



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 07:47 PM EDT

PDB ID : 3CCM
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2611U
Authors : Blaha, G.; Gurel, G.
Deposited on : unknown
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

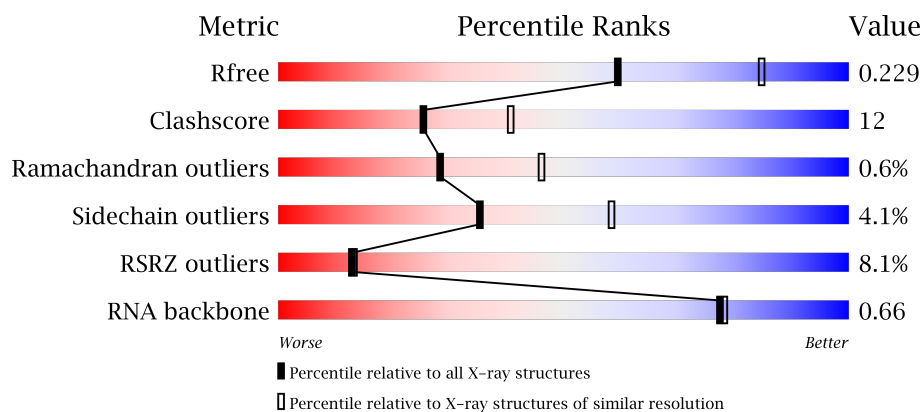
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)
RNA backbone	2435	1023 (2.96-2.12)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>8%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
2	B	338	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>.</div> </div> </div>
3	C	246	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>.</div> </div> </div>
4	D	177	<div> <div>40%</div> <div> <div></div> <div>52%</div> <div>25%</div> <div>.</div> <div>21%</div> </div> </div>



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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8001	-	-	-	X
32	MG	0	8004	-	-	-	X
32	MG	0	8006	-	-	-	X
32	MG	0	8008	-	-	-	X
32	MG	0	8009	-	-	-	X
32	MG	0	8012	-	-	-	X
32	MG	0	8014	-	-	-	X
32	MG	0	8015	-	-	-	X
32	MG	0	8020	-	-	-	X
32	MG	0	8028	-	-	-	X
32	MG	0	8041	-	-	-	X
32	MG	0	8044	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8062	-	-	-	X
32	MG	0	8065	-	-	-	X
32	MG	0	8085	-	-	-	X
32	MG	A	8051	-	-	-	X
33	CL	B	8819	-	-	-	X
34	SR	0	8910	-	-	-	X
34	SR	0	8918	-	-	-	X
34	SR	0	8987	-	-	-	X
35	NA	0	8504	-	-	-	X
35	NA	0	8508	-	-	-	X
35	NA	0	8512	-	-	-	X
35	NA	0	8513	-	-	-	X
35	NA	0	8517	-	-	-	X
35	NA	0	8520	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8523	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8530	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8547	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8558	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8569	-	-	-	X
35	NA	0	8575	-	-	-	X
35	NA	C	8503	-	-	-	X
37	K	0	8401	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99119 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L2P.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

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

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 38 is water.

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

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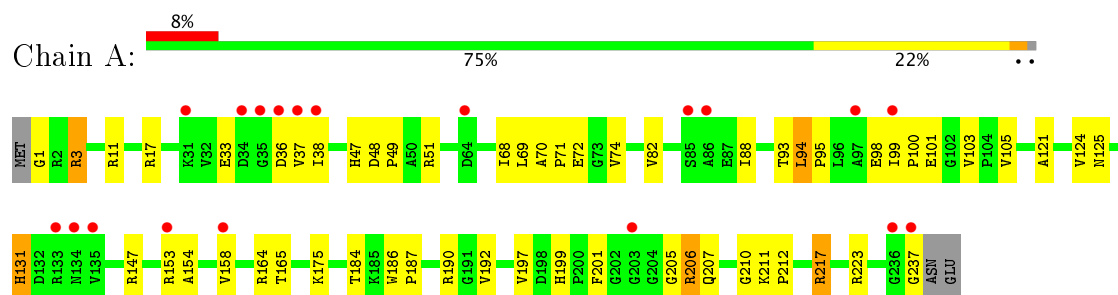
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	W	68	Total 68	O 68	0	0
38	X	24	Total 24	O 24	0	0
38	Y	97	Total 97	O 97	0	0
38	Z	29	Total 29	O 29	0	0
38	1	51	Total 51	O 51	0	0
38	2	37	Total 37	O 37	0	0
38	3	72	Total 72	O 72	0	0
38	0	5938	Total 5938	O 5938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

