



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:23 AM UTC

PDB ID : 3CC2 / pdb_00003cc2
Title : The Refined Crystal Structure of the Haloarcula Marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution with rrnA Sequence for the 23S rRNA and Genome-derived Sequences for r-Proteins
Authors : Gurel, G.; Blaha, G.
Deposited on : 2008-02-23
Resolution : 2.40 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

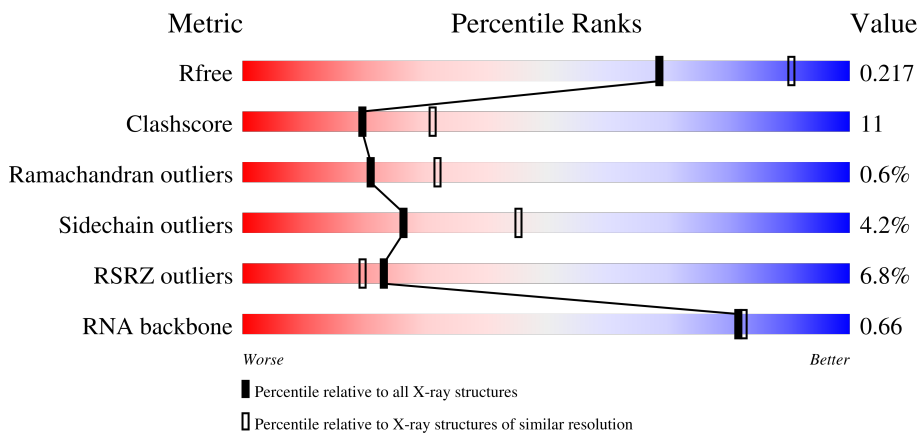
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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	5% (Poor fit) 68% (0 outliers) 25% (1 outlier) 5% (2 outliers)
2	B	338	4% (Poor fit) 66% (0 outliers) 28% (1 outlier) 5% (2 outliers)
3	C	246	2% (Poor fit) 73% (0 outliers) 22% (1 outlier) 5% (2 outliers)
4	D	177	41% (Poor fit) 46% (0 outliers) 31% (1 outlier) 21% (2 outliers)

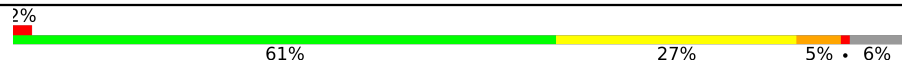

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Mol	Chain	Length	Quality of chain
5	E	178	11% 66% 30% ..
6	F	120	15% 71% 28% ..
7	G	348	4% 92%
8	H	177	7% 65% 24% 10%
9	I	162	38% 22% 21% 57%
10	J	145	5% 71% 25% ..
11	K	132	2% 73% 26% .
12	L	165	17% 65% 22% 12%
13	M	196	75% 21% ..
14	N	187	18% 63% 31% 5% ..
15	O	116	5% 80% 17% ..
16	P	149	3% 81% 15% .
17	Q	96	2% 80% 15% ..
18	R	155	0% 74% 20% ...
19	S	85	6% 73% 22% 5%
20	T	120	6% 73% 22% ..
21	U	67	9% 49% 28% 21%
22	V	71	17% 59% 28% 8%
23	W	154	2% 62% 32% 5% .
24	X	92	16% 61% 24% 11%
25	Y	241	2% 45% 12% 41%
26	Z	116	6% 44% 19% 37%
27	1	57	72% 25% ..
28	2	50	24% 52% 38% 8%
29	3	92	3% 76% 22% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	NA	0	8370	-	-	-	X
33	NA	R	8386	-	-	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 99049 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
			Total	C	N	O	S			
1	A	237	1753	1072	352	324	5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S			
28	2	46	396	239	89	67	1	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
30	0	2754	59021	26349	10873	19054	2745	0	0	0

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	3	1	Total	Mg	0	0
			1	1		
32	0	109	Total	Mg	0	0
			109	109		
32	9	1	Total	Mg	0	0
			1	1		

- Molecule 33 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total Na 1 1	0	0
33	C	1	Total Na 1 1	0	0
33	H	1	Total Na 1 1	0	0
33	J	1	Total Na 1 1	0	0
33	L	1	Total Na 1 1	0	0
33	M	1	Total Na 1 1	0	0
33	Q	1	Total Na 1 1	0	0
33	R	2	Total Na 2 2	0	0
33	S	1	Total Na 1 1	0	0
33	0	73	Total Na 73 73	0	0
33	9	3	Total Na 3 3	0	0

- Molecule 34 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	3	1	Total Cl 1 1	0	0
34	0	10	Total Cl 10 10	0	0

- Molecule 35 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	O	1	Total Cd 1 1	0	0
35	U	1	Total Cd 1 1	0	0
35	Z	1	Total Cd 1 1	0	0
35	1	1	Total Cd 1 1	0	0
35	3	1	Total Cd 1 1	0	0

- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	2	Total K 2 2	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	117	Total O 117 117	0	0
37	B	146	Total O 146 146	0	0
37	C	170	Total O 170 170	0	0
37	D	47	Total O 47 47	0	0
37	E	42	Total O 42 42	0	0
37	F	24	Total O 24 24	0	0
37	G	19	Total O 19 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	H	72	Total 72	O 72	0	0
37	I	9	Total 9	O 9	0	0
37	J	51	Total 51	O 51	0	0
37	K	56	Total 56	O 56	0	0
37	L	72	Total 72	O 72	0	0
37	M	119	Total 119	O 119	0	0
37	N	65	Total 65	O 65	0	0
37	O	39	Total 39	O 39	0	0
37	P	63	Total 63	O 63	0	0
37	Q	52	Total 52	O 52	0	0
37	R	80	Total 80	O 80	0	0
37	S	33	Total 33	O 33	0	0
37	T	38	Total 38	O 38	0	0
37	U	27	Total 27	O 27	0	0
37	V	14	Total 14	O 14	0	0
37	W	66	Total 66	O 66	0	0
37	X	29	Total 29	O 29	0	0
37	Y	94	Total 94	O 94	0	0
37	Z	26	Total 26	O 26	0	0
37	1	53	Total 53	O 53	0	0
37	2	40	Total 40	O 40	0	0

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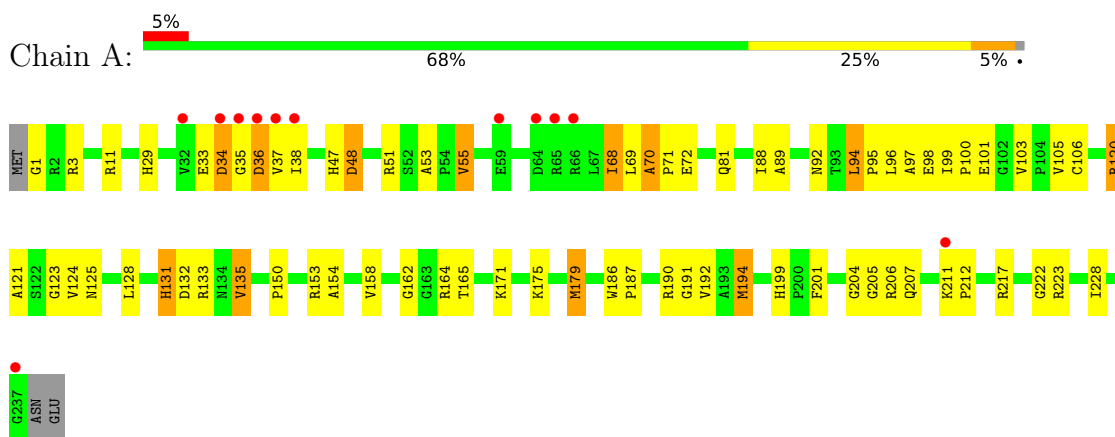
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	3	72	Total O 72 72	0	0
37	0	5949	Total O 5949 5949	0	0
37	9	139	Total O 139 139	0	0

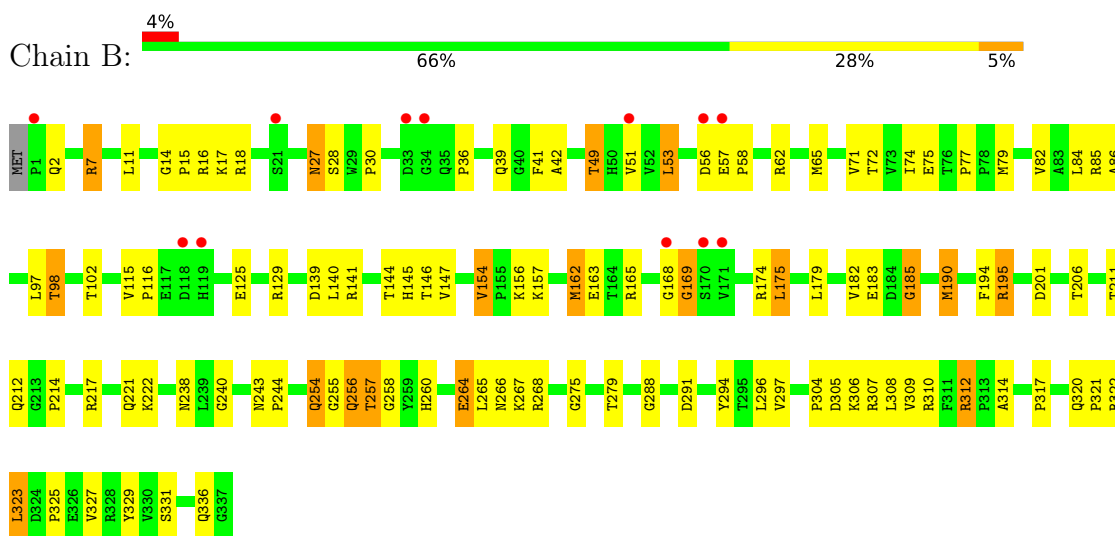
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

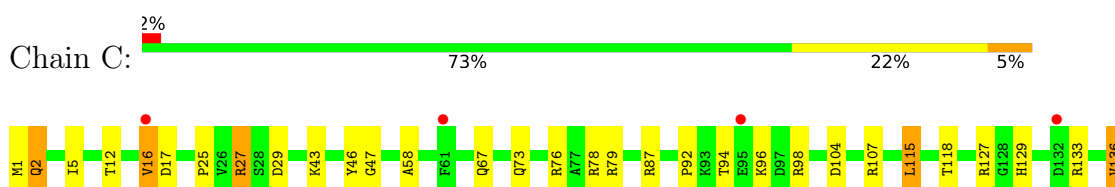
- Molecule 1: 50S ribosomal protein L2P

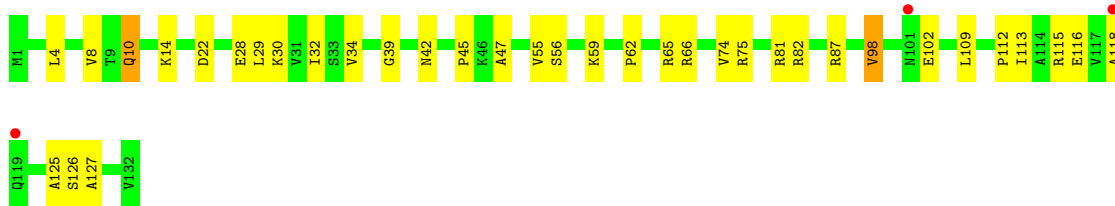


- Molecule 2: 50S ribosomal protein L3P

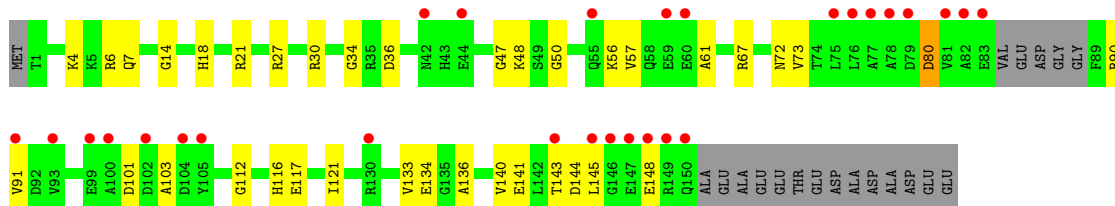


- Molecule 3: 50S ribosomal protein L4P

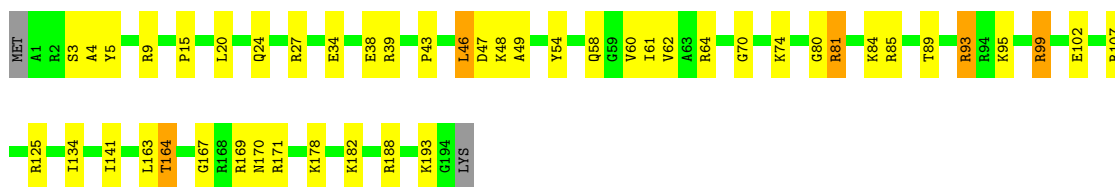
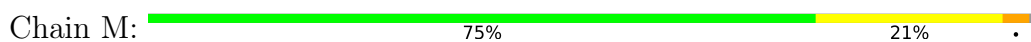




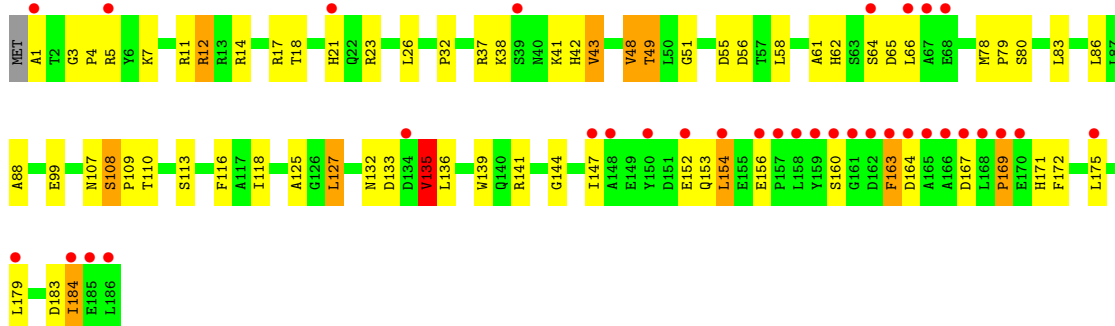
- Molecule 12: 50S ribosomal protein L15P



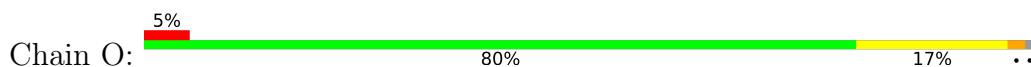
- Molecule 13: 50S ribosomal protein L15e



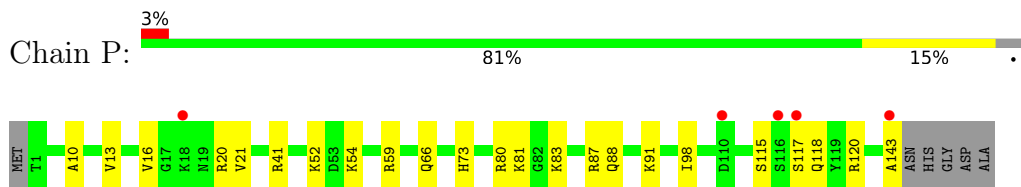
- Molecule 14: 50S ribosomal protein L18P



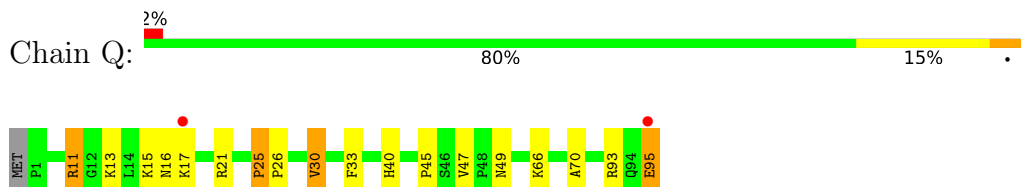
- Molecule 15: 50S ribosomal protein L18e



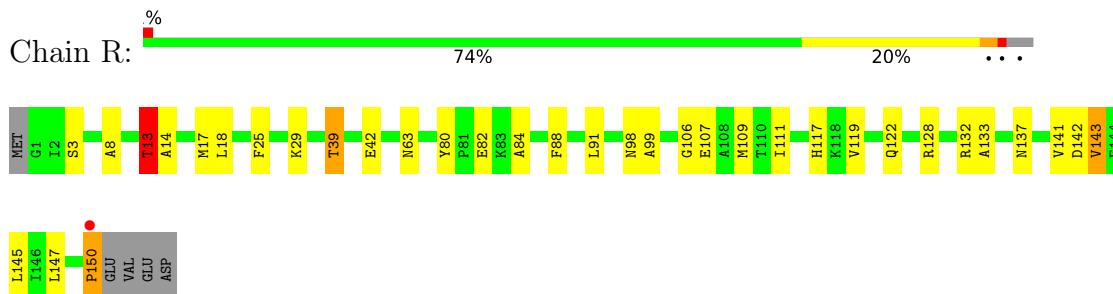
- Molecule 16: 50S ribosomal protein L19e



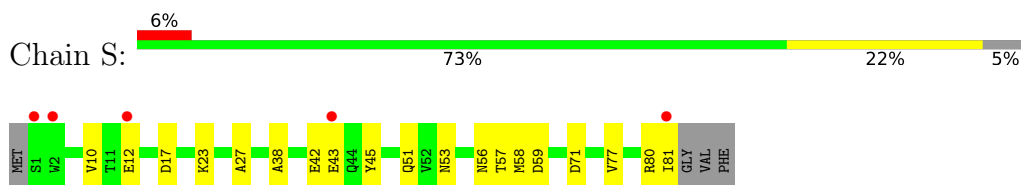
- Molecule 17: 50S ribosomal protein L21e



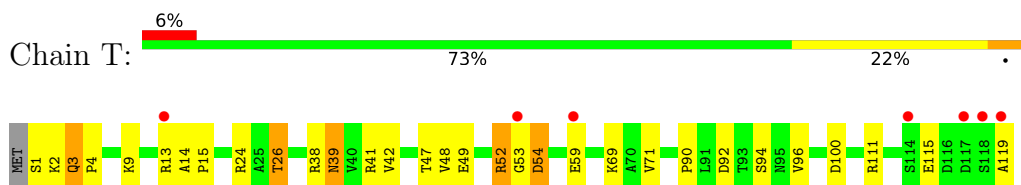
- Molecule 18: 50S ribosomal protein L22P



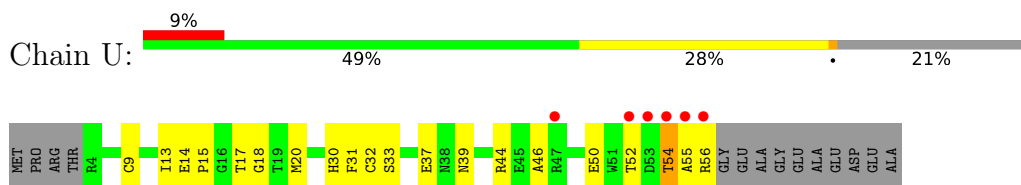
- Molecule 19: 50S ribosomal protein L23P



- Molecule 20: 50S ribosomal protein L24P



- Molecule 21: 50S ribosomal protein L24e



- Molecule 22: 50S ribosomal protein L29P

- Molecule 27: 50S ribosomal protein L37e

Chain 1:  72% 25% ..




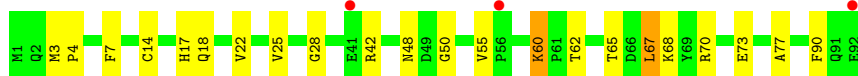
- Molecule 28: 50S ribosomal protein L39e

Chain 2:  24% 52% 38% 8%



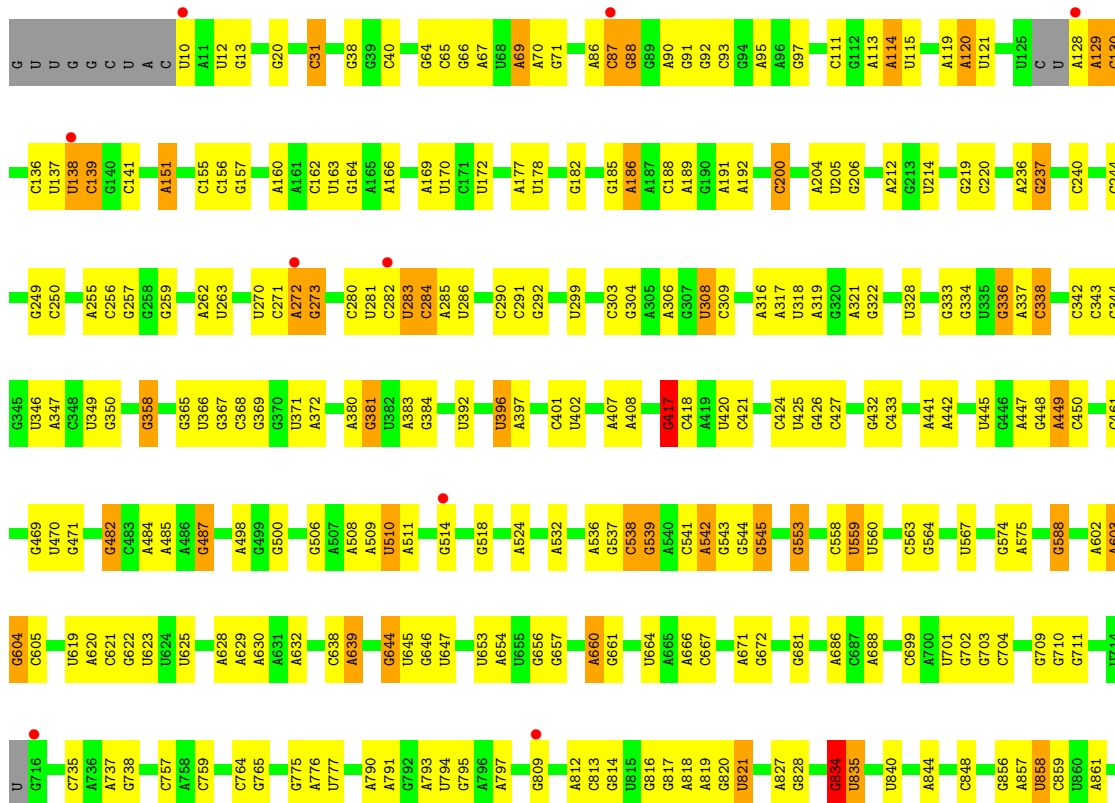
- Molecule 29: 50S ribosomal protein L44E

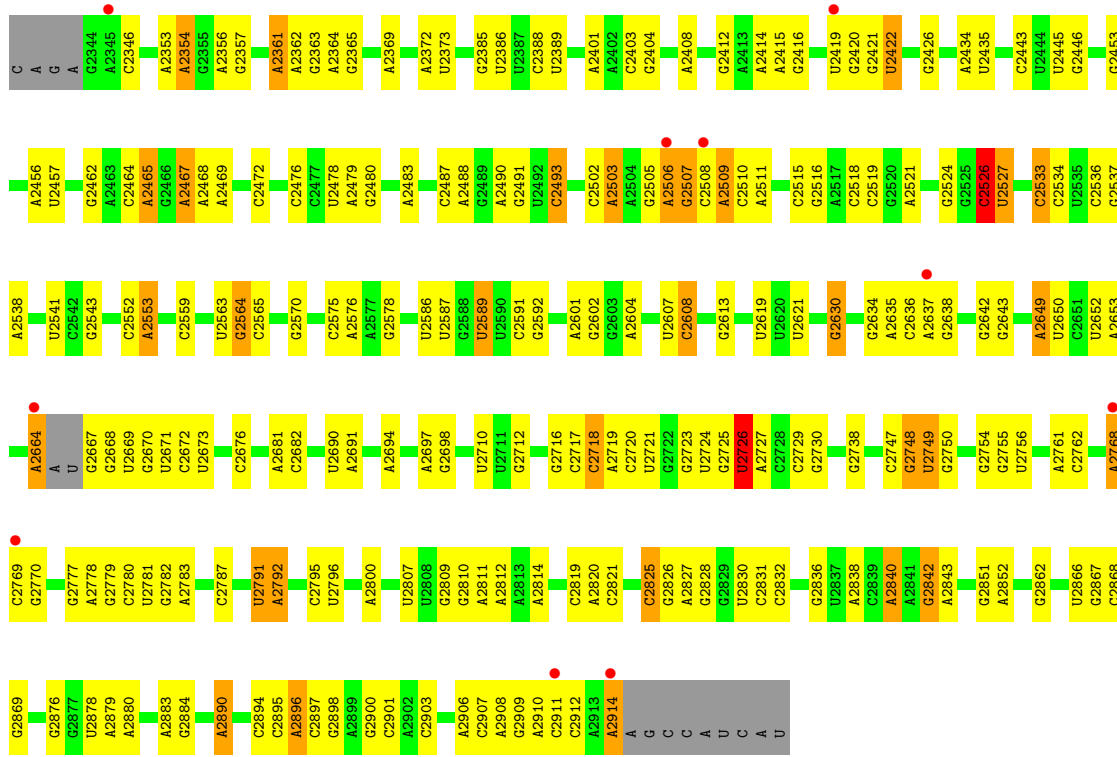
Chain 3:  3% 76% 22%



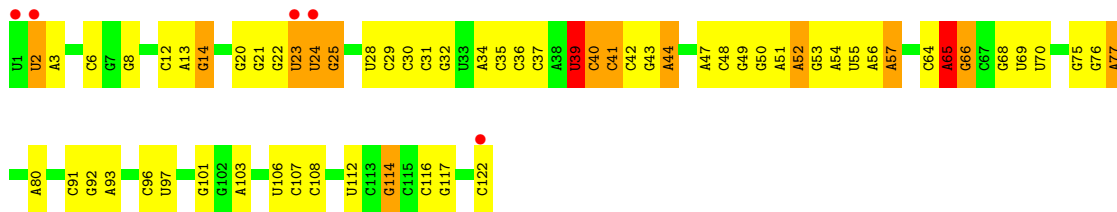
- Molecule 30: 23S RIBOSOMAL RNA

Chain 0:  2% 61% 27% 5% 6%





• Molecule 31: 5S RIBOSOMAL RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.65Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.40 49.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.5 (49.95-2.40) 90.6 (49.95-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.40Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.231 0.185 , 0.217	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtrriage
Anisotropy	0.263	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99049	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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 i

