54,54,54	0
34	SR	0	8936	1/1	0.99	0.02	44,44,44,44	0
32	MG	0	8061	1/1	0.99	0.07	17,17,17,17	0
33	CL	0	8817	1/1	0.99	0.09	33,33,33,33	0
36	CD	3	8704	1/1	0.99	0.06	63,63,63,63	0
34	SR	0	8940	1/1	0.99	0.03	62,62,62,62	0
33	CL	J	8801	1/1	0.99	0.07	42,42,42,42	0
32	MG	0	8009	1/1	1.00	0.16	1,1,1,1	0
34	SR	0	8901	1/1	1.00	0.04	35,35,35,35	0
32	MG	0	8028	1/1	1.00	0.11	1,1,1,1	0
34	SR	0	8903	1/1	1.00	0.07	36,36,36,36	0
32	MG	0	8004	1/1	1.00	0.04	13,13,13,13	0
34	SR	0	8905	1/1	1.00	0.11	43,43,43,43	0
34	SR	0	8918	1/1	1.00	0.10	45,45,45,45	0
34	SR	1	8913	1/1	1.00	0.02	32,32,32,32	0
32	MG	0	8006	1/1	1.00	0.14	1,1,1,1	0
36	CD	U	8701	1/1	1.00	0.08	62,62,62,62	0
36	CD	Z	8703	1/1	1.00	0.10	67,67,67,67	0
36	CD	1	8702	1/1	1.00	0.04	54,54,54,54	0
34	SR	3	8932	1/1	1.00	0.03	65,65,65,65	0
34	SR	0	8909	1/1	1.00	0.02	44,44,44,44	0
34	SR	0	8937	1/1	1.00	0.01	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.