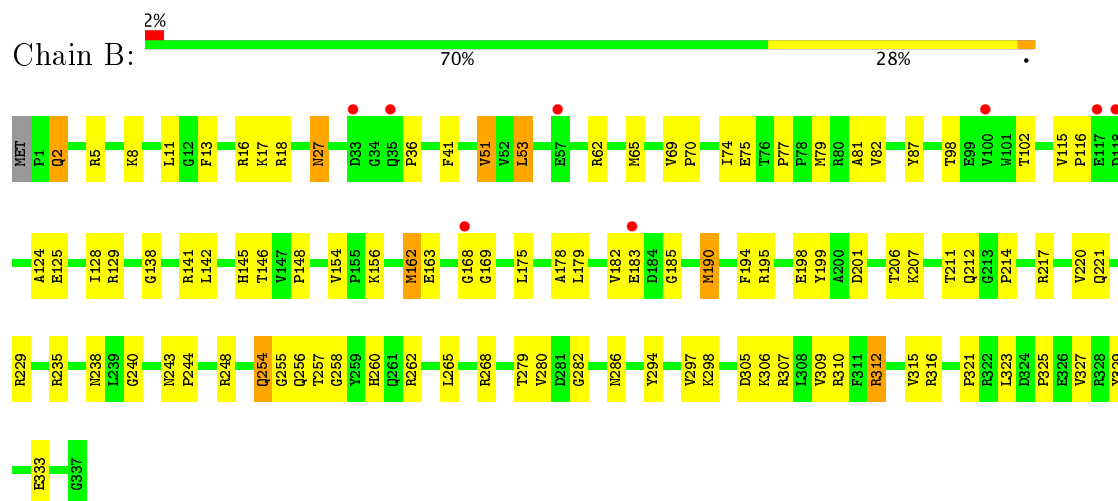
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



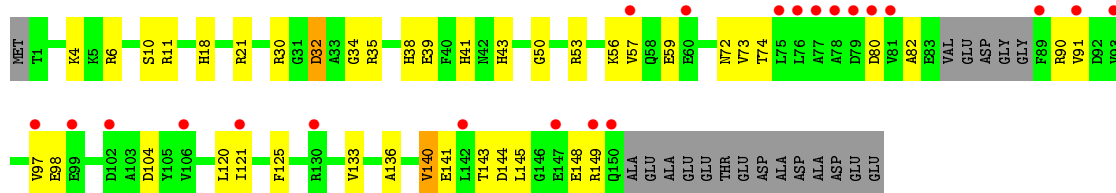
• Molecule 2: 50S ribosomal protein L3P



L132

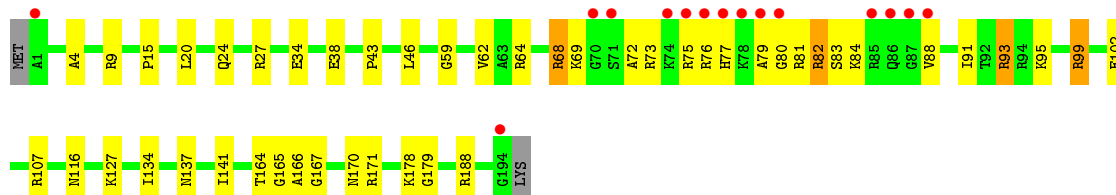
- Molecule 12: 50S ribosomal protein L15P

