



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 10:11 AM UTC

PDB ID : 3CD6 / pdb_00003cd6
Title : Co-cystal of large Ribosomal Subunit mutant G2616A with CC-Puromycin
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.75 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

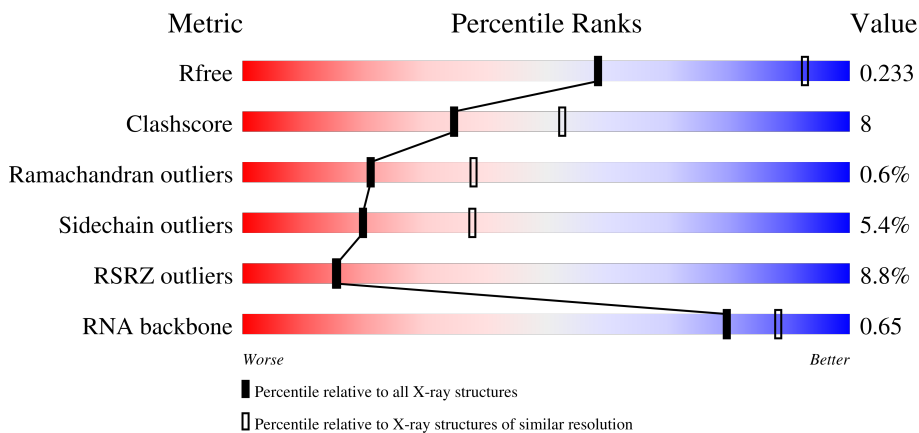
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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.



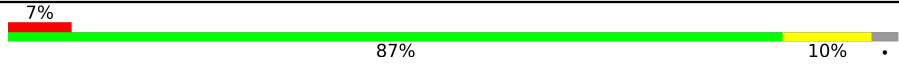

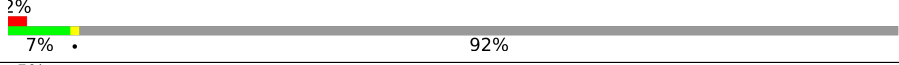

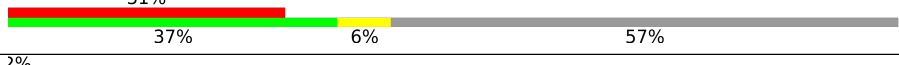
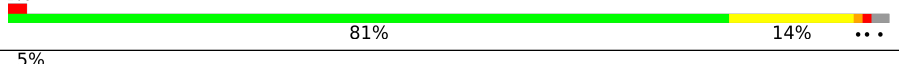
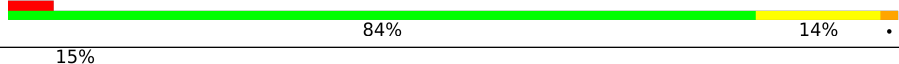

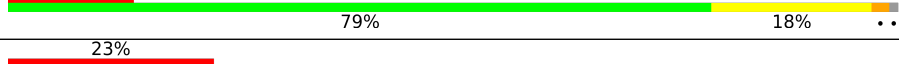


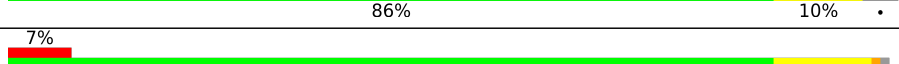
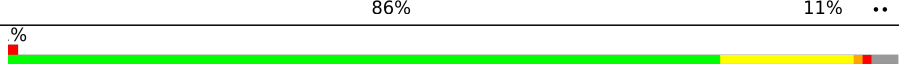
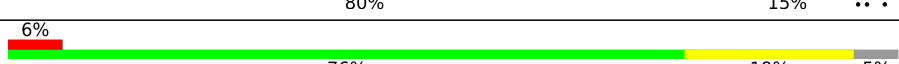

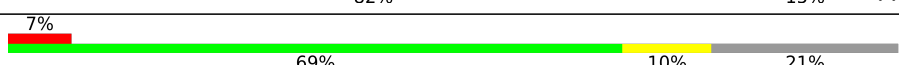
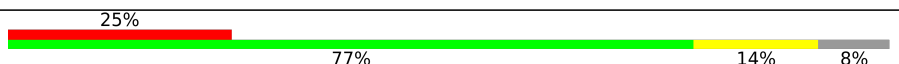
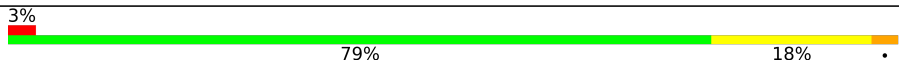
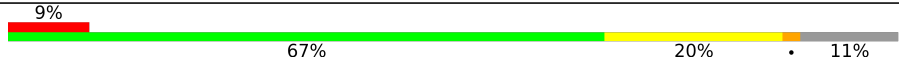


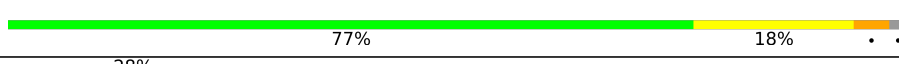
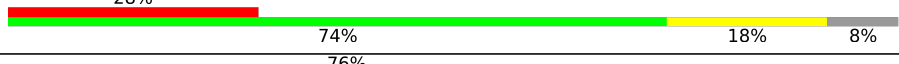


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)
RNA backbone	3983	1179 (3.00-2.52)

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	 12% 85% 13% ..
2	B	338	 5% 81% 16% .
3	C	246	 2% 83% 15% .
4	D	177	 36% 61% 16% .. 21%

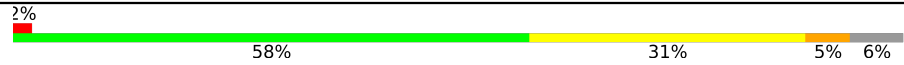

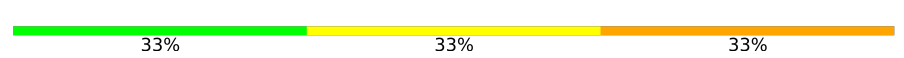
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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1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

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	
32	4	3	

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
36	NA	0	8555	-	-	-	X
36	NA	0	8559	-	-	-	X
36	NA	0	8567	-	-	-	X
36	NA	0	8571	-	-	-	X
36	NA	0	8574	-	-	-	X
36	NA	9	8572	-	-	-	X
37	CD	3	8704	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99180 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
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59019	26349	10873	19052	2745			

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

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

- Molecule 32 is a RNA chain called RNA (5'-R(*CP*CP*(PPU))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	4	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	A	2	Total	Mg	0	0
			2	2		
33	B	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	0	86	Total	Mg	0	0
			86	86		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	9	1	Total 1	Mg 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	1	Total 1	Cl 1	0	0
34	B	1	Total 1	Cl 1	0	0
34	J	3	Total 3	Cl 3	0	0
34	L	1	Total 1	Cl 1	0	0
34	M	1	Total 1	Cl 1	0	0
34	N	1	Total 1	Cl 1	0	0
34	O	1	Total 1	Cl 1	0	0
34	R	1	Total 1	Cl 1	0	0
34	Y	1	Total 1	Cl 1	0	0
34	3	1	Total 1	Cl 1	0	0
34	0	10	Total 10	Cl 10	0	0

- Molecule 35 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	2	Total 2	Sr 2	0	0
35	B	1	Total 1	Sr 1	0	0
35	F	1	Total 1	Sr 1	0	0
35	J	1	Total 1	Sr 1	0	0
35	R	1	Total 1	Sr 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	S	1	Total 1	Sr 1	0	0
35	1	2	Total 2	Sr 2	0	0
35	3	2	Total 2	Sr 2	0	0
35	0	93	Total 93	Sr 93	0	0
35	9	3	Total 3	Sr 3	0	0

- Molecule 36 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	B	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	H	1	Total 1	Na 1	0	0
36	J	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0
36	Q	1	Total 1	Na 1	0	0
36	R	1	Total 1	Na 1	0	0
36	S	1	Total 1	Na 1	0	0
36	0	65	Total 65	Na 65	0	0
36	9	2	Total 2	Na 2	0	0

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

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

- Molecule 38 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	2	Total 2	K 2	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	A	115	Total 115	O 115	0	0
39	B	136	Total 136	O 136	0	0
39	C	167	Total 167	O 167	0	0
39	D	45	Total 45	O 45	0	0
39	E	46	Total 46	O 46	0	0
39	F	28	Total 28	O 28	0	0
39	G	17	Total 17	O 17	0	0
39	H	65	Total 65	O 65	0	0
39	I	7	Total 7	O 7	0	0
39	J	49	Total 49	O 49	0	0
39	K	53	Total 53	O 53	0	0
39	L	92	Total 92	O 92	0	0
39	M	123	Total 123	O 123	0	0

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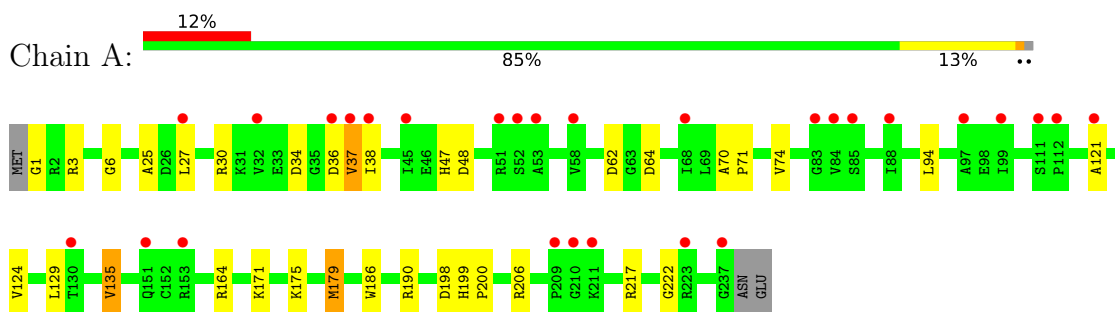
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	N	55	Total 55	O 55	0	0
39	O	37	Total 37	O 37	0	0
39	P	63	Total 63	O 63	0	0
39	Q	51	Total 51	O 51	0	0
39	R	78	Total 78	O 78	0	0
39	S	31	Total 31	O 31	0	0
39	T	38	Total 38	O 38	0	0
39	U	30	Total 30	O 30	0	0
39	V	10	Total 10	O 10	0	0
39	W	67	Total 67	O 67	0	0
39	X	23	Total 23	O 23	0	0
39	Y	93	Total 93	O 93	0	0
39	Z	25	Total 25	O 25	0	0
39	1	60	Total 60	O 60	0	0
39	2	46	Total 46	O 46	0	0
39	3	62	Total 62	O 62	0	0
39	0	5949	Total 5949	O 5949	0	0
39	9	148	Total 148	O 148	0	0

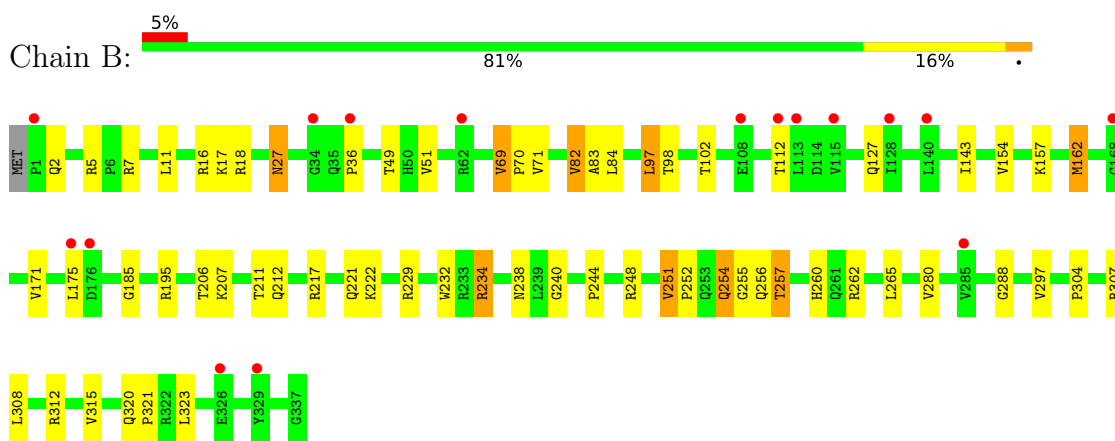
3 Residue-property plots [i](#)

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.

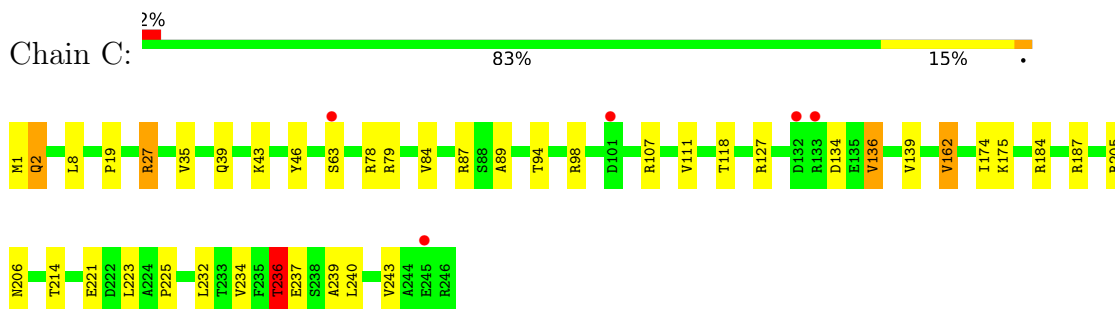
- Molecule 1: 50S ribosomal protein L2P



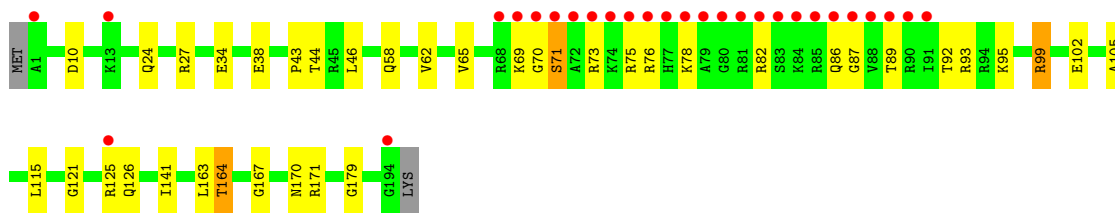
- Molecule 2: 50S ribosomal protein L3P



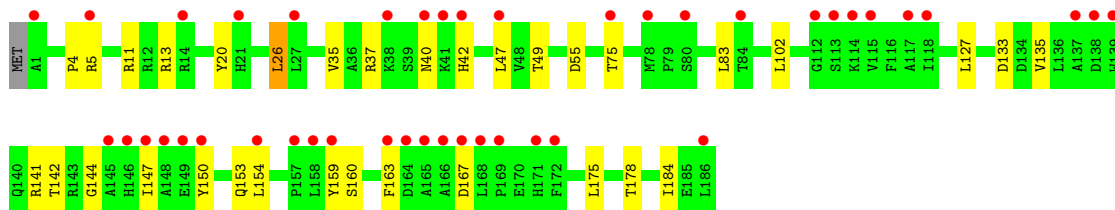
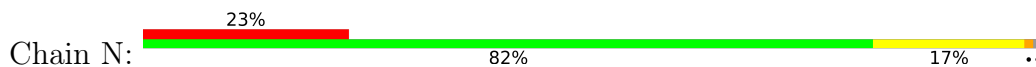
- Molecule 3: 50S ribosomal protein L4P



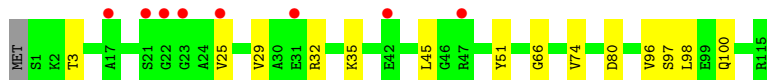
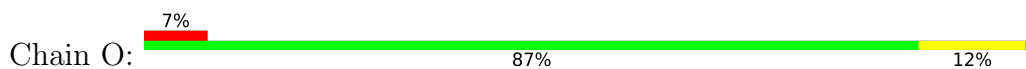
- Molecule 4: 50S ribosomal protein L5P



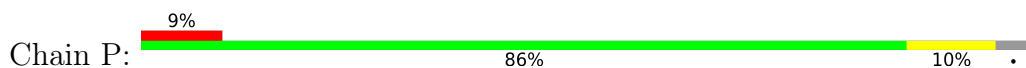
- Molecule 14: 50S ribosomal protein L18P



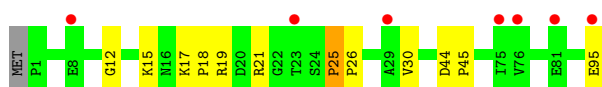
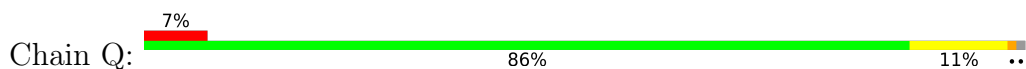
- Molecule 15: 50S ribosomal protein L18e



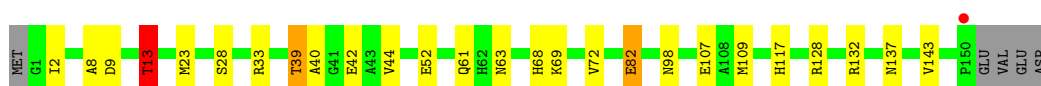
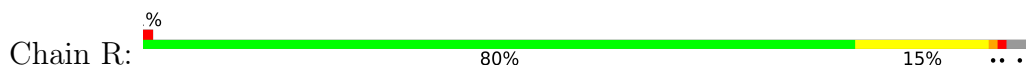
- Molecule 16: 50S ribosomal protein L19e



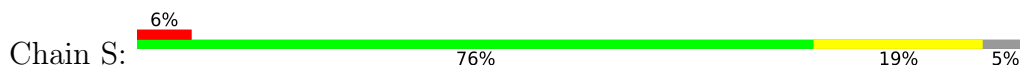
- Molecule 17: 50S ribosomal protein L21e



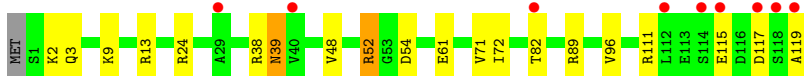
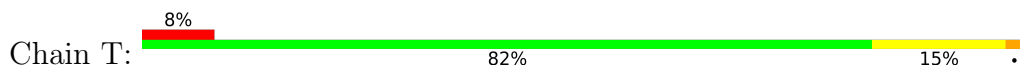
- Molecule 18: 50S ribosomal protein L22P



- Molecule 19: 50S ribosomal protein L23P



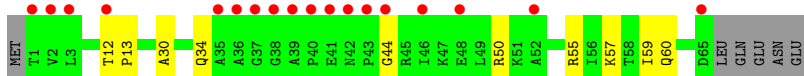
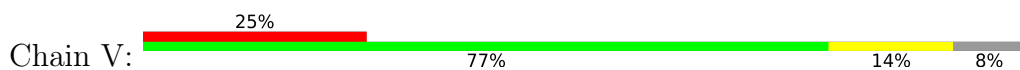
- Molecule 20: 50S ribosomal protein L24P



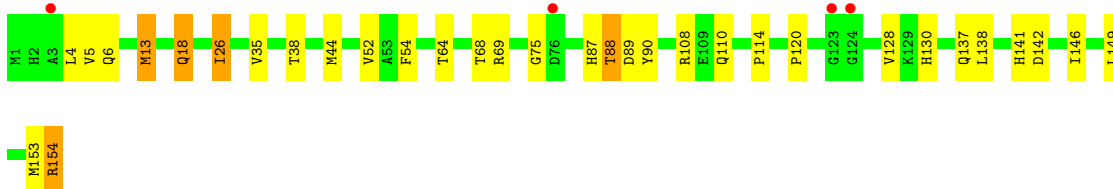
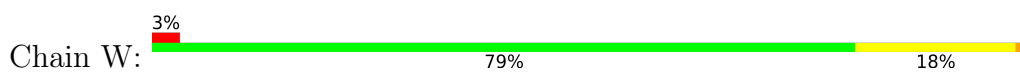
- Molecule 21: 50S ribosomal protein L24e



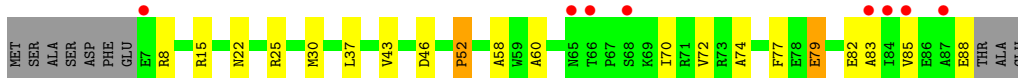
- Molecule 22: 50S ribosomal protein L29P



- Molecule 23: 50S ribosomal protein L30P

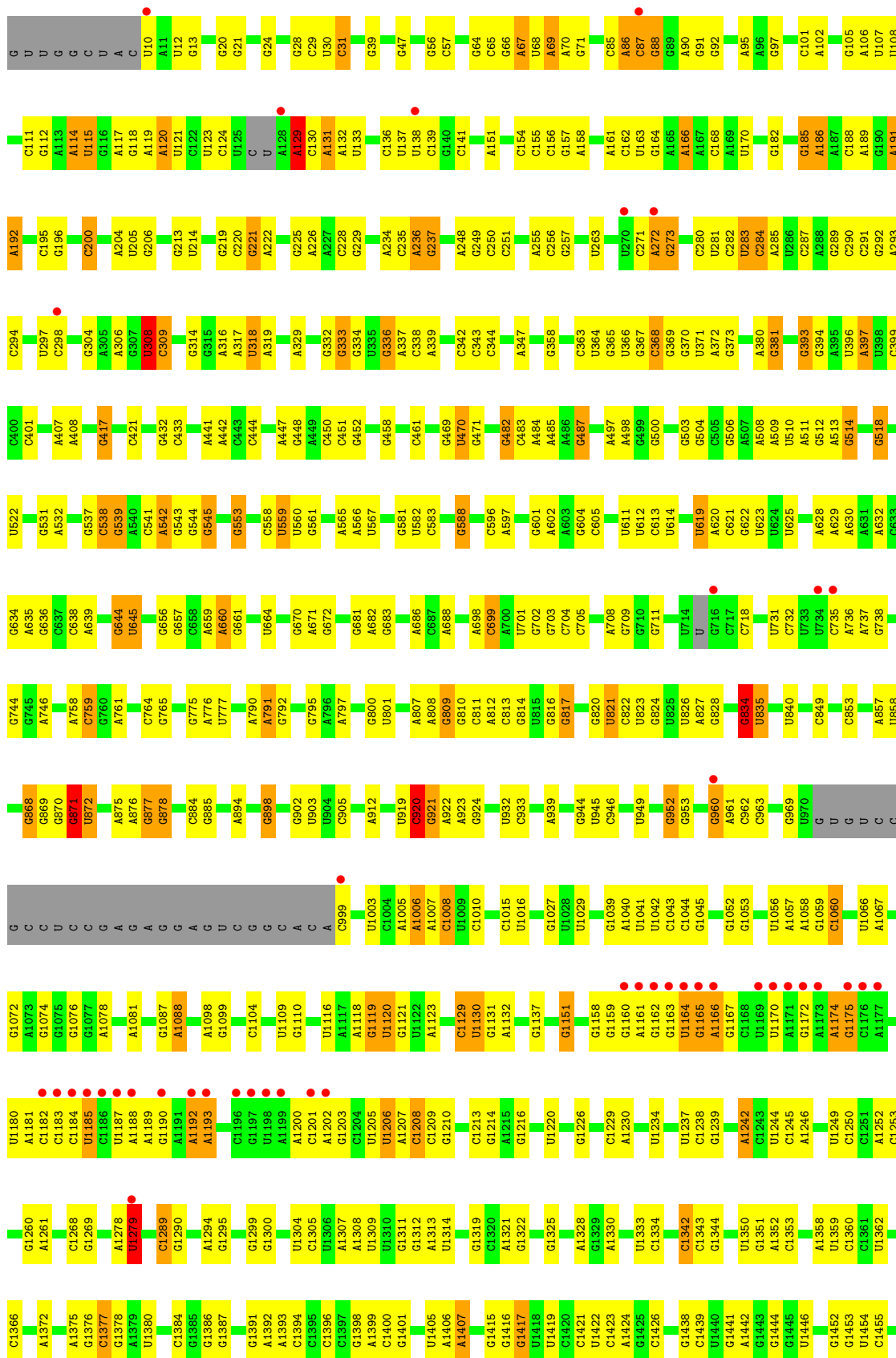


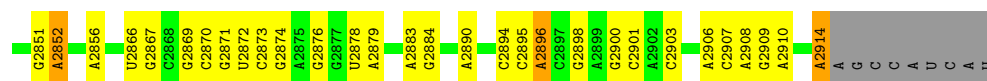
- Molecule 24: 50S ribosomal protein L31e



