



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 11:24 PM UTC

PDB ID : 3CC7 / pdb_00003cc7
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation C2487U
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-25
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

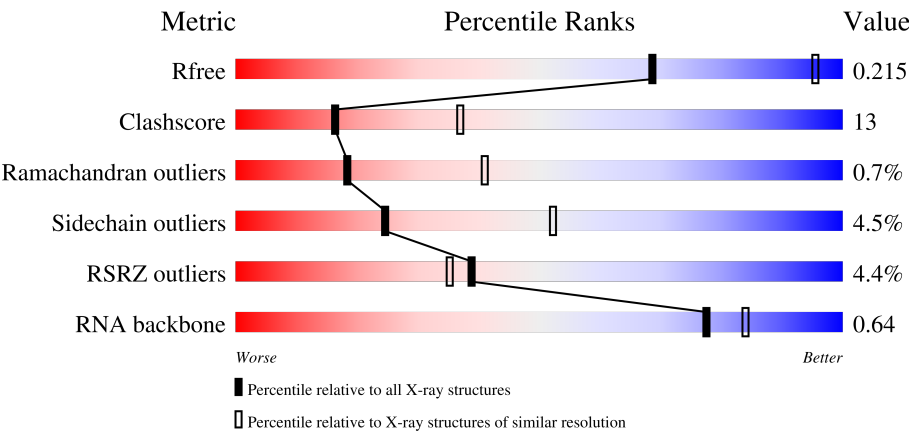
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	3% 68% 26% • •
2	B	338	2% 62% 33% •
3	C	246	% 72% 24% •
4	D	177	21% 46% 29% • • 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	2% 53% 35% 6% 6%
31	9	122	3% 38% 49% 13%

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99122 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
			59020	26349	10872	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	2	Total	Mg	0	0
			2	2		
32	B	2	Total	Mg	0	0
			2	2		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	0	85	Total	Mg	0	0
			85	85		
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	2	Total Sr 2 2	0	0
34	F	1	Total Sr 1 1	0	0
34	J	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	93	Total Sr 93 93	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	9	2	Total	Sr	0	0
			2	2		

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

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

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

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

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	111	Total O 111 111	0	0
38	B	153	Total O 153 153	0	0
38	C	165	Total O 165 165	0	0
38	D	46	Total O 46 46	0	0
38	E	44	Total O 44 44	0	0
38	F	23	Total O 23 23	0	0
38	G	19	Total O 19 19	0	0
38	H	71	Total O 71 71	0	0
38	I	10	Total O 10 10	0	0
38	J	54	Total O 54 54	0	0
38	K	56	Total O 56 56	0	0
38	L	80	Total O 80 80	0	0
38	M	130	Total O 130 130	0	0
38	N	59	Total O 59 59	0	0
38	O	41	Total O 41 41	0	0
38	P	61	Total O 61 61	0	0
38	Q	51	Total O 51 51	0	0
38	R	78	Total O 78 78	0	0
38	S	33	Total O 33 33	0	0
38	T	37	Total O 37 37	0	0
38	U	25	Total O 25 25	0	0

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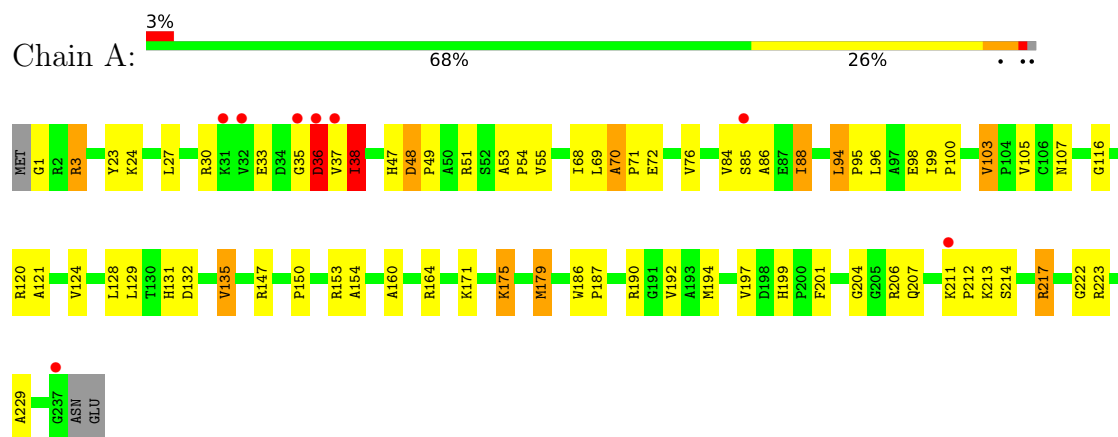
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	V	11	Total 11	O 11	0	0
38	W	63	Total 63	O 63	0	0
38	X	28	Total 28	O 28	0	0
38	Y	91	Total 91	O 91	0	0
38	Z	28	Total 28	O 28	0	0
38	1	52	Total 52	O 52	0	0
38	2	37	Total 37	O 37	0	0
38	3	68	Total 68	O 68	0	0
38	0	5951	Total 5951	O 5951	0	0
38	9	147	Total 147	O 147	0	0

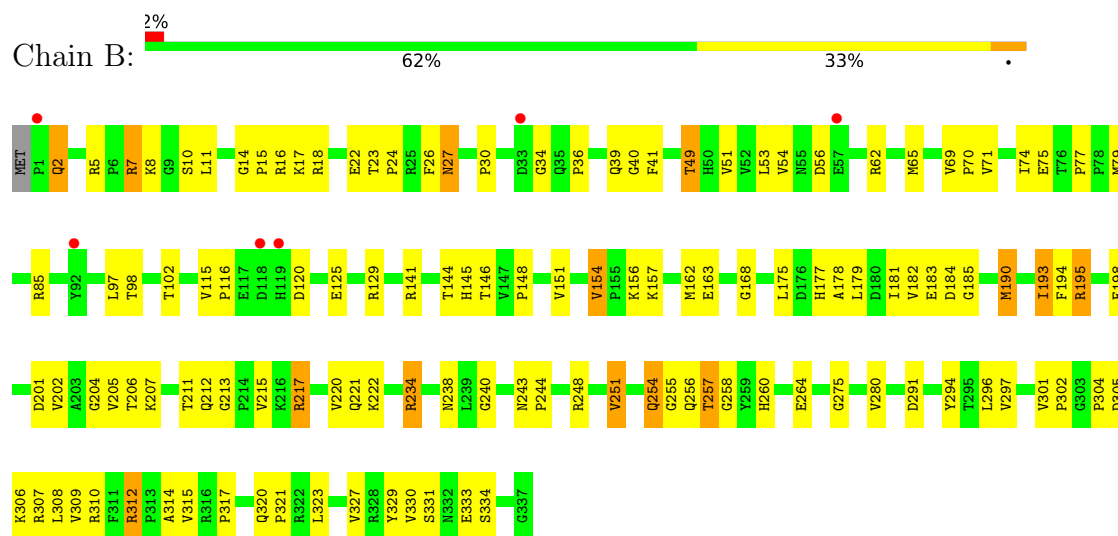
3 Residue-property plots

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

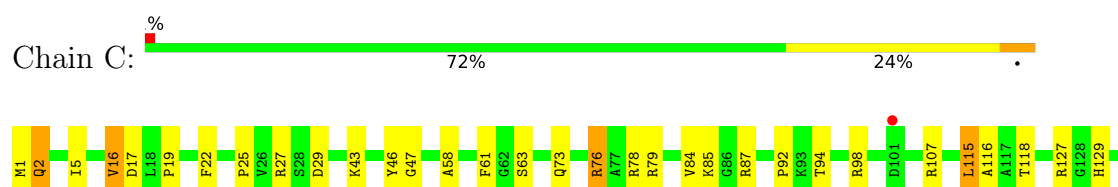
• Molecule 1: 50S ribosomal protein L2P

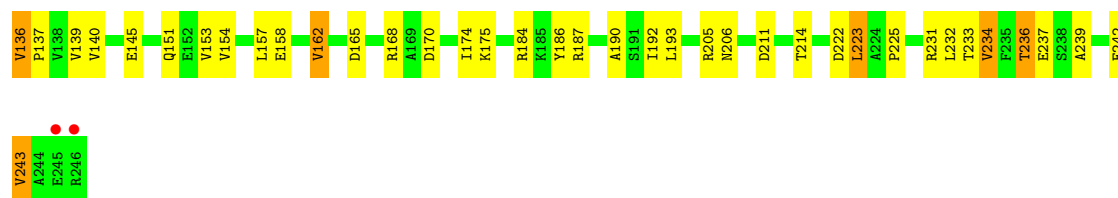


• Molecule 2: 50S ribosomal protein L3P

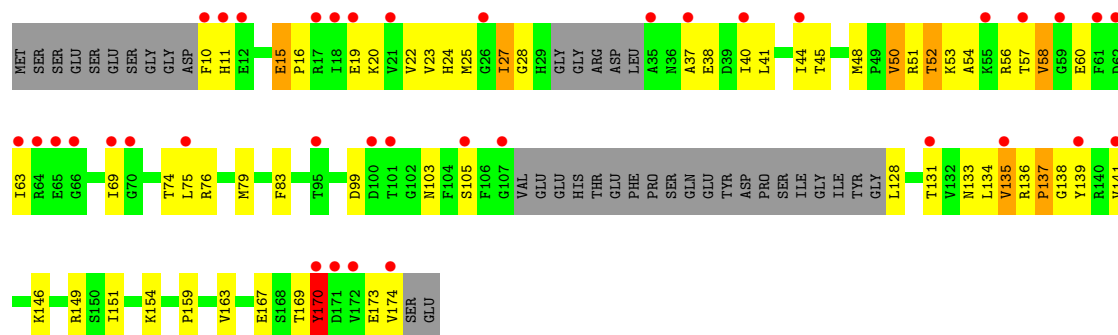


• Molecule 3: 50S ribosomal protein L4P

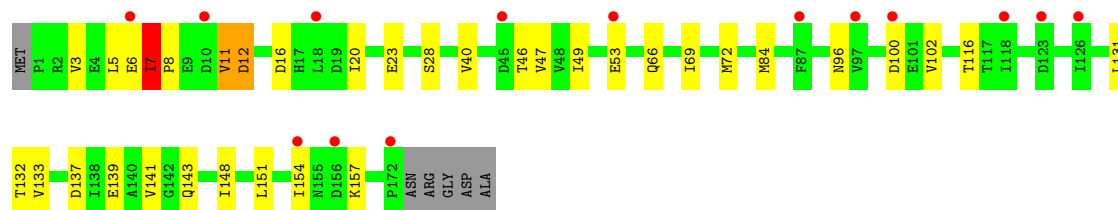
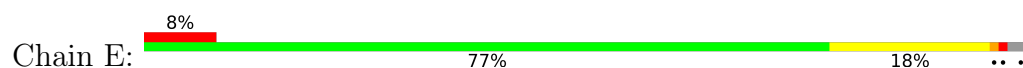




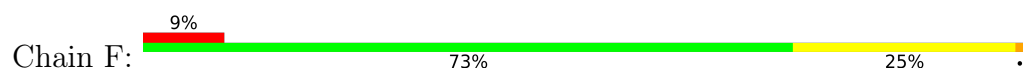
• Molecule 4: 50S ribosomal protein L5P



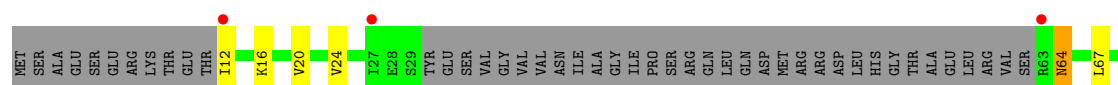
• Molecule 5: 50S ribosomal protein L6P

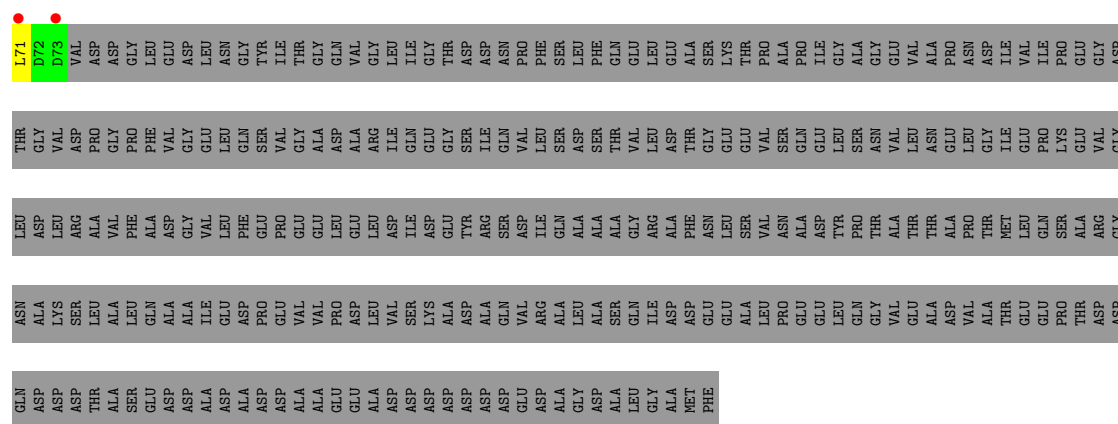


• Molecule 6: 50S ribosomal protein L7Ae

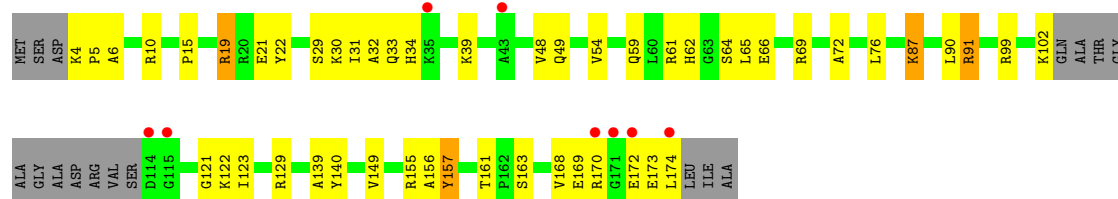


• Molecule 7: 50S ribosomal protein L10E

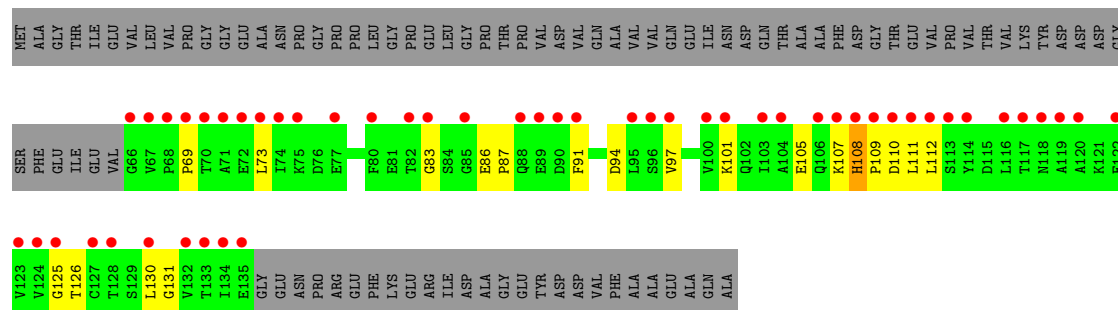




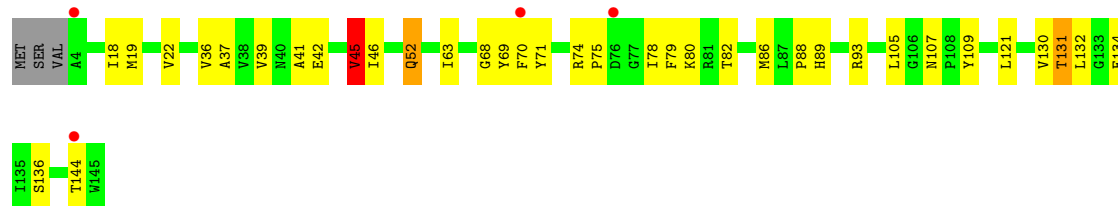
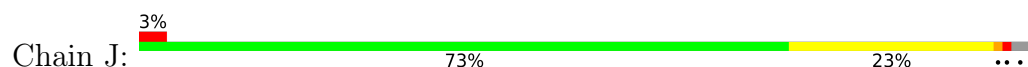
- Molecule 8: 50S ribosomal protein L10e



- Molecule 9: 50S ribosomal protein L11P

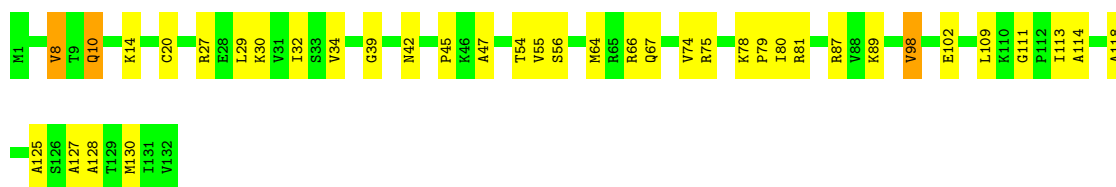


- Molecule 10: 50S ribosomal protein L13P



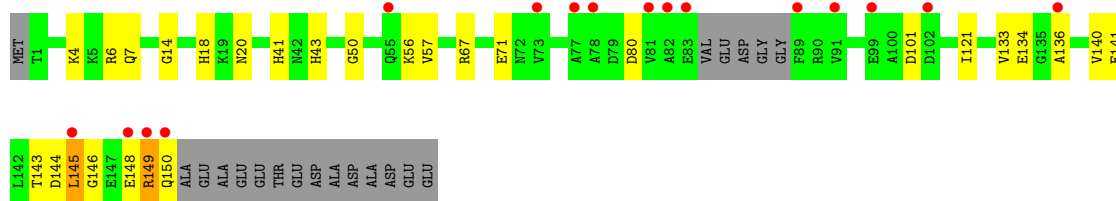
- Molecule 11: 50S ribosomal protein L14P

Chain K:  71% 27% .



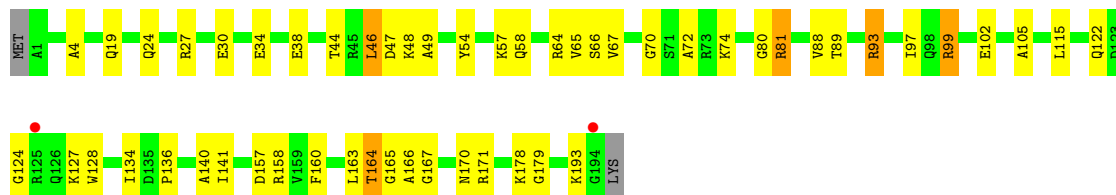
- Molecule 12: 50S ribosomal protein L15P

Chain L:  10% 71% 16% 12% .



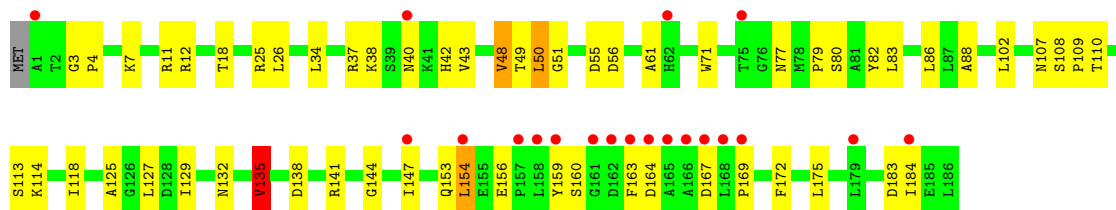
- Molecule 13: 50S ribosomal protein L15e

Chain M:  72% 24% . .



- Molecule 14: 50S ribosomal protein L18P

Chain N:  11% 68% 29% . . .

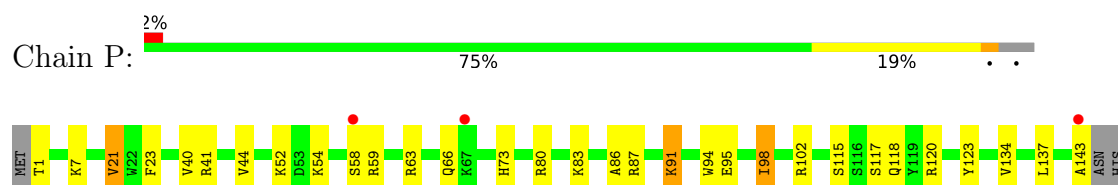


- Molecule 15: 50S ribosomal protein L18e

Chain O:  2% 78% 19% . .

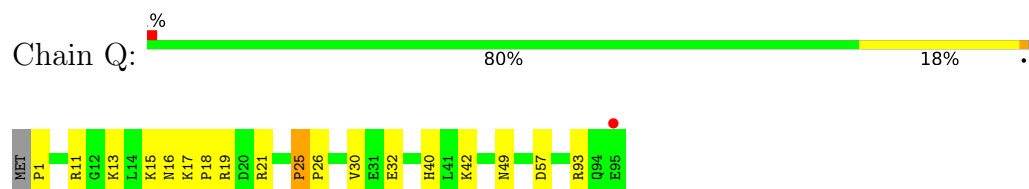


- Molecule 16: 50S ribosomal protein L19e

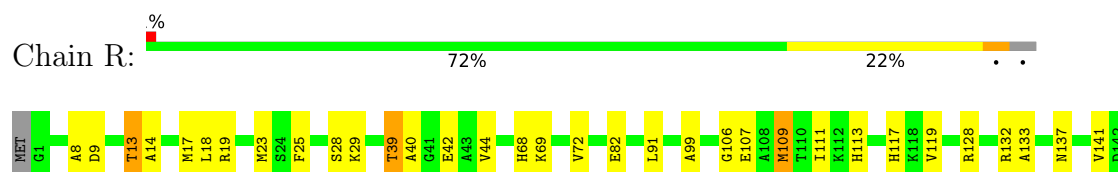


GLY
ASP
ALA

- Molecule 17: 50S ribosomal protein L21e

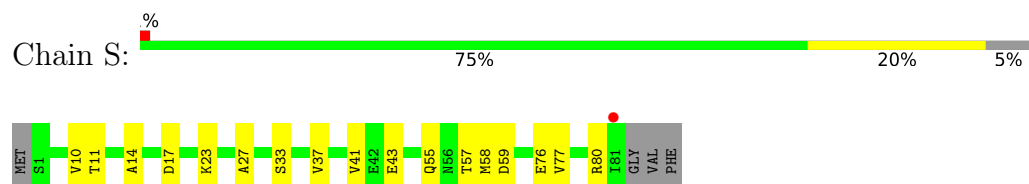


- Molecule 18: 50S ribosomal protein L22P

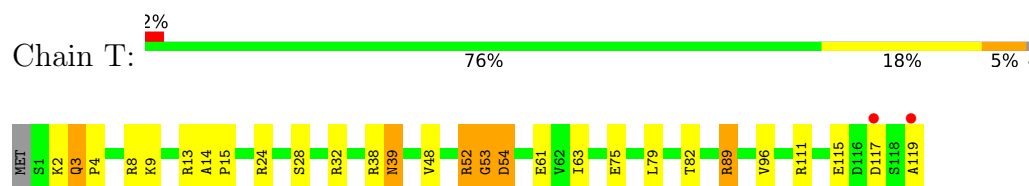


V143
E144
L145
I146
L147
E148
E149
P150
GLU
VAL
GLU
ASP

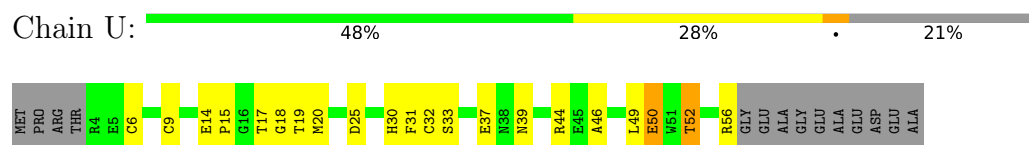
- Molecule 19: 50S ribosomal protein L23P



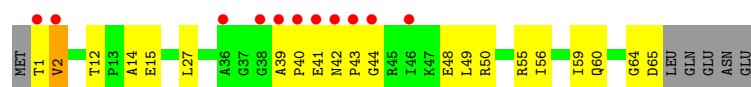
- Molecule 20: 50S ribosomal protein L24P



- Molecule 21: 50S ribosomal protein L24e



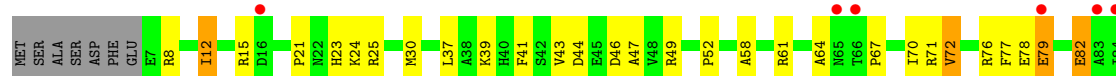
- Molecule 22: 50S ribosomal protein L29P



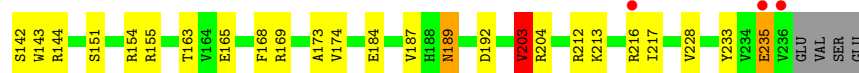
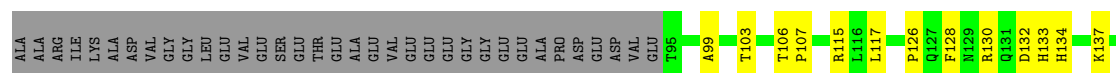
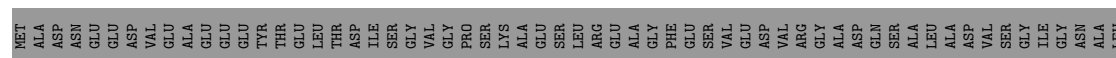
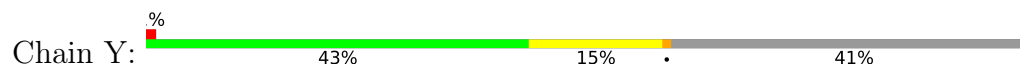
- Molecule 23: 50S ribosomal protein L30P



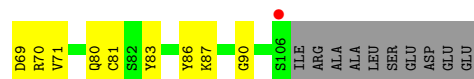
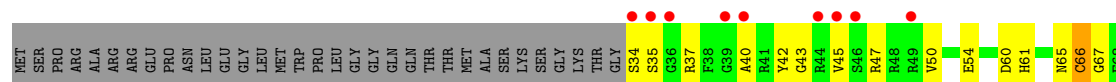
- Molecule 24: 50S ribosomal protein L31e



- Molecule 25: 50S ribosomal protein L32e



- Molecule 26: 50S ribosomal protein L37Ae



- Molecule 27: 50S ribosomal protein L37e

Chain 1: 



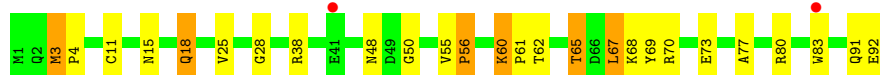
- Molecule 28: 50S ribosomal protein L39e

Chain 2: 



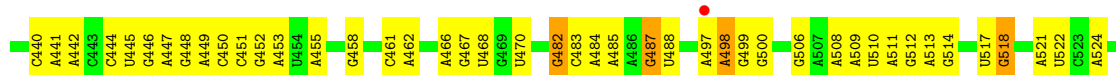
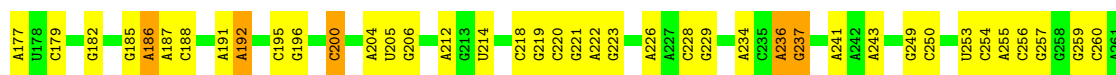
- Molecule 29: 50S ribosomal protein L44E