Chain L:



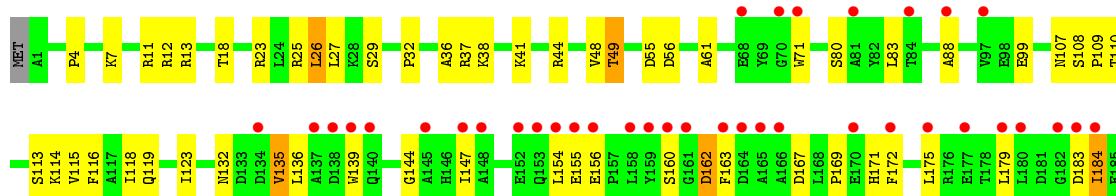
- Molecule 13: 50S ribosomal protein L15e

Chain M:



- Molecule 14: 50S ribosomal protein L18P

Chain N:



L186

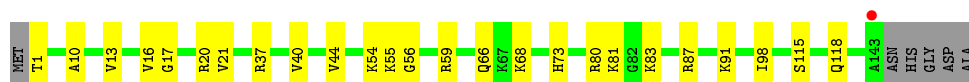
- Molecule 15: 50S ribosomal protein L18e

Chain O:



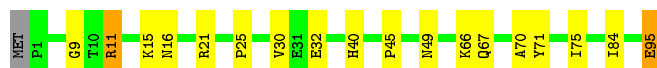
- Molecule 16: 50S ribosomal protein L19e

Chain P:



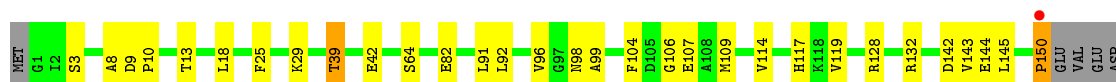
- Molecule 17: 50S ribosomal protein L21e

Chain Q: 80% 17% ..



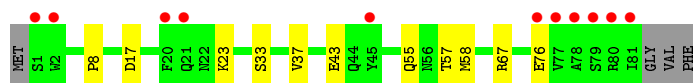
- Molecule 18: 50S ribosomal protein L22P

Chain R: .% 77% 19% ..



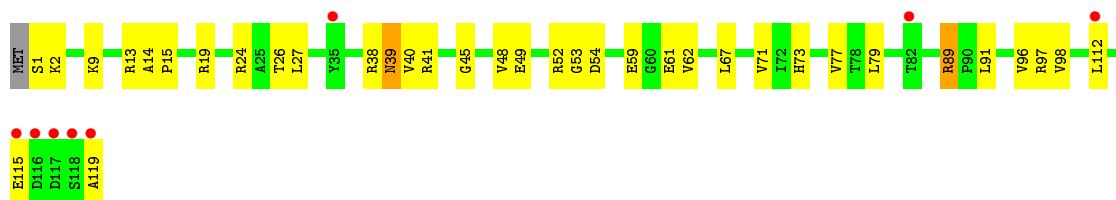
- Molecule 19: 50S ribosomal protein L23P

Chain S: 13% 82% 13% 5%



- Molecule 20: 50S ribosomal protein L24P

Chain T: 7% 69% 28% ..