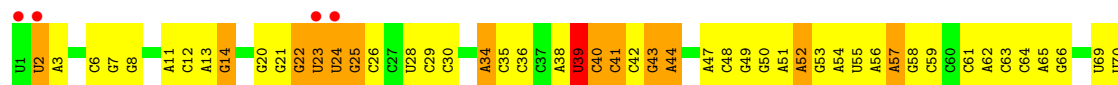
- Molecule 25: 50S ribosomal protein L32e







- Molecule 31: 5S RIBOSOMAL RNA



- Molecule 32: RNA (5'-R(*CP*CP*(PPU))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.81Å 300.00Å 576.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.75 49.95 – 2.75	Depositor EDS
% Data completeness (in resolution range)	91.0 (49.95-2.75) 91.1 (49.95-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.193 , 0.241 0.188 , 0.233	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtrriage
Anisotropy	0.243	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99180	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: 1MA, PPU, PSU, SR, OMU, K, NA, OMG, MG, CD, CL, UR3

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	0.64	0/1786	1.10	6/2408 (0.2%)
2	B	0.62	3/2690 (0.1%)	1.09	9/3652 (0.2%)
3	C	0.62	0/1885	1.10	7/2552 (0.3%)
4	D	0.71	0/1111	1.06	8/1498 (0.5%)
5	E	0.67	0/1382	0.97	2/1880 (0.1%)
6	F	0.70	1/901 (0.1%)	1.14	1/1224 (0.1%)
7	G	0.59	0/241	1.06	0/324
8	H	0.66	0/1302	1.09	7/1743 (0.4%)
9	I	0.72	0/526	1.07	1/716 (0.1%)
10	J	0.66	1/1136 (0.1%)	1.12	5/1530 (0.3%)
11	K	0.60	0/1004	1.13	7/1351 (0.5%)
12	L	0.59	0/1130	1.09	9/1509 (0.6%)
13	M	0.59	0/1582	1.03	3/2116 (0.1%)
14	N	0.65	0/1474	1.16	9/1999 (0.5%)
15	O	0.59	0/874	1.08	3/1181 (0.3%)
16	P	0.53	0/1147	1.05	0/1528
17	Q	0.59	0/749	1.13	5/1005 (0.5%)
18	R	0.64	1/1172 (0.1%)	1.08	4/1578 (0.3%)
19	S	0.58	0/648	0.99	0/875
20	T	0.57	0/958	1.14	4/1289 (0.3%)
21	U	0.63	0/417	1.09	2/562 (0.4%)
22	V	0.57	0/502	1.14	1/675 (0.1%)
23	W	0.69	1/1219 (0.1%)	1.16	4/1655 (0.2%)
24	X	0.66	0/664	1.20	6/895 (0.7%)
25	Y	0.61	0/1146	1.05	2/1536 (0.1%)
26	Z	0.78	0/584	1.17	2/781 (0.3%)
27	1	0.56	0/438	1.03	2/578 (0.3%)
28	2	0.54	0/401	1.04	0/529
29	3	0.78	0/771	1.07	2/1024 (0.2%)
30	0	0.38	0/65956	0.60	15/102865 (0.0%)
31	9	0.37	0/2904	0.56	1/4526 (0.0%)
32	4	0.44	0/40	0.61	0/60

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.47	7/98740 (0.0%)	0.76	127/147644 (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
23	W	0	1
30	0	0	40
All	All	0	41

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	63	ILE	CA-CB	9.37	1.58	1.54
18	R	109	MET	SD-CE	-7.85	1.59	1.79
23	W	13	MET	SD-CE	-6.79	1.62	1.79
2	B	162	MET	SD-CE	-6.55	1.63	1.79
10	J	19	MET	SD-CE	-6.01	1.64	1.79
2	B	69	VAL	CA-CB	5.32	1.58	1.54
2	B	251	VAL	CA-CB	5.09	1.60	1.53

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	52	ARG	N-CA-C	10.68	126.89	113.43
17	Q	17	LYS	N-CA-C	-8.38	99.54	109.93
14	N	163	PHE	N-CA-C	-8.00	100.69	111.96
23	W	75	GLY	N-CA-C	7.65	119.95	111.85
10	J	89	HIS	N-CA-C	7.62	122.25	112.34
24	X	22	ASN	N-CA-C	7.54	120.46	111.33
3	C	205	ARG	N-CA-C	7.52	120.42	111.33
8	H	10	ARG	N-CA-C	7.52	120.35	111.71
9	I	127	CYS	N-CA-C	7.45	119.09	110.97
2	B	222	LYS	N-CA-C	-7.36	99.02	110.42
4	D	136	ARG	CA-C-N	7.13	128.75	119.84
4	D	136	ARG	C-N-CA	7.13	128.75	119.84
5	E	11	VAL	N-CA-C	7.11	120.00	108.97
8	H	161	THR	N-CA-C	7.00	122.26	112.75
30	0	834	G	C2'-C3'-O3'	-6.88	103.38	113.70
4	D	171	ASP	N-CA-C	6.80	118.45	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	42	HIS	N-CA-C	6.76	120.16	109.81
17	Q	25	PRO	CA-C-N	6.73	126.42	119.56
17	Q	25	PRO	C-N-CA	6.73	126.42	119.56
12	L	73	VAL	N-CA-C	6.70	117.45	110.62
11	K	46	LYS	N-CA-C	6.69	121.19	109.96
1	A	129	LEU	N-CA-C	6.64	121.22	112.13
24	X	79	GLU	N-CA-C	6.62	118.16	111.07
4	D	170	TYR	N-CA-C	6.57	124.79	110.80
26	Z	42	TYR	N-CA-C	6.40	124.43	110.80
8	H	119	ALA	N-CA-C	6.34	120.27	112.54
14	N	13	ARG	N-CA-C	-6.31	105.72	113.41
20	T	3	GLN	CA-C-N	6.29	126.49	119.32
20	T	3	GLN	C-N-CA	6.29	126.49	119.32
12	L	149	ARG	N-CA-C	6.22	118.95	109.62
30	0	1504	A	N9-C1'-C2'	6.20	121.30	112.00
1	A	37	VAL	N-CA-C	6.20	122.23	109.34
30	0	1120	U	C5'-C4'-C3'	-6.11	106.83	116.00
1	A	135	VAL	N-CA-C	6.08	117.68	108.80
24	X	77	PHE	N-CA-C	6.05	116.07	108.45
26	Z	88	PHE	N-CA-C	6.05	119.06	109.81
3	C	134	ASP	N-CA-C	-6.03	105.83	113.43
6	F	59	ILE	N-CA-C	5.95	116.61	110.36
30	0	1819	G	C5'-C4'-C3'	5.95	124.92	116.00
30	0	2726	U	N1-C1'-C2'	5.94	120.90	112.00
23	W	87	HIS	N-CA-C	5.92	119.69	112.23
22	V	30	ALA	N-CA-C	-5.92	106.09	113.55
24	X	25	ARG	N-CA-C	5.91	117.73	111.28
2	B	323	LEU	N-CA-C	5.90	118.38	110.35
1	A	222	GLY	N-CA-C	-5.86	107.50	114.48
12	L	7	GLN	N-CA-C	5.86	119.69	112.54
24	X	60	ALA	N-CA-C	5.85	118.41	111.33
11	K	94	ALA	N-CA-C	5.84	118.06	109.24
23	W	69	ARG	N-CA-C	5.84	121.31	113.72
12	L	55	GLN	N-CA-C	5.82	119.19	111.75
15	O	51	TYR	N-CA-C	5.81	120.53	113.38
14	N	75	THR	N-CA-C	5.80	121.26	113.72
3	C	84	VAL	N-CA-C	-5.79	102.06	109.30
14	N	153	GLN	N-CA-C	-5.79	100.94	109.62
11	K	74	VAL	CB-CA-C	5.78	116.15	111.06
2	B	157	LYS	N-CA-C	-5.77	106.09	114.12
1	A	25	ALA	N-CA-C	5.77	118.05	108.99
4	D	137	PRO	N-CA-C	5.74	124.30	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	3	60	LYS	N-CA-C	-5.73	102.85	110.07
20	T	72	ILE	N-CA-C	5.71	117.64	108.85
3	C	89	ALA	N-CA-C	5.69	117.96	111.02
21	U	50	GLU	N-CA-C	5.67	119.00	111.75
1	A	198	ASP	N-CA-C	5.64	120.22	113.23
3	C	19	PRO	N-CA-C	5.63	120.06	111.34
23	W	26	ILE	CB-CA-C	5.60	118.27	110.99
30	0	2291	A	N9-C1'-C2'	5.57	120.36	112.00
18	R	63	ASN	N-CA-C	5.57	120.06	112.88
3	C	236	THR	N-CA-C	-5.55	101.23	110.17
18	R	82	GLU	N-CA-C	5.53	118.24	111.82
30	0	871	G	C5'-C4'-O4'	-5.53	101.50	109.80
30	0	920	C	C2'-C3'-O3'	-5.51	105.43	113.70
11	K	111	GLY	CA-C-N	5.51	125.50	120.21
11	K	111	GLY	C-N-CA	5.51	125.50	120.21
17	Q	12	GLY	N-CA-C	5.50	119.14	112.49
2	B	82	VAL	N-CA-C	5.49	119.73	112.04
2	B	143	ILE	N-CA-C	-5.47	101.67	108.89
12	L	145	LEU	N-CA-C	-5.45	105.37	112.23
15	O	66	GLY	N-CA-C	5.42	126.02	113.18
14	N	133	ASP	N-CA-C	5.41	116.85	111.07
8	H	34	HIS	N-CA-C	-5.39	107.35	114.04
25	Y	203	VAL	N-CA-C	5.38	116.34	108.53
13	M	121	GLY	N-CA-C	5.38	119.70	112.17
27	1	42	SER	N-CA-C	5.36	117.54	109.23
12	L	80	ASP	N-CA-C	5.35	122.20	110.80
12	L	12	THR	N-CA-C	5.35	119.65	113.18
11	K	54	THR	N-CA-C	-5.33	101.01	109.96
12	L	118	LEU	N-CA-C	5.32	118.08	109.40
13	M	125	ARG	N-CA-C	5.32	120.95	113.02
10	J	47	THR	N-CA-C	5.32	117.58	110.35
30	0	129	A	C2'-C3'-O3'	5.29	121.63	113.70
8	H	124	VAL	N-CA-C	5.29	118.25	112.96
14	N	150	TYR	N-CA-C	-5.28	107.01	113.50
14	N	20	TYR	N-CA-C	5.27	117.77	111.71
2	B	175	LEU	N-CA-C	-5.27	105.62	111.36
27	1	11	LYS	N-CA-C	5.27	117.72	108.56
5	E	91	PHE	N-CA-C	5.26	117.04	109.04
18	R	137	ASN	N-CA-C	5.26	118.30	110.52
30	0	2301	A	N9-C1'-C2'	5.25	119.88	112.00
8	H	164	CYS	N-CA-C	5.23	117.63	109.52
8	H	143	VAL	N-CA-C	5.22	115.94	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	9	39	U	N1-C1'-C2'	5.20	119.80	112.00
12	L	20	ASN	N-CA-C	5.19	119.09	111.04
30	0	308	U	C2'-C3'-O3'	-5.18	105.92	113.70
14	N	102	LEU	N-CA-C	5.18	117.20	109.59
3	C	175	LYS	N-CA-C	5.16	116.95	110.24
29	3	8	ASN	N-CA-C	5.16	117.17	108.96
30	0	1279	U	N1-C1'-C2'	5.16	119.74	112.00
4	D	15	GLU	CA-C-N	5.15	125.43	119.92
4	D	15	GLU	C-N-CA	5.15	125.43	119.92
10	J	75	PRO	CA-C-N	5.14	127.44	120.65
10	J	75	PRO	C-N-CA	5.14	127.44	120.65
18	R	13	THR	N-CA-C	5.12	117.17	109.23
17	Q	44	ASP	N-CA-C	-5.09	102.17	109.24
30	0	1819	G	C4'-C3'-C2'	-5.09	97.51	102.60
15	O	45	LEU	N-CA-C	5.08	117.56	111.71
2	B	83	ALA	N-CA-C	5.07	116.00	108.60
30	0	206	G	C5'-C4'-C3'	-5.04	108.44	116.00
13	M	87	GLY	N-CA-C	5.02	118.60	110.87
11	K	122	GLY	N-CA-C	5.02	118.75	112.73
2	B	154	VAL	CA-C-N	5.02	124.80	119.28
2	B	154	VAL	C-N-CA	5.02	124.80	119.28
4	D	16	PRO	N-CA-C	5.02	119.12	111.34
24	X	83	ALA	N-CA-C	5.02	116.57	108.34
10	J	45	VAL	N-CA-C	5.01	116.57	108.85
25	Y	143	TRP	N-CA-C	5.01	117.56	110.10
30	0	1261	A	N9-C1'-C2'	5.01	119.51	112.00
21	U	46	ALA	N-CA-C	5.01	117.39	111.33

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	115	U	Sidechain
30	0	1309	U	Sidechain
30	0	1417	G	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1878	G	Sidechain
30	0	1970	G	Sidechain
30	0	1978	A	Sidechain
30	0	1979	G	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2012	U	Sidechain
30	0	221	G	Sidechain
30	0	2308	U	Sidechain
30	0	2316	G	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2552	C	Sidechain
30	0	2557	U	Sidechain
30	0	2607	U	Sidechain
30	0	2681	A	Sidechain
30	0	2726	U	Sidechain
30	0	2774	U	Sidechain
30	0	2842	G	Sidechain
30	0	333	G	Sidechain
30	0	393	G	Sidechain
30	0	458	G	Sidechain
30	0	469	G	Sidechain
30	0	470	U	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	791	A	Sidechain
30	0	795	G	Sidechain
30	0	817	G	Sidechain
30	0	868	G	Sidechain
30	0	872	U	Sidechain
30	0	903	U	Sidechain
30	0	952	G	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	18	0
2	B	2625	0	2533	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1860	0	1813	19	0
4	D	1094	0	1085	11	0
5	E	1357	0	1266	8	0
6	F	890	0	843	5	0
7	G	240	0	231	2	0
8	H	1282	0	1292	11	0
9	I	519	0	500	5	0
10	J	1120	0	1098	18	0
11	K	994	0	1027	10	0
12	L	1118	0	1076	8	0
13	M	1558	0	1573	23	0
14	N	1445	0	1401	17	0
15	O	865	0	873	6	0
16	P	1136	0	1123	9	0
17	Q	735	0	729	7	0
18	R	1149	0	1122	15	0
19	S	641	0	605	9	0
20	T	950	0	924	8	0
21	U	410	0	364	2	0
22	V	499	0	511	6	0
23	W	1196	0	1137	19	0
24	X	654	0	653	5	0
25	Y	1130	0	1133	10	0
26	Z	573	0	534	11	0
27	1	431	0	426	11	0
28	2	396	0	413	10	0
29	3	755	0	732	14	0
30	0	59019	0	29812	902	0
31	9	2599	0	1325	69	0
32	4	74	0	51	7	0
33	0	86	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	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	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	93	0	0	0	0
35	1	2	0	0	0	0
35	3	2	0	0	0	0
35	9	3	0	0	0	0
35	A	2	0	0	0	0
35	B	1	0	0	0	0
35	F	1	0	0	0	0
35	J	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	0	65	0	0	0	0
36	9	2	0	0	0	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	2	0	0	0	0
39	0	5949	0	0	114	0
39	1	60	0	0	0	0
39	2	46	0	0	0	0
39	3	62	0	0	0	0
39	9	148	0	0	6	0
39	A	115	0	0	2	0
39	B	136	0	0	5	0
39	C	167	0	0	2	0
39	D	45	0	0	1	0
39	E	46	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	F	28	0	0	0	0
39	G	17	0	0	0	0
39	H	65	0	0	0	0
39	I	7	0	0	1	0
39	J	49	0	0	2	0
39	K	53	0	0	0	0
39	L	92	0	0	2	0
39	M	123	0	0	1	0
39	N	55	0	0	0	0
39	O	37	0	0	0	0
39	P	63	0	0	0	0
39	Q	51	0	0	0	0
39	R	78	0	0	2	0
39	S	31	0	0	0	0
39	T	38	0	0	0	0
39	U	30	0	0	1	0
39	V	10	0	0	0	0
39	W	67	0	0	0	0
39	X	23	0	0	0	0
39	Y	93	0	0	1	0
39	Z	25	0	0	1	0
All	All	99180	0	59971	1130	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 8.