5.1 Standard geometry i

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

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	0.44	1/1786 (0.1%)	0.98	7/2408 (0.3%)
2	B	0.40	0/2690	0.98	9/3652 (0.2%)
3	C	0.45	0/1885	0.95	5/2552 (0.2%)
4	D	0.40	0/1111	0.93	6/1498 (0.4%)
5	E	0.38	0/1382	0.85	2/1880 (0.1%)
6	F	0.39	0/901	0.91	1/1224 (0.1%)
7	G	0.55	0/241	0.98	0/324
8	H	0.44	0/1302	1.00	8/1743 (0.5%)
9	I	0.43	0/526	1.01	2/716 (0.3%)
10	J	0.38	0/1136	0.91	3/1530 (0.2%)
11	K	0.39	0/1004	0.96	1/1351 (0.1%)
12	L	0.39	0/1130	0.95	5/1509 (0.3%)
13	M	0.41	0/1582	0.89	3/2116 (0.1%)
14	N	0.36	0/1474	1.04	13/1999 (0.7%)
15	O	0.41	0/874	0.93	4/1181 (0.3%)
16	P	0.38	0/1147	0.83	0/1528
17	Q	0.41	0/749	1.06	7/1005 (0.7%)
18	R	1.32	7/1172 (0.6%)	1.37	11/1578 (0.7%)
19	S	0.37	0/648	0.90	1/875 (0.1%)
20	T	0.38	0/958	0.94	4/1289 (0.3%)
21	U	0.38	0/417	0.89	1/562 (0.2%)
22	V	0.43	0/502	1.04	2/675 (0.3%)
23	W	0.47	1/1219 (0.1%)	0.99	5/1655 (0.3%)
24	X	0.45	0/664	0.99	4/895 (0.4%)
25	Y	0.43	0/1146	0.92	1/1536 (0.1%)
26	Z	0.38	0/584	1.00	2/781 (0.3%)
27	1	0.46	0/438	0.90	2/578 (0.3%)
28	2	0.38	0/401	0.78	0/529
29	3	0.39	0/771	0.88	4/1024 (0.4%)
30	0	0.37	0/65958	0.60	27/102869 (0.0%)
31	9	0.36	0/2904	0.58	3/4526 (0.1%)
All	All	0.41	9/98702 (0.0%)	0.72	143/147588 (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	39
31	9	0	1
All	All	1	40

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CA-C	-28.27	0.93	1.52
18	R	150	PRO	N-CA	16.81	1.72	1.47
18	R	150	PRO	CB-CG	16.25	2.31	1.49
18	R	150	PRO	CA-CB	12.17	1.77	1.53
18	R	150	PRO	C-O	11.46	1.46	1.23
18	R	150	PRO	CG-CD	11.41	1.89	1.50
18	R	150	PRO	N-CD	9.32	1.60	1.47
1	A	194	MET	SD-CE	-6.05	1.64	1.79
23	W	13	MET	SD-CE	-5.23	1.66	1.79

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-25.23	62.16	110.10
18	R	150	PRO	N-CA-C	-24.97	49.68	112.10
18	R	150	PRO	CA-C-O	-12.91	80.28	119.00
30	0	1979	G	C2'-C3'-O3'	9.58	123.87	109.50
17	Q	17	LYS	N-CA-C	-8.96	98.46	109.83
30	0	1942	A	C5'-C4'-C3'	8.70	129.05	116.00
9	I	86	GLU	CA-C-N	8.64	128.68	119.78
9	I	86	GLU	C-N-CA	8.64	128.68	119.78
20	T	52	ARG	N-CA-C	8.63	124.66	113.18
14	N	163	PHE	N-CA-C	-8.34	100.86	112.45
2	B	157	LYS	N-CA-C	-7.93	104.21	114.04
1	A	70	ALA	N-CA-C	7.86	119.56	109.65
8	H	173	GLU	N-CA-C	-7.83	99.80	110.68
18	R	141	VAL	N-CA-C	7.77	118.99	108.11
18	R	150	PRO	N-CA-CB	7.76	111.54	103.00
18	R	150	PRO	CA-N-CD	7.71	122.80	112.00
22	V	42	ASN	CA-C-N	7.56	129.29	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	42	ASN	C-N-CA	7.56	129.29	119.84
29	3	55	VAL	CA-C-N	7.52	129.24	119.84
29	3	55	VAL	C-N-CA	7.52	129.24	119.84
30	0	2103	A	C2'-C3'-O3'	7.46	120.69	109.50
1	A	222	GLY	N-CA-C	-7.46	104.97	114.37
12	L	47	GLY	N-CA-C	7.45	119.74	111.85
30	0	1819	G	C5'-C4'-C3'	7.19	126.79	116.00
31	9	39	U	N1-C1'-C2'	6.94	122.41	112.00
14	N	51	GLY	CA-C-N	6.93	126.91	119.28
14	N	51	GLY	C-N-CA	6.93	126.91	119.28
14	N	169	PRO	N-CA-C	-6.86	105.00	114.27
30	0	834	G	C2'-C3'-O3'	-6.83	103.45	113.70
25	Y	143	TRP	N-CA-C	6.83	120.20	109.96
8	H	121	GLY	N-CA-C	6.77	119.77	112.33
13	M	89	THR	N-CA-C	6.76	118.31	111.07
17	Q	25	PRO	CA-C-N	6.66	126.25	119.19
17	Q	25	PRO	C-N-CA	6.66	126.25	119.19
3	C	205	ARG	N-CA-C	6.65	119.38	111.33
30	0	920	C	C2'-C3'-O3'	-6.63	103.75	113.70
4	D	170	TYR	N-CA-C	6.60	120.76	111.52
17	Q	47	VAL	CA-C-N	6.58	125.82	118.97
17	Q	47	VAL	C-N-CA	6.58	125.82	118.97
10	J	68	GLY	N-CA-C	6.54	120.94	112.18
30	0	2291	A	N9-C1'-C2'	6.47	121.71	112.00
30	0	206	G	C5'-C4'-C3'	-6.45	106.32	116.00
14	N	135	VAL	N-CA-C	-6.42	106.98	113.47
19	S	27	ALA	N-CA-C	-6.39	97.27	108.20
24	X	77	PHE	N-CA-C	6.39	116.29	107.73
17	Q	49	ASN	N-CA-C	6.37	118.74	110.53
12	L	145	LEU	N-CA-C	-6.37	104.42	111.36
2	B	222	LYS	N-CA-C	-6.36	101.11	110.52
30	0	2316	G	C5'-C4'-C3'	-6.33	105.71	115.20
13	M	74	LYS	N-CA-C	6.32	119.77	109.59
2	B	323	LEU	N-CA-C	6.28	118.90	110.35
14	N	3	GLY	CA-C-N	6.28	126.19	119.28
14	N	3	GLY	C-N-CA	6.28	126.19	119.28
21	U	54	THR	N-CA-C	-6.26	103.02	112.04
30	0	1592	G	N9-C1'-C2'	6.24	121.36	112.00
30	0	871	G	C5'-C4'-O4'	-6.23	100.46	109.80
5	E	11	VAL	N-CA-C	6.22	118.84	109.20
3	C	175	LYS	N-CA-C	6.20	118.30	110.24
8	H	163	SER	N-CA-C	-6.20	101.31	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	3	GLN	CA-C-N	6.16	126.35	119.32
20	T	3	GLN	C-N-CA	6.16	126.35	119.32
23	W	9	GLY	N-CA-C	6.12	120.46	112.25
15	O	24	ALA	N-CA-C	-6.10	106.44	114.31
4	D	15	GLU	CA-C-N	6.01	127.36	119.84
4	D	15	GLU	C-N-CA	6.01	127.36	119.84
24	X	12	ILE	N-CA-C	6.00	113.82	107.76
29	3	67	LEU	N-CA-C	5.96	119.26	109.85
30	0	1504	A	N9-C1'-C2'	5.89	120.83	112.00
14	N	48	VAL	N-CA-C	5.86	116.38	108.17
18	R	137	ASN	N-CA-C	5.86	119.13	110.46
14	N	153	GLN	N-CA-C	-5.83	103.42	111.81
1	A	133	ARG	N-CA-C	-5.82	106.01	113.23
1	A	135	VAL	N-CA-C	5.74	116.95	108.45
8	H	10	ARG	N-CA-C	5.73	118.30	111.71
18	R	122	GLN	N-CA-C	-5.71	99.82	108.67
8	H	162	PRO	N-CA-C	5.70	119.62	111.13
8	H	119	ALA	N-CA-C	5.69	119.49	112.54
27	1	54	ALA	N-CA-C	5.61	118.12	111.33
24	X	79	GLU	N-CA-C	5.60	118.32	111.82
23	W	75	GLY	N-CA-C	5.60	119.11	112.33
1	A	228	ILE	N-CA-C	5.54	116.16	108.84
13	M	70	GLY	N-CA-C	5.54	121.04	112.45
8	H	161	THR	N-CA-C	5.53	120.43	113.25
12	L	7	GLN	N-CA-C	5.52	118.22	111.82
2	B	154	VAL	CA-C-N	5.52	125.35	119.28
2	B	154	VAL	C-N-CA	5.52	125.35	119.28
18	R	3	SER	N-CA-C	-5.52	100.96	109.52
4	D	136	ARG	CA-C-N	5.50	126.72	119.84
4	D	136	ARG	C-N-CA	5.50	126.72	119.84
8	H	91	ARG	N-CA-C	5.50	119.71	112.89
12	L	57	VAL	N-CA-C	-5.50	107.62	112.90
2	B	175	LEU	N-CA-C	-5.49	105.21	111.14
30	0	2726	U	N1-C1'-C2'	5.47	120.20	112.00
27	1	21	ARG	N-CA-C	5.45	118.39	111.69
26	Z	42	TYR	N-CA-C	5.44	122.39	110.80
30	0	1942	A	C4'-C3'-C2'	-5.44	97.16	102.60
3	C	192	ILE	N-CA-C	5.44	116.61	109.21
14	N	133	ASP	N-CA-C	5.42	117.89	111.33
14	N	108	SER	CA-C-N	5.42	126.62	119.84
14	N	108	SER	C-N-CA	5.42	126.62	119.84
15	O	66	GLY	N-CA-C	5.41	126.01	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	921	G	N9-C1'-C2'	5.39	120.08	112.00
11	K	8	VAL	N-CA-C	5.37	115.62	108.11
26	Z	44	ARG	N-CA-C	5.36	117.56	111.02
30	0	1120	U	C5'-C4'-C3'	-5.36	107.97	116.00
4	D	48	MET	N-CA-C	5.32	116.40	109.64
18	R	13	THR	N-CA-C	5.30	117.45	109.23
3	C	219	ASN	N-CA-C	5.29	117.30	109.69
20	T	54	ASP	N-CA-C	-5.27	106.35	112.89
30	0	2301	A	N9-C1'-C2'	5.25	119.88	112.00
3	C	177	GLY	N-CA-C	5.24	117.39	112.04
30	0	1504	A	C1'-O4'-C4'	-5.24	104.67	109.90
15	O	43	VAL	N-CA-C	5.22	115.48	108.17
30	0	1878	G	O4'-C1'-C2'	-5.22	102.38	107.60
30	0	2291	A	C4'-C3'-O3'	-5.22	105.17	113.00
2	B	147	VAL	CA-C-N	5.21	124.88	119.56
2	B	147	VAL	C-N-CA	5.21	124.88	119.56
23	W	35	VAL	CA-C-N	5.21	125.15	119.78
23	W	35	VAL	C-N-CA	5.21	125.15	119.78
23	W	142	ASP	N-CA-C	-5.20	103.53	110.55
30	0	874	A	C4'-C3'-O3'	-5.20	105.21	113.00
10	J	71	TYR	CA-C-N	5.19	125.11	119.76
10	J	71	TYR	C-N-CA	5.19	125.11	119.76
1	A	48	ASP	CA-C-N	5.19	124.85	119.56
1	A	48	ASP	C-N-CA	5.19	124.85	119.56
30	0	1878	G	C2'-C3'-O3'	-5.18	105.92	113.70
6	F	79	GLN	N-CA-C	5.17	117.92	109.59
5	E	37	ASP	N-CA-C	5.15	119.14	112.86
30	0	2313	C	C5'-C4'-C3'	5.13	123.70	116.00
30	0	1819	G	C2'-C3'-O3'	-5.12	106.02	113.70
31	9	65	A	N9-C1'-C2'	5.12	119.67	112.00
17	Q	13	LYS	N-CA-C	5.10	118.60	112.38
18	R	63	ASN	N-CA-C	5.09	119.03	112.41
31	9	39	U	C4'-C3'-O3'	-5.09	105.36	113.00
30	0	2526	C	N1-C1'-C2'	5.07	119.60	112.00
30	0	1819	G	C4'-C3'-C2'	-5.05	97.55	102.60
14	N	42	HIS	N-CA-C	5.04	117.08	109.41
15	O	82	SER	N-CA-C	-5.04	103.75	110.55
12	L	91	VAL	N-CA-C	5.02	115.35	108.12
24	X	60	ALA	N-CA-C	5.02	117.13	111.11
2	B	266	ASN	N-CA-C	5.01	118.23	111.17
30	0	138	U	C2'-C3'-O3'	-5.01	106.19	113.70
29	3	60	LYS	N-CA-C	-5.00	103.18	110.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain
30	0	1340	G	Sidechain
30	0	1342	C	Sidechain
30	0	1417	G	Sidechain
30	0	1450	C	Sidechain
30	0	1829	A	Sidechain
30	0	1845	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	1972	U	Sidechain
30	0	2103	A	Sidechain
30	0	2316	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2543	G	Sidechain
30	0	2552	C	Sidechain
30	0	2564	G	Sidechain
30	0	2607	U	Sidechain
30	0	2630	G	Sidechain
30	0	270	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	417	G	Sidechain
30	0	449	A	Sidechain
30	0	469	G	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	639	A	Sidechain

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Mol	Chain	Res	Type	Group
30	0	795	G	Sidechain
30	0	867	A	Sidechain
31	9	39	U	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	79	0
2	B	2625	0	2533	85	0
3	C	1860	0	1813	65	0
4	D	1094	0	1085	46	0
5	E	1357	0	1266	46	0
6	F	890	0	843	27	0
7	G	240	0	231	11	0
8	H	1282	0	1292	34	0
9	I	519	0	500	25	0
10	J	1120	0	1098	39	0
11	K	994	0	1027	40	0
12	L	1118	0	1076	28	0
13	M	1558	0	1572	47	0
14	N	1445	0	1401	57	0
15	O	865	0	873	19	0
16	P	1136	0	1123	20	0
17	Q	735	0	728	11	0
18	R	1149	0	1122	32	0
19	S	641	0	605	14	0
20	T	950	0	923	24	0
21	U	410	0	364	16	0
22	V	499	0	511	20	0
23	W	1196	0	1137	65	0
24	X	654	0	653	20	0
25	Y	1130	0	1133	31	0
26	Z	573	0	532	15	0
27	1	431	0	426	16	0
28	2	396	0	413	24	0
29	3	755	0	728	16	0
30	0	59021	0	29809	873	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	9	2599	0	1325	72	0
32	0	109	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	73	0	0	0	0
33	9	3	0	0	0	0
33	A	1	0	0	0	0
33	C	1	0	0	0	0
33	H	1	0	0	0	0
33	J	1	0	0	0	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	2	0	0	0	0
33	S	1	0	0	0	0
34	0	10	0	0	0	0
34	3	1	0	0	0	0
34	A	1	0	0	0	0
34	B	1	0	0	0	0
34	J	3	0	0	1	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	O	1	0	0	0	0
34	R	1	0	0	0	0
34	Y	1	0	0	0	0
35	1	1	0	0	0	0
35	3	1	0	0	0	0
35	O	1	0	0	0	0
35	U	1	0	0	0	0
35	Z	1	0	0	1	0
36	0	2	0	0	0	0
37	0	5949	0	0	148	0
37	1	53	0	0	2	0
37	2	40	0	0	4	0
37	3	72	0	0	6	0
37	9	139	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	A	117	0	0	15	0
37	B	146	0	0	13	0
37	C	170	0	0	18	0
37	D	47	0	0	5	0
37	E	42	0	0	4	0
37	F	24	0	0	2	0
37	G	19	0	0	1	0
37	H	72	0	0	5	0
37	I	9	0	0	3	0
37	J	51	0	0	2	0
37	K	56	0	0	4	0
37	L	72	0	0	9	0
37	M	119	0	0	9	0
37	N	65	0	0	10	0
37	O	39	0	0	3	0
37	P	63	0	0	1	0
37	Q	52	0	0	3	0
37	R	80	0	0	2	0
37	S	33	0	0	2	0
37	T	38	0	0	2	0
37	U	27	0	0	1	0
37	V	14	0	0	1	0
37	W	66	0	0	5	0
37	X	29	0	0	5	0
37	Y	94	0	0	10	0
37	Z	26	0	0	2	0
All	All	99049	0	59908	1724	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 11.