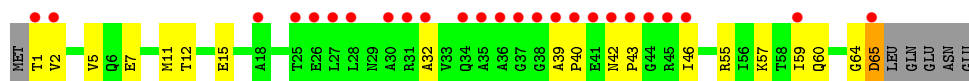
- Molecule 21: 50S ribosomal protein L24e

Chain U: 4% 52% 25% 21%

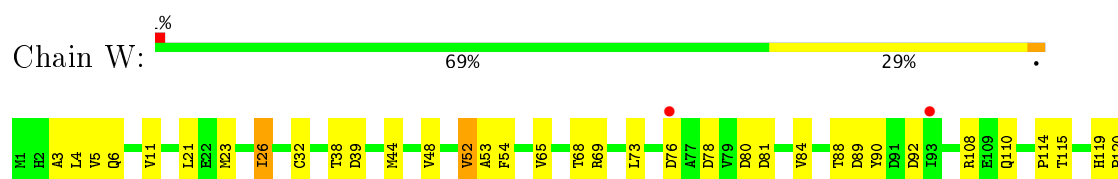


- Molecule 22: 50S ribosomal protein L29P

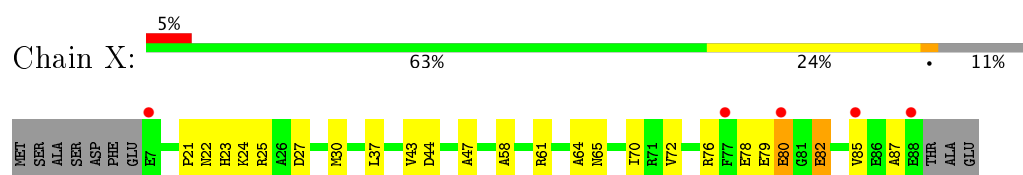
Chain V: 35% 65% 25% 8%



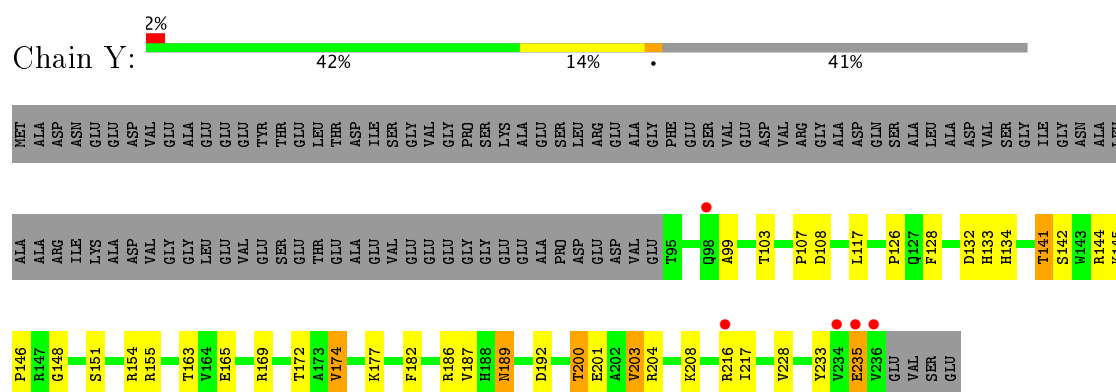
- Molecule 23: 50S ribosomal protein L30P



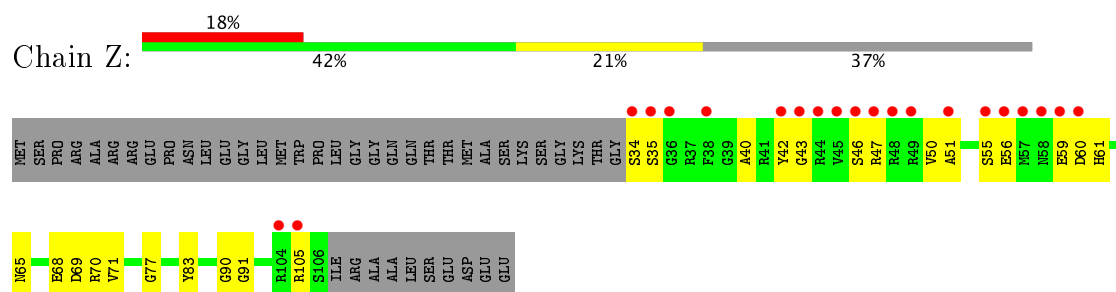
• Molecule 24: 50S ribosomal protein L31e