All (1130) 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)
30:0:1160:G:H5'	30:0:1161:A:H5'	1.17	1.08
30:0:1559:A:H1'	39:0:5885:HOH:O	1.55	1.05
31:9:76:G:H3'	31:9:77:A:H5''	1.41	1.00
30:0:871:G:H5'	30:0:871:G:H8	1.25	0.99
30:0:871:G:H5'	30:0:871:G:C8	1.97	0.98
30:0:1701:A:H4'	30:0:1702:U:H5''	1.47	0.96
10:J:82:THR:HG23	30:0:1242:A:H5'	1.49	0.94
30:0:870:G:H2'	30:0:871:G:H5''	1.51	0.91
13:M:171:ARG:HD3	30:0:156:C:H5''	1.49	0.91
16:P:115:SER:H	16:P:118:GLN:HE21	1.19	0.90
30:0:2717:C:C2'	30:0:2718:C:H5''	2.03	0.89
30:0:1160:G:C5'	30:0:1161:A:H5'	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:56:A:H2'	31:9:57:A:H5''	1.52	0.88
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.88	0.88
30:0:1160:G:H5'	30:0:1161:A:C5'	2.02	0.87
30:0:1118:A:H62	30:0:1244:U:H3	1.21	0.87
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.40	0.86
30:0:1835:U:H5	30:0:1840:A:N7	1.73	0.86
30:0:2533:C:H6	30:0:2533:C:H5'	1.41	0.86
30:0:2321:A:H2	30:0:2378:U:H3	1.21	0.85
31:9:29:C:H2'	31:9:30:C:H5'	1.59	0.85
30:0:1603:A:H5'	30:0:1605:G:O4'	1.77	0.84
30:0:2717:C:H2'	30:0:2718:C:H5''	1.59	0.84
11:K:10:GLN:H	11:K:10:GLN:HE21	1.22	0.84
30:0:545:G:H5'	30:0:545:G:H8	1.39	0.84
30:0:2506:A:HO2'	30:0:2507:G:H8	0.87	0.84
30:0:1116:U:HO2'	30:0:1118:A:H2	0.86	0.84
30:0:1116:U:O2'	30:0:1118:A:H2	1.64	0.81
30:0:1118:A:H3'	30:0:1118:A:H8	1.47	0.79
13:M:163:LEU:HD21	30:0:188:C:H5''	1.62	0.79
30:0:871:G:H8	30:0:871:G:C5'	1.96	0.79
30:0:1300:G:H1'	39:0:4703:HOH:O	1.82	0.79
39:B:9053:HOH:O	30:0:2672:C:H1'	1.82	0.78
31:9:14:G:H5'	31:9:14:G:H8	1.47	0.78
30:0:2421:G:H1'	39:0:7053:HOH:O	1.83	0.78
30:0:2812:A:H2	30:0:2814:A:H62	1.32	0.78
30:0:2506:A:O2'	30:0:2507:G:H8	1.66	0.78
30:0:1118:A:H3'	30:0:1118:A:C8	2.19	0.77
30:0:1666:C:O2'	30:0:1667:A:H5''	1.85	0.77
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.65	0.77
30:0:1474:C:H5'	30:0:1474:C:H6	1.50	0.77
30:0:1667:A:H5'	30:0:1667:A:H8	1.49	0.77
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.31	0.77
2:B:206:THR:HG21	30:0:2716:G:H5''	1.67	0.76
30:0:542:A:H5'	30:0:542:A:H8	1.51	0.76
30:0:282:C:H1'	30:0:368:C:N4	2.01	0.76
30:0:1164:U:H3	30:0:1192:A:H2	1.32	0.76
15:O:3:THR:HG22	30:0:656:G:H5'	1.68	0.76
30:0:506:G:H22	30:0:509:A:C5'	1.98	0.76
30:0:2908:A:H2'	30:0:2909:G:O4'	1.85	0.76
31:9:92:G:H2'	31:9:93:A:C8	2.21	0.75
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.69	0.75
30:0:1183:C:H2'	39:0:6265:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.35	0.74
30:0:1116:U:H3	30:0:1246:A:H62	1.34	0.73
3:C:139:VAL:HG13	39:C:8643:HOH:O	1.88	0.73
30:0:969:G:H1	30:0:999:C:H42	1.37	0.73
30:0:1205:U:H2'	30:0:1206:U:H5'	1.71	0.73
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.70	0.72
30:0:1741:U:O2'	30:0:2723:G:H4'	1.88	0.72
30:0:544:G:H2'	30:0:545:G:H5''	1.68	0.72
23:W:44:MET:HE2	30:0:944:G:H21	1.54	0.72
30:0:559:U:H6	30:0:559:U:H5'	1.53	0.72
30:0:2717:C:O2'	30:0:2718:C:H5''	1.88	0.72
30:0:2420:G:O2'	30:0:2421:G:H5'	1.89	0.71
30:0:1183:C:N4	30:0:1184:C:H41	1.88	0.71
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.88	0.71
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.88	0.71
30:0:2637:A:H4'	39:0:4955:HOH:O	1.91	0.71
30:0:558:C:C2'	30:0:559:U:H5''	2.21	0.71
30:0:1666:C:C2'	30:0:1667:A:H5''	2.21	0.71
31:9:7:G:H5'	39:9:9100:HOH:O	1.89	0.71
30:0:2578:G:H5'	30:0:2578:G:H8	1.56	0.70
30:0:823:U:H3'	39:0:4468:HOH:O	1.90	0.70
30:0:1189:A:H1'	30:0:1209:C:O4'	1.91	0.70
30:0:870:G:C2'	30:0:871:G:H5''	2.19	0.70
25:Y:204:ARG:HH22	30:0:553:G:P	2.15	0.70
30:0:1119:G:N2	30:0:1246:A:C2	2.58	0.70
30:0:1206:U:H5'	30:0:1206:U:H6	1.56	0.70
3:C:184:ARG:NH2	30:0:450:C:OP1	2.25	0.70
30:0:506:G:H22	30:0:509:A:H5''	1.57	0.70
30:0:2073:G:H5''	39:0:3843:HOH:O	1.91	0.70
30:0:2502:C:C2'	30:0:2503:A:H5'	2.22	0.70
31:9:56:A:C2'	31:9:57:A:H5''	2.22	0.70
30:0:2534:C:H1'	39:0:3506:HOH:O	1.91	0.70
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.69
30:0:1372:A:H3'	39:0:7222:HOH:O	1.92	0.69
30:0:1838:U:O2'	30:0:2644:C:H5'	1.92	0.69
4:D:140:ARG:HB3	31:9:29:C:H5''	1.75	0.69
30:0:2321:A:H8	30:0:2322:U:HO2'	1.40	0.69
30:0:2491:G:H1'	39:0:6897:HOH:O	1.92	0.69
30:0:1189:A:H3'	39:0:7712:HOH:O	1.92	0.69
30:0:1205:U:H2'	30:0:1206:U:C5'	2.23	0.69
31:9:24:U:H3'	31:9:25:G:H5'	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:545:G:H5'	30:0:545:G:C8	2.25	0.69
3:C:27:ARG:NH2	30:0:657:G:OP1	2.25	0.68
30:0:1183:C:H42	30:0:1184:C:H41	1.40	0.68
30:0:2712:G:H5'	39:0:5248:HOH:O	1.92	0.68
30:0:308:U:H5'	30:0:309:C:OP1	1.93	0.68
30:0:960:G:H3'	30:0:960:G:N3	2.08	0.68
30:0:2502:C:H2'	30:0:2503:A:H5'	1.75	0.68
30:0:2073:G:OP2	30:0:2490:A:H5'	1.93	0.68
30:0:2419:U:H5''	30:0:2420:G:H5'	1.74	0.68
30:0:541:C:H2'	30:0:542:A:C5'	2.23	0.68
30:0:635:A:H2'	30:0:636:G:H5''	1.76	0.68
30:0:853:C:H3'	39:0:4574:HOH:O	1.94	0.67
30:0:1474:C:H5'	30:0:1474:C:C6	2.29	0.67
30:0:1641:A:H2'	30:0:1642:A:H5'	1.76	0.67
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.42	0.67
30:0:2586:U:H3	30:0:2592:G:H22	1.42	0.67
30:0:281:U:H2'	30:0:282:C:O4'	1.94	0.67
30:0:31:C:H4'	39:0:7452:HOH:O	1.94	0.67
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.77	0.67
30:0:1130:U:H2'	30:0:1131:G:O4'	1.95	0.67
30:0:541:C:C2'	30:0:542:A:H5''	2.24	0.67
22:V:50:ARG:HH12	30:0:56:G:H5''	1.60	0.66
30:0:1942:A:H3'	39:0:7377:HOH:O	1.95	0.66
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.43	0.66
30:0:2613:G:O2'	30:0:2614:C:H5'	1.95	0.66
30:0:1330:A:H4'	39:0:7478:HOH:O	1.95	0.66
13:M:27:ARG:NH2	13:M:44:THR:HG23	2.09	0.66
30:0:182:G:H5'	39:0:5187:HOH:O	1.93	0.66
18:R:128:ARG:NH2	30:0:2054:A:N3	2.43	0.66
30:0:2635:A:O2'	30:0:2636:C:H5'	1.95	0.66
39:Z:395:HOH:O	30:0:1886:A:H4'	1.96	0.66
30:0:541:C:H2'	30:0:542:A:H5''	1.77	0.65
30:0:558:C:H2'	30:0:559:U:H5''	1.77	0.65
30:0:877:G:H5'	30:0:878:G:OP1	1.96	0.65
30:0:2756:U:H3	30:0:2896:A:H2	1.44	0.65
30:0:1666:C:H2'	30:0:1667:A:C5'	2.26	0.65
30:0:2533:C:H5'	30:0:2533:C:C6	2.29	0.65
30:0:659:A:H5''	39:0:7132:HOH:O	1.97	0.65
30:0:2291:A:C8	30:0:2309:C:H5'	2.31	0.65
30:0:2769:C:H2'	30:0:2770:G:O4'	1.97	0.65
30:0:681:G:N3	30:0:681:G:H5'	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.62	0.65
30:0:318:U:H5'	30:0:339:A:C2	2.32	0.65
30:0:812:A:H2'	30:0:813:C:C6	2.32	0.65
30:0:969:G:H1	30:0:999:C:N4	1.95	0.65
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.78	0.64
30:0:1835:U:C5	30:0:1840:A:N7	2.62	0.64
14:N:40:ASN:ND2	31:9:28:U:H5''	2.13	0.64
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.61	0.64
30:0:544:G:C2'	30:0:545:G:H5''	2.26	0.64
30:0:814:G:H4'	39:0:3146:HOH:O	1.97	0.64
30:0:2795:C:O2'	30:0:2796:U:H5'	1.97	0.64
30:0:282:C:O2'	30:0:283:U:H5'	1.98	0.64
30:0:1279:U:H2'	30:0:1279:U:O2	1.98	0.64
26:Z:44:ARG:NH1	30:0:1887:U:H4'	2.12	0.64
30:0:2005:G:OP2	30:0:2005:G:H3'	1.97	0.64
30:0:2827:A:H2'	30:0:2828:G:O4'	1.97	0.63
2:B:238:ASN:HD22	2:B:240:GLY:H	1.47	0.63
30:0:1170:U:H2'	30:0:1172:G:OP2	1.99	0.63
30:0:1701:A:H5''	30:0:1702:U:H3'	1.81	0.63
30:0:2401:A:H2'	30:0:2402:A:C8	2.34	0.63
30:0:2896:A:H5''	39:0:6123:HOH:O	1.99	0.62
18:R:98:ASN:HD21	30:0:500:G:H21	1.47	0.62
30:0:871:G:C8	30:0:871:G:C5'	2.74	0.62
30:0:1087:G:H4'	30:0:1088:A:OP1	1.99	0.62
30:0:2563:U:H2'	30:0:2565:C:O5'	1.99	0.62
30:0:2824:C:H5''	30:0:2825:C:H5'	1.82	0.62
30:0:2851:G:C2'	30:0:2852:A:H5'	2.30	0.62
31:9:13:A:O2'	31:9:14:G:H5''	2.00	0.62
22:V:50:ARG:NH1	30:0:56:G:H5''	2.13	0.62
30:0:506:G:H22	30:0:509:A:H5'	1.65	0.62
30:0:381:G:H5''	39:0:4338:HOH:O	1.98	0.62
30:0:2505:G:O2'	30:0:2506:A:H5'	2.00	0.62
30:0:221:G:H5''	39:0:5759:HOH:O	1.99	0.62
31:9:2:U:OP2	31:9:3:A:H5'	1.99	0.62
30:0:821:U:H3'	39:0:3785:HOH:O	1.99	0.62
30:0:2511:A:H2'	30:0:2512:U:O4'	2.00	0.61
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.99	0.61
30:0:69:A:H5'	30:0:69:A:C8	2.35	0.61
30:0:582:U:H2'	30:0:583:C:C6	2.35	0.61
30:0:625:U:H5''	30:0:1044:C:N4	2.16	0.61
18:R:39:THR:HG22	18:R:42:GLU:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1919:A:H4'	39:0:4875:HOH:O	1.99	0.61
10:J:41:ALA:HB3	39:J:9025:HOH:O	1.99	0.61
30:0:10:U:O4	30:0:531:G:H2'	2.01	0.61
7:G:64:ASN:N	7:G:64:ASN:HD22	1.99	0.61
30:0:2336:G:H2'	39:0:6318:HOH:O	2.01	0.61
30:0:1455:C:H3'	39:0:7908:HOH:O	2.01	0.61
28:2:41:HIS:H	28:2:45:ASN:HD22	1.48	0.61
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.47	0.60
30:0:363:C:H1'	39:0:5308:HOH:O	2.00	0.60
31:9:49:G:O2'	31:9:50:G:H5'	2.01	0.60
13:M:27:ARG:HH22	13:M:44:THR:HG23	1.66	0.60
30:0:2002:C:H2'	30:0:2003:U:H5'	1.83	0.60
30:0:1278:A:H4'	30:0:1279:U:C4	2.36	0.60
30:0:1666:C:H2'	30:0:1667:A:H5'	1.84	0.60
14:N:37:ARG:NH1	31:9:6:C:OP1	2.34	0.60
30:0:2426:G:H1'	39:0:6116:HOH:O	2.01	0.60
11:K:39:GLY:HA2	39:0:5248:HOH:O	2.02	0.60
29:3:80:ARG:NH2	30:0:2381:C:H4'	2.15	0.60
30:0:1120:U:H5'	30:0:1121:G:OP2	2.02	0.60
30:0:1667:A:H5'	30:0:1667:A:C8	2.36	0.60
31:9:12:C:H5'	31:9:70:U:O4'	2.01	0.59
30:0:1132:A:N6	30:0:1229:C:H2'	2.18	0.59
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.18	0.59
23:W:154:ARG:NH1	30:0:588:G:O6	2.35	0.59
30:0:703:G:O2'	30:0:704:C:H5'	2.03	0.59
30:0:821:U:H2'	30:0:822:C:H6	1.68	0.59
30:0:119:A:H2'	30:0:120:A:H5''	1.85	0.59
30:0:485:A:N3	30:0:487:G:H5''	2.17	0.59
30:0:1189:A:H1'	30:0:1209:C:C1'	2.32	0.59
30:0:1528:A:H2'	30:0:1529:G:O4'	2.03	0.59
30:0:2769:C:O2'	30:0:2770:G:H5'	2.03	0.59
30:0:596:C:H2'	30:0:597:A:H8	1.68	0.59
30:0:2820:A:H2'	30:0:2821:C:C6	2.37	0.59
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.03	0.58
30:0:2748:G:H2'	39:0:7572:HOH:O	2.02	0.58
5:E:143:GLN:HE21	30:0:2780:C:C1'	2.16	0.58
30:0:1377:C:H6	30:0:1377:C:H5'	1.68	0.58
30:0:164:G:H3'	39:0:3657:HOH:O	2.03	0.58
30:0:195:C:H2'	30:0:196:G:H5'	1.85	0.58
31:9:29:C:C2'	31:9:30:C:H5'	2.29	0.58
2:B:18:ARG:HE	2:B:256:GLN:NE2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1778:A:H2'	30:0:1779:A:H5'	1.85	0.58
30:0:12:U:H2'	30:0:13:G:H5'	1.85	0.58
30:0:1701:A:H4'	30:0:1702:U:C5'	2.25	0.58
31:9:54:A:O2'	31:9:55:U:H5'	2.03	0.58
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.84	0.58
30:0:2239:C:H2'	30:0:2240:U:C6	2.39	0.58
1:A:199:HIS:HE1	30:0:1881:A:OP1	1.88	0.57
30:0:10:U:O4	30:0:532:A:OP2	2.22	0.57
30:0:256:C:H2'	30:0:257:G:O4'	2.04	0.57
30:0:1741:U:H5'	30:0:1742:A:OP1	2.04	0.57
30:0:2852:A:H5''	39:0:5259:HOH:O	2.04	0.57
1:A:48:ASP:HB3	39:A:9020:HOH:O	2.03	0.57
23:W:149:LEU:HG	23:W:153:MET:HE2	1.86	0.57
30:0:558:C:H2'	30:0:559:U:C5'	2.33	0.57
30:0:1206:U:H2'	30:0:1207:A:O4'	2.04	0.57
29:3:47:GLY:HA2	30:0:2121:G:H4'	1.87	0.57
30:0:1268:C:O2'	30:0:1269:G:H5'	2.05	0.57
29:3:42:ARG:NH1	30:0:396:U:H5'	2.20	0.57
30:0:371:U:H2'	30:0:372:A:H8	1.69	0.57
30:0:1595:G:O2'	30:0:1596:U:H5'	2.05	0.57
30:0:2644:C:O2'	30:0:2645:U:H5'	2.04	0.57
14:N:141:ARG:NH2	31:9:48:C:H4'	2.19	0.57
30:0:1592:G:H2'	30:0:1593:C:C6	2.40	0.57
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.57
30:0:69:A:H5'	30:0:69:A:H8	1.70	0.57
30:0:282:C:H1'	30:0:368:C:H41	1.68	0.57
30:0:1426:C:H2'	39:0:9601:HOH:O	2.04	0.57
30:0:1562:C:H3'	30:0:1563:G:C8	2.40	0.57
30:0:1759:A:N3	30:0:1818:C:H2'	2.20	0.57
30:0:2415:A:H2'	30:0:2416:G:H5'	1.86	0.57
26:Z:44:ARG:HH11	30:0:1887:U:H4'	1.69	0.56
12:L:6:ARG:HD3	30:0:1299:G:O6	2.05	0.56
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.85	0.56
30:0:1118:A:H8	30:0:1119:G:H5''	1.70	0.56
16:P:115:SER:H	16:P:118:GLN:NE2	1.97	0.56
30:0:1166:A:H1'	30:0:1192:A:C2	2.40	0.56
30:0:2597:U:H2'	30:0:2598:U:H5'	1.86	0.56
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.70	0.56
10:J:19:MET:HE1	10:J:78:ILE:HG22	1.86	0.56
30:0:214:U:H5'	39:0:6165:HOH:O	2.04	0.56
30:0:735:C:H5	30:0:736:A:C4	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:ILE:CD1	30:0:338:C:H4'	2.35	0.56
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.87	0.56
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.86	0.56
30:0:1213:C:O2'	30:0:1214:G:H5'	2.06	0.56
31:9:20:G:O2'	31:9:21:G:H5'	2.05	0.56
30:0:1118:A:C8	30:0:1118:A:C3'	2.84	0.56
30:0:1506:U:H6	30:0:1506:U:H5'	1.71	0.56
30:0:2414:A:H2'	30:0:2415:A:C8	2.41	0.56
30:0:1603:A:H5''	30:0:1604:G:H3'	1.88	0.56
30:0:2505:G:C2'	30:0:2506:A:H5'	2.36	0.56
30:0:2769:C:C2'	30:0:2770:G:H5'	2.36	0.56
30:0:613:C:H2'	30:0:614:U:H6	1.71	0.56
30:0:1666:C:C2'	30:0:1667:A:C5'	2.83	0.55
19:S:51:GLN:NE2	19:S:53:ASN:HD21	2.04	0.55
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.88	0.55
30:0:2090:G:H2'	30:0:2091:G:C8	2.41	0.55
30:0:2344:G:N3	30:0:2344:G:H2'	2.21	0.55
30:0:2851:G:O2'	30:0:2852:A:H5'	2.06	0.55
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.06	0.55
17:Q:19:ARG:HH21	31:9:11:A:P	2.28	0.55
18:R:117:HIS:HD2	30:0:20:G:H21	1.53	0.55
29:3:31:THR:O	30:0:1923:G:H4'	2.07	0.55
31:9:91:C:H2'	31:9:92:G:O4'	2.06	0.55
30:0:28:G:H1'	39:0:4701:HOH:O	2.06	0.55
3:C:174:ILE:HD11	30:0:338:C:H4'	1.87	0.55
10:J:45:VAL:HG11	10:J:121:LEU:HD22	1.88	0.55
20:T:52:ARG:O	30:0:317:A:OP1	2.25	0.55
30:0:421:C:H4'	30:0:1919:A:C6	2.41	0.55
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.53	0.55
30:0:559:U:H2'	30:0:560:U:O4'	2.06	0.55
30:0:31:C:H2'	39:0:7721:HOH:O	2.07	0.55
30:0:64:G:H2'	30:0:65:C:O4'	2.07	0.55
30:0:660:A:H4'	30:0:661:G:O5'	2.07	0.55
30:0:2524:G:H21	30:0:2526:C:N4	2.04	0.55
30:0:2791:U:H1'	30:0:2792:A:H5''	1.88	0.55
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.89	0.55
30:0:1189:A:O2'	30:0:1208:C:H2'	2.07	0.55
30:0:2900:G:H2'	30:0:2901:C:O4'	2.06	0.55
1:A:70:ALA:HB1	26:Z:89:THR:HG21	1.88	0.54
30:0:670:G:H2'	30:0:671:A:C8	2.41	0.54
30:0:1159:G:H21	30:0:1189:A:H8	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2239:C:H2'	30:0:2240:U:H6	1.72	0.54
30:0:2748:G:H1'	39:0:7934:HOH:O	2.07	0.54
30:0:1596:U:H2'	30:0:1598:A:OP2	2.06	0.54
30:0:2241:C:O2'	30:0:2242:U:H5'	2.07	0.54
30:0:834:G:H3'	30:0:835:U:H4'	1.89	0.54
30:0:2064:U:H5'	30:0:2652:U:H4'	1.90	0.54
30:0:2717:C:H2'	30:0:2718:C:C5'	2.33	0.54
31:9:75:G:H1	31:9:106:U:H3	1.55	0.54
30:0:2248:C:H3'	39:0:5468:HOH:O	2.06	0.54
30:0:1973:A:H2'	30:0:1974:G:O4'	2.08	0.54
31:9:49:G:H5''	39:9:9090:HOH:O	2.06	0.54
32:4:76:PPU:C	32:4:76:PPU:H5''	2.37	0.54
30:0:90:A:H2'	30:0:91:G:O4'	2.06	0.54
30:0:596:C:H2'	30:0:597:A:C8	2.42	0.54
30:0:1130:U:H5'	39:0:7704:HOH:O	2.07	0.54
30:0:1184:C:H1'	39:0:7498:HOH:O	2.07	0.54
30:0:1477:C:O2'	30:0:1478:U:H5'	2.08	0.54
30:0:2329:C:O2'	30:0:2330:U:H5'	2.07	0.54
31:9:76:G:C3'	31:9:77:A:H5''	2.28	0.54
39:L:8813:HOH:O	30:0:220:C:H2'	2.08	0.54
27:1:9:GLY:HA2	30:0:1687:C:O2	2.08	0.54
30:0:1042:U:O2'	30:0:1043:C:H5'	2.08	0.54
22:V:34:GLN:HE22	30:0:57:C:H4'	1.72	0.54
30:0:10:U:H3'	30:0:10:U:H6	1.73	0.54
30:0:1377:C:H1'	39:0:7305:HOH:O	2.08	0.54
13:M:179:GLY:O	30:0:399:C:H5'	2.07	0.54
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.07	0.54
30:0:1304:U:H2'	30:0:1305:C:C6	2.43	0.54
30:0:2032:U:H2'	30:0:2033:G:C5'	2.39	0.54
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.73	0.53
30:0:582:U:H2'	30:0:583:C:H6	1.73	0.53
30:0:1118:A:C8	30:0:1119:G:H5''	2.43	0.53
30:0:1657:A:H2'	30:0:1658:A:C8	2.44	0.53
30:0:2335:C:H2'	30:0:2336:G:C8	2.42	0.53
30:0:2372:A:H2'	30:0:2373:U:C6	2.44	0.53
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.74	0.53
30:0:200:C:H2'	39:0:3455:HOH:O	2.07	0.53
30:0:2256:G:O2'	30:0:2257:G:H5'	2.08	0.53
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.24	0.53
29:3:48:ASN:HD21	30:0:2468:A:H61	1.56	0.53
30:0:558:C:O2'	30:0:559:U:H5''	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:88:THR:HG22	23:W:89:ASP:H	1.74	0.53
30:0:1594:C:O2'	30:0:1607:A:H4'	2.07	0.53
30:0:2559:C:H4'	39:0:7287:HOH:O	2.09	0.53
27:1:28:HIS:HE1	30:0:776:A:OP1	1.92	0.53
30:0:1441:G:O2'	30:0:1442:A:H5'	2.07	0.53
30:0:2004:U:H4'	39:0:5336:HOH:O	2.09	0.53
30:0:2636:C:H3'	30:0:2637:A:H5'	1.91	0.53
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.91	0.53
30:0:1555:G:H4'	30:0:1630:A:H2	1.74	0.53
30:0:2377:U:O2'	30:0:2378:U:H5'	2.09	0.53
30:0:945:U:H2'	30:0:946:C:C6	2.44	0.53
30:0:1730:G:H5''	30:0:1731:C:H6	1.73	0.53
31:9:92:G:H2'	31:9:93:A:H8	1.73	0.53
2:B:229:ARG:NH2	30:0:1753:C:O2	2.41	0.52
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.49	0.52
30:0:1702:U:H1'	39:0:5793:HOH:O	2.08	0.52
30:0:2445:U:H2'	30:0:2446:G:C8	2.44	0.52
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.90	0.52
30:0:952:G:N3	30:0:2302:A:H2'	2.25	0.52
30:0:1973:A:H5'	30:0:1973:A:H8	1.74	0.52
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.74	0.52
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.07	0.52
30:0:1342:C:C2'	30:0:1343:C:H5'	2.39	0.52
30:0:1904:A:H2'	30:0:1905:U:O4'	2.09	0.52
30:0:2353:A:H4'	30:0:2354:A:O5'	2.09	0.52
30:0:2781:U:H2'	30:0:2782:G:H5'	1.91	0.52
30:0:482:G:H4'	30:0:508:A:N1	2.25	0.52
30:0:736:A:H2'	30:0:737:A:O4'	2.09	0.52
30:0:1181:A:H2'	30:0:1182:C:H5'	1.91	0.52
30:0:2542:C:H5''	30:0:2608:C:N4	2.24	0.52
1:A:179:MET:HG2	1:A:186:TRP:HB2	1.91	0.52
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.09	0.52
13:M:95:LYS:HE2	30:0:157:G:H4'	1.91	0.52
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.90	0.52
29:3:36:ILE:HG21	30:0:2433:A:OP1	2.09	0.52
30:0:541:C:H2'	30:0:542:A:H5'	1.89	0.52
30:0:611:U:H2'	30:0:612:U:C6	2.43	0.52
30:0:1066:U:H2'	30:0:1067:A:C8	2.44	0.52
30:0:1116:U:O2'	30:0:1118:A:C2	2.48	0.52
30:0:2718:C:H5'	30:0:2718:C:H6	1.75	0.52
31:9:23:U:O2'	31:9:24:U:H4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.41	0.52
25:Y:169:ARG:HD2	30:0:1328:A:OP1	2.10	0.52
30:0:702:G:O2'	30:0:703:G:H5'	2.10	0.52
30:0:1878:G:H1'	39:0:6145:HOH:O	2.10	0.52
3:C:27:ARG:HH22	30:0:657:G:P	2.33	0.52
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.25	0.52
30:0:1471:A:H2'	30:0:1472:C:C6	2.44	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.92	0.52
31:9:108:C:H2'	31:9:109:G:C8	2.45	0.52
39:D:6783:HOH:O	31:9:59:C:H4'	2.10	0.52
23:W:44:MET:CE	30:0:944:G:H21	2.21	0.52
29:3:80:ARG:O	30:0:2457:U:H4'	2.10	0.52
30:0:1174:A:C6	30:0:1201:C:H4'	2.45	0.52
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.91	0.52
20:T:38:ARG:NH1	39:0:6710:HOH:O	2.43	0.52
30:0:1187:U:O2'	30:0:1189:A:H2	1.93	0.52
30:0:1377:C:H5'	30:0:1377:C:C6	2.45	0.52
31:9:38:A:H2'	31:9:39:U:C6	2.45	0.52
20:T:9:LYS:HE2	20:T:13:ARG:NH1	2.25	0.52
30:0:704:C:H2'	30:0:705:C:H6	1.75	0.52
30:0:1245:C:H6	30:0:1245:C:O5'	1.93	0.52
30:0:1268:C:H2'	30:0:1269:G:H8	1.75	0.52
30:0:1819:G:H2'	30:0:1820:G:C5'	2.40	0.52
4:D:25:MET:HE3	4:D:41:LEU:HG	1.92	0.51
16:P:1:THR:O	30:0:1396:C:H1'	2.10	0.51
30:0:162:C:H2'	30:0:163:U:H5'	1.92	0.51
30:0:192:A:H5'	39:0:7678:HOH:O	2.10	0.51
30:0:297:U:H2'	30:0:298:C:C6	2.45	0.51
30:0:1819:G:H5'	39:0:4730:HOH:O	2.09	0.51
30:0:2781:U:C2'	30:0:2782:G:H5'	2.40	0.51
30:0:2872:U:H2'	30:0:2873:C:H6	1.76	0.51
30:0:1736:A:H1'	39:0:7617:HOH:O	2.10	0.51
16:P:105:LEU:HD21	16:P:137:LEU:HD11	1.92	0.51
30:0:221:G:H2'	30:0:222:A:C8	2.46	0.51
14:N:11:ARG:HD3	31:9:114:G:O6	2.10	0.51
30:0:236:A:H4'	30:0:237:G:OP1	2.09	0.51
30:0:565:A:H4'	39:0:3972:HOH:O	2.11	0.51
30:0:1453:G:H2'	30:0:1454:U:O4'	2.10	0.51
31:9:24:U:H3'	31:9:25:G:C5'	2.38	0.51
11:K:66:ARG:HH22	30:0:1994:A:P	2.34	0.51
30:0:1123:A:C2	30:0:1129:C:H4'	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1165:G:H4'	30:0:1174:A:O2'	2.11	0.51
30:0:1386:G:O2'	30:0:1387:G:H5'	2.10	0.51
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.58	0.51
18:R:2:ILE:HG22	30:0:21:G:H4'	1.91	0.51
30:0:291:C:H2'	30:0:292:G:O4'	2.11	0.51
30:0:1592:G:H2'	30:0:1593:C:H6	1.76	0.51
30:0:2002:C:C2'	30:0:2003:U:H5'	2.40	0.51
30:0:522:U:O2'	30:0:1366:C:H5'	2.10	0.51
2:B:212:GLN:HA	30:0:1733:A:H4'	1.92	0.51
14:N:35:VAL:HG11	31:9:6:C:H4'	1.91	0.51
14:N:144:GLY:O	14:N:147:ILE:HG22	2.10	0.51
30:0:1289:C:O2'	30:0:1290:G:H5'	2.11	0.51
30:0:2883:A:H2'	30:0:2884:G:O4'	2.11	0.51
14:N:55:ASP:OD2	31:9:7:G:H4'	2.11	0.51
23:W:64:THR:O	23:W:68:THR:HG22	2.10	0.51
28:2:42:TRP:HZ2	30:0:1438:G:H1'	1.75	0.51
30:0:185:G:O3'	30:0:186:A:H4'	2.11	0.51
30:0:1202:A:C2'	30:0:1203:G:H5'	2.40	0.51
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.91	0.51
20:T:38:ARG:HH21	30:0:306:A:P	2.33	0.51
29:3:2:GLN:O	30:0:2320:U:H2'	2.10	0.51
30:0:1201:C:H2'	30:0:1202:A:H5'	1.93	0.51
30:0:1249:U:H2'	30:0:1250:C:C6	2.46	0.51
30:0:2016:U:H2'	30:0:2017:U:O4'	2.11	0.51
31:9:108:C:H2'	31:9:109:G:H8	1.76	0.51
30:0:638:C:H2'	30:0:639:A:C8	2.47	0.50
30:0:2276:U:H2'	30:0:2277:U:C6	2.46	0.50
30:0:2618:G:N3	32:4:76:PPU:H2	2.25	0.50
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.07	0.50
3:C:118:THR:O	3:C:136:VAL:HG13	2.12	0.50
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.94	0.50
30:0:1768:C:H2'	30:0:1769:C:O4'	2.11	0.50
30:0:2256:G:C2'	30:0:2257:G:H5'	2.41	0.50
30:0:2510:C:H42	30:0:2564:G:H22	1.59	0.50
30:0:2703:A:H2'	30:0:2704:C:H6	1.76	0.50
31:9:63:C:O2'	31:9:64:C:H5'	2.12	0.50
15:O:3:THR:CG2	30:0:656:G:H5'	2.39	0.50
30:0:1484:G:H2'	39:0:9108:HOH:O	2.11	0.50
30:0:1174:A:C5	30:0:1201:C:H4'	2.46	0.50
31:9:36:C:H5'	39:9:9050:HOH:O	2.11	0.50
4:D:105:SER:OG	30:0:2338:G:H1'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:137:ASP:O	5:E:141:VAL:HG23	2.12	0.50
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.47	0.50
30:0:849:C:H1'	39:0:6642:HOH:O	2.10	0.50
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.27	0.50
30:0:2296:C:H4'	30:0:2362:A:H2	1.77	0.50
30:0:2670:G:O2'	30:0:2671:U:H5'	2.11	0.50
30:0:2768:A:O2'	30:0:2769:C:H5'	2.11	0.50
30:0:1681:G:H5''	30:0:1682:A:H5'	1.93	0.50
30:0:2578:G:H5'	30:0:2578:G:C8	2.43	0.50
2:B:252:PRO:HD2	30:0:2548:C:H5'	1.94	0.50
4:D:141:VAL:HG21	31:9:57:A:H8	1.77	0.50
12:L:111:ALA:HB2	30:0:698:A:H5''	1.92	0.50
30:0:366:U:H2'	30:0:367:G:O4'	2.11	0.50
30:0:1535:G:H2'	30:0:1536:C:C6	2.47	0.50
39:B:9053:HOH:O	30:0:2818:A:H2	1.95	0.49
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.92	0.49
30:0:407:A:H2'	30:0:408:A:C8	2.47	0.49
30:0:363:C:O2'	30:0:364:U:H5'	2.12	0.49
30:0:1741:U:H3'	39:0:9773:HOH:O	2.11	0.49
30:0:1819:G:H2'	30:0:1820:G:H4'	1.93	0.49
10:J:107:ASN:HD22	10:J:109:TYR:H	1.60	0.49
30:0:371:U:H2'	30:0:372:A:C8	2.47	0.49
30:0:514:G:OP1	30:0:514:G:H2'	2.11	0.49
30:0:1393:A:H2'	30:0:1394:C:C6	2.47	0.49
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.49
4:D:76:ARG:NE	31:9:44:A:O4'	2.44	0.49
24:X:15:ARG:NH2	30:0:2856:A:OP1	2.44	0.49
30:0:1180:U:H2'	30:0:1181:A:C8	2.48	0.49
30:0:1419:U:H2'	30:0:1685:A:C2	2.47	0.49
30:0:2608:C:H3'	39:0:7840:HOH:O	2.13	0.49
26:Z:43:GLY:HA2	30:0:1771:U:O2	2.12	0.49
30:0:711:G:C2	30:0:718:C:C2	3.00	0.49
30:0:1702:U:H5'	39:0:3437:HOH:O	2.12	0.49
30:0:2379:G:N3	30:0:2418:G:H2'	2.28	0.49
30:0:1527:A:H1'	30:0:1528:A:C8	2.48	0.49
30:0:1834:C:H2'	30:0:1840:A:N6	2.27	0.49
11:K:32:ILE:HD11	11:K:56:SER:HB2	1.95	0.49
26:Z:63:CYS:SG	26:Z:81:CYS:HB2	2.52	0.49
30:0:107:U:H2'	30:0:108:U:H5'	1.95	0.49
30:0:2266:A:H2'	30:0:2267:G:C8	2.47	0.49
3:C:39:GLN:O	3:C:43:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:4:PRO:HG3	31:9:69:U:OP1	2.13	0.49
29:3:48:ASN:HB3	30:0:170:U:H5'	1.95	0.49
30:0:1226:G:H5'	39:0:4554:HOH:O	2.11	0.49
30:0:1625:U:H4'	39:0:4685:HOH:O	2.13	0.49
30:0:1666:C:H2'	30:0:1667:A:H5''	1.89	0.49
30:0:1946:C:H2'	30:0:1971:G:C8	2.48	0.49
30:0:2348:C:H2'	30:0:2349:G:H8	1.78	0.49
30:0:2507:G:H2'	30:0:2510:C:H42	1.78	0.49
30:0:2542:C:H4'	32:4:75:C:O2'	2.12	0.49
30:0:2758:G:H2'	30:0:2759:C:C6	2.48	0.49
30:0:441:A:H1'	30:0:442:A:N7	2.28	0.49
27:1:12:ASN:O	30:0:1415:G:H5'	2.13	0.49
29:3:79:LEU:HD13	30:0:2457:U:H1'	1.94	0.49
30:0:1006:A:N1	30:0:2311:A:H1'	2.28	0.48
30:0:2421:G:H3'	30:0:2422:U:C5'	2.44	0.48
30:0:2644:C:H5''	39:0:3408:HOH:O	2.13	0.48
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.12	0.48
13:M:65:VAL:HG21	13:M:105:ALA:HB2	1.94	0.48
30:0:601:G:O2'	30:0:602:A:H5'	2.13	0.48
30:0:2320:U:H4'	30:0:2321:A:O4'	2.13	0.48
30:0:2509:A:H2'	30:0:2510:C:O4'	2.13	0.48
2:B:17:LYS:O	2:B:260:HIS:HD2	1.96	0.48
30:0:432:G:O2'	30:0:433:C:H5'	2.13	0.48
30:0:1058:A:H2'	30:0:1060:C:H5''	1.94	0.48
30:0:1131:G:C6	30:0:1230:A:C4	3.01	0.48
30:0:1205:U:C2'	30:0:1206:U:C5'	2.91	0.48
30:0:1452:G:O2'	30:0:1453:G:H5'	2.13	0.48
30:0:2469:A:H1'	39:0:3254:HOH:O	2.13	0.48
30:0:2619:UR3:H5	39:0:5872:HOH:O	2.13	0.48
12:L:27:ARG:HH21	12:L:30:ARG:HG2	1.78	0.48
30:0:249:G:O2'	30:0:250:C:H5'	2.14	0.48
30:0:1589:G:N2	30:0:1605:G:H1'	2.28	0.48
11:K:10:GLN:H	11:K:10:GLN:NE2	2.00	0.48
27:1:16:HIS:HD2	30:0:470:U:O2'	1.96	0.48
30:0:372:A:H2'	30:0:373:G:H8	1.78	0.48
30:0:629:A:H2'	30:0:630:A:O4'	2.14	0.48
29:3:33:MET:HG2	30:0:1922:A:H2'	1.96	0.48
30:0:553:G:O4'	30:0:1325:G:H5'	2.14	0.48
30:0:1667:A:H2'	30:0:1668:U:C6	2.48	0.48
30:0:1766:U:O2	30:0:1778:A:H5'	2.14	0.48
30:0:2256:G:H2'	30:0:2257:G:C5'	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2445:U:H2'	30:0:2446:G:H8	1.77	0.48
30:0:2783:A:H2'	30:0:2784:A:C8	2.49	0.48
1:A:206:ARG:NH2	30:0:2630:G:O6	2.46	0.48
30:0:661:G:C5	30:0:686:A:C2	3.02	0.48
30:0:2851:G:H2'	30:0:2852:A:H5'	1.96	0.48
31:9:34:A:H2'	31:9:35:C:O4'	2.14	0.48
30:0:2878:U:H2'	30:0:2879:A:O4'	2.14	0.48
20:T:2:LYS:HG2	30:0:447:A:OP1	2.14	0.48
23:W:88:THR:HG22	23:W:110:GLN:HE21	1.79	0.48
30:0:920:C:H5''	30:0:921:G:O5'	2.13	0.48
30:0:2001:G:O2'	30:0:2002:C:H5'	2.14	0.48
30:0:2812:A:C2	30:0:2814:A:N6	2.79	0.48
2:B:211:THR:HG21	39:0:7486:HOH:O	2.14	0.48
30:0:1477:C:H5'	30:0:1868:G:C5'	2.44	0.48
30:0:1972:U:H2'	30:0:1973:A:C5'	2.44	0.48
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.28	0.47
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.95	0.47
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.96	0.47
30:0:158:A:H3'	39:0:7591:HOH:O	2.14	0.47
30:0:1375:A:C2'	30:0:1376:G:H5'	2.43	0.47
30:0:2105:C:H2'	30:0:2106:C:C6	2.49	0.47
30:0:2689:A:H2'	30:0:2690:U:H5'	1.96	0.47
31:9:3:A:H2	31:9:21:G:N3	2.12	0.47
23:W:128:VAL:HG22	30:0:1098:A:OP1	2.14	0.47
30:0:1878:G:O2'	30:0:1879:U:OP2	2.32	0.47
30:0:2374:G:H2'	30:0:2375:A:C8	2.49	0.47
30:0:2506:A:O2'	30:0:2507:G:O5'	2.32	0.47
31:9:55:U:H4'	31:9:56:A:C8	2.49	0.47
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.50	0.47
22:V:44:GLY:HA3	30:0:92:G:H4'	1.95	0.47