All (1724) 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:CD	18:R:150:PRO:CG	1.89	1.50
14:N:37:ARG:NH1	31:9:6:C:H5'	1.61	1.14
18:R:150:PRO:CG	18:R:150:PRO:C	2.21	1.12
30:0:871:G:H5'	30:0:871:G:C8	1.86	1.10
30:0:960:G:H4'	37:0:6980:HOH:O	1.49	1.09
18:R:150:PRO:CG	18:R:150:PRO:CB	2.30	1.08
15:O:3:THR:HG22	30:0:656:G:H5'	1.38	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1160:G:C5'	30:0:1161:A:H5'	1.85	1.06
10:J:82:THR:HG23	30:0:1242:A:H5'	1.37	1.05
13:M:171:ARG:HD3	30:0:156:C:H5''	1.37	1.05
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.39	1.02
30:0:2812:A:H2	30:0:2814:A:H62	1.08	1.02
30:0:1160:G:H5'	30:0:1161:A:H5'	1.02	1.01
31:9:56:A:H2'	31:9:57:A:H5''	1.42	1.01
30:0:1372:A:H3'	37:0:6737:HOH:O	1.60	1.00
30:0:1160:G:H5'	30:0:1161:A:C5'	1.91	1.00
30:0:2717:C:H2'	30:0:2718:C:H5''	1.43	0.99
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.44	0.99
31:9:76:G:H3'	31:9:77:A:H5''	1.44	0.98
30:0:2710:U:H1'	37:0:7172:HOH:O	1.62	0.98
30:0:1474:C:H5'	30:0:1474:C:H6	1.30	0.97
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.46	0.96
30:0:542:A:H5'	30:0:542:A:H8	1.28	0.96
30:0:871:G:H5'	30:0:871:G:H8	1.25	0.95
2:B:62:ARG:HA	2:B:65:MET:HE3	1.48	0.95
30:0:2717:C:C2'	30:0:2718:C:H5''	1.96	0.95
28:2:41:HIS:H	28:2:45:ASN:HD22	1.11	0.95
4:D:134:LEU:HD11	4:D:166:ILE:HD11	1.49	0.94
30:0:214:U:H5'	37:0:5687:HOH:O	1.67	0.94
30:0:541:C:H2'	30:0:542:A:H5''	1.50	0.94
11:K:10:GLN:H	11:K:10:GLN:HE21	0.96	0.93
23:W:149:LEU:HG	23:W:153:MET:HE2	1.48	0.93
30:0:1835:U:H5	30:0:1840:A:N7	1.66	0.93
3:C:236:THR:HG22	3:C:239:ALA:H	1.30	0.93
30:0:1625:U:H4'	37:0:4207:HOH:O	1.68	0.93
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.17	0.92
13:M:164:THR:HG22	13:M:167:GLY:H	1.33	0.92
30:0:381:G:H5''	37:0:3859:HOH:O	1.67	0.92
30:0:282:C:H1'	30:0:368:C:N4	1.85	0.91
30:0:871:G:H8	30:0:871:G:C5'	1.83	0.91
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.53	0.90
30:0:1184:C:H1'	37:0:7015:HOH:O	1.70	0.90
30:0:870:G:H2'	30:0:871:G:H5''	1.51	0.90
30:0:2291:A:C8	30:0:2309:C:H5'	2.06	0.90
21:U:52:THR:HG22	21:U:54:THR:H	1.35	0.90
30:0:1116:U:O2'	30:0:1118:A:H2	1.55	0.89
30:0:1667:A:H5'	30:0:1667:A:H8	1.36	0.89
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2748:G:H2'	37:0:7089:HOH:O	1.72	0.89
30:0:1666:C:O2'	30:0:1667:A:H5''	1.70	0.89
30:0:1701:A:H4'	30:0:1702:U:H5''	1.53	0.89
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.54	0.88
30:0:236:A:H4'	30:0:237:G:H5'	1.55	0.87
2:B:140:LEU:HA	37:B:8581:HOH:O	1.74	0.87
30:0:541:C:C2'	30:0:542:A:H5''	2.03	0.87
11:K:39:GLY:HA2	37:0:4763:HOH:O	1.73	0.87
30:0:871:G:C8	30:0:871:G:C5'	2.58	0.87
30:0:1116:U:H3	30:0:1246:A:H62	1.23	0.86
16:P:115:SER:H	16:P:118:GLN:HE21	1.19	0.86
4:D:154:LYS:H	4:D:154:LYS:HD2	1.38	0.86
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.19	0.86
30:0:69:A:H5'	30:0:69:A:C8	2.10	0.86
30:0:2506:A:O2'	30:0:2507:G:H8	1.59	0.86
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.55	0.85
30:0:1300:G:H1'	37:0:4223:HOH:O	1.77	0.85
14:N:37:ARG:HH12	31:9:6:C:H5''	1.39	0.85
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.42	0.85
31:9:39:U:H1'	31:9:44:A:H61	1.42	0.85
30:0:282:C:O2'	30:0:283:U:H5'	1.77	0.84
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.58	0.84
30:0:545:G:H5'	30:0:545:G:H8	1.40	0.84
23:W:88:THR:HB	37:W:6679:HOH:O	1.77	0.84
30:0:506:G:H22	30:0:509:A:C5'	1.91	0.83
30:0:69:A:H5'	30:0:69:A:H8	1.42	0.83
30:0:1119:G:N2	30:0:1246:A:C2	2.46	0.83
31:9:14:G:H5'	31:9:14:G:H8	1.43	0.83
2:B:206:THR:HG21	30:0:2716:G:H5''	1.60	0.83
30:0:1730:G:H5'	30:0:1731:C:C5	2.14	0.82
26:Z:34:SER:HB2	37:Z:8414:HOH:O	1.77	0.82
4:D:25:MET:HE2	4:D:41:LEU:HG	1.60	0.82
30:0:1862:C:H1'	37:0:6768:HOH:O	1.80	0.82
30:0:2586:U:H3	30:0:2592:G:H22	1.28	0.82
30:0:1118:A:H3'	30:0:1118:A:H8	1.44	0.82
30:0:272:A:H3'	37:0:7079:HOH:O	1.79	0.81
30:0:2769:C:C2'	30:0:2770:G:H5'	2.10	0.81
37:I:5128:HOH:O	30:0:1168:C:H4'	1.81	0.81
25:Y:200:THR:HG22	25:Y:201:GLU:HG3	1.61	0.81
30:0:506:G:H22	30:0:509:A:H5''	1.45	0.81
30:0:564:G:H1'	37:0:5857:HOH:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.26	0.81
30:0:346:U:H4'	37:0:6392:HOH:O	1.80	0.81
11:K:10:GLN:HE21	11:K:10:GLN:N	1.79	0.81
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.63	0.81
30:0:2851:G:O2'	30:0:2852:A:H5'	1.81	0.81
8:H:170:ARG:HD2	37:H:8342:HOH:O	1.79	0.80
31:9:56:A:C2'	31:9:57:A:H5''	2.11	0.80
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.46	0.80
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.63	0.80
30:0:1474:C:H5'	30:0:1474:C:C6	2.17	0.80
30:0:1973:A:H5'	30:0:1973:A:H8	1.47	0.80
30:0:2908:A:H2'	30:0:2909:G:O4'	1.82	0.80
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.63	0.80
30:0:1118:A:H3'	30:0:1118:A:C8	2.16	0.80
30:0:2637:A:H5'	37:0:8794:HOH:O	1.80	0.79
1:A:199:HIS:HD2	1:A:201:PHE:H	1.27	0.79
2:B:238:ASN:HD22	2:B:240:GLY:H	1.26	0.79
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.98	0.79
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.47	0.79
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.64	0.79
30:0:544:G:H2'	30:0:545:G:H5''	1.65	0.78
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.18	0.78
31:9:29:C:H2'	31:9:30:C:H5'	1.66	0.78
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.83	0.78
15:O:3:THR:CG2	30:0:656:G:H5'	2.12	0.78
30:0:541:C:H2'	30:0:542:A:C5'	2.14	0.78
30:0:1119:G:H22	30:0:1246:A:H2	1.32	0.78
11:K:81:ARG:HB2	11:K:87:ARG:HH11	1.49	0.78
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.65	0.78
23:W:122:ARG:NH2	23:W:154:ARG:HB3	1.99	0.78
30:0:182:G:H5'	37:0:4697:HOH:O	1.83	0.78
8:H:30:LYS:H	8:H:62:HIS:HD2	1.31	0.77
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.81	0.77
30:0:1919:A:H4'	37:0:4389:HOH:O	1.85	0.77
30:0:2896:A:H5''	37:0:5645:HOH:O	1.84	0.77
1:A:179:MET:HE3	1:A:179:MET:HA	1.67	0.77
3:C:1:MET:HG2	3:C:2:GLN:H	1.49	0.77
30:0:1206:U:H6	30:0:1206:U:H5'	1.50	0.76
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.66	0.76
30:0:1165:G:H4'	30:0:1174:A:O2'	1.86	0.76
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:1:THR:HG23	22:V:2:VAL:H	1.50	0.76
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.68	0.76
30:0:1080:C:H4'	30:0:1081:A:OP1	1.84	0.76
14:N:144:GLY:O	14:N:147:ILE:HG22	1.85	0.76
30:0:542:A:H5'	30:0:542:A:C8	2.18	0.76
30:0:2004:U:H4'	37:0:4853:HOH:O	1.85	0.76
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.66	0.75
30:0:603:A:H5''	30:0:604:G:OP1	1.86	0.75
30:0:2769:C:H2'	30:0:2770:G:H5'	1.68	0.75
30:0:2506:A:HO2'	30:0:2507:G:H8	0.81	0.75
14:N:37:ARG:NH1	31:9:6:C:C5'	2.48	0.75
30:0:1701:A:H4'	30:0:1702:U:C5'	2.16	0.75
2:B:321:PRO:HA	37:B:8656:HOH:O	1.85	0.75
30:0:877:G:H5'	30:0:878:G:OP1	1.86	0.74
29:3:65:THR:HG22	29:3:67:LEU:HG	1.69	0.74
30:0:2635:A:O2'	30:0:2636:C:H5'	1.88	0.74
4:D:99:ASP:HB3	4:D:103:ASN:H	1.53	0.74
30:0:559:U:H6	30:0:559:U:H5'	1.53	0.74
30:0:870:G:C2'	30:0:871:G:H5''	2.18	0.74
31:9:39:U:H1'	31:9:44:A:N6	2.03	0.74
2:B:86:ALA:HA	37:B:8581:HOH:O	1.87	0.73
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.69	0.73
30:0:1603:A:H5'	30:0:1605:G:O4'	1.88	0.73
37:B:8634:HOH:O	30:0:2672:C:H1'	1.87	0.73
30:0:2323:G:H5''	37:0:4318:HOH:O	1.88	0.73
5:E:143:GLN:NE2	30:0:2779:G:H21	1.86	0.73
30:0:558:C:O2'	30:0:559:U:H5''	1.89	0.73
14:N:113:SER:HB2	37:N:8558:HOH:O	1.87	0.73
30:0:1497:G:H4'	30:0:1627:G:O2'	1.88	0.72
1:A:35:GLY:O	1:A:36:ASP:HB3	1.90	0.72
30:0:1666:C:H2'	30:0:1667:A:H5'	1.70	0.72
30:0:1130:U:H5'	37:0:7223:HOH:O	1.89	0.72
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.71	0.72
3:C:174:ILE:CD1	30:0:338:C:H4'	2.19	0.72
15:O:3:THR:HG22	30:0:656:G:C5'	2.18	0.72
30:0:2505:G:O2'	30:0:2506:A:H5'	1.89	0.72
30:0:2507:G:H2'	30:0:2510:C:H42	1.55	0.72
30:0:1180:U:H1'	37:0:9766:HOH:O	1.90	0.71
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.54	0.71
14:N:23:ARG:HD3	37:N:8546:HOH:O	1.90	0.71
9:I:127:CYS:HB3	9:I:132:VAL:HB	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.71	0.71
11:K:10:GLN:H	11:K:10:GLN:NE2	1.80	0.71
1:A:211:LYS:HB2	37:A:8612:HOH:O	1.91	0.71
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.71	0.71
30:0:2756:U:H3	30:0:2896:A:H2	1.34	0.71
21:U:9:CYS:HA	21:U:52:THR:HG23	1.73	0.71
1:A:51:ARG:HB2	37:A:8599:HOH:O	1.91	0.71
26:Z:34:SER:OG	30:0:797:A:H4'	1.90	0.71
30:0:299:U:H5'	37:0:6885:HOH:O	1.91	0.70
30:0:1667:A:H5'	30:0:1667:A:C8	2.25	0.70
28:2:41:HIS:N	28:2:45:ASN:HD22	1.88	0.70
30:0:1835:U:C5	30:0:1840:A:N7	2.56	0.70
30:0:1634:G:H3'	37:0:3430:HOH:O	1.90	0.70
30:0:558:C:C2'	30:0:559:U:H5''	2.21	0.70
30:0:1166:A:H61	30:0:1180:U:H3	1.38	0.70
30:0:1183:C:N4	30:0:1184:C:H41	1.90	0.70
31:9:14:G:H5'	31:9:14:G:C8	2.26	0.70
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.27	0.70
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.73	0.70
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.90	0.70
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.74	0.70
13:M:171:ARG:CD	30:0:156:C:H5''	2.19	0.69
13:M:178:LYS:HB2	37:0:6424:HOH:O	1.90	0.69
18:R:128:ARG:NH2	30:0:2054:A:N3	2.40	0.69
28:2:39:ARG:HG2	37:2:3143:HOH:O	1.92	0.69
30:0:2426:G:H1'	37:0:5638:HOH:O	1.92	0.69
30:0:2533:C:H6	30:0:2533:C:H5'	1.57	0.69
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.07	0.69
1:A:191:GLY:HA2	1:A:194:MET:CE	2.22	0.69
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.69
30:0:951:A:C2'	30:0:952:G:H5'	2.22	0.69
10:J:76:ASP:HA	37:J:5907:HOH:O	1.93	0.69
30:0:536:A:H3'	37:0:4588:HOH:O	1.92	0.69
30:0:1603:A:H5''	30:0:1605:G:H5'	1.75	0.69
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.74	0.69
30:0:558:C:H2'	30:0:559:U:C5'	2.23	0.69
30:0:1058:A:H2'	30:0:1060:C:H5''	1.74	0.68
30:0:1632:A:H2'	30:0:1633:C:H5'	1.74	0.68
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.74	0.68
30:0:2812:A:C2	30:0:2814:A:N6	2.59	0.68
2:B:211:THR:HG21	37:0:7003:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2756:U:N3	30:0:2896:A:C2	2.59	0.68
30:0:2769:C:H2'	30:0:2770:G:C5'	2.23	0.68
30:0:2787:C:H5	37:0:4174:HOH:O	1.76	0.68
30:0:1166:A:H1'	30:0:1192:A:C2	2.28	0.68
30:0:1730:G:C5'	30:0:1731:C:C6	2.77	0.68
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.08	0.68
28:2:41:HIS:H	28:2:45:ASN:ND2	1.89	0.68
5:E:69:ILE:HA	5:E:72:MET:HE3	1.74	0.68
30:0:1766:U:O2	30:0:1778:A:H5'	1.94	0.68
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.76	0.67
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.76	0.67
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.94	0.67
30:0:1701:A:H5'	37:0:5830:HOH:O	1.93	0.67
30:0:1730:G:H5'	30:0:1731:C:H5	1.58	0.67
19:S:57:THR:HG22	19:S:59:ASP:H	1.58	0.67
30:0:1189:A:H3'	37:0:7231:HOH:O	1.93	0.67
30:0:1878:G:H1'	37:0:5667:HOH:O	1.94	0.67
18:R:98:ASN:HD21	30:0:500:G:H21	1.41	0.67
23:W:125:HIS:HD2	23:W:127:GLY:H	1.42	0.67
30:0:272:A:H5'	30:0:273:G:OP2	1.94	0.67
30:0:1441:G:O2'	30:0:1442:A:H5'	1.94	0.67
2:B:190:MET:HE2	2:B:194:PHE:HD1	1.57	0.67
3:C:140:VAL:HB	37:C:8449:HOH:O	1.93	0.67
30:0:2064:U:H5'	30:0:2652:U:O3'	1.94	0.67
30:0:1377:C:H6	30:0:1377:C:H5'	1.60	0.67
10:J:74:ARG:HH11	10:J:74:ARG:HB3	1.58	0.67
30:0:1187:U:O2'	30:0:1189:A:H2	1.77	0.67
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.10	0.67
29:3:48:ASN:HD21	30:0:2468:A:H61	1.41	0.67
30:0:1819:G:H2'	30:0:1820:G:H4'	1.76	0.67
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.09	0.66
1:A:199:HIS:CD2	1:A:201:PHE:H	2.11	0.66
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.78	0.66
30:0:31:C:H4'	37:0:6974:HOH:O	1.94	0.66
30:0:856:G:H2'	37:0:4975:HOH:O	1.94	0.66
30:0:2827:A:H2'	30:0:2828:G:O4'	1.95	0.66
6:F:91:VAL:HG12	6:F:92:GLY:H	1.60	0.66
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.78	0.66
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.11	0.66
23:W:21:LEU:HD22	23:W:26:ILE:HD11	1.77	0.66
30:0:545:G:H5'	30:0:545:G:C8	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:GLN:HE22	30:0:1119:G:H8	1.42	0.66
30:0:711:G:H1'	37:0:6640:HOH:O	1.95	0.66
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.77	0.66
30:0:1205:U:H2'	30:0:1206:U:C5'	2.25	0.66
3:C:139:VAL:HG13	37:C:8446:HOH:O	1.95	0.66
3:C:236:THR:HG21	37:C:8373:HOH:O	1.96	0.66
30:0:1209:C:H2'	30:0:1210:G:H8	1.61	0.66
30:0:2783:A:H3'	37:0:4774:HOH:O	1.95	0.66
3:C:236:THR:HG22	3:C:239:ALA:N	2.08	0.66
4:D:135:VAL:HG22	4:D:136:ARG:H	1.60	0.66
30:0:544:G:C2'	30:0:545:G:H5''	2.24	0.66
30:0:1185:U:H2'	30:0:1186:C:C6	2.31	0.66
12:L:30:ARG:HD3	30:0:164:G:H4'	1.78	0.65
22:V:1:THR:HB	30:0:93:C:H5''	1.76	0.65
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.26	0.65
30:0:1205:U:H2'	30:0:1206:U:H5''	1.76	0.65
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.78	0.65
23:W:21:LEU:HD22	23:W:26:ILE:CD1	2.26	0.65
23:W:122:ARG:HH11	23:W:122:ARG:CG	2.08	0.65
30:0:856:G:C8	37:0:4975:HOH:O	2.48	0.65
30:0:2414:A:H2'	30:0:2415:A:C8	2.31	0.65
31:9:64:C:H2'	31:9:65:A:H5'	1.79	0.65
3:C:5:ILE:HD11	3:C:16:VAL:HG23	1.78	0.65
14:N:5:ARG:NH1	30:0:962:C:H1'	2.10	0.65
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.78	0.65
30:0:1741:U:H5'	30:0:1742:A:OP1	1.96	0.65
31:9:54:A:O2'	31:9:55:U:H5'	1.96	0.65
18:R:29:LYS:HE2	30:0:524:A:C5'	2.26	0.65
3:C:5:ILE:HD11	3:C:16:VAL:CG2	2.27	0.65
6:F:96:ALA:HA	37:F:3111:HOH:O	1.97	0.65
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.42	0.65
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.11	0.65
30:0:1878:G:O2'	30:0:1879:U:C6	2.48	0.65
2:B:185:GLY:HA2	37:B:8633:HOH:O	1.97	0.65
16:P:117:SER:HB3	30:0:1593:C:OP1	1.98	0.64
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.05	0.64
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.78	0.64
30:0:2608:C:H2'	37:0:3110:HOH:O	1.96	0.64
5:E:97:VAL:HG12	37:E:4191:HOH:O	1.97	0.64
12:L:133:VAL:HA	37:L:8562:HOH:O	1.95	0.64
12:L:18:HIS:HD2	30:0:902:G:N7	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:42:ASN:HB3	37:V:7247:HOH:O	1.97	0.64
10:J:19:MET:HE1	10:J:78:ILE:HG22	1.80	0.64
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.09	0.64
27:1:16:HIS:HD2	30:0:470:U:O2'	1.81	0.64
30:0:1632:A:C2'	30:0:1633:C:H5'	2.28	0.64
30:0:31:C:H2'	37:0:7238:HOH:O	1.97	0.64
8:H:49:GLN:HE21	8:H:140:TYR:HE2	1.46	0.64
30:0:1666:C:C2'	30:0:1667:A:H5''	2.27	0.64
30:0:1666:C:H2'	30:0:1667:A:C5'	2.27	0.64
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.12	0.63
14:N:4:PRO:HG3	31:9:69:U:OP1	1.98	0.63
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.34	0.63
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.45	0.63
30:0:1641:A:H2'	30:0:1642:A:H5'	1.79	0.63
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.78	0.63
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.45	0.63
30:0:2649:A:H5'	30:0:2649:A:H8	1.63	0.63
30:0:2717:C:H2'	30:0:2718:C:C5'	2.24	0.63
30:0:1330:A:H2	37:0:4223:HOH:O	1.81	0.63
30:0:2769:C:O2'	30:0:2770:G:H5'	1.97	0.63
5:E:139:GLU:OE2	30:0:2781:U:H1'	1.99	0.63
25:Y:141:THR:HG23	37:Y:8586:HOH:O	1.99	0.63
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.81	0.63
25:Y:187:VAL:HG12	25:Y:205:ILE:HA	1.81	0.63
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.81	0.63
30:0:281:U:O2'	30:0:282:C:H5'	1.99	0.63
30:0:558:C:H2'	30:0:559:U:H5'	1.81	0.63
18:R:39:THR:HG23	18:R:107:GLU:O	1.98	0.62
20:T:9:LYS:HB2	37:0:6974:HOH:O	1.98	0.62
30:0:506:G:H22	30:0:509:A:H5'	1.64	0.62
30:0:1116:U:HO2'	30:0:1118:A:H2	0.74	0.62
27:1:20:ARG:HG2	30:0:111:C:O2'	1.99	0.62
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.34	0.62
27:1:25:LYS:HE2	37:2:7213:HOH:O	1.98	0.62
25:Y:185:VAL:HG12	37:Y:8567:HOH:O	1.99	0.62
30:0:2832:C:H5	37:0:6762:HOH:O	1.82	0.62
9:I:120:ALA:O	9:I:124:VAL:HG23	1.99	0.62
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.80	0.62
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.64	0.62
1:A:192:VAL:HB	37:A:8587:HOH:O	1.99	0.62
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.81	0.62
30:0:138:U:H5''	30:0:139:C:OP2	1.99	0.62
30:0:1666:C:C2'	30:0:1667:A:C5'	2.78	0.62
30:0:2717:C:O2'	30:0:2718:C:H5''	1.99	0.62
30:0:2768:A:H2'	30:0:2769:C:O4'	1.99	0.62
4:D:57:THR:HG23	4:D:63:ILE:HA	1.82	0.62
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.80	0.62
10:J:47:THR:HB	37:0:4375:HOH:O	2.00	0.62
18:R:99:ALA:CB	18:R:109:MET:HE1	2.23	0.62
2:B:145:HIS:HD2	2:B:146:THR:O	1.83	0.62
4:D:99:ASP:HA	37:0:5842:HOH:O	2.00	0.62
30:0:1730:G:H5''	30:0:1731:C:H6	1.65	0.62
30:0:1118:A:C8	30:0:1118:A:C3'	2.79	0.61
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.82	0.61
29:3:73:GLU:HB3	37:3:8559:HOH:O	2.00	0.61
31:9:2:U:OP2	31:9:3:A:H5'	2.00	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.30	0.61
2:B:179:LEU:O	2:B:183:GLU:HG2	1.99	0.61
2:B:211:THR:HG23	30:0:2840:A:OP1	2.00	0.61
6:F:91:VAL:HG12	6:F:92:GLY:N	2.14	0.61
12:L:136:ALA:HB3	37:L:8562:HOH:O	1.99	0.61
13:M:80:GLY:O	13:M:81:ARG:HD3	1.99	0.61
30:0:396:U:O2'	30:0:418:C:H4'	2.00	0.61
30:0:1130:U:H2'	30:0:1131:G:O4'	2.00	0.61
3:C:236:THR:H	3:C:239:ALA:HB3	1.65	0.61
18:R:39:THR:HG22	18:R:42:GLU:H	1.65	0.61
30:0:1778:A:H2'	30:0:1779:A:H5'	1.82	0.61
30:0:2346:C:H6	30:0:2346:C:O5'	1.83	0.61
30:0:2533:C:H5'	30:0:2533:C:C6	2.34	0.61
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.83	0.61
30:0:1189:A:H1'	30:0:1209:C:H1'	1.83	0.61
2:B:16:ARG:NH1	37:B:8617:HOH:O	2.34	0.61
30:0:951:A:O2'	30:0:952:G:H5'	2.01	0.61
30:0:960:G:N3	30:0:960:G:H2'	2.16	0.61
30:0:1201:C:H2'	30:0:1202:A:H5'	1.82	0.61
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.33	0.61
15:O:42:GLU:HB2	37:O:2176:HOH:O	2.00	0.61
30:0:1189:A:H1'	30:0:1209:C:C1'	2.30	0.61
30:0:2502:C:C2'	30:0:2503:A:H5'	2.30	0.61
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.81	0.61
31:9:13:A:O2'	31:9:14:G:H5''	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:82:THR:HG23	30:0:1242:A:C5'	2.24	0.60
2:B:238:ASN:HD22	2:B:240:GLY:N	1.98	0.60
12:L:143:THR:HG22	12:L:144:ASP:N	2.16	0.60
4:D:163:VAL:HA	37:D:6326:HOH:O	2.02	0.60
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.81	0.60
21:U:20:MET:HE2	21:U:30:HIS:NE2	2.17	0.60
23:W:21:LEU:HB3	23:W:26:ILE:HG12	1.82	0.60
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.67	0.60
13:M:61:ILE:HG13	37:M:8617:HOH:O	1.99	0.60
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.46	0.60
1:A:48:ASP:HB3	37:A:8599:HOH:O	2.02	0.60
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.31	0.60
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.65	0.60
12:L:4:LYS:HE2	30:0:645:U:OP2	2.01	0.60
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.83	0.60
9:I:110:ASP:O	30:0:1163:G:H5'	2.02	0.60
10:J:19:MET:HE2	10:J:79:PHE:HA	1.82	0.60
14:N:37:ARG:NH1	31:9:6:C:OP1	2.34	0.60
30:0:2415:A:H2'	30:0:2416:G:H5'	1.82	0.60
30:0:2768:A:O2'	30:0:2769:C:H5'	2.01	0.60
30:0:1528:A:H2'	30:0:1529:G:O4'	2.01	0.60
2:B:267:LYS:HD3	37:B:8526:HOH:O	2.01	0.60
18:R:117:HIS:HD2	30:0:20:G:H21	1.50	0.60
23:W:88:THR:HG22	23:W:89:ASP:N	2.17	0.60
30:0:1172:G:H5''	37:0:6809:HOH:O	2.01	0.60
30:0:1377:C:H5'	30:0:1377:C:C6	2.37	0.60
30:0:1559:A:H1'	37:0:5413:HOH:O	2.02	0.60
22:V:39:ALA:C	22:V:41:GLU:H	2.09	0.59
30:0:1205:U:C2'	30:0:1206:U:H5''	2.32	0.59
30:0:1350:U:H4'	37:0:4662:HOH:O	2.02	0.59
30:0:2670:G:O2'	30:0:2671:U:H5'	2.02	0.59
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.29	0.59
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.02	0.59
22:V:8:ILE:HA	22:V:11:MET:HE3	1.84	0.59
25:Y:133:HIS:HD2	37:Y:8579:HOH:O	1.85	0.59
30:0:2578:G:H5'	30:0:2578:G:H8	1.67	0.59
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.32	0.59
30:0:1175:G:H1'	30:0:1193:A:H2'	1.84	0.59
30:0:2488:A:H2	37:0:6826:HOH:O	1.84	0.59
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.35	0.59
6:F:58:GLU:HA	6:F:61:MET:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:49:G:O2'	31:9:50:G:H5'	2.01	0.59
23:W:4:LEU:O	23:W:32:CYS:HA	2.03	0.59
23:W:88:THR:HG22	23:W:89:ASP:H	1.67	0.59
30:0:2756:U:N3	30:0:2896:A:H2	1.98	0.59
31:9:23:U:O2'	31:9:24:U:H4'	2.02	0.59
23:W:84:VAL:HG12	37:W:6679:HOH:O	2.02	0.59
30:0:567:U:H5''	37:0:5949:HOH:O	2.01	0.59
3:C:27:ARG:NH2	30:0:657:G:OP1	2.31	0.59
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.68	0.59
23:W:139:GLY:O	23:W:141:HIS:HD2	1.85	0.59
30:0:2420:G:O2'	30:0:2421:G:H5'	2.02	0.59
30:0:204:A:C2'	30:0:205:U:H5'	2.32	0.59
30:0:1159:G:H1	30:0:1208:C:H42	1.50	0.59
30:0:2649:A:H5'	30:0:2649:A:C8	2.38	0.59
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.84	0.58
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.85	0.58
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.85	0.58
23:W:122:ARG:HH11	23:W:122:ARG:HG2	1.68	0.58
30:0:1120:U:C6	30:0:1120:U:H5''	2.37	0.58
18:R:17:MET:SD	37:R:8542:HOH:O	2.57	0.58
30:0:1182:C:H1'	30:0:1192:A:H8	1.68	0.58
30:0:1667:A:H2'	30:0:1668:U:C6	2.38	0.58
30:0:2316:G:H4'	37:0:5638:HOH:O	2.03	0.58
31:9:64:C:C2'	31:9:65:A:H5'	2.33	0.58
8:H:48:VAL:HA	8:H:170:ARG:O	2.03	0.58
18:R:29:LYS:HE2	30:0:524:A:H5'	1.85	0.58
31:9:75:G:H1	31:9:106:U:H3	1.51	0.58
3:C:236:THR:CG2	3:C:239:ALA:H	2.11	0.58
20:T:52:ARG:HD2	30:0:317:A:H5''	1.84	0.58
30:0:1730:G:C5'	30:0:1731:C:H6	2.16	0.58
30:0:2604:A:H5'	37:0:5339:HOH:O	2.04	0.58
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.84	0.58
3:C:76:ARG:HD3	37:C:8366:HOH:O	2.04	0.58
5:E:100:ASP:HB2	37:E:2789:HOH:O	2.03	0.58
23:W:64:THR:O	23:W:68:THR:HG22	2.04	0.58
23:W:80:ASP:O	23:W:84:VAL:HG23	2.02	0.58
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.01	0.58
9:I:87:PRO:C	9:I:89:GLU:H	2.10	0.58
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.87	0.58
30:0:2320:U:H4'	30:0:2321:A:O4'	2.03	0.58
30:0:2718:C:H5'	30:0:2718:C:H6	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:80:SER:HB2	37:N:8535:HOH:O	2.02	0.58
19:S:51:GLN:NE2	19:S:53:ASN:HD21	2.02	0.58
12:L:148:GLU:HA	37:L:8561:HOH:O	2.04	0.58
14:N:43:VAL:HG13	14:N:118:ILE:HD11	1.84	0.58
30:0:1118:A:H8	30:0:1119:G:H5''	1.67	0.58
31:9:92:G:H2'	31:9:93:A:C8	2.39	0.58
10:J:107:ASN:ND2	10:J:109:TYR:H	2.01	0.57
29:3:60:LYS:HG3	37:0:7104:HOH:O	2.04	0.57
30:0:2064:U:H4'	30:0:2653:A:OP1	2.04	0.57
31:9:20:G:O2'	31:9:21:G:H5'	2.04	0.57
3:C:78:ARG:HG3	3:C:78:ARG:HH11	1.67	0.57
30:0:2878:U:H2'	30:0:2879:A:O4'	2.04	0.57
31:9:35:C:H5''	37:9:8455:HOH:O	2.04	0.57
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.86	0.57
4:D:25:MET:HE1	4:D:37:ALA:HB1	1.85	0.57
18:R:29:LYS:HE2	30:0:524:A:H5''	1.87	0.57
3:C:76:ARG:HG2	3:C:78:ARG:HH12	1.68	0.57
4:D:103:ASN:ND2	4:D:134:LEU:H	2.02	0.57
19:S:57:THR:HG22	19:S:59:ASP:N	2.18	0.57
30:0:1119:G:N2	30:0:1246:A:H2	1.95	0.57
31:9:28:U:H2'	31:9:29:C:C6	2.39	0.57
23:W:38:THR:HG22	37:W:3580:HOH:O	2.03	0.57
30:0:1819:G:H5'	37:0:4250:HOH:O	2.05	0.57
30:0:1972:U:H2'	30:0:1973:A:H5''	1.85	0.57
30:0:432:G:O2'	30:0:433:C:H5'	2.05	0.57
30:0:1679:C:H5'	37:0:8846:HOH:O	2.04	0.57
30:0:1701:A:H5''	30:0:1702:U:H3'	1.86	0.57
30:0:1834:C:H2'	30:0:1840:A:N6	2.18	0.57
12:L:6:ARG:HD3	30:0:1299:G:O6	2.04	0.57
30:0:1289:C:O2'	30:0:1290:G:H5'	2.05	0.57
30:0:2064:U:H5'	30:0:2652:U:H4'	1.85	0.57
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.87	0.57
23:W:125:HIS:CD2	23:W:127:GLY:H	2.23	0.57
30:0:558:C:C2'	30:0:559:U:C5'	2.82	0.57
30:0:1730:G:C5'	30:0:1731:C:C5	2.87	0.57
1:A:121:ALA:O	1:A:124:VAL:HG22	2.04	0.56
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.35	0.56
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.03	0.56
13:M:182:LYS:HE2	30:0:392:U:O2'	2.05	0.56
25:Y:144:ARG:NH1	37:Y:8573:HOH:O	2.37	0.56
30:0:558:C:H2'	30:0:559:U:H5''	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:681:G:N3	30:0:681:G:H5'	2.20	0.56
27:1:42:SER:HB2	37:1:8409:HOH:O	2.05	0.56
30:0:282:C:O2'	30:0:283:U:C5'	2.51	0.56
30:0:1181:A:C2'	30:0:1182:C:H5'	2.36	0.56
30:0:2467:A:H1'	37:0:4272:HOH:O	2.04	0.56
1:A:192:VAL:HG13	37:A:8553:HOH:O	2.05	0.56
10:J:103:VAL:HG12	37:J:5907:HOH:O	2.04	0.56
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.53	0.56
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.05	0.56
19:S:43:GLU:HB3	37:S:7106:HOH:O	2.05	0.56
21:U:14:GLU:O	21:U:17:THR:HB	2.05	0.56
25:Y:204:ARG:HH22	30:0:553:G:P	2.28	0.56
30:0:703:G:O2'	30:0:704:C:H5'	2.06	0.56
30:0:1878:G:O2'	30:0:1879:U:H6	1.89	0.56
30:0:2435:U:H1'	37:0:4978:HOH:O	2.06	0.56
3:C:1:MET:HG2	3:C:2:GLN:N	2.20	0.56
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.86	0.56
30:0:2488:A:H61	30:0:2534:C:H42	1.53	0.56
30:0:2851:G:C2'	30:0:2852:A:H5'	2.35	0.56
16:P:143:ALA:HA	37:P:184:HOH:O	2.03	0.56
30:0:2300:A:H4'	30:0:2301:A:O5'	2.06	0.56
1:A:153:ARG:HB2	1:A:153:ARG:HH11	1.71	0.56
6:F:38:LYS:HE3	30:0:244:C:OP2	2.06	0.56
10:J:107:ASN:HD22	10:J:109:TYR:H	1.53	0.56
30:0:282:C:H1'	30:0:368:C:H42	1.70	0.56
30:0:1118:A:H62	30:0:1244:U:H3	1.54	0.56
2:B:139:ASP:HB2	2:B:165:ARG:HE	1.70	0.56
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.36	0.56
22:V:39:ALA:N	22:V:40:PRO:HD2	2.21	0.56
30:0:1278:A:H4'	30:0:1279:U:C4	2.41	0.56
30:0:899:C:H5'	37:0:9733:HOH:O	2.05	0.56
30:0:1477:C:H5'	30:0:1868:G:C5'	2.35	0.56
1:A:223:ARG:HG3	37:A:8595:HOH:O	2.05	0.56
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.71	0.56
11:K:55:VAL:HG12	11:K:56:SER:N	2.21	0.56
13:M:95:LYS:HE2	30:0:157:G:H4'	1.88	0.56
14:N:37:ARG:NE	37:N:8533:HOH:O	2.39	0.56
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.04	0.56
30:0:2251:G:H2'	30:0:2252:A:C8	2.41	0.56
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.70	0.56
4:D:50:VAL:HG22	31:9:41:C:O4'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2502:C:H2'	30:0:2503:A:H5'	1.87	0.56
20:T:53:GLY:HA3	37:T:6384:HOH:O	2.05	0.55
30:0:396:U:H1'	37:0:7180:HOH:O	2.06	0.55
30:0:1120:U:H5'	30:0:1121:G:OP2	2.05	0.55
30:0:1250:C:O2'	30:0:1251:C:H5'	2.05	0.55
30:0:2825:C:H4'	30:0:2826:G:O5'	2.06	0.55
31:9:91:C:H2'	31:9:92:G:O4'	2.05	0.55
1:A:96:LEU:HD22	1:A:128:LEU:HD13	1.87	0.55
5:E:68:HIS:O	5:E:72:MET:HG3	2.06	0.55
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.86	0.55
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.35	0.55
37:N:8545:HOH:O	31:9:49:G:H5''	2.05	0.55
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.07	0.55
21:U:37:GLU:HB3	37:U:408:HOH:O	2.06	0.55
30:0:2361:A:H5''	37:0:8523:HOH:O	2.07	0.55
4:D:25:MET:CE	4:D:37:ALA:HB1	2.36	0.55
5:E:84:MET:HE2	5:E:133:VAL:CG2	2.35	0.55
14:N:110:THR:HB	14:N:113:SER:OG	2.06	0.55
14:N:141:ARG:HH21	31:9:48:C:H4'	1.71	0.55
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.36	0.55
23:W:115:THR:HG23	37:W:5420:HOH:O	2.06	0.55
30:0:88:G:H5'	30:0:88:G:H8	1.72	0.55
30:0:1783:A:O2'	30:0:1784:U:H5'	2.06	0.55
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.87	0.55
13:M:188:ARG:HD3	30:0:155:C:OP2	2.06	0.55
18:R:25:PHE:CE2	18:R:29:LYS:HE3	2.41	0.55
30:0:204:A:H2'	30:0:205:U:H5'	1.88	0.55
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.42	0.55
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.07	0.55
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.87	0.55
23:W:122:ARG:HG3	23:W:152:ALA:O	2.06	0.55
30:0:1636:G:O2'	30:0:1637:A:H5'	2.07	0.55
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.41	0.55
2:B:17:LYS:O	2:B:260:HIS:HD2	1.90	0.55
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.36	0.55
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.89	0.55
27:1:16:HIS:HE1	30:0:775:G:OP1	1.90	0.55
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.88	0.55
30:0:1595:G:O2'	30:0:1596:U:H5'	2.07	0.55
13:M:84:LYS:HE2	37:M:8571:HOH:O	2.06	0.54
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:41:LYS:HD3	37:9:8439:HOH:O	2.08	0.54
30:0:661:G:C5	30:0:686:A:C2	2.95	0.54
30:0:1135:G:H5'	37:0:5475:HOH:O	2.05	0.54
30:0:1165:G:O2'	30:0:1174:A:H1'	2.07	0.54
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.72	0.54
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.43	0.54
30:0:1972:U:H2'	30:0:1973:A:C5'	2.37	0.54
30:0:2467:A:O2'	30:0:2468:A:H2'	2.06	0.54
30:0:485:A:N3	30:0:487:G:H5''	2.22	0.54
30:0:1181:A:H2'	30:0:1182:C:H5'	1.89	0.54
30:0:2419:U:H5''	30:0:2420:G:H5'	1.89	0.54
2:B:125:GLU:O	2:B:129:ARG:HG3	2.07	0.54
3:C:79:ARG:O	3:C:87:ARG:HG2	2.08	0.54
9:I:100:VAL:HG11	9:I:124:VAL:HG22	1.89	0.54
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.28	0.54
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.88	0.54
30:0:1158:G:O2'	30:0:1159:G:H5'	2.08	0.54
30:0:2712:G:H5'	37:0:4763:HOH:O	2.07	0.54
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.89	0.54
2:B:254:GLN:HG3	37:0:9223:HOH:O	2.08	0.54
9:I:69:PRO:HA	30:0:1164:U:OP1	2.08	0.54
30:0:343:C:O2'	30:0:344:C:H5'	2.06	0.54
30:0:1299:G:H5'	37:0:3611:HOH:O	2.06	0.54
30:0:1926:G:H2'	30:0:1927:A:C8	2.43	0.54
30:0:2524:G:H21	30:0:2526:C:N4	2.05	0.54
31:9:76:G:C3'	31:9:77:A:H5''	2.28	0.54
3:C:115:LEU:O	3:C:118:THR:HB	2.08	0.54
4:D:159:PRO:O	4:D:163:VAL:HG23	2.07	0.54
25:Y:187:VAL:HG22	25:Y:192:ASP:HB2	1.89	0.54
30:0:200:C:H2'	37:0:9976:HOH:O	2.08	0.54
30:0:1615:A:H5'	37:0:3722:HOH:O	2.06	0.54
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.88	0.54
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.23	0.54
30:0:644:G:N3	30:0:644:G:H5'	2.22	0.54
30:0:1279:U:H2'	30:0:1279:U:O2	2.06	0.54
24:X:43:VAL:HG12	24:X:44:ASP:N	2.23	0.54
30:0:1268:C:O2'	30:0:1269:G:H5'	2.07	0.54
30:0:1973:A:H5'	30:0:1973:A:C8	2.35	0.54
30:0:2638:G:H5'	37:0:4469:HOH:O	2.08	0.54
2:B:51:VAL:CG2	2:B:327:VAL:HG13	2.38	0.54
4:D:54:ALA:CB	4:D:69:ILE:HD12	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:80:ASP:HB2	12:L:90:ARG:O	2.08	0.54
17:Q:95:GLU:HA	30:0:949:U:H4'	1.89	0.54
30:0:280:C:H2'	30:0:281:U:O4'	2.08	0.54
30:0:1972:U:C2'	30:0:1973:A:H5''	2.37	0.54
2:B:336:GLN:O	30:0:2862:G:H4'	2.07	0.53
24:X:25:ARG:HD2	37:X:3861:HOH:O	2.07	0.53
3:C:184:ARG:HD2	30:0:1306:U:OP1	2.08	0.53
14:N:4:PRO:HD2	37:0:6319:HOH:O	2.08	0.53
14:N:160:SER:HB3	31:9:51:A:H5'	1.89	0.53
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.89	0.53
9:I:113:SER:HB2	9:I:118:ASN:HB2	1.89	0.53
13:M:169:ARG:HD2	37:M:8587:HOH:O	2.08	0.53
1:A:36:ASP:O	1:A:38:ILE:N	2.34	0.53
20:T:1:SER:HB2	30:0:447:A:OP2	2.08	0.53
30:0:95:A:H5''	30:0:97:G:O4'	2.08	0.53
30:0:1730:G:H5''	30:0:1731:C:C6	2.41	0.53
30:0:2001:G:O2'	30:0:2002:C:H5'	2.08	0.53
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.44	0.53
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.89	0.53
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.90	0.53
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.73	0.53
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.48	0.53
30:0:814:G:H4'	37:0:9664:HOH:O	2.08	0.53
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.90	0.53
5:E:11:VAL:HG12	5:E:12:ASP:N	2.23	0.53
21:U:39:ASN:ND2	21:U:44:ARG:HH11	2.06	0.53
30:0:172:U:H5'	37:0:3697:HOH:O	2.09	0.53
30:0:1116:U:O2'	30:0:1118:A:C2	2.40	0.53
1:A:97:ALA:HB2	1:A:150:PRO:HB2	1.91	0.53
2:B:51:VAL:HG23	2:B:329:TYR:O	2.09	0.53
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.43	0.53
6:F:101:ALA:HA	37:F:5413:HOH:O	2.09	0.53
13:M:81:ARG:HG3	13:M:85:ARG:HB2	1.91	0.53
31:9:24:U:H3'	31:9:25:G:H5'	1.90	0.53
13:M:58:GLN:NE2	30:0:259:G:H21	2.08	0.52
16:P:73:HIS:HE1	30:0:1789:G:O6	1.91	0.52
30:0:2563:U:H2'	30:0:2565:C:O5'	2.08	0.52
31:9:107:C:H5	37:9:8435:HOH:O	1.91	0.52
1:A:194:MET:HE3	1:A:199:HIS:HB2	1.91	0.52
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.20	0.52
14:N:163:PHE:HZ	14:N:171:HIS:HD1	1.55	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.74	0.52
29:3:17:HIS:O	29:3:18:GLN:HG3	2.10	0.52
30:0:1189:A:H1'	30:0:1209:C:O4'	2.09	0.52
30:0:1525:G:H5'	30:0:1526:A:OP2	2.09	0.52
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.91	0.52
7:G:64:ASN:N	7:G:64:ASN:HD22	2.06	0.52
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.09	0.52
16:P:83:LYS:HG2	30:0:793:A:H5''	1.92	0.52
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.92	0.52
30:0:2866:U:H4'	30:0:2867:G:H5'	1.90	0.52
1:A:81:GLN:HB2	1:A:92:ASN:ND2	2.23	0.52
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.09	0.52
16:P:41:ARG:HH22	30:0:1500:U:P	2.32	0.52
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.90	0.52
30:0:2256:G:H2'	30:0:2257:G:C5'	2.39	0.52
4:D:135:VAL:HG22	4:D:136:ARG:N	2.24	0.52
30:0:794:U:H3	30:0:819:A:H61	1.57	0.52
30:0:2241:C:O2'	30:0:2242:U:H5'	2.09	0.52
1:A:123:GLY:HA3	1:A:162:GLY:HA2	1.92	0.52
3:C:246:ARG:NH1	37:C:8369:HOH:O	2.42	0.52
13:M:163:LEU:HD21	30:0:188:C:H5''	1.91	0.52
17:Q:25:PRO:HB2	37:Q:4350:HOH:O	2.10	0.52
23:W:151:GLU:O	23:W:154:ARG:HB2	2.09	0.52
30:0:1211:G:O2'	30:0:1212:C:H5'	2.10	0.52
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.91	0.52
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.75	0.52
5:E:69:ILE:HA	5:E:72:MET:CE	2.40	0.52
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.92	0.52
23:W:130:HIS:O	23:W:136:GLY:HA3	2.10	0.52
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.10	0.52
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.10	0.52
30:0:319:A:H4'	30:0:338:C:C4	2.45	0.52
14:N:11:ARG:NH1	31:9:8:G:O6	2.42	0.52
20:T:1:SER:HB2	30:0:447:A:P	2.50	0.52
30:0:65:C:O2'	30:0:66:G:H5'	2.09	0.52
30:0:820:G:O2'	30:0:856:G:H4'	2.10	0.52
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.74	0.51
1:A:179:MET:HG2	1:A:186:TRP:CB	2.40	0.51
9:I:108:HIS:N	9:I:109:PRO:HD2	2.25	0.51
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.91	0.51
30:0:291:C:H2'	30:0:292:G:O4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1118:A:C8	30:0:1119:G:H5''	2.45	0.51
30:0:1120:U:H5''	30:0:1120:U:H6	1.75	0.51
30:0:2329:C:O2'	30:0:2330:U:H5'	2.10	0.51
2:B:305:ASP:O	2:B:306:LYS:HB2	2.11	0.51
8:H:66:GLU:HA	37:H:8381:HOH:O	2.09	0.51
15:O:25:VAL:HG12	30:0:709:G:O2'	2.10	0.51
17:Q:11:ARG:HD3	37:Q:5620:HOH:O	2.09	0.51
19:S:51:GLN:HE21	19:S:53:ASN:ND2	2.08	0.51
24:X:71:ARG:HD3	37:X:2171:HOH:O	2.10	0.51
25:Y:187:VAL:HB	25:Y:203:VAL:HG22	1.91	0.51
30:0:256:C:H2'	30:0:257:G:O4'	2.11	0.51
30:0:1406:A:H4'	30:0:1407:A:H5''	1.92	0.51
30:0:2507:G:H2'	30:0:2510:C:N4	2.23	0.51
3:C:236:THR:HA	37:C:8449:HOH:O	2.10	0.51
9:I:124:VAL:HG12	9:I:124:VAL:O	2.11	0.51
14:N:154:LEU:C	14:N:156:GLU:H	2.19	0.51
28:2:31:ARG:NH2	37:2:7177:HOH:O	2.43	0.51
30:0:951:A:H2'	30:0:952:G:H5'	1.92	0.51
30:0:1165:G:O2'	30:0:1174:A:C1'	2.59	0.51
30:0:1942:A:H3'	37:0:6896:HOH:O	2.11	0.51
30:0:1996:U:O2'	30:0:1997:A:H5'	2.11	0.51
30:0:2769:C:H2'	30:0:2770:G:O4'	2.11	0.51
8:H:12:ILE:HG23	8:H:129:ARG:CZ	2.41	0.51
14:N:48:VAL:HG11	14:N:55:ASP:HB3	1.93	0.51
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.11	0.51
30:0:920:C:H5'	30:0:921:G:C4	2.45	0.51
30:0:2795:C:O2'	30:0:2796:U:H5'	2.09	0.51
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.91	0.51
19:S:10:VAL:HG11	22:V:36:ALA:HA	1.92	0.51
30:0:969:G:H1	30:0:999:C:H42	1.59	0.51
30:0:1527:A:H1'	30:0:1528:A:C8	2.45	0.51
30:0:2072:G:C6	30:0:2533:C:H1'	2.46	0.51
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.41	0.51
29:3:48:ASN:ND2	29:3:50:GLY:H	2.09	0.51
30:0:90:A:H2'	30:0:91:G:O4'	2.11	0.51
30:0:1342:C:O2'	30:0:1343:C:H5'	2.10	0.51
30:0:2830:U:H3'	37:0:4770:HOH:O	2.09	0.51
4:D:84:LEU:HA	4:D:87:ALA:HB3	1.93	0.51
4:D:104:PHE:CE2	4:D:132:VAL:HB	2.46	0.51
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.93	0.51
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:30:ARG:HD2	37:0:8538:HOH:O	2.11	0.51
22:V:55:ARG:O	22:V:59:ILE:HG12	2.11	0.51
24:X:15:ARG:NH1	30:0:2896:A:OP1	2.44	0.51
30:0:848:C:H5'	37:0:6823:HOH:O	2.10	0.51
30:0:2301:A:H5''	30:0:2302:A:H5'	1.91	0.51
30:0:2591:C:H2'	30:0:2592:G:O4'	2.11	0.51
31:9:49:G:H2'	31:9:50:G:O4'	2.11	0.51
1:A:53:ALA:HB3	37:A:8599:HOH:O	2.10	0.51
23:W:65:VAL:HA	23:W:68:THR:HG22	1.92	0.51
11:K:30:LYS:O	11:K:55:VAL:HG13	2.11	0.51
21:U:33:SER:O	21:U:37:GLU:HG3	2.10	0.51
30:0:1180:U:H2'	30:0:1181:A:C8	2.46	0.51
30:0:2478:U:O2'	30:0:2479:A:H5'	2.10	0.51
3:C:214:THR:HG23	37:C:8435:HOH:O	2.10	0.50
5:E:84:MET:HE1	5:E:148:ILE:HD12	1.92	0.50
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.46	0.50
30:0:960:G:N3	30:0:960:G:C2'	2.74	0.50
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.50
30:0:1503:U:H2'	30:0:1504:A:O4'	2.12	0.50
30:0:2445:U:H2'	30:0:2446:G:C8	2.46	0.50
30:0:2756:U:C2	30:0:2896:A:H2	2.28	0.50
31:9:56:A:C3'	31:9:57:A:H5''	2.40	0.50
2:B:264:GLU:HG2	2:B:267:LYS:CE	2.41	0.50
28:2:35:ARG:HB2	37:2:2691:HOH:O	2.11	0.50
30:0:2265:U:H2'	30:0:2266:A:C8	2.47	0.50
2:B:212:GLN:HA	30:0:1733:A:H4'	1.92	0.50
2:B:288:GLY:HA2	30:0:2898:G:H4'	1.93	0.50
7:G:16:LYS:O	7:G:20:VAL:HG23	2.12	0.50
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.10	0.50
8:H:41:LYS:HE2	8:H:45:ASP:HB3	1.93	0.50
27:1:28:HIS:HE1	30:0:776:A:OP1	1.94	0.50
30:0:1741:U:O2'	30:0:2723:G:H4'	2.11	0.50
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.94	0.50
30:0:2415:A:C2'	30:0:2416:G:H5'	2.41	0.50
30:0:2472:C:O2'	30:0:2634:G:H4'	2.12	0.50
2:B:214:PRO:HD2	37:B:8521:HOH:O	2.12	0.50
4:D:76:ARG:NE	31:9:44:A:O4'	2.45	0.50
5:E:15:GLN:HG2	5:E:19:ASP:O	2.12	0.50
5:E:84:MET:HE1	5:E:148:ILE:CD1	2.41	0.50
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.41	0.50
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:122:ARG:NH2	37:0:4835:HOH:O	2.45	0.50
24:X:76:ARG:HG3	24:X:76:ARG:HH11	1.74	0.50
30:0:447:A:O2'	30:0:448:G:H5'	2.12	0.50
30:0:1603:A:C5'	30:0:1605:G:O4'	2.60	0.50
30:0:1921:A:C6	30:0:1922:A:C2	3.00	0.50
30:0:2842:G:H2'	30:0:2843:A:H5'	1.93	0.50
3:C:174:ILE:HD11	30:0:338:C:H4'	1.94	0.50
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.46	0.50
20:T:24:ARG:HH21	20:T:39:ASN:ND2	2.09	0.50
14:N:164:ASP:CG	14:N:167:ASP:HA	2.37	0.50
20:T:38:ARG:NH1	37:T:6217:HOH:O	2.44	0.50
25:Y:187:VAL:HG23	37:Y:8567:HOH:O	2.11	0.50
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.43	0.50
29:3:62:THR:HB	37:3:8549:HOH:O	2.10	0.50
30:0:861:A:C8	37:0:5228:HOH:O	2.55	0.50
30:0:1342:C:C2'	30:0:1343:C:H5'	2.42	0.50
30:0:1419:U:H5'	30:0:1420:C:OP2	2.11	0.50
2:B:254:GLN:HG2	2:B:255:GLY:N	2.25	0.50
22:V:44:GLY:HA3	30:0:92:G:H4'	1.94	0.50
30:0:308:U:C4	30:0:342:C:H1'	2.46	0.50
30:0:702:G:O2'	30:0:703:G:H5'	2.12	0.50
30:0:2505:G:C2'	30:0:2506:A:H5'	2.41	0.50
6:F:59:ILE:HD13	30:0:263:U:O4'	2.11	0.50
8:H:14:LYS:HE2	37:0:3382:HOH:O	2.11	0.50
8:H:49:GLN:HG3	8:H:140:TYR:CE2	2.47	0.50
11:K:62:PRO:HG3	11:K:65:ARG:NH2	2.26	0.50
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.12	0.50
29:3:3:MET:O	29:3:90:PHE:HA	2.12	0.50
1:A:3:ARG:HD3	30:0:870:G:OP2	2.11	0.49
10:J:52:GLN:NE2	30:0:1119:G:H8	2.06	0.49
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.93	0.49
2:B:102:THR:HG21	2:B:182:VAL:O	2.11	0.49
3:C:98:ARG:NH1	37:C:8355:HOH:O	2.44	0.49
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.94	0.49
14:N:179:LEU:HA	14:N:184:ILE:HD12	1.93	0.49
37:R:8545:HOH:O	30:0:1370:G:H5''	2.12	0.49
23:W:13:MET:CE	23:W:17:ILE:HG22	2.42	0.49
30:0:2256:G:H2'	30:0:2257:G:H5'	1.95	0.49
1:A:128:LEU:HG	37:A:8568:HOH:O	2.11	0.49
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.95	0.49
7:G:20:VAL:O	7:G:24:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:164:THR:HG22	13:M:167:GLY:N	2.14	0.49
30:0:185:G:H4'	30:0:186:A:H4'	1.94	0.49
30:0:542:A:H2'	30:0:543:G:O4'	2.13	0.49
30:0:2061:C:C2'	30:0:2062:A:H5'	2.42	0.49
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.47	0.49
15:O:24:ALA:HB3	30:0:710:G:OP1	2.11	0.49
20:T:49:GLU:HB3	20:T:59:GLU:HG2	1.95	0.49
23:W:11:VAL:HG11	30:0:1086:A:C6	2.46	0.49
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.94	0.49
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.76	0.49
27:1:16:HIS:CD2	30:0:470:U:O2'	2.65	0.49
30:0:602:A:O2'	30:0:605:C:H4'	2.11	0.49
30:0:941:G:O2'	30:0:942:U:H5'	2.12	0.49
30:0:1127:C:C5	30:0:1128:U:C4	3.00	0.49
1:A:33:GLU:CD	1:A:33:GLU:H	2.20	0.49
3:C:43:LYS:HG2	30:0:449:A:N7	2.27	0.49
4:D:154:LYS:H	4:D:154:LYS:CD	2.18	0.49
22:V:16:ARG:NH1	22:V:65:ASP:O	2.46	0.49
30:0:858:U:C6	37:0:4975:HOH:O	2.66	0.49
30:0:1137:G:H1'	37:0:3414:HOH:O	2.12	0.49
30:0:1206:U:H2'	30:0:1207:A:O4'	2.13	0.49
30:0:1189:A:O2'	30:0:1208:C:H2'	2.11	0.49
30:0:1787:C:H4'	30:0:2883:A:O4'	2.12	0.49
30:0:1819:G:H2'	30:0:1820:G:C4'	2.43	0.49
30:0:2010:A:H2'	37:0:5505:HOH:O	2.11	0.49
1:A:211:LYS:O	30:0:1943:C:H4'	2.13	0.49
4:D:23:VAL:HG22	4:D:73:VAL:HB	1.95	0.49
26:Z:37:ARG:NH1	37:Z:8419:HOH:O	2.45	0.49
30:0:407:A:H5'	37:0:5572:HOH:O	2.13	0.49
4:D:65:GLU:HG3	37:D:6752:HOH:O	2.12	0.49
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.42	0.49