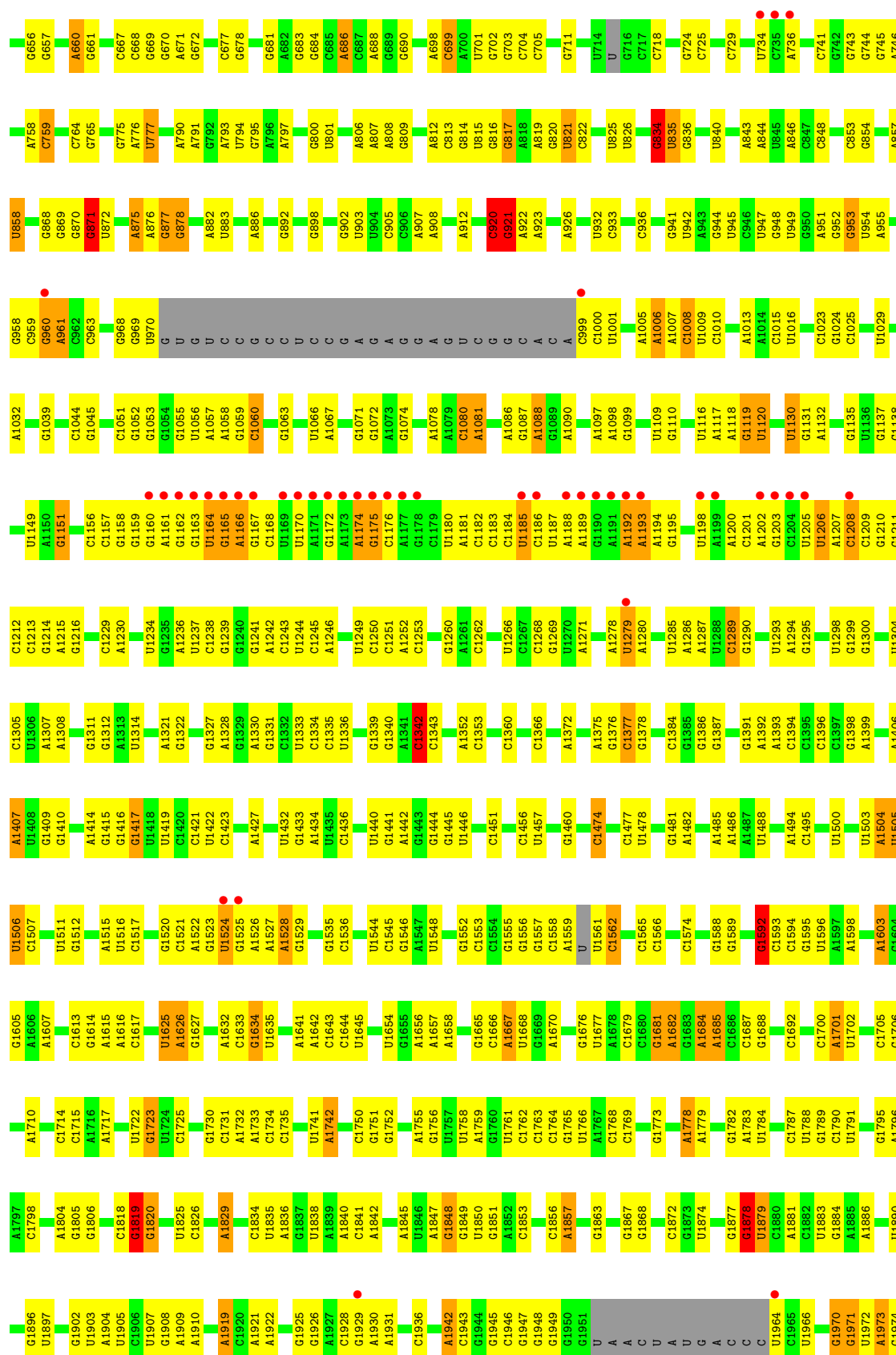
Chain 3: 

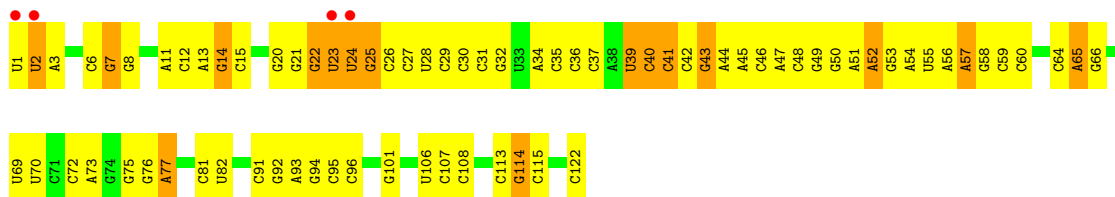


- Molecule 30: 23S ribosomal RNA

Chain 0: 







4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.83Å 299.90Å 576.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 2.70 49.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.83-2.70) 92.7 (49.83-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.184 , 0.226 0.175 , 0.215	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 74.5	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	99122	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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: NA, UR3, OMG, PSU, CL, 1MA, MG, SR, K, CD, OMU

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	0.42	0/1786	0.99	9/2408 (0.4%)
2	B	0.42	0/2690	1.02	16/3652 (0.4%)
3	C	0.44	0/1885	0.94	5/2552 (0.2%)
4	D	0.39	0/1111	0.93	6/1498 (0.4%)
5	E	0.38	0/1382	0.87	3/1880 (0.2%)
6	F	0.39	0/901	0.95	2/1224 (0.2%)
7	G	0.36	0/241	0.85	0/324
8	H	0.38	0/1302	0.92	4/1743 (0.2%)
9	I	0.36	0/526	0.86	0/716
10	J	0.42	0/1136	0.95	7/1530 (0.5%)
11	K	0.40	0/1004	0.95	4/1351 (0.3%)
12	L	0.38	0/1130	0.94	4/1509 (0.3%)
13	M	0.42	0/1582	0.89	3/2116 (0.1%)
14	N	0.37	0/1474	1.01	10/1999 (0.5%)
15	O	0.42	0/874	0.94	3/1181 (0.3%)
16	P	0.39	0/1147	0.85	0/1528
17	Q	0.42	0/749	1.02	5/1005 (0.5%)
18	R	1.29	7/1172 (0.6%)	1.40	8/1578 (0.5%)
19	S	0.36	0/648	0.89	2/875 (0.2%)
20	T	0.39	0/958	0.94	4/1289 (0.3%)
21	U	0.40	0/417	0.86	1/562 (0.2%)
22	V	0.39	0/502	0.97	3/675 (0.4%)
23	W	0.47	1/1219 (0.1%)	0.98	4/1655 (0.2%)
24	X	0.45	0/664	0.99	3/895 (0.3%)
25	Y	0.43	0/1146	0.91	3/1536 (0.2%)
26	Z	0.38	0/584	0.94	1/781 (0.1%)
27	1	0.40	0/438	0.84	0/578
28	2	0.41	0/401	0.77	0/529
29	3	0.38	0/771	0.87	6/1024 (0.6%)
30	0	0.37	0/65957	0.60	14/102867 (0.0%)
31	9	0.36	0/2904	0.59	2/4526 (0.0%)
All	All	0.41	8/98701 (0.0%)	0.72	132/147586 (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	42
31	9	0	1
All	All	1	43

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.40	2.86	1.49
18	R	150	PRO	CA-C	-17.39	1.16	1.52
18	R	150	PRO	CG-CD	13.53	1.96	1.50
18	R	150	PRO	N-CA	12.91	1.66	1.47
18	R	150	PRO	C-O	11.73	1.47	1.23
18	R	150	PRO	N-CD	10.87	1.62	1.47
18	R	150	PRO	CA-CB	7.63	1.68	1.53
23	W	13	MET	SD-CE	-5.00	1.67	1.79

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-28.56	55.83	110.10
18	R	150	PRO	N-CA-C	-20.16	61.69	112.10
18	R	150	PRO	N-CA-CB	12.25	116.48	103.00
18	R	150	PRO	CA-N-CD	12.10	128.94	112.00
14	N	163	PHE	N-CA-C	-8.93	102.18	113.43
17	Q	17	LYS	N-CA-C	-7.65	99.53	110.08
5	E	11	VAL	N-CA-C	7.55	119.95	109.45
2	B	157	LYS	N-CA-C	-7.47	104.78	114.04
24	X	79	GLU	N-CA-C	7.11	119.03	111.28
12	L	7	GLN	N-CA-C	7.08	120.03	111.82
20	T	3	GLN	CA-C-N	7.05	126.57	119.24
20	T	3	GLN	C-N-CA	7.05	126.57	119.24
24	X	77	PHE	N-CA-C	7.01	117.13	107.73
2	B	154	VAL	CA-C-N	6.96	126.21	118.97
2	B	154	VAL	C-N-CA	6.96	126.21	118.97
1	A	135	VAL	N-CA-C	6.90	117.46	108.35
18	R	141	VAL	N-CA-C	6.88	118.51	108.53
10	J	68	GLY	N-CA-C	6.87	121.38	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	GLY	N-CA-C	-6.82	105.78	114.37
29	3	55	VAL	CA-C-N	6.81	128.35	119.84
29	3	55	VAL	C-N-CA	6.81	128.35	119.84
14	N	51	GLY	CA-C-N	6.67	126.93	119.32
14	N	51	GLY	C-N-CA	6.67	126.93	119.32
20	T	52	ARG	N-CA-C	6.66	124.97	110.80
2	B	175	LEU	N-CA-C	-6.64	103.97	111.14
14	N	42	HIS	N-CA-C	6.63	118.59	109.18
25	Y	143	TRP	N-CA-C	6.47	119.66	109.96
18	R	150	PRO	CA-C-O	-6.41	99.77	119.00
18	R	150	PRO	CA-CB-CG	-6.36	92.41	104.50
3	C	205	ARG	N-CA-C	6.36	119.02	111.33
14	N	135	VAL	N-CA-C	-6.32	106.54	113.43
1	A	70	ALA	N-CA-C	6.30	118.75	109.50
30	0	920	C	C2'-C3'-O3'	-6.27	104.29	113.70
4	D	15	GLU	CA-C-N	6.27	127.68	119.84
4	D	15	GLU	C-N-CA	6.27	127.68	119.84
8	H	10	ARG	N-CA-C	6.26	118.91	111.71
13	M	89	THR	N-CA-C	6.25	117.76	111.07
6	F	62	HIS	N-CA-C	6.16	118.97	111.82
30	0	2291	A	N9-C1'-C2'	6.16	121.24	112.00
14	N	102	LEU	N-CA-C	6.15	118.01	109.15
31	9	39	U	N1-C1'-C2'	6.08	121.12	112.00
22	V	42	ASN	CA-C-N	6.07	127.43	119.84
22	V	42	ASN	C-N-CA	6.07	127.43	119.84
6	F	79	GLN	N-CA-C	6.06	118.77	108.90
2	B	222	LYS	N-CA-C	-6.05	101.04	110.42
14	N	153	GLN	N-CA-C	-6.00	101.40	110.70
12	L	80	ASP	N-CA-C	5.99	118.68	110.24
2	B	2	GLN	CA-C-N	5.91	125.92	119.89
2	B	2	GLN	C-N-CA	5.91	125.92	119.89
13	M	74	LYS	N-CA-C	5.88	119.05	109.59
30	0	1504	A	N9-C1'-C2'	5.87	120.80	112.00
8	H	161	THR	N-CA-C	5.84	120.84	113.25
30	0	2301	A	N9-C1'-C2'	5.79	120.69	112.00
4	D	170	TYR	N-CA-C	5.76	119.05	111.28
30	0	834	G	C2'-C3'-O3'	-5.75	105.08	113.70
20	T	54	ASP	N-CA-C	-5.72	106.26	113.18
11	K	54	THR	N-CA-C	-5.70	102.05	110.48
2	B	22	GLU	N-CA-C	-5.67	105.86	112.89
10	J	88	PRO	N-CA-C	-5.67	104.83	112.48
22	V	42	ASN	N-CA-C	-5.67	100.60	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	175	LYS	N-CA-C	5.63	117.56	110.24
17	Q	13	LYS	N-CA-C	5.63	118.96	111.75
1	A	213	LYS	N-CA-C	5.63	118.36	111.82
30	0	1819	G	C5'-C4'-C3'	5.62	124.42	116.00
30	0	1592	G	N9-C1'-C2'	5.61	120.41	112.00
30	0	2726	U	N1-C1'-C2'	5.59	120.38	112.00
1	A	129	LEU	N-CA-C	5.58	119.83	111.96
12	L	145	LEU	N-CA-C	-5.56	105.30	111.36
2	B	213	GLY	CA-C-N	5.53	125.19	119.05
2	B	213	GLY	C-N-CA	5.53	125.19	119.05
3	C	78	ARG	N-CA-C	5.53	116.37	108.74
4	D	135	VAL	N-CA-C	5.50	114.41	107.70
24	X	12	ILE	N-CA-C	5.48	112.97	107.55
13	M	70	GLY	N-CA-C	5.45	119.80	112.17
8	H	163	SER	N-CA-C	-5.45	102.42	110.48
11	K	8	VAL	N-CA-C	5.42	115.70	108.11
1	A	48	ASP	CA-C-N	5.42	125.24	119.28
1	A	48	ASP	C-N-CA	5.42	125.24	119.28
19	S	27	ALA	N-CA-C	-5.42	99.69	108.41
30	0	922	A	C4'-C3'-O3'	-5.39	104.92	113.00
14	N	48	VAL	N-CA-C	5.38	116.33	108.53
1	A	103	VAL	N-CA-C	5.37	114.39	108.05
18	R	137	ASN	N-CA-C	5.37	118.41	110.46
26	Z	42	TYR	N-CA-C	5.37	122.24	110.80
10	J	22	VAL	N-CA-C	-5.37	105.48	110.53
8	H	121	GLY	N-CA-C	5.37	118.23	112.33
29	3	67	LEU	N-CA-C	5.34	118.29	109.85
30	0	1120	U	C5'-C4'-C3'	-5.34	107.99	116.00
15	O	66	GLY	N-CA-C	5.33	125.81	113.18
5	E	7	ILE	CA-C-N	5.32	125.31	119.89
5	E	7	ILE	C-N-CA	5.32	125.31	119.89
2	B	120	ASP	CA-C-N	5.31	124.94	119.05
2	B	120	ASP	C-N-CA	5.31	124.94	119.05
21	U	50	GLU	N-CA-C	5.31	117.75	111.33
30	0	921	G	N9-C1'-C2'	5.30	119.96	112.00
4	D	151	ILE	CA-C-N	5.29	125.21	119.76
4	D	151	ILE	C-N-CA	5.29	125.21	119.76
3	C	192	ILE	N-CA-C	5.29	116.91	108.87
29	3	11	CYS	CA-C-N	5.28	124.95	119.56
29	3	11	CYS	C-N-CA	5.28	124.95	119.56
15	O	69	VAL	N-CA-C	5.26	115.54	108.17
23	W	9	GLY	N-CA-C	5.26	119.30	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	25	PRO	CA-C-N	5.26	125.06	119.28
17	Q	25	PRO	C-N-CA	5.26	125.06	119.28
30	0	871	G	C5'-C4'-O4'	-5.26	101.91	109.80
23	W	35	VAL	N-CA-C	5.25	113.61	107.89
25	Y	203	VAL	N-CA-C	5.24	117.09	108.97
29	3	60	LYS	N-CA-C	-5.23	102.60	110.24
23	W	142	ASP	N-CA-C	-5.23	103.78	110.53
10	J	89	HIS	N-CA-C	5.22	119.14	112.87
25	Y	173	ALA	N-CA-C	5.17	117.66	111.71
30	0	308	U	C2'-C3'-O3'	-5.17	105.94	113.70
11	K	111	GLY	CA-C-N	5.17	125.17	120.21
11	K	111	GLY	C-N-CA	5.17	125.17	120.21
2	B	151	VAL	CA-C-N	5.16	124.77	119.05
2	B	151	VAL	C-N-CA	5.16	124.77	119.05
2	B	193	ILE	N-CA-C	5.15	116.07	111.90
14	N	3	GLY	CA-C-N	5.14	124.64	119.19
14	N	3	GLY	C-N-CA	5.14	124.64	119.19
19	S	10	VAL	N-CA-C	5.13	114.14	106.85
3	C	186	TYR	N-CA-C	5.12	118.08	110.14
23	W	25	ASN	N-CA-C	5.12	118.66	111.90
17	Q	49	ASN	N-CA-C	5.08	117.96	110.59
12	L	20	ASN	N-CA-C	5.08	118.91	111.04
10	J	45	VAL	N-CA-C	5.05	117.09	108.86
1	A	24	LYS	N-CA-C	5.05	118.86	111.04
10	J	71	TYR	CA-C-N	5.04	124.96	119.76
10	J	71	TYR	C-N-CA	5.04	124.96	119.76
31	9	39	U	C4'-C3'-O3'	-5.04	105.44	113.00
30	0	206	G	C5'-C4'-C3'	-5.03	108.45	116.00
15	O	43	VAL	N-CA-C	5.03	115.21	108.17
2	B	217	ARG	N-CA-C	5.03	116.84	111.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1262	C	Sidechain

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Mol	Chain	Res	Type	Group
30	0	1342	C	Sidechain
30	0	1417	G	Sidechain
30	0	1432	U	Sidechain
30	0	1681	G	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1970	G	Sidechain
30	0	1979	G	Sidechain
30	0	2036	C	Sidechain
30	0	2115	U	Sidechain
30	0	221	G	Sidechain
30	0	2301	A	Sidechain
30	0	2312	G	Sidechain
30	0	2316	G	Sidechain
30	0	2412	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2524	G	Sidechain
30	0	2551	C	Sidechain
30	0	2564	G	Sidechain
30	0	26	U	Sidechain
30	0	2607	U	Sidechain
30	0	2679	G	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	686	A	Sidechain
30	0	817	G	Sidechain
30	0	903	U	Sidechain
31	9	94	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	77	0
2	B	2625	0	2533	95	0
3	C	1860	0	1813	57	0
4	D	1094	0	1085	44	0
5	E	1357	0	1266	26	0
6	F	890	0	843	26	0
7	G	240	0	231	6	0
8	H	1282	0	1292	39	0
9	I	519	0	500	15	0
10	J	1120	0	1098	32	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	23	0
13	M	1558	0	1573	43	0
14	N	1445	0	1401	46	0
15	O	865	0	873	15	0
16	P	1136	0	1123	28	0
17	Q	735	0	729	14	0
18	R	1149	0	1122	33	0
19	S	641	0	605	10	0
20	T	950	0	924	19	0
21	U	410	0	364	19	0
22	V	499	0	511	17	0
23	W	1196	0	1137	57	0
24	X	654	0	653	23	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	17	0
27	1	431	0	426	22	0
28	2	396	0	413	18	0
29	3	755	0	728	20	0
30	0	59020	0	29806	1146	0
31	9	2599	0	1325	104	0
32	0	85	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	10	0	0	2	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	0	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	93	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	2	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	J	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	2	0	0	0	0
35	S	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	5951	0	0	153	0
38	1	52	0	0	3	0
38	2	37	0	0	2	0
38	3	68	0	0	5	0
38	9	147	0	0	8	0
38	A	111	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	B	153	0	0	13	0
38	C	165	0	0	11	0
38	D	46	0	0	2	0
38	E	44	0	0	2	0
38	F	23	0	0	1	0
38	G	19	0	0	0	0
38	H	71	0	0	6	0
38	I	10	0	0	2	0
38	J	54	0	0	2	0
38	K	56	0	0	2	0
38	L	80	0	0	6	0
38	M	130	0	0	5	0
38	N	59	0	0	5	0
38	O	41	0	0	3	0
38	P	61	0	0	1	0
38	Q	51	0	0	2	0
38	R	78	0	0	3	0
38	S	33	0	0	2	0
38	T	37	0	0	2	0
38	U	25	0	0	3	0
38	V	11	0	0	0	0
38	W	63	0	0	4	0
38	X	28	0	0	1	0
38	Y	91	0	0	6	0
38	Z	28	0	0	3	0
All	All	99122	0	59907	1956	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 13.