30:0:287:C:H42	30:0:365:G:H1	1.62	0.47
30:0:380:A:H2'	39:0:7258:HOH:O	2.14	0.47
30:0:827:A:H2'	30:0:828:G:O4'	2.15	0.47
30:0:2411:C:H4'	39:0:4981:HOH:O	2.13	0.47
18:R:39:THR:HG23	18:R:107:GLU:O	2.14	0.47
30:0:67:A:H5''	30:0:69:A:C8	2.50	0.47
30:0:161:A:H2'	30:0:162:C:C6	2.49	0.47
30:0:105:G:O2'	30:0:106:A:H5'	2.14	0.47
30:0:542:A:H5'	30:0:542:A:C8	2.39	0.47
30:0:1187:U:H2'	39:0:6925:HOH:O	2.13	0.47
30:0:2321:A:H8	30:0:2322:U:O2'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2587:OMU:O5'	30:0:2587:OMU:H6	2.14	0.47
30:0:2909:G:H2'	30:0:2910:A:H8	1.80	0.47
31:9:78:G:H5'	39:9:9095:HOH:O	2.13	0.47
12:L:6:ARG:NH1	30:0:1299:G:N7	2.62	0.47
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.96	0.47
30:0:451:C:O2'	30:0:452:G:H5'	2.14	0.47
30:0:821:U:H2'	30:0:822:C:C6	2.47	0.47
30:0:2757:A:H2'	30:0:2758:G:O4'	2.14	0.47
2:B:217:ARG:HG3	2:B:257:THR:HG23	1.97	0.47
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.15	0.47
6:F:77:VAL:HG21	6:F:83:LEU:HD13	1.96	0.47
30:0:88:G:H5'	30:0:88:G:H8	1.80	0.47
30:0:304:G:H1'	30:0:347:A:N6	2.30	0.47
30:0:308:U:C4	30:0:342:C:H1'	2.50	0.47
30:0:790:A:H2'	30:0:791:A:O4'	2.15	0.47
30:0:1016:U:H1'	39:0:3672:HOH:O	2.13	0.47
30:0:2002:C:H2'	30:0:2003:U:C5'	2.44	0.47
30:0:2266:A:H2'	30:0:2267:G:H8	1.79	0.47
2:B:27:ASN:HD22	2:B:27:ASN:H	1.63	0.47
4:D:159:PRO:O	4:D:163:VAL:HG23	2.15	0.47
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.96	0.47
30:0:136:C:H2'	30:0:137:U:O4'	2.15	0.47
30:0:1815:A:H4'	30:0:2751:C:O4'	2.15	0.47
30:0:1903:U:O2'	30:0:1904:A:N7	2.43	0.47
31:9:95:C:O2'	31:9:96:C:H5'	2.15	0.47
2:B:297:VAL:HG23	39:B:9029:HOH:O	2.13	0.47
25:Y:144:ARG:NH1	39:0:7478:HOH:O	2.47	0.47
30:0:137:U:H2'	30:0:139:C:C5	2.50	0.47
30:0:807:A:O2'	30:0:808:A:H5'	2.15	0.47
30:0:1160:G:H2'	39:0:5654:HOH:O	2.15	0.47
30:0:2816:A:H5''	30:0:2817:G:H5'	1.97	0.47
3:C:236:THR:HG22	3:C:239:ALA:H	1.80	0.47
12:L:18:HIS:HD2	30:0:902:G:N7	2.12	0.47
30:0:24:G:N2	30:0:518:G:H1'	2.30	0.47
30:0:272:A:H5'	30:0:273:G:OP2	2.15	0.47
30:0:731:U:H2'	30:0:732:C:C6	2.50	0.47
30:0:1619:G:H2'	30:0:1620:C:O4'	2.15	0.47
31:9:3:A:N6	31:9:22:G:H1'	2.29	0.47
31:9:80:A:H2'	31:9:81:C:O4'	2.14	0.47
3:C:79:ARG:O	3:C:87:ARG:HG2	2.15	0.46
12:L:14:GLY:O	30:0:1295:G:H5''	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:25:LYS:HG3	28:2:49:GLU:H	1.80	0.46
30:0:816:G:H5'	30:0:1598:A:H4'	1.97	0.46
30:0:1202:A:H2'	30:0:1203:G:H5'	1.97	0.46
30:0:1804:A:H2'	30:0:1805:G:C8	2.50	0.46
30:0:372:A:H2'	30:0:373:G:C8	2.51	0.46
30:0:2252:A:H2'	30:0:2253:G:O4'	2.15	0.46
30:0:2563:U:O2'	30:0:2564:G:H3'	2.16	0.46
30:0:2619:UR3:H5'	32:4:76:PPU:H103	1.98	0.46
3:C:46:TYR:CE1	30:0:450:C:H4'	2.50	0.46
30:0:800:G:H2'	30:0:801:U:C6	2.50	0.46
30:0:1188:A:C6	30:0:1189:A:C6	3.03	0.46
30:0:1803:C:H2'	30:0:1804:A:C8	2.50	0.46
30:0:2300:A:H4'	30:0:2301:A:O5'	2.16	0.46
30:0:1515:A:H2'	30:0:1516:U:C6	2.50	0.46
30:0:1765:G:H1'	30:0:1780:G:N2	2.30	0.46
30:0:2764:C:H2'	30:0:2765:C:H6	1.80	0.46
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.44	0.46
30:0:101:C:H2'	30:0:102:A:C8	2.51	0.46
30:0:660:A:N6	30:0:746:A:O4'	2.49	0.46
30:0:708:A:H2'	30:0:709:G:O4'	2.14	0.46
30:0:1398:G:O2'	30:0:1399:A:H5'	2.15	0.46
30:0:2387:U:H2'	30:0:2388:C:C6	2.51	0.46
13:M:69:LYS:O	13:M:73:ARG:NH2	2.49	0.46
14:N:159:TYR:HE1	31:9:50:G:H5''	1.80	0.46
30:0:319:A:H4'	30:0:338:C:C4	2.50	0.46
30:0:542:A:H2'	30:0:543:G:O4'	2.16	0.46
30:0:644:G:N3	30:0:644:G:H5'	2.31	0.46
30:0:1189:A:H1'	30:0:1209:C:H1'	1.97	0.46
30:0:2133:U:H4'	30:0:2134:G:H5'	1.98	0.46
30:0:2591:C:H2'	30:0:2592:G:O4'	2.16	0.46
30:0:2691:A:H5'	30:0:2693:U:H1'	1.97	0.46
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.98	0.46
30:0:834:G:H4'	30:0:835:U:OP2	2.16	0.46
30:0:1166:A:H61	30:0:1180:U:H3	1.64	0.46
30:0:1589:G:H22	30:0:1605:G:H1'	1.81	0.46
3:C:63:SER:OG	30:0:2101:A:H2'	2.16	0.46
30:0:876:A:H2'	30:0:876:A:N3	2.31	0.46
31:9:29:C:H2'	31:9:30:C:C5'	2.40	0.46
31:9:57:A:H2'	31:9:58:G:O4'	2.16	0.46
23:W:88:THR:CG2	23:W:110:GLN:HE21	2.29	0.46
25:Y:208:LYS:O	30:0:1313:A:H5'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1056:U:H2'	30:0:1057:A:O4'	2.15	0.46
30:0:1158:G:O2'	30:0:1159:G:H5'	2.15	0.46
30:0:1330:A:H2	39:0:4703:HOH:O	1.99	0.46
30:0:1495:C:H1'	30:0:1573:A:H1'	1.98	0.46
30:0:1555:G:H4'	30:0:1630:A:C2	2.51	0.46
30:0:2481:G:H5''	39:0:4569:HOH:O	2.15	0.46
3:C:87:ARG:NH2	30:0:894:A:N1	2.63	0.46
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.46	0.46
25:Y:174:VAL:HG23	25:Y:177:LYS:HD2	1.98	0.46
30:0:226:A:H1'	30:0:393:G:C5	2.51	0.46
30:0:542:A:H1'	39:0:4696:HOH:O	2.15	0.46
30:0:560:U:H2'	30:0:561:G:H8	1.80	0.46
30:0:671:A:O2'	30:0:672:G:H2'	2.16	0.46
30:0:699:C:H2'	30:0:744:G:O4'	2.16	0.46
30:0:960:G:N3	30:0:960:G:C3'	2.79	0.46
30:0:1400:C:O2'	30:0:1401:G:H5'	2.16	0.46
30:0:1634:G:H3'	39:0:3912:HOH:O	2.14	0.46
30:0:1929:G:H1'	39:0:5188:HOH:O	2.15	0.46
30:0:2112:A:H2'	30:0:2113:G:C8	2.51	0.46
30:0:2421:G:H3'	30:0:2422:U:H5''	1.97	0.46
31:9:35:C:H5''	39:9:9078:HOH:O	2.15	0.46
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.49	0.45
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.64	0.45
30:0:343:C:O2'	30:0:344:C:H5'	2.16	0.45
30:0:541:C:O2'	30:0:542:A:H5''	2.17	0.45
30:0:1120:U:C6	30:0:1120:U:H5''	2.52	0.45
30:0:2636:C:H3'	30:0:2637:A:C5'	2.46	0.45
17:Q:26:PRO:O	17:Q:30:VAL:HG22	2.17	0.45
29:3:58:GLY:O	30:0:2460:A:H4'	2.16	0.45
30:0:396:U:O2'	30:0:397:A:P	2.74	0.45
30:0:922:A:N7	30:0:2281:C:H5'	2.31	0.45
30:0:1380:U:H5'	39:0:9222:HOH:O	2.15	0.45
30:0:2659:U:H5''	39:0:4146:HOH:O	2.16	0.45
31:9:114:G:H2'	31:9:115:C:C6	2.51	0.45
1:A:121:ALA:O	1:A:124:VAL:HG22	2.15	0.45
22:V:55:ARG:O	22:V:59:ILE:HG12	2.15	0.45
30:0:1183:C:N3	30:0:1184:C:C5	2.85	0.45
30:0:1342:C:H2'	30:0:1343:C:H5'	1.98	0.45
30:0:1625:U:H5''	39:0:6044:HOH:O	2.16	0.45
30:0:2825:C:H4'	30:0:2826:G:O4'	2.17	0.45
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.52	0.45
30:0:204:A:C2'	30:0:205:U:H5'	2.46	0.45
30:0:503:G:H2'	30:0:504:G:H8	1.81	0.45
30:0:932:U:H2'	30:0:933:C:C6	2.51	0.45
30:0:1183:C:H41	30:0:1192:A:P	2.40	0.45
30:0:2668:G:H2'	30:0:2669:U:C6	2.51	0.45
30:0:2756:U:N3	30:0:2896:A:H2	2.13	0.45
13:M:70:GLY:HA3	30:0:2263:G:H4'	1.97	0.45
16:P:88:GLN:NE2	30:0:1800:G:H1'	2.32	0.45
30:0:29:C:O2'	30:0:30:U:H5'	2.17	0.45
1:A:171:LYS:HB2	30:0:820:G:C6	2.51	0.45
2:B:244:PRO:HB3	30:0:1234:U:N3	2.31	0.45
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.15	0.45
15:O:97:SER:H	15:O:100:GLN:NE2	2.14	0.45
30:0:47:G:N3	30:0:114:A:C2	2.85	0.45
30:0:1244:U:H4'	30:0:1246:A:O4'	2.17	0.45
30:0:1583:U:H2'	30:0:1584:C:O4'	2.17	0.45
3:C:107:ARG:O	3:C:111:VAL:HG23	2.16	0.45
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.98	0.45
30:0:39:G:N2	30:0:444:C:C2	2.85	0.45
30:0:154:C:H2'	30:0:155:C:C6	2.52	0.45
30:0:255:A:H2'	30:0:256:C:C6	2.52	0.45
30:0:1278:A:O2'	30:0:1279:U:H3'	2.17	0.45
30:0:1925:G:O2'	30:0:1926:G:H5'	2.17	0.45
30:0:2281:C:C2'	30:0:2282:U:H5'	2.46	0.45
30:0:2584:G:H4'	39:0:7151:HOH:O	2.16	0.45
30:0:2697:A:H2'	30:0:2698:G:O4'	2.16	0.45
31:9:52:A:H2'	31:9:53:G:O4'	2.17	0.45
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.82	0.45
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.14	0.45
29:3:17:HIS:CG	30:0:2409:C:H4'	2.52	0.45
30:0:129:A:O2'	30:0:131:A:OP1	2.34	0.45
30:0:297:U:H2'	30:0:298:C:H6	1.81	0.45
30:0:1362:U:H5'	39:0:3278:HOH:O	2.16	0.45
30:0:2469:A:H2'	39:0:7506:HOH:O	2.16	0.45
30:0:2505:G:H2'	30:0:2506:A:H5'	1.98	0.45
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.98	0.45
30:0:317:A:H4'	39:0:3787:HOH:O	2.16	0.45
30:0:629:A:C2	30:0:2074:A:C2	3.05	0.45
30:0:699:C:C2	30:0:744:G:C2	3.05	0.45
30:0:2348:C:H2'	30:0:2349:G:C8	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2437:A:H2'	30:0:2438:G:C8	2.52	0.45
31:9:55:U:H4'	31:9:56:A:H8	1.81	0.45
30:0:1205:U:H2'	30:0:1206:U:H5''	1.97	0.45
30:0:1743:G:H1'	39:0:4916:HOH:O	2.16	0.45
30:0:2256:G:H2'	30:0:2257:G:H5'	1.98	0.45
14:N:26:LEU:HD13	30:0:2415:A:N3	2.32	0.44
14:N:40:ASN:HD21	31:9:28:U:H5''	1.81	0.44
26:Z:47:ARG:HH21	30:0:1771:U:H1'	1.82	0.44
30:0:634:G:O2'	30:0:1358:A:OP1	2.31	0.44
30:0:1556:G:O2'	30:0:1557:G:H5'	2.16	0.44
30:0:1849:G:H1'	30:0:2011:A:N1	2.33	0.44
30:0:2598:U:O2	30:0:2600:A:H8	1.99	0.44
30:0:2748:G:H5'	39:0:7572:HOH:O	2.16	0.44
30:0:2781:U:H2'	30:0:2782:G:C5'	2.47	0.44
3:C:35:VAL:HG13	3:C:221:GLU:HG2	1.99	0.44
19:S:50:GLU:HB3	19:S:67:ARG:HH21	1.82	0.44
28:2:10:ARG:NH2	30:0:121:U:OP2	2.35	0.44
30:0:154:C:H2'	30:0:155:C:H6	1.81	0.44
30:0:234:A:H2'	30:0:235:C:O4'	2.17	0.44
30:0:1166:A:N3	30:0:1166:A:H2'	2.33	0.44
30:0:1566:C:H2'	30:0:1567:G:H8	1.83	0.44
30:0:1610:G:H2'	30:0:1611:G:O4'	2.17	0.44
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.53	0.44
30:0:332:G:O2'	30:0:333:G:H5'	2.17	0.44
30:0:566:A:H2'	30:0:567:U:O4'	2.16	0.44
30:0:1641:A:C2'	30:0:1642:A:H5'	2.45	0.44
30:0:1682:A:O2'	30:0:1683:G:H5''	2.17	0.44
30:0:2089:A:O2'	30:0:2090:G:H5'	2.18	0.44
2:B:16:ARG:NH1	39:B:9041:HOH:O	2.49	0.44
30:0:962:C:H5''	39:0:4940:HOH:O	2.18	0.44
30:0:1343:C:H2'	30:0:1344:G:O5'	2.17	0.44
30:0:1391:G:H2'	30:0:1392:A:H5'	2.00	0.44
30:0:1634:G:H2'	30:0:1635:U:C6	2.52	0.44
30:0:1636:G:O2'	30:0:1637:A:H5'	2.17	0.44
30:0:2073:G:C6	30:0:2489:G:H4'	2.53	0.44
30:0:2420:G:H4'	39:0:4115:HOH:O	2.18	0.44
30:0:2507:G:H2'	30:0:2510:C:N4	2.33	0.44
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.87	0.44
9:I:93:ALA:HB3	9:I:132:VAL:HG22	2.00	0.44
19:S:57:THR:HG22	19:S:58:MET:N	2.32	0.44
29:3:64:LYS:HA	29:3:84:ARG:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:228:C:H2'	30:0:229:G:H5'	2.00	0.44
2:B:232:TRP:CZ3	30:0:2614:C:H5''	2.52	0.44
28:2:28:LYS:O	30:0:87:C:H2'	2.18	0.44
30:0:65:C:O2'	30:0:66:G:H5'	2.17	0.44
30:0:397:A:O2'	30:0:417:G:N3	2.50	0.44
30:0:447:A:O2'	30:0:448:G:H5'	2.17	0.44
30:0:541:C:C2'	30:0:542:A:C5'	2.89	0.44
30:0:816:G:C6	30:0:817:G:N1	2.86	0.44
30:0:1878:G:H5''	39:0:9802:HOH:O	2.18	0.44
30:0:2724:U:H2'	30:0:2725:G:O4'	2.17	0.44
13:M:58:GLN:HE22	30:0:251:C:H1'	1.83	0.44
13:M:82:ARG:O	13:M:86:GLN:HG3	2.18	0.44
30:0:120:A:N3	30:0:120:A:H2'	2.33	0.44
30:0:1202:A:O2'	30:0:1203:G:H5'	2.18	0.44
30:0:2252:A:C5	30:0:2253:G:H1'	2.52	0.44
30:0:2768:A:H5''	39:0:4447:HOH:O	2.16	0.44
11:K:30:LYS:HB3	11:K:56:SER:HB3	2.00	0.44
30:0:213:G:N2	30:0:225:G:H2'	2.33	0.44
30:0:919:U:H5'	30:0:2465:A:O2'	2.18	0.44
30:0:1202:A:H2'	30:0:1203:G:C5'	2.47	0.44
30:0:1314:U:H2'	39:0:5894:HOH:O	2.18	0.44
30:0:2894:C:O2'	30:0:2895:C:H5'	2.18	0.44
14:N:11:ARG:NH1	31:9:8:G:O6	2.51	0.44
30:0:101:C:H2'	30:0:102:A:H8	1.83	0.44
30:0:1268:C:H2'	30:0:1269:G:C8	2.52	0.44
30:0:1552:G:H2'	30:0:1553:C:C6	2.52	0.44
30:0:2533:C:H6	30:0:2533:C:C5'	2.22	0.44
30:0:2703:A:O2'	30:0:2704:C:H5'	2.17	0.44
32:4:76:PPU:N7	32:4:76:PPU:C9	2.79	0.44
30:0:293:A:O2'	30:0:294:C:H5'	2.18	0.43
30:0:912:A:C4	30:0:1294:A:C2	3.06	0.43
30:0:1130:U:H4'	39:0:6150:HOH:O	2.18	0.43
30:0:1307:A:H2'	30:0:1308:A:C8	2.53	0.43
30:0:1706:G:C6	30:0:1707:G:C6	3.06	0.43
30:0:2564:G:OP2	30:0:2565:C:H5''	2.18	0.43
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.51	0.43
10:J:80:LYS:HE3	10:J:101:VAL:O	2.18	0.43
18:R:69:LYS:HB2	18:R:72:VAL:HG23	1.99	0.43
30:0:168:C:H6	30:0:168:C:O5'	2.01	0.43
30:0:1730:G:C5'	30:0:1731:C:C6	3.00	0.43
30:0:1819:G:H2'	30:0:1820:G:H5'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1883:U:H5'	30:0:2012:U:OP2	2.17	0.43
30:0:2419:U:H5''	30:0:2420:G:C5'	2.44	0.43
2:B:238:ASN:HD22	2:B:240:GLY:N	2.13	0.43
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.83	0.43
18:R:23:MET:HE3	18:R:28:SER:OG	2.18	0.43
30:0:68:U:H4'	39:0:6784:HOH:O	2.19	0.43
30:0:2032:U:H5'	39:0:4537:HOH:O	2.18	0.43
30:0:2281:C:H2'	30:0:2282:U:H5'	2.00	0.43
30:0:2313:C:H4'	39:0:6597:HOH:O	2.19	0.43
30:0:2514:U:H2'	30:0:2515:C:H6	1.83	0.43
31:9:39:U:H3'	31:9:40:C:H5''	2.00	0.43
4:D:141:VAL:HG21	31:9:57:A:C8	2.54	0.43
30:0:132:A:H2'	30:0:133:U:C6	2.53	0.43
30:0:1568:G:O2'	30:0:1569:U:H5'	2.18	0.43
14:N:160:SER:HB3	31:9:51:A:H5'	1.99	0.43
27:1:1:THR:O	30:0:1836:A:H1'	2.18	0.43
30:0:1790:C:H2'	30:0:1791:U:H6	1.82	0.43
30:0:1878:G:O2'	30:0:1879:U:P	2.77	0.43
30:0:2764:C:H2'	30:0:2765:C:C6	2.54	0.43
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.18	0.43
9:I:87:PRO:HD2	30:0:1180:U:H1'	2.01	0.43
30:0:1632:A:H2'	30:0:1633:C:H5'	2.00	0.43
30:0:1659:A:H2'	30:0:1660:G:O4'	2.18	0.43
30:0:1743:G:H2'	30:0:1744:G:O4'	2.19	0.43
30:0:2301:A:H5''	30:0:2302:A:H5'	2.00	0.43
39:I:6825:HOH:O	30:0:1167:G:H1'	2.17	0.43
10:J:52:GLN:HE22	30:0:1119:G:H8	1.65	0.43
30:0:483:C:C4	30:0:484:A:C6	3.07	0.43
30:0:612:U:H2'	30:0:613:C:C6	2.54	0.43
30:0:645:U:O2	30:0:761:A:H2	2.02	0.43
30:0:1175:G:H1'	30:0:1193:A:H2'	2.00	0.43
30:0:2325:U:H1'	39:0:4167:HOH:O	2.19	0.43
26:Z:76:THR:HG21	30:0:1652:C:H4'	2.00	0.43
28:2:41:HIS:HE1	30:0:1439:C:H5''	1.84	0.43
30:0:1406:A:H4'	30:0:1407:A:H5''	2.01	0.43
30:0:1992:U:H2'	30:0:1994:A:OP2	2.18	0.43
30:0:2065:C:O2'	30:0:2066:C:H5'	2.19	0.43
31:9:53:G:O2'	31:9:54:A:H5'	2.19	0.43
19:S:33:SER:O	19:S:37:VAL:HG23	2.19	0.43
26:Z:40:ALA:HA	30:0:1773:G:C8	2.54	0.43
30:0:1181:A:C2'	30:0:1182:C:H5'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2064:U:H5'	30:0:2652:U:O3'	2.19	0.43
30:0:2644:C:O2'	30:0:2645:U:C5'	2.66	0.43
30:0:2689:A:C2'	30:0:2690:U:H5'	2.49	0.43
30:0:2832:C:H5	39:0:7245:HOH:O	2.01	0.43
31:9:39:U:H1'	31:9:44:A:H61	1.83	0.43
2:B:248:ARG:NH1	39:B:9040:HOH:O	2.51	0.43
30:0:1375:A:H2'	30:0:1376:G:H5'	2.00	0.43
30:0:2253:G:H2'	30:0:2254:G:H8	1.83	0.43
30:0:2502:C:H2'	30:0:2503:A:C5'	2.47	0.43
3:C:1:MET:HG2	3:C:2:GLN:H	1.84	0.42
11:K:8:VAL:HG13	11:K:80:ILE:HG22	2.01	0.42
18:R:40:ALA:O	18:R:44:VAL:HG23	2.18	0.42
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.42
30:0:2026:C:O2'	30:0:2027:U:H5'	2.19	0.42
30:0:2291:A:N9	30:0:2309:C:H5'	2.34	0.42
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.84	0.42
30:0:1057:A:H1'	30:0:2492:U:O2'	2.18	0.42
30:0:1503:U:H2'	30:0:1504:A:O4'	2.18	0.42
30:0:1700:C:H5''	30:0:1701:A:OP2	2.19	0.42
30:0:2429:A:H4'	39:0:7769:HOH:O	2.19	0.42
32:4:75:C:H2'	32:4:76:PPU:N9	2.34	0.42
2:B:254:GLN:HG2	2:B:255:GLY:N	2.34	0.42
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.91	0.42
30:0:85:C:H5''	30:0:86:A:OP2	2.18	0.42
30:0:248:A:H5'	30:0:249:G:OP2	2.20	0.42
30:0:1015:C:H6	30:0:1015:C:O5'	2.02	0.42
30:0:1730:G:H5'	30:0:1731:C:C5	2.54	0.42
30:0:2769:C:H2'	30:0:2770:G:C5'	2.49	0.42
30:0:2874:G:H3'	39:0:9585:HOH:O	2.20	0.42
3:C:206:ASN:HB2	30:0:329:A:OP2	2.19	0.42
24:X:30:MET:HG2	30:0:1384:C:H5'	2.02	0.42
30:0:622:G:O2'	30:0:623:U:H5'	2.19	0.42
30:0:1730:G:H5''	30:0:1731:C:C6	2.53	0.42
30:0:2385:G:H2'	30:0:2386:U:C6	2.54	0.42
30:0:2436:U:H2'	30:0:2437:A:C8	2.55	0.42
30:0:2758:G:H2'	30:0:2759:C:H6	1.84	0.42
1:A:190:ARG:NH2	39:A:9008:HOH:O	2.52	0.42
17:Q:45:PRO:O	30:0:2365:G:H4'	2.19	0.42
30:0:10:U:H3'	30:0:10:U:C6	2.54	0.42
30:0:289:G:O2'	30:0:290:C:H5'	2.20	0.42
30:0:1624:A:H5'	30:0:1626:A:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2416:G:H2'	30:0:2417:C:C6	2.55	0.42
31:9:47:A:C2	31:9:48:C:C2	3.08	0.42
4:D:172:VAL:HG12	4:D:173:GLU:H	1.85	0.42
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.84	0.42
28:2:42:TRP:CZ2	30:0:1438:G:H1'	2.53	0.42
30:0:204:A:H2'	30:0:205:U:H5'	2.01	0.42
30:0:363:C:H2'	30:0:364:U:C6	2.55	0.42
30:0:1209:C:H2'	30:0:1210:G:H8	1.84	0.42
30:0:1422:U:H2'	30:0:1423:C:C6	2.55	0.42
30:0:1762:C:H2'	30:0:1763:C:H6	1.84	0.42
30:0:1829:A:C8	30:0:1885:A:C8	3.08	0.42
30:0:2039:A:H2'	30:0:2040:C:C6	2.54	0.42
30:0:2667:G:H1'	30:0:2914:A:N3	2.34	0.42
30:0:2896:A:H2'	30:0:2896:A:N3	2.35	0.42
31:9:61:C:H2'	31:9:62:A:H8	1.85	0.42
9:I:112:LEU:HD11	30:0:1162:G:H1'	2.02	0.42
25:Y:204:ARG:NH2	30:0:553:G:P	2.88	0.42
30:0:166:A:O2'	30:0:898:G:O6	2.33	0.42
30:0:1015:C:H2'	30:0:1016:U:H6	1.84	0.42
30:0:1557:G:O2'	30:0:1558:C:H5'	2.20	0.42
6:F:59:ILE:HD13	30:0:263:U:C2	2.54	0.42
16:P:120:ARG:HD2	30:0:1594:C:OP2	2.19	0.42
30:0:333:G:O2'	30:0:334:G:H5'	2.19	0.42
30:0:758:A:H2'	30:0:759:C:O4'	2.19	0.42
30:0:812:A:H1'	39:0:3977:HOH:O	2.19	0.42
30:0:1497:G:H2'	30:0:1498:G:H8	1.85	0.42
30:0:1588:G:C6	30:0:1589:G:N1	2.88	0.42
30:0:1741:U:HO2'	30:0:2723:G:H4'	1.79	0.42
30:0:1769:C:O2'	30:0:1770:U:H5'	2.20	0.42
30:0:2533:C:O2'	30:0:2534:C:H5'	2.20	0.42
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.53	0.42
2:B:288:GLY:HA2	30:0:2898:G:H4'	2.02	0.42
8:H:59:GLN:HE21	8:H:129:ARG:NE	2.09	0.42
13:M:71:SER:HB2	13:M:92:THR:HG22	2.02	0.42
17:Q:95:GLU:HA	30:0:949:U:H4'	2.02	0.42
30:0:95:A:H5''	30:0:97:G:O4'	2.20	0.42
30:0:1185:U:H5'	39:0:7498:HOH:O	2.20	0.42
30:0:1883:U:H5''	30:0:2013:G:OP2	2.20	0.42
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.42
30:0:2321:A:H2	30:0:2378:U:N3	2.02	0.42
30:0:2871:G:H2'	30:0:2872:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:C:8655:HOH:O	30:0:2100:A:H5'	2.19	0.42
18:R:9:ASP:O	18:R:13:THR:HB	2.20	0.42
27:1:10:LYS:HG3	39:0:4369:HOH:O	2.19	0.42
30:0:363:C:H2'	30:0:364:U:H6	1.84	0.42
30:0:1319:G:H1'	39:0:4712:HOH:O	2.20	0.42
30:0:1321:A:H2'	30:0:1322:G:C8	2.55	0.42
30:0:2430:A:O2'	30:0:2431:C:H5'	2.20	0.42
1:A:36:ASP:O	1:A:38:ILE:N	2.48	0.41
1:A:190:ARG:HH11	30:0:1845:A:P	2.43	0.41
30:0:191:A:H2'	30:0:237:G:O6	2.20	0.41
30:0:960:G:H8	39:0:5994:HOH:O	2.02	0.41
30:0:1165:G:C4'	30:0:1174:A:O2'	2.68	0.41
30:0:1181:A:H2'	30:0:1182:C:C5'	2.50	0.41
30:0:1205:U:C2'	30:0:1206:U:H5''	2.50	0.41
30:0:1252:A:H2'	30:0:1253:C:O4'	2.19	0.41
30:0:1664:A:H8	30:0:1664:A:OP1	2.02	0.41
30:0:2135:A:O4'	30:0:2243:C:N4	2.53	0.41
30:0:2135:A:O2'	30:0:2136:G:H5'	2.19	0.41
30:0:2636:C:C3'	30:0:2637:A:C5'	2.98	0.41
30:0:2724:U:O5'	30:0:2724:U:H6	2.03	0.41
30:0:2869:G:H2'	30:0:2870:C:C6	2.55	0.41
15:O:29:VAL:HG11	15:O:98:LEU:HD21	2.02	0.41
18:R:33:ARG:NH1	39:R:8934:HOH:O	2.52	0.41
30:0:228:C:C2'	30:0:229:G:H5'	2.50	0.41
30:0:538:C:H5''	30:0:539:G:C8	2.55	0.41
30:0:619:U:H3'	39:0:3295:HOH:O	2.19	0.41
30:0:920:C:H2'	30:0:2109:U:C2	2.55	0.41
30:0:939:A:C2	30:0:1027:G:N3	2.88	0.41
30:0:1592:G:O2'	30:0:1593:C:O4'	2.36	0.41
30:0:1855:G:H4'	30:0:1856:C:O5'	2.19	0.41
30:0:2011:A:H4'	30:0:2012:U:O5'	2.20	0.41
30:0:2479:A:H3'	39:0:9847:HOH:O	2.18	0.41
10:J:82:THR:CG2	30:0:1242:A:H5'	2.36	0.41
19:S:17:ASP:HB3	19:S:23:LYS:HB2	2.02	0.41
27:1:16:HIS:HE1	30:0:775:G:OP1	2.03	0.41
30:0:824:G:H2'	30:0:826:U:OP1	2.20	0.41
30:0:1041:U:H2'	30:0:1042:U:H5'	2.01	0.41
30:0:1311:G:C2	30:0:1312:G:C8	3.08	0.41
30:0:2580:G:N3	30:0:2600:A:H2	2.17	0.41
2:B:234:ARG:HD3	30:0:1734:C:OP1	2.20	0.41
4:D:50:VAL:HG13	31:9:41:C:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:76:ARG:HH21	30:0:2122:C:H1'	1.86	0.41
14:N:5:ARG:NH1	30:0:1010:C:OP1	2.53	0.41
21:U:47:ARG:HG3	39:U:4381:HOH:O	2.19	0.41
25:Y:216:ARG:HD2	39:Y:8867:HOH:O	2.20	0.41
30:0:284:C:H4'	30:0:285:A:H8	1.85	0.41
30:0:314:G:N1	30:0:317:A:OP2	2.52	0.41
30:0:613:C:H2'	30:0:614:U:C6	2.54	0.41
30:0:1039:G:H2'	30:0:1040:A:O4'	2.21	0.41
30:0:1377:C:H6	30:0:1377:C:C5'	2.32	0.41
30:0:1615:A:H4'	39:0:5906:HOH:O	2.20	0.41
30:0:1762:C:O2'	30:0:1763:C:H5'	2.20	0.41
30:0:2064:U:H4'	30:0:2653:A:OP1	2.19	0.41
30:0:2768:A:H2'	30:0:2769:C:O4'	2.20	0.41
30:0:2781:U:O2'	30:0:2782:G:H5'	2.20	0.41
30:0:2793:A:H2'	30:0:2794:G:H5'	2.03	0.41
1:A:6:GLY:O	30:0:1861:C:H4'	2.20	0.41
2:B:238:ASN:HD21	30:0:2609:G:N2	2.18	0.41
4:D:52:THR:HG21	30:0:2347:C:H5'	2.03	0.41
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.16	0.41
15:O:25:VAL:O	15:O:29:VAL:HG23	2.20	0.41
25:Y:148:GLY:HA3	30:0:622:G:P	2.60	0.41
26:Z:47:ARG:NH2	30:0:1771:U:H1'	2.36	0.41
30:0:512:G:O3'	30:0:513:A:H8	2.04	0.41
30:0:737:A:H2'	30:0:738:G:O4'	2.19	0.41
30:0:963:C:O2	30:0:1005:A:N1	2.52	0.41
30:0:1350:U:H4'	39:0:5154:HOH:O	2.21	0.41
30:0:1616:A:H5''	30:0:1617:C:OP1	2.21	0.41
30:0:1754:A:H2'	30:0:1755:A:O4'	2.20	0.41
30:0:2610:U:H4'	39:0:9485:HOH:O	2.20	0.41
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.92	0.41
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.86	0.41
10:J:105:LEU:HD23	39:J:9025:HOH:O	2.20	0.41
18:R:61:GLN:NE2	39:R:8942:HOH:O	2.54	0.41
18:R:68:HIS:O	30:0:2842:G:H5'	2.20	0.41
30:0:111:C:H2'	30:0:112:G:O4'	2.20	0.41
30:0:1805:G:O2'	30:0:1806:G:H5'	2.19	0.41
30:0:1942:A:H5'	39:0:7377:HOH:O	2.21	0.41
30:0:2731:G:H2'	30:0:2732:U:O4'	2.20	0.41
9:I:110:ASP:O	30:0:1163:G:H5'	2.21	0.41
12:L:56:LYS:HE3	30:0:2443:C:H1'	2.02	0.41
30:0:682:A:H2'	30:0:683:G:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:705:C:O2	30:0:705:C:H2'	2.19	0.41
30:0:1421:C:O2'	30:0:1422:U:H5'	2.20	0.41
30:0:1566:C:H2'	30:0:1567:G:C8	2.56	0.41
30:0:2842:G:H2'	30:0:2843:A:H5'	2.02	0.41
2:B:97:LEU:HD22	2:B:127:GLN:HE21	1.85	0.41
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.19	0.41
23:W:13:MET:SD	23:W:18:GLN:HG3	2.60	0.41
23:W:128:VAL:O	23:W:138:LEU:HD11	2.21	0.41
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	2.01	0.41
30:0:791:A:H2'	30:0:792:G:O4'	2.21	0.41
30:0:921:G:H4'	30:0:924:G:N1	2.36	0.41
30:0:1279:U:O2	30:0:1279:U:C2'	2.67	0.41
30:0:1819:G:H2'	30:0:1820:G:C4'	2.50	0.41
30:0:2061:C:C2'	30:0:2062:A:H5'	2.51	0.41
30:0:2651:C:H2'	30:0:2652:U:O4'	2.20	0.41
1:A:164:ARG:NH2	30:0:1877:G:OP1	2.53	0.41
2:B:162:MET:HE1	2:B:308:LEU:HD21	2.02	0.41
12:L:6:ARG:NH2	39:L:8852:HOH:O	2.54	0.41
14:N:141:ARG:HH21	31:9:48:C:H4'	1.86	0.41
20:T:54:ASP:OD2	30:0:316:A:H5'	2.19	0.41
30:0:369:G:O2'	30:0:370:G:H5'	2.21	0.41
30:0:664:U:O4	30:0:681:G:H5''	2.21	0.41
30:0:809:G:H2'	30:0:810:G:H8	1.86	0.41
30:0:810:G:H2'	30:0:811:C:C6	2.55	0.41
30:0:1074:G:H4'	30:0:1260:G:C6	2.54	0.41
30:0:1076:G:H1'	39:0:4473:HOH:O	2.20	0.41
30:0:1160:G:O2'	30:0:1190:G:H1'	2.21	0.41
30:0:1181:A:N1	30:0:1192:A:O2'	2.51	0.41
30:0:1200:A:H3'	39:0:5773:HOH:O	2.20	0.41
30:0:1631:A:H2'	30:0:1632:A:C8	2.56	0.41
30:0:2474:A:N7	30:0:2621:PSU:H4'	2.35	0.41
30:0:2639:G:O2'	30:0:2640:U:H5'	2.21	0.41
30:0:2766:A:H5'	39:0:9570:HOH:O	2.20	0.41
30:0:2791:U:C1'	30:0:2792:A:H5''	2.49	0.41
30:0:2866:U:H4'	30:0:2867:G:H5'	2.03	0.41
8:H:91:ARG:O	30:0:1003:U:H4'	2.20	0.41
30:0:280:C:H2'	30:0:281:U:O4'	2.21	0.41
30:0:394:G:H1'	30:0:417:G:H22	1.85	0.41
30:0:764:C:H2'	30:0:765:G:O4'	2.21	0.41
30:0:1626:A:H2'	30:0:1627:G:O4'	2.21	0.41
30:0:1714:C:O2'	30:0:1715:C:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2478:U:O2'	30:0:2479:A:H5'	2.20	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.21	0.41
30:0:2825:C:H4'	30:0:2826:G:O5'	2.21	0.41
30:0:2836:G:H1'	39:0:6867:HOH:O	2.20	0.41
8:H:174:LEU:HD21	30:0:1220:U:H4'	2.02	0.40
16:P:81:LYS:O	30:0:1761:U:H5'	2.21	0.40
19:S:73:ASP:O	19:S:77:VAL:HG23	2.22	0.40
23:W:130:HIS:NE2	31:9:88:G:OP1	2.52	0.40
28:2:41:HIS:CE1	30:0:1439:C:H5''	2.56	0.40
30:0:797:A:N6	30:0:816:G:H1'	2.35	0.40
30:0:1333:U:H2'	30:0:1334:C:C6	2.57	0.40
30:0:1359:U:C5	30:0:2101:A:C8	3.09	0.40
30:0:2072:G:H3'	30:0:2073:G:H5''	2.03	0.40
31:9:26:C:H4'	39:9:9052:HOH:O	2.21	0.40
31:9:42:C:H5'	31:9:43:G:OP2	2.21	0.40
31:9:56:A:C3'	31:9:57:A:H5''	2.51	0.40
3:C:162:VAL:HG22	3:C:232:LEU:HD21	2.03	0.40
13:M:92:THR:HB	30:0:401:C:O2'	2.22	0.40
19:S:11:THR:HG22	30:0:1444:G:H5''	2.02	0.40
32:4:76:PPU:HE1	32:4:76:PPU:HM3	1.81	0.40
2:B:27:ASN:HD21	30:0:2807:U:P	2.44	0.40
10:J:80:LYS:NZ	30:0:2815:G:N7	2.70	0.40
13:M:34:GLU:HB3	13:M:38:GLU:HG3	2.04	0.40
13:M:75:ARG:HG3	39:M:8868:HOH:O	2.21	0.40
26:Z:49:ARG:O	26:Z:53:ILE:HD12	2.21	0.40
30:0:876:A:N3	30:0:876:A:C2'	2.85	0.40
30:0:1006:A:H5''	39:0:3536:HOH:O	2.22	0.40
30:0:1201:C:H5''	39:0:6256:HOH:O	2.21	0.40
30:0:1405:U:H4'	30:0:1406:A:H5''	2.03	0.40
30:0:1416:G:C2'	30:0:1417:G:H5'	2.51	0.40
30:0:1603:A:H5'	30:0:1605:G:C4'	2.51	0.40
30:0:1921:A:O2'	30:0:1922:A:H5'	2.21	0.40
30:0:2415:A:C2'	30:0:2416:G:H5'	2.51	0.40
30:0:2438:G:H2'	30:0:2439:C:O4'	2.22	0.40
5:E:100:ASP:HB2	39:E:2789:HOH:O	2.20	0.40
30:0:117:A:H2'	30:0:118:G:O4'	2.22	0.40
30:0:812:A:H2'	30:0:813:C:H6	1.79	0.40
30:0:1052:G:H2'	30:0:1052:G:N3	2.37	0.40
30:0:1735:C:H2'	30:0:1736:A:C8	2.55	0.40
30:0:2084:C:H2'	30:0:2085:A:C8	2.56	0.40
30:0:2299:G:H4'	39:0:6506:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2906:A:H5'	30:0:2907:C:O4'	2.21	0.40
4:D:67:ASP:HA	4:D:68:PRO:HD3	1.99	0.40
13:M:171:ARG:NH2	30:0:189:A:OP1	2.55	0.40
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.87	0.40
30:0:123:U:O2'	30:0:124:C:H5'	2.22	0.40
30:0:316:A:N3	30:0:336:G:O2'	2.46	0.40
30:0:544:G:C3'	30:0:545:G:H5''	2.51	0.40
30:0:1423:C:O2'	30:0:1424:A:H5'	2.21	0.40
30:0:1706:G:C6	30:0:1707:G:N1	2.89	0.40
30:0:1842:A:C4	30:0:1979:G:C6	3.10	0.40
30:0:1980:U:O2	30:0:2008:U:H4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	221 (94%)	11 (5%)	3 (1%)	9	18
2	B	335/338 (99%)	310 (92%)	23 (7%)	2 (1%)	21	38
3	C	244/246 (99%)	228 (93%)	15 (6%)	1 (0%)	30	50
4	D	134/177 (76%)	114 (85%)	17 (13%)	3 (2%)	5	10
5	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
6	F	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	14	28
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	148 (95%)	7 (4%)	1 (1%)	21	38
9	I	68/162 (42%)	61 (90%)	5 (7%)	2 (3%)	3	6
10	J	140/145 (97%)	134 (96%)	6 (4%)	0	100	100
11	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	141/165 (86%)	131 (93%)	10 (7%)	0	100	100
13	M	192/196 (98%)	184 (96%)	7 (4%)	1 (0%)	24	43
14	N	184/187 (98%)	167 (91%)	14 (8%)	3 (2%)	7	14
15	O	113/116 (97%)	112 (99%)	1 (1%)	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%)	76 (96%)	3 (4%)	0	100	100
20	T	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
21	U	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
22	V	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
23	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
24	X	80/92 (87%)	76 (95%)	2 (2%)	2 (2%)	4	8
25	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
26	Z	71/116 (61%)	59 (83%)	10 (14%)	2 (3%)	4	6
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%)	83 (92%)	5 (6%)	2 (2%)	5	10
All	All	3705/4472 (83%)	3502 (94%)	180 (5%)	23 (1%)	21	38