30:0:1205:U:H2'	30:0:1206:U:H5'	1.95	0.49
28:2:5:LYS:HD2	30:0:1675:C:H5''	1.95	0.49
30:0:441:A:H1'	30:0:442:A:N7	2.28	0.49
30:0:1641:A:C2'	30:0:1642:A:H5'	2.43	0.49
30:0:2289:G:N2	30:0:2291:A:C2	2.71	0.49
31:9:20:G:H3'	37:9:8434:HOH:O	2.13	0.49
1:A:194:MET:SD	30:0:875:A:C2	3.06	0.49
2:B:79:MET:HE3	2:B:144:THR:HG21	1.93	0.49
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.95	0.49
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.03	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ARG:NH1	3:C:78:ARG:HG3	2.27	0.49
8:H:49:GLN:NE2	8:H:140:TYR:HE2	2.11	0.49
10:J:88:PRO:O	10:J:94:GLY:HA3	2.13	0.49
22:V:1:THR:CB	30:0:93:C:H5''	2.43	0.49
30:0:482:G:H4'	30:0:508:A:N1	2.28	0.49
30:0:1167:G:H2'	30:0:1168:C:O4'	2.13	0.49
30:0:2089:A:O2'	30:0:2090:G:H5'	2.13	0.49
30:0:2896:A:H2'	30:0:2896:A:N3	2.28	0.49
24:X:80:GLU:HB3	37:X:5564:HOH:O	2.12	0.48
30:0:559:U:H2'	30:0:560:U:O4'	2.13	0.48
30:0:871:G:H4'	37:0:3951:HOH:O	2.12	0.48
30:0:1314:U:H5''	30:0:1316:G:O4'	2.13	0.48
1:A:211:LYS:NZ	37:A:8613:HOH:O	2.46	0.48
30:0:1291:A:H2	37:0:4838:HOH:O	1.96	0.48
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.96	0.48
10:J:107:ASN:HD22	10:J:107:ASN:C	2.20	0.48
30:0:737:A:H2'	30:0:738:G:O4'	2.13	0.48
30:0:1730:G:H5'	30:0:1731:C:C6	2.43	0.48
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.29	0.48
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.79	0.48
7:G:12:ILE:N	7:G:13:PRO:HD3	2.28	0.48
12:L:18:HIS:CD2	30:0:902:G:N7	2.79	0.48
30:0:1014:A:H2'	30:0:1015:C:H5'	1.95	0.48
30:0:1506:U:H6	30:0:1506:U:H5'	1.79	0.48
2:B:264:GLU:HG2	2:B:267:LYS:HE2	1.95	0.48
2:B:297:VAL:HB	37:B:8606:HOH:O	2.12	0.48
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.78	0.48
13:M:107:ARG:NH1	37:M:8573:HOH:O	2.46	0.48
16:P:81:LYS:HG2	37:0:9060:HOH:O	2.14	0.48
30:0:1339:G:C6	30:0:1340:G:N1	2.80	0.48
30:0:1667:A:H2'	30:0:1668:U:H6	1.77	0.48
30:0:2911:C:H2'	30:0:2912:C:C6	2.49	0.48
1:A:125:ASN:HB3	1:A:158:VAL:HG12	1.95	0.48
14:N:58:LEU:HD12	14:N:58:LEU:N	2.29	0.48
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.43	0.48
22:V:39:ALA:N	22:V:40:PRO:CD	2.77	0.48
30:0:1044:C:H3'	30:0:1045:G:H5''	1.95	0.48
30:0:1377:C:H6	30:0:1377:C:C5'	2.25	0.48
30:0:1588:G:C6	30:0:1589:G:N1	2.82	0.48
30:0:2314:G:C2'	30:0:2315:C:H5'	2.43	0.48
2:B:82:VAL:HG12	2:B:82:VAL:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:ARG:NH1	37:B:8634:HOH:O	2.46	0.48
3:C:233:THR:HG22	3:C:234:VAL:N	2.26	0.48
4:D:166:ILE:HD12	37:D:6326:HOH:O	2.13	0.48
13:M:99:ARG:HH21	13:M:170:ASN:ND2	2.11	0.48
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.96	0.48
30:0:871:G:H8	30:0:871:G:H5'	1.74	0.48
30:0:1159:G:H21	30:0:1189:A:H8	1.62	0.48
30:0:1772:C:H5'	30:0:1773:G:C5	2.49	0.48
30:0:2421:G:H4'	37:0:4318:HOH:O	2.13	0.48
31:9:2:U:OP2	31:9:2:U:H4'	2.14	0.48
1:A:29:HIS:HB2	1:A:153:ARG:HH12	1.79	0.48
2:B:268:ARG:NH2	2:B:325:PRO:HG3	2.28	0.48
3:C:12:THR:HB	37:C:8439:HOH:O	2.13	0.48
4:D:137:PRO:O	31:9:30:C:OP1	2.32	0.48
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.28	0.48
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.95	0.48
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.95	0.48
23:W:108:ARG:HE	23:W:114:PRO:HG3	1.78	0.48
24:X:25:ARG:HG2	37:X:5356:HOH:O	2.13	0.48
30:0:255:A:H2'	30:0:256:C:C6	2.49	0.48
30:0:1409:G:H5'	37:0:3263:HOH:O	2.14	0.48
30:0:2754:G:C2'	30:0:2755:G:H5'	2.44	0.48
31:9:55:U:H4'	31:9:56:A:C8	2.48	0.48
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.14	0.48
14:N:11:ARG:HD3	31:9:114:G:O6	2.13	0.48
18:R:29:LYS:HD3	37:0:4262:HOH:O	2.14	0.48
30:0:236:A:C4'	30:0:237:G:H5'	2.38	0.48
30:0:1202:A:C2'	30:0:1203:G:H5'	2.44	0.48
30:0:1419:U:H2'	30:0:1685:A:C2	2.49	0.48
30:0:2134:G:C6	30:0:2258:A:C8	3.01	0.48
30:0:2909:G:H2'	30:0:2910:A:H8	1.78	0.48
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.48
13:M:125:ARG:HD3	37:0:4520:HOH:O	2.13	0.48
23:W:38:THR:HG22	23:W:39:ASP:N	2.29	0.48
23:W:154:ARG:NH1	30:0:588:G:O6	2.46	0.48
26:Z:35:SER:CB	26:Z:47:ARG:HB2	2.44	0.48
30:0:1484:G:H2'	37:0:8620:HOH:O	2.14	0.48
1:A:212:PRO:HB2	37:A:8556:HOH:O	2.14	0.47
3:C:87:ARG:NH2	30:0:894:A:C2	2.82	0.47
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.96	0.47
30:0:10:U:O4	30:0:532:A:OP2	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2668:G:H2'	30:0:2669:U:C6	2.49	0.47
30:0:2768:A:H5''	37:0:3966:HOH:O	2.13	0.47
5:E:111:LYS:HE3	30:0:2690:U:O2'	2.14	0.47
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.26	0.47
14:N:132:ASN:O	14:N:135:VAL:HG12	2.13	0.47
16:P:115:SER:OG	16:P:118:GLN:HG3	2.15	0.47
30:0:764:C:H2'	30:0:765:G:O4'	2.14	0.47
30:0:1202:A:H2'	30:0:1203:G:H5'	1.96	0.47
30:0:1735:C:O2'	30:0:1736:A:H5'	2.12	0.47
30:0:1883:U:O2'	30:0:1884:G:H5'	2.13	0.47
30:0:2487:C:H5	37:0:4427:HOH:O	1.97	0.47
9:I:84:SER:HB3	9:I:92:VAL:CG2	2.44	0.47
10:J:45:VAL:HG23	10:J:130:VAL:O	2.14	0.47
10:J:131:THR:HG22	10:J:134:GLU:H	1.79	0.47
11:K:125:ALA:C	11:K:127:ALA:H	2.23	0.47
12:L:50:GLY:C	30:0:2453:G:H4'	2.39	0.47
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.14	0.47
23:W:4:LEU:HD22	23:W:52:VAL:CG2	2.40	0.47
23:W:38:THR:O	23:W:42:ARG:HB2	2.14	0.47
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.97	0.47
30:0:285:A:H2'	30:0:286:U:O4'	2.14	0.47
30:0:920:C:H5''	30:0:921:G:O5'	2.14	0.47
30:0:1474:C:H6	30:0:1474:C:C5'	2.15	0.47
30:0:1878:G:O2'	30:0:1879:U:P	2.73	0.47
1:A:164:ARG:NE	37:A:8580:HOH:O	2.47	0.47
23:W:38:THR:HG22	23:W:39:ASP:H	1.79	0.47
30:0:407:A:H8	37:0:4000:HOH:O	1.96	0.47
30:0:816:G:C6	30:0:817:G:N1	2.82	0.47
30:0:1450:C:H4'	30:0:1493:A:C5	2.49	0.47
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.97	0.47
21:U:17:THR:HG22	21:U:18:GLY:N	2.29	0.47
29:3:70:ARG:HD3	37:3:8571:HOH:O	2.14	0.47
30:0:426:G:H2'	30:0:427:C:O4'	2.14	0.47
30:0:834:G:H4'	30:0:835:U:OP2	2.15	0.47
30:0:2724:U:H2'	30:0:2725:G:O4'	2.14	0.47
1:A:211:LYS:HD3	37:A:8604:HOH:O	2.14	0.47
11:K:87:ARG:NH1	37:K:4066:HOH:O	2.47	0.47
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.96	0.47
22:V:12:THR:HG23	22:V:14:ALA:H	1.80	0.47
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.94	0.47
30:0:603:A:H4'	30:0:604:G:O5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1006:A:N1	30:0:2311:A:H1'	2.29	0.47
30:0:1132:A:N6	30:0:1229:C:H2'	2.30	0.47
3:C:214:THR:HB	37:0:9200:HOH:O	2.13	0.47
4:D:94:ALA:HB3	4:D:97:GLN:HG3	1.96	0.47
13:M:61:ILE:HA	37:M:8617:HOH:O	2.15	0.47
13:M:107:ARG:HG3	13:M:107:ARG:HH11	1.80	0.47
25:Y:122:ARG:NH2	37:Y:8535:HOH:O	2.48	0.47
25:Y:144:ARG:NE	37:Y:8610:HOH:O	2.47	0.47
30:0:162:C:H2'	30:0:163:U:H5'	1.96	0.47
30:0:506:G:N2	30:0:509:A:H5''	2.22	0.47
30:0:1056:U:H2'	30:0:1057:A:O4'	2.15	0.47
30:0:1681:G:H5''	30:0:1682:A:H5'	1.96	0.47
30:0:2900:G:H2'	30:0:2901:C:O4'	2.15	0.47
5:E:35:TYR:HA	10:J:127:ILE:HD12	1.96	0.47
5:E:132:THR:HB	37:E:2227:HOH:O	2.14	0.47
14:N:1:ALA:HB2	31:9:14:G:O2'	2.15	0.47
20:T:71:VAL:HG11	20:T:90:PRO:CB	2.36	0.47
30:0:1187:U:HO2'	30:0:1188:A:H8	1.62	0.47
30:0:2291:A:N9	30:0:2309:C:H5'	2.29	0.47
30:0:2831:C:C2'	30:0:2832:C:H5'	2.45	0.47
10:J:75:PRO:HD3	10:J:136:SER:OG	2.15	0.47
30:0:1181:A:H2'	30:0:1182:C:C5'	2.45	0.47
30:0:2019:A:H5'	37:0:4079:HOH:O	2.15	0.47
30:0:2506:A:O2'	30:0:2507:G:O5'	2.33	0.47
11:K:66:ARG:HD2	30:0:1992:U:OP2	2.15	0.47
30:0:417:G:P	37:0:6968:HOH:O	2.71	0.47
30:0:1562:C:H2'	30:0:1562:C:O2	2.14	0.47
30:0:1657:A:H2'	30:0:1658:A:C8	2.50	0.47
31:9:24:U:H3'	31:9:25:G:C5'	2.45	0.47
4:D:172:VAL:HG12	4:D:173:GLU:N	2.30	0.46
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.30	0.46
30:0:1205:U:C2'	30:0:1206:U:C5'	2.93	0.46
30:0:1213:C:O2'	30:0:1214:G:H5'	2.15	0.46
30:0:1353:C:P	37:0:4219:HOH:O	2.73	0.46
30:0:2361:A:H2'	30:0:2362:A:C8	2.50	0.46
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.76	0.46
1:A:179:MET:HA	1:A:179:MET:CE	2.42	0.46
2:B:27:ASN:HB2	37:0:3602:HOH:O	2.16	0.46
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.97	0.46
20:T:54:ASP:OD2	30:0:316:A:H5'	2.16	0.46
20:T:92:ASP:OD1	20:T:94:SER:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:189:ASN:ND2	25:Y:192:ASP:H	2.14	0.46
26:Z:41:ARG:NH1	30:0:821:U:H4'	2.31	0.46
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.46
30:0:2256:G:C2'	30:0:2257:G:H5'	2.44	0.46
30:0:2419:U:H5''	30:0:2420:G:C5'	2.45	0.46
31:9:31:C:H2'	31:9:32:G:O4'	2.16	0.46
12:L:73:VAL:HG21	12:L:116:HIS:CD2	2.50	0.46
14:N:147:ILE:HB	37:N:8545:HOH:O	2.14	0.46
21:U:14:GLU:OE1	21:U:15:PRO:HD2	2.16	0.46
30:0:1441:G:H1'	37:0:7314:HOH:O	2.15	0.46
4:D:27:ILE:HD11	4:D:37:ALA:HB3	1.98	0.46
7:G:19:GLU:O	7:G:23:ILE:HG13	2.15	0.46
15:O:87:THR:O	15:O:91:GLN:HG3	2.16	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.98	0.46
30:0:445:U:H1'	37:0:6885:HOH:O	2.14	0.46
30:0:1200:A:H4'	37:0:6890:HOH:O	2.14	0.46
30:0:2112:A:H2'	30:0:2113:G:C8	2.51	0.46
30:0:2456:A:H5'	37:0:5242:HOH:O	2.15	0.46
12:L:61:ALA:HA	37:L:8553:HOH:O	2.15	0.46
16:P:41:ARG:NH2	30:0:1500:U:OP2	2.48	0.46
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.30	0.46
30:0:69:A:H8	30:0:69:A:C5'	2.20	0.46
30:0:136:C:H2'	30:0:137:U:O4'	2.15	0.46
30:0:1044:C:H5	37:0:6150:HOH:O	1.96	0.46
30:0:1174:A:C5	30:0:1201:C:H4'	2.50	0.46
30:0:1625:U:H5''	37:0:5568:HOH:O	2.15	0.46
31:9:31:C:C2	31:9:50:G:N2	2.84	0.46
7:G:23:ILE:O	7:G:27:ILE:HG13	2.15	0.46
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.40	0.46
30:0:284:C:H4'	30:0:285:A:H8	1.80	0.46
30:0:538:C:H5''	30:0:539:G:C8	2.50	0.46
30:0:2010:A:C2'	37:0:5505:HOH:O	2.62	0.46
30:0:2256:G:O2'	30:0:2257:G:H5'	2.16	0.46
31:9:55:U:H4'	31:9:56:A:H8	1.78	0.46
3:C:118:THR:O	3:C:136:VAL:HG13	2.16	0.46
24:X:30:MET:HG2	30:0:1384:C:H5'	1.98	0.46
30:0:821:U:H5''	37:0:9582:HOH:O	2.15	0.46
30:0:1181:A:N1	30:0:1192:A:O2'	2.48	0.46
30:0:1252:A:H2'	30:0:1253:C:O4'	2.15	0.46
30:0:1947:G:H2'	30:0:1948:G:H8	1.81	0.46
5:E:143:GLN:HE22	30:0:2779:G:H21	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.15	0.46
20:T:69:LYS:O	20:T:71:VAL:HG23	2.16	0.46
22:V:38:GLY:C	22:V:40:PRO:HD2	2.41	0.46
25:Y:220:GLU:HG3	37:Y:8546:HOH:O	2.15	0.46
30:0:876:A:H2'	30:0:876:A:N3	2.31	0.46
30:0:1393:A:H2'	30:0:1394:C:C6	2.51	0.46
1:A:88:ILE:O	1:A:88:ILE:HG22	2.16	0.46
3:C:104:ASP:HA	3:C:107:ARG:NH1	2.31	0.46
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.96	0.46
4:D:96:SER:C	4:D:98:PHE:H	2.23	0.46
5:E:36:PRO:HD3	10:J:127:ILE:HD12	1.97	0.46
8:H:102:LYS:HD3	8:H:122:LYS:HD3	1.97	0.46
11:K:81:ARG:HD3	11:K:87:ARG:NH1	2.31	0.46
23:W:3:ALA:O	23:W:54:PHE:HA	2.16	0.46
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.96	0.46
30:0:304:G:H1'	30:0:347:A:N6	2.31	0.46
30:0:1165:G:H4'	30:0:1174:A:HO2'	1.81	0.46
30:0:1592:G:O2'	30:0:1593:C:O5'	2.34	0.46
30:0:2570:G:H5''	37:0:4452:HOH:O	2.15	0.46
31:9:36:C:C5	31:9:37:C:C5	3.04	0.46
30:0:1249:U:H2'	30:0:1250:C:C6	2.51	0.46
30:0:2672:C:O2'	30:0:2673:U:H5'	2.16	0.46
30:0:2831:C:H2'	30:0:2832:C:H5'	1.97	0.46
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.46	0.45
6:F:58:GLU:HG3	6:F:61:MET:HE2	1.97	0.45
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.46	0.45
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.15	0.45
30:0:574:G:O2'	30:0:575:A:H5'	2.16	0.45
30:0:1314:U:H2'	37:0:5422:HOH:O	2.15	0.45
30:0:2726:U:O2	30:0:2749:U:O5'	2.34	0.45
2:B:98:THR:HG22	30:0:2820:A:OP1	2.16	0.45
19:S:45:TYR:HD2	37:S:4527:HOH:O	1.99	0.45
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.82	0.45
30:0:69:A:C8	30:0:69:A:C5'	2.92	0.45
30:0:119:A:H2'	30:0:120:A:H5''	1.96	0.45
30:0:138:U:OP2	30:0:139:C:H5	1.98	0.45
30:0:2716:G:O2'	30:0:2717:C:H5'	2.17	0.45
31:9:52:A:H2'	31:9:53:G:O4'	2.16	0.45
3:C:168:ARG:NH2	3:C:190:ALA:O	2.49	0.45
37:C:8357:HOH:O	15:O:3:THR:HG21	2.15	0.45
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1119:G:C6	30:0:1244:U:C5	3.04	0.45
30:0:1559:A:C1'	37:0:5413:HOH:O	2.62	0.45
30:0:2061:C:H2'	30:0:2062:A:H5'	1.98	0.45
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.81	0.45
5:E:31:ARG:NH1	37:E:5919:HOH:O	2.49	0.45
9:I:87:PRO:C	9:I:89:GLU:N	2.75	0.45
19:S:38:ALA:O	19:S:42:GLU:HG3	2.15	0.45
30:0:130:C:H5'	37:0:4755:HOH:O	2.16	0.45
30:0:1183:C:H42	30:0:1184:C:H41	1.62	0.45
5:E:7:ILE:HG22	5:E:45:ASP:O	2.16	0.45
8:H:69:ARG:HD3	37:H:8381:HOH:O	2.16	0.45
14:N:108:SER:HA	14:N:109:PRO:HD3	1.76	0.45
15:O:35:LYS:HD3	37:0:4157:HOH:O	2.17	0.45
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.46	0.45
20:T:2:LYS:HG2	30:0:447:A:OP1	2.17	0.45
28:2:41:HIS:HE1	30:0:1439:C:OP1	1.99	0.45
30:0:844:A:C6	30:0:882:A:C5	3.04	0.45
13:M:171:ARG:NH2	30:0:189:A:OP1	2.49	0.45
14:N:127:LEU:HD13	37:N:8556:HOH:O	2.16	0.45
16:P:115:SER:H	16:P:118:GLN:NE2	2.00	0.45
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.99	0.45
26:Z:84:CYS:O	26:Z:85:ASP:HB2	2.15	0.45
30:0:1505:U:H1'	37:0:7139:HOH:O	2.16	0.45
30:0:1925:G:O2'	30:0:1926:G:H5'	2.17	0.45
30:0:2289:G:N2	30:0:2291:A:H2	2.13	0.45
30:0:2326:C:H4'	30:0:2412:G:H4'	1.99	0.45
1:A:194:MET:HE3	1:A:199:HIS:CB	2.47	0.45
3:C:104:ASP:HA	3:C:107:ARG:HH12	1.80	0.45
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.99	0.45
30:0:816:G:H5'	30:0:1598:A:H4'	1.98	0.45
30:0:1188:A:N7	30:0:1189:A:C2	2.85	0.45
30:0:1545:C:H2'	30:0:1546:G:O4'	2.17	0.45
30:0:2526:C:H5'	30:0:2526:C:C6	2.51	0.45
1:A:100:PRO:HG2	1:A:103:VAL:CG2	2.44	0.45
2:B:72:THR:HB	37:B:8606:HOH:O	2.16	0.45
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.45	0.45
9:I:133:THR:HG22	9:I:134:ILE:N	2.32	0.45
15:O:96:VAL:HG13	15:O:100:GLN:HB2	1.98	0.45
16:P:13:VAL:HG21	16:P:41:ARG:HG2	1.99	0.45
18:R:80:TYR:O	30:0:2050:G:H5''	2.17	0.45
30:0:1060:C:H6	30:0:1060:C:H5'	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1200:A:H3'	37:0:5302:HOH:O	2.16	0.45
30:0:1596:U:H2'	30:0:1598:A:OP2	2.16	0.45
30:0:2667:G:H1'	30:0:2914:A:N3	2.31	0.45
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.17	0.45
4:D:52:THR:HG21	30:0:2346:C:O2'	2.16	0.45
6:F:60:VAL:O	6:F:60:VAL:HG12	2.17	0.45
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.47	0.45
15:O:39:THR:O	15:O:115:ARG:NH2	2.49	0.45
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.99	0.45
30:0:484:A:N1	30:0:506:G:H4'	2.32	0.45
30:0:541:C:C2'	30:0:542:A:C5'	2.82	0.45
30:0:1183:C:H2'	37:0:5790:HOH:O	2.17	0.45
30:0:2361:A:H5'	30:0:2361:A:H8	1.82	0.45
30:0:2509:A:OP2	30:0:2510:C:H5	2.00	0.45
30:0:2515:C:H2'	30:0:2516:G:O4'	2.16	0.45
30:0:2781:U:C2'	30:0:2782:G:H5'	2.46	0.45
2:B:14:GLY:HA2	2:B:15:PRO:C	2.42	0.45
12:L:14:GLY:O	30:0:1295:G:H5''	2.17	0.45
23:W:13:MET:HE2	23:W:18:GLN:HA	1.98	0.45
30:0:1209:C:H2'	30:0:1210:G:C8	2.48	0.45
30:0:2883:A:H2'	30:0:2884:G:O4'	2.17	0.45
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.16	0.44
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.81	0.44
6:F:16:ALA:HA	6:F:111:ILE:HD13	1.99	0.44
8:H:23:ILE:HG23	8:H:123:ILE:HD11	1.99	0.44
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.82	0.44
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.98	0.44
27:1:10:LYS:HG3	37:1:8431:HOH:O	2.17	0.44
30:0:999:C:O2'	30:0:1000:C:H5'	2.18	0.44
30:0:1979:G:O2'	30:0:1980:U:OP1	2.29	0.44
3:C:16:VAL:HG12	3:C:17:ASP:H	1.81	0.44
37:I:5128:HOH:O	30:0:1168:C:C5'	2.64	0.44
11:K:75:ARG:HD3	11:K:112:PRO:O	2.16	0.44
13:M:164:THR:HB	37:M:8519:HOH:O	2.17	0.44
13:M:167:GLY:O	13:M:171:ARG:HG3	2.17	0.44
15:O:37:ARG:HD2	30:0:656:G:OP2	2.17	0.44
28:2:42:TRP:HB3	30:0:1418:U:OP1	2.18	0.44
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.99	0.44
30:0:292:G:H2'	30:0:358:G:N2	2.33	0.44
30:0:316:A:N3	30:0:336:G:O2'	2.43	0.44
30:0:1044:C:H5''	37:0:8543:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1058:A:H2'	30:0:1060:C:C5'	2.44	0.44
30:0:1942:A:O2'	30:0:1943:C:H5'	2.18	0.44
30:0:2553:A:H2'	30:0:2553:A:N3	2.31	0.44
30:0:2781:U:H2'	30:0:2782:G:H5'	2.00	0.44
3:C:25:PRO:HG2	37:C:8322:HOH:O	2.17	0.44
8:H:59:GLN:HE21	8:H:129:ARG:NE	2.00	0.44
18:R:128:ARG:HH22	30:0:2054:A:H2	1.61	0.44
27:1:25:LYS:HD2	28:2:48:ASP:HA	1.98	0.44
30:0:212:A:O4'	30:0:214:U:C6	2.71	0.44
30:0:958:G:H2'	30:0:959:C:C6	2.52	0.44
30:0:1477:C:H5'	30:0:1868:G:H5''	1.98	0.44
30:0:2090:G:H2'	30:0:2091:G:C8	2.51	0.44
30:0:2103:A:N7	30:0:2538:A:N6	2.65	0.44
30:0:2135:A:O2'	30:0:2136:G:H5'	2.16	0.44
30:0:2642:G:H2'	30:0:2643:G:O4'	2.17	0.44
30:0:2712:G:P	37:0:4763:HOH:O	2.75	0.44
30:0:2791:U:H1'	30:0:2792:A:H5''	1.99	0.44
31:9:57:A:N6	37:9:8441:HOH:O	2.47	0.44
2:B:75:GLU:C	2:B:77:PRO:HD3	2.42	0.44
2:B:243:ASN:HA	2:B:244:PRO:C	2.41	0.44
3:C:236:THR:HG22	3:C:239:ALA:CB	2.47	0.44
4:D:88:LEU:HB2	4:D:89:PRO:HD3	1.98	0.44
5:E:3:VAL:CG2	5:E:49:ILE:HB	2.48	0.44
10:J:90:LYS:HB2	34:J:8502:CL:CL	2.54	0.44
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.81	0.44
12:L:21:ARG:N	37:L:8524:HOH:O	2.50	0.44
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.48	0.44
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.17	0.44
18:R:111:ILE:HG23	18:R:145:LEU:CD1	2.48	0.44
25:Y:144:ARG:NH2	37:Y:8610:HOH:O	2.49	0.44
30:0:2812:A:N7	37:0:7067:HOH:O	2.36	0.44
31:9:2:U:C4'	37:9:8480:HOH:O	2.66	0.44
31:9:39:U:HO2'	31:9:42:C:H5	1.56	0.44
2:B:244:PRO:HB3	30:0:1234:U:N3	2.32	0.44
3:C:2:GLN:HB3	37:C:8333:HOH:O	2.17	0.44
3:C:2:GLN:HB3	37:C:8384:HOH:O	2.18	0.44
4:D:50:VAL:O	4:D:71:ALA:HA	2.18	0.44
4:D:56:ARG:N	37:D:6752:HOH:O	2.50	0.44
8:H:62:HIS:HA	8:H:65:LEU:HD23	1.99	0.44
12:L:133:VAL:HB	37:L:8547:HOH:O	2.17	0.44
18:R:106:GLY:HA2	18:R:109:MET:CE	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:281:U:H3'	37:0:6755:HOH:O	2.17	0.44
30:0:2115:U:H2'	30:0:2116:U:C6	2.53	0.44
2:B:57:GLU:HA	2:B:58:PRO:HD2	1.89	0.44
3:C:153:VAL:O	3:C:157:LEU:HG	2.18	0.44
5:E:116:THR:HG22	5:E:151:LEU:HD22	2.00	0.44
13:M:193:LYS:HB3	30:0:392:U:C5'	2.48	0.44
22:V:7:GLU:O	22:V:11:MET:HG3	2.18	0.44
29:3:28:GLY:HA3	30:0:2434:A:O3'	2.17	0.44
30:0:559:U:H5'	30:0:559:U:C6	2.42	0.44
30:0:834:G:H3'	30:0:835:U:H4'	1.99	0.44
30:0:1014:A:H5''	31:9:101:G:O2'	2.18	0.44
30:0:1940:C:H4'	37:0:6896:HOH:O	2.16	0.44
30:0:1948:G:H2'	30:0:1949:G:O4'	2.18	0.44
30:0:2004:U:H2'	30:0:2005:G:OP1	2.16	0.44
2:B:71:VAL:HG11	2:B:296:LEU:HD22	1.99	0.44
4:D:167:GLU:C	4:D:169:THR:H	2.25	0.44
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.50	0.44
11:K:45:PRO:HB2	37:0:6920:HOH:O	2.17	0.44
21:U:13:ILE:HG12	21:U:32:CYS:HB3	1.99	0.44
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.52	0.44
30:0:737:A:H2	37:0:6249:HOH:O	1.98	0.44
30:0:1423:C:O2'	30:0:1424:A:H5'	2.18	0.44
30:0:2353:A:H4'	30:0:2354:A:O5'	2.17	0.44
3:C:184:ARG:NH2	30:0:450:C:OP1	2.35	0.44
3:C:235:PHE:HE2	3:C:243:VAL:HG21	1.82	0.44
3:C:237:GLU:HB2	37:C:8428:HOH:O	2.16	0.44
5:E:31:ARG:NH1	5:E:68:HIS:CG	2.86	0.44
8:H:172:GLU:HB3	37:H:8392:HOH:O	2.18	0.44
12:L:143:THR:HG22	12:L:144:ASP:H	1.78	0.44
14:N:160:SER:CB	31:9:51:A:H5'	2.48	0.44
30:0:113:A:OP2	30:0:114:A:H2'	2.17	0.44
30:0:660:A:H4'	30:0:661:G:O5'	2.18	0.44
30:0:1299:G:N2	37:0:4223:HOH:O	2.49	0.44
5:E:84:MET:HE2	5:E:133:VAL:HG23	2.00	0.44
29:3:14:CYS:SG	37:3:8559:HOH:O	2.62	0.44
30:0:2403:C:H2'	30:0:2404:G:O5'	2.17	0.44
31:9:34:A:H2'	31:9:35:C:O4'	2.18	0.44
1:A:171:LYS:HB2	30:0:820:G:C5	2.53	0.43
8:H:41:LYS:HE2	8:H:45:ASP:CB	2.47	0.43
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.53	0.43
14:N:169:PRO:O	14:N:172:PHE:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:12:THR:HG22	22:V:15:GLU:CG	2.46	0.43
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.99	0.43
30:0:240:C:O2	30:0:240:C:H2'	2.18	0.43
30:0:2031:C:H2'	30:0:2032:U:O4'	2.17	0.43
30:0:2326:C:H4'	30:0:2412:G:C4'	2.48	0.43
30:0:2401:A:H5'	37:0:9014:HOH:O	2.18	0.43
31:9:49:G:C2'	31:9:50:G:H5'	2.48	0.43
3:C:107:ARG:NH1	37:C:8429:HOH:O	2.51	0.43
5:E:20:ILE:CD1	5:E:40:VAL:HG11	2.44	0.43
12:L:27:ARG:HD2	30:0:757:C:OP1	2.18	0.43
19:S:56:ASN:O	28:2:8:LYS:NZ	2.46	0.43
22:V:44:GLY:O	22:V:48:GLU:HG2	2.18	0.43
23:W:125:HIS:HE1	37:W:3071:HOH:O	2.01	0.43
24:X:74:ALA:HB2	24:X:85:VAL:HG13	2.00	0.43
28:2:20:ARG:HG2	28:2:21:VAL:N	2.33	0.43
30:0:653:U:H2'	30:0:654:A:C8	2.53	0.43
30:0:1592:G:O2'	30:0:1593:C:O4'	2.34	0.43
30:0:2820:A:H2'	30:0:2821:C:O4'	2.18	0.43
2:B:14:GLY:HA3	37:B:8609:HOH:O	2.17	0.43
13:M:64:ARG:HD2	37:M:8581:HOH:O	2.17	0.43
14:N:116:PHE:HB3	14:N:136:LEU:HD23	2.00	0.43
30:0:333:G:O2'	30:0:334:G:H5'	2.19	0.43
30:0:510:U:H6	37:0:6987:HOH:O	2.01	0.43
30:0:1825:U:O2'	30:0:1826:C:H5'	2.18	0.43
30:0:2073:G:OP2	30:0:2490:A:H5'	2.19	0.43
30:0:2508:C:H2'	37:0:6301:HOH:O	2.17	0.43
30:0:2697:A:H2'	30:0:2698:G:O4'	2.18	0.43
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.33	0.43
3:C:140:VAL:HG12	3:C:141:SER:N	2.33	0.43
3:C:242:GLU:HG3	37:C:8381:HOH:O	2.19	0.43
7:G:12:ILE:HA	37:0:5006:HOH:O	2.17	0.43
15:O:38:ARG:NH1	37:O:7674:HOH:O	2.50	0.43
21:U:9:CYS:CA	21:U:52:THR:HG23	2.47	0.43
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.82	0.43
28:2:48:ASP:O	28:2:49:GLU:HB2	2.18	0.43
30:0:1367:A:H2'	30:0:1368:U:O4'	2.18	0.43
30:0:1684:A:O2'	30:0:1685:A:H5''	2.18	0.43
30:0:2754:G:O2'	30:0:2755:G:H5'	2.17	0.43
30:0:2768:A:H3'	37:0:3966:HOH:O	2.17	0.43
31:9:65:A:N6	31:9:112:U:C6	2.86	0.43
31:9:80:A:C2	31:9:103:A:C4	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLU:O	1:A:34:ASP:HB2	2.18	0.43
5:E:93:MET:HE1	5:E:165:GLY:N	2.33	0.43
10:J:74:ARG:O	10:J:78:ILE:HG12	2.18	0.43
13:M:39:ARG:NH2	37:M:8617:HOH:O	2.51	0.43
18:R:111:ILE:HG23	18:R:145:LEU:HD11	2.01	0.43
20:T:41:ARG:NH1	20:T:42:VAL:O	2.51	0.43
30:0:941:G:C5	30:0:942:U:C4	3.06	0.43
30:0:2464:C:H5'	30:0:2465:A:OP1	2.18	0.43
1:A:153:ARG:HD3	37:A:8528:HOH:O	2.18	0.43
1:A:206:ARG:NH2	30:0:2630:G:O6	2.48	0.43
2:B:314:ALA:HB3	2:B:317:PRO:HG3	2.00	0.43
5:E:137:ASP:O	5:E:141:VAL:HG23	2.19	0.43
13:M:9:ARG:HD2	30:0:380:A:OP2	2.18	0.43
14:N:11:ARG:NH2	37:N:8519:HOH:O	2.51	0.43
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.48	0.43
23:W:119:HIS:HD2	23:W:120:PRO:O	2.01	0.43
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.32	0.43
25:Y:117:LEU:HA	25:Y:174:VAL:HG11	2.01	0.43
26:Z:37:ARG:HD3	30:0:818:A:O2'	2.19	0.43
30:0:380:A:H4'	30:0:381:G:OP1	2.19	0.43
30:0:876:A:N3	30:0:876:A:C2'	2.82	0.43
30:0:1406:A:H4'	30:0:1407:A:C5'	2.49	0.43
30:0:2072:G:H3'	30:0:2073:G:C5'	2.49	0.43
30:0:2269:C:C2'	30:0:2270:G:H5'	2.49	0.43
5:E:31:ARG:HH12	5:E:68:HIS:CG	2.36	0.43
6:F:59:ILE:CD1	30:0:263:U:C2	3.01	0.43
9:I:84:SER:HB2	9:I:90:ASP:HB2	1.99	0.43
11:K:28:GLU:HB3	11:K:59:LYS:HB2	2.00	0.43
19:S:57:THR:CG2	19:S:58:MET:N	2.82	0.43
23:W:108:ARG:HE	23:W:114:PRO:CG	2.32	0.43
23:W:126:ASP:HB3	23:W:135:GLY:O	2.18	0.43
24:X:25:ARG:HD3	24:X:64:ALA:O	2.18	0.43
30:0:249:G:O2'	30:0:250:C:H5'	2.18	0.43
30:0:1535:G:H2'	30:0:1536:C:C6	2.54	0.43
1:A:105:VAL:HG12	1:A:106:CYS:N	2.33	0.43
6:F:36:THR:HG23	6:F:97:ALA:HB2	2.00	0.43
18:R:132:ARG:HG2	18:R:133:ALA:N	2.34	0.43
22:V:1:THR:HG23	22:V:2:VAL:N	2.28	0.43
25:Y:189:ASN:C	25:Y:189:ASN:HD22	2.26	0.43
30:0:567:U:C5'	37:0:5949:HOH:O	2.65	0.43
30:0:1556:G:O2'	30:0:1557:G:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1701:A:H1'	37:0:5924:HOH:O	2.18	0.43
30:0:2456:A:H2'	30:0:2457:U:C6	2.53	0.43
5:E:11:VAL:HG13	5:E:23:GLU:O	2.19	0.43
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.91	0.43
30:0:303:C:H2'	30:0:304:G:O4'	2.19	0.43
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.43
30:0:1163:G:H2'	30:0:1164:U:C5	2.54	0.43
30:0:2842:G:C2'	30:0:2843:A:H5'	2.48	0.43
30:0:2868:C:H2'	30:0:2869:G:O4'	2.19	0.43
1:A:171:LYS:HB2	30:0:820:G:C6	2.54	0.43
1:A:186:TRP:CG	1:A:187:PRO:HA	2.54	0.43
2:B:36:PRO:HA	2:B:168:GLY:CA	2.46	0.43
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.48	0.43
6:F:50:VAL:CG2	6:F:63:ILE:HG21	2.49	0.43
8:H:149:VAL:HG22	37:H:8378:HOH:O	2.18	0.43
17:Q:45:PRO:O	30:0:2365:G:H4'	2.18	0.43
27:1:28:HIS:HD2	27:1:30:LYS:H	1.65	0.43
30:0:407:A:H2'	30:0:408:A:C8	2.54	0.43
30:0:1883:U:C2'	30:0:1884:G:H5'	2.49	0.43
1:A:55:VAL:HG22	1:A:68:ILE:O	2.19	0.42
2:B:49:THR:HG21	2:B:331:SER:O	2.19	0.42
9:I:129:SER:O	9:I:130:LEU:HD23	2.19	0.42
12:L:143:THR:CG2	12:L:144:ASP:N	2.80	0.42
14:N:62:HIS:HB3	14:N:65:ASP:OD1	2.19	0.42
37:Q:5998:HOH:O	30:0:2296:C:H5	2.01	0.42
28:2:28:LYS:O	30:0:87:C:H2'	2.19	0.42
28:2:40:ARG:HG3	28:2:45:ASN:CB	2.49	0.42
30:0:283:U:C5	30:0:284:C:N3	2.87	0.42
30:0:559:U:H6	30:0:559:U:C5'	2.28	0.42
30:0:818:A:H5''	37:0:6135:HOH:O	2.18	0.42
1:A:11:ARG:HD3	37:0:8736:HOH:O	2.19	0.42
37:I:3512:HOH:O	30:0:1163:G:N2	2.52	0.42
12:L:72:ASN:HB2	37:L:8570:HOH:O	2.17	0.42
13:M:81:ARG:HD2	30:0:160:A:O3'	2.19	0.42
23:W:119:HIS:HE1	37:0:9078:HOH:O	2.02	0.42
24:X:74:ALA:CB	24:X:85:VAL:HG22	2.49	0.42
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.53	0.42
29:3:3:MET:HG3	29:3:4:PRO:HD2	2.01	0.42
30:0:128:A:O2'	30:0:129:A:H5'	2.19	0.42
30:0:946:C:H2'	30:0:947:U:C6	2.54	0.42
30:0:1165:G:H1'	30:0:1174:A:H1'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1202:A:H2'	30:0:1203:G:C5'	2.50	0.42
30:0:1427:A:H61	30:0:1440:U:H1'	1.84	0.42
30:0:1562:C:H42	30:0:2738:G:H1	1.67	0.42
4:D:173:GLU:HG3	4:D:174:VAL:HG23	2.02	0.42
6:F:49:PHE:HE1	6:F:98:VAL:HG23	1.84	0.42
6:F:91:VAL:HG11	30:0:262:A:OP2	2.19	0.42
8:H:34:HIS:HD2	8:H:90:LEU:O	2.01	0.42
9:I:96:SER:H	9:I:99:GLN:CD	2.27	0.42
23:W:13:MET:HE2	23:W:18:GLN:CA	2.49	0.42
23:W:23:MET:O	30:0:1025:C:H5'	2.19	0.42
30:0:907:A:H4'	30:0:1328:A:C2	2.54	0.42
30:0:1641:A:H2'	30:0:1642:A:C5'	2.48	0.42
4:D:76:ARG:NH1	31:9:42:C:O2	2.51	0.42
5:E:21:THR:HG23	5:E:30:THR:OG1	2.19	0.42
14:N:32:PRO:HD2	14:N:99:GLU:O	2.20	0.42
17:Q:33:PHE:HE2	17:Q:93:ARG:HG3	1.83	0.42
30:0:1183:C:N4	30:0:1184:C:N4	2.64	0.42
30:0:1980:U:O2	30:0:2008:U:H4'	2.19	0.42
30:0:2290:U:H2'	37:0:6681:HOH:O	2.18	0.42
30:0:2372:A:H2'	30:0:2373:U:C6	2.55	0.42
30:0:2493:C:O2	30:0:2493:C:H2'	2.17	0.42
30:0:2526:C:O2'	30:0:2527:U:H5'	2.19	0.42
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.20	0.42
5:E:6:GLU:HG2	5:E:46:THR:HG22	2.01	0.42
10:J:130:VAL:HG12	10:J:131:THR:N	2.35	0.42
13:M:47:ASP:CG	13:M:48:LYS:N	2.78	0.42
23:W:11:VAL:HG11	30:0:1086:A:N6	2.34	0.42
23:W:73:LEU:HD12	23:W:73:LEU:HA	1.77	0.42
24:X:18:ARG:NH1	37:X:4132:HOH:O	2.52	0.42
30:0:1462:C:O2'	30:0:1463:U:H5'	2.19	0.42
30:0:1701:A:H4'	30:0:1702:U:O5'	2.18	0.42
4:D:166:ILE:HB	37:D:6326:HOH:O	2.18	0.42
13:M:43:PRO:HG3	13:M:62:VAL:HG21	2.00	0.42
19:S:57:THR:C	19:S:59:ASP:H	2.28	0.42
24:X:43:VAL:HG12	24:X:44:ASP:H	1.84	0.42
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.01	0.42
26:Z:84:CYS:HG	35:Z:8403:CD:CD	1.52	0.42
29:3:18:GLN:HG2	37:3:8514:HOH:O	2.19	0.42
37:3:8515:HOH:O	30:0:2408:A:H2	2.02	0.42
30:0:349:U:O2'	30:0:350:G:H5'	2.20	0.42
30:0:366:U:H2'	30:0:367:G:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:912:A:C4	30:0:1294:A:C2	3.08	0.42
30:0:1433:G:O2'	30:0:1434:A:H5'	2.20	0.42
30:0:2243:C:H5''	37:0:3288:HOH:O	2.19	0.42
30:0:2323:G:H5'	37:0:6566:HOH:O	2.19	0.42
30:0:2421:G:H3'	30:0:2422:U:C5'	2.50	0.42
30:0:2769:C:C2'	30:0:2770:G:C5'	2.86	0.42
31:9:39:U:C2'	31:9:40:C:OP1	2.68	0.42
31:9:116:C:O2'	31:9:117:G:H5'	2.20	0.42
2:B:258:GLY:H	2:B:260:HIS:CE1	2.36	0.42
3:C:133:ARG:NH1	37:C:8406:HOH:O	2.51	0.42
3:C:202:THR:HG22	30:0:328:U:O4'	2.20	0.42
9:I:101:LYS:O	9:I:105:GLU:HG3	2.19	0.42
13:M:5:TYR:HE2	13:M:46:LEU:HD13	1.84	0.42
14:N:23:ARG:NH1	37:N:8546:HOH:O	2.52	0.42
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.49	0.42
25:Y:208:LYS:O	30:0:1313:A:H5'	2.19	0.42
30:0:177:A:H2'	30:0:178:U:O4'	2.19	0.42
30:0:790:A:H2'	30:0:791:A:O4'	2.20	0.42
30:0:1482:A:O2'	30:0:1483:C:H5'	2.20	0.42
30:0:1624:A:H4'	30:0:1625:U:H5'	2.02	0.42
30:0:1878:G:O2'	30:0:1879:U:OP2	2.37	0.42
30:0:2271:G:H2'	30:0:2271:G:N3	2.34	0.42
30:0:2831:C:H2'	30:0:2832:C:C5'	2.49	0.42
30:0:2894:C:O2'	30:0:2895:C:H5'	2.19	0.42
1:A:132:ASP:HB3	1:A:135:VAL:H	1.85	0.42
1:A:199:HIS:HE1	30:0:1881:A:OP1	2.02	0.42
5:E:84:MET:HB2	5:E:131:LEU:HB2	2.01	0.42
8:H:30:LYS:N	8:H:62:HIS:HD2	2.07	0.42
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.76	0.42
10:J:131:THR:HG22	10:J:133:GLY:N	2.35	0.42
16:P:88:GLN:HE22	30:0:1799:G:H21	1.67	0.42
30:0:282:C:O2'	30:0:283:U:C4'	2.68	0.42
30:0:420:U:H2'	30:0:421:C:C6	2.55	0.42
30:0:441:A:O5'	30:0:441:A:H8	2.03	0.42
30:0:1042:U:O2'	30:0:1043:C:H5'	2.20	0.42
30:0:1565:C:O4'	30:0:2738:G:H1'	2.20	0.42
30:0:1589:G:N2	30:0:1605:G:H1'	2.35	0.42
30:0:1771:U:O2'	30:0:1773:G:N7	2.51	0.42
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.87	0.42
12:L:134:GLU:HG3	37:L:8547:HOH:O	2.18	0.42
13:M:60:VAL:C	13:M:61:ILE:HD12	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:84:ALA:O	18:R:88:PHE:HD1	2.02	0.42
30:0:870:G:C3'	30:0:871:G:H5''	2.50	0.42
30:0:883:U:O2	30:0:883:U:C2'	2.68	0.42
30:0:1119:G:N2	30:0:1246:A:N1	2.67	0.42
30:0:1304:U:H2'	30:0:1305:C:C6	2.55	0.42
30:0:1453:G:N2	30:0:1675:C:C2	2.88	0.42
30:0:2467:A:HO2'	30:0:2468:A:H2'	1.84	0.42
30:0:2909:G:O2'	30:0:2910:A:H5'	2.20	0.42
31:9:65:A:O2'	31:9:66:G:P	2.78	0.42
3:C:118:THR:CG2	3:C:137:PRO:HB3	2.50	0.42
37:L:8533:HOH:O	30:0:2453:G:H5''	2.19	0.42
13:M:49:ALA:C	13:M:54:TYR:HB3	2.45	0.42
20:T:26:THR:HA	20:T:39:ASN:HB3	2.01	0.42
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.55	0.42
21:U:50:GLU:HB3	30:0:2866:U:C4	2.55	0.42
30:0:12:U:H2'	30:0:13:G:H5'	2.02	0.42
30:0:151:A:C2	30:0:442:A:C8	3.08	0.42
30:0:290:C:O2'	30:0:291:C:H5'	2.20	0.42
30:0:1218:U:H2'	30:0:1219:U:C6	2.54	0.42
30:0:1634:G:H2'	30:0:1635:U:C6	2.54	0.42
30:0:2070:G:H5''	37:0:3318:HOH:O	2.20	0.42
30:0:2403:C:C2'	30:0:2404:G:O5'	2.68	0.42
30:0:2491:G:H1'	37:0:6418:HOH:O	2.19	0.42
30:0:2559:C:H4'	37:0:6805:HOH:O	2.19	0.42
30:0:2664:A:H8	30:0:2664:A:OP1	2.03	0.42
30:0:2879:A:H2'	30:0:2880:A:O4'	2.20	0.42
1:A:11:ARG:HA	37:0:6768:HOH:O	2.20	0.41
2:B:294:TYR:HE2	37:B:8649:HOH:O	2.02	0.41
3:C:133:ARG:NE	3:C:138:VAL:HG22	2.35	0.41
7:G:67:LEU:O	7:G:71:LEU:HG	2.20	0.41
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.20	0.41
13:M:93:ARG:HD2	30:0:1470:A:OP1	2.20	0.41
27:1:28:HIS:HD2	27:1:31:LYS:H	1.68	0.41
28:2:18:ASN:HD21	28:2:40:ARG:H	1.68	0.41
28:2:36:ASN:HB3	28:2:39:ARG:HG3	2.01	0.41
30:0:383:A:H2'	30:0:384:G:O4'	2.20	0.41
30:0:638:C:H2'	30:0:639:A:C8	2.54	0.41
30:0:1131:G:C6	30:0:1230:A:C4	3.07	0.41
30:0:1613:C:H2'	30:0:1614:G:O4'	2.19	0.41
30:0:1615:A:H4'	37:0:5434:HOH:O	2.20	0.41
30:0:1697:G:O2'	30:0:1698:U:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1947:G:H2'	30:0:1948:G:C8	2.54	0.41
30:0:1993:C:C4	30:0:1994:A:C6	3.08	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.19	0.41
11:K:4:LEU:HD22	11:K:116:GLU:HB3	2.02	0.41
30:0:284:C:N4	37:0:6734:HOH:O	2.52	0.41
30:0:1842:A:C4	30:0:1979:G:C6	3.09	0.41
30:0:1909:A:N1	30:0:2128:G:H1'	2.34	0.41
30:0:1946:C:H2'	30:0:1971:G:C8	2.55	0.41
30:0:1985:U:C2	30:0:1996:U:O4'	2.73	0.41
30:0:2356:A:H2'	30:0:2357:G:O4'	2.19	0.41
30:0:2385:G:H2'	30:0:2386:U:C6	2.56	0.41
30:0:2388:C:O2'	30:0:2389:U:H5'	2.21	0.41
31:9:47:A:C2	31:9:48:C:C2	3.08	0.41
1:A:89:ALA:HB3	37:A:8616:HOH:O	2.19	0.41
1:A:153:ARG:HB2	1:A:153:ARG:NH1	2.35	0.41
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.34	0.41
23:W:21:LEU:HD13	23:W:26:ILE:HD11	2.02	0.41
30:0:283:U:H5	30:0:284:C:N3	2.18	0.41
30:0:321:A:O2'	30:0:322:G:H5'	2.20	0.41
30:0:542:A:C5'	30:0:542:A:C8	2.99	0.41
30:0:629:A:H2'	30:0:630:A:O4'	2.21	0.41
30:0:827:A:H2'	30:0:828:G:O4'	2.20	0.41
30:0:932:U:H2'	30:0:933:C:C6	2.55	0.41
30:0:1103:C:C2	30:0:1241:G:N2	2.88	0.41
30:0:2312:G:H2'	30:0:2313:C:H5'	2.02	0.41
31:9:65:A:C2'	31:9:66:G:OP2	2.67	0.41
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.50	0.41
5:E:108:LEU:HD11	5:E:164:ASP:HB2	2.02	0.41
7:G:65:THR:O	7:G:69:ARG:HB2	2.19	0.41
18:R:98:ASN:ND2	30:0:500:G:H21	2.14	0.41
28:2:18:ASN:ND2	28:2:40:ARG:H	2.17	0.41
30:0:664:U:O4	30:0:681:G:H5''	2.20	0.41
30:0:1257:C:H2'	30:0:1258:G:O4'	2.20	0.41
30:0:1819:G:H2'	30:0:1820:G:C5'	2.51	0.41
30:0:2518:C:H2'	30:0:2519:C:O4'	2.20	0.41
30:0:2809:G:H2'	30:0:2810:G:O4'	2.21	0.41
1:A:36:ASP:O	1:A:36:ASP:CG	2.64	0.41
2:B:41:PHE:HB3	2:B:190:MET:HE1	2.03	0.41
7:G:63:ARG:N	37:G:2569:HOH:O	2.53	0.41
14:N:152:GLU:C	14:N:154:LEU:H	2.29	0.41
20:T:2:LYS:HE2	37:0:6955:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.19	0.41
27:1:2:GLY:O	27:1:6:PRO:HG2	2.20	0.41
30:0:1171:A:H2'	30:0:1172:G:H5'	2.02	0.41
30:0:1926:G:H2'	30:0:1927:A:H8	1.82	0.41
30:0:2003:U:H4'	30:0:2004:U:H5	1.84	0.41
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.20	0.41
1:A:204:GLY:N	30:0:2634:G:OP2	2.41	0.41
2:B:217:ARG:HG3	2:B:257:THR:HG22	2.01	0.41
5:E:154:ILE:HD11	5:E:157:LYS:HE2	2.03	0.41
9:I:94:ASP:OD1	9:I:133:THR:HB	2.21	0.41
9:I:123:VAL:C	9:I:125:GLY:H	2.27	0.41
10:J:52:GLN:NE2	30:0:1119:G:C8	2.87	0.41
11:K:65:ARG:HD3	37:K:5358:HOH:O	2.20	0.41
12:L:34:GLY:C	12:L:36:ASP:H	2.29	0.41
12:L:48:LYS:HE2	30:0:220:C:C2	2.56	0.41
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.16	0.41
25:Y:186:ARG:HG2	25:Y:186:ARG:HH11	1.86	0.41
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.21	0.41
29:3:7:PHE:HE2	29:3:22:VAL:HG21	1.86	0.41
30:0:371:U:H2'	30:0:372:A:H8	1.86	0.41
30:0:666:A:H2'	30:0:667:C:O4'	2.21	0.41
30:0:1185:U:H2'	30:0:1186:C:H6	1.82	0.41
30:0:1413:A:H2'	30:0:1414:A:O4'	2.20	0.41
30:0:2729:C:O2'	30:0:2730:G:H5'	2.20	0.41
30:0:2897:C:H2'	30:0:2898:G:H8	1.85	0.41
31:9:68:G:C6	31:9:69:U:C4	3.08	0.41
31:9:107:C:H2'	31:9:108:C:C6	2.55	0.41
1:A:95:PRO:HA	1:A:153:ARG:HA	2.02	0.41
5:E:47:VAL:HG11	5:E:69:ILE:HD13	2.03	0.41
15:O:25:VAL:HG23	15:O:26:TRP:N	2.36	0.41
30:0:255:A:H2'	30:0:256:C:H6	1.84	0.41
30:0:401:C:H2'	30:0:402:U:C6	2.55	0.41
30:0:558:C:H5'	37:0:4803:HOH:O	2.20	0.41
30:0:625:U:H5''	30:0:1044:C:N4	2.35	0.41
30:0:940:G:C5	30:0:1027:G:C2	3.08	0.41
30:0:1172:G:H1'	37:0:4513:HOH:O	2.20	0.41
30:0:2015:A:H2'	30:0:2016:U:O4'	2.21	0.41
3:C:214:THR:HG21	37:C:8399:HOH:O	2.20	0.41
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.95	0.41
12:L:121:ILE:HG12	12:L:141:GLU:HB2	2.01	0.41
30:0:368:C:H2'	30:0:369:G:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:646:G:H2'	30:0:647:U:C6	2.56	0.41
30:0:1529:G:H5'	37:0:6937:HOH:O	2.20	0.41
30:0:1626:A:H2'	30:0:1627:G:O4'	2.20	0.41
30:0:1815:A:H2'	30:0:1816:C:O4'	2.21	0.41
1:A:36:ASP:C	1:A:38:ILE:H	2.26	0.41
1:A:165:THR:HG22	37:A:8611:HOH:O	2.21	0.41
1:A:205:GLY:HA3	37:0:5905:HOH:O	2.21	0.41
2:B:28:SER:HB2	30:0:2807:U:OP2	2.21	0.41
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.89	0.41
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.03	0.41
6:F:111:ILE:O	6:F:115:VAL:HG23	2.20	0.41
9:I:133:THR:HG22	9:I:134:ILE:H	1.86	0.41
10:J:26:VAL:HG13	10:J:36:VAL:HG11	2.02	0.41
10:J:63:ILE:HD11	30:0:1236:A:C8	2.56	0.41
11:K:22:ASP:HB2	37:K:5264:HOH:O	2.21	0.41
13:M:169:ARG:NH2	37:M:8548:HOH:O	2.51	0.41
14:N:171:HIS:CE1	37:N:8566:HOH:O	2.74	0.41
20:T:38:ARG:HH21	30:0:306:A:P	2.44	0.41
20:T:47:THR:HB	20:T:100:ASP:HB3	2.01	0.41
30:0:38:G:N2	37:0:6885:HOH:O	2.54	0.41
30:0:282:C:C2'	30:0:283:U:H5'	2.51	0.41
30:0:290:C:H1'	37:0:5650:HOH:O	2.20	0.41
30:0:365:G:C6	30:0:366:U:C4	3.09	0.41
30:0:424:C:H2'	30:0:425:U:C6	2.55	0.41
30:0:603:A:H1'	30:0:605:C:C2	2.56	0.41
30:0:1023:C:H2'	30:0:1024:G:O4'	2.20	0.41
30:0:1611:G:O2'	30:0:1612:A:H5'	2.21	0.41
30:0:1883:U:H5'	30:0:2012:U:OP2	2.20	0.41
30:0:2718:C:H5'	30:0:2718:C:C6	2.53	0.41
30:0:2756:U:O2	30:0:2896:A:H2	2.03	0.41
30:0:2906:A:H5'	30:0:2907:C:O4'	2.21	0.41
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	2.03	0.41
6:F:38:LYS:NZ	13:M:3:SER:HA	2.36	0.41
8:H:31:ILE:HA	8:H:66:GLU:OE1	2.20	0.41
14:N:64:SER:C	14:N:66:LEU:H	2.28	0.41
18:R:39:THR:HB	18:R:42:GLU:CD	2.45	0.41
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.55	0.41
30:0:661:G:C6	30:0:686:A:C2	3.08	0.41
30:0:1139:U:H2'	30:0:1140:C:C6	2.56	0.41
30:0:1159:G:H1	30:0:1208:C:N4	2.18	0.41
30:0:1429:U:C2'	30:0:1430:G:H5'	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2362:A:H2'	30:0:2363:G:C8	2.56	0.41
31:9:96:C:H2'	31:9:97:U:C6	2.56	0.41
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.50	0.40
2:B:116:PRO:HG3	30:0:2821:C:H4'	2.03	0.40
10:J:80:LYS:HE2	10:J:98:PHE:CE1	2.56	0.40
15:O:26:TRP:HB2	37:O:3062:HOH:O	2.19	0.40
25:Y:155:ARG:NH1	37:Y:8556:HOH:O	2.53	0.40
30:0:812:A:H2'	30:0:813:C:O4'	2.20	0.40
30:0:999:C:H2'	30:0:1000:C:O4'	2.21	0.40
30:0:1080:C:O5'	30:0:1080:C:H6	2.03	0.40
30:0:2237:G:H1'	37:O:4393:HOH:O	2.20	0.40
30:0:2691:A:H8	30:0:2691:A:OP1	2.04	0.40
30:0:2836:G:O2'	30:0:2838:A:N7	2.48	0.40
31:9:12:C:H5'	31:9:70:U:O4'	2.21	0.40
11:K:62:PRO:HG3	11:K:65:ARG:HH21	1.85	0.40
11:K:115:ARG:NH2	37:K:3160:HOH:O	2.53	0.40
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.77	0.40
30:0:40:C:H6	30:0:40:C:O5'	2.04	0.40
30:0:1076:G:C2	30:0:1084:C:C2	3.09	0.40
30:0:1191:A:H2'	30:0:1193:A:H5'	2.03	0.40
30:0:1976:G:O2'	30:0:1977:U:H5'	2.21	0.40
30:0:2103:A:O2'	30:0:2104:C:H5'	2.21	0.40
30:0:2819:C:H2'	30:0:2820:A:C8	2.56	0.40
1:A:69:LEU:HD21	1:A:120:ARG:HB3	2.03	0.40
2:B:56:ASP:OD1	2:B:322:ARG:HB3	2.21	0.40
2:B:141:ARG:HG2	2:B:165:ARG:HA	2.03	0.40
4:D:58:VAL:HB	4:D:62:ASP:HB3	2.02	0.40
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.92	0.40
8:H:12:ILE:HD12	8:H:57:THR:HG22	2.03	0.40
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.56	0.40
12:L:101:ASP:C	12:L:103:ALA:H	2.30	0.40
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.78	0.40
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.55	0.40
24:X:78:GLU:HG2	24:X:79:GLU:H	1.86	0.40
25:Y:184:GLU:OE1	25:Y:204:ARG:NH1	2.55	0.40
28:2:10:ARG:NH2	30:0:121:U:OP2	2.40	0.40
30:0:64:G:H2'	30:0:65:C:O4'	2.22	0.40
30:0:383:A:C2	30:0:407:A:C4	3.09	0.40
30:0:858:U:H2'	30:0:859:C:C6	2.56	0.40
30:0:1181:A:O2'	30:0:1182:C:H5'	2.20	0.40
30:0:1444:G:O2'	30:0:1502:A:N1	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1632:A:H2'	30:0:1633:C:C5'	2.46	0.40
30:0:1714:C:O2'	30:0:1715:C:H5'	2.21	0.40
31:9:107:C:O2'	31:9:108:C:H5'	2.22	0.40
1:A:153:ARG:HH11	1:A:153:ARG:CB	2.33	0.40
2:B:42:ALA:HB2	2:B:162:MET:HE2	2.04	0.40
2:B:53:LEU:HD11	2:B:327:VAL:HG22	2.03	0.40
6:F:91:VAL:CG1	6:F:92:GLY:N	2.84	0.40
9:I:70:THR:OG1	9:I:107:LYS:HE2	2.22	0.40
14:N:37:ARG:HH12	31:9:6:C:C5'	2.23	0.40
14:N:78:MET:HB2	14:N:79:PRO:HD3	2.02	0.40
28:2:40:ARG:HG3	28:2:45:ASN:HB2	2.04	0.40
30:0:10:U:C4	30:0:532:A:N7	2.89	0.40
30:0:1046:G:N3	30:0:1082:A:H2	2.19	0.40
30:0:1434:A:H2'	30:0:1436:C:C5	2.56	0.40
30:0:2314:G:H2'	30:0:2315:C:H5'	2.03	0.40
31:9:2:U:H4'	37:9:8480:HOH:O	2.20	0.40
2:B:36:PRO:HG3	2:B:169:GLY:H	1.86	0.40
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.56	0.40
2:B:162:MET:HE1	2:B:308:LEU:HD21	2.03	0.40
2:B:275:GLY:O	2:B:291:ASP:HA	2.21	0.40
3:C:138:VAL:O	3:C:234:VAL:HA	2.21	0.40
5:E:22:VAL:O	5:E:28:SER:HA	2.22	0.40
14:N:21:HIS:HD2	37:0:4268:HOH:O	2.05	0.40
14:N:38:LYS:HE3	14:N:38:LYS:HB2	1.81	0.40
15:O:38:ARG:HD3	30:0:654:A:OP2	2.22	0.40
19:S:77:VAL:O	19:S:80:ARG:HG2	2.22	0.40
23:W:88:THR:CG2	23:W:89:ASP:H	2.34	0.40
30:0:553:G:O4'	30:0:1325:G:H5'	2.20	0.40
30:0:563:C:H2'	30:0:564:G:O4'	2.22	0.40
30:0:622:G:O2'	30:0:623:U:H5'	2.21	0.40
30:0:671:A:O2'	30:0:672:G:H2'	2.22	0.40
30:0:1333:U:H2'	30:0:1334:C:H6	1.86	0.40
30:0:1571:G:C2'	30:0:1626:A:H61	2.34	0.40
30:0:1656:A:H2'	30:0:1657:A:O4'	2.21	0.40
30:0:2002:C:H2'	30:0:2003:U:H5'	2.03	0.40
30:0:2575:C:H2'	30:0:2576:A:O4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	14	22
2	B	335/338 (99%)	315 (94%)	17 (5%)	3 (1%)	14	22
3	C	244/246 (99%)	231 (95%)	13 (5%)	0	100	100
4	D	134/177 (76%)	115 (86%)	15 (11%)	4 (3%)	3	3
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	106 (91%)	9 (8%)	2 (2%)	7	10
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	148 (95%)	8 (5%)	0	100	100
9	I	68/162 (42%)	57 (84%)	11 (16%)	0	100	100
10	J	140/145 (97%)	132 (94%)	7 (5%)	1 (1%)	18	28
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	16	25
12	L	141/165 (86%)	126 (89%)	14 (10%)	1 (1%)	18	28
13	M	192/196 (98%)	187 (97%)	5 (3%)	0	100	100
14	N	184/187 (98%)	170 (92%)	11 (6%)	3 (2%)	7	11
15	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
21	U	51/67 (76%)	48 (94%)	2 (4%)	1 (2%)	6	7
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	7	11
23	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	18	28
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	9	14
25	Y	140/241 (58%)	140 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	63 (89%)	6 (8%)	2 (3%)	4	3
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
All	All	3705/4472 (83%)	3505 (95%)	177 (5%)	23 (1%)	21	32