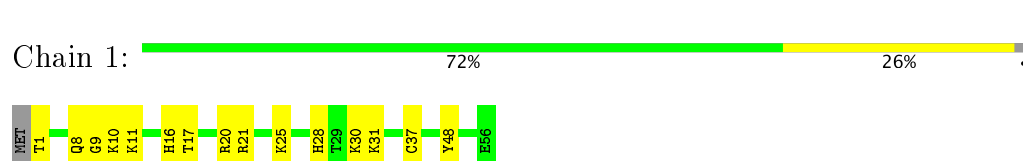
• Molecule 25: 50S ribosomal protein L32e



• Molecule 26: 50S ribosomal protein L37Ae



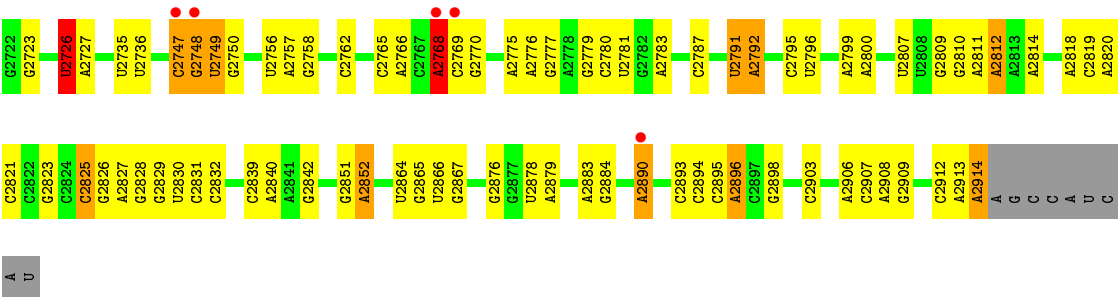
• Molecule 27: 50S ribosomal protein L37e



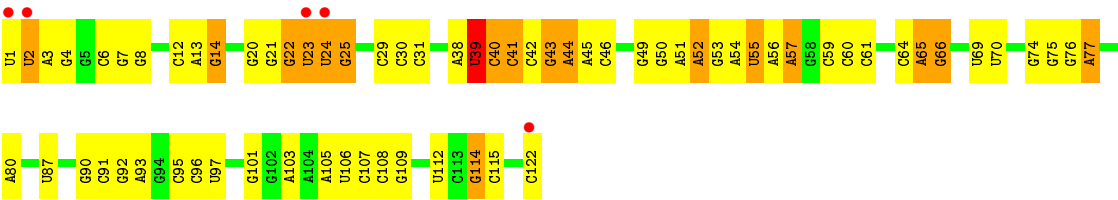
• Molecule 28: 50S ribosomal protein L39e