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
14	N	154	LEU
1	A	27	LEU
8	H	19	ARG
13	M	71	SER
4	D	56	ARG
14	N	167	ASP
26	Z	70	ARG
1	A	74	VAL
2	B	2	GLN
2	B	185	GLY
3	C	8	LEU

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Mol	Chain	Res	Type
6	F	100	ASP
26	Z	44	ARG
4	D	27	ILE
9	I	108	HIS
29	3	64	LYS
14	N	184	ILE
9	I	131	GLY
24	X	70	ILE
29	3	61	PRO
24	X	52	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	168 (94%)	11 (6%)	17	31
2	B	282/283 (100%)	261 (93%)	21 (7%)	13	24
3	C	193/193 (100%)	178 (92%)	15 (8%)	11	21
4	D	117/148 (79%)	104 (89%)	13 (11%)	6	11
5	E	152/156 (97%)	148 (97%)	4 (3%)	40	63
6	F	93/94 (99%)	91 (98%)	2 (2%)	45	67
7	G	27/282 (10%)	25 (93%)	2 (7%)	13	24
8	H	134/145 (92%)	128 (96%)	6 (4%)	24	46
9	I	58/130 (45%)	57 (98%)	1 (2%)	53	71
10	J	118/121 (98%)	112 (95%)	6 (5%)	21	40
11	K	106/106 (100%)	99 (93%)	7 (7%)	15	29
12	L	113/127 (89%)	108 (96%)	5 (4%)	25	47
13	M	158/160 (99%)	148 (94%)	10 (6%)	16	30
14	N	149/150 (99%)	142 (95%)	7 (5%)	23	45
15	O	93/94 (99%)	90 (97%)	3 (3%)	34	58
16	P	113/117 (97%)	108 (96%)	5 (4%)	25	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	79/80 (99%)	78 (99%)	1 (1%)	61	76
18	R	117/122 (96%)	112 (96%)	5 (4%)	26	47
19	S	71/74 (96%)	69 (97%)	2 (3%)	38	61
20	T	105/106 (99%)	96 (91%)	9 (9%)	10	18
21	U	44/53 (83%)	42 (96%)	2 (4%)	24	46
22	V	51/57 (90%)	49 (96%)	2 (4%)	28	51
23	W	130/130 (100%)	121 (93%)	9 (7%)	14	26
24	X	66/74 (89%)	58 (88%)	8 (12%)	5	8
25	Y	120/196 (61%)	117 (98%)	3 (2%)	42	64
26	Z	60/94 (64%)	59 (98%)	1 (2%)	53	71
27	1	46/47 (98%)	45 (98%)	1 (2%)	45	67
28	2	42/46 (91%)	41 (98%)	1 (2%)	43	65
29	3	79/79 (100%)	73 (92%)	6 (8%)	12	23
All	All	3095/3646 (85%)	2927 (95%)	168 (5%)	20	38