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
6	F	101	ALA
10	J	5	GLU
12	L	80	ASP
14	N	154	LEU
14	N	184	ILE
4	D	27	ILE
14	N	183	ASP
22	V	43	PRO
23	W	77	ALA
26	Z	105	ARG
2	B	185	GLY
4	D	56	ARG
4	D	65	GLU
21	U	55	ALA
26	Z	66	CYS
1	A	34	ASP
4	D	171	ASP
2	B	169	GLY
11	K	126	SER
6	F	100	ASP
2	B	2	GLN
24	X	70	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	170 (95%)	9 (5%)	22	38
2	B	282/283 (100%)	262 (93%)	20 (7%)	13	23
3	C	193/193 (100%)	176 (91%)	17 (9%)	9	15
4	D	117/148 (79%)	114 (97%)	3 (3%)	40	63
5	E	152/156 (97%)	149 (98%)	3 (2%)	48	70
6	F	93/94 (99%)	91 (98%)	2 (2%)	45	67
7	G	27/282 (10%)	26 (96%)	1 (4%)	30	51
8	H	134/145 (92%)	129 (96%)	5 (4%)	30	51
9	I	58/130 (45%)	57 (98%)	1 (2%)	53	74
10	J	118/121 (98%)	113 (96%)	5 (4%)	26	45
11	K	106/106 (100%)	104 (98%)	2 (2%)	50	71
12	L	113/127 (89%)	111 (98%)	2 (2%)	51	73
13	M	158/160 (99%)	153 (97%)	5 (3%)	34	56
14	N	149/150 (99%)	142 (95%)	7 (5%)	23	41
15	O	93/94 (99%)	90 (97%)	3 (3%)	34	56
16	P	113/117 (97%)	109 (96%)	4 (4%)	32	53
17	Q	79/80 (99%)	75 (95%)	4 (5%)	21	37
18	R	117/122 (96%)	113 (97%)	4 (3%)	32	54
19	S	71/74 (96%)	68 (96%)	3 (4%)	26	45
20	T	105/106 (99%)	100 (95%)	5 (5%)	23	40
21	U	44/53 (83%)	44 (100%)	0	100	100
22	V	51/57 (90%)	49 (96%)	2 (4%)	28	48
23	W	130/130 (100%)	123 (95%)	7 (5%)	20	35
24	X	66/74 (89%)	61 (92%)	5 (8%)	12	21
25	Y	120/196 (61%)	111 (92%)	9 (8%)	12	21
26	Z	60/94 (64%)	59 (98%)	1 (2%)	53	74
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	43	65
29	3	79/79 (100%)	78 (99%)	1 (1%)	61	80
All	All	3095/3646 (85%)	2964 (96%)	131 (4%)	26	45