G2612	A2509	G2314	C	U	U2063	A	G1849	A1736	A1630	A1501	A1369	G1290	G1197
G2613	C2510	C2315	U	A	U2064	A	U1850	A1737	A1631	A1502	A1372	A1294	U1198
G2614	A2511	G2316	C	G	G2070	C	A1851	G1738	A1632	U1503	A1372	A1294	A1199
G2615	U2512	C2317	A	U	G2071	U	A1852	G1739	G1633	A1504	A1377	U1298	A1200
G2616	G2513	U2320	C	U	G2072	A	C1856	U1740	C1634	U1505	G1377	U1299	C1201
G2617	C2515	A2321	C	A	G2073	U	C1856	U1741	G1634	U1506	A1378	G1300	A1202
G2626	G2516	U2322	U	G	G2074	G	C1862	G1744	A1641	U1511	U1380	U1304	G1203
G2627	A2521	G2323	C	G	A2081	C	G1863	G1745	A1642	G1512	U1305	U1304	C1204
A2635	G2522	C2326	G	U	A2089	C	C1864	C1750	U1654	A1518	C1384	C1305	U1206
C2636	G2523	A2327	U	U	A2089	C	U1866	G1751	G1655	U1519	G1391	U1309	A1207
A2637	G2524	U2328	G	C	G2090	C	G1867	G1752	A1656	G1520	A1392	U1310	G1208
G2644	G2525	C2329	A	U	G2091	U	G1868	G1755	A1657	C1521	G1311	G1311	G1210
U2645	C2526	U2330	C	U	G2094	U	U1871	G1756	A1658	A1522	C1396	G1312	G1211
G2646	G2428	A2332	G	C	A2095	C	G1872	G1756	A1659	G1523	G1397	A1313	C1212
A2649	A2430	G2333	C	A	A2096	C	G1873	A1759	G1660	U1524	G1398	U1314	C1213
U2652	G2438	G2338	A	G	A2099	C	G1877	G1760	C1666	A1526	A1399	G1315	G1214
U2661	C2443	C	A	A	A2100	C	G1878	U1761	A1667	A1527	A1406	A1321	G1216
A2664	G2453	G2344	G	A	A2101	C	U1879	C1762	U1668	A1528	A1407	G1322	U1218
A	C2454	A2345	C	C	G2102	U	U1883	U1766	C1675	G1529	G1415	G1325	U1219
U	A2455	A2346	C	C	A2103	A	A1886	C1768	C1679	G1535	A1414	G1325	U1220
G2667	U2457	C2347	C	C	C2105	C	U1985	C1769	G1680	A1536	G1415	A1328	C1229
G2670	C2552	C2247	G	A	C2106	C	U1992	G1773	G1681	G1552	G1417	G1331	A1230
U2671	A2553	C2248	C	G	G2110	C	G1902	G1777	A1682	C1553	U1418	A1231	A1232
C2672	U2461	G2249	C	G	A2111	C	U1903	G1778	G1683	G1554	U1419	C1332	A1233
G2676	G2462	G2250	U	U	A2112	C	A1909	A1778	A1684	G1555	U1422	U1333	A1233
G2679	A2465	G2251	C	A	G2113	C	A1910	A1779	A1685	U	C1423	C1334	U1234
A2680	G2466	G2252	C	U	C2114	C	A1919	C1787	G1686	A1559	U1426	C1335	G1235
A2681	A2467	A2253	C	C	G2128	C	G1920	U1788	C1687	C1562	G1426	U1336	A1236
G2682	A2468	A2254	G	G	A2135	C	A1921	C1789	C1692	C1562	G1441	G1339	U1237
A2694	C2476	A2255	C	C	G2136	C	A1922	U1791	G1697	A1573	A1442	G1340	G1239
A2697	G2482	U2256	C	C	A	C	G1925	C1798	C1700	C1574	U1446	G1341	G1240
G2698	U2483	A2266	C	C	G	C	G1926	C1799	A1701	G1588	G1451	C1342	G1241
A2699	U2484	G2271	C	U	U2007	A	A1927	U1791	U1702	G1589	U1452	G1343	A1242
G2700	C2487	G2272	C	C	U2008	C	G1928	C1816	U1702	G1589	G1452	G1344	C1243
C2704	A2490	G2281	C	C	C	C	G1929	U1817	A1710	G1592	U1452	U1346	U1244
U2705	U2491	U2282	C	C	C	C	U1939	C1818	C1714	C1593	U1471	U1350	A1246
U2710	U2492	G2283	A	U	U2032	C	C1940	G1819	C1715	C1594	U1472	G1351	U1249
U2711	C2493	G2284	G	G	U2033	C	U1941	G1820	C1716	G1595	C1474	A1352	C1250
G2712	A2502	U2289	C	C	C2035	C	A1942	U1835	A1717	U1596	G1475	C1353	G1251
G2716	C2503	U2290	C	C	U2036	C	C1943	U1838	C1722	G1597	C1476	G1354	A1252
C2717	A2504	A2302	U	U	C2037	C	C1946	U1839	U1722	A1598	U1477	A1355	C1253
G2718	G2505	G2309	A	A	A2038	C	G1947	A1840	G1730	A1603	A1482	A1357	C1257
A2719	U2506	G2310	A	A	C2039	C	G1948	C1841	C1731	G1604	C1483	A1358	G1258
C2608	G2507	A2311	A	A	A2054	C	G1949	A1842	A1732	U1724	G1484	C1360	C1268
C2720	G2507	G2312	U	U	C2061	C	U1951	A1847	C1733	G1605	U1488	G1363	A1278
U2721	G2407	G2313	A	A	A2062	C	U	G1948	C1735	A1626	A1497	C1366	A1280