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	34	ASP
1	A	62	ASP
1	A	64	ASP
1	A	94	LEU
1	A	135	VAL
1	A	175	LYS
1	A	179	MET
1	A	200	PRO
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN
2	B	36	PRO
2	B	49	THR
2	B	51	VAL
2	B	71	VAL
2	B	82	VAL

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Mol	Chain	Res	Type
2	B	84	LEU
2	B	97	LEU
2	B	98	THR
2	B	102	THR
2	B	112	THR
2	B	171	VAL
2	B	195	ARG
2	B	234	ARG
2	B	251	VAL
2	B	254	GLN
2	B	257	THR
2	B	265	LEU
2	B	280	VAL
3	C	2	GLN
3	C	27	ARG
3	C	78	ARG
3	C	94	THR
3	C	98	ARG
3	C	136	VAL
3	C	162	VAL
3	C	187	ARG
3	C	214	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	240	LEU
3	C	243	VAL
4	D	19	GLU
4	D	23	VAL
4	D	24	HIS
4	D	29	HIS
4	D	48	MET
4	D	50	VAL
4	D	58	VAL
4	D	86	THR
4	D	101	THR
4	D	137	PRO
4	D	149	ARG
4	D	161	ASP
4	D	172	VAL
5	E	36	PRO

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Mol	Chain	Res	Type
5	E	102	VAL
5	E	126	ILE
5	E	156	ASP
6	F	12	LEU
6	F	91	VAL
7	G	64	ASN
7	G	73	ASP
8	H	62	HIS
8	H	65	LEU
8	H	80	LEU
8	H	87	LYS
8	H	157	TYR
8	H	173	GLU
9	I	94	ASP
10	J	39	VAL
10	J	45	VAL
10	J	46	ILE
10	J	107	ASN
10	J	130	VAL
10	J	131	THR
11	K	10	GLN
11	K	16	SER
11	K	55	VAL
11	K	62	PRO
11	K	74	VAL
11	K	98	VAL
11	K	120	ARG
12	L	93	VAL
12	L	97	VAL
12	L	114	VAL
12	L	140	VAL
12	L	143	THR
13	M	10	ASP
13	M	46	LEU
13	M	78	LYS
13	M	89	THR
13	M	93	ARG
13	M	99	ARG
13	M	115	LEU
13	M	126	GLN
13	M	141	ILE
13	M	164	THR

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Mol	Chain	Res	Type
14	N	26	LEU
14	N	47	LEU
14	N	49	THR
14	N	127	LEU
14	N	135	VAL
14	N	142	THR
14	N	178	THR
15	O	74	VAL
15	O	80	ASP
15	O	96	VAL
16	P	16	VAL
16	P	21	VAL
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE
17	Q	18	PRO
18	R	13	THR
18	R	39	THR
18	R	52	GLU
18	R	82	GLU
18	R	143	VAL
19	S	10	VAL
19	S	81	ILE
20	T	39	ASN
20	T	48	VAL
20	T	61	GLU
20	T	71	VAL
20	T	82	THR
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	28	THR
21	U	52	THR
22	V	12	THR
22	V	13	PRO
23	W	18	GLN
23	W	35	VAL
23	W	38	THR
23	W	52	VAL
23	W	88	THR
23	W	120	PRO

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Mol	Chain	Res	Type
23	W	142	ASP
23	W	146	ILE
23	W	154	ARG
24	X	8	ARG
24	X	43	VAL
24	X	46	ASP
24	X	52	PRO
24	X	72	VAL
24	X	79	GLU
24	X	82	GLU
24	X	88	GLU
25	Y	154	ARG
25	Y	189	ASN
25	Y	203	VAL
26	Z	94	LYS
27	1	25	LYS
28	2	18	ASN
29	3	3	MET
29	3	17	HIS
29	3	56	PRO
29	3	65	THR
29	3	84	ARG
29	3	88	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	127	GLN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	243	ASN
2	B	256	GLN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	67	GLN
3	C	73	GLN

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Mol	Chain	Res	Type
3	C	129	HIS
4	D	85	GLN
4	D	103	ASN
5	E	96	ASN
5	E	106	ASN
5	E	143	GLN
6	F	80	GLN
7	G	64	ASN
8	H	59	GLN
8	H	73	ASN
8	H	75	HIS
10	J	25	GLN
10	J	52	GLN
10	J	89	HIS
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
11	K	119	GLN
12	L	18	HIS
12	L	41	HIS
13	M	24	GLN
13	M	28	GLN
13	M	58	GLN
13	M	137	ASN
13	M	143	ASN
13	M	170	ASN
14	N	107	ASN
14	N	140	GLN
15	O	53	GLN
15	O	100	GLN
16	P	50	GLN
16	P	66	GLN
16	P	88	GLN
16	P	101	GLN
16	P	118	GLN
17	Q	16	ASN
18	R	94	ASN
18	R	98	ASN
18	R	102	GLN
18	R	117	HIS
19	S	7	HIS
19	S	44	GLN

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Mol	Chain	Res	Type
19	S	53	ASN
19	S	55	GLN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	34	GLN
22	V	60	GLN
23	W	6	GLN
23	W	110	GLN
23	W	119	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	98	GLN
25	Y	119	GLN
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	41	HIS
28	2	45	ASN
29	3	15	ASN
29	3	20	HIS
29	3	43	ASN
29	3	48	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	246 (8%)	23 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
32	4	1/3 (33%)	0	0
All	All	2867/3048 (94%)	264 (9%)	24 (0%)

All (264) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A

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Mol	Chain	Res	Type
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	131	A
30	0	138	U
30	0	141	C
30	0	151	A
30	0	166	A
30	0	185	G
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	219	G
30	0	236	A
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	368	C
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	497	A
30	0	498	A
30	0	510	U

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Mol	Chain	Res	Type
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
30	0	588	G
30	0	604	G
30	0	605	C
30	0	620	A
30	0	632	A
30	0	644	G
30	0	645	U
30	0	660	A
30	0	688	A
30	0	699	C
30	0	701	U
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G

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Mol	Chain	Res	Type
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1129	C
30	0	1130	U
30	0	1137	G
30	0	1151	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1242	A
30	0	1279	U
30	0	1289	C
30	0	1342	C
30	0	1351	G
30	0	1353	C
30	0	1360	C
30	0	1377	C

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Mol	Chain	Res	Type
30	0	1378	G
30	0	1407	A
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1592	G
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	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1968	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1996	U
30	0	2006	C

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Mol	Chain	Res	Type
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	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	2322	U
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	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	2542	C
30	0	2553	A

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Mol	Chain	Res	Type
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2634	G
30	0	2637	A
30	0	2649	A
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	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	34	A
31	9	39	U
31	9	40	C

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Mol	Chain	Res	Type
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 (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	604	G
30	0	644	G
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1237	U
30	0	1352	A
30	0	1377	C
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1730	G
30	0	1856	C
30	0	2011	A
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2791	U
31	9	65	A

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

6 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	1MA	0	628	30,36	21,25,26	0.73	1 (4%)	30,37,40	0.86	2 (6%)
32	PPU	4	76	30,32	37,40,41	2.60	6 (16%)	47,57,60	2.08	14 (29%)
30	PSU	0	2621	30	18,21,22	1.57	2 (11%)	21,30,33	1.37	3 (14%)
30	UR3	0	2619	30	19,22,23	0.43	0	26,32,35	0.69	1 (3%)
30	OMU	0	2587	30,36	19,22,23	0.31	0	25,31,34	0.40	0
30	OMG	0	2588	30,32	23,26,27	0.28	0	32,38,41	0.38	0

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	1MA	0	628	30,36	-	2/7/25/26	0/3/3/3
32	PPU	4	76	30,32	-	6/25/43/44	0/4/4/4
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30,36	-	0/9/27/28	0/2/2/2
30	OMG	0	2588	30,32	-	0/9/27/28	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	4	76	PPU	O-C	10.46	1.43	1.23
32	4	76	PPU	C-N3'	6.29	1.47	1.34
32	4	76	PPU	C9-N6	-5.99	1.32	1.45
32	4	76	PPU	C10-N6	-5.89	1.32	1.45
30	0	2621	PSU	C2-N1	5.18	1.43	1.36
32	4	76	PPU	C5-N7	-3.17	1.33	1.39
30	0	2621	PSU	C6-C5	2.85	1.38	1.35
32	4	76	PPU	C8-N9	-2.54	1.33	1.37
30	0	628	1MA	C6-N6	2.43	1.33	1.28

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	4	76	PPU	C3'-N3'-C	-7.08	112.43	123.20
32	4	76	PPU	C5-C4-N3	-4.88	119.99	126.72
32	4	76	PPU	N3-C2-N1	-4.62	121.59	128.58
32	4	76	PPU	C2-N1-C6	3.90	121.36	111.83
32	4	76	PPU	C2-N3-C4	3.49	120.35	111.83
30	0	2621	PSU	C6-C5-C4	3.44	120.49	118.17
32	4	76	PPU	N3-C4-N9	3.41	132.96	127.17
32	4	76	PPU	CM-OC-CZ	-3.14	110.76	117.50
30	0	2621	PSU	C6-N1-C2	-3.07	119.84	122.69
32	4	76	PPU	N9-C8-N7	-3.02	109.66	113.94
30	0	2621	PSU	O2-C2-N1	2.94	125.81	122.79
30	0	628	1MA	N1-C2-N3	2.89	129.43	126.00
32	4	76	PPU	C5-N7-C8	2.88	107.98	103.45
32	4	76	PPU	C4-C5-N7	-2.78	107.40	110.58
30	0	2619	UR3	C4-N3-C2	2.75	126.79	124.58
30	0	628	1MA	CM1-N1-C6	2.33	123.76	120.15
32	4	76	PPU	C4-C5-C6	2.18	118.16	115.91
32	4	76	PPU	N1-C6-N6	2.13	119.45	116.86
32	4	76	PPU	C5-C6-N6	-2.10	122.01	125.33
32	4	76	PPU	C4-N9-C8	2.08	107.92	105.74

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	4	76	PPU	O-C-CA-CB
32	4	76	PPU	O-C-N3'-C3'
32	4	76	PPU	CE2-CZ-OC-CM
32	4	76	PPU	CE1-CZ-OC-CM
30	0	628	1MA	C2'-C1'-N9-C8
32	4	76	PPU	N3'-C-CA-N
30	0	628	1MA	C2'-C1'-N9-C4
32	4	76	PPU	C4'-C5'-O5'-P