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASP
1	A	55	VAL
1	A	68	ILE
1	A	94	LEU
1	A	120	ARG
1	A	131	HIS
1	A	175	LYS
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN
2	B	49	THR
2	B	53	LEU
2	B	84	LEU
2	B	97	LEU
2	B	98	THR
2	B	162	MET
2	B	174	ARG
2	B	175	LEU
2	B	190	MET
2	B	195	ARG
2	B	254	GLN
2	B	256	GLN
2	B	257	THR
2	B	264	GLU
2	B	265	LEU
2	B	279	THR
2	B	312	ARG
3	C	2	GLN
3	C	16	VAL
3	C	27	ARG
3	C	67	GLN
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

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Mol	Chain	Res	Type
3	C	237	GLU
3	C	240	LEU
3	C	243	VAL
4	D	24	HIS
4	D	136	ARG
4	D	137	PRO
5	E	16	ASP
5	E	86	VAL
5	E	102	VAL
6	F	12	LEU
6	F	46	GLU
7	G	73	ASP
8	H	87	LYS
8	H	91	ARG
8	H	149	VAL
8	H	157	TYR
8	H	174	LEU
9	I	135	GLU
10	J	39	VAL
10	J	46	ILE
10	J	74	ARG
10	J	127	ILE
10	J	131	THR
11	K	10	GLN
11	K	98	VAL
12	L	117	GLU
12	L	140	VAL
13	M	46	LEU
13	M	81	ARG
13	M	93	ARG
13	M	99	ARG
13	M	164	THR
14	N	12	ARG
14	N	17	ARG
14	N	26	LEU
14	N	43	VAL
14	N	49	THR
14	N	127	LEU
14	N	135	VAL
15	O	3	THR
15	O	98	LEU
15	O	111	VAL