● Molecule 31: 5S RIBOSOMAL RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.53Å 298.18Å 573.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.55 85.30 – 2.39	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.70-2.55) 90.6 (85.30-2.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.240 0.194 , 0.229	Depositor DCC
R_{free} test set	5365 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99119	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.33	0/1786	0.65	0/2408
2	B	0.33	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.65	0/2552
4	D	0.30	0/1111	0.56	1/1498 (0.1%)
5	E	0.31	0/1382	0.56	0/1880
6	F	0.33	0/901	0.56	0/1224
7	G	0.29	0/241	0.45	0/324
8	H	0.33	0/1302	0.64	0/1743
9	I	0.29	0/526	0.47	0/716
10	J	0.36	0/1136	0.58	0/1530
11	K	0.32	0/1004	0.66	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.35	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.63	0/1999
15	O	0.32	0/874	0.60	0/1181
16	P	0.33	0/1147	0.53	0/1528
17	Q	0.35	0/749	0.69	0/1005
18	R	1.26	7/1172 (0.6%)	1.11	6/1578 (0.4%)
19	S	0.33	0/648	0.56	0/875
20	T	0.32	0/958	0.64	0/1289
21	U	0.34	0/417	0.55	0/562
22	V	0.30	0/502	0.51	0/675
23	W	0.33	0/1219	0.60	0/1655
24	X	0.32	0/664	0.57	0/895
25	Y	0.36	0/1146	0.63	0/1536
26	Z	0.36	0/584	0.60	0/781
27	1	0.39	0/438	0.65	0/578
28	2	0.35	0/401	0.56	0/529
29	3	0.38	0/771	0.57	0/1024
30	0	0.35	0/65953	0.69	25/102860 (0.0%)
31	9	0.30	0/2904	0.70	1/4526 (0.0%)
All	All	0.37	7/98697 (0.0%)	0.68	33/147579 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
30	0	0	46
31	9	0	3
All	All	1	49