All (1956) 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	1.96	1.44
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.12
30:0:1160:G:C5'	30:0:1161:A:H5'	1.81	1.10
31:9:56:A:H2'	31:9:57:A:H5''	1.33	1.08
30:0:871:G:C8	30:0:871:G:H5'	1.87	1.07
14:N:37:ARG:NH1	31:9:6:C:H5''	1.71	1.05
30:0:1160:G:H5'	30:0:1161:A:C5'	1.88	1.03
30:0:381:G:H5''	38:0:4345:HOH:O	1.58	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1160:G:H5'	30:0:1161:A:H5'	1.02	1.02
30:0:2812:A:H2	30:0:2814:A:H62	1.03	1.02
13:M:171:ARG:HD3	30:0:156:C:H5''	1.40	1.00
10:J:82:THR:HG23	30:0:1242:A:H5'	1.44	1.00
30:0:2717:C:C2'	30:0:2718:C:H5''	1.92	0.99
11:K:10:GLN:HE21	11:K:10:GLN:H	1.06	0.99
31:9:76:G:H3'	31:9:77:A:H5''	1.42	0.99
30:0:182:G:H5'	38:0:5188:HOH:O	1.63	0.98
30:0:871:G:H5'	30:0:871:G:H8	1.23	0.98
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.44	0.98
30:0:1666:C:O2'	30:0:1667:A:H5''	1.61	0.98
30:0:1118:A:H8	30:0:1118:A:H3'	1.29	0.97
30:0:2717:C:H2'	30:0:2718:C:H5''	1.46	0.97
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.46	0.96
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.47	0.96
30:0:1474:C:H6	30:0:1474:C:H5'	1.29	0.96
15:O:3:THR:HG22	30:0:656:G:H5'	1.46	0.96
30:0:1243:C:H3'	38:0:4869:HOH:O	1.65	0.95
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.12	0.94
30:0:1187:U:HO2'	30:0:1189:A:H2	1.07	0.94
3:C:236:THR:HG22	3:C:239:ALA:H	1.31	0.94
30:0:282:C:O2'	30:0:283:U:H5'	1.68	0.93
2:B:62:ARG:HA	2:B:65:MET:HE3	1.51	0.92
16:P:115:SER:H	16:P:118:GLN:HE21	0.95	0.92
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.84	0.92
30:0:69:A:H5'	30:0:69:A:H8	1.33	0.92
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.14	0.92
30:0:871:G:H8	30:0:871:G:C5'	1.83	0.91
30:0:1205:U:H2'	30:0:1206:U:C5'	2.00	0.91
30:0:2491:G:H1'	38:0:6910:HOH:O	1.70	0.91
30:0:69:A:H5'	30:0:69:A:C8	2.06	0.91
30:0:1118:A:H3'	30:0:1118:A:C8	2.04	0.91
23:W:149:LEU:HG	23:W:153:MET:HE2	1.50	0.91
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.51	0.91
30:0:2533:C:H5'	30:0:2533:C:H6	1.35	0.90
8:H:49:GLN:HE21	8:H:140:TYR:HE2	1.15	0.90
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.53	0.90
4:D:154:LYS:H	4:D:154:LYS:HD2	1.37	0.89
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.89
30:0:1603:A:H5'	30:0:1605:G:O4'	1.72	0.89
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1474:C:H5'	30:0:1474:C:C6	2.08	0.89
30:0:1701:A:H5'	38:0:6316:HOH:O	1.73	0.89
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.19	0.89
30:0:1183:C:H2'	38:0:6276:HOH:O	1.73	0.89
30:0:1184:C:H1'	38:0:7504:HOH:O	1.71	0.88
30:0:542:A:H5'	30:0:542:A:H8	1.38	0.88
30:0:282:C:H1'	30:0:368:C:N4	1.88	0.88
30:0:1666:C:C2'	30:0:1667:A:H5''	2.03	0.88
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.88
30:0:877:G:H5'	30:0:878:G:OP1	1.74	0.88
30:0:2251:G:H2'	30:0:2252:A:C8	2.09	0.87
2:B:238:ASN:HD22	2:B:240:GLY:H	1.20	0.87
30:0:558:C:C2'	30:0:559:U:H5''	2.04	0.87
30:0:1206:U:H5'	30:0:1206:U:H6	1.40	0.87
31:9:56:A:C2'	31:9:57:A:H5''	2.05	0.86
31:9:14:G:H5'	31:9:14:G:H8	1.39	0.86
2:B:162:MET:HE1	2:B:308:LEU:HD21	1.56	0.86
30:0:10:U:H3'	30:0:10:U:H6	1.40	0.86
14:N:37:ARG:HH12	31:9:6:C:H5''	1.37	0.86
30:0:1372:A:H3'	38:0:7227:HOH:O	1.76	0.85
30:0:1701:A:H4'	30:0:1702:U:H5''	1.56	0.85
16:P:117:SER:HB3	30:0:1593:C:OP1	1.77	0.85
30:0:506:G:H22	30:0:509:A:C5'	1.88	0.85
30:0:871:G:C8	30:0:871:G:C5'	2.59	0.85
30:0:1205:U:H2'	30:0:1206:U:H5'	1.56	0.84
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.59	0.84
30:0:545:G:H5'	30:0:545:G:H8	1.39	0.84
30:0:1118:A:H62	30:0:1244:U:H3	1.25	0.84
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.60	0.84
30:0:1667:A:H8	30:0:1667:A:H5'	1.41	0.84
30:0:1116:U:H3	30:0:1246:A:H62	1.26	0.84
30:0:2502:C:C2'	30:0:2503:A:H5'	2.08	0.83
30:0:2506:A:HO2'	30:0:2507:G:H8	0.88	0.83
30:0:541:C:C2'	30:0:542:A:H5''	2.08	0.83
30:0:2769:C:C2'	30:0:2770:G:H5'	2.07	0.83
30:0:214:U:H5'	38:0:6173:HOH:O	1.77	0.83
30:0:1300:G:H1'	38:0:4714:HOH:O	1.78	0.83
30:0:506:G:H22	30:0:509:A:H5'	1.42	0.82
30:0:541:C:H2'	30:0:542:A:H5''	1.60	0.82
30:0:1189:A:H1'	30:0:1209:C:O4'	1.79	0.82
30:0:396:U:H1'	38:0:7666:HOH:O	1.77	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:41:HIS:H	28:2:45:ASN:HD22	1.25	0.82
30:0:1878:G:H1'	38:0:6153:HOH:O	1.79	0.82
30:0:2502:C:H2'	30:0:2503:A:H5'	1.60	0.82
30:0:2506:A:O2'	30:0:2507:G:H8	1.61	0.82
23:W:88:THR:HB	38:W:6679:HOH:O	1.80	0.82
30:0:1183:C:N4	30:0:1184:C:H41	1.78	0.81
30:0:236:A:H4'	30:0:237:G:H5'	1.62	0.81
30:0:1116:U:O2'	30:0:1118:A:H2	1.63	0.81
30:0:1116:U:HO2'	30:0:1118:A:H2	0.82	0.81
30:0:544:G:H2'	30:0:545:G:H5''	1.63	0.81
11:K:39:GLY:HA2	38:0:5251:HOH:O	1.79	0.81
30:0:2783:A:H3'	38:0:5262:HOH:O	1.80	0.81
30:0:559:U:H6	30:0:559:U:H5'	1.43	0.81
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.61	0.81
30:0:558:C:O2'	30:0:559:U:H5''	1.79	0.81
30:0:380:A:H2'	38:0:7266:HOH:O	1.81	0.80
30:0:1632:A:H2'	30:0:1633:C:H5'	1.63	0.80
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.28	0.80
30:0:1189:A:H3'	38:0:7718:HOH:O	1.80	0.80
30:0:2291:A:C8	30:0:2309:C:H5'	2.16	0.80
30:0:2586:U:H3	30:0:2592:G:H22	1.26	0.80
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.78	0.80
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.64	0.80
30:0:2426:G:H1'	38:0:6125:HOH:O	1.82	0.80
30:0:1603:A:H5''	30:0:1605:G:H5'	1.63	0.80
16:P:115:SER:H	16:P:118:GLN:NE2	1.77	0.80
30:0:1741:U:H5'	30:0:1742:A:OP1	1.82	0.80
30:0:1119:G:N2	30:0:1246:A:C2	2.49	0.79
30:0:2533:C:H5'	30:0:2533:C:C6	2.15	0.79
3:C:139:VAL:HG13	38:C:8641:HOH:O	1.82	0.79
15:O:3:THR:CG2	30:0:656:G:H5'	2.11	0.79
30:0:541:C:H2'	30:0:542:A:C5'	2.12	0.79
30:0:2851:G:O2'	30:0:2852:A:H5'	1.83	0.79
20:T:9:LYS:HE3	20:T:13:ARG:NH1	1.98	0.79
30:0:2896:A:H5''	38:0:6132:HOH:O	1.81	0.78
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.18	0.78
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.65	0.78
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.48	0.78
30:0:2827:A:H2'	30:0:2828:G:O4'	1.83	0.78
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.13	0.78
33:0:8813:CL:CL	38:0:4714:HOH:O	2.39	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.63	0.77
30:0:1634:G:H3'	38:0:3915:HOH:O	1.84	0.77
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.49	0.77
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.99	0.77
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.33	0.77
30:0:2769:C:O2'	30:0:2770:G:H5'	1.85	0.77
30:0:1666:C:H2'	30:0:1667:A:C5'	2.14	0.77
13:M:164:THR:HG22	13:M:167:GLY:H	1.50	0.77
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.76
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.50	0.76
22:V:50:ARG:HH12	30:0:56:G:H5''	1.48	0.76
5:E:143:GLN:NE2	30:0:2779:G:H21	1.82	0.76
30:0:1209:C:H2'	30:0:1210:G:H8	1.50	0.76
30:0:2908:A:H2'	30:0:2909:G:O4'	1.85	0.76
30:0:282:C:H1'	30:0:368:C:H42	1.50	0.76
3:C:174:ILE:HD11	30:0:338:C:H4'	1.66	0.76
30:0:558:C:H2'	30:0:559:U:C5'	2.15	0.76
30:0:1080:C:H4'	30:0:1081:A:OP1	1.85	0.76
31:9:2:U:OP2	31:9:3:A:H5'	1.86	0.76
30:0:2768:A:O2'	30:0:2769:C:H5'	1.86	0.76
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.68	0.76
30:0:2004:U:H4'	38:0:5338:HOH:O	1.86	0.76
30:0:31:C:H4'	38:0:7463:HOH:O	1.87	0.75
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.68	0.75
30:0:2637:A:H5'	38:0:4961:HOH:O	1.85	0.75
30:0:2717:C:O2'	30:0:2718:C:H5''	1.86	0.75
30:0:283:U:H5	30:0:284:C:C4	2.05	0.74
30:0:1973:A:H5'	30:0:1973:A:H8	1.52	0.74
30:0:2239:C:H2'	30:0:2240:U:H6	1.52	0.74
30:0:603:A:H5''	30:0:604:G:OP1	1.87	0.74
10:J:19:MET:HE2	10:J:79:PHE:HA	1.69	0.74
28:2:41:HIS:HD2	28:2:44:ARG:H	1.35	0.74
30:0:2748:G:H5'	38:0:7579:HOH:O	1.85	0.74
30:0:2851:G:C2'	30:0:2852:A:H5'	2.17	0.74
30:0:179:C:H5''	38:0:9320:HOH:O	1.86	0.74
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.69	0.74
30:0:1118:A:C8	30:0:1118:A:C3'	2.69	0.74
30:0:2559:C:H4'	38:0:7294:HOH:O	1.86	0.74
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.69	0.74
14:N:113:SER:HB2	38:N:8854:HOH:O	1.87	0.74
30:0:272:A:H5'	30:0:273:G:OP2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:14:G:H5'	31:9:14:G:C8	2.23	0.74
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.69	0.73
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.69	0.73
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.71	0.73
30:0:1942:A:H3'	38:0:7386:HOH:O	1.88	0.73
30:0:1180:U:H2'	30:0:1181:A:O4'	1.89	0.73
16:P:115:SER:N	16:P:118:GLN:HE21	1.79	0.73
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.88	0.73
30:0:10:U:H3'	30:0:10:U:C6	2.23	0.73
30:0:1183:C:H42	30:0:1184:C:H41	1.35	0.73
30:0:2717:C:H2'	30:0:2718:C:C5'	2.19	0.73
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.71	0.72
11:K:10:GLN:H	11:K:10:GLN:NE2	1.83	0.72
30:0:338:C:H5''	38:0:3821:HOH:O	1.89	0.72
30:0:1205:U:H2'	30:0:1206:U:H5''	1.70	0.72
31:9:49:G:O2'	31:9:50:G:H5'	1.88	0.72
30:0:1279:U:O2	30:0:1279:U:H2'	1.88	0.72
30:0:2256:G:O2'	30:0:2257:G:H5'	1.88	0.72
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.87	0.72
18:R:39:THR:HG22	18:R:42:GLU:H	1.53	0.72
30:0:2420:G:O2'	30:0:2421:G:H5'	1.90	0.72
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.70	0.71
30:0:1666:C:H2'	30:0:1667:A:H5'	1.72	0.71
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.73	0.71
30:0:544:G:C2'	30:0:545:G:H5''	2.20	0.71
30:0:1666:C:C2'	30:0:1667:A:C5'	2.68	0.71
18:R:9:ASP:O	18:R:13:THR:HB	1.89	0.71
30:0:558:C:H2'	30:0:559:U:H5''	1.70	0.71
30:0:1632:A:C2'	30:0:1633:C:H5'	2.19	0.71
30:0:2679:G:H2'	30:0:2681:A:OP2	1.91	0.71
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.37	0.71
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.72	0.71
30:0:2010:A:H2'	38:0:5990:HOH:O	1.90	0.71
30:0:2578:G:H5'	30:0:2578:G:H8	1.54	0.71
30:0:1964:U:H2'	30:0:1964:U:O2	1.91	0.71
31:9:92:G:H2'	31:9:93:A:C8	2.26	0.71
2:B:190:MET:HE2	2:B:194:PHE:HD1	1.53	0.70
30:0:1157:C:H2'	30:0:1158:G:H8	1.56	0.70
30:0:2635:A:O2'	30:0:2636:C:H5'	1.90	0.70
30:0:2769:C:H2'	30:0:2770:G:O4'	1.91	0.70
31:9:39:U:H1'	31:9:44:A:H61	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.27	0.70
30:0:1527:A:H1'	30:0:1528:A:C8	2.27	0.70
3:C:174:ILE:CD1	30:0:338:C:H4'	2.21	0.70
30:0:1174:A:C5	30:0:1201:C:H4'	2.26	0.70
30:0:31:C:H2'	38:0:7726:HOH:O	1.89	0.70
30:0:1701:A:H4'	30:0:1702:U:C5'	2.20	0.70
22:V:1:THR:HG23	22:V:2:VAL:H	1.56	0.70
30:0:2852:A:H5''	38:0:5264:HOH:O	1.91	0.70
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.05	0.69
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.07	0.69
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.74	0.69
12:L:148:GLU:HA	38:L:8870:HOH:O	1.92	0.69
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.73	0.69
30:0:308:U:H5'	30:0:309:C:OP1	1.91	0.69
30:0:1165:G:O2'	30:0:1174:A:H1'	1.92	0.69
30:0:2507:G:H2'	30:0:2510:C:H42	1.57	0.69
31:9:29:C:H2'	31:9:30:C:H5'	1.73	0.69
3:C:1:MET:HG2	3:C:2:GLN:H	1.55	0.69
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.92	0.69
30:0:814:G:H4'	38:0:3155:HOH:O	1.91	0.69
30:0:1603:A:C5'	30:0:1605:G:H5'	2.22	0.69
31:9:1:U:H4'	31:9:3:A:OP1	1.92	0.69
12:L:133:VAL:HA	38:L:8871:HOH:O	1.92	0.69
30:0:545:G:H5'	30:0:545:G:C8	2.25	0.69
2:B:217:ARG:HG3	2:B:257:THR:HB	1.75	0.68
30:0:281:U:H2'	30:0:282:C:O4'	1.94	0.68
31:9:7:G:H5'	38:9:9099:HOH:O	1.93	0.68
38:Y:8852:HOH:O	33:0:8817:CL:CL	2.49	0.68
14:N:37:ARG:NH1	31:9:6:C:C5'	2.53	0.68
2:B:258:GLY:H	2:B:260:HIS:CE1	2.12	0.68
10:J:70:PHE:HD1	30:0:2676:C:HO2'	1.39	0.68
30:0:1120:U:H5''	30:0:1120:U:C6	2.29	0.68
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.07	0.68
30:0:1819:G:H2'	30:0:1820:G:H4'	1.74	0.68
30:0:870:G:C2'	30:0:871:G:H5''	2.23	0.68
30:0:2256:G:C2'	30:0:2257:G:H5'	2.23	0.68
2:B:244:PRO:HB3	30:0:1234:U:N3	2.09	0.67
13:M:171:ARG:CD	30:0:156:C:H5''	2.20	0.67
14:N:144:GLY:O	14:N:147:ILE:HG22	1.94	0.67
18:R:150:PRO:CG	18:R:150:PRO:O	2.41	0.67
30:0:292:G:H2'	30:0:358:G:N2	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.94	0.67
14:N:11:ARG:HD3	31:9:114:G:O6	1.94	0.67
27:1:42:SER:HB2	38:1:354:HOH:O	1.93	0.67
30:0:297:U:H2'	30:0:298:C:C6	2.28	0.67
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.76	0.67
20:T:24:ARG:HH21	20:T:39:ASN:ND2	1.93	0.67
30:0:2812:A:C2	30:0:2814:A:N6	2.58	0.67
31:9:39:U:H1'	31:9:44:A:N6	2.08	0.67
30:0:564:G:H1'	38:0:6342:HOH:O	1.94	0.67
30:0:1667:A:H5'	30:0:1667:A:C8	2.27	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.28	0.66
30:0:1060:C:H6	30:0:1060:C:H5'	1.60	0.66
30:0:1474:C:H6	30:0:1474:C:C5'	2.07	0.66
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.58	0.66
12:L:6:ARG:HD3	30:0:1299:G:O6	1.95	0.66
30:0:2681:A:H4'	30:0:2682:C:H5'	1.75	0.66
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.26	0.66
30:0:1116:U:O2'	30:0:1118:A:C2	2.44	0.66
30:0:1205:U:C2'	30:0:1206:U:C5'	2.72	0.66
12:L:136:ALA:HB3	38:L:8871:HOH:O	1.96	0.66
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.78	0.66
30:0:1289:C:H3'	38:0:6443:HOH:O	1.95	0.66
22:V:50:ARG:NH1	30:0:56:G:H5''	2.10	0.66
30:0:2239:C:H2'	30:0:2240:U:C6	2.30	0.66
3:C:236:THR:HG22	3:C:239:ALA:N	2.09	0.66
30:0:960:G:N3	30:0:960:G:H2'	2.11	0.66
30:0:1016:U:H1'	38:0:3678:HOH:O	1.96	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.44	0.66
30:0:125:U:H2'	38:0:3785:HOH:O	1.96	0.65
30:0:2769:C:H2'	30:0:2770:G:H5'	1.77	0.65
30:0:2836:G:H1'	38:0:6880:HOH:O	1.95	0.65
1:A:199:HIS:HD2	1:A:201:PHE:H	1.44	0.65
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.96	0.65
30:0:2795:C:O2'	30:0:2796:U:H5'	1.95	0.65
30:0:283:U:C5	30:0:284:C:C4	2.85	0.65
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.37	0.65
30:0:960:G:N3	30:0:960:G:C2'	2.59	0.65
2:B:212:GLN:HA	30:0:1733:A:H4'	1.79	0.65
16:P:59:ARG:HH22	16:P:66:GLN:NE2	1.94	0.65
30:0:1183:C:N3	30:0:1184:C:C5	2.65	0.65
30:0:1189:A:O2'	30:0:1208:C:H2'	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1451:C:H5'	30:0:1505:U:C5	2.32	0.65
30:0:704:C:O2'	30:0:705:C:H5'	1.97	0.65
4:D:103:ASN:ND2	4:D:134:LEU:H	1.95	0.64
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.32	0.64
30:0:363:C:H1'	38:0:5312:HOH:O	1.97	0.64
30:0:1058:A:H2'	30:0:1060:C:H5''	1.78	0.64
30:0:1925:G:O2'	30:0:1926:G:H5'	1.97	0.64
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.32	0.64
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.62	0.64
30:0:2414:A:H2'	30:0:2415:A:C8	2.32	0.64
2:B:206:THR:HG21	30:0:2716:G:H5''	1.80	0.64
30:0:256:C:H2'	30:0:257:G:O4'	1.96	0.64
30:0:2505:G:O2'	30:0:2506:A:H5'	1.97	0.64
30:0:280:C:H2'	30:0:281:U:O4'	1.97	0.64
30:0:558:C:C2'	30:0:559:U:C5'	2.74	0.64
30:0:1189:A:H1'	30:0:1209:C:C1'	2.28	0.64
30:0:1441:G:O2'	30:0:1442:A:H5'	1.97	0.64
30:0:1741:U:O2'	30:0:2723:G:H4'	1.97	0.64
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.63	0.64
25:Y:204:ARG:HH22	30:0:553:G:P	2.21	0.64
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.78	0.64
3:C:184:ARG:NH2	30:0:450:C:OP1	2.30	0.64
23:W:125:HIS:HD2	23:W:127:GLY:H	1.46	0.64
1:A:33:GLU:H	1:A:33:GLU:CD	2.04	0.64
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.26	0.64
30:0:297:U:H2'	30:0:298:C:H6	1.63	0.64
30:0:2769:C:H2'	30:0:2770:G:C5'	2.28	0.64
1:A:199:HIS:CD2	1:A:201:PHE:H	2.15	0.63
30:0:10:U:C6	30:0:10:U:C3'	2.80	0.63
30:0:1205:U:C2'	30:0:1206:U:H5''	2.28	0.63
30:0:2256:G:H2'	30:0:2257:G:C5'	2.27	0.63
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.81	0.63
23:W:13:MET:HE2	23:W:18:GLN:HA	1.81	0.63
29:3:65:THR:HG23	29:3:67:LEU:HG	1.79	0.63
30:0:1187:U:H2'	38:0:6939:HOH:O	1.98	0.63
18:R:128:ARG:NH2	30:0:2054:A:N3	2.46	0.63
21:U:46:ALA:O	21:U:52:THR:HG21	1.98	0.63
24:X:71:ARG:HD3	38:X:2171:HOH:O	1.98	0.63
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.64	0.63
30:0:2533:C:H6	30:0:2533:C:C5'	2.09	0.63
13:M:27:ARG:NH2	13:M:44:THR:HG23	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1120:U:H5''	30:0:1120:U:H6	1.63	0.63
30:0:1278:A:H4'	30:0:1279:U:C4	2.33	0.63
30:0:1878:G:O2'	30:0:1879:U:C6	2.49	0.63
31:9:75:G:H1	31:9:106:U:H3	1.47	0.63
9:I:110:ASP:O	30:0:1163:G:H5'	1.99	0.63
30:0:317:A:H4'	38:0:3791:HOH:O	1.98	0.63
30:0:2524:G:H21	30:0:2526:C:N4	1.96	0.63
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.81	0.63
30:0:1835:U:C5	30:0:1840:A:N7	2.60	0.63
30:0:2509:A:H2'	30:0:2510:C:O4'	1.99	0.63
30:0:2649:A:H5'	30:0:2649:A:H8	1.64	0.63
2:B:162:MET:CE	2:B:308:LEU:HD21	2.27	0.63
2:B:264:GLU:HG3	2:B:302:PRO:HD3	1.79	0.63
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.64	0.63
30:0:2604:A:H5'	38:0:5822:HOH:O	1.99	0.62
31:9:54:A:O2'	31:9:55:U:H5'	1.98	0.62
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.96	0.62
30:0:853:C:H3'	38:0:4580:HOH:O	2.00	0.62
30:0:2250:G:C2	30:0:2251:G:H1'	2.34	0.62
30:0:2256:G:H2'	30:0:2257:G:H5'	1.81	0.62
15:O:73:ASP:HA	15:O:92:VAL:O	2.00	0.62
13:M:178:LYS:HB2	38:0:6916:HOH:O	1.99	0.62
30:0:2421:G:H1'	38:0:7060:HOH:O	1.98	0.62
8:H:168:VAL:HG13	38:H:211:HOH:O	1.98	0.62
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.81	0.62
30:0:1701:A:H5''	30:0:1702:U:H3'	1.82	0.62
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.81	0.62
30:0:1198:U:H1'	30:0:1201:C:H5	1.63	0.62
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.82	0.62
7:G:64:ASN:HD22	7:G:64:ASN:N	1.96	0.62
27:1:16:HIS:HD2	30:0:470:U:O2'	1.83	0.62
27:1:20:ARG:HG2	30:0:111:C:O2'	2.00	0.62
30:0:567:U:H5''	38:0:6435:HOH:O	1.99	0.62
31:9:2:U:P	31:9:3:A:H5'	2.40	0.62
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.80	0.62
11:K:10:GLN:HE21	11:K:10:GLN:N	1.87	0.62
29:3:48:ASN:HD21	30:0:2468:A:H61	1.47	0.62
30:0:960:G:N3	30:0:960:G:H3'	2.14	0.62
30:0:1166:A:H61	30:0:1180:U:H3	1.46	0.62
30:0:2404:G:H5''	38:0:5241:HOH:O	2.00	0.62
30:0:2670:G:O2'	30:0:2671:U:H5'	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:91:VAL:HG12	6:F:92:GLY:N	2.14	0.61
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.82	0.61
25:Y:216:ARG:HD2	38:Y:8865:HOH:O	2.00	0.61
30:0:1170:U:H2'	30:0:1172:G:OP2	2.00	0.61
30:0:1314:U:H2'	38:0:5904:HOH:O	2.00	0.61
11:K:32:ILE:HD11	11:K:56:SER:HB2	1.82	0.61
30:0:848:C:H5'	38:0:7311:HOH:O	2.00	0.61
30:0:958:G:O2'	30:0:959:C:H5'	2.00	0.61
13:M:157:ASP:HB3	13:M:160:PHE:HD1	1.65	0.61
30:0:506:G:H22	30:0:509:A:H5''	1.63	0.61
30:0:2083:A:H3'	38:0:7616:HOH:O	1.99	0.61
30:0:2613:G:O2'	30:0:2614:C:H5'	2.00	0.61
31:9:20:G:O2'	31:9:21:G:H5'	2.00	0.61
2:B:162:MET:HG3	2:B:310:ARG:HD3	1.83	0.61
14:N:4:PRO:HG3	31:9:69:U:OP1	2.00	0.61
23:W:88:THR:HG22	23:W:89:ASP:H	1.65	0.61
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.82	0.61
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.81	0.61
30:0:1679:C:H5'	38:0:9334:HOH:O	2.00	0.61
30:0:1759:A:N3	30:0:1818:C:H2'	2.16	0.61
31:9:64:C:C2'	31:9:65:A:H5'	2.30	0.61
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.83	0.61
22:V:1:THR:HB	30:0:93:C:H5''	1.82	0.61
30:0:1506:U:H6	30:0:1506:U:H5'	1.66	0.61
30:0:1641:A:H2'	30:0:1642:A:H5'	1.83	0.61
30:0:1948:G:H2'	30:0:1949:G:O4'	2.01	0.61
27:1:10:LYS:HG3	38:1:2979:HOH:O	2.00	0.61
30:0:2787:C:H5	38:0:4664:HOH:O	1.83	0.61
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.16	0.61
30:0:558:C:H2'	30:0:559:U:H5'	1.82	0.61
3:C:16:VAL:HG12	3:C:17:ASP:H	1.66	0.61
3:C:236:THR:HG21	38:C:8569:HOH:O	2.00	0.61
1:A:36:ASP:CB	1:A:85:SER:H	2.14	0.60
14:N:141:ARG:HH21	31:9:48:C:H4'	1.66	0.60
23:W:84:VAL:HG12	38:W:6679:HOH:O	2.01	0.60
30:0:2505:G:C2'	30:0:2506:A:H5'	2.31	0.60
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.82	0.60
14:N:40:ASN:ND2	31:9:28:U:H5''	2.16	0.60
30:0:936:C:H5	38:0:5991:HOH:O	1.82	0.60
30:0:2637:A:H4'	38:0:6094:HOH:O	2.00	0.60
30:0:1515:A:H2'	30:0:1516:U:C6	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:B:9109:HOH:O	30:0:2672:C:H1'	2.02	0.60
30:0:236:A:H4'	30:0:237:G:OP1	2.01	0.60
30:0:542:A:H5'	30:0:542:A:C8	2.28	0.60
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.84	0.60
23:W:88:THR:HG22	23:W:89:ASP:N	2.17	0.60
30:0:836:G:H5''	38:0:9288:HOH:O	1.99	0.60
4:D:57:THR:HG23	4:D:63:ILE:HA	1.82	0.60
11:K:27:ARG:HD2	38:K:4747:HOH:O	2.01	0.60
10:J:41:ALA:HB3	38:J:5907:HOH:O	2.00	0.60
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.84	0.60
30:0:702:G:O2'	30:0:703:G:H5'	2.02	0.60
30:0:1080:C:O5'	30:0:1080:C:H6	1.85	0.60
30:0:2563:U:H2'	30:0:2565:C:O5'	2.01	0.60
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.84	0.60
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	1.84	0.60
14:N:164:ASP:CG	14:N:167:ASP:HA	2.26	0.60
30:0:2089:A:O2'	30:0:2090:G:H5'	2.02	0.60
31:9:3:A:N6	31:9:22:G:H1'	2.16	0.60
6:F:101:ALA:HA	38:F:5413:HOH:O	2.02	0.59
8:H:102:LYS:HD3	8:H:122:LYS:HD3	1.83	0.59
30:0:2419:U:H5''	30:0:2420:G:H5'	1.83	0.59
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.84	0.59
9:I:87:PRO:HB3	38:I:6825:HOH:O	2.02	0.59
30:0:368:C:H2'	30:0:369:G:H5'	1.84	0.59
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.83	0.59
13:M:80:GLY:O	13:M:81:ARG:HD3	2.01	0.59
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.32	0.59
30:0:567:U:H5''	38:0:5320:HOH:O	2.02	0.59
30:0:271:C:H41	30:0:378:A:H2	1.47	0.59
30:0:1132:A:N6	30:0:1229:C:H2'	2.17	0.59
30:0:1790:C:H2'	30:0:1791:U:H6	1.67	0.59
30:0:2329:C:O2'	30:0:2330:U:H5'	2.01	0.59
2:B:254:GLN:HG3	38:0:9714:HOH:O	2.01	0.59
8:H:29:SER:HA	8:H:62:HIS:HD2	1.68	0.59
8:H:49:GLN:NE2	8:H:140:TYR:HE2	1.95	0.59
38:Z:8706:HOH:O	30:0:1886:A:H4'	2.03	0.59
30:0:2237:G:H1'	38:0:4887:HOH:O	2.02	0.59
30:0:2718:C:H6	30:0:2718:C:H5'	1.68	0.59
3:C:236:THR:CG2	3:C:239:ALA:H	2.11	0.59
8:H:174:LEU:HA	38:H:222:HOH:O	2.02	0.59
9:I:108:HIS:H	9:I:109:PRO:HD2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:39:THR:HG23	18:R:107:GLU:O	2.02	0.59
30:0:119:A:H2'	30:0:120:A:H5''	1.83	0.59
30:0:1377:C:H5'	30:0:1377:C:H6	1.68	0.59
30:0:1595:G:O2'	30:0:1596:U:H5'	2.03	0.59
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.32	0.59
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.37	0.59
23:W:44:MET:HE2	30:0:944:G:H21	1.66	0.59
30:0:308:U:C4	30:0:342:C:H1'	2.38	0.59
30:0:2344:G:H2'	30:0:2344:G:N3	2.17	0.59
30:0:2756:U:H3	30:0:2896:A:H2	1.43	0.59
1:A:48:ASP:HB3	38:A:9060:HOH:O	2.03	0.59
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.85	0.59
7:G:16:LYS:O	7:G:20:VAL:HG23	2.03	0.59
23:W:125:HIS:CD2	23:W:127:GLY:H	2.21	0.59
7:G:12:ILE:HG23	38:0:5490:HOH:O	2.03	0.59
18:R:23:MET:HE3	18:R:28:SER:OG	2.03	0.59
31:9:64:C:H2'	31:9:65:A:H5'	1.84	0.59
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.85	0.58
2:B:248:ARG:O	2:B:251:VAL:HG13	2.03	0.58
38:C:8655:HOH:O	30:0:2100:A:H5'	2.03	0.58
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.04	0.58
30:0:468:U:H3'	38:0:7607:HOH:O	2.03	0.58
30:0:2812:A:H2	30:0:2814:A:N6	1.87	0.58
31:9:24:U:H3'	31:9:25:G:C5'	2.32	0.58
1:A:171:LYS:HB2	30:0:820:G:C6	2.37	0.58
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.67	0.58
30:0:2534:C:H1'	38:0:3513:HOH:O	2.01	0.58