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Mol	Chain	Res	Type
16	P	21	VAL
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	16	ASN
17	Q	30	VAL
17	Q	95	GLU
18	R	13	THR
18	R	39	THR
18	R	82	GLU
18	R	143	VAL
19	S	12	GLU
19	S	71	ASP
19	S	81	ILE
20	T	26	THR
20	T	39	ASN
20	T	48	VAL
20	T	96	VAL
20	T	115	GLU
22	V	43	PRO
22	V	65	ASP
23	W	26	ILE
23	W	35	VAL
23	W	52	VAL
23	W	73	LEU
23	W	122	ARG
23	W	142	ASP
23	W	146	ILE
24	X	15	ARG
24	X	49	ARG
24	X	72	VAL
24	X	80	GLU
24	X	82	GLU
25	Y	103	THR
25	Y	141	THR
25	Y	154	ARG
25	Y	172	THR
25	Y	187	VAL
25	Y	189	ASN
25	Y	200	THR
25	Y	203	VAL

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Mol	Chain	Res	Type
25	Y	235	GLU
26	Z	68	GLU
28	2	18	ASN
29	3	42	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
1	A	218	ASN
2	B	27	ASN
2	B	55	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
3	C	39	GLN
3	C	67	GLN
3	C	73	GLN
3	C	129	HIS
4	D	47	GLN
4	D	103	ASN
4	D	133	ASN
5	E	106	ASN
5	E	119	HIS
5	E	143	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	75	HIS
8	H	131	GLN
10	J	25	GLN
10	J	52	GLN
10	J	107	ASN
10	J	142	ASN
11	K	10	GLN
12	L	18	HIS
12	L	41	HIS

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Mol	Chain	Res	Type
12	L	116	HIS
13	M	24	GLN
13	M	58	GLN
13	M	170	ASN
14	N	21	HIS
14	N	22	GLN
14	N	107	ASN
14	N	140	GLN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	40	HIS
17	Q	67	GLN
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	101	HIS
18	R	117	HIS
18	R	122	GLN
18	R	140	GLN
19	S	9	HIS
19	S	51	GLN
19	S	53	ASN
19	S	55	GLN
20	T	39	ASN
20	T	73	HIS
21	U	39	ASN
22	V	4	HIS
22	V	60	GLN
23	W	28	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
27	1	8	GLN

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Mol	Chain	Res	Type
27	1	16	HIS
27	1	28	HIS
28	2	18	ASN
28	2	37	HIS
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN
29	3	48	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	239 (8%)	32 (1%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	255 (8%)	33 (1%)

All (255) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	169	A
30	0	170	U
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C

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Mol	Chain	Res	Type
30	0	219	G
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	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	735	C
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U

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Mol	Chain	Res	Type
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	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A

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Mol	Chain	Res	Type
30	0	1193	A
30	0	1206	U
30	0	1216	G
30	0	1232	A
30	0	1233	A
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1279	U
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	1409	G
30	0	1474	C
30	0	1485	A
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
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	1693	A
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1731	C

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Mol	Chain	Res	Type
30	0	1752	G
30	0	1778	A
30	0	1779	A
30	0	1798	C
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	1943	C
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1980	U
30	0	1996	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
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2103	A
30	0	2104	C
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	2321	A
30	0	2354	A

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Mol	Chain	Res	Type
30	0	2361	A
30	0	2369	A
30	0	2422	U
30	0	2462	G
30	0	2469	A
30	0	2476	C
30	0	2480	G
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	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	2649	A
30	0	2650	U
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2718	C
30	0	2719	A
30	0	2726	U
30	0	2727	A
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2761	A
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A

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Mol	Chain	Res	Type
30	0	2825	C
30	0	2840	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (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	338	C
30	0	603	A
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A

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Mol	Chain	Res	Type
30	0	1377	C
30	0	1506	U
30	0	1692	C
30	0	1856	C
30	0	1942	A
30	0	1979	G
30	0	2011	A
30	0	2103	A
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	2726	U
30	0	2761	A
30	0	2791	U
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
30	PSU	0	2621	30	18,21,22	1.45	2 (11%)	21,30,33	1.28	3 (14%)
30	OMU	0	2587	30	19,22,23	0.25	0	25,31,34	0.35	0
30	1MA	0	628	30,33	21,25,26	0.70	1 (4%)	30,37,40	0.68	1 (3%)
30	OMG	0	2588	30	23,26,27	0.30	0	32,38,41	0.37	0
30	UR3	0	2619	30	19,22,23	0.38	0	26,32,35	0.72	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	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2
30	1MA	0	628	30,33	-	1/7/25/26	0/3/3/3
30	OMG	0	2588	30	-	0/9/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	4.98	1.43	1.36
30	0	2621	PSU	C6-C5	2.46	1.38	1.35
30	0	628	1MA	C6-N6	2.37	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	3.23	120.35	118.17
30	0	2621	PSU	O2-C2-N1	2.88	125.76	122.79
30	0	2619	UR3	C4-N3-C2	2.86	126.88	124.58
30	0	2621	PSU	C6-N1-C2	-2.77	120.12	122.69
30	0	628	1MA	N1-C2-N3	2.72	129.23	126.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

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

Of 231 ligands modelled in this entry, 231 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.21	12 (5%) 33 30	19, 38, 77, 98	0
2	B	337/338 (99%)	0.45	12 (3%) 46 42	21, 46, 74, 84	0
3	C	246/246 (100%)	0.11	4 (1%) 70 66	15, 36, 60, 71	0
4	D	140/177 (79%)	2.19	72 (51%) 0 0	47, 90, 115, 123	0
5	E	172/178 (96%)	0.90	19 (11%) 10 8	39, 61, 81, 85	0
6	F	119/120 (99%)	1.12	18 (15%) 5 4	34, 61, 90, 104	0
7	G	29/348 (8%)	2.22	13 (44%) 0 0	69, 86, 95, 98	0
8	H	160/177 (90%)	0.56	12 (7%) 20 17	30, 48, 83, 90	0
9	I	70/162 (43%)	3.74	62 (88%) 0 0	122, 136, 154, 155	0
10	J	142/145 (97%)	0.36	7 (4%) 35 31	29, 43, 66, 89	0
11	K	132/132 (100%)	0.20	3 (2%) 61 57	27, 42, 65, 77	0
12	L	145/165 (87%)	0.86	28 (19%) 3 2	18, 55, 101, 117	0
13	M	194/196 (98%)	-0.23	0 100 100	20, 31, 47, 55	0
14	N	186/187 (99%)	1.10	34 (18%) 3 3	32, 53, 102, 112	0
15	O	115/116 (99%)	0.52	6 (5%) 33 29	29, 44, 62, 70	0
16	P	143/149 (95%)	0.38	5 (3%) 47 43	31, 45, 57, 68	0
17	Q	95/96 (98%)	0.08	2 (2%) 63 59	26, 35, 54, 66	0
18	R	150/155 (96%)	-0.15	1 (0%) 84 81	22, 37, 58, 71	0
19	S	81/85 (95%)	0.53	5 (6%) 26 23	31, 48, 72, 82	0
20	T	119/120 (99%)	0.64	7 (5%) 28 24	29, 46, 78, 98	0
21	U	53/67 (79%)	0.53	6 (11%) 10 7	34, 48, 66, 76	0
22	V	65/71 (91%)	1.26	12 (18%) 3 3	40, 62, 106, 113	0
23	W	154/154 (100%)	0.25	3 (1%) 66 62	28, 42, 59, 71	0
24	X	82/92 (89%)	1.07	15 (18%) 3 3	36, 50, 78, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.11	4 (2%) 55 51	22, 36, 60, 80	0
26	Z	73/116 (62%)	0.71	7 (9%) 13 10	34, 48, 68, 87	0
27	1	56/57 (98%)	-0.62	0 100 100	19, 24, 31, 40	0
28	2	46/50 (92%)	1.01	12 (26%) 1 1	26, 50, 75, 89	0
29	3	92/92 (100%)	0.29	3 (3%) 49 45	22, 45, 62, 76	0
30	0	2749/2923 (94%)	-0.61	66 (2%) 59 55	16, 36, 81, 155	0
31	9	122/122 (100%)	0.06	5 (4%) 41 37	31, 54, 77, 138	0
All	All	6646/7517 (88%)	0.07	455 (6%) 23 20	15, 42, 89, 155	0

All (455) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	9.9
9	I	128	THR	9.0
4	D	10	PHE	8.9
24	X	88	GLU	8.2
4	D	174	VAL	6.6
9	I	113	SER	6.5
2	B	1	PRO	6.5
1	A	237	GLY	6.4
22	V	39	ALA	6.4
22	V	40	PRO	6.3
9	I	134	ILE	6.1
26	Z	34	SER	6.1
28	2	49	GLU	6.1
14	N	168	LEU	6.1
1	A	37	VAL	6.1
9	I	116	LEU	6.0
9	I	67	VAL	5.8
9	I	97	VAL	5.8
4	D	63	ILE	5.8
14	N	166	ALA	5.6
9	I	88	GLN	5.6
8	H	174	LEU	5.6
30	0	10	U	5.4
9	I	119	ALA	5.4
22	V	2	VAL	5.3
7	G	71	LEU	5.3
9	I	124	VAL	5.2
14	N	161	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
9	I	95	LEU	5.2
9	I	111	LEU	5.2
9	I	133	THR	5.2
9	I	91	PHE	5.2
26	Z	106	SER	5.0
9	I	74	ILE	5.0
14	N	154	LEU	5.0
4	D	172	VAL	4.9
31	9	1	U	4.9
12	L	78	ALA	4.9
9	I	112	LEU	4.8
25	Y	235	GLU	4.8
4	D	61	PHE	4.8
4	D	44	ILE	4.7
9	I	71	ALA	4.7
9	I	83	GLY	4.7
5	E	10	ASP	4.7
7	G	26	MET	4.6
9	I	80	PHE	4.6
7	G	12	ILE	4.6
9	I	114	TYR	4.6
12	L	82	ALA	4.6
9	I	132	VAL	4.5
24	X	83	ALA	4.5
24	X	87	ALA	4.5
9	I	72	GLU	4.5
9	I	100	VAL	4.4
4	D	107	GLY	4.4
9	I	68	PRO	4.4
9	I	73	LEU	4.4
14	N	165	ALA	4.3
12	L	99	GLU	4.3
9	I	85	GLY	4.3
9	I	101	LYS	4.3
16	P	143	ALA	4.3
1	A	36	ASP	4.2
9	I	66	GLY	4.2
12	L	75	LEU	4.2
24	X	85	VAL	4.1
4	D	170	TYR	4.1
30	0	2637	A	4.1
6	F	101	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
4	D	171	ASP	4.1
5	E	45	ASP	4.1
9	I	123	VAL	4.1
12	L	149	ARG	4.0
19	S	81	ILE	4.0
7	G	27	ILE	4.0
18	R	150	PRO	4.0
14	N	158	LEU	4.0
9	I	106	GLN	4.0
4	D	55	LYS	4.0
9	I	108	HIS	3.9
28	2	35	ARG	3.9
14	N	159	TYR	3.9
5	E	154	ILE	3.9
7	G	73	ASP	3.9
14	N	160	SER	3.9
9	I	120	ALA	3.9
9	I	130	LEU	3.8
4	D	35	ALA	3.8
14	N	167	ASP	3.8
14	N	186	LEU	3.8
25	Y	108	ASP	3.8
9	I	109	PRO	3.8
14	N	152	GLU	3.8
4	D	135	VAL	3.7
10	J	4	ALA	3.7
12	L	148	GLU	3.7
30	0	960	G	3.7
22	V	43	PRO	3.6
30	0	1165	G	3.6
8	H	171	GLY	3.6
14	N	164	ASP	3.6
4	D	75	LEU	3.6
12	L	150	GLN	3.6
8	H	13	ASP	3.6
4	D	54	ALA	3.6
12	L	77	ALA	3.6
28	2	39	ARG	3.6
9	I	69	PRO	3.6
4	D	11	HIS	3.5
5	E	53	GLU	3.5
9	I	135	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
9	I	82	THR	3.5
9	I	110	ASP	3.5
14	N	162	ASP	3.5
31	9	24	U	3.5
4	D	101	THR	3.5
9	I	104	ALA	3.5
30	0	1173	A	3.5
9	I	127	CYS	3.5
4	D	18	ILE	3.5
14	N	163	PHE	3.5
12	L	102	ASP	3.4
22	V	65	ASP	3.4
4	D	17	ARG	3.4
9	I	70	THR	3.4
12	L	105	TYR	3.4
8	H	172	GLU	3.4
30	0	128	A	3.4
16	P	18	LYS	3.4
15	O	1	SER	3.4
4	D	106	PHE	3.4
11	K	119	GLN	3.4
4	D	59	GLY	3.4
2	B	171	VAL	3.4
4	D	40	ILE	3.4
8	H	114	ASP	3.3
4	D	57	THR	3.3
6	F	119	ARG	3.3
9	I	129	SER	3.3
5	E	87	PHE	3.3
9	I	103	ILE	3.3
28	2	31	ARG	3.3
19	S	2	TRP	3.3
20	T	119	ALA	3.3
19	S	1	SER	3.3
31	9	2	U	3.3
9	I	89	GLU	3.3
21	U	56	ARG	3.2
4	D	68	PRO	3.2
14	N	68	GLU	3.2
28	2	37	HIS	3.2
1	A	35	GLY	3.2
6	F	99	THR	3.2