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	4	76	PPU	6	0
30	0	2621	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2619	UR3	2	0
30	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 304 ligands modelled in this entry, 304 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	0.72	28 (11%) 9 7	32, 66, 104, 124	0
2	B	337/338 (99%)	0.59	16 (4%) 36 36	31, 59, 87, 104	0
3	C	246/246 (100%)	0.32	5 (2%) 65 63	19, 47, 71, 81	0
4	D	140/177 (79%)	2.07	64 (45%) 0 0	83, 112, 135, 143	0
5	E	172/178 (96%)	0.73	12 (6%) 22 22	47, 72, 92, 97	0
6	F	119/120 (99%)	1.02	13 (10%) 10 9	58, 81, 111, 122	0
7	G	29/348 (8%)	1.52	7 (24%) 2 1	76, 97, 108, 110	0
8	H	160/177 (90%)	0.57	8 (5%) 34 34	50, 72, 105, 117	0
9	I	70/162 (43%)	2.84	50 (71%) 0 0	130, 150, 167, 169	0
10	J	142/145 (97%)	0.37	3 (2%) 63 61	35, 54, 76, 86	0
11	K	132/132 (100%)	0.55	7 (5%) 32 31	38, 55, 83, 87	0
12	L	145/165 (87%)	1.03	25 (17%) 4 3	32, 80, 121, 130	0
13	M	194/196 (98%)	0.86	28 (14%) 6 5	31, 48, 108, 117	0
14	N	186/187 (99%)	1.42	43 (23%) 2 1	61, 85, 128, 133	0
15	O	115/116 (99%)	0.86	8 (6%) 22 22	39, 58, 75, 79	0
16	P	143/149 (95%)	0.68	13 (9%) 15 14	42, 60, 83, 90	0
17	Q	95/96 (98%)	0.59	7 (7%) 20 20	45, 57, 75, 83	0
18	R	150/155 (96%)	-0.05	1 (0%) 84 84	29, 49, 70, 78	0
19	S	81/85 (95%)	0.66	5 (6%) 26 26	42, 63, 84, 95	0
20	T	119/120 (99%)	0.61	9 (7%) 20 19	40, 58, 87, 122	0
21	U	53/67 (79%)	0.66	5 (9%) 14 13	59, 73, 93, 97	0
22	V	65/71 (91%)	1.29	18 (27%) 1 1	51, 77, 123, 129	0
23	W	154/154 (100%)	0.45	4 (2%) 57 55	35, 52, 66, 81	0
24	X	82/92 (89%)	0.66	8 (9%) 13 12	48, 64, 88, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.13	2 (1%) 73 73	26, 45, 69, 90	0
26	Z	73/116 (62%)	3.39	48 (65%) 0 0	99, 121, 131, 134	0
27	1	56/57 (98%)	-0.36	0 100 100	23, 32, 45, 57	0
28	2	46/50 (92%)	1.08	14 (30%) 1 1	33, 65, 97, 106	0
29	3	92/92 (100%)	3.43	70 (76%) 0 0	112, 127, 133, 140	0
30	0	2749/2923 (94%)	-0.29	63 (2%) 61 59	18, 50, 98, 167	0
31	9	122/122 (100%)	0.32	4 (3%) 49 47	41, 80, 105, 152	0
32	4	2/3 (66%)	0.65	0 100 100	70, 70, 70, 74	0
All	All	6648/7520 (88%)	0.38	588 (8%) 15 15	18, 57, 120, 169	0

All (588) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	12.4
13	M	89	THR	11.0
9	I	128	THR	10.5
26	Z	46	SER	10.5
13	M	70	GLY	10.2
13	M	80	GLY	9.9
26	Z	36	GLY	9.9
26	Z	35	SER	8.9
29	3	83	TRP	8.8
29	3	34	LYS	8.2
26	Z	40	ALA	8.1
13	M	81	ARG	8.1
29	3	84	ARG	8.0
26	Z	42	TYR	8.0
26	Z	50	VAL	8.0
26	Z	39	GLY	7.8
29	3	82	GLY	7.6
26	Z	38	PHE	7.6
26	Z	45	VAL	7.5
13	M	88	VAL	7.2
13	M	71	SER	7.1
13	M	74	LYS	7.1
26	Z	37	ARG	7.1
13	M	78	LYS	6.9
29	3	33	MET	6.8
31	9	1	U	6.7

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Mol	Chain	Res	Type	RSRZ
29	3	61	PRO	6.7
29	3	60	LYS	6.6
29	3	7	PHE	6.2
26	Z	58	ASN	6.2
29	3	79	LEU	6.1
13	M	82	ARG	6.1
26	Z	53	ILE	6.0
29	3	46	ILE	6.0
9	I	127	CYS	5.9
13	M	90	ARG	5.9
4	D	18	ILE	5.7
9	I	113	SER	5.7
29	3	54	LYS	5.7
9	I	120	ALA	5.6
13	M	83	SER	5.6
29	3	9	THR	5.5
29	3	31	THR	5.5
26	Z	43	GLY	5.5
4	D	135	VAL	5.4
13	M	87	GLY	5.4
4	D	174	VAL	5.4
29	3	55	VAL	5.4
13	M	79	ALA	5.4
29	3	36	ILE	5.4
13	M	73	ARG	5.3
30	0	735	C	5.3
4	D	40	ILE	5.2
28	2	49	GLU	5.2
4	D	10	PHE	5.1
26	Z	51	ALA	5.1
29	3	56	PRO	5.1
1	A	51	ARG	5.1
26	Z	64	PRO	5.1
26	Z	44	ARG	5.1
9	I	100	VAL	5.0
22	V	2	VAL	4.9
9	I	71	ALA	4.9
4	D	107	GLY	4.9
30	0	1171	A	4.9
26	Z	78	ILE	4.8
31	9	2	U	4.8
14	N	154	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
29	3	39	GLN	4.8
29	3	51	LYS	4.7
29	3	63	LYS	4.7
17	Q	76	VAL	4.7
13	M	86	GLN	4.7
9	I	85	GLY	4.7
29	3	65	THR	4.7
26	Z	41	ARG	4.6
29	3	4	PRO	4.6
14	N	168	LEU	4.6
29	3	67	LEU	4.6
26	Z	34	SER	4.6
29	3	43	ASN	4.6
13	M	68	ARG	4.5
29	3	38	ARG	4.5
17	Q	81	GLU	4.5
13	M	75	ARG	4.5
13	M	72	ALA	4.5
29	3	35	TRP	4.5
25	Y	235	GLU	4.5
29	3	48	ASN	4.4
4	D	57	THR	4.4
29	3	85	ALA	4.4
9	I	74	ILE	4.3
29	3	28	GLY	4.3
4	D	139	TYR	4.3
5	E	154	ILE	4.2
4	D	141	VAL	4.2
29	3	64	LYS	4.2
30	0	10	U	4.2
22	V	39	ALA	4.2
4	D	63	ILE	4.2
29	3	88	LEU	4.2
14	N	169	PRO	4.1
14	N	166	ALA	4.1
9	I	134	ILE	4.1
4	D	172	VAL	4.1
9	I	123	VAL	4.1
26	Z	106	SER	4.1
7	G	12	ILE	4.0
29	3	57	GLY	4.0
14	N	1	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
8	H	171	GLY	4.0
4	D	35	ALA	4.0
24	X	87	ALA	4.0
14	N	147	ILE	4.0
9	I	112	LEU	4.0
12	L	48	LYS	4.0
9	I	132	VAL	4.0
29	3	62	THR	3.9
9	I	119	ALA	3.9
19	S	81	ILE	3.9
29	3	52	PHE	3.9
9	I	70	THR	3.9
30	0	734	U	3.9
9	I	118	ASN	3.9
4	D	17	ARG	3.9
29	3	77	ALA	3.9
24	X	85	VAL	3.9
13	M	77	HIS	3.9
11	K	6	ALA	3.9
1	A	36	ASP	3.9
7	G	73	ASP	3.8
30	0	138	U	3.8
14	N	75	THR	3.8
13	M	76	ARG	3.8
29	3	13	HIS	3.8
30	0	1176	C	3.8
26	Z	47	ARG	3.8
4	D	90	LEU	3.7
9	I	95	LEU	3.7
29	3	3	MET	3.7
12	L	146	GLY	3.7
3	C	101	ASP	3.7
7	G	71	LEU	3.7
9	I	111	LEU	3.7
22	V	40	PRO	3.7
14	N	158	LEU	3.7
30	0	1186	C	3.7
4	D	142	ALA	3.7
1	A	85	SER	3.7
12	L	81	VAL	3.7
9	I	130	LEU	3.6
8	H	114	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
4	D	55	LYS	3.6
4	D	26	GLY	3.6
1	A	37	VAL	3.6
9	I	91	PHE	3.6
6	F	17	LEU	3.6
14	N	38	LYS	3.6
26	Z	77	GLY	3.6
26	Z	57	MET	3.6
9	I	80	PHE	3.6
1	A	52	SER	3.6
29	3	17	HIS	3.5
8	H	174	LEU	3.5
28	2	35	ARG	3.5
13	M	91	ILE	3.5
28	2	38	LYS	3.5
26	Z	82	SER	3.5
30	0	1175	G	3.5
14	N	114	LYS	3.5
14	N	159	TYR	3.4
1	A	112	PRO	3.4
29	3	32	GLY	3.4
4	D	134	LEU	3.4
16	P	114	LEU	3.4
26	Z	73	ARG	3.4
26	Z	103	VAL	3.4
6	F	101	ALA	3.4
4	D	58	VAL	3.4
9	I	97	VAL	3.4
30	0	1172	G	3.4
29	3	41	GLU	3.4
26	Z	87	LYS	3.4
29	3	69	TYR	3.4
14	N	145	ALA	3.4
10	J	70	PHE	3.4
1	A	88	ILE	3.3
29	3	58	GLY	3.3
7	G	27	ILE	3.3
9	I	103	ILE	3.3
26	Z	49	ARG	3.3
9	I	117	THR	3.3
12	L	143	THR	3.3
13	M	84	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
14	N	165	ALA	3.3
20	T	119	ALA	3.3
30	0	2769	C	3.2
4	D	16	PRO	3.2
30	0	1161	A	3.2
1	A	237	GLY	3.2
15	O	22	GLY	3.2
1	A	53	ALA	3.2
29	3	37	ASP	3.2
1	A	211	LYS	3.2
29	3	1	MET	3.2
30	0	1185	U	3.2
30	0	2541	U	3.2
4	D	44	ILE	3.2
12	L	97	VAL	3.2
29	3	59	ASP	3.2
26	Z	70	ARG	3.2
9	I	88	GLN	3.2
9	I	84	SER	3.2
5	E	108	LEU	3.1
22	V	48	GLU	3.1
29	3	11	CYS	3.1
6	F	102	GLY	3.1
29	3	75	GLY	3.1
4	D	27	ILE	3.1
29	3	22	VAL	3.1
24	X	83	ALA	3.1
29	3	10	TYR	3.1
12	L	99	GLU	3.1
29	3	76	LYS	3.1
30	0	1524	U	3.1
8	H	43	ALA	3.1
1	A	32	VAL	3.1
28	2	37	HIS	3.0
9	I	107	LYS	3.0
4	D	59	GLY	3.0
4	D	70	GLY	3.0
6	F	75	ILE	3.0
15	O	23	GLY	3.0
20	T	114	SER	3.0
29	3	12	PRO	3.0
28	2	46	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
30	0	2103	A	3.0
4	D	143	LYS	3.0
16	P	67	LYS	3.0
23	W	124	GLY	3.0
1	A	111	SER	3.0
12	L	148	GLU	3.0
14	N	40	ASN	3.0
30	0	1190	G	3.0
30	0	1197	G	3.0
6	F	106	ALA	3.0
9	I	104	ALA	3.0
28	2	42	TRP	3.0
16	P	64	GLU	3.0
1	A	210	GLY	3.0
19	S	74	ALA	3.0
30	0	1162	G	3.0
2	B	285	VAL	3.0
13	M	85	ARG	2.9
24	X	66	THR	2.9
9	I	124	VAL	2.9
2	B	140	LEU	2.9
30	0	2664	A	2.9
20	T	118	SER	2.9
29	3	8	ASN	2.9
12	L	47	GLY	2.9
4	D	37	ALA	2.9
11	K	118	ALA	2.9
6	F	91	VAL	2.9
20	T	40	VAL	2.9
30	0	1184	C	2.9
26	Z	63	CYS	2.9
4	D	77	ASP	2.9
4	D	138	GLY	2.9
22	V	38	GLY	2.9
29	3	50	GLY	2.9
22	V	35	ALA	2.9
30	0	716	G	2.9
28	2	44	ARG	2.8
31	9	24	U	2.8
30	0	1196	C	2.8
12	L	150	GLN	2.8
9	I	129	SER	2.8