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.85	0.58
28:2:38:LYS:HE3	38:0:4254:HOH:O	2.01	0.58
30:0:1603:A:H5'	30:0:1605:G:C4'	2.33	0.58
30:0:1972:U:H2'	30:0:1973:A:C5'	2.32	0.58
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.03	0.58
23:W:13:MET:HE2	23:W:18:GLN:CA	2.33	0.58
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.19	0.58
1:A:36:ASP:HB2	1:A:85:SER:H	1.68	0.58
16:P:115:SER:OG	16:P:118:GLN:HG3	2.03	0.58
30:0:1304:U:H2'	30:0:1305:C:C6	2.39	0.58
30:0:2252:A:C5	30:0:2253:G:H1'	2.38	0.58
30:0:2649:A:H5'	30:0:2649:A:C8	2.39	0.58
4:D:103:ASN:HD22	4:D:134:LEU:H	1.49	0.58
28:2:10:ARG:NH2	30:0:121:U:OP2	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:407:A:H5'	38:0:6057:HOH:O	2.04	0.58
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.34	0.58
30:0:660:A:H4'	30:0:661:G:O5'	2.04	0.58
2:B:238:ASN:HD22	2:B:240:GLY:N	1.96	0.58
23:W:139:GLY:O	23:W:141:HIS:HD2	1.87	0.58
30:0:441:A:H1'	30:0:442:A:N7	2.19	0.58
30:0:2346:C:H6	30:0:2346:C:O5'	1.86	0.58
5:E:69:ILE:HA	5:E:72:MET:HE3	1.86	0.58
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.85	0.58
12:L:145:LEU:O	12:L:148:GLU:HG3	2.03	0.57
17:Q:11:ARG:HG3	30:0:2363:G:O2'	2.04	0.57
30:0:1819:G:H5'	38:0:5847:HOH:O	2.04	0.57
30:0:192:A:H5'	38:0:7682:HOH:O	2.03	0.57
30:0:567:U:C5'	38:0:6435:HOH:O	2.52	0.57
30:0:947:U:H2'	30:0:948:G:C8	2.39	0.57
30:0:1477:C:H5'	30:0:1868:G:C5'	2.34	0.57
3:C:79:ARG:O	3:C:87:ARG:HG2	2.04	0.57
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.86	0.57
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.03	0.57
22:V:39:ALA:N	22:V:40:PRO:HD2	2.19	0.57
30:0:88:G:H2'	30:0:89:G:C8	2.39	0.57
30:0:228:C:H2'	30:0:229:G:H5'	1.86	0.57
30:0:644:G:H5'	30:0:644:G:N3	2.19	0.57
30:0:711:G:C2	30:0:718:C:C2	2.92	0.57
31:9:1:U:O3'	31:9:3:A:H5'	2.03	0.57
30:0:2894:C:O2'	30:0:2895:C:H5'	2.05	0.57
30:0:1183:C:C2	30:0:1184:C:C5	2.93	0.57
1:A:51:ARG:HB2	38:A:9060:HOH:O	2.04	0.57
24:X:25:ARG:HD3	24:X:64:ALA:O	2.05	0.57
25:Y:235:GLU:CD	25:Y:235:GLU:H	2.12	0.57
30:0:512:G:O3'	30:0:513:A:H8	1.87	0.57
30:0:1592:G:H2'	30:0:1593:C:H6	1.69	0.57
30:0:1714:C:O2'	30:0:1715:C:H5'	2.05	0.57
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.86	0.57
18:R:68:HIS:O	30:0:2842:G:H5'	2.05	0.57
30:0:2372:A:H2'	30:0:2373:U:C6	2.39	0.57
12:L:41:HIS:HD2	30:0:926:A:O2'	1.88	0.57
30:0:396:U:O2'	30:0:418:C:H4'	2.04	0.57
30:0:541:C:H2'	30:0:542:A:H5'	1.87	0.57
30:0:1768:C:H2'	30:0:1769:C:O4'	2.05	0.57
30:0:1942:A:H5'	38:0:7386:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.87	0.56
10:J:19:MET:HE1	10:J:78:ILE:HG22	1.86	0.56
10:J:74:ARG:NH1	10:J:144:THR:HG21	2.20	0.56
18:R:117:HIS:HD2	30:0:20:G:H21	1.53	0.56
30:0:1477:C:O2'	30:0:1478:U:H5'	2.05	0.56
31:9:49:G:H5''	38:9:9090:HOH:O	2.05	0.56
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.87	0.56
30:0:283:U:C5	30:0:284:C:N3	2.73	0.56
30:0:366:U:H2'	30:0:367:G:O4'	2.05	0.56
30:0:2269:C:H2'	30:0:2270:G:H5'	1.86	0.56
30:0:2320:U:H4'	30:0:2321:A:O4'	2.04	0.56
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.87	0.56
30:0:485:A:N3	30:0:487:G:H5''	2.20	0.56
30:0:2005:G:H3'	30:0:2005:G:OP2	2.06	0.56
30:0:2668:G:H2'	30:0:2669:U:C6	2.40	0.56
31:9:1:U:O3'	31:9:3:A:C5'	2.53	0.56
2:B:71:VAL:HG21	2:B:296:LEU:HB3	1.87	0.56
25:Y:189:ASN:C	25:Y:189:ASN:HD22	2.14	0.56
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.86	0.56
30:0:255:A:H2'	30:0:256:C:H6	1.71	0.56
30:0:542:A:H2'	30:0:543:G:O4'	2.05	0.56
31:9:12:C:H5'	31:9:70:U:O4'	2.04	0.56
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.70	0.56
12:L:134:GLU:HG3	38:L:8854:HOH:O	2.06	0.56
23:W:44:MET:CE	30:0:944:G:H21	2.19	0.56
30:0:319:A:H4'	30:0:338:C:C4	2.40	0.56
3:C:63:SER:OG	30:0:2101:A:H2'	2.05	0.56
10:J:74:ARG:HH12	10:J:144:THR:HG21	1.71	0.56
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.71	0.56
30:0:1206:U:C5'	30:0:1206:U:H6	2.15	0.56
2:B:145:HIS:HD2	2:B:146:THR:O	1.89	0.56
12:L:143:THR:HG22	12:L:144:ASP:H	1.71	0.56
30:0:363:C:H2'	30:0:364:U:H6	1.69	0.56
30:0:2472:C:O2'	30:0:2634:G:H4'	2.05	0.56
30:0:2880:A:H2'	30:0:2881:C:H5'	1.88	0.56
31:9:76:G:C3'	31:9:77:A:H5''	2.28	0.56
31:9:114:G:H2'	31:9:115:C:C6	2.41	0.56
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.41	0.56
29:3:70:ARG:HB3	38:3:9064:HOH:O	2.06	0.56
30:0:2002:C:H2'	30:0:2003:U:H5'	1.87	0.56
2:B:17:LYS:O	2:B:260:HIS:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.41	0.56
27:1:9:GLY:HA2	30:0:1687:C:O2	2.05	0.56
27:1:28:HIS:HE1	30:0:776:A:OP1	1.89	0.56
30:0:1213:C:O2'	30:0:1214:G:H5'	2.06	0.56
30:0:2064:U:H5'	30:0:2652:U:H4'	1.87	0.56
7:G:20:VAL:O	7:G:24:VAL:HG23	2.06	0.56
30:0:583:C:H2'	30:0:584:U:H6	1.70	0.56
4:D:25:MET:HE1	4:D:37:ALA:HB1	1.88	0.55
30:0:681:G:N3	30:0:681:G:H5'	2.21	0.55
30:0:834:G:H4'	30:0:835:U:OP2	2.05	0.55
30:0:1209:C:H2'	30:0:1210:G:C8	2.36	0.55
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.39	0.55
30:0:1766:U:O2	30:0:1778:A:H5'	2.06	0.55
30:0:2316:G:H4'	38:0:6125:HOH:O	2.05	0.55
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.89	0.55
30:0:281:U:O2'	30:0:282:C:H5'	2.06	0.55
30:0:283:U:H5	30:0:284:C:N3	2.04	0.55
30:0:1904:A:H2'	30:0:1905:U:O4'	2.05	0.55
30:0:2269:C:C2'	30:0:2270:G:H5'	2.36	0.55
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.07	0.55
30:0:65:C:O2'	30:0:66:G:H5'	2.06	0.55
30:0:236:A:C4'	30:0:237:G:H5'	2.36	0.55
30:0:1676:G:O2'	30:0:1677:U:H5'	2.06	0.55
30:0:1834:C:H2'	30:0:1840:A:N6	2.20	0.55
2:B:125:GLU:O	2:B:129:ARG:HG3	2.06	0.55
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.88	0.55
30:0:1973:A:H5'	30:0:1973:A:C8	2.39	0.55
12:L:18:HIS:HD2	30:0:902:G:N7	2.05	0.55
14:N:80:SER:HB2	38:N:8833:HOH:O	2.07	0.55
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	1.89	0.55
30:0:249:G:H2'	30:0:250:C:H6	1.71	0.55
30:0:2748:G:H1'	38:0:7936:HOH:O	2.05	0.55
30:0:2756:U:N3	30:0:2896:A:C2	2.71	0.55
31:9:22:G:H5'	31:9:23:U:OP1	2.06	0.55
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.89	0.55
5:E:11:VAL:HG12	5:E:12:ASP:N	2.22	0.55
30:0:1592:G:H2'	30:0:1593:C:C6	2.42	0.55
15:O:37:ARG:HD2	30:0:656:G:OP2	2.07	0.55
26:Z:40:ALA:HA	30:0:1773:G:C8	2.41	0.55
30:0:282:C:C2'	30:0:283:U:H5'	2.35	0.55
30:0:2748:G:H2'	38:0:7579:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:49:G:C2'	31:9:50:G:H5'	2.37	0.55
12:L:41:HIS:CD2	30:0:926:A:O2'	2.60	0.55
14:N:37:ARG:NH1	31:9:6:C:OP1	2.39	0.55
30:0:1200:A:H3'	38:0:5786:HOH:O	2.06	0.55
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.89	0.55
15:O:35:LYS:HD3	38:0:4645:HOH:O	2.06	0.55
21:U:20:MET:HE2	21:U:30:HIS:NE2	2.22	0.55
30:0:2768:A:H5''	38:0:4453:HOH:O	2.07	0.55
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.37	0.54
13:M:163:LEU:HD21	30:0:188:C:H5''	1.89	0.54
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.07	0.54
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.42	0.54
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.05	0.54
30:0:1157:C:H2'	30:0:1158:G:C8	2.40	0.54
30:0:2064:U:H5'	30:0:2652:U:O3'	2.08	0.54
14:N:110:THR:HB	14:N:113:SER:OG	2.08	0.54
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.90	0.54
30:0:1165:G:O2'	30:0:1174:A:C1'	2.54	0.54
30:0:1681:G:H5''	30:0:1682:A:H5'	1.88	0.54
30:0:1819:G:H2'	30:0:1820:G:C4'	2.38	0.54
30:0:1878:G:O2'	30:0:1879:U:P	2.66	0.54
2:B:177:HIS:O	2:B:181:ILE:HG13	2.07	0.54
5:E:132:THR:HB	38:E:2227:HOH:O	2.07	0.54
38:I:1549:HOH:O	30:0:1180:U:H1'	2.07	0.54
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.79	0.54
30:0:350:G:H1'	38:0:5705:HOH:O	2.06	0.54
31:9:47:A:C2	31:9:48:C:C2	2.94	0.54
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.89	0.54
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.90	0.54
29:3:73:GLU:HB3	38:3:9053:HOH:O	2.08	0.54
30:0:363:C:O2'	30:0:364:U:H5'	2.07	0.54
31:9:23:U:O2'	31:9:24:U:H4'	2.07	0.54
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.08	0.54
8:H:69:ARG:HD3	38:H:231:HOH:O	2.07	0.54
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.73	0.54
30:0:661:G:C5	30:0:686:A:C2	2.96	0.54
30:0:1947:G:H2'	30:0:1948:G:H8	1.73	0.54
9:I:126:THR:O	9:I:130:LEU:HG	2.08	0.54
23:W:130:HIS:O	23:W:136:GLY:HA3	2.08	0.54
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.89	0.54
30:0:1193:A:H2	30:0:1194:A:N6	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1559:A:H4'	38:0:5895:HOH:O	2.07	0.54
30:0:1594:C:O2'	30:0:1607:A:H4'	2.08	0.54
30:0:1755:A:H2'	30:0:1756:G:O4'	2.07	0.54
30:0:1842:A:C4	30:0:1979:G:C6	2.95	0.54
30:0:2135:A:O2'	30:0:2136:G:H5'	2.06	0.54
31:9:3:A:H2	31:9:21:G:N3	2.06	0.54
4:D:138:GLY:HA2	31:9:29:C:O3'	2.08	0.54
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.08	0.54
30:0:2415:A:H2'	30:0:2416:G:H5'	1.88	0.54
30:0:2505:G:H2'	30:0:2506:A:H5'	1.89	0.54
30:0:2507:G:H2'	30:0:2510:C:N4	2.23	0.54
30:0:2781:U:C2'	30:0:2782:G:H5'	2.37	0.54
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.90	0.54
16:P:58:SER:HB3	38:0:5659:HOH:O	2.08	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.08	0.54
30:0:877:G:C5'	30:0:878:G:OP1	2.53	0.54
30:0:1878:G:O2'	30:0:1879:U:H6	1.89	0.54
30:0:10:U:O4	30:0:531:G:H2'	2.08	0.54
30:0:1535:G:H2'	30:0:1536:C:C6	2.43	0.54
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.73	0.53
14:N:160:SER:HB2	31:9:51:A:H5'	1.90	0.53
30:0:2073:G:OP2	30:0:2490:A:H5'	2.08	0.53
2:B:198:GLU:HA	38:B:9133:HOH:O	2.07	0.53
10:J:107:ASN:C	10:J:107:ASN:HD22	2.17	0.53
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.90	0.53
30:0:407:A:H3'	38:0:4486:HOH:O	2.08	0.53
31:9:49:G:H2'	31:9:50:G:O4'	2.09	0.53
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.73	0.53
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.38	0.53
20:T:2:LYS:HG2	30:0:447:A:OP1	2.08	0.53
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.09	0.53
30:0:24:G:N2	30:0:518:G:H1'	2.23	0.53
30:0:1130:U:H2'	30:0:1131:G:O4'	2.08	0.53
30:0:2371:G:H5'	38:0:5041:HOH:O	2.08	0.53
30:0:2502:C:H2'	30:0:2503:A:C5'	2.37	0.53
5:E:84:MET:HE1	5:E:148:ILE:HD13	1.90	0.53
5:E:137:ASP:O	5:E:141:VAL:HG23	2.08	0.53
17:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.08	0.53
30:0:953:G:H4'	30:0:954:U:OP1	2.08	0.53
30:0:1819:G:H2'	30:0:1820:G:C5'	2.38	0.53
30:0:1850:U:H2'	30:0:1851:G:H8	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2756:U:N3	30:0:2896:A:H2	2.06	0.53
2:B:294:TYR:HE2	38:B:9124:HOH:O	1.89	0.53
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.09	0.53
30:0:2783:A:H2'	30:0:2784:A:C8	2.44	0.53
21:U:17:THR:HG22	21:U:18:GLY:N	2.24	0.53
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.91	0.53
30:0:138:U:OP2	30:0:139:C:H5	1.91	0.53
30:0:368:C:C2'	30:0:369:G:H5'	2.39	0.53
30:0:1333:U:H2'	30:0:1334:C:C6	2.44	0.53
30:0:1523:G:C6	30:0:1524:U:C4	2.96	0.53
30:0:1787:C:H4'	30:0:2883:A:O4'	2.08	0.53
31:9:2:U:H4'	38:9:9103:HOH:O	2.08	0.53
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.90	0.53
21:U:14:GLU:O	21:U:17:THR:HB	2.08	0.53
30:0:67:A:H5''	30:0:69:A:C8	2.44	0.53
30:0:947:U:H2'	30:0:948:G:H8	1.72	0.53
30:0:2249:G:C2	30:0:2253:G:C6	2.96	0.53
31:9:39:U:O2'	31:9:42:C:C5	2.61	0.53
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.90	0.53
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.39	0.53
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.88	0.53
30:0:123:U:H5'	38:0:6694:HOH:O	2.09	0.53
30:0:1206:U:H2'	30:0:1207:A:O4'	2.09	0.53
30:0:1556:G:O2'	30:0:1557:G:H5'	2.09	0.53
30:0:2597:U:H2'	30:0:2598:U:H5'	1.90	0.53
3:C:5:ILE:HD11	3:C:16:VAL:CG2	2.39	0.53
13:M:57:LYS:HE2	13:M:140:ALA:O	2.09	0.53
30:0:960:G:N3	30:0:960:G:C3'	2.72	0.53
30:0:2897:C:O2'	30:0:2898:G:H5'	2.09	0.53
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.23	0.53
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.39	0.53
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.23	0.53
30:0:876:A:H2'	30:0:876:A:N3	2.23	0.53
30:0:1206:U:H5'	30:0:1206:U:C6	2.32	0.53
2:B:23:THR:HG23	2:B:162:MET:HE3	1.91	0.52
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.91	0.52
23:W:80:ASP:O	23:W:84:VAL:HG23	2.09	0.52
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.91	0.52
30:0:1524:U:OP1	30:0:1524:U:H4'	2.09	0.52
30:0:2781:U:O2'	30:0:2782:G:H5'	2.07	0.52
12:L:4:LYS:HE2	30:0:645:U:OP2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.90	0.52
30:0:241:A:C2	30:0:378:A:H4'	2.44	0.52
30:0:1702:U:H1'	38:0:5805:HOH:O	2.08	0.52
30:0:2314:G:C2'	30:0:2315:C:H5'	2.39	0.52
18:R:150:PRO:CG	18:R:150:PRO:CB	2.86	0.52
4:D:159:PRO:O	4:D:163:VAL:HG23	2.09	0.52
13:M:30:GLU:O	13:M:34:GLU:HG3	2.10	0.52
30:0:1174:A:C6	30:0:1201:C:H4'	2.45	0.52
30:0:1377:C:H5'	30:0:1377:C:C6	2.45	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.90	0.52
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.92	0.52
3:C:153:VAL:O	3:C:157:LEU:HG	2.09	0.52
4:D:50:VAL:HG13	31:9:41:C:O4'	2.10	0.52
17:Q:25:PRO:HB2	38:9:9082:HOH:O	2.10	0.52
19:S:43:GLU:HB3	38:S:8991:HOH:O	2.10	0.52
30:0:113:A:OP2	30:0:114:A:H2'	2.09	0.52
30:0:2478:U:O2'	30:0:2479:A:H5'	2.08	0.52
12:L:143:THR:HG22	12:L:144:ASP:N	2.25	0.52
20:T:38:ARG:NH1	38:0:6725:HOH:O	2.42	0.52
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.45	0.52
28:2:39:ARG:HG2	38:2:3143:HOH:O	2.08	0.52
30:0:1135:G:H5'	38:0:5960:HOH:O	2.09	0.52
1:A:36:ASP:HB2	1:A:84:VAL:N	2.25	0.52
4:D:138:GLY:N	38:D:7597:HOH:O	2.42	0.52
8:H:48:VAL:HA	8:H:170:ARG:O	2.10	0.52
30:0:602:A:O2'	30:0:605:C:H4'	2.09	0.52
30:0:2105:C:H2'	30:0:2106:C:C6	2.44	0.52
30:0:2250:G:H2'	30:0:2251:G:O4'	2.09	0.52
30:0:2664:A:H8	30:0:2664:A:OP1	1.93	0.52
30:0:2681:A:H4'	30:0:2682:C:C5'	2.39	0.52
30:0:2509:A:OP2	30:0:2510:C:H5	1.93	0.52
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.91	0.52
27:1:20:ARG:HG2	30:0:111:C:HO2'	1.75	0.52
30:0:968:G:O2'	30:0:969:G:H5'	2.10	0.52
30:0:1444:G:O2'	30:0:1445:G:H5'	2.09	0.52
30:0:1921:A:C6	30:0:1922:A:C2	2.98	0.52
30:0:1930:A:H2'	30:0:1931:A:C8	2.45	0.52
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.10	0.52
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.10	0.52
30:0:12:U:H2'	30:0:13:G:H5'	1.91	0.52
30:0:704:C:H2'	30:0:705:C:H6	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1279:U:O2	30:0:1279:U:C2'	2.58	0.52
30:0:1289:C:O2'	30:0:1290:G:H5'	2.10	0.52
30:0:1805:G:O2'	30:0:1806:G:H5'	2.10	0.52
30:0:2237:G:O2'	30:0:2238:A:C8	2.62	0.52
30:0:2878:U:H2'	30:0:2879:A:O4'	2.10	0.52
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.91	0.51
13:M:179:GLY:O	30:0:399:C:H5'	2.10	0.51
23:W:64:THR:O	23:W:68:THR:HG22	2.10	0.51
30:0:185:G:H4'	30:0:186:A:OP1	2.10	0.51
30:0:200:C:H2'	38:0:3463:HOH:O	2.09	0.51
30:0:1130:U:H5'	38:0:7710:HOH:O	2.10	0.51
30:0:1188:A:C6	30:0:1189:A:C6	2.99	0.51
30:0:2531:U:O2'	30:0:2532:A:H5'	2.10	0.51
31:9:24:U:H3'	31:9:25:G:H5'	1.91	0.51
2:B:148:PRO:HD2	38:B:9049:HOH:O	2.10	0.51
6:F:57:GLU:O	6:F:61:MET:HG3	2.10	0.51
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.26	0.51
22:V:12:THR:HG23	22:V:14:ALA:H	1.75	0.51
23:W:119:HIS:HD2	23:W:120:PRO:O	1.92	0.51
30:0:299:U:H5'	38:0:7375:HOH:O	2.09	0.51
30:0:2250:G:N2	30:0:2251:G:H1'	2.25	0.51
30:0:2830:U:O2'	30:0:2831:C:H5'	2.09	0.51
3:C:145:GLU:HG3	38:C:8569:HOH:O	2.09	0.51
23:W:24:LEU:O	23:W:26:ILE:HG22	2.10	0.51
30:0:10:U:O4	30:0:532:A:OP2	2.28	0.51
30:0:363:C:H2'	30:0:364:U:C6	2.46	0.51
30:0:541:C:O2'	30:0:542:A:H5''	2.11	0.51
30:0:1762:C:O2'	30:0:1763:C:H5'	2.10	0.51
31:9:39:U:O2'	31:9:42:C:H5	1.92	0.51
2:B:211:THR:HG21	38:0:7492:HOH:O	2.11	0.51
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.92	0.51
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.92	0.51
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.41	0.51
30:0:228:C:C2'	30:0:229:G:H5'	2.41	0.51
30:0:285:A:H2'	30:0:286:U:O4'	2.10	0.51
30:0:2252:A:H2'	30:0:2253:G:H5'	1.92	0.51
30:0:2825:C:H4'	30:0:2826:G:O5'	2.10	0.51
31:9:1:U:C4'	31:9:3:A:OP1	2.59	0.51
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.44	0.51
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.93	0.51
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:414:C:H5'	38:0:9667:HOH:O	2.11	0.51
30:0:958:G:H2'	30:0:959:C:C6	2.45	0.51
30:0:1386:G:O2'	30:0:1387:G:H5'	2.11	0.51
1:A:179:MET:HA	1:A:179:MET:HE3	1.92	0.51
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.11	0.51
30:0:69:A:H8	30:0:69:A:C5'	2.15	0.51
30:0:1205:U:O2'	30:0:1206:U:H5''	2.11	0.51
30:0:2421:G:H3'	30:0:2422:U:H5''	1.92	0.51
30:0:2781:U:H2'	30:0:2782:G:C5'	2.40	0.51
30:0:2826:G:C6	30:0:2913:A:N6	2.78	0.51
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.79	0.51
24:X:23:HIS:HD2	38:0:9973:HOH:O	1.93	0.51
30:0:541:C:C2'	30:0:542:A:C5'	2.79	0.51
30:0:790:A:H2'	30:0:791:A:O4'	2.10	0.51
30:0:1398:G:O2'	30:0:1399:A:H5'	2.11	0.51
30:0:2241:C:O2'	30:0:2242:U:H5'	2.11	0.51
31:9:91:C:H2'	31:9:92:G:O4'	2.10	0.51
2:B:256:GLN:HG2	38:B:9132:HOH:O	2.11	0.51
12:L:14:GLY:O	30:0:1295:G:H5''	2.11	0.51
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.59	0.51
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.41	0.51
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.93	0.51
19:S:33:SER:O	19:S:37:VAL:HG23	2.11	0.51
30:0:282:C:O2'	30:0:283:U:C5'	2.50	0.51
30:0:346:U:H4'	38:0:6884:HOH:O	2.11	0.51
30:0:2764:C:O2'	30:0:2765:C:H5'	2.10	0.51
30:0:2781:U:H2'	30:0:2782:G:H5'	1.92	0.51
29:3:15:ASN:O	30:0:2408:A:H4'	2.11	0.51
30:0:397:A:O2'	30:0:417:G:N3	2.42	0.51
30:0:952:G:N3	30:0:2302:A:H2'	2.26	0.51
30:0:2251:G:H2'	30:0:2252:A:H8	1.72	0.51
3:C:233:THR:HG22	3:C:234:VAL:N	2.26	0.51
25:Y:184:GLU:OE2	25:Y:204:ARG:HD2	2.11	0.51
30:0:1419:U:H2'	30:0:1685:A:C2	2.46	0.51
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.76	0.50
30:0:120:A:H2'	30:0:120:A:N3	2.27	0.50
2:B:85:ARG:NH1	38:B:9109:HOH:O	2.44	0.50
22:V:56:ILE:O	22:V:60:GLN:HG3	2.11	0.50
30:0:249:G:H2'	30:0:250:C:C6	2.46	0.50
30:0:289:G:O2'	30:0:290:C:H5'	2.12	0.50
30:0:383:A:H4'	38:0:5359:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:683:G:O2'	30:0:684:G:H5'	2.11	0.50
30:0:1167:G:H2'	30:0:1168:C:C6	2.46	0.50
30:0:1186:C:N4	30:0:1187:U:C4	2.79	0.50
4:D:48:MET:HE2	31:9:41:C:C5'	2.40	0.50
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.94	0.50
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.94	0.50
30:0:1183:C:H2'	30:0:1183:C:O2	2.10	0.50
30:0:1202:A:C2'	30:0:1203:G:H5'	2.40	0.50
30:0:1494:A:H1'	30:0:1495:C:C6	2.47	0.50
30:0:1557:G:O2'	30:0:1558:C:H5'	2.11	0.50
30:0:1972:U:C2'	30:0:1973:A:H5''	2.41	0.50
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.27	0.50
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.94	0.50
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.12	0.50
15:O:39:THR:O	15:O:115:ARG:NH2	2.44	0.50
22:V:44:GLY:O	22:V:48:GLU:HG2	2.12	0.50
30:0:559:U:H6	30:0:559:U:C5'	2.20	0.50
30:0:1183:C:H42	30:0:1184:C:N4	2.05	0.50
1:A:135:VAL:HA	1:A:150:PRO:HD3	1.93	0.50
5:E:7:ILE:HG13	5:E:11:VAL:HB	1.93	0.50
8:H:66:GLU:HA	38:H:231:HOH:O	2.11	0.50
11:K:66:ARG:HH22	30:0:1994:A:P	2.35	0.50
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.94	0.50
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.95	0.50
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.11	0.50
30:0:69:A:C8	30:0:69:A:C5'	2.89	0.50
30:0:95:A:H5''	30:0:97:G:O4'	2.11	0.50
30:0:858:U:H5	38:0:5459:HOH:O	1.93	0.50
30:0:2610:U:H4'	38:0:9491:HOH:O	2.12	0.50
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.47	0.50
10:J:42:GLU:O	10:J:131:THR:HG23	2.12	0.50
24:X:61:ARG:NH1	24:X:67:PRO:HD3	2.27	0.50
27:1:16:HIS:HE1	30:0:775:G:OP1	1.94	0.50
30:0:1588:G:C6	30:0:1589:G:N1	2.80	0.50
30:0:1795:G:H2'	30:0:1796:A:O4'	2.12	0.50
30:0:1878:G:C1'	38:0:6153:HOH:O	2.47	0.50
31:9:13:A:O2'	31:9:14:G:H5''	2.12	0.50
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.47	0.50
5:E:143:GLN:HE22	30:0:2779:G:H21	1.55	0.50
13:M:49:ALA:C	13:M:54:TYR:HB3	2.37	0.50
18:R:111:ILE:HG23	18:R:145:LEU:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.30	0.50
23:W:65:VAL:HG12	23:W:116:LEU:HD13	1.94	0.50
30:0:1118:A:H8	30:0:1119:G:H5''	1.76	0.50
30:0:2421:G:H3'	30:0:2422:U:C5'	2.42	0.50
30:0:2793:A:N6	38:0:5912:HOH:O	2.44	0.50
30:0:2883:A:H2'	30:0:2884:G:O4'	2.12	0.50
2:B:310:ARG:HD2	38:B:9122:HOH:O	2.12	0.50
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.93	0.50
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.93	0.50
14:N:132:ASN:O	14:N:135:VAL:HG12	2.12	0.50
23:W:139:GLY:O	23:W:141:HIS:CD2	2.64	0.50
30:0:154:C:H2'	30:0:155:C:H6	1.76	0.50
30:0:264:G:H1'	30:0:265:U:H5	1.77	0.50
30:0:912:A:C4	30:0:1294:A:C2	2.99	0.50
30:0:1667:A:H2'	30:0:1668:U:C6	2.47	0.50
31:9:36:C:C5	31:9:37:C:C5	3.00	0.50
1:A:35:GLY:O	1:A:36:ASP:HB3	2.12	0.50
5:E:69:ILE:HA	5:E:72:MET:CE	2.41	0.50
5:E:84:MET:HB2	5:E:131:LEU:HB2	1.94	0.50
8:H:123:ILE:HD12	8:H:123:ILE:N	2.27	0.50
11:K:125:ALA:C	11:K:127:ALA:H	2.20	0.50
30:0:79:G:H22	30:0:97:G:H1'	1.77	0.50
30:0:79:G:N2	30:0:97:G:H1'	2.27	0.50
30:0:968:G:C2	30:0:1001:U:O2	2.65	0.50
30:0:969:G:H1	30:0:999:C:N4	2.10	0.50
30:0:2820:A:H2'	30:0:2821:C:C6	2.47	0.50
30:0:2896:A:N3	30:0:2896:A:H2'	2.27	0.50
4:D:52:THR:HG21	30:0:2347:C:H5'	1.94	0.49
19:S:76:GLU:HB3	38:S:8992:HOH:O	2.11	0.49
22:V:39:ALA:H	22:V:40:PRO:HD2	1.76	0.49
30:0:886:A:OP2	30:0:2113:G:H5'	2.11	0.49
30:0:941:G:C5	30:0:942:U:C4	3.00	0.49
30:0:1149:U:H5''	30:0:1151:G:O4'	2.12	0.49
30:0:1644:C:H2'	30:0:1645:U:H6	1.77	0.49
30:0:1848:G:O2'	30:0:1849:G:H5'	2.12	0.49
30:0:2010:A:C2'	38:0:5990:HOH:O	2.56	0.49
30:0:2577:A:H8	38:0:9613:HOH:O	1.95	0.49
31:9:95:C:O2'	31:9:96:C:H5'	2.12	0.49
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.77	0.49
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.94	0.49
29:3:60:LYS:HG3	38:0:7595:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2256:G:C2'	30:0:2257:G:C5'	2.89	0.49
30:0:2793:A:H2'	30:0:2794:G:H5'	1.94	0.49
2:B:254:GLN:HG2	2:B:255:GLY:N	2.27	0.49
3:C:236:THR:HA	38:C:8644:HOH:O	2.12	0.49
4:D:103:ASN:ND2	4:D:133:ASN:HD22	2.10	0.49
12:L:50:GLY:C	30:0:2453:G:H4'	2.37	0.49
14:N:37:ARG:NH2	38:N:8831:HOH:O	2.45	0.49
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.11	0.49
10:J:131:THR:HB	10:J:134:GLU:HG3	1.95	0.49
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.13	0.49
16:P:41:ARG:HH22	30:0:1500:U:P	2.35	0.49
25:Y:154:ARG:NH1	25:Y:155:ARG:HG3	2.28	0.49
30:0:2092:G:H2'	30:0:2613:G:OP1	2.13	0.49
1:A:51:ARG:NH1	1:A:120:ARG:O	2.46	0.49
2:B:54:VAL:HB	38:B:9087:HOH:O	2.11	0.49
3:C:43:LYS:HG2	30:0:449:A:N7	2.28	0.49
30:0:301:C:O2'	30:0:302:A:H5'	2.13	0.49
30:0:1972:U:H2'	30:0:1973:A:H5''	1.92	0.49
30:0:2724:U:H2'	30:0:2725:G:O4'	2.12	0.49
30:0:2851:G:H2'	30:0:2852:A:H5'	1.91	0.49
2:B:26:PHE:HE1	38:B:9122:HOH:O	1.96	0.49
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.93	0.49
13:M:193:LYS:HB3	30:0:392:U:H4'	1.94	0.49
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.93	0.49
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.95	0.49
20:T:54:ASP:OD2	30:0:316:A:H5'	2.12	0.49
21:U:33:SER:O	21:U:37:GLU:HG3	2.13	0.49