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Mol	Chain	Res	Type	RSRZ
17	Q	17	LYS	3.2
14	N	1	ALA	3.2
12	L	60	GLU	3.2
20	T	53	GLY	3.2
4	D	150	SER	3.2
29	3	56	PRO	3.2
12	L	44	GLU	3.2
7	G	24	VAL	3.2
11	K	118	ALA	3.2
9	I	77	GLU	3.2
2	B	34	GLY	3.2
30	0	1171	A	3.1
4	D	69	ILE	3.1
8	H	169	GLU	3.1
30	0	87	C	3.1
3	C	132	ASP	3.1
9	I	94	ASP	3.1
12	L	145	LEU	3.1
9	I	92	VAL	3.1
22	V	36	ALA	3.0
4	D	62	ASP	3.0
22	V	44	GLY	3.0
30	0	1175	G	3.0
15	O	23	GLY	3.0
4	D	86	THR	3.0
30	0	1160	G	3.0
2	B	119	HIS	3.0
24	X	46	ASP	3.0
30	0	1191	A	3.0
9	I	87	PRO	2.9
28	2	44	ARG	2.9
9	I	107	LYS	2.9
30	0	1279	U	2.9
30	0	2103	A	2.9
12	L	81	VAL	2.9
21	U	55	ALA	2.9
1	A	64	ASP	2.9
9	I	115	ASP	2.9
7	G	29	SER	2.9
30	0	2911	C	2.9
10	J	62	ASP	2.9
4	D	104	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
12	L	55	GLN	2.9
20	T	114	SER	2.9
24	X	84	ILE	2.9
1	A	211	LYS	2.9
4	D	169	THR	2.9
2	B	57	GLU	2.9
4	D	19	GLU	2.9
9	I	118	ASN	2.8
20	T	118	SER	2.8
14	N	169	PRO	2.8
9	I	78	ALA	2.8
3	C	61	PHE	2.8
12	L	147	GLU	2.8
30	0	1525	G	2.8
30	0	2237	G	2.8
30	0	1524	U	2.8
4	D	153	THR	2.8
30	0	2345	A	2.8
5	E	126	ILE	2.8
30	0	1561	U	2.8
30	0	1161	A	2.8
24	X	61	ARG	2.8
4	D	165	PHE	2.8
5	E	6	GLU	2.8
30	0	1199	A	2.8
24	X	65	ASN	2.7
25	Y	236	VAL	2.7
4	D	74	THR	2.7
9	I	117	THR	2.7
21	U	52	THR	2.7
30	0	1198	U	2.7
30	0	1176	C	2.7
4	D	166	ILE	2.7
14	N	157	PRO	2.7
5	E	12	ASP	2.7
28	2	38	LYS	2.7
30	0	1964	U	2.7
14	N	184	ILE	2.7
1	A	65	ARG	2.7
4	D	134	LEU	2.7
28	2	20	ARG	2.7
6	F	16	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
8	H	173	GLU	2.7
19	S	43	GLU	2.7
30	0	1164	U	2.7
4	D	56	ARG	2.6
21	U	47	ARG	2.6
26	Z	48	ARG	2.6
14	N	150	TYR	2.6
30	0	138	U	2.6
5	E	32	ARG	2.6
5	E	11	VAL	2.6
30	0	1626	A	2.6
30	0	1172	G	2.6
2	B	33	ASP	2.6
4	D	66	GLY	2.6
12	L	146	GLY	2.6
21	U	53	ASP	2.6
6	F	1	PRO	2.6
30	0	1169	U	2.6
5	E	20	ILE	2.6
12	L	42	ASN	2.6
12	L	83	GLU	2.6
4	D	58	VAL	2.6
4	D	156	ARG	2.6
12	L	104	ASP	2.6
31	9	23	U	2.6
24	X	7	GLU	2.6
9	I	99	GLN	2.6
6	F	44	SER	2.6
4	D	64	ARG	2.5
26	Z	104	ARG	2.5
30	0	2769	C	2.5
6	F	102	GLY	2.5
30	0	716	G	2.5
30	0	1167	G	2.5
15	O	24	ALA	2.5
8	H	165	ARG	2.5
2	B	56	ASP	2.5
15	O	22	GLY	2.5
4	D	60	GLU	2.5
4	D	157	LEU	2.5
7	G	67	LEU	2.5
30	0	1130	U	2.5

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Mol	Chain	Res	Type	RSRZ
30	0	1170	U	2.5
9	I	126	THR	2.5
30	0	1951	G	2.5
7	G	70	ALA	2.5
8	H	43	ALA	2.5
4	D	52	THR	2.5
4	D	105	SER	2.5
14	N	175	LEU	2.5
2	B	21	SER	2.5
24	X	66	THR	2.5
1	A	34	ASP	2.4
9	I	76	ASP	2.4
12	L	76	LEU	2.4
15	O	104	ASN	2.4
4	D	95	THR	2.4
2	B	168	GLY	2.4
4	D	53	LYS	2.4
4	D	128	LEU	2.4
8	H	170	ARG	2.4
30	0	2768	A	2.4
30	0	2914	A	2.4
4	D	48	MET	2.4
6	F	103	GLU	2.4
6	F	117	GLU	2.4
12	L	59	GLU	2.4
14	N	185	GLU	2.4
7	G	72	ASP	2.4
10	J	70	PHE	2.4
22	V	41	GLU	2.4
30	0	1185	U	2.4
4	D	41	LEU	2.4
4	D	47	GLN	2.4
23	W	142	ASP	2.4
25	Y	216	ARG	2.4
30	0	514	G	2.4
14	N	156	GLU	2.4
24	X	79	GLU	2.4
4	D	89	PRO	2.3
9	I	96	SER	2.3
30	0	1184	C	2.3
1	A	38	ILE	2.3
5	E	7	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	51	VAL	2.3
11	K	101	ASN	2.3
30	0	1162	G	2.3
30	0	1203	G	2.3
9	I	122	GLU	2.3
24	X	80	GLU	2.3
5	E	172	PRO	2.3
30	0	1188	A	2.3
30	0	2664	A	2.3
23	W	86	GLU	2.3
30	0	1929	G	2.3
30	0	1187	U	2.3
5	E	39	ASP	2.3
12	L	79	ASP	2.3
4	D	154	LYS	2.3
30	0	999	C	2.3
30	0	1204	C	2.3
1	A	59	GLU	2.3
4	D	91	ALA	2.3
22	V	45	ARG	2.3
4	D	102	GLY	2.3
2	B	170	SER	2.3
14	N	39	SER	2.3
16	P	116	SER	2.3
6	F	118	LEU	2.3
7	G	23	ILE	2.3
30	0	272	A	2.3
30	0	1174	A	2.3
30	0	1559	A	2.3
9	I	75	LYS	2.3
30	0	2419	U	2.3
5	E	9	GLU	2.3
1	A	66	ARG	2.3
4	D	139	TYR	2.3
14	N	5	ARG	2.3
12	L	100	ALA	2.2
26	Z	65	ASN	2.2
6	F	26	THR	2.2
4	D	29	HIS	2.2
4	D	93	LEU	2.2
6	F	39	SER	2.2
10	J	63	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	118	ASP	2.2
4	D	23	VAL	2.2
4	D	149	ARG	2.2
30	0	282	C	2.2
28	2	28	LYS	2.2
9	I	84	SER	2.2
14	N	147	ILE	2.2
22	V	46	ILE	2.2
24	X	71	ARG	2.2
6	F	98	VAL	2.2
12	L	93	VAL	2.2
28	2	27	LEU	2.2
24	X	82	GLU	2.2
30	0	1202	A	2.2
1	A	32	VAL	2.2
6	F	91	VAL	2.2
30	0	809	G	2.2
30	0	1178	G	2.2
21	U	54	THR	2.2
14	N	179	LEU	2.2
4	D	12	GLU	2.2
5	E	156	ASP	2.2
24	X	78	GLU	2.2
29	3	92	GLU	2.2
4	D	21	VAL	2.1
6	F	104	ALA	2.1
14	N	67	ALA	2.1
14	N	66	LEU	2.1
30	0	1195	G	2.1
31	9	122	C	2.1
14	N	64	SER	2.1
20	T	13	ARG	2.1
20	T	117	ASP	2.1
4	D	50	VAL	2.1
7	G	15	TRP	2.1
9	I	102	GLN	2.1
30	0	970	U	2.1
4	D	133	ASN	2.1
10	J	47	THR	2.1
17	Q	95	GLU	2.1
23	W	60	GLU	2.1
30	0	1196	C	2.1

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Mol	Chain	Res	Type	RSRZ
30	0	2508	C	2.1
3	C	16	VAL	2.1
6	F	29	VAL	2.1
5	E	13	ALA	2.1
7	G	64	ASN	2.1
30	0	1166	A	2.1
12	L	143	THR	2.1
22	V	64	GLY	2.1
12	L	130	ARG	2.1
9	I	86	GLU	2.1
29	3	41	GLU	2.1
15	O	8	SER	2.1
28	2	48	ASP	2.1
30	0	1190	G	2.1
10	J	92	GLN	2.1
6	F	17	LEU	2.1
28	2	36	ASN	2.1
8	H	115	GLY	2.1
3	C	95	GLU	2.1
4	D	38	GLU	2.1
14	N	170	GLU	2.1
19	S	12	GLU	2.1
4	D	67	ASP	2.1
4	D	99	ASP	2.1
5	E	100	ASP	2.1
16	P	110	ASP	2.1
16	P	117	SER	2.1
26	Z	35	SER	2.1
30	0	1182	C	2.1
6	F	19	ALA	2.0
4	D	36	ASN	2.0
9	I	131	GLY	2.0
20	T	59	GLU	2.0
4	D	45	THR	2.0
5	E	169	THR	2.0
10	J	46	ILE	2.0
4	D	159	PRO	2.0
12	L	91	VAL	2.0
26	Z	105	ARG	2.0
30	0	1168	C	2.0
4	D	37	ALA	2.0
4	D	88	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
14	N	148	ALA	2.0
8	H	12	ILE	2.0
4	D	49	PRO	2.0
14	N	134	ASP	2.0
30	0	1200	A	2.0
30	0	2506	A	2.0
14	N	21	HIS	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(Å ²)	Q<0.9
30	OMU	0	2587	21/22	0.98	0.06	22,25,27,28	0
30	OMG	0	2588	24/25	0.98	0.05	22,25,27,28	0
30	UR3	0	2619	21/22	0.98	0.06	24,27,31,36	0
30	PSU	0	2621	20/21	0.98	0.05	20,23,27,27	0
30	1MA	0	628	23/24	0.99	0.05	20,22,23,25	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(Å ²)	Q<0.9
33	NA	R	8386	1/1	0.59	0.56	80,80,80,80	0
33	NA	0	8370	1/1	0.66	0.53	70,70,70,70	0
32	MG	9	8095	1/1	0.72	0.23	64,64,64,64	0
32	MG	0	8087	1/1	0.78	0.17	57,57,57,57	0
32	MG	0	8090	1/1	0.82	0.14	56,56,56,56	0
33	NA	0	8329	1/1	0.82	0.15	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	MG	0	8050	1/1	0.82	0.16	66,66,66,66	0
33	NA	0	8376	1/1	0.83	0.16	42,42,42,42	0
33	NA	0	8314	1/1	0.85	0.10	38,38,38,38	0
33	NA	9	8351	1/1	0.85	0.23	45,45,45,45	0
32	MG	0	8094	1/1	0.86	0.18	59,59,59,59	0
32	MG	0	8082	1/1	0.87	0.21	62,62,62,62	0
33	NA	0	8340	1/1	0.87	0.17	49,49,49,49	0
32	MG	0	8047	1/1	0.87	0.11	59,59,59,59	0
33	NA	0	8311	1/1	0.87	0.14	52,52,52,52	0
33	NA	0	8384	1/1	0.87	0.14	53,53,53,53	0
32	MG	0	8104	1/1	0.87	0.13	50,50,50,50	0
32	MG	0	8070	1/1	0.88	0.08	44,44,44,44	0
33	NA	0	8324	1/1	0.88	0.22	48,48,48,48	0
33	NA	0	8307	1/1	0.88	0.11	42,42,42,42	0
33	NA	H	8322	1/1	0.88	0.21	54,54,54,54	0
33	NA	0	8371	1/1	0.89	0.12	48,48,48,48	0
32	MG	0	8105	1/1	0.89	0.06	45,45,45,45	0
33	NA	0	8369	1/1	0.90	0.15	42,42,42,42	0
32	MG	0	8102	1/1	0.90	0.07	48,48,48,48	0
33	NA	0	8366	1/1	0.90	0.13	63,63,63,63	0
33	NA	0	8373	1/1	0.91	0.06	44,44,44,44	0
33	NA	0	8363	1/1	0.91	0.14	50,50,50,50	0
33	NA	0	8381	1/1	0.91	0.08	43,43,43,43	0
33	NA	0	8364	1/1	0.91	0.12	40,40,40,40	0
33	NA	0	8341	1/1	0.91	0.13	41,41,41,41	0
32	MG	0	8066	1/1	0.92	0.16	88,88,88,88	0
33	NA	0	8374	1/1	0.92	0.11	47,47,47,47	0
33	NA	9	8383	1/1	0.92	0.11	46,46,46,46	0
33	NA	0	8372	1/1	0.93	0.25	60,60,60,60	0
33	NA	0	8382	1/1	0.93	0.09	67,67,67,67	0
32	MG	0	8100	1/1	0.93	0.14	63,63,63,63	0
33	NA	0	8385	1/1	0.93	0.19	44,44,44,44	0
32	MG	0	8053	1/1	0.93	0.16	33,33,33,33	0
32	MG	0	8103	1/1	0.93	0.13	55,55,55,55	0
33	NA	0	8368	1/1	0.94	0.10	48,48,48,48	0
33	NA	R	8337	1/1	0.94	0.05	33,33,33,33	0
33	NA	0	8326	1/1	0.94	0.08	37,37,37,37	0
33	NA	0	8327	1/1	0.94	0.09	36,36,36,36	0
32	MG	0	8046	1/1	0.94	0.05	39,39,39,39	0
33	NA	0	8335	1/1	0.94	0.06	31,31,31,31	0
32	MG	0	8107	1/1	0.94	0.09	68,68,68,68	0
32	MG	0	8043	1/1	0.94	0.05	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	NA	0	8377	1/1	0.94	0.12	50,50,50,50	0
33	NA	0	8342	1/1	0.94	0.06	35,35,35,35	0
33	NA	0	8356	1/1	0.94	0.09	35,35,35,35	0
32	MG	0	8049	1/1	0.94	0.09	54,54,54,54	0
33	NA	0	8316	1/1	0.94	0.08	38,38,38,38	0
33	NA	0	8365	1/1	0.94	0.21	31,31,31,31	0
33	NA	0	8318	1/1	0.94	0.10	47,47,47,47	0
33	NA	0	8360	1/1	0.95	0.10	41,41,41,41	0
33	NA	0	8362	1/1	0.95	0.12	46,46,46,46	0
32	MG	0	8076	1/1	0.95	0.04	44,44,44,44	0
33	NA	0	8313	1/1	0.95	0.06	55,55,55,55	0
32	MG	0	8112	1/1	0.95	0.08	39,39,39,39	0
32	MG	0	8113	1/1	0.95	0.07	31,31,31,31	0
33	NA	0	8367	1/1	0.95	0.14	46,46,46,46	0
32	MG	0	8115	1/1	0.95	0.05	41,41,41,41	0
32	MG	0	8116	1/1	0.95	0.07	35,35,35,35	0
32	MG	0	8101	1/1	0.95	0.06	44,44,44,44	0
32	MG	0	8080	1/1	0.95	0.06	40,40,40,40	0
32	MG	0	8092	1/1	0.95	0.10	66,66,66,66	0
33	NA	0	8330	1/1	0.95	0.07	37,37,37,37	0
33	NA	0	8331	1/1	0.95	0.07	35,35,35,35	0
32	MG	0	8062	1/1	0.95	0.05	42,42,42,42	0
33	NA	S	8312	1/1	0.95	0.09	28,28,28,28	0
33	NA	0	8379	1/1	0.95	0.12	46,46,46,46	0
33	NA	0	8302	1/1	0.95	0.09	44,44,44,44	0
32	MG	0	8099	1/1	0.95	0.05	40,40,40,40	0
33	NA	0	8349	1/1	0.95	0.07	32,32,32,32	0
33	NA	0	8350	1/1	0.95	0.12	41,41,41,41	0
33	NA	0	8308	1/1	0.95	0.10	45,45,45,45	0
33	NA	9	8352	1/1	0.95	0.10	41,41,41,41	0
33	NA	0	8358	1/1	0.95	0.18	73,73,73,73	0
33	NA	0	8319	1/1	0.96	0.04	31,31,31,31	0
33	NA	0	8301	1/1	0.96	0.07	34,34,34,34	0
33	NA	0	8325	1/1	0.96	0.08	50,50,50,50	0
32	MG	0	8072	1/1	0.96	0.04	47,47,47,47	0
33	NA	0	8359	1/1	0.96	0.09	39,39,39,39	0
33	NA	0	8375	1/1	0.96	0.15	38,38,38,38	0
33	NA	C	8304	1/1	0.96	0.06	29,29,29,29	0
33	NA	0	8361	1/1	0.96	0.08	41,41,41,41	0
33	NA	0	8378	1/1	0.96	0.12	40,40,40,40	0
32	MG	0	8085	1/1	0.96	0.05	37,37,37,37	0
33	NA	M	8347	1/1	0.96	0.04	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	NA	Q	8348	1/1	0.96	0.06	30,30,30,30	0
33	NA	0	8334	1/1	0.96	0.12	36,36,36,36	0
32	MG	0	8096	1/1	0.96	0.06	34,34,34,34	0
33	NA	0	8315	1/1	0.96	0.07	30,30,30,30	0
32	MG	B	8055	1/1	0.96	0.06	42,42,42,42	0
32	MG	0	8045	1/1	0.96	0.10	55,55,55,55	0
34	CL	J	8502	1/1	0.96	0.07	55,55,55,55	0
34	CL	J	8521	1/1	0.96	0.08	47,47,47,47	0
34	CL	0	8515	1/1	0.96	0.11	53,53,53,53	0
34	CL	0	8517	1/1	0.96	0.06	47,47,47,47	0
36	K	0	8201	1/1	0.96	0.20	60,60,60,60	0
32	MG	0	8089	1/1	0.97	0.05	43,43,43,43	0
33	NA	0	8333	1/1	0.97	0.06	23,23,23,23	0
33	NA	0	8305	1/1	0.97	0.05	33,33,33,33	0
32	MG	0	8063	1/1	0.97	0.06	60,60,60,60	0
32	MG	0	8114	1/1	0.97	0.03	38,38,38,38	0
33	NA	0	8309	1/1	0.97	0.03	25,25,25,25	0
32	MG	0	8064	1/1	0.97	0.05	26,26,26,26	0
33	NA	0	8344	1/1	0.97	0.06	24,24,24,24	0
32	MG	Y	8108	1/1	0.97	0.08	25,25,25,25	0
32	MG	0	8067	1/1	0.97	0.10	28,28,28,28	0
33	NA	0	8354	1/1	0.97	0.04	23,23,23,23	0
33	NA	0	8355	1/1	0.97	0.17	53,53,53,53	0
33	NA	A	8345	1/1	0.97	0.09	43,43,43,43	0
33	NA	0	8357	1/1	0.97	0.07	39,39,39,39	0
32	MG	0	8014	1/1	0.97	0.06	25,25,25,25	0
32	MG	0	8024	1/1	0.97	0.03	22,22,22,22	0
33	NA	J	8346	1/1	0.97	0.04	37,37,37,37	0
33	NA	0	8320	1/1	0.97	0.10	37,37,37,37	0
32	MG	0	8075	1/1	0.97	0.06	27,27,27,27	0
34	CL	A	8509	1/1	0.97	0.07	49,49,49,49	0
34	CL	J	8501	1/1	0.97	0.08	46,46,46,46	0
32	MG	0	8041	1/1	0.97	0.12	34,34,34,34	0
32	MG	0	8051	1/1	0.97	0.07	54,54,54,54	0
34	CL	L	8510	1/1	0.97	0.10	40,40,40,40	0
34	CL	0	8514	1/1	0.97	0.07	39,39,39,39	0
32	MG	0	8052	1/1	0.97	0.04	48,48,48,48	0
32	MG	A	8065	1/1	0.97	0.04	23,23,23,23	0
32	MG	K	8069	1/1	0.97	0.04	47,47,47,47	0
33	NA	0	8332	1/1	0.98	0.06	31,31,31,31	0
32	MG	0	8111	1/1	0.98	0.04	23,23,23,23	0
33	NA	0	8306	1/1	0.98	0.16	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	3	8078	1/1	0.98	0.04	37,37,37,37	0
33	NA	0	8336	1/1	0.98	0.03	37,37,37,37	0
33	NA	0	8338	1/1	0.98	0.03	41,41,41,41	0
33	NA	0	8339	1/1	0.98	0.03	19,19,19,19	0
32	MG	0	8088	1/1	0.98	0.03	24,24,24,24	0
32	MG	0	8026	1/1	0.98	0.03	23,23,23,23	0
33	NA	0	8310	1/1	0.98	0.04	30,30,30,30	0
32	MG	0	8048	1/1	0.98	0.04	41,41,41,41	0
32	MG	0	8037	1/1	0.98	0.03	35,35,35,35	0
32	MG	0	8093	1/1	0.98	0.05	37,37,37,37	0
33	NA	0	8353	1/1	0.98	0.04	17,17,17,17	0
32	MG	0	8006	1/1	0.98	0.04	29,29,29,29	0
32	MG	0	8071	1/1	0.98	0.05	61,61,61,61	0
33	NA	0	8317	1/1	0.98	0.04	28,28,28,28	0
32	MG	0	8098	1/1	0.98	0.11	25,25,25,25	0
32	MG	0	8042	1/1	0.98	0.06	31,31,31,31	0
33	NA	L	8380	1/1	0.98	0.31	44,44,44,44	0
33	NA	0	8321	1/1	0.98	0.11	42,42,42,42	0
32	MG	0	8012	1/1	0.98	0.05	30,30,30,30	0
32	MG	0	8044	1/1	0.98	0.03	33,33,33,33	0
32	MG	0	8079	1/1	0.98	0.03	20,20,20,20	0
34	CL	N	8507	1/1	0.98	0.07	44,44,44,44	0
34	CL	R	8506	1/1	0.98	0.08	40,40,40,40	0
34	CL	Y	8520	1/1	0.98	0.05	35,35,35,35	0
34	CL	0	8505	1/1	0.98	0.06	41,41,41,41	0
34	CL	0	8511	1/1	0.98	0.06	37,37,37,37	0
34	CL	0	8513	1/1	0.98	0.06	44,44,44,44	0
32	MG	0	8057	1/1	0.98	0.07	34,34,34,34	0
32	MG	0	8060	1/1	0.98	0.06	33,33,33,33	0
34	CL	0	8516	1/1	0.98	0.13	41,41,41,41	0
32	MG	T	8073	1/1	0.98	0.04	40,40,40,40	0
34	CL	0	8522	1/1	0.98	0.25	44,44,44,44	0
32	MG	0	8086	1/1	0.98	0.04	37,37,37,37	0
32	MG	0	8007	1/1	0.99	0.06	21,21,21,21	0
32	MG	0	8059	1/1	0.99	0.06	22,22,22,22	0
32	MG	0	8027	1/1	0.99	0.02	36,36,36,36	0
32	MG	0	8061	1/1	0.99	0.04	30,30,30,30	0
32	MG	0	8028	1/1	0.99	0.03	27,27,27,27	0
32	MG	0	8029	1/1	0.99	0.03	34,34,34,34	0
32	MG	0	8030	1/1	0.99	0.03	21,21,21,21	0
32	MG	0	8106	1/1	0.99	0.02	31,31,31,31	0
33	NA	0	8323	1/1	0.99	0.09	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8031	1/1	0.99	0.02	24,24,24,24	0
32	MG	0	8109	1/1	0.99	0.02	25,25,25,25	0
32	MG	0	8034	1/1	0.99	0.04	30,30,30,30	0
32	MG	0	8068	1/1	0.99	0.03	46,46,46,46	0
33	NA	0	8328	1/1	0.99	0.10	31,31,31,31	0
32	MG	0	8035	1/1	0.99	0.02	34,34,34,34	0
32	MG	0	8036	1/1	0.99	0.02	31,31,31,31	0
32	MG	0	8010	1/1	0.99	0.02	24,24,24,24	0
32	MG	0	8074	1/1	0.99	0.04	35,35,35,35	0
32	MG	0	8038	1/1	0.99	0.02	21,21,21,21	0
32	MG	0	8040	1/1	0.99	0.03	38,38,38,38	0
32	MG	0	8011	1/1	0.99	0.02	21,21,21,21	0
32	MG	0	8003	1/1	0.99	0.03	21,21,21,21	0
32	MG	0	8081	1/1	0.99	0.04	39,39,39,39	0
32	MG	0	8013	1/1	0.99	0.03	22,22,22,22	0
32	MG	0	8083	1/1	0.99	0.02	33,33,33,33	0
34	CL	B	8519	1/1	0.99	0.07	34,34,34,34	0
32	MG	0	8084	1/1	0.99	0.02	38,38,38,38	0
32	MG	0	8004	1/1	0.99	0.02	19,19,19,19	0
33	NA	0	8343	1/1	0.99	0.06	28,28,28,28	0
32	MG	0	8016	1/1	0.99	0.06	30,30,30,30	0
34	CL	M	8518	1/1	0.99	0.04	32,32,32,32	0
32	MG	0	8017	1/1	0.99	0.02	11,11,11,11	0
34	CL	O	8508	1/1	0.99	0.06	51,51,51,51	0
32	MG	0	8019	1/1	0.99	0.02	23,23,23,23	0
32	MG	0	8020	1/1	0.99	0.02	22,22,22,22	0
34	CL	3	8504	1/1	0.99	0.03	43,43,43,43	0
34	CL	0	8503	1/1	0.99	0.05	38,38,38,38	0
33	NA	0	8303	1/1	0.99	0.03	32,32,32,32	0
32	MG	0	8021	1/1	0.99	0.02	25,25,25,25	0
34	CL	0	8512	1/1	0.99	0.04	35,35,35,35	0
32	MG	0	8091	1/1	0.99	0.06	41,41,41,41	0
32	MG	0	8022	1/1	0.99	0.03	31,31,31,31	0
32	MG	0	8023	1/1	0.99	0.04	28,28,28,28	0
32	MG	0	8002	1/1	0.99	0.06	25,25,25,25	0
32	MG	0	8025	1/1	0.99	0.02	32,32,32,32	0
32	MG	0	8097	1/1	0.99	0.04	30,30,30,30	0
35	CD	O	8405	1/1	0.99	0.06	71,71,71,71	0
35	CD	U	8401	1/1	0.99	0.02	48,48,48,48	0
32	MG	0	8054	1/1	0.99	0.03	16,16,16,16	0
36	K	0	8202	1/1	0.99	0.16	37,37,37,37	0
32	MG	0	8018	1/1	1.00	0.02	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8039	1/1	1.00	0.01	33,33,33,33	0
32	MG	0	8009	1/1	1.00	0.02	25,25,25,25	0
32	MG	0	8032	1/1	1.00	0.04	26,26,26,26	0
32	MG	0	8077	1/1	1.00	0.01	22,22,22,22	0
32	MG	0	8033	1/1	1.00	0.03	19,19,19,19	0
32	MG	0	8001	1/1	1.00	0.01	24,24,24,24	0
32	MG	0	8015	1/1	1.00	0.02	25,25,25,25	0
32	MG	0	8005	1/1	1.00	0.01	25,25,25,25	0
32	MG	0	8056	1/1	1.00	0.02	34,34,34,34	0
32	MG	0	8110	1/1	1.00	0.03	29,29,29,29	0
35	CD	Z	8403	1/1	1.00	0.02	43,43,43,43	0
35	CD	1	8402	1/1	1.00	0.05	45,45,45,45	0
35	CD	3	8404	1/1	1.00	0.03	45,45,45,45	0
32	MG	0	8008	1/1	1.00	0.02	26,26,26,26	0
32	MG	0	8058	1/1	1.00	0.03	29,29,29,29	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.