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Mol	Chain	Res	Type	RSRZ
4	D	66	GLY	2.8
28	2	48	ASP	2.8
1	A	27	LEU	2.8
12	L	46	LEU	2.8
9	I	133	THR	2.8
29	3	14	CYS	2.8
13	M	125	ARG	2.8
30	0	2645	U	2.8
14	N	118	ILE	2.8
29	3	68	LYS	2.8
6	F	16	ALA	2.8
14	N	84	THR	2.8
4	D	19	GLU	2.8
14	N	78	MET	2.8
14	N	172	PHE	2.8
29	3	42	ARG	2.8
2	B	128	ILE	2.8
9	I	131	GLY	2.8
14	N	115	VAL	2.8
22	V	52	ALA	2.8
26	Z	76	THR	2.8
15	O	47	ARG	2.8
30	0	1164	U	2.7
30	0	1964	U	2.7
4	D	42	GLY	2.7
7	G	26	MET	2.7
29	3	20	HIS	2.7
30	0	2345	A	2.7
5	E	172	PRO	2.7
22	V	43	PRO	2.7
5	E	126	ILE	2.7
4	D	11	HIS	2.7
13	M	194	GLY	2.7
30	0	1169	U	2.7
3	C	245	GLU	2.7
15	O	42	GLU	2.7
9	I	67	VAL	2.7
28	2	31	ARG	2.7
26	Z	88	PHE	2.7
26	Z	83	TYR	2.7
29	3	24	LYS	2.7
4	D	128	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
28	2	41	HIS	2.7
30	0	1160	G	2.7
24	X	65	ASN	2.7
29	3	26	ARG	2.7
29	3	25	VAL	2.7
20	T	117	ASP	2.7
26	Z	66	CYS	2.7
1	A	153	ARG	2.7
14	N	112	GLY	2.7
15	O	21	SER	2.7
29	3	15	ASN	2.7
9	I	101	LYS	2.7
12	L	55	GLN	2.6
30	0	1163	G	2.6
30	0	2344	G	2.6
29	3	78	HIS	2.6
9	I	66	GLY	2.6
26	Z	56	GLU	2.6
29	3	81	GLU	2.6
1	A	84	VAL	2.6
16	P	143	ALA	2.6
29	3	44	SER	2.6
26	Z	74	GLN	2.6
16	P	35	ILE	2.6
4	D	41	LEU	2.6
26	Z	54	GLU	2.6
14	N	138	ASP	2.6
4	D	69	ILE	2.6
21	U	13	ILE	2.6
2	B	329	TYR	2.6
4	D	72	LYS	2.6
6	F	117	GLU	2.6
6	F	6	PHE	2.6
5	E	45	ASP	2.6
30	0	2637	A	2.6
4	D	79	MET	2.6
2	B	113	LEU	2.6
2	B	175	LEU	2.6
2	B	326	GLU	2.6
5	E	53	GLU	2.6
9	I	83	GLY	2.6
9	I	92	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
26	Z	95	PRO	2.6
30	0	1170	U	2.6
30	0	1279	U	2.6
14	N	137	ALA	2.6
14	N	148	ALA	2.6
17	Q	23	THR	2.5
14	N	167	ASP	2.5
30	0	960	G	2.5
11	K	109	LEU	2.5
30	0	1173	A	2.5
29	3	80	ARG	2.5
4	D	61	PHE	2.5
12	L	100	ALA	2.5
14	N	163	PHE	2.5
5	E	10	ASP	2.5
26	Z	85	ASP	2.5
4	D	166	ILE	2.5
6	F	111	ILE	2.5
5	E	18	LEU	2.5
7	G	63	ARG	2.5
22	V	3	LEU	2.5
9	I	77	GLU	2.5
30	0	1166	A	2.5
9	I	69	PRO	2.5
1	A	151	GLN	2.5
12	L	77	ALA	2.5
9	I	96	SER	2.5
29	3	27	SER	2.5
7	G	23	ILE	2.5
12	L	149	ARG	2.5
1	A	83	GLY	2.5
9	I	125	GLY	2.5
26	Z	71	VAL	2.5
30	0	272	A	2.5
30	0	1199	A	2.5
4	D	140	ARG	2.5
14	N	27	LEU	2.5
4	D	65	GLU	2.5
2	B	1	PRO	2.5
22	V	12	THR	2.4
28	2	47	THR	2.4
16	P	120	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
26	Z	48	ARG	2.4
12	L	145	LEU	2.4
16	P	58	SER	2.4
16	P	116	SER	2.4
26	Z	55	SER	2.4
6	F	15	ASP	2.4
22	V	44	GLY	2.4
30	0	1198	U	2.4
2	B	62	ARG	2.4
22	V	46	ILE	2.4
30	0	1525	G	2.4
30	0	1947	G	2.4
4	D	46	GLY	2.4
26	Z	67	GLY	2.4
1	A	121	ALA	2.4
14	N	117	ALA	2.4
15	O	17	ALA	2.4
12	L	36	ASP	2.4
12	L	102	ASP	2.4
15	O	31	GLU	2.4
9	I	121	LYS	2.4
30	0	1177	A	2.4
5	E	131	LEU	2.4
11	K	4	LEU	2.4
21	U	52	THR	2.4
30	0	2004	U	2.4
29	3	74	CYS	2.4
23	W	123	GLY	2.4
3	C	133	ARG	2.4
5	E	102	VAL	2.4
11	K	73	VAL	2.4
14	N	14	ARG	2.4
12	L	82	ALA	2.4
8	H	133	GLY	2.3
8	H	132	ALA	2.3
14	N	186	LEU	2.3
4	D	131	THR	2.3
30	0	2511	A	2.3
9	I	72	GLU	2.3
3	C	63	SER	2.3
9	I	87	PRO	2.3
10	J	4	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
11	K	47	ALA	2.3
14	N	150	TYR	2.3
2	B	108	GLU	2.3
13	M	69	LYS	2.3
9	I	90	ASP	2.3
21	U	51	TRP	2.3
30	0	1561	U	2.3
30	0	2322	U	2.3
4	D	132	VAL	2.3
20	T	112	LEU	2.3
1	A	99	ILE	2.3
13	M	1	ALA	2.3
17	Q	75	ILE	2.3
26	Z	62	ALA	2.3
14	N	21	HIS	2.3
30	0	1165	G	2.3
30	0	2247	C	2.3
1	A	130	THR	2.3
4	D	89	PRO	2.3
4	D	149	ARG	2.3
12	L	45	PRO	2.3
14	N	5	ARG	2.3
14	N	139	TRP	2.3
4	D	21	VAL	2.3
5	E	11	VAL	2.3
1	A	97	ALA	2.2
31	9	23	U	2.2
1	A	223	ARG	2.2
12	L	96	VAL	2.2
1	A	45	ILE	2.2
1	A	68	ILE	2.2
22	V	36	ALA	2.2
24	X	84	ILE	2.2
29	3	90	PHE	2.2
30	0	1193	A	2.2
9	I	82	THR	2.2
17	Q	95	GLU	2.2
12	L	67	ARG	2.2
30	0	298	C	2.2
10	J	62	ASP	2.2
14	N	113	SER	2.2
14	N	164	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
29	3	53	SER	2.2
17	Q	29	ALA	2.2
4	D	101	THR	2.2
20	T	82	THR	2.2
4	D	144	ARG	2.2
4	D	97	GLN	2.2
2	B	168	GLY	2.2
30	0	1201	C	2.2
26	Z	52	GLU	2.2
26	Z	97	THR	2.2
4	D	14	ARG	2.2
19	S	67	ARG	2.2
28	2	39	ARG	2.2
9	I	68	PRO	2.2
9	I	114	TYR	2.2
30	0	1202	A	2.2
13	M	13	LYS	2.2
16	P	54	LYS	2.2
26	Z	75	GLY	2.2
1	A	58	VAL	2.2
12	L	57	VAL	2.2
14	N	42	HIS	2.2
14	N	146	HIS	2.2
24	X	7	GLU	2.1
16	P	63	ARG	2.1
21	U	54	THR	2.1
29	3	6	ARG	2.1
30	0	87	C	2.1
18	R	150	PRO	2.1
22	V	42	ASN	2.1
28	2	45	ASN	2.1
8	H	157	TYR	2.1
4	D	13	MET	2.1
9	I	73	LEU	2.1
16	P	108	LEU	2.1
22	V	65	ASP	2.1
23	W	76	ASP	2.1
30	0	1187	U	2.1
11	K	3	ALA	2.1
19	S	12	GLU	2.1
4	D	153	THR	2.1
1	A	209	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	137	PRO	2.1
14	N	157	PRO	2.1
28	2	28	LYS	2.1
30	0	1183	C	2.1
4	D	36	ASN	2.1
4	D	133	ASN	2.1
9	I	116	LEU	2.1
14	N	47	LEU	2.1
2	B	34	GLY	2.1
22	V	37	GLY	2.1
2	B	115	VAL	2.1
21	U	55	ALA	2.1
23	W	3	ALA	2.1
30	0	1188	A	2.1
5	E	6	GLU	2.1
14	N	149	GLU	2.1
17	Q	8	GLU	2.1
22	V	41	GLU	2.1
26	Z	59	GLU	2.1
4	D	154	LYS	2.1
2	B	36	PRO	2.1
14	N	171	HIS	2.1
12	L	91	VAL	2.1
15	O	25	VAL	2.1
30	0	1182	C	2.1
9	I	110	ASP	2.1
29	3	49	ASP	2.1
4	D	91	ALA	2.1
12	L	78	ALA	2.1
4	D	53	LYS	2.1
30	0	1192	A	2.1
30	0	1559	A	2.1
4	D	170	TYR	2.1
2	B	176	ASP	2.0
3	C	132	ASP	2.0
4	D	104	PHE	2.1
4	D	171	ASP	2.0
16	P	62	ALA	2.0
19	S	78	ALA	2.0
24	X	68	SER	2.0
30	0	999	C	2.0
6	F	12	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
30	0	270	U	2.0
30	0	128	A	2.0
1	A	38	ILE	2.0
8	H	143	VAL	2.0
25	Y	236	VAL	2.0
16	P	121	ASP	2.0
20	T	115	GLU	2.0
14	N	41	LYS	2.0
20	T	29	ALA	2.0
14	N	80	SER	2.0
2	B	112	THR	2.0
4	D	25	MET	2.0
4	D	68	PRO	2.0
6	F	2	VAL	2.0
12	L	130	ARG	2.0
30	0	1527	A	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
32	PPU	4	76	37/38	0.92	0.14	67,75,88,91	0
30	PSU	0	2621	20/21	0.96	0.07	30,37,55,56	0
30	UR3	0	2619	21/22	0.96	0.08	46,49,53,55	0
30	1MA	0	628	23/24	0.98	0.06	28,32,34,36	0
30	OMU	0	2587	21/22	0.98	0.06	37,38,41,42	0
30	OMG	0	2588	24/25	0.98	0.07	37,39,41,45	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
34	CL	3	8804	1/1	0.47	0.14	114,114,114,114	0
35	SR	3	8999	1/1	0.47	0.29	200,200,200,200	0
35	SR	0	9001	1/1	0.54	0.12	186,186,186,186	0
36	NA	0	8548	1/1	0.55	0.37	65,65,65,65	0
36	NA	0	8555	1/1	0.56	0.43	79,79,79,79	0
37	CD	3	8704	1/1	0.61	0.41	200,200,200,200	0
36	NA	0	8511	1/1	0.67	0.27	75,75,75,75	0
36	NA	0	8571	1/1	0.67	0.43	90,90,90,90	0
35	SR	0	9006	1/1	0.67	0.24	194,194,194,194	0
35	SR	0	8979	1/1	0.68	0.18	200,200,200,200	0
36	NA	0	8573	1/1	0.68	0.30	79,79,79,79	0
36	NA	0	8557	1/1	0.68	0.27	58,58,58,58	0
35	SR	9	9003	1/1	0.69	0.15	180,180,180,180	0
35	SR	0	8983	1/1	0.69	0.22	183,183,183,183	0
36	NA	0	8525	1/1	0.69	0.25	70,70,70,70	0
35	SR	0	8959	1/1	0.70	0.15	200,200,200,200	0
36	NA	0	8509	1/1	0.70	0.36	67,67,67,67	0
35	SR	0	8997	1/1	0.71	0.26	185,185,185,185	0
33	MG	0	8080	1/1	0.71	0.17	92,92,92,92	0
36	NA	0	8559	1/1	0.71	0.52	81,81,81,81	0
36	NA	9	8572	1/1	0.72	0.43	98,98,98,98	0
35	SR	J	8986	1/1	0.73	0.23	200,200,200,200	0
33	MG	A	8051	1/1	0.74	0.20	81,81,81,81	0
35	SR	9	8980	1/1	0.74	0.11	185,185,185,185	0
35	SR	0	8953	1/1	0.75	0.17	200,200,200,200	0
37	CD	Z	8703	1/1	0.75	0.23	200,200,200,200	0
36	NA	0	8567	1/1	0.75	0.77	81,81,81,81	0
35	SR	0	8991	1/1	0.76	0.19	182,182,182,182	0
35	SR	0	8947	1/1	0.77	0.27	194,194,194,194	0
36	NA	9	8543	1/1	0.78	0.36	68,68,68,68	0
36	NA	0	8522	1/1	0.78	0.40	78,78,78,78	0
33	MG	0	8031	1/1	0.78	0.14	55,55,55,55	0
35	SR	0	8971	1/1	0.78	0.14	174,174,174,174	0
35	SR	0	8976	1/1	0.79	0.20	181,181,181,181	0
33	MG	0	8083	1/1	0.79	0.13	70,70,70,70	0
35	SR	0	8944	1/1	0.79	0.22	167,167,167,167	0
35	SR	0	8956	1/1	0.80	0.12	141,141,141,141	0
35	SR	0	8938	1/1	0.80	0.23	200,200,200,200	0
36	NA	0	8512	1/1	0.80	0.54	89,89,89,89	0
36	NA	0	8574	1/1	0.80	0.54	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	SR	9	8978	1/1	0.81	0.20	171,171,171,171	0
33	MG	0	8063	1/1	0.81	0.30	81,81,81,81	0
35	SR	0	8977	1/1	0.81	0.09	177,177,177,177	0
35	SR	0	8933	1/1	0.81	0.16	134,134,134,134	0
35	SR	3	8932	1/1	0.81	0.15	167,167,167,167	0
35	SR	0	8920	1/1	0.82	0.13	138,138,138,138	0
36	NA	0	8556	1/1	0.82	0.29	51,51,51,51	0
33	MG	0	8066	1/1	0.82	0.27	76,76,76,76	0
36	NA	0	8541	1/1	0.83	0.30	73,73,73,73	0
36	NA	0	8569	1/1	0.83	0.23	61,61,61,61	0
36	NA	0	8531	1/1	0.83	0.22	46,46,46,46	0
35	SR	0	8922	1/1	0.84	0.17	141,141,141,141	0
35	SR	0	8982	1/1	0.84	0.30	200,200,200,200	0
35	SR	0	8927	1/1	0.84	0.15	161,161,161,161	0
35	SR	0	8988	1/1	0.84	0.10	166,166,166,166	0
33	MG	0	8038	1/1	0.84	0.15	96,96,96,96	0
33	MG	0	8047	1/1	0.84	0.21	72,72,72,72	0
34	CL	J	8802	1/1	0.84	0.11	67,67,67,67	0
33	MG	0	8073	1/1	0.84	0.45	105,105,105,105	0
35	SR	0	8968	1/1	0.85	0.15	175,175,175,175	0
35	SR	0	8987	1/1	0.85	0.37	200,200,200,200	0
33	MG	9	8074	1/1	0.85	0.10	79,79,79,79	0
36	NA	0	8520	1/1	0.85	0.17	48,48,48,48	0
35	SR	0	9004	1/1	0.85	0.24	200,200,200,200	0
36	NA	Q	8540	1/1	0.85	0.28	74,74,74,74	0
36	NA	0	8561	1/1	0.85	0.41	67,67,67,67	0
36	NA	0	8506	1/1	0.85	0.18	63,63,63,63	0
38	K	0	8402	1/1	0.85	0.20	86,86,86,86	0
35	SR	0	8958	1/1	0.86	0.13	128,128,128,128	0
36	NA	0	8519	1/1	0.86	0.18	54,54,54,54	0
33	MG	0	8092	1/1	0.86	0.08	74,74,74,74	0
35	SR	0	8955	1/1	0.86	0.22	200,200,200,200	0
36	NA	H	8518	1/1	0.86	0.13	69,69,69,69	0
36	NA	0	8528	1/1	0.86	0.11	56,56,56,56	0
33	MG	0	8040	1/1	0.86	0.40	84,84,84,84	0
36	NA	0	8536	1/1	0.86	0.16	65,65,65,65	0
35	SR	0	9002	1/1	0.86	0.19	182,182,182,182	0
36	NA	0	8544	1/1	0.86	0.22	71,71,71,71	0
36	NA	0	8507	1/1	0.86	0.19	48,48,48,48	0
35	SR	0	8974	1/1	0.86	0.18	163,163,163,163	0
35	SR	0	8975	1/1	0.86	0.19	144,144,144,144	0
35	SR	0	8992	1/1	0.87	0.28	136,136,136,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	NA	0	8527	1/1	0.87	0.24	67,67,67,67	0
36	NA	0	8514	1/1	0.87	0.17	46,46,46,46	0
35	SR	F	9005	1/1	0.87	0.14	144,144,144,144	0
36	NA	0	8533	1/1	0.87	0.20	70,70,70,70	0
35	SR	0	8998	1/1	0.87	0.23	186,186,186,186	0
33	MG	0	8090	1/1	0.87	0.17	87,87,87,87	0
36	NA	0	8562	1/1	0.87	0.26	73,73,73,73	0
36	NA	0	8563	1/1	0.87	0.46	86,86,86,86	0
36	NA	0	8564	1/1	0.87	0.15	62,62,62,62	0
35	SR	0	8942	1/1	0.88	0.12	126,126,126,126	0
35	SR	0	8996	1/1	0.88	0.23	200,200,200,200	0
36	NA	0	8553	1/1	0.88	0.26	84,84,84,84	0
36	NA	0	8554	1/1	0.88	0.32	61,61,61,61	0
35	SR	0	8915	1/1	0.88	0.12	127,127,127,127	0
33	MG	0	8089	1/1	0.88	0.07	49,49,49,49	0
36	NA	0	8513	1/1	0.88	0.31	46,46,46,46	0
33	MG	T	8057	1/1	0.88	0.23	76,76,76,76	0
36	NA	0	8534	1/1	0.88	0.46	84,84,84,84	0
35	SR	0	8990	1/1	0.88	0.19	164,164,164,164	0
35	SR	0	8939	1/1	0.88	0.11	133,133,133,133	0
35	SR	0	9000	1/1	0.89	0.18	168,168,168,168	0
34	CL	0	8815	1/1	0.89	0.20	69,69,69,69	0
36	NA	0	8529	1/1	0.89	0.12	43,43,43,43	0
36	NA	0	8530	1/1	0.89	0.15	48,48,48,48	0
36	NA	0	8508	1/1	0.89	0.11	47,47,47,47	0
35	SR	0	8989	1/1	0.89	0.26	157,157,157,157	0
35	SR	0	8957	1/1	0.89	0.24	200,200,200,200	0
36	NA	0	8535	1/1	0.89	0.15	59,59,59,59	0
33	MG	0	8060	1/1	0.89	0.19	69,69,69,69	0
35	SR	0	8934	1/1	0.89	0.23	133,133,133,133	0
35	SR	0	8993	1/1	0.89	0.12	167,167,167,167	0
36	NA	0	8575	1/1	0.89	0.30	89,89,89,89	0
36	NA	0	8516	1/1	0.89	0.30	53,53,53,53	0
35	SR	0	8949	1/1	0.89	0.16	113,113,113,113	0
33	MG	0	8049	1/1	0.89	0.23	56,56,56,56	0
33	MG	0	8056	1/1	0.89	0.16	59,59,59,59	0
36	NA	0	8502	1/1	0.89	0.12	49,49,49,49	0
35	SR	0	8916	1/1	0.90	0.14	112,112,112,112	0
35	SR	B	8950	1/1	0.90	0.11	112,112,112,112	0
35	SR	0	8995	1/1	0.90	0.16	141,141,141,141	0
36	NA	C	8503	1/1	0.90	0.08	36,36,36,36	0
33	MG	0	8046	1/1	0.90	0.16	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8039	1/1	0.90	0.13	62,62,62,62	0
36	NA	R	8532	1/1	0.90	0.13	56,56,56,56	0
36	NA	0	8549	1/1	0.90	0.20	53,53,53,53	0
35	SR	0	8962	1/1	0.90	0.22	194,194,194,194	0
35	SR	0	8967	1/1	0.90	0.14	125,125,125,125	0
34	CL	N	8807	1/1	0.90	0.15	71,71,71,71	0
35	SR	0	8951	1/1	0.90	0.11	142,142,142,142	0
33	MG	0	8030	1/1	0.90	0.21	85,85,85,85	0
36	NA	0	8558	1/1	0.90	0.28	63,63,63,63	0
33	MG	0	8082	1/1	0.90	0.14	73,73,73,73	0
36	NA	0	8560	1/1	0.91	0.20	87,87,87,87	0
36	NA	0	8537	1/1	0.91	0.08	40,40,40,40	0
36	NA	B	8552	1/1	0.91	0.27	78,78,78,78	0
36	NA	0	8542	1/1	0.91	0.15	45,45,45,45	0
35	SR	0	8981	1/1	0.91	0.14	148,148,148,148	0
36	NA	0	8547	1/1	0.91	0.28	59,59,59,59	0
33	MG	0	8071	1/1	0.91	0.21	67,67,67,67	0
36	NA	M	8539	1/1	0.91	0.10	38,38,38,38	0
36	NA	0	8550	1/1	0.91	0.20	63,63,63,63	0
35	SR	0	8969	1/1	0.91	0.26	184,184,184,184	0
33	MG	0	8075	1/1	0.91	0.07	62,62,62,62	0
36	NA	S	8510	1/1	0.91	0.15	47,47,47,47	0
36	NA	0	8501	1/1	0.91	0.23	39,39,39,39	0
36	NA	0	8517	1/1	0.91	0.19	56,56,56,56	0
35	SR	0	8924	1/1	0.91	0.17	124,124,124,124	0
38	K	0	8401	1/1	0.91	0.37	147,147,147,147	0
35	SR	0	8994	1/1	0.91	0.30	200,200,200,200	0
35	SR	0	8960	1/1	0.92	0.12	138,138,138,138	0
33	MG	0	8064	1/1	0.92	0.10	48,48,48,48	0
36	NA	J	8538	1/1	0.92	0.13	57,57,57,57	0
35	SR	0	8965	1/1	0.92	0.10	118,118,118,118	0
36	NA	0	8504	1/1	0.92	0.16	37,37,37,37	0
34	CL	O	8808	1/1	0.92	0.20	62,62,62,62	0
36	NA	0	8523	1/1	0.92	0.07	30,30,30,30	0
35	SR	0	8910	1/1	0.93	0.10	94,94,94,94	0
35	SR	0	8963	1/1	0.93	0.07	129,129,129,129	0
35	SR	0	8941	1/1	0.93	0.10	114,114,114,114	0
33	MG	0	8010	1/1	0.93	0.07	47,47,47,47	0
33	MG	0	8036	1/1	0.93	0.15	47,47,47,47	0
33	MG	0	8078	1/1	0.93	0.11	59,59,59,59	0
36	NA	0	8566	1/1	0.93	0.11	38,38,38,38	0
35	SR	A	8930	1/1	0.93	0.08	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8067	1/1	0.93	0.12	54,54,54,54	0
34	CL	A	8809	1/1	0.93	0.32	88,88,88,88	0
35	SR	0	8928	1/1	0.93	0.13	141,141,141,141	0
35	SR	0	8931	1/1	0.93	0.08	100,100,100,100	0
36	NA	0	8524	1/1	0.93	0.10	45,45,45,45	0
33	MG	0	8069	1/1	0.93	0.12	75,75,75,75	0
34	CL	L	8810	1/1	0.93	0.09	70,70,70,70	0
35	SR	0	8936	1/1	0.93	0.10	95,95,95,95	0
33	MG	0	8037	1/1	0.93	0.20	75,75,75,75	0
35	SR	0	8984	1/1	0.93	0.09	107,107,107,107	0
35	SR	0	8985	1/1	0.93	0.14	121,121,121,121	0
35	SR	0	8954	1/1	0.94	0.08	94,94,94,94	0
35	SR	0	8970	1/1	0.94	0.10	113,113,113,113	0
33	MG	0	8068	1/1	0.94	0.15	59,59,59,59	0
35	SR	0	8972	1/1	0.94	0.22	143,143,143,143	0
35	SR	0	8973	1/1	0.94	0.12	124,124,124,124	0
36	NA	0	8515	1/1	0.94	0.05	36,36,36,36	0
34	CL	0	8805	1/1	0.94	0.11	71,71,71,71	0
33	MG	0	8024	1/1	0.94	0.15	44,44,44,44	0
35	SR	0	8917	1/1	0.94	0.10	110,110,110,110	0
36	NA	0	8546	1/1	0.94	0.11	64,64,64,64	0
33	MG	0	8035	1/1	0.94	0.11	62,62,62,62	0
34	CL	J	8801	1/1	0.94	0.10	68,68,68,68	0
33	MG	0	8072	1/1	0.94	0.18	58,58,58,58	0
33	MG	0	8088	1/1	0.94	0.12	41,41,41,41	0
36	NA	0	8551	1/1	0.94	0.13	36,36,36,36	0
35	SR	0	8964	1/1	0.94	0.09	121,121,121,121	0
35	SR	S	8961	1/1	0.94	0.08	118,118,118,118	0
33	MG	0	8059	1/1	0.94	0.16	47,47,47,47	0
33	MG	0	8017	1/1	0.94	0.13	29,29,29,29	0
35	SR	0	9007	1/1	0.94	0.44	200,200,200,200	0
36	NA	0	8565	1/1	0.95	0.16	71,71,71,71	0
35	SR	0	8966	1/1	0.95	0.10	103,103,103,103	0
35	SR	0	8937	1/1	0.95	0.09	102,102,102,102	0
33	MG	0	8052	1/1	0.95	0.07	50,50,50,50	0
36	NA	0	8521	1/1	0.95	0.09	50,50,50,50	0
33	MG	B	8042	1/1	0.95	0.14	55,55,55,55	0
35	SR	0	8926	1/1	0.95	0.09	118,118,118,118	0
33	MG	0	8076	1/1	0.95	0.04	31,31,31,31	0
35	SR	0	8914	1/1	0.95	0.11	108,108,108,108	0
33	MG	0	8032	1/1	0.95	0.09	42,42,42,42	0
35	SR	0	8948	1/1	0.95	0.11	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8079	1/1	0.95	0.10	60,60,60,60	0
33	MG	0	8033	1/1	0.95	0.06	50,50,50,50	0
33	MG	0	8081	1/1	0.95	0.17	68,68,68,68	0
35	SR	0	8946	1/1	0.96	0.07	102,102,102,102	0
35	SR	0	8923	1/1	0.96	0.08	94,94,94,94	0
33	MG	0	8034	1/1	0.96	0.06	44,44,44,44	0
33	MG	0	8008	1/1	0.96	0.11	26,26,26,26	0
33	MG	0	8007	1/1	0.96	0.10	50,50,50,50	0
35	SR	1	8952	1/1	0.96	0.05	73,73,73,73	0
34	CL	Y	8820	1/1	0.96	0.04	41,41,41,41	0
36	NA	0	8545	1/1	0.96	0.30	42,42,42,42	0
33	MG	0	8043	1/1	0.96	0.10	44,44,44,44	0
36	NA	0	8568	1/1	0.96	0.11	58,58,58,58	0
33	MG	0	8045	1/1	0.96	0.05	38,38,38,38	0
36	NA	0	8570	1/1	0.96	0.28	50,50,50,50	0
34	CL	0	8811	1/1	0.96	0.12	64,64,64,64	0
34	CL	0	8813	1/1	0.96	0.06	44,44,44,44	0
34	CL	B	8819	1/1	0.96	0.14	53,53,53,53	0
35	SR	A	8929	1/1	0.96	0.16	119,119,119,119	0
36	NA	0	8505	1/1	0.96	0.39	37,37,37,37	0
35	SR	0	8918	1/1	0.96	0.09	84,84,84,84	0
33	MG	0	8085	1/1	0.96	0.16	71,71,71,71	0
35	SR	0	8943	1/1	0.96	0.10	75,75,75,75	0
33	MG	0	8016	1/1	0.96	0.08	46,46,46,46	0
35	SR	0	8945	1/1	0.96	0.06	99,99,99,99	0
33	MG	0	8048	1/1	0.97	0.10	25,25,25,25	0
33	MG	0	8029	1/1	0.97	0.18	43,43,43,43	0
33	MG	0	8009	1/1	0.97	0.10	31,31,31,31	0
36	NA	0	8526	1/1	0.97	0.04	34,34,34,34	0
33	MG	0	8055	1/1	0.97	0.05	59,59,59,59	0
34	CL	M	8818	1/1	0.97	0.10	40,40,40,40	0
33	MG	Y	8086	1/1	0.97	0.05	36,36,36,36	0
35	SR	0	8935	1/1	0.97	0.07	92,92,92,92	0
33	MG	0	8087	1/1	0.97	0.04	24,24,24,24	0
33	MG	0	8014	1/1	0.97	0.12	31,31,31,31	0
35	SR	0	8901	1/1	0.97	0.08	57,57,57,57	0
35	SR	0	8908	1/1	0.97	0.06	87,87,87,87	0
35	SR	0	8940	1/1	0.97	0.05	89,89,89,89	0
33	MG	0	8002	1/1	0.97	0.06	33,33,33,33	0
35	SR	0	8911	1/1	0.97	0.06	82,82,82,82	0
34	CL	0	8803	1/1	0.97	0.12	51,51,51,51	0
33	MG	K	8054	1/1	0.97	0.14	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8077	1/1	0.97	0.04	42,42,42,42	0
33	MG	0	8093	1/1	0.97	0.05	37,37,37,37	0
33	MG	A	8050	1/1	0.97	0.08	60,60,60,60	0
34	CL	0	8816	1/1	0.97	0.12	61,61,61,61	0
35	SR	0	8921	1/1	0.97	0.08	84,84,84,84	0
34	CL	0	8817	1/1	0.97	0.06	58,58,58,58	0
34	CL	0	8822	1/1	0.97	0.20	87,87,87,87	0
33	MG	0	8028	1/1	0.97	0.09	27,27,27,27	0
35	SR	0	8925	1/1	0.97	0.07	89,89,89,89	0
33	MG	0	8061	1/1	0.98	0.07	30,30,30,30	0
33	MG	0	8062	1/1	0.98	0.14	49,49,49,49	0
33	MG	0	8025	1/1	0.98	0.08	42,42,42,42	0
33	MG	0	8027	1/1	0.98	0.08	38,38,38,38	0
34	CL	J	8821	1/1	0.98	0.04	56,56,56,56	0
33	MG	0	8065	1/1	0.98	0.08	37,37,37,37	0
35	SR	R	8912	1/1	0.98	0.06	72,72,72,72	0
33	MG	0	8015	1/1	0.98	0.08	37,37,37,37	0
35	SR	1	8913	1/1	0.98	0.05	79,79,79,79	0
35	SR	0	9008	1/1	0.98	0.05	79,79,79,79	0
33	MG	0	8020	1/1	0.98	0.10	42,42,42,42	0
33	MG	0	8021	1/1	0.98	0.10	26,26,26,26	0
33	MG	0	8022	1/1	0.98	0.12	33,33,33,33	0
33	MG	0	8070	1/1	0.98	0.09	58,58,58,58	0
33	MG	0	8053	1/1	0.98	0.09	55,55,55,55	0
33	MG	0	8023	1/1	0.98	0.12	24,24,24,24	0
33	MG	0	8091	1/1	0.98	0.04	47,47,47,47	0
34	CL	0	8812	1/1	0.98	0.07	49,49,49,49	0
33	MG	0	8041	1/1	0.98	0.09	35,35,35,35	0
37	CD	O	8705	1/1	0.98	0.04	88,88,88,88	0
34	CL	0	8814	1/1	0.98	0.09	56,56,56,56	0
33	MG	0	8006	1/1	0.98	0.09	33,33,33,33	0
33	MG	0	8001	1/1	0.98	0.16	20,20,20,20	0
33	MG	0	8044	1/1	0.98	0.06	54,54,54,54	0
33	MG	0	8018	1/1	0.99	0.14	37,37,37,37	0
33	MG	0	8026	1/1	0.99	0.09	38,38,38,38	0
34	CL	R	8806	1/1	0.99	0.04	47,47,47,47	0
33	MG	0	8084	1/1	0.99	0.17	33,33,33,33	0
33	MG	0	8019	1/1	0.99	0.14	33,33,33,33	0
35	SR	0	8902	1/1	0.99	0.09	53,53,53,53	0
35	SR	0	8903	1/1	0.99	0.10	49,49,49,49	0
35	SR	0	8904	1/1	0.99	0.07	54,54,54,54	0
35	SR	0	8905	1/1	0.99	0.12	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	SR	0	8906	1/1	0.99	0.07	56,56,56,56	0
35	SR	0	8907	1/1	0.99	0.06	53,53,53,53	0
33	MG	0	8013	1/1	0.99	0.05	30,30,30,30	0
35	SR	0	8909	1/1	0.99	0.06	84,84,84,84	0
33	MG	0	8058	1/1	0.99	0.07	28,28,28,28	0
37	CD	U	8701	1/1	0.99	0.03	78,78,78,78	0
33	MG	0	8005	1/1	0.99	0.09	28,28,28,28	0
33	MG	0	8003	1/1	0.99	0.04	30,30,30,30	0
33	MG	0	8004	1/1	0.99	0.07	24,24,24,24	0
33	MG	0	8012	1/1	0.99	0.08	23,23,23,23	0
37	CD	1	8702	1/1	1.00	0.03	54,54,54,54	0
33	MG	0	8011	1/1	1.00	0.10	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.