30:0:671:A:O2'	30:0:672:G:H2'	2.13	0.49
30:0:1198:U:C6	30:0:1200:A:OP2	2.65	0.49
31:9:39:U:HO2'	31:9:42:C:H5	1.52	0.49
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.42	0.49
30:0:255:A:C4	30:0:256:C:C6	3.00	0.49
30:0:2265:U:H2'	30:0:2266:A:C8	2.48	0.49
30:0:2356:A:H5'	38:0:5666:HOH:O	2.12	0.49
30:0:2467:A:H2'	38:0:5488:HOH:O	2.12	0.49
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.95	0.49
20:T:52:ARG:O	30:0:317:A:OP1	2.29	0.49
30:0:1008:C:O2'	30:0:1009:U:H5'	2.13	0.49
30:0:1552:G:H2'	30:0:1553:C:C6	2.47	0.49
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.94	0.49
8:H:30:LYS:H	8:H:62:HIS:CD2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.93	0.49
25:Y:154:ARG:HH21	30:0:1293:U:H5'	1.78	0.49
30:0:255:A:H2'	30:0:256:C:C6	2.47	0.49
30:0:304:G:H1'	30:0:347:A:N6	2.28	0.49
30:0:790:A:H1'	30:0:1710:A:H2'	1.95	0.49
30:0:2453:G:H5''	38:0:4755:HOH:O	2.13	0.49
30:0:2717:C:C2'	30:0:2718:C:C5'	2.79	0.49
30:0:2769:C:C2'	30:0:2770:G:C5'	2.84	0.49
18:R:17:MET:HE1	18:R:19:ARG:NH2	2.28	0.49
30:0:154:C:H2'	30:0:155:C:C6	2.48	0.49
30:0:513:A:N3	38:0:3679:HOH:O	2.35	0.49
30:0:1857:A:H5''	38:0:6744:HOH:O	2.12	0.49
30:0:2002:C:C2'	30:0:2003:U:H5'	2.42	0.49
30:0:2316:G:OP1	30:0:2317:C:H1'	2.13	0.49
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.94	0.48
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.95	0.48
7:G:67:LEU:O	7:G:71:LEU:HG	2.12	0.48
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.42	0.48
21:U:37:GLU:HB3	38:U:408:HOH:O	2.11	0.48
22:V:1:THR:HG23	22:V:2:VAL:HG23	1.94	0.48
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.94	0.48
30:0:282:C:O2	30:0:282:C:H2'	2.13	0.48
30:0:1158:G:O2'	30:0:1159:G:H5'	2.13	0.48
30:0:1391:G:H2'	30:0:1392:A:H5'	1.95	0.48
30:0:1562:C:O2	30:0:1562:C:H2'	2.12	0.48
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.45	0.48
10:J:75:PRO:HB3	10:J:132:LEU:HB3	1.95	0.48
12:L:6:ARG:NH1	30:0:1299:G:N7	2.62	0.48
16:P:83:LYS:HG2	30:0:793:A:H5''	1.94	0.48
24:X:43:VAL:HG12	24:X:44:ASP:N	2.28	0.48
27:1:1:THR:O	30:0:1836:A:H1'	2.13	0.48
30:0:195:C:H2'	30:0:196:G:H5'	1.95	0.48
30:0:1159:G:H1	30:0:1208:C:H42	1.58	0.48
30:0:1825:U:O2'	30:0:1826:C:H5'	2.12	0.48
2:B:205:VAL:O	2:B:307:ARG:NE	2.47	0.48
3:C:136:VAL:HG22	3:C:137:PRO:HA	1.95	0.48
15:O:32:ARG:O	15:O:32:ARG:HD3	2.12	0.48
19:S:37:VAL:O	19:S:41:VAL:HG23	2.13	0.48
23:W:23:MET:O	30:0:1025:C:H5'	2.12	0.48
25:Y:212:ARG:HD2	38:Y:8896:HOH:O	2.12	0.48
26:Z:80:GLN:HA	26:Z:86:TYR:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:137:U:H2'	30:0:139:C:C5	2.47	0.48
30:0:1087:G:H4'	30:0:1088:A:OP1	2.13	0.48
30:0:1528:A:H2'	30:0:1529:G:O4'	2.13	0.48
30:0:1632:A:C3'	30:0:1633:C:H5'	2.43	0.48
1:A:121:ALA:O	1:A:124:VAL:HG22	2.13	0.48
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.95	0.48
20:T:8:ARG:HD2	30:0:31:C:OP2	2.13	0.48
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.48
30:0:1321:A:H2'	30:0:1322:G:C8	2.48	0.48
30:0:2300:A:H4'	30:0:2301:A:O5'	2.13	0.48
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.48
2:B:49:THR:HG21	2:B:331:SER:O	2.14	0.48
2:B:255:GLY:O	2:B:257:THR:HG22	2.14	0.48
3:C:236:THR:H	3:C:239:ALA:HB3	1.78	0.48
6:F:48:VAL:HG23	6:F:74:PHE:CB	2.42	0.48
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.95	0.48
18:R:113:HIS:HE1	18:R:144:GLU:CD	2.22	0.48
30:0:961:A:H4'	38:0:6814:HOH:O	2.12	0.48
30:0:1883:U:O2'	30:0:1884:G:H5'	2.13	0.48
30:0:2301:A:H5''	30:0:2302:A:H5'	1.95	0.48
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.96	0.48
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.95	0.48
30:0:447:A:O2'	30:0:448:G:H5'	2.14	0.48
30:0:1165:G:H4'	30:0:1174:A:O2'	2.13	0.48
30:0:2269:C:H2'	30:0:2270:G:C5'	2.44	0.48
30:0:222:A:H2'	30:0:223:G:O4'	2.14	0.48
30:0:2564:G:OP2	30:0:2565:C:H5''	2.14	0.48
6:F:21:GLU:O	6:F:24:ARG:HG2	2.14	0.48
30:0:484:A:N1	30:0:506:G:H4'	2.28	0.48
30:0:920:C:H5'	30:0:921:G:C4	2.49	0.48
30:0:1130:U:H4'	38:0:6158:HOH:O	2.13	0.48
31:9:45:A:H2'	31:9:46:C:H6	1.79	0.48
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.94	0.48
3:C:140:VAL:HB	38:C:8644:HOH:O	2.13	0.48
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.46	0.48
15:O:57:THR:HB	15:O:111:VAL:HG23	1.95	0.48
29:3:48:ASN:ND2	29:3:50:GLY:H	2.11	0.48
30:0:734:U:O2'	30:0:736:A:N7	2.43	0.48
30:0:960:G:H3'	30:0:960:G:C4	2.49	0.48
30:0:1051:C:H2'	30:0:1052:G:O4'	2.14	0.48
30:0:1131:G:C6	30:0:1230:A:C4	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1545:C:H2'	30:0:1546:G:O4'	2.14	0.48
30:0:2912:C:H2'	30:0:2913:A:O4'	2.14	0.48
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.44	0.48
2:B:275:GLY:O	2:B:291:ASP:HA	2.14	0.48
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.79	0.48
12:L:121:ILE:HG12	12:L:141:GLU:HB2	1.96	0.48
30:0:1477:C:H5'	30:0:1868:G:H5''	1.96	0.48
30:0:1625:U:H5''	38:0:6053:HOH:O	2.13	0.48
30:0:2439:C:H5'	38:0:5518:HOH:O	2.12	0.48
1:A:3:ARG:HD3	30:0:870:G:OP2	2.14	0.47
3:C:22:PHE:HA	3:C:116:ALA:HA	1.94	0.47
13:M:64:ARG:HD2	38:M:8881:HOH:O	2.14	0.47
14:N:43:VAL:HG13	14:N:118:ILE:HD11	1.96	0.47
14:N:114:LYS:O	14:N:118:ILE:HG13	2.14	0.47
14:N:169:PRO:O	14:N:172:PHE:HB3	2.14	0.47
23:W:65:VAL:HA	23:W:68:THR:HG22	1.95	0.47
27:1:28:HIS:HD2	27:1:30:LYS:H	1.60	0.47
30:0:90:A:H2'	30:0:91:G:O4'	2.14	0.47
30:0:2314:G:H2'	30:0:2315:C:H5'	1.96	0.47
4:D:76:ARG:NE	31:9:44:A:O4'	2.47	0.47
21:U:9:CYS:HA	21:U:52:THR:OG1	2.14	0.47
30:0:398:U:H2'	30:0:399:C:C6	2.49	0.47
30:0:1666:C:H2'	30:0:1667:A:H5''	1.78	0.47
30:0:1838:U:O2'	30:0:2644:C:H5'	2.14	0.47
30:0:1850:U:H2'	30:0:1851:G:C8	2.48	0.47
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.27	0.47
8:H:61:ARG:HG3	8:H:61:ARG:NH1	2.29	0.47
27:1:25:LYS:HD2	28:2:48:ASP:HA	1.96	0.47
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.47
30:0:1422:U:H2'	30:0:1423:C:C6	2.50	0.47
30:0:1641:A:C2'	30:0:1642:A:H5'	2.44	0.47
30:0:1788:U:O2'	30:0:1789:G:H5'	2.14	0.47
30:0:2264:A:H2'	30:0:2265:U:C6	2.48	0.47
30:0:2506:A:H1'	38:0:3766:HOH:O	2.13	0.47
1:A:30:ARG:NH2	1:A:38:ILE:HG13	2.28	0.47
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.79	0.47
2:B:14:GLY:HA2	2:B:15:PRO:C	2.39	0.47
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.50	0.47
4:D:48:MET:HE2	31:9:41:C:H5'	1.96	0.47
6:F:107:ASP:O	6:F:111:ILE:HG13	2.14	0.47
16:P:143:ALA:HA	38:P:184:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:154:ARG:NH1	30:0:588:G:O6	2.47	0.47
30:0:955:A:C2	30:0:1013:A:C4	3.03	0.47
30:0:1268:C:O2'	30:0:1269:G:H5'	2.14	0.47
30:0:1280:A:OP1	30:0:1280:A:H3'	2.15	0.47
30:0:2064:U:H4'	30:0:2653:A:OP1	2.13	0.47
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.30	0.47
8:H:39:LYS:HA	8:H:87:LYS:HZ1	1.79	0.47
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.47
14:N:40:ASN:HD21	31:9:28:U:H5''	1.80	0.47
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.49	0.47
30:0:137:U:OP1	30:0:259:G:O2'	2.33	0.47
30:0:1193:A:C2	30:0:1194:A:N6	2.78	0.47
30:0:1252:A:H2'	30:0:1253:C:O4'	2.14	0.47
31:9:56:A:C3'	31:9:57:A:H5''	2.44	0.47
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.97	0.47
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.48	0.47
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.15	0.47
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.45	0.47
16:P:120:ARG:NH1	30:0:1594:C:C5	2.82	0.47
18:R:109:MET:HG2	18:R:148:GLU:C	2.40	0.47
24:X:85:VAL:HG12	24:X:86:GLU:N	2.30	0.47
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	1.97	0.47
30:0:407:A:H2'	30:0:408:A:C8	2.50	0.47
30:0:1393:A:H2'	30:0:1394:C:C6	2.49	0.47
30:0:2271:G:H5'	38:0:4783:HOH:O	2.14	0.47
30:0:2469:A:H2'	38:0:7512:HOH:O	2.15	0.47
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.47	0.47
4:D:10:PHE:CG	4:D:11:HIS:N	2.81	0.47
12:L:149:ARG:O	12:L:150:GLN:HB2	2.14	0.47
17:Q:32:GLU:O	17:Q:93:ARG:NH2	2.48	0.47
30:0:283:U:H5	30:0:284:C:N4	2.12	0.47
30:0:440:C:H2'	30:0:441:A:C8	2.50	0.47
30:0:1118:A:C8	30:0:1119:G:H5''	2.49	0.47
30:0:1176:C:N4	38:0:5775:HOH:O	2.48	0.47
30:0:1762:C:H2'	30:0:1763:C:H6	1.80	0.47
30:0:2353:A:H4'	30:0:2354:A:O5'	2.14	0.47
13:M:164:THR:HG22	13:M:166:ALA:N	2.29	0.47
23:W:11:VAL:HG11	30:0:1086:A:C6	2.49	0.47
27:1:22:CYS:SG	27:1:24:GLU:HB2	2.55	0.47
29:3:65:THR:HB	29:3:83:TRP:H	1.79	0.47
30:0:426:G:H2'	30:0:427:C:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:483:C:C4	30:0:484:A:C6	3.03	0.47
30:0:2791:U:H1'	30:0:2792:A:H5''	1.97	0.47
31:9:52:A:H2'	31:9:53:G:O4'	2.15	0.47
6:F:91:VAL:HG12	6:F:92:GLY:H	1.78	0.47
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.45	0.47
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.44	0.47
30:0:1682:A:H2'	38:0:9820:HOH:O	2.14	0.47
30:0:2533:C:C6	30:0:2533:C:C5'	2.92	0.47
31:9:55:U:H4'	31:9:56:A:C8	2.49	0.47
2:B:297:VAL:HB	38:B:9080:HOH:O	2.15	0.47
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.97	0.47
30:0:816:G:C6	30:0:817:G:N1	2.83	0.47
30:0:1249:U:H2'	30:0:1250:C:C6	2.50	0.47
30:0:1477:C:C5'	30:0:1868:G:H5''	2.44	0.47
30:0:1928:C:H2'	30:0:1929:G:H5'	1.96	0.47
30:0:2281:C:H2'	30:0:2282:U:H5'	1.97	0.47
30:0:2372:A:H2'	30:0:2373:U:H6	1.78	0.47
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.30	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.15	0.46
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.35	0.46
26:Z:34:SER:HB3	30:0:797:A:H4'	1.96	0.46
30:0:170:U:H2'	30:0:171:C:H5'	1.95	0.46
30:0:2011:A:H4'	30:0:2012:U:O5'	2.15	0.46
30:0:2238:A:H3'	38:0:6711:HOH:O	2.15	0.46
30:0:2589:U:H2'	30:0:2590:U:C6	2.50	0.46
1:A:175:LYS:HG3	30:0:1847:A:OP1	2.16	0.46
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.19	0.46
8:H:172:GLU:HB3	38:H:243:HOH:O	2.15	0.46
21:U:50:GLU:HB2	30:0:2866:U:C5	2.50	0.46
24:X:43:VAL:HG12	24:X:47:ALA:HB3	1.97	0.46
25:Y:165:GLU:HB3	38:0:6747:HOH:O	2.15	0.46
27:1:11:LYS:HG2	30:0:777:U:O2'	2.15	0.46
31:9:28:U:H2'	31:9:29:C:C6	2.50	0.46
14:N:141:ARG:NH2	31:9:48:C:H4'	2.30	0.46
16:P:1:THR:O	30:0:1396:C:H1'	2.15	0.46
30:0:304:G:H1'	30:0:347:A:H61	1.80	0.46
30:0:559:U:C5	30:0:560:U:C5	3.03	0.46
30:0:800:G:H2'	30:0:801:U:C6	2.50	0.46
30:0:969:G:H1	30:0:999:C:H42	1.62	0.46
30:0:1907:U:O2'	30:0:1908:G:H5'	2.15	0.46
1:A:88:ILE:O	1:A:88:ILE:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASP:HB3	1:A:135:VAL:H	1.80	0.46
2:B:75:GLU:C	2:B:77:PRO:HD3	2.40	0.46
3:C:129:HIS:HD2	3:C:165:ASP:OD2	1.99	0.46
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.15	0.46
23:W:122:ARG:NH2	38:0:5320:HOH:O	2.48	0.46
25:Y:115:ARG:NH2	30:0:1266:U:H4'	2.30	0.46
30:0:105:G:O2'	30:0:106:A:H5'	2.15	0.46
30:0:690:G:H4'	30:0:741:C:O2	2.15	0.46
30:0:699:C:C2	30:0:744:G:C2	3.03	0.46
30:0:2103:A:H2'	30:0:2104:C:H5'	1.96	0.46
2:B:320:GLN:HE21	2:B:321:PRO:CD	2.24	0.46
8:H:139:ALA:HB3	8:H:149:VAL:HG21	1.97	0.46
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.31	0.46
10:J:82:THR:CG2	30:0:1242:A:H5'	2.30	0.46
10:J:107:ASN:HD22	10:J:109:TYR:H	1.64	0.46
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.96	0.46
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.51	0.46
30:0:343:C:O2'	30:0:344:C:H5'	2.15	0.46
30:0:638:C:H2'	30:0:639:A:C8	2.51	0.46
30:0:920:C:H5''	30:0:921:G:O5'	2.15	0.46
30:0:1117:A:C2	30:0:1244:U:C2	3.04	0.46
30:0:1657:A:H2'	30:0:1658:A:C8	2.51	0.46
31:9:101:G:H5''	38:9:9140:HOH:O	2.15	0.46
1:A:51:ARG:HD2	30:0:1874:U:OP1	2.15	0.46
2:B:243:ASN:HA	2:B:244:PRO:C	2.40	0.46
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.95	0.46
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.82	0.46
20:T:28:SER:O	20:T:32:ARG:HG3	2.15	0.46
30:0:11:A:H5'	30:0:12:U:OP2	2.15	0.46
30:0:583:C:C2	30:0:584:U:C5	3.03	0.46
30:0:1503:U:H2'	30:0:1504:A:O4'	2.15	0.46
30:0:1596:U:H2'	30:0:1598:A:OP2	2.15	0.46
30:0:2712:G:H5'	38:0:5251:HOH:O	2.15	0.46
27:1:1:THR:HA	38:0:9368:HOH:O	2.16	0.46
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.54	0.46
30:0:613:C:H2'	30:0:614:U:H6	1.80	0.46
30:0:812:A:H2'	30:0:813:C:O4'	2.16	0.46
30:0:1883:U:C2'	30:0:1884:G:H5'	2.46	0.46
31:9:39:U:C2'	31:9:40:C:OP1	2.63	0.46
1:A:214:SER:HB2	38:0:4392:HOH:O	2.15	0.46
3:C:206:ASN:HB2	30:0:329:A:OP2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:27:ILE:HB	4:D:69:ILE:O	2.15	0.46
8:H:61:ARG:HG3	38:0:5004:HOH:O	2.15	0.46
18:R:132:ARG:NH1	38:R:8984:HOH:O	2.48	0.46
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.98	0.46
30:0:1202:A:O2'	30:0:1203:G:H5'	2.16	0.46
30:0:1928:C:C2'	30:0:1929:G:H5'	2.46	0.46
6:F:91:VAL:HG11	30:0:262:A:OP2	2.16	0.46
10:J:63:ILE:CD1	30:0:1236:A:C8	2.99	0.46
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.97	0.46
18:R:29:LYS:HD3	30:0:524:A:H5''	1.98	0.46
28:2:20:ARG:HD3	38:0:6163:HOH:O	2.16	0.46
30:0:71:G:H5''	38:0:3932:HOH:O	2.16	0.46
30:0:622:G:O2'	30:0:623:U:H5'	2.16	0.46
30:0:711:G:H1'	38:0:7133:HOH:O	2.14	0.46
30:0:2065:C:O2'	30:0:2066:C:H5'	2.16	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.51	0.46
30:0:2758:G:H2'	30:0:2759:C:C6	2.51	0.46
31:9:29:C:C2'	31:9:30:C:H5'	2.42	0.46
1:A:206:ARG:NH2	30:0:2630:G:O6	2.49	0.46
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.51	0.46
2:B:141:ARG:N	38:B:9048:HOH:O	2.48	0.46
19:S:57:THR:C	19:S:59:ASP:H	2.24	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.98	0.46
30:0:1311:G:C2	30:0:1312:G:C8	3.04	0.46
30:0:1790:C:H2'	30:0:1791:U:C6	2.50	0.46
30:0:2241:C:H2'	30:0:2242:U:C6	2.51	0.46
30:0:2379:G:N7	30:0:2408:A:N1	2.63	0.46
1:A:194:MET:HG2	30:0:875:A:C2	2.52	0.45
5:E:84:MET:HE1	5:E:148:ILE:CD1	2.46	0.45
5:E:84:MET:HE2	5:E:133:VAL:CG2	2.46	0.45
29:3:62:THR:HB	38:3:9044:HOH:O	2.15	0.45
30:0:78:G:C6	30:0:79:G:C6	3.04	0.45
30:0:162:C:H2'	30:0:163:U:H5'	1.98	0.45
30:0:278:A:H2'	30:0:279:C:O4'	2.16	0.45
30:0:372:A:H2'	30:0:373:G:C8	2.51	0.45
30:0:876:A:N3	30:0:876:A:C2'	2.80	0.45
30:0:1511:U:O2'	30:0:1512:G:H5'	2.16	0.45
30:0:1522:A:C2	30:0:1665:G:C6	3.04	0.45
30:0:2415:A:C2'	30:0:2416:G:H5'	2.46	0.45
30:0:2831:C:H42	30:0:2909:G:H1	1.64	0.45
30:0:2872:U:H2'	30:0:2873:C:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2880:A:C2'	30:0:2881:C:H5'	2.46	0.45
10:J:75:PRO:HD3	10:J:136:SER:OG	2.16	0.45
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.31	0.45
20:T:63:ILE:HD11	20:T:75:GLU:HB2	1.99	0.45
22:V:39:ALA:C	22:V:41:GLU:H	2.23	0.45
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.98	0.45
30:0:53:C:H2'	30:0:54:G:O4'	2.16	0.45
30:0:412:C:O2'	30:0:413:G:H5'	2.16	0.45
30:0:669:G:O2'	30:0:670:G:H5'	2.16	0.45
30:0:758:A:H2'	30:0:759:C:O4'	2.17	0.45
30:0:1074:G:H4'	30:0:1260:G:C6	2.51	0.45
30:0:1194:A:O2'	30:0:1195:G:H5'	2.16	0.45
30:0:1339:G:C6	30:0:1340:G:N1	2.85	0.45
30:0:1778:A:H2'	30:0:1779:A:H5'	1.97	0.45
3:C:19:PRO:HG2	3:C:22:PHE:CD1	2.51	0.45
23:W:38:THR:HG22	23:W:39:ASP:N	2.31	0.45
30:0:407:A:H8	38:0:4486:HOH:O	2.00	0.45
30:0:445:U:H2'	30:0:446:G:H8	1.81	0.45
30:0:2456:A:H2'	30:0:2457:U:C6	2.51	0.45
6:F:91:VAL:CG1	6:F:92:GLY:N	2.80	0.45
30:0:253:U:H1'	30:0:256:C:H41	1.82	0.45
30:0:281:U:H2'	30:0:282:C:H6	1.82	0.45
30:0:506:G:N2	30:0:509:A:H5'	2.22	0.45
30:0:522:U:O2'	30:0:1366:C:H5'	2.16	0.45
30:0:1333:U:H2'	30:0:1334:C:H6	1.82	0.45
30:0:2271:G:N3	30:0:2271:G:H2'	2.31	0.45
31:9:3:A:OP2	31:9:25:G:N2	2.49	0.45
31:9:53:G:O2'	31:9:54:A:H5'	2.16	0.45
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.35	0.45
11:K:113:ILE:HG22	11:K:114:ALA:N	2.32	0.45
14:N:154:LEU:C	14:N:156:GLU:H	2.24	0.45
15:O:10:LEU:HD13	15:O:99:GLU:HG3	1.99	0.45
30:0:1919:A:H4'	38:0:4883:HOH:O	2.15	0.45
30:0:2493:C:O2	30:0:2493:C:H2'	2.15	0.45
31:9:40:C:H2'	31:9:41:C:OP1	2.17	0.45
31:9:57:A:N6	38:9:9066:HOH:O	2.47	0.45
2:B:79:MET:HE3	2:B:144:THR:HG21	1.98	0.45
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.51	0.45
4:D:20:LYS:HG2	4:D:133:ASN:HB3	1.97	0.45
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.51	0.45
18:R:132:ARG:HG2	18:R:133:ALA:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:78:GLU:HG2	24:X:79:GLU:H	1.81	0.45
30:0:603:A:H1'	30:0:605:C:C2	2.52	0.45
30:0:1202:A:H2'	30:0:1203:G:H5'	1.99	0.45
30:0:1588:G:C6	30:0:1589:G:C6	3.05	0.45
30:0:1947:G:H2'	30:0:1948:G:C8	2.52	0.45
30:0:2598:U:O2	30:0:2600:A:H8	2.00	0.45
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.99	0.45
1:A:164:ARG:NE	38:A:9043:HOH:O	2.49	0.45
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.99	0.45
13:M:99:ARG:HG3	38:M:8855:HOH:O	2.16	0.45
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.99	0.45
16:P:134:VAL:O	16:P:137:LEU:HB3	2.17	0.45
17:Q:1:PRO:HA	30:0:2299:G:O6	2.16	0.45
30:0:42:C:H1'	38:0:4707:HOH:O	2.15	0.45
30:0:821:U:H3'	38:0:3789:HOH:O	2.15	0.45
30:0:1183:C:N3	30:0:1184:C:H5	2.15	0.45
30:0:2090:G:H2'	30:0:2091:G:C8	2.51	0.45
30:0:2281:C:C2'	30:0:2282:U:H5'	2.47	0.45
30:0:2812:A:N7	38:0:7555:HOH:O	2.36	0.45
31:9:54:A:HO2'	31:9:55:U:H5'	1.82	0.45
1:A:96:LEU:HD22	1:A:128:LEU:HD13	1.99	0.45
1:A:99:ILE:O	1:A:131:HIS:HE1	2.00	0.45
1:A:186:TRP:CG	1:A:187:PRO:HA	2.52	0.45
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.98	0.45
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.99	0.45
8:H:34:HIS:HD2	8:H:90:LEU:O	2.00	0.45
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.97	0.45
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.32	0.45
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.52	0.45
30:0:1987:C:H2'	30:0:1988:C:C6	2.51	0.45
3:C:84:VAL:O	3:C:85:LYS:HB2	2.17	0.45
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.99	0.45
18:R:113:HIS:O	18:R:145:LEU:HD12	2.17	0.45
19:S:77:VAL:O	19:S:80:ARG:HG2	2.16	0.45
23:W:119:HIS:HE1	38:0:9565:HOH:O	2.00	0.45
30:0:128:A:C8	30:0:128:A:H3'	2.52	0.45
30:0:1902:G:N2	30:0:1936:C:C2	2.85	0.45
30:0:2506:A:O2'	30:0:2507:G:P	2.75	0.45
31:9:81:C:O2'	31:9:82:U:H5'	2.17	0.45
3:C:168:ARG:NH2	3:C:190:ALA:O	2.50	0.45
23:W:74:GLU:OE1	30:0:1285:U:H4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:137:LYS:HD2	30:0:521:A:H5''	1.99	0.45
27:1:2:GLY:O	27:1:6:PRO:HG2	2.17	0.45
30:0:77:G:C2'	30:0:78:G:H5'	2.47	0.45
30:0:951:A:O2'	30:0:952:G:H5'	2.17	0.45
30:0:969:G:N2	30:0:1000:C:C2	2.84	0.45
30:0:1615:A:H5'	38:0:4210:HOH:O	2.16	0.45
30:0:1626:A:H2'	30:0:1627:G:O4'	2.17	0.45
31:9:1:U:O3'	31:9:3:A:OP1	2.35	0.45
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.00	0.44
13:M:164:THR:HB	38:M:8819:HOH:O	2.15	0.44
30:0:542:A:O2'	30:0:543:G:H5'	2.16	0.44
30:0:1783:A:O2'	30:0:1784:U:H5'	2.16	0.44
30:0:1896:G:C6	30:0:1897:U:C4	3.05	0.44
30:0:1942:A:O2'	30:0:1943:C:H5'	2.17	0.44
30:0:2754:G:H2'	30:0:2755:G:O4'	2.17	0.44
1:A:53:ALA:HB3	38:A:9060:HOH:O	2.16	0.44
4:D:135:VAL:HG22	4:D:136:ARG:N	2.32	0.44
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.98	0.44
26:Z:37:ARG:HD2	38:Z:8719:HOH:O	2.17	0.44
29:3:65:THR:CG2	29:3:67:LEU:HG	2.46	0.44
30:0:291:C:H2'	30:0:292:G:O4'	2.17	0.44
30:0:812:A:H2'	30:0:813:C:C6	2.52	0.44
30:0:1406:A:H4'	30:0:1407:A:H5''	1.99	0.44
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.76	0.44
1:A:171:LYS:NZ	30:0:820:G:OP2	2.42	0.44
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.38	0.44
11:K:14:LYS:HG3	11:K:32:ILE:O	2.18	0.44
14:N:108:SER:HA	14:N:109:PRO:HD3	1.81	0.44
30:0:187:A:H3'	30:0:188:C:H6	1.82	0.44
30:0:204:A:H2'	30:0:205:U:H5'	1.98	0.44
30:0:582:U:H2'	30:0:583:C:C6	2.53	0.44
30:0:1182:C:HO2'	30:0:1183:C:H5	1.64	0.44
30:0:2032:U:H2'	30:0:2033:G:C5'	2.47	0.44
4:D:38:GLU:CD	4:D:51:ARG:HE	2.26	0.44
13:M:58:GLN:HG3	38:M:8906:HOH:O	2.18	0.44
25:Y:144:ARG:NH2	38:Y:8907:HOH:O	2.51	0.44
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.44
30:0:451:C:O2'	30:0:452:G:H5'	2.18	0.44
30:0:453:A:H4'	30:0:455:A:N7	2.32	0.44
30:0:2385:G:H2'	30:0:2386:U:C6	2.52	0.44
30:0:2464:C:H5''	30:0:2465:A:OP1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2473:U:O3'	30:0:2474:A:H3'	2.17	0.44
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.47	0.44
16:P:120:ARG:NH2	16:P:123:TYR:CD2	2.85	0.44
30:0:185:G:H4'	30:0:186:A:H4'	1.99	0.44
30:0:815:U:O2'	30:0:1598:A:H4'	2.17	0.44
30:0:825:U:H5''	30:0:826:U:OP1	2.18	0.44
30:0:947:U:O2'	30:0:948:G:H5'	2.16	0.44
30:0:1342:C:C2'	30:0:1343:C:H5'	2.47	0.44
30:0:1973:A:H2'	30:0:1974:G:O4'	2.18	0.44
30:0:2635:A:C2'	30:0:2636:C:H5'	2.46	0.44
2:B:74:ILE:HG13	38:B:9080:HOH:O	2.17	0.44
4:D:53:LYS:HE3	31:9:40:C:H42	1.82	0.44
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.17	0.44
13:M:46:LEU:HG	38:M:8922:HOH:O	2.18	0.44
28:2:2:LYS:HG3	30:0:1486:A:C5	2.52	0.44
30:0:77:G:H2'	30:0:78:G:H5'	1.99	0.44
30:0:218:C:C5	30:0:220:C:C4	3.06	0.44
30:0:816:G:H5'	30:0:1598:A:H4'	1.99	0.44
30:0:1427:A:H61	30:0:1440:U:C1'	2.30	0.44
30:0:1592:G:C4	30:0:1593:C:C5	3.06	0.44
30:0:1592:G:O2'	30:0:1593:C:O5'	2.35	0.44
30:0:2276:U:H2'	30:0:2277:U:C6	2.53	0.44
30:0:2636:C:H4'	38:0:6666:HOH:O	2.18	0.44
31:9:76:G:H3'	31:9:77:A:C5'	2.31	0.44
10:J:19:MET:CE	10:J:132:LEU:HD11	2.39	0.44
14:N:11:ARG:NH1	31:9:8:G:O6	2.50	0.44
16:P:91:LYS:O	16:P:95:GLU:HG3	2.17	0.44
30:0:204:A:C2'	30:0:205:U:H5'	2.47	0.44
30:0:764:C:H2'	30:0:765:G:O4'	2.17	0.44
30:0:794:U:C2'	30:0:795:G:H5'	2.48	0.44
30:0:1603:A:C5'	30:0:1605:G:C5'	2.94	0.44
30:0:1878:G:O2'	30:0:1879:U:OP2	2.36	0.44
1:A:204:GLY:N	30:0:2634:G:OP2	2.48	0.44
2:B:280:VAL:HG13	2:B:333:GLU:O	2.17	0.44
4:D:131:THR:HG21	30:0:2348:C:H1'	1.99	0.44
4:D:135:VAL:HG22	4:D:136:ARG:H	1.82	0.44
5:E:6:GLU:HG2	5:E:46:THR:HG22	1.99	0.44
6:F:60:VAL:HG13	6:F:63:ILE:HG13	1.99	0.44
8:H:30:LYS:H	8:H:62:HIS:HD2	1.65	0.44
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.83	0.44
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:441:A:H8	30:0:441:A:O5'	1.99	0.44
30:0:497:A:H2'	30:0:498:A:C5'	2.48	0.44
30:0:807:A:O2'	30:0:808:A:H5'	2.17	0.44
30:0:1006:A:N1	30:0:2311:A:H1'	2.33	0.44
30:0:1044:C:H5''	38:0:9028:HOH:O	2.18	0.44
30:0:2461:U:O2	30:0:2466:G:H1'	2.18	0.44
30:0:2511:A:H2'	30:0:2512:U:O4'	2.17	0.44
30:0:2565:C:H4'	38:0:4868:HOH:O	2.18	0.44
31:9:107:C:O2'	31:9:108:C:H5'	2.18	0.44
1:A:76:VAL:HG23	26:Z:87:LYS:HB3	2.00	0.44
4:D:146:LYS:NZ	14:N:107:ASN:ND2	2.66	0.44
11:K:89:LYS:HE2	21:U:19:THR:HG21	2.00	0.44
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.49	0.44
21:U:49:LEU:HG	38:U:3805:HOH:O	2.17	0.44
30:0:66:G:C2	30:0:109:U:C4	3.06	0.44
30:0:88:G:H2'	30:0:89:G:H8	1.83	0.44
30:0:383:A:H2'	30:0:384:G:O4'	2.18	0.44
30:0:629:A:C2	30:0:2074:A:C2	3.06	0.44
30:0:1066:U:H2'	30:0:1067:A:C8	2.52	0.44
30:0:1189:A:H1'	30:0:1209:C:H1'	1.99	0.44
30:0:1375:A:C2'	30:0:1376:G:H5'	2.47	0.44
30:0:1588:G:C5	30:0:1589:G:C6	3.06	0.44
30:0:1903:U:O2'	30:0:1904:A:N7	2.50	0.44
30:0:2015:A:H2'	30:0:2016:U:O4'	2.18	0.44
30:0:2238:A:O2'	30:0:2239:C:H5'	2.18	0.44
30:0:2506:A:O2'	30:0:2507:G:O5'	2.36	0.44
30:0:2569:A:H2'	30:0:2570:G:O5'	2.18	0.44
1:A:190:ARG:HH11	30:0:1845:A:P	2.41	0.43
2:B:53:LEU:HD11	2:B:327:VAL:HG22	1.99	0.43
3:C:170:ASP:OD2	30:0:330:C:H5	2.01	0.43
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.99	0.43
10:J:70:PHE:HD1	30:0:2676:C:O2'	2.00	0.43
14:N:37:ARG:HH12	31:9:6:C:C5'	2.21	0.43
14:N:37:ARG:NE	38:N:8831:HOH:O	2.51	0.43
16:P:73:HIS:HE1	30:0:1789:G:O6	2.01	0.43
17:Q:19:ARG:HH21	31:9:11:A:P	2.41	0.43
30:0:177:A:O2'	30:0:892:G:H4'	2.17	0.43
30:0:499:G:O2'	30:0:500:G:H5'	2.16	0.43
30:0:594:C:C4	30:0:595:U:C4	3.06	0.43
30:0:1632:A:H2'	30:0:1633:C:C5'	2.42	0.43
30:0:2842:G:H2'	30:0:2843:A:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:55:U:H4'	31:9:56:A:H8	1.83	0.43
2:B:10:SER:HB2	30:0:2714:U:H4'	1.99	0.43
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.51	0.43
13:M:134:ILE:O	13:M:136:PRO:HD3	2.19	0.43
14:N:50:LEU:HD12	14:N:50:LEU:HA	1.86	0.43
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.53	0.43
29:3:91:GLN:O	29:3:92:GLU:HB2	2.18	0.43
30:0:963:C:O2	30:0:1005:A:N1	2.51	0.43
30:0:1119:G:N2	30:0:1246:A:H2	2.13	0.43
31:9:31:C:H2'	31:9:32:G:O4'	2.18	0.43
31:9:114:G:H2'	31:9:115:C:H6	1.81	0.43
1:A:1:GLY:HA2	1:A:197:VAL:HG23	1.99	0.43
1:A:95:PRO:O	1:A:99:ILE:HG12	2.19	0.43
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.84	0.43
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.16	0.43
18:R:40:ALA:O	18:R:44:VAL:HG23	2.18	0.43
28:2:16:ASN:HB2	38:2:5203:HOH:O	2.17	0.43
30:0:271:C:C2	30:0:273:G:O4'	2.70	0.43
30:0:1056:U:H2'	30:0:1057:A:O4'	2.18	0.43
30:0:1156:C:O5'	30:0:1156:C:H6	2.01	0.43
30:0:1517:C:O2	30:0:1670:A:C2	2.71	0.43
30:0:1565:C:H2'	30:0:1566:C:H6	1.83	0.43
30:0:2870:C:O2'	30:0:2871:G:H5'	2.19	0.43
31:9:3:A:C2	31:9:21:G:N3	2.85	0.43
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.43
3:C:61:PHE:HB3	38:C:8639:HOH:O	2.18	0.43
7:G:12:ILE:HG12	38:0:5490:HOH:O	2.19	0.43
30:0:17:G:H2'	30:0:18:C:C6	2.53	0.43
30:0:212:A:O4'	30:0:214:U:C6	2.72	0.43
30:0:294:C:H2'	30:0:295:C:O4'	2.18	0.43
30:0:559:U:H2'	30:0:560:U:O4'	2.18	0.43
30:0:677:C:O2'	30:0:678:G:H5'	2.18	0.43
30:0:960:G:C3'	30:0:960:G:C4	3.01	0.43
30:0:1434:A:H2'	30:0:1436:C:C5	2.53	0.43
30:0:1456:C:H2'	30:0:1457:U:C6	2.54	0.43
30:0:1789:G:H2'	30:0:1790:C:O5'	2.18	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.96	0.43
2:B:305:ASP:O	2:B:306:LYS:HB2	2.19	0.43
3:C:242:GLU:HB2	38:C:8577:HOH:O	2.17	0.43
8:H:157:TYR:CD1	8:H:157:TYR:C	2.96	0.43
11:K:8:VAL:HG13	11:K:80:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:146:GLY:C	12:L:148:GLU:H	2.26	0.43
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.89	0.43
22:V:1:THR:HG23	22:V:2:VAL:N	2.30	0.43
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.48	0.43
28:2:41:HIS:CD2	28:2:44:ARG:H	2.26	0.43
30:0:365:G:C6	30:0:366:U:C4	3.06	0.43
30:0:424:C:H2'	30:0:425:U:C6	2.53	0.43
30:0:951:A:C2'	30:0:952:G:H5'	2.48	0.43
30:0:1946:C:H2'	30:0:1971:G:C8	2.53	0.43
13:M:47:ASP:CG	13:M:48:LYS:N	2.77	0.43
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.82	0.43
30:0:35:U:H2'	30:0:36:C:C6	2.53	0.43
30:0:226:A:H1'	30:0:393:G:C5	2.54	0.43
31:9:42:C:H5'	31:9:43:G:OP2	2.19	0.43
31:9:58:G:H3'	31:9:59:C:C6	2.54	0.43
1:A:94:LEU:HG	1:A:99:ILE:HD13	2.01	0.43
6:F:59:ILE:CD1	30:0:263:U:C2	3.01	0.43
8:H:64:SER:OG	30:0:2520:G:H5'	2.17	0.43
30:0:130:C:H5'	38:0:5243:HOH:O	2.19	0.43
30:0:512:G:O3'	30:0:513:A:C8	2.71	0.43
30:0:794:U:H2'	30:0:795:G:H5'	2.01	0.43
30:0:794:U:H3	30:0:819:A:H61	1.65	0.43
30:0:844:A:C6	30:0:882:A:C5	3.06	0.43
30:0:1764:C:H2'	30:0:1765:G:O4'	2.18	0.43
30:0:1970:G:H2'	30:0:1970:G:N3	2.33	0.43
30:0:1992:U:H2'	30:0:1994:A:OP2	2.18	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.34	0.43
30:0:2523:U:O2'	30:0:2524:G:H5'	2.19	0.43
3:C:98:ARG:NH1	38:C:8554:HOH:O	2.51	0.43
6:F:59:ILE:HD13	30:0:263:U:O4'	2.19	0.43
6:F:99:THR:HG23	6:F:99:THR:O	2.19	0.43
11:K:130:MET:SD	21:U:25:ASP:O	2.77	0.43
19:S:57:THR:HG22	19:S:58:MET:N	2.33	0.43
22:V:55:ARG:O	22:V:59:ILE:HG12	2.19	0.43
30:0:1250:C:O2'	30:0:1251:C:H5'	2.19	0.43
30:0:1589:G:N2	30:0:1605:G:H1'	2.34	0.43
30:0:2387:U:H2'	30:0:2388:C:C6	2.54	0.43
3:C:151:GLN:HG3	30:0:327:A:OP2	2.19	0.43
4:D:128:LEU:HB2	38:D:6007:HOH:O	2.19	0.43
4:D:167:GLU:C	4:D:169:THR:H	2.27	0.43
11:K:64:MET:HA	11:K:67:GLN:HE21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.49	0.43
16:P:40:VAL:O	16:P:44:VAL:HG23	2.19	0.43
21:U:49:LEU:O	21:U:52:THR:HG22	2.17	0.43
25:Y:133:HIS:HD2	38:Y:8877:HOH:O	2.02	0.43
25:Y:168:PHE:CE2	30:0:1090:A:H4'	2.54	0.43
30:0:537:G:O4'	30:0:538:C:C5	2.71	0.43
30:0:941:G:C6	30:0:942:U:C4	3.07	0.43
30:0:1245:C:O5'	30:0:1245:C:H6	2.02	0.43
30:0:1421:C:O2'	30:0:1422:U:H5'	2.18	0.43
30:0:1616:A:H5''	30:0:1617:C:OP1	2.19	0.43
31:9:59:C:H2'	31:9:60:C:C6	2.54	0.43
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.90	0.43
2:B:162:MET:HE2	2:B:310:ARG:CD	2.48	0.43
4:D:99:ASP:HB3	4:D:103:ASN:H	1.84	0.43
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.43
14:N:38:LYS:HB2	14:N:38:LYS:HE3	1.77	0.43
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.19	0.43
27:1:25:LYS:O	27:1:25:LYS:HG2	2.19	0.43
30:0:488:U:H2'	38:0:4031:HOH:O	2.18	0.43
30:0:1032:A:H2'	30:0:1032:A:N3	2.33	0.43
30:0:1160:G:H5'	30:0:1161:A:C4'	2.46	0.43
30:0:1187:U:O2'	30:0:1189:A:H2	1.85	0.43
30:0:1555:G:O2'	30:0:1556:G:H5'	2.19	0.43
30:0:1644:C:C2	30:0:1645:U:C6	3.07	0.43
30:0:1996:U:O2'	30:0:1997:A:H5'	2.18	0.43
30:0:2524:G:N2	30:0:2526:C:H41	2.17	0.43
31:9:52:A:O2'	31:9:53:G:H5'	2.19	0.43
2:B:5:ARG:NH1	2:B:8:LYS:HE2	2.34	0.42
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.34	0.42
9:I:86:GLU:HG2	30:0:1180:U:H4'	2.01	0.42
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.18	0.42
30:0:39:G:N2	30:0:444:C:C2	2.87	0.42
30:0:332:G:O2'	30:0:333:G:H5'	2.19	0.42
30:0:1202:A:H2'	30:0:1203:G:C5'	2.48	0.42
30:0:1788:U:C2	30:0:1805:G:N2	2.87	0.42
30:0:2252:A:C6	30:0:2253:G:H1'	2.53	0.42
30:0:2435:U:H1'	38:0:5462:HOH:O	2.19	0.42
31:9:45:A:H2'	31:9:46:C:C6	2.54	0.42
1:A:99:ILE:O	1:A:131:HIS:CE1	2.72	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.18	0.42
3:C:25:PRO:HG2	38:C:8520:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.20	0.42
14:N:82:TYR:CD2	14:N:82:TYR:C	2.97	0.42
30:0:1015:C:O5'	30:0:1015:C:H6	2.02	0.42
30:0:1761:U:H2'	30:0:1762:C:C6	2.54	0.42
31:9:2:U:OP2	31:9:2:U:H4'	2.19	0.42
31:9:2:U:C4'	38:9:9103:HOH:O	2.67	0.42
31:9:14:G:H2'	31:9:15:C:H5'	2.01	0.42
31:9:72:C:O2'	31:9:73:A:H5'	2.19	0.42
1:A:179:MET:HG2	1:A:186:TRP:CG	2.55	0.42
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.51	0.42
8:H:31:ILE:HG23	38:H:231:HOH:O	2.18	0.42
12:L:67:ARG:O	12:L:71:GLU:HG3	2.20	0.42
38:Q:2875:HOH:O	30:0:2392:C:H4'	2.20	0.42
29:3:3:MET:HG3	29:3:4:PRO:HD2	2.01	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.46	0.42
30:0:1634:G:C6	30:0:1635:U:C4	3.07	0.42
30:0:1762:C:H2'	30:0:1763:C:C6	2.54	0.42
30:0:2004:U:H2'	30:0:2005:G:OP1	2.19	0.42
30:0:2423:C:H2'	30:0:2424:U:C6	2.54	0.42
30:0:2819:C:H2'	30:0:2820:A:C8	2.54	0.42
1:A:179:MET:HG2	1:A:186:TRP:CB	2.49	0.42
2:B:178:ALA:O	2:B:182:VAL:HG23	2.20	0.42
6:F:118:LEU:O	6:F:119:ARG:HB3	2.19	0.42
9:I:111:LEU:HD23	30:0:1163:G:H4'	2.01	0.42
16:P:59:ARG:NH2	16:P:66:GLN:HE22	2.10	0.42
23:W:43:GLY:HA3	30:0:945:U:O2'	2.19	0.42
24:X:15:ARG:HH22	30:0:2856:A:P	2.42	0.42
30:0:254:C:O2	30:0:254:C:H2'	2.19	0.42
30:0:1175:G:H1'	30:0:1193:A:H2'	2.02	0.42
30:0:1416:G:C2'	30:0:1417:G:H5'	2.49	0.42
30:0:1561:U:O2	30:0:1561:U:H2'	2.18	0.42
30:0:2104:C:O2	30:0:2485:A:N1	2.53	0.42
10:J:36:VAL:HG12	10:J:37:ALA:N	2.34	0.42
10:J:93:ARG:HB3	10:J:93:ARG:HH11	1.83	0.42
20:T:32:ARG:NH1	20:T:38:ARG:HH12	2.17	0.42
23:W:13:MET:CE	23:W:17:ILE:HG22	2.49	0.42
23:W:80:ASP:HB2	38:W:3312:HOH:O	2.18	0.42
30:0:344:C:H2'	30:0:345:G:O4'	2.20	0.42
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.42
30:0:2134:G:N2	30:0:2242:U:C2	2.87	0.42
30:0:2414:A:N1	30:0:2415:A:C6	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2719:A:H5''	38:0:3702:HOH:O	2.19	0.42
4:D:23:VAL:HG11	4:D:83:PHE:CZ	2.55	0.42
14:N:34:LEU:HD22	14:N:129:ILE:HD13	2.01	0.42
21:U:17:THR:CG2	21:U:18:GLY:N	2.83	0.42
30:0:243:A:H61	30:0:269:G:H1'	1.84	0.42
30:0:284:C:H4'	30:0:285:A:H8	1.84	0.42
30:0:544:G:C3'	30:0:545:G:H5''	2.48	0.42
30:0:603:A:H4'	30:0:604:G:O5'	2.20	0.42
30:0:843:A:C2	30:0:846:A:C8	3.08	0.42
30:0:1206:U:C6	30:0:1206:U:C3'	3.02	0.42
30:0:1211:G:O2'	30:0:1212:C:H5'	2.19	0.42
30:0:1451:C:H5'	30:0:1505:U:C4	2.54	0.42
30:0:1987:C:H2'	30:0:1988:C:H6	1.85	0.42
30:0:2134:G:C6	30:0:2258:A:C8	3.08	0.42
30:0:2361:A:H2'	30:0:2362:A:O4'	2.19	0.42
30:0:2578:G:H5'	30:0:2578:G:C8	2.44	0.42
30:0:2754:G:C2'	30:0:2755:G:H5'	2.49	0.42
31:9:14:G:H2'	31:9:15:C:C5'	2.50	0.42
2:B:314:ALA:CB	2:B:317:PRO:HG3	2.50	0.42
14:N:25:ARG:HB3	30:0:2415:A:C2	2.54	0.42
23:W:7:LEU:HD12	23:W:53:ALA:HB2	2.00	0.42
26:Z:45:VAL:HG12	38:Z:8713:HOH:O	2.19	0.42
30:0:369:G:C2	30:0:370:G:C8	3.08	0.42
30:0:466:A:H2'	30:0:467:G:O4'	2.20	0.42
30:0:1307:A:H2'	30:0:1308:A:C8	2.55	0.42
30:0:2505:G:H2'	30:0:2506:A:C5'	2.50	0.42
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.85	0.42
3:C:85:LYS:HA	3:C:85:LYS:HD2	1.90	0.42
4:D:170:TYR:CD1	4:D:170:TYR:N	2.87	0.42
8:H:4:LYS:HA	8:H:5:PRO:HD3	1.86	0.42
8:H:87:LYS:NZ	8:H:87:LYS:HB2	2.35	0.42
13:M:124:GLY:HA3	30:0:2132:C:H1'	2.02	0.42
15:O:96:VAL:HG12	15:O:97:SER:O	2.20	0.42
18:R:69:LYS:HB2	18:R:72:VAL:HG23	2.01	0.42
22:V:12:THR:HG22	22:V:15:GLU:CG	2.47	0.42
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.30	0.42
24:X:37:LEU:O	24:X:41:PHE:HB2	2.19	0.42
30:0:539:G:H2'	30:0:540:A:C8	2.54	0.42
30:0:790:A:H8	38:0:6134:HOH:O	2.01	0.42
30:0:1023:C:H2'	30:0:1024:G:O4'	2.20	0.42
30:0:1244:U:H4'	30:0:1246:A:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1298:U:H2'	30:0:1299:G:C8	2.54	0.42
30:0:1782:G:O2'	30:0:1783:A:H5'	2.19	0.42
30:0:2252:A:C2'	30:0:2253:G:H5'	2.49	0.42
30:0:2756:U:C2	30:0:2896:A:H2	2.38	0.42
30:0:2909:G:H2'	30:0:2910:A:H8	1.84	0.42
1:A:23:TYR:HD1	30:0:1872:C:H2'	1.85	0.42
1:A:94:LEU:HD23	1:A:94:LEU:N	2.34	0.42
2:B:27:ASN:HD22	2:B:27:ASN:H	1.67	0.42
14:N:159:TYR:HE1	31:9:50:G:H5''	1.85	0.42
15:O:44:ASN:OD1	15:O:65:LEU:HB2	2.19	0.42
24:X:8:ARG:NH1	30:0:2904:U:H4'	2.35	0.42
24:X:37:LEU:HD21	24:X:72:VAL:HG11	2.02	0.42
30:0:417:G:P	38:0:7457:HOH:O	2.77	0.42
30:0:1198:U:H1'	30:0:1201:C:C5	2.50	0.42
30:0:1433:G:O2'	30:0:1434:A:H5'	2.20	0.42
30:0:1676:G:C2'	30:0:1677:U:H5'	2.50	0.42
30:0:2783:A:O2'	30:0:2784:A:H5'	2.19	0.42
1:A:54:PRO:HG2	1:A:160:ALA:HB3	2.02	0.42
1:A:107:ASN:OD1	1:A:116:GLY:HA3	2.20	0.42
1:A:211:LYS:HB2	38:A:9075:HOH:O	2.19	0.42
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.85	0.42
3:C:5:ILE:HD11	3:C:16:VAL:HG23	2.01	0.42
10:J:45:VAL:HG11	10:J:121:LEU:HD22	2.02	0.42
18:R:29:LYS:NZ	38:R:8944:HOH:O	2.53	0.42
30:0:128:A:C8	30:0:128:A:C3'	3.03	0.42
30:0:1334:C:H2'	30:0:1335:C:H6	1.85	0.42
30:0:2509:A:OP2	30:0:2510:C:C5	2.72	0.42
30:0:2712:G:P	38:0:5251:HOH:O	2.77	0.42
30:0:2718:C:H5'	30:0:2718:C:C6	2.53	0.42
30:0:2908:A:C2'	30:0:2909:G:H5'	2.49	0.42
4:D:105:SER:OG	30:0:2338:G:H1'	2.20	0.41
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.20	0.41
6:F:39:SER:HB3	6:F:45:ALA:HB2	2.02	0.41
10:J:131:THR:HG22	10:J:134:GLU:H	1.85	0.41
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.17	0.41
14:N:147:ILE:HB	38:9:9090:HOH:O	2.19	0.41
25:Y:154:ARG:HH22	30:0:1071:G:H4'	1.85	0.41
29:3:18:GLN:HG3	38:3:9009:HOH:O	2.20	0.41
30:0:129:A:O2'	30:0:131:A:OP1	2.36	0.41
30:0:259:G:O2'	30:0:260:C:H5'	2.20	0.41
30:0:821:U:H2'	30:0:822:C:H6	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:883:U:O2	30:0:883:U:C2'	2.67	0.41
30:0:960:G:H2'	30:0:961:A:OP2	2.19	0.41
30:0:1335:C:H2'	30:0:1336:U:C6	2.55	0.41
30:0:1406:A:H4'	30:0:1407:A:C5'	2.50	0.41
30:0:1562:C:N4	38:0:5895:HOH:O	2.53	0.41
30:0:1789:G:C2'	30:0:1790:C:O5'	2.68	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.20	0.41
30:0:2727:A:C6	30:0:2756:U:C2	3.08	0.41
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.51	0.41
2:B:40:GLY:O	2:B:193:ILE:HD13	2.20	0.41
3:C:193:LEU:HD12	3:C:211:ASP:O	2.20	0.41
4:D:22:VAL:HG22	4:D:74:THR:HG22	2.00	0.41
4:D:37:ALA:O	4:D:40:ILE:HG12	2.20	0.41
10:J:80:LYS:NZ	38:J:7377:HOH:O	2.52	0.41
12:L:150:GLN:HB3	38:L:8868:HOH:O	2.20	0.41
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.44	0.41
19:S:11:THR:H	19:S:14:ALA:HB3	1.84	0.41
25:Y:142:SER:OG	30:0:1331:G:OP2	2.34	0.41
30:0:64:G:H2'	30:0:65:C:O4'	2.20	0.41
30:0:420:U:H2'	30:0:421:C:C6	2.55	0.41
30:0:1052:G:C5	30:0:1063:G:C6	3.09	0.41
31:9:47:A:H2'	31:9:48:C:O4'	2.20	0.41
2:B:248:ARG:NH1	38:B:9090:HOH:O	2.53	0.41
4:D:141:VAL:HG21	31:9:57:A:H8	1.85	0.41
9:I:69:PRO:HA	30:0:1164:U:OP1	2.21	0.41
14:N:37:ARG:HD3	33:N:8807:CL:CL	2.57	0.41
27:1:45:ARG:HB3	38:1:988:HOH:O	2.20	0.41
28:2:41:HIS:CD2	28:2:43:ARG:H	2.39	0.41
30:0:506:G:N2	30:0:509:A:H5''	2.32	0.41
30:0:1167:G:C2	30:0:1168:C:C2	3.08	0.41
30:0:1185:U:H5'	38:0:7504:HOH:O	2.20	0.41
30:0:1840:A:H4'	30:0:1841:C:O5'	2.20	0.41
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.41
9:I:101:LYS:O	9:I:105:GLU:HG3	2.21	0.41
13:M:158:ARG:HB2	13:M:163:LEU:HB2	2.01	0.41
28:2:41:HIS:N	28:2:45:ASN:HD22	2.03	0.41
30:0:151:A:C2	30:0:442:A:C8	3.09	0.41
30:0:635:A:H2'	30:0:636:G:H5''	2.02	0.41
30:0:729:C:C2	30:0:743:G:C2	3.08	0.41
30:0:1422:U:O2'	30:0:1423:C:H5'	2.20	0.41
30:0:1474:C:C6	30:0:1474:C:C5'	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1909:A:H2'	30:0:1910:A:C8	2.54	0.41
31:9:45:A:C5	31:9:46:C:C5	3.08	0.41
1:A:36:ASP:O	1:A:38:ILE:N	2.53	0.41
3:C:223:LEU:HD12	3:C:223:LEU:HA	1.91	0.41
16:P:7:LYS:HG2	16:P:23:PHE:CE2	2.55	0.41
24:X:39:LYS:HE2	30:0:2834:G:OP1	2.20	0.41
28:2:37:HIS:CE1	30:0:462:A:C8	3.08	0.41
30:0:834:G:H3'	30:0:835:U:H4'	2.01	0.41
30:0:1138:G:H4'	38:0:5739:HOH:O	2.18	0.41
30:0:1342:C:O2'	30:0:1343:C:H5'	2.20	0.41
30:0:1667:A:C2	30:0:1668:U:C2	3.08	0.41
30:0:1903:U:O2'	30:0:1904:A:C8	2.68	0.41
30:0:2421:G:H4'	38:0:4814:HOH:O	2.20	0.41
30:0:2704:C:H2'	30:0:2705:U:O4'	2.20	0.41
2:B:215:VAL:HA	2:B:220:VAL:HG22	2.02	0.41
3:C:154:VAL:O	3:C:158:GLU:HG3	2.21	0.41
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.20	0.41
10:J:52:GLN:HE22	30:0:1119:G:H8	1.69	0.41
16:P:59:ARG:O	16:P:63:ARG:HG3	2.21	0.41
23:W:41:TYR:HA	23:W:44:MET:HE3	2.02	0.41
24:X:43:VAL:HG11	24:X:82:GLU:HA	2.01	0.41
29:3:38:ARG:HD2	30:0:396:U:OP2	2.21	0.41
30:0:243:A:H61	30:0:269:G:C1'	2.34	0.41
30:0:290:C:H1'	38:0:6136:HOH:O	2.21	0.41
30:0:318:U:H5'	30:0:339:A:C2	2.56	0.41
30:0:482:G:H4'	30:0:508:A:N1	2.36	0.41
30:0:2102:G:C2	30:0:2104:C:C4	3.08	0.41
30:0:2361:A:H5'	30:0:2361:A:H8	1.86	0.41
30:0:2419:U:H5''	30:0:2420:G:C5'	2.50	0.41
30:0:2637:A:C5'	38:0:4961:HOH:O	2.59	0.41
30:0:2791:U:H4'	30:0:2792:A:OP1	2.20	0.41
30:0:2802:C:H2'	30:0:2803:C:C6	2.55	0.41
1:A:212:PRO:HB2	38:0:4392:HOH:O	2.20	0.41
1:A:217:ARG:HG2	1:A:229:ALA:HB2	2.03	0.41
2:B:280:VAL:CG1	2:B:334:SER:HA	2.50	0.41
13:M:67:VAL:HB	13:M:97:ILE:HG23	2.03	0.41
16:P:94:TRP:CZ2	16:P:98:ILE:HG13	2.56	0.41
25:Y:213:LYS:HE3	25:Y:213:LYS:HB2	1.90	0.41
27:1:5:THR:HG23	30:0:1688:G:O2'	2.20	0.41
29:3:69:TYR:CZ	29:3:80:ARG:HD2	2.56	0.41
30:0:290:C:O2'	30:0:291:C:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:559:U:H5'	30:0:559:U:C6	2.35	0.41
30:0:1377:C:H6	30:0:1377:C:C5'	2.33	0.41
30:0:1481:G:H2'	30:0:1482:A:O4'	2.20	0.41
30:0:1548:U:H1'	38:0:6897:HOH:O	2.19	0.41
30:0:2089:A:C2'	30:0:2090:G:H5'	2.49	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.20	0.41
1:A:95:PRO:HA	1:A:153:ARG:HA	2.03	0.41
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.48	0.41
11:K:30:LYS:HB3	11:K:56:SER:HB3	2.03	0.41
13:M:167:GLY:O	13:M:171:ARG:HG3	2.21	0.41
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.21	0.41
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.56	0.41
14:N:160:SER:CB	31:9:51:A:H5'	2.50	0.41
15:O:98:LEU:O	15:O:102:ILE:HG13	2.21	0.41
16:P:83:LYS:O	16:P:86:ALA:HB3	2.21	0.41
18:R:17:MET:SD	38:R:8951:HOH:O	2.62	0.41
22:V:27:LEU:HA	22:V:49:LEU:HD13	2.02	0.41
23:W:48:VAL:HG12	23:W:48:VAL:O	2.19	0.41
26:Z:37:ARG:HH22	26:Z:54:GLU:CD	2.29	0.41
30:0:81:G:N3	30:0:98:A:C2	2.88	0.41
30:0:667:C:H2'	30:0:668:C:H6	1.85	0.41
30:0:1544:U:O2'	30:0:1545:C:H5'	2.20	0.41
30:0:1714:C:C2'	30:0:1715:C:H5'	2.51	0.41
30:0:1804:A:H2'	30:0:1805:G:C8	2.56	0.41
30:0:2617:G:C2	30:0:2618:G:C8	3.08	0.41
30:0:2802:C:H2'	30:0:2803:C:H6	1.84	0.41
31:9:13:A:OP1	31:9:113:C:H5'	2.21	0.41
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.85	0.41
2:B:154:VAL:CG1	2:B:156:LYS:HG2	2.51	0.41
3:C:76:ARG:HB3	3:C:76:ARG:NH1	2.36	0.41
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.49	0.41
13:M:164:THR:CG2	13:M:165:GLY:N	2.83	0.41
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.51	0.41
38:N:8830:HOH:O	30:0:2368:A:H8	2.04	0.41
15:O:115:ARG:NH1	38:O:6194:HOH:O	2.54	0.41
20:T:79:LEU:HG	20:T:89:ARG:HB2	2.03	0.41
26:Z:50:VAL:O	26:Z:54:GLU:HG3	2.20	0.41
30:0:23:G:C6	30:0:24:G:N1	2.89	0.41
30:0:130:C:H2'	38:0:3183:HOH:O	2.20	0.41
30:0:969:G:H2'	30:0:970:U:C6	2.56	0.41
30:0:1166:A:N3	30:0:1166:A:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1184:C:O2'	30:0:1185:U:OP2	2.36	0.41
30:0:1634:G:C5	30:0:1635:U:C4	3.08	0.41
30:0:1909:A:N1	30:0:2128:G:H1'	2.35	0.41
30:0:1945:G:O2'	30:0:1946:C:H5'	2.20	0.41
30:0:2039:A:H2'	30:0:2040:C:C6	2.56	0.41
30:0:2246:U:N3	30:0:2256:G:C2	2.89	0.41
31:9:34:A:H2'	31:9:35:C:O4'	2.21	0.41
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.02	0.41
29:3:70:ARG:HD3	38:3:9064:HOH:O	2.21	0.41
30:0:595:U:O2'	30:0:596:C:H5'	2.21	0.41
30:0:1119:G:N2	30:0:1246:A:N1	2.69	0.41
30:0:1163:G:N2	38:0:6078:HOH:O	2.54	0.41
30:0:1271:A:C2	30:0:1286:A:C2	3.09	0.41
30:0:1522:A:C2'	30:0:1523:G:H5'	2.51	0.41
30:0:1574:C:O5'	30:0:1574:C:H6	2.04	0.41
30:0:1613:C:H2'	30:0:1614:G:O4'	2.21	0.41
30:0:2072:G:N2	38:0:6910:HOH:O	2.54	0.41
30:0:2251:G:C6	30:0:2252:A:C6	3.09	0.41
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.86	0.40
2:B:154:VAL:HG12	2:B:156:LYS:HG2	2.02	0.40
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.03	0.40
25:Y:106:THR:HG23	25:Y:107:PRO:HD2	2.03	0.40
25:Y:189:ASN:ND2	25:Y:192:ASP:H	2.19	0.40
30:0:106:A:H2'	30:0:107:U:O4'	2.21	0.40
30:0:369:G:O2'	30:0:370:G:H5'	2.21	0.40
30:0:401:C:H2'	30:0:402:U:C6	2.56	0.40
30:0:745:G:H5''	30:0:746:A:OP1	2.21	0.40
30:0:1098:A:H2'	30:0:1099:G:O4'	2.21	0.40
30:0:1182:C:O2'	30:0:1183:C:H5	2.04	0.40
30:0:1515:A:H2'	30:0:1516:U:H6	1.82	0.40
30:0:1520:G:C6	30:0:1521:C:C4	3.09	0.40
30:0:1536:C:H6	30:0:1536:C:O5'	2.03	0.40
30:0:1750:C:N4	30:0:1751:G:C6	2.89	0.40
30:0:1758:U:H2'	30:0:1759:A:O4'	2.22	0.40
30:0:2332:A:C2	30:0:2355:G:C5	3.09	0.40
30:0:2334:C:O2'	30:0:2335:C:H5'	2.21	0.40
31:9:64:C:O2'	31:9:65:A:H5'	2.21	0.40
2:B:234:ARG:HD3	30:0:1734:C:OP1	2.21	0.40
12:L:143:THR:HG21	38:L:8837:HOH:O	2.21	0.40
30:0:74:G:H2'	30:0:75:U:C6	2.56	0.40
30:0:278:A:C6	30:0:279:C:C4	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1192:A:H3'	30:0:1193:A:H5'	2.02	0.40
30:0:1327:G:N1	30:0:1330:A:OP2	2.52	0.40
30:0:1377:C:H2'	30:0:1723:G:O6	2.21	0.40
30:0:1617:C:C4	30:0:1643:C:H4'	2.56	0.40
30:0:1700:C:H5''	30:0:1701:A:OP2	2.22	0.40
30:0:1947:G:C8	30:0:1970:G:C8	3.09	0.40
30:0:2253:G:C2	30:0:2254:G:C8	3.09	0.40
30:0:2524:G:H21	30:0:2526:C:H41	1.67	0.40
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.80	0.40
8:H:76:LEU:HD21	8:H:149:VAL:HA	2.02	0.40
8:H:91:ARG:H	8:H:91:ARG:HG2	1.59	0.40
10:J:86:MET:HE2	30:0:1241:G:N3	2.35	0.40
20:T:24:ARG:NH2	20:T:39:ASN:HD22	2.07	0.40
30:0:111:C:O2'	30:0:112:G:H5'	2.21	0.40
30:0:200:C:H6	38:0:3463:HOH:O	2.03	0.40
30:0:255:A:C5	30:0:256:C:C5	3.09	0.40
30:0:932:U:H2'	30:0:933:C:C6	2.57	0.40
30:0:1163:G:C4	30:0:1164:U:C5	3.09	0.40
30:0:1183:C:O2	30:0:1183:C:C2'	2.69	0.40
30:0:1409:G:C2	30:0:1410:G:C8	3.10	0.40
30:0:1896:G:H1'	38:0:4284:HOH:O	2.21	0.40
30:0:1947:G:N2	30:0:1966:U:C2	2.90	0.40
30:0:2626:C:H2'	30:0:2627:G:C8	2.56	0.40
30:0:2727:A:N1	30:0:2756:U:C2	2.90	0.40
30:0:2782:G:O6	30:0:2790:C:H5''	2.21	0.40
31:9:26:C:H2'	31:9:27:C:C6	2.57	0.40
1:A:86:ALA:HB3	1:A:94:LEU:HD22	2.03	0.40
2:B:202:VAL:HG11	2:B:301:VAL:HG13	2.04	0.40
3:C:107:ARG:HB3	3:C:107:ARG:NH1	2.37	0.40
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.95	0.40
23:W:90:TYR:CE2	23:W:99:ALA:HB2	2.56	0.40
25:Y:154:ARG:NH2	30:0:1071:G:H4'	2.37	0.40
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.21	0.40
30:0:445:U:H2'	30:0:446:G:C8	2.56	0.40
30:0:724:G:O2'	30:0:725:C:H5'	2.22	0.40
30:0:806:A:H2'	30:0:807:A:O4'	2.22	0.40
30:0:853:C:H2'	30:0:854:G:O4'	2.21	0.40
30:0:1149:U:C5	30:0:1215:A:C5	3.09	0.40
30:0:1414:A:H2'	30:0:1415:G:O4'	2.21	0.40
30:0:1503:U:H6	30:0:1503:U:H3'	1.86	0.40
30:0:1741:U:C5'	30:0:1742:A:OP1	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2112:A:H2'	30:0:2113:G:C8	2.56	0.40
30:0:2726:U:O2	30:0:2749:U:O5'	2.40	0.40
30:0:2842:G:C2'	30:0:2843:A:H5'	2.51	0.40
31:9:39:U:H3'	31:9:40:C:H5''	2.02	0.40
3:C:2:GLN:HB3	38:C:8530:HOH:O	2.21	0.40
3:C:16:VAL:HG12	3:C:17:ASP:N	2.36	0.40
3:C:118:THR:O	3:C:136:VAL:HG13	2.22	0.40
3:C:236:THR:HG22	3:C:239:ALA:CB	2.51	0.40
4:D:25:MET:HE2	4:D:41:LEU:HG	2.03	0.40
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.36	0.40
20:T:82:THR:HG21	30:0:488:U:O2'	2.21	0.40
25:Y:144:ARG:NH1	38:Y:8871:HOH:O	2.53	0.40
28:2:5:LYS:O	28:2:9:LYS:HG3	2.22	0.40
30:0:47:G:N3	30:0:114:A:C2	2.90	0.40
30:0:138:U:OP2	30:0:139:C:C5	2.73	0.40
30:0:234:A:H4'	30:0:437:A:O4'	2.22	0.40
30:0:517:U:H1'	38:0:7614:HOH:O	2.21	0.40
30:0:907:A:H2'	30:0:908:A:H8	1.85	0.40
30:0:1705:C:H2'	30:0:1706:G:O4'	2.20	0.40
30:0:1878:G:H2'	38:0:3278:HOH:O	2.21	0.40
30:0:2016:U:O5'	30:0:2016:U:H6	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	212 (90%)	18 (8%)	5 (2%)	5	15
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	14	35
3	C	244/246 (99%)	228 (93%)	16 (7%)	0	100	100
4	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	5	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
6	F	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	14	35
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	149 (96%)	6 (4%)	1 (1%)	21	44
9	I	68/162 (42%)	55 (81%)	10 (15%)	3 (4%)	2	4
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
11	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
12	L	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	18	41
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	24	48
14	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	7	20
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	141 (100%)	0	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
19	S	79/85 (93%)	78 (99%)	1 (1%)	0	100	100
20	T	117/120 (98%)	110 (94%)	6 (5%)	1 (1%)	14	35
21	U	51/67 (76%)	47 (92%)	4 (8%)	0	100	100
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	7	20
23	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
24	X	80/92 (87%)	73 (91%)	6 (8%)	1 (1%)	9	25
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
26	Z	71/116 (61%)	61 (86%)	8 (11%)	2 (3%)	4	9
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	11	29
All	All	3705/4472 (83%)	3458 (93%)	220 (6%)	27 (1%)	18	41

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	VAL
14	N	154	LEU

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Mol	Chain	Res	Type
14	N	183	ASP
14	N	184	ILE
2	B	34	GLY
6	F	101	ALA
12	L	149	ARG
20	T	53	GLY
26	Z	66	CYS
2	B	185	GLY
4	D	27	ILE
4	D	137	PRO
8	H	19	ARG
2	B	2	GLN
22	V	43	PRO
1	A	36	ASP
4	D	56	ARG
9	I	108	HIS
29	3	56	PRO
26	Z	65	ASN
9	I	83	GLY
24	X	70	ILE
1	A	88	ILE
9	I	125	GLY
1	A	38	ILE
13	M	88	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	169 (94%)	10 (6%)	19	44
2	B	282/283 (100%)	266 (94%)	16 (6%)	18	43
3	C	193/193 (100%)	178 (92%)	15 (8%)	11	29
4	D	117/148 (79%)	109 (93%)	8 (7%)	14	35
5	E	152/156 (97%)	146 (96%)	6 (4%)	28	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	93/94 (99%)	93 (100%)	0	100	100
7	G	27/282 (10%)	26 (96%)	1 (4%)	30	59
8	H	134/145 (92%)	125 (93%)	9 (7%)	15	36
9	I	58/130 (45%)	57 (98%)	1 (2%)	53	79
10	J	118/121 (98%)	112 (95%)	6 (5%)	21	48
11	K	106/106 (100%)	103 (97%)	3 (3%)	38	68
12	L	113/127 (89%)	110 (97%)	3 (3%)	39	69
13	M	158/160 (99%)	152 (96%)	6 (4%)	29	58
14	N	149/150 (99%)	142 (95%)	7 (5%)	23	51
15	O	93/94 (99%)	90 (97%)	3 (3%)	34	64
16	P	113/117 (97%)	109 (96%)	4 (4%)	32	61
17	Q	79/80 (99%)	77 (98%)	2 (2%)	42	71
18	R	117/122 (96%)	111 (95%)	6 (5%)	21	48
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	99 (94%)	6 (6%)	18	43
21	U	44/53 (83%)	43 (98%)	1 (2%)	44	73
22	V	51/57 (90%)	50 (98%)	1 (2%)	48	76
23	W	130/130 (100%)	123 (95%)	7 (5%)	20	45
24	X	66/74 (89%)	59 (89%)	7 (11%)	6	17
25	Y	120/196 (61%)	115 (96%)	5 (4%)	26	55
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	43	72
29	3	79/79 (100%)	75 (95%)	4 (5%)	21	48
All	All	3095/3646 (85%)	2957 (96%)	138 (4%)	24	52

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

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	38	ILE
1	A	55	VAL
1	A	68	ILE

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Mol	Chain	Res	Type
1	A	69	LEU
1	A	94	LEU
1	A	175	LYS
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	16	ARG
2	B	27	ASN
2	B	49	THR
2	B	56	ASP
2	B	97	LEU
2	B	98	THR
2	B	184	ASP
2	B	190	MET
2	B	195	ARG
2	B	234	ARG
2	B	251	VAL
2	B	254	GLN
2	B	257	THR
2	B	312	ARG
3	C	2	GLN
3	C	16	VAL
3	C	76	ARG
3	C	94	THR
3	C	115	LEU
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	243	VAL
4	D	19	GLU
4	D	24	HIS
4	D	50	VAL
4	D	52	THR
4	D	58	VAL
4	D	137	PRO

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Mol	Chain	Res	Type
4	D	149	ARG
4	D	170	TYR
5	E	7	ILE
5	E	12	ASP
5	E	16	ASP
5	E	53	GLU
5	E	96	ASN
5	E	102	VAL
7	G	64	ASN
8	H	21	GLU
8	H	33	GLN
8	H	54	VAL
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	169	GLU
8	H	173	GLU
9	I	94	ASP
10	J	39	VAL
10	J	45	VAL
10	J	46	ILE
10	J	52	GLN
10	J	130	VAL
10	J	131	THR
11	K	10	GLN
11	K	55	VAL
11	K	98	VAL
12	L	43	HIS
12	L	101	ASP
12	L	140	VAL
13	M	46	LEU
13	M	81	ARG
13	M	93	ARG
13	M	99	ARG
13	M	115	LEU
13	M	164	THR
14	N	26	LEU
14	N	49	THR
14	N	50	LEU
14	N	56	ASP
14	N	127	LEU

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Mol	Chain	Res	Type
14	N	135	VAL
14	N	138	ASP
15	O	43	VAL
15	O	87	THR
15	O	98	LEU
16	P	21	VAL
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
17	Q	16	ASN
17	Q	57	ASP
18	R	13	THR
18	R	39	THR
18	R	82	GLU
18	R	109	MET
18	R	119	VAL
18	R	143	VAL
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	52	THR
22	V	2	VAL
23	W	4	LEU
23	W	26	ILE
23	W	35	VAL
23	W	52	VAL
23	W	73	LEU
23	W	142	ASP
23	W	146	ILE
24	X	12	ILE
24	X	46	ASP
24	X	49	ARG
24	X	52	PRO
24	X	72	VAL
24	X	82	GLU
24	X	88	GLU
25	Y	103	THR
25	Y	163	THR
25	Y	189	ASN

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Mol	Chain	Res	Type
25	Y	203	VAL
25	Y	235	GLU
28	2	18	ASN
29	3	3	MET
29	3	18	GLN
29	3	56	PRO
29	3	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	188	ASN
1	A	199	HIS
1	A	218	ASN
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	243	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
3	C	2	GLN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	47	GLN
4	D	85	GLN
4	D	97	GLN
4	D	103	ASN
4	D	133	ASN
5	E	143	GLN
5	E	150	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	75	HIS
10	J	25	GLN

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Mol	Chain	Res	Type
10	J	52	GLN
10	J	89	HIS
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
12	L	42	ASN
12	L	116	HIS
13	M	19	GLN
13	M	24	GLN
13	M	58	GLN
13	M	170	ASN
14	N	22	GLN
14	N	40	ASN
14	N	107	ASN
14	N	140	GLN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	118	GLN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
18	R	140	GLN
19	S	53	ASN
19	S	55	GLN
19	S	56	ASN
20	T	39	ASN
20	T	73	HIS
21	U	39	ASN
22	V	4	HIS
22	V	42	ASN
22	V	60	GLN
23	W	6	GLN
23	W	27	HIS
23	W	28	HIS
23	W	110	GLN

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Mol	Chain	Res	Type
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
24	X	36	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
26	Z	61	HIS
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	20	HIS
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	244 (8%)	32 (1%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	260 (9%)	33 (1%)

All (260) 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

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Mol	Chain	Res	Type
30	0	120	A
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
30	0	236	A
30	0	237	G
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	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	588	G
30	0	604	G
30	0	605	C

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Mol	Chain	Res	Type
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	698	A
30	0	701	U
30	0	759	C
30	0	777	U
30	0	809	G
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	898	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	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G

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Mol	Chain	Res	Type
30	0	1130	U
30	0	1137	G
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
30	0	1193	A
30	0	1206	U
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	1287	A
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1460	G
30	0	1474	C
30	0	1485	A
30	0	1488	U
30	0	1505	U
30	0	1506	U
30	0	1507	C
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

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Mol	Chain	Res	Type
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	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1732	A
30	0	1742	A
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	1857	A
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1996	U
30	0	2004	U
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

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Mol	Chain	Res	Type
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2320	U
30	0	2321	A
30	0	2345	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	2469	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2513	A
30	0	2526	C
30	0	2527	U
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2645	U
30	0	2649	A
30	0	2650	U

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Mol	Chain	Res	Type
30	0	2664	A
30	0	2676	C
30	0	2681	A
30	0	2682	C
30	0	2718	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
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	2867	G
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	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
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 (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	169	A
30	0	603	A
30	0	604	G
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	869	G
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1237	U
30	0	1352	A
30	0	1377	C
30	0	1474	C
30	0	1506	U
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1856	C
30	0	1878	G
30	0	1979	G
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2761	A
30	0	2791	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	0.32	0	32,38,41	0.36	0
30	OMU	0	2587	30	19,22,23	0.33	0	25,31,34	0.36	0
30	1MA	0	628	35,30	21,25,26	0.69	1 (4%)	30,37,40	0.69	1 (3%)
30	PSU	0	2621	30	18,21,22	1.53	2 (11%)	21,30,33	1.37	3 (14%)
30	UR3	0	2619	30	19,22,23	0.45	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	OMU	0	2587	30	-	0/9/27/28	0/2/2/2
30	1MA	0	628	35,30	-	2/7/25/26	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	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	5.08	1.43	1.36
30	0	2621	PSU	C6-C5	2.61	1.38	1.35
30	0	628	1MA	C6-N6	2.32	1.33	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C6-C5-C4	3.62	120.62	118.17
30	0	2621	PSU	O2-C2-N1	2.92	125.80	122.79
30	0	2621	PSU	C6-N1-C2	-2.84	120.06	122.69
30	0	2619	UR3	C4-N3-C2	2.81	126.84	124.58
30	0	628	1MA	N1-C2-N3	2.76	129.27	126.00

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

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	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%)	0.09	8 (3%) 48 44	26, 50, 86, 109	0
2	B	337/338 (99%)	0.17	6 (1%) 67 65	28, 51, 79, 93	0
3	C	246/246 (100%)	-0.02	3 (1%) 76 75	21, 43, 69, 77	0
4	D	140/177 (79%)	1.61	37 (26%) 1 1	56, 98, 124, 134	0
5	E	172/178 (96%)	0.56	14 (8%) 18 15	43, 66, 87, 91	0
6	F	119/120 (99%)	0.78	11 (9%) 14 12	47, 70, 99, 114	0
7	G	29/348 (8%)	1.38	5 (17%) 4 3	75, 93, 103, 106	0
8	H	160/177 (90%)	0.27	8 (5%) 34 30	34, 54, 92, 100	0
9	I	70/162 (43%)	2.79	51 (72%) 0 0	129, 145, 162, 163	0
10	J	142/145 (97%)	0.14	4 (2%) 55 51	34, 48, 70, 91	0
11	K	132/132 (100%)	0.00	0 100 100	31, 49, 72, 78	0
12	L	145/165 (87%)	0.61	16 (11%) 10 9	24, 63, 111, 125	0
13	M	194/196 (98%)	-0.16	2 (1%) 79 78	28, 40, 55, 64	0
14	N	186/187 (99%)	0.75	20 (10%) 11 9	39, 61, 111, 121	0
15	O	115/116 (99%)	0.30	2 (1%) 69 67	36, 51, 69, 79	0
16	P	143/149 (95%)	0.22	3 (2%) 63 61	37, 53, 67, 76	0
17	Q	95/96 (98%)	-0.04	1 (1%) 78 76	33, 43, 59, 76	0
18	R	150/155 (96%)	-0.24	1 (0%) 84 83	30, 43, 62, 77	0
19	S	81/85 (95%)	0.16	1 (1%) 76 75	38, 57, 78, 89	0
20	T	119/120 (99%)	0.28	2 (1%) 69 67	37, 54, 86, 111	0
21	U	53/67 (79%)	0.16	0 100 100	40, 54, 72, 80	0
22	V	65/71 (91%)	1.02	11 (16%) 4 3	51, 71, 116, 122	0
23	W	154/154 (100%)	0.12	2 (1%) 75 73	32, 48, 64, 77	0
24	X	82/92 (89%)	0.46	8 (9%) 13 11	39, 58, 83, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.06	3 (2%) 63 61	23, 43, 66, 86	0
26	Z	73/116 (62%)	0.96	10 (13%) 6 5	49, 67, 83, 95	0
27	1	56/57 (98%)	-0.68	0 100 100	25, 31, 39, 47	0
28	2	46/50 (92%)	0.68	5 (10%) 10 9	31, 59, 88, 100	0
29	3	92/92 (100%)	0.15	2 (2%) 62 59	33, 55, 68, 83	0
30	0	2749/2923 (94%)	-0.51	55 (2%) 65 62	19, 42, 87, 162	0
31	9	122/122 (100%)	0.05	4 (3%) 49 45	35, 61, 85, 146	0
All	All	6646/7517 (88%)	-0.02	295 (4%) 39 35	19, 49, 98, 163	0

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	10.8
9	I	128	THR	8.5
31	9	1	U	7.4
4	D	174	VAL	6.1
9	I	113	SER	6.0
9	I	74	ILE	5.9
22	V	43	PRO	5.8
4	D	10	PHE	5.6
4	D	63	ILE	5.6
22	V	40	PRO	5.6
8	H	171	GLY	5.2
9	I	71	ALA	5.2
30	0	735	C	5.1
30	0	1190	G	5.1
22	V	39	ALA	5.1
9	I	112	LEU	5.0
22	V	2	VAL	5.0
30	0	1161	A	5.0
31	9	2	U	5.0
30	0	138	U	4.8
30	0	1175	G	4.7
30	0	10	U	4.7
9	I	70	THR	4.7
8	H	174	LEU	4.6
9	I	111	LEU	4.6
26	Z	106	SER	4.6
14	N	168	LEU	4.6
28	2	49	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
14	N	169	PRO	4.4
30	0	1172	G	4.4
30	0	2769	C	4.4
30	0	1173	A	4.3
9	I	132	VAL	4.2
30	0	1171	A	4.1
14	N	154	LEU	4.1
12	L	81	VAL	4.1
30	0	1279	U	4.0
9	I	101	LYS	4.0
29	3	41	GLU	3.9
12	L	82	ALA	3.9
9	I	124	VAL	3.9
9	I	97	VAL	3.9
14	N	166	ALA	3.9
9	I	133	THR	3.9
30	0	2345	A	3.9
5	E	154	ILE	3.9
7	G	12	ILE	3.9
9	I	116	LEU	3.8
30	0	2004	U	3.8
14	N	1	ALA	3.8
5	E	10	ASP	3.7
30	0	1162	G	3.7
4	D	57	THR	3.7
30	0	1160	G	3.7
9	I	134	ILE	3.7
24	X	87	ALA	3.7
28	2	35	ARG	3.7
4	D	17	ARG	3.6
12	L	78	ALA	3.6
9	I	95	LEU	3.6
4	D	59	GLY	3.6
24	X	83	ALA	3.6
9	I	85	GLY	3.6
26	Z	46	SER	3.6
4	D	69	ILE	3.5
9	I	120	ALA	3.5
9	I	104	ALA	3.5
30	0	1169	U	3.5
4	D	19	GLU	3.5
30	0	1176	C	3.5

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Mol	Chain	Res	Type	RSRZ
4	D	35	ALA	3.4
5	E	45	ASP	3.4
10	J	70	PHE	3.4
1	A	237	GLY	3.4
7	G	71	LEU	3.4
1	A	37	VAL	3.4
4	D	18	ILE	3.4
26	Z	34	SER	3.4
14	N	147	ILE	3.4
9	I	80	PHE	3.4
4	D	44	ILE	3.3
4	D	172	VAL	3.3
24	X	85	VAL	3.3
6	F	106	ALA	3.3
7	G	73	ASP	3.3
18	R	150	PRO	3.3
1	A	36	ASP	3.3
19	S	81	ILE	3.3
14	N	162	ASP	3.3
2	B	1	PRO	3.2
30	O	1177	A	3.2
13	M	194	GLY	3.2
9	I	72	GLU	3.2
14	N	75	THR	3.2
14	N	161	GLY	3.2
9	I	67	VAL	3.2
14	N	167	ASP	3.2
25	Y	235	GLU	3.2
30	O	960	G	3.2
9	I	106	GLN	3.1
4	D	101	THR	3.1
9	I	127	CYS	3.1
9	I	96	SER	3.1
30	O	1186	C	3.1
16	P	143	ALA	3.1
6	F	90	GLU	3.1
31	9	24	U	3.1
14	N	62	HIS	3.1
26	Z	36	GLY	3.1
9	I	107	LYS	3.1
14	N	165	ALA	3.1
14	N	164	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
14	N	163	PHE	3.0
30	0	1165	G	3.0
5	E	6	GLU	3.0
4	D	55	LYS	3.0
9	I	83	GLY	3.0
6	F	105	ASP	3.0
5	E	172	PRO	3.0
8	H	114	ASP	3.0
28	2	37	HIS	2.9
9	I	69	PRO	2.9
24	X	84	ILE	2.9
4	D	26	GLY	2.9
4	D	135	VAL	2.9
12	L	150	GLN	2.9
4	D	40	ILE	2.9
5	E	123	ASP	2.9
4	D	107	GLY	2.9
10	J	4	ALA	2.9
12	L	91	VAL	2.8
12	L	83	GLU	2.8
14	N	157	PRO	2.8
4	D	70	GLY	2.8
14	N	158	LEU	2.8
2	B	119	HIS	2.8
12	L	99	GLU	2.8
30	0	1164	U	2.8
30	0	1185	U	2.8
9	I	88	GLN	2.8
30	0	1166	A	2.8
30	0	1204	C	2.8
4	D	61	PHE	2.8
4	D	65	GLU	2.8
6	F	91	VAL	2.8
9	I	91	PHE	2.8
9	I	122	GLU	2.8
9	I	123	VAL	2.8
14	N	159	TYR	2.8
1	A	211	LYS	2.8
30	0	2664	A	2.8
16	P	58	SER	2.8
6	F	101	ALA	2.8
8	H	43	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
9	I	82	THR	2.8
9	I	108	HIS	2.7
30	0	1192	A	2.7
30	0	1193	A	2.7
9	I	114	TYR	2.7
30	0	1163	G	2.7
30	0	1929	G	2.7
9	I	119	ALA	2.7
25	Y	236	VAL	2.7
5	E	126	ILE	2.7
9	I	130	LEU	2.7
6	F	102	GLY	2.7
12	L	149	ARG	2.7
20	T	119	ALA	2.7
20	T	117	ASP	2.7
30	0	1191	A	2.6
4	D	11	HIS	2.6
28	2	38	LYS	2.6
15	O	24	ALA	2.6
30	0	1524	U	2.6
9	I	135	GLU	2.6
30	0	130	C	2.6
7	G	63	ARG	2.6
22	V	41	GLU	2.6
30	0	2344	G	2.6
9	I	118	ASN	2.6
9	I	90	ASP	2.6
1	A	85	SER	2.5
6	F	47	LEU	2.5
28	2	31	ARG	2.5
4	D	170	TYR	2.5
10	J	144	THR	2.5
26	Z	35	SER	2.5
30	0	1170	U	2.5
3	C	101	ASP	2.5
2	B	57	GLU	2.5
4	D	139	TYR	2.5
12	L	89	PHE	2.5
9	I	75	LYS	2.5
3	C	246	ARG	2.5
12	L	145	LEU	2.5
26	Z	45	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
24	X	65	ASN	2.4
4	D	171	ASP	2.4
12	L	148	GLU	2.4
4	D	95	THR	2.4
26	Z	44	ARG	2.4
4	D	75	LEU	2.4
30	0	1174	A	2.4
30	0	1188	A	2.4
30	0	1178	G	2.4
9	I	68	PRO	2.4
22	V	36	ALA	2.4
26	Z	40	ALA	2.4
2	B	118	ASP	2.4
5	E	18	LEU	2.4
17	Q	95	GLU	2.4
12	L	73	VAL	2.4
22	V	46	ILE	2.3
9	I	77	GLU	2.3
24	X	79	GLU	2.3
31	9	23	U	2.3
5	E	100	ASP	2.3
5	E	156	ASP	2.3
9	I	109	PRO	2.3
1	A	35	GLY	2.3
30	0	1205	U	2.3
5	E	97	VAL	2.3
12	L	77	ALA	2.3
5	E	53	GLU	2.3
8	H	170	ARG	2.3
16	P	67	LYS	2.3
8	H	172	GLU	2.3
30	0	128	A	2.3
30	0	1208	C	2.2
4	D	100	ASP	2.2
6	F	17	LEU	2.2
9	I	73	LEU	2.2
9	I	117	THR	2.2
30	0	1964	U	2.2
9	I	110	ASP	2.2
14	N	179	LEU	2.2
4	D	21	VAL	2.2
5	E	87	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	12	GLU	2.2
4	D	62	ASP	2.2
4	D	66	GLY	2.2
4	D	105	SER	2.2
23	W	76	ASP	2.2
30	0	999	C	2.2
4	D	37	ALA	2.2
12	L	136	ALA	2.2
15	O	31	GLU	2.2
30	0	1203	G	2.2
14	N	40	ASN	2.2
30	0	734	U	2.2
9	I	66	GLY	2.2
22	V	44	GLY	2.2
4	D	141	VAL	2.2
6	F	103	GLU	2.1
24	X	66	THR	2.1
30	0	1167	G	2.1
30	0	1525	G	2.1
30	0	2237	G	2.1
12	L	55	GLN	2.1
3	C	245	GLU	2.1
29	3	83	TRP	2.1
6	F	119	ARG	2.1
13	M	125	ARG	2.1
6	F	26	THR	2.1
1	A	31	LYS	2.1
8	H	35	LYS	2.1
22	V	42	ASN	2.1
2	B	92	TYR	2.1
9	I	125	GLY	2.1
30	0	497	A	2.1
30	0	1202	A	2.1
4	D	64	ARG	2.1
8	H	115	GLY	2.1
26	Z	39	GLY	2.1
7	G	27	ILE	2.1
9	I	100	VAL	2.1
12	L	102	ASP	2.1
9	I	89	GLU	2.1
26	Z	49	ARG	2.1
4	D	131	THR	2.1

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Mol	Chain	Res	Type	RSRZ
30	0	736	A	2.1
30	0	1189	A	2.1
30	0	1198	U	2.1
30	0	1199	A	2.1
22	V	38	GLY	2.1
1	A	32	VAL	2.1
2	B	33	ASP	2.0
5	E	118	ILE	2.0
25	Y	216	ARG	2.0
10	J	76	ASP	2.0
23	W	78	ASP	2.0
24	X	16	ASP	2.0
30	0	284	C	2.0
9	I	103	ILE	2.0
14	N	184	ILE	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	0.97	0.07	34,37,39,43	0
30	OMU	0	2587	21/22	0.98	0.06	29,32,34,36	0
30	OMG	0	2588	24/25	0.98	0.06	28,32,34,36	0
30	1MA	0	628	23/24	0.98	0.06	22,25,28,28	0
30	PSU	0	2621	20/21	0.98	0.05	24,26,33,33	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
35	NA	0	8548	1/1	0.65	0.38	59,59,59,59	0
35	NA	0	8573	1/1	0.68	0.24	69,69,69,69	0
34	SR	0	9001	1/1	0.69	0.14	171,171,171,171	0
34	SR	0	8976	1/1	0.73	0.24	194,194,194,194	0
34	SR	9	9003	1/1	0.75	0.19	169,169,169,169	0
34	SR	0	9006	1/1	0.76	0.27	200,200,200,200	0
34	SR	0	8983	1/1	0.76	0.18	177,177,177,177	0
35	NA	0	8557	1/1	0.77	0.34	68,68,68,68	0
35	NA	0	8571	1/1	0.77	0.24	73,73,73,73	0
34	SR	9	8980	1/1	0.77	0.14	177,177,177,177	0
34	SR	J	8986	1/1	0.79	0.30	200,200,200,200	0
34	SR	0	8979	1/1	0.79	0.20	199,199,199,199	0
34	SR	0	8971	1/1	0.79	0.18	165,165,165,165	0
34	SR	0	8991	1/1	0.79	0.23	188,188,188,188	0
34	SR	0	9004	1/1	0.80	0.34	200,200,200,200	0
35	NA	0	8559	1/1	0.81	0.39	71,71,71,71	0
34	SR	0	8997	1/1	0.81	0.24	190,190,190,190	0
34	SR	0	8922	1/1	0.81	0.21	160,160,160,160	0
35	NA	0	8546	1/1	0.82	0.30	77,77,77,77	0
35	NA	R	8575	1/1	0.82	0.29	82,82,82,82	0
34	SR	0	8947	1/1	0.83	0.19	178,178,178,178	0
34	SR	0	8919	1/1	0.83	0.17	173,173,173,173	0
34	SR	0	8996	1/1	0.83	0.27	200,200,200,200	0
32	MG	9	8074	1/1	0.83	0.21	74,74,74,74	0
34	SR	0	8944	1/1	0.83	0.20	161,161,161,161	0
35	NA	0	8525	1/1	0.83	0.20	79,79,79,79	0
35	NA	9	8543	1/1	0.83	0.21	47,47,47,47	0
35	NA	0	8554	1/1	0.84	0.25	63,63,63,63	0
35	NA	0	8574	1/1	0.84	0.39	61,61,61,61	0
34	SR	A	8977	1/1	0.84	0.12	158,158,158,158	0
32	MG	0	8071	1/1	0.85	0.30	53,53,53,53	0
35	NA	0	8567	1/1	0.86	0.37	65,65,65,65	0
32	MG	A	8051	1/1	0.86	0.12	72,72,72,72	0
35	NA	0	8506	1/1	0.86	0.16	66,66,66,66	0
34	SR	0	8939	1/1	0.86	0.14	146,146,146,146	0
34	SR	0	8959	1/1	0.86	0.17	159,159,159,159	0
34	SR	0	8988	1/1	0.87	0.10	158,158,158,158	0
34	SR	0	9002	1/1	0.87	0.21	175,175,175,175	0
35	NA	0	8562	1/1	0.87	0.42	62,62,62,62	0
34	SR	0	8974	1/1	0.87	0.18	166,166,166,166	0
32	MG	0	8073	1/1	0.88	0.27	79,79,79,79	0
34	SR	B	8987	1/1	0.88	0.37	200,200,200,200	0
32	MG	0	8037	1/1	0.88	0.19	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	9000	1/1	0.88	0.23	157,157,157,157	0
35	NA	0	8564	1/1	0.89	0.14	63,63,63,63	0
32	MG	T	8057	1/1	0.89	0.11	58,58,58,58	0
32	MG	0	8083	1/1	0.89	0.11	55,55,55,55	0
35	NA	0	8522	1/1	0.89	0.18	58,58,58,58	0
34	SR	0	8993	1/1	0.89	0.12	165,165,165,165	0
34	SR	0	8927	1/1	0.89	0.14	150,150,150,150	0
34	SR	0	8968	1/1	0.90	0.12	146,146,146,146	0
32	MG	0	8092	1/1	0.90	0.16	51,51,51,51	0
34	SR	0	8960	1/1	0.90	0.17	141,141,141,141	0
34	SR	0	8998	1/1	0.90	0.21	171,171,171,171	0
35	NA	0	8558	1/1	0.90	0.17	44,44,44,44	0
34	SR	0	8962	1/1	0.90	0.19	164,164,164,164	0
35	NA	0	8561	1/1	0.90	0.37	68,68,68,68	0
32	MG	0	8049	1/1	0.91	0.21	65,65,65,65	0
32	MG	0	8031	1/1	0.91	0.12	55,55,55,55	0
33	CL	N	8807	1/1	0.91	0.12	68,68,68,68	0
34	SR	0	8951	1/1	0.91	0.10	132,132,132,132	0
34	SR	0	8955	1/1	0.91	0.20	189,189,189,189	0
35	NA	0	8560	1/1	0.91	0.26	92,92,92,92	0
34	SR	0	8957	1/1	0.91	0.15	188,188,188,188	0
35	NA	0	8511	1/1	0.91	0.22	63,63,63,63	0
35	NA	0	8518	1/1	0.91	0.27	65,65,65,65	0
34	SR	0	8958	1/1	0.91	0.08	86,86,86,86	0
35	NA	0	8523	1/1	0.91	0.08	29,29,29,29	0
34	SR	0	8981	1/1	0.91	0.17	153,153,153,153	0
35	NA	0	8541	1/1	0.91	0.12	50,50,50,50	0
34	SR	0	8933	1/1	0.91	0.15	127,127,127,127	0
35	NA	0	8514	1/1	0.92	0.11	41,41,41,41	0
34	SR	0	8994	1/1	0.92	0.46	198,198,198,198	0
34	SR	0	8982	1/1	0.92	0.42	189,189,189,189	0
34	SR	0	8924	1/1	0.92	0.14	134,134,134,134	0
34	SR	0	8965	1/1	0.92	0.10	117,117,117,117	0
35	NA	0	8533	1/1	0.92	0.08	55,55,55,55	0
35	NA	0	8535	1/1	0.92	0.18	46,46,46,46	0
35	NA	R	8532	1/1	0.92	0.11	48,48,48,48	0
35	NA	0	8544	1/1	0.92	0.21	64,64,64,64	0
34	SR	0	8989	1/1	0.92	0.19	168,168,168,168	0
34	SR	F	9005	1/1	0.92	0.13	122,122,122,122	0
34	SR	0	8915	1/1	0.92	0.10	115,115,115,115	0
35	NA	0	8555	1/1	0.93	0.23	61,61,61,61	0
32	MG	0	8033	1/1	0.93	0.10	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8036	1/1	0.93	0.11	49,49,49,49	0
34	SR	0	8953	1/1	0.93	0.12	143,143,143,143	0
34	SR	0	8970	1/1	0.93	0.09	115,115,115,115	0
32	MG	0	8081	1/1	0.93	0.13	64,64,64,64	0
34	SR	0	9007	1/1	0.93	0.26	200,200,200,200	0
32	MG	0	8063	1/1	0.93	0.14	69,69,69,69	0
35	NA	0	8565	1/1	0.93	0.13	57,57,57,57	0
34	SR	0	8975	1/1	0.93	0.10	120,120,120,120	0
35	NA	0	8569	1/1	0.93	0.17	53,53,53,53	0
34	SR	0	8995	1/1	0.93	0.10	117,117,117,117	0
34	SR	0	8916	1/1	0.93	0.13	98,98,98,98	0
34	SR	B	8950	1/1	0.93	0.10	101,101,101,101	0
34	SR	0	8946	1/1	0.93	0.10	102,102,102,102	0
35	NA	9	8572	1/1	0.93	0.12	64,64,64,64	0
37	K	0	8401	1/1	0.93	0.14	88,88,88,88	0
37	K	0	8402	1/1	0.93	0.15	62,62,62,62	0
33	CL	L	8810	1/1	0.94	0.11	50,50,50,50	0
35	NA	0	8552	1/1	0.94	0.11	59,59,59,59	0
35	NA	0	8553	1/1	0.94	0.16	67,67,67,67	0
32	MG	0	8068	1/1	0.94	0.08	64,64,64,64	0
32	MG	0	8069	1/1	0.94	0.19	65,65,65,65	0
35	NA	0	8556	1/1	0.94	0.22	41,41,41,41	0
34	SR	0	8985	1/1	0.94	0.22	118,118,118,118	0
32	MG	0	8040	1/1	0.94	0.20	84,84,84,84	0
34	SR	0	8938	1/1	0.94	0.09	139,139,139,139	0
35	NA	0	8505	1/1	0.94	0.41	45,45,45,45	0
34	SR	0	8963	1/1	0.94	0.09	105,105,105,105	0
35	NA	0	8509	1/1	0.94	0.14	50,50,50,50	0
34	SR	0	8992	1/1	0.94	0.32	125,125,125,125	0
34	SR	0	8964	1/1	0.94	0.08	110,110,110,110	0
32	MG	0	8030	1/1	0.94	0.15	60,60,60,60	0
34	SR	0	8967	1/1	0.94	0.08	116,116,116,116	0
34	SR	0	8941	1/1	0.94	0.09	113,113,113,113	0
32	MG	0	8053	1/1	0.94	0.10	53,53,53,53	0
32	MG	0	8060	1/1	0.94	0.09	54,54,54,54	0
32	MG	0	8089	1/1	0.94	0.10	40,40,40,40	0
32	MG	0	8039	1/1	0.94	0.07	64,64,64,64	0
32	MG	0	8066	1/1	0.94	0.09	57,57,57,57	0
34	SR	0	8920	1/1	0.94	0.08	113,113,113,113	0
34	SR	0	8969	1/1	0.95	0.18	134,134,134,134	0
35	NA	0	8508	1/1	0.95	0.07	39,39,39,39	0
34	SR	0	8943	1/1	0.95	0.09	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8082	1/1	0.95	0.07	56,56,56,56	0
34	SR	0	8973	1/1	0.95	0.09	121,121,121,121	0
35	NA	0	8516	1/1	0.95	0.07	28,28,28,28	0
33	CL	0	8805	1/1	0.95	0.12	58,58,58,58	0
35	NA	0	8520	1/1	0.95	0.14	54,54,54,54	0
35	NA	0	8521	1/1	0.95	0.12	54,54,54,54	0
34	SR	0	8928	1/1	0.95	0.11	125,125,125,125	0
32	MG	0	8080	1/1	0.95	0.07	66,66,66,66	0
33	CL	B	8819	1/1	0.95	0.08	50,50,50,50	0
35	NA	0	8527	1/1	0.95	0.12	43,43,43,43	0
35	NA	0	8531	1/1	0.95	0.07	41,41,41,41	0
35	NA	J	8538	1/1	0.95	0.12	57,57,57,57	0
34	SR	0	8954	1/1	0.95	0.07	94,94,94,94	0
33	CL	J	8801	1/1	0.95	0.08	54,54,54,54	0
35	NA	0	8542	1/1	0.95	0.13	42,42,42,42	0
35	NA	S	8510	1/1	0.95	0.08	34,34,34,34	0
35	NA	0	8502	1/1	0.95	0.12	55,55,55,55	0
35	NA	0	8547	1/1	0.95	0.22	51,51,51,51	0
32	MG	0	8079	1/1	0.95	0.09	50,50,50,50	0
33	CL	O	8808	1/1	0.96	0.11	62,62,62,62	0
35	NA	0	8545	1/1	0.96	0.14	38,38,38,38	0
33	CL	Y	8820	1/1	0.96	0.08	38,38,38,38	0
32	MG	0	8085	1/1	0.96	0.17	73,73,73,73	0
34	SR	0	8931	1/1	0.96	0.06	94,94,94,94	0
35	NA	0	8549	1/1	0.96	0.17	58,58,58,58	0
35	NA	0	8550	1/1	0.96	0.11	55,55,55,55	0
33	CL	0	8813	1/1	0.96	0.06	44,44,44,44	0
34	SR	0	8934	1/1	0.96	0.19	108,108,108,108	0
34	SR	0	8937	1/1	0.96	0.05	103,103,103,103	0
34	SR	A	8929	1/1	0.96	0.13	113,113,113,113	0
35	NA	0	8513	1/1	0.96	0.12	45,45,45,45	0
32	MG	0	8038	1/1	0.96	0.05	68,68,68,68	0
32	MG	0	8090	1/1	0.96	0.09	55,55,55,55	0
32	MG	0	8076	1/1	0.96	0.07	32,32,32,32	0
35	NA	0	8519	1/1	0.96	0.07	36,36,36,36	0
32	MG	0	8093	1/1	0.96	0.04	29,29,29,29	0
34	SR	0	8972	1/1	0.96	0.18	112,112,112,112	0
32	MG	0	8018	1/1	0.96	0.11	36,36,36,36	0
34	SR	0	8914	1/1	0.96	0.13	107,107,107,107	0
32	MG	0	8035	1/1	0.96	0.12	62,62,62,62	0
35	NA	0	8568	1/1	0.96	0.08	53,53,53,53	0
32	MG	B	8042	1/1	0.96	0.07	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8528	1/1	0.96	0.09	40,40,40,40	0
35	NA	0	8530	1/1	0.96	0.10	47,47,47,47	0
33	CL	J	8821	1/1	0.96	0.07	59,59,59,59	0
32	MG	0	8017	1/1	0.96	0.10	23,23,23,23	0
34	SR	0	8956	1/1	0.96	0.07	128,128,128,128	0
35	NA	Q	8540	1/1	0.96	0.10	41,41,41,41	0
32	MG	0	8059	1/1	0.96	0.05	35,35,35,35	0
34	SR	0	8990	1/1	0.97	0.07	113,113,113,113	0
32	MG	0	8088	1/1	0.97	0.04	34,34,34,34	0
35	NA	0	8507	1/1	0.97	0.06	40,40,40,40	0
34	SR	0	8942	1/1	0.97	0.07	115,115,115,115	0
34	SR	0	8966	1/1	0.97	0.06	100,100,100,100	0
35	NA	0	8551	1/1	0.97	0.12	47,47,47,47	0
34	SR	0	8917	1/1	0.97	0.06	95,95,95,95	0
33	CL	0	8815	1/1	0.97	0.09	58,58,58,58	0
34	SR	0	8945	1/1	0.97	0.06	105,105,105,105	0
33	CL	0	8816	1/1	0.97	0.12	54,54,54,54	0
35	NA	0	8517	1/1	0.97	0.14	31,31,31,31	0
34	SR	0	8921	1/1	0.97	0.06	84,84,84,84	0
34	SR	0	8949	1/1	0.97	0.08	90,90,90,90	0
33	CL	0	8817	1/1	0.97	0.05	50,50,50,50	0
32	MG	0	8062	1/1	0.97	0.10	47,47,47,47	0
34	SR	0	8926	1/1	0.97	0.08	107,107,107,107	0
33	CL	J	8802	1/1	0.97	0.04	56,56,56,56	0
35	NA	0	8563	1/1	0.97	0.11	65,65,65,65	0
34	SR	0	8978	1/1	0.97	0.06	108,108,108,108	0
32	MG	0	8024	1/1	0.97	0.22	61,61,61,61	0
35	NA	0	8566	1/1	0.97	0.18	58,58,58,58	0
32	MG	0	8091	1/1	0.97	0.17	54,54,54,54	0
35	NA	C	8503	1/1	0.97	0.04	31,31,31,31	0
32	MG	0	8077	1/1	0.97	0.04	35,35,35,35	0
32	MG	0	8078	1/1	0.97	0.04	43,43,43,43	0
34	SR	0	8984	1/1	0.97	0.06	105,105,105,105	0
35	NA	0	8537	1/1	0.97	0.04	32,32,32,32	0
34	SR	S	8961	1/1	0.97	0.06	113,113,113,113	0
32	MG	0	8056	1/1	0.97	0.07	41,41,41,41	0
33	CL	A	8809	1/1	0.97	0.08	60,60,60,60	0
35	NA	0	8504	1/1	0.97	0.06	33,33,33,33	0
34	SR	A	8930	1/1	0.98	0.05	100,100,100,100	0
32	MG	0	8034	1/1	0.98	0.06	36,36,36,36	0
32	MG	0	8070	1/1	0.98	0.04	40,40,40,40	0
32	MG	0	8055	1/1	0.98	0.03	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	K	8054	1/1	0.98	0.03	37,37,37,37	0
34	SR	0	8936	1/1	0.98	0.03	84,84,84,84	0
32	MG	0	8075	1/1	0.98	0.04	49,49,49,49	0
35	NA	0	8512	1/1	0.98	0.06	38,38,38,38	0
34	SR	R	8912	1/1	0.98	0.05	73,73,73,73	0
32	MG	0	8032	1/1	0.98	0.04	36,36,36,36	0
35	NA	0	8515	1/1	0.98	0.07	35,35,35,35	0
34	SR	3	8999	1/1	0.98	0.05	93,93,93,93	0
34	SR	0	8908	1/1	0.98	0.04	80,80,80,80	0
34	SR	0	8910	1/1	0.98	0.09	84,84,84,84	0
33	CL	3	8804	1/1	0.98	0.05	53,53,53,53	0
32	MG	0	8044	1/1	0.98	0.05	46,46,46,46	0
33	CL	0	8811	1/1	0.98	0.07	58,58,58,58	0
32	MG	0	8046	1/1	0.98	0.04	28,28,28,28	0
34	SR	0	8948	1/1	0.98	0.06	77,77,77,77	0
35	NA	0	8524	1/1	0.98	0.09	41,41,41,41	0
34	SR	0	8918	1/1	0.98	0.06	76,76,76,76	0
35	NA	0	8526	1/1	0.98	0.06	46,46,46,46	0
33	CL	0	8814	1/1	0.98	0.05	48,48,48,48	0
32	MG	0	8047	1/1	0.98	0.16	44,44,44,44	0
35	NA	0	8529	1/1	0.98	0.15	38,38,38,38	0
35	NA	M	8539	1/1	0.98	0.05	33,33,33,33	0
35	NA	0	8570	1/1	0.98	0.05	44,44,44,44	0
32	MG	0	8064	1/1	0.98	0.05	43,43,43,43	0
32	MG	0	8016	1/1	0.98	0.04	43,43,43,43	0
34	SR	0	8923	1/1	0.98	0.04	85,85,85,85	0
35	NA	0	8536	1/1	0.98	0.08	44,44,44,44	0
33	CL	0	8822	1/1	0.98	0.23	74,74,74,74	0
36	CD	O	8705	1/1	0.98	0.04	83,83,83,83	0
35	NA	0	8501	1/1	0.98	0.08	24,24,24,24	0
32	MG	0	8052	1/1	0.98	0.04	38,38,38,38	0
32	MG	B	8043	1/1	0.99	0.03	48,48,48,48	0
32	MG	Y	8086	1/1	0.99	0.03	33,33,33,33	0
34	SR	0	8940	1/1	0.99	0.03	70,70,70,70	0
32	MG	0	8001	1/1	0.99	0.04	29,29,29,29	0
32	MG	0	8048	1/1	0.99	0.04	27,27,27,27	0
32	MG	0	8019	1/1	0.99	0.05	20,20,20,20	0
32	MG	0	8084	1/1	0.99	0.06	27,27,27,27	0
35	NA	0	8534	1/1	0.99	0.03	25,25,25,25	0
32	MG	0	8020	1/1	0.99	0.09	38,38,38,38	0
32	MG	0	8087	1/1	0.99	0.03	31,31,31,31	0
32	MG	0	8022	1/1	0.99	0.04	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8023	1/1	0.99	0.03	18,18,18,18	0
32	MG	0	8002	1/1	0.99	0.02	21,21,21,21	0
32	MG	0	8026	1/1	0.99	0.02	27,27,27,27	0
34	SR	1	8913	1/1	0.99	0.07	78,78,78,78	0
34	SR	0	9008	1/1	0.99	0.04	85,85,85,85	0
34	SR	1	8952	1/1	0.99	0.05	74,74,74,74	0
32	MG	0	8027	1/1	0.99	0.03	39,39,39,39	0
34	SR	0	8901	1/1	0.99	0.03	73,73,73,73	0
34	SR	0	8904	1/1	0.99	0.06	49,49,49,49	0
34	SR	0	8905	1/1	0.99	0.14	54,54,54,54	0
34	SR	0	8906	1/1	0.99	0.08	52,52,52,52	0
34	SR	0	8907	1/1	0.99	0.11	53,53,53,53	0
32	MG	0	8061	1/1	0.99	0.04	29,29,29,29	0
34	SR	0	8909	1/1	0.99	0.04	75,75,75,75	0
32	MG	0	8029	1/1	0.99	0.15	52,52,52,52	0
34	SR	0	8911	1/1	0.99	0.03	74,74,74,74	0
32	MG	0	8003	1/1	0.99	0.04	26,26,26,26	0
32	MG	0	8006	1/1	0.99	0.04	23,23,23,23	0
32	MG	0	8065	1/1	0.99	0.04	47,47,47,47	0
32	MG	0	8007	1/1	0.99	0.03	27,27,27,27	0
32	MG	0	8067	1/1	0.99	0.02	26,26,26,26	0
32	MG	0	8008	1/1	0.99	0.04	23,23,23,23	0
33	CL	M	8818	1/1	0.99	0.03	33,33,33,33	0
32	MG	0	8009	1/1	0.99	0.08	19,19,19,19	0
32	MG	0	8010	1/1	0.99	0.02	23,23,23,23	0
33	CL	R	8806	1/1	0.99	0.03	42,42,42,42	0
32	MG	0	8011	1/1	0.99	0.04	24,24,24,24	0
34	SR	0	8925	1/1	0.99	0.06	84,84,84,84	0
32	MG	0	8072	1/1	0.99	0.05	53,53,53,53	0
33	CL	0	8803	1/1	0.99	0.09	50,50,50,50	0
32	MG	0	8012	1/1	0.99	0.05	22,22,22,22	0
32	MG	0	8013	1/1	0.99	0.04	24,24,24,24	0
33	CL	0	8812	1/1	0.99	0.06	40,40,40,40	0
32	MG	0	8014	1/1	0.99	0.03	19,19,19,19	0
34	SR	0	8935	1/1	0.99	0.04	68,68,68,68	0
36	CD	Z	8703	1/1	0.99	0.03	71,71,71,71	0
32	MG	0	8015	1/1	0.99	0.03	27,27,27,27	0
32	MG	0	8041	1/1	0.99	0.04	19,19,19,19	0
34	SR	3	8932	1/1	1.00	0.02	67,67,67,67	0
32	MG	0	8004	1/1	1.00	0.03	21,21,21,21	0
32	MG	0	8005	1/1	1.00	0.06	29,29,29,29	0
34	SR	0	8902	1/1	1.00	0.02	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	8903	1/1	1.00	0.07	45,45,45,45	0
32	MG	0	8045	1/1	1.00	0.04	39,39,39,39	0
32	MG	0	8025	1/1	1.00	0.02	31,31,31,31	0
32	MG	0	8058	1/1	1.00	0.02	25,25,25,25	0
36	CD	U	8701	1/1	1.00	0.02	51,51,51,51	0
32	MG	0	8021	1/1	1.00	0.03	31,31,31,31	0
36	CD	1	8702	1/1	1.00	0.05	53,53,53,53	0
36	CD	3	8704	1/1	1.00	0.02	64,64,64,64	0
32	MG	A	8050	1/1	1.00	0.02	24,24,24,24	0
32	MG	0	8028	1/1	1.00	0.01	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.