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	26.57	2.82	1.50
18	R	150	PRO	CA-C	-19.00	1.14	1.52
18	R	150	PRO	CG-CD	14.11	1.97	1.50
18	R	150	PRO	C-O	11.94	1.47	1.23
18	R	150	PRO	N-CA	11.60	1.67	1.47
18	R	150	PRO	N-CD	10.77	1.62	1.47
18	R	150	PRO	CA-CB	7.91	1.69	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.33	56.17	112.00
18	R	150	PRO	N-CA-C	-19.61	61.12	112.10
18	R	150	PRO	CA-N-CD	12.19	128.76	111.70
18	R	150	PRO	N-CA-CB	10.92	116.40	103.30
30	0	1942	A	C5'-C4'-C3'	8.23	129.17	116.00
18	R	150	PRO	CA-C-O	-8.07	100.83	120.20
30	0	871	G	C5'-C4'-O4'	-7.66	99.91	109.10
30	0	1942	A	C5'-C4'-O4'	6.92	117.41	109.10
30	0	1592	G	N9-C1'-C2'	6.74	122.76	114.00
30	0	1504	A	C1'-O4'-C4'	-6.26	104.89	109.90
30	0	1819	G	C5'-C4'-C3'	6.22	125.96	116.00
31	9	39	U	N1-C1'-C2'	6.17	122.03	114.00
30	0	777	U	O4'-C1'-N1	5.90	112.92	108.20
30	0	921	G	N9-C1'-C2'	5.80	121.54	114.00
30	0	1942	A	C1'-O4'-C4'	-5.80	105.26	109.90
18	R	150	PRO	CA-CB-CG	-5.79	93.00	104.00
30	0	2316	G	C5'-C4'-C3'	-5.76	106.78	116.00
30	0	1737	A	C5'-C4'-C3'	-5.68	106.91	116.00
30	0	1819	G	C1'-O4'-C4'	-5.67	105.37	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1819	G	C4'-C3'-C2'	-5.63	96.97	102.60
30	0	1452	G	C5'-C4'-C3'	-5.53	107.15	116.00
30	0	1942	A	C4'-C3'-C2'	-5.52	97.08	102.60
30	0	2467	A	C1'-O4'-C4'	-5.52	105.48	109.90
30	0	206	G	C5'-C4'-C3'	-5.41	107.34	116.00
30	0	2536	C	N1-C1'-C2'	5.37	120.98	114.00
4	D	170	TYR	N-CA-C	5.32	125.35	111.00
30	0	1504	A	N9-C1'-C2'	5.28	120.87	114.00
30	0	1878	G	N9-C1'-C2'	-5.20	106.28	112.00
30	0	1615	A	C5'-C4'-C3'	5.12	124.19	116.00
30	0	1342	C	N1-C1'-C2'	-5.10	106.39	112.00
30	0	2726	U	N1-C1'-C2'	5.08	120.61	114.00
30	0	2313	C	C5'-C4'-O4'	5.07	115.18	109.10
30	0	841	A	C1'-O4'-C4'	-5.03	105.87	109.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1122	U	Sidechain
30	0	1237	U	Sidechain
30	0	1340	G	Sidechain
30	0	1342	C	Sidechain
30	0	1417	G	Sidechain
30	0	1488	U	Sidechain
30	0	1714	C	Sidechain
30	0	1744	G	Sidechain
30	0	1777	G	Sidechain
30	0	1819	G	Sidechain
30	0	182	G	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1979	G	Sidechain
30	0	2036	C	Sidechain
30	0	2316	G	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2552	C	Sidechain
30	0	2597	U	Sidechain
30	0	2599	A	Sidechain
30	0	26	U	Sidechain
30	0	2607	U	Sidechain
30	0	270	U	Sidechain
30	0	2768	A	Sidechain
30	0	2842	G	Sidechain
30	0	332	G	Sidechain
30	0	396	U	Sidechain
30	0	460	A	Sidechain
30	0	462	A	Sidechain
30	0	469	G	Sidechain
30	0	470	U	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	664	U	Sidechain
30	0	795	G	Sidechain
30	0	817	G	Sidechain
30	0	867	A	Sidechain
30	0	868	G	Sidechain
31	9	39	U	Sidechain
31	9	87	U	Sidechain
31	9	90	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	51	0
2	B	2625	0	2533	86	0
3	C	1860	0	1813	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1094	0	1085	37	0
5	E	1357	0	1266	35	0
6	F	890	0	843	25	0
7	G	240	0	231	6	0
8	H	1282	0	1292	31	0
9	I	519	0	500	19	0
10	J	1120	0	1098	37	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	35	0
13	M	1558	0	1572	48	0
14	N	1445	0	1401	50	0
15	O	865	0	873	24	0
16	P	1136	0	1123	23	0
17	Q	735	0	729	16	0
18	R	1149	0	1122	32	0
19	S	641	0	605	9	0
20	T	950	0	924	25	0
21	U	410	0	364	15	0
22	V	499	0	511	15	0
23	W	1196	0	1137	52	0
24	X	654	0	653	15	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	15	0
27	1	431	0	426	22	0
28	2	396	0	413	19	0
29	3	755	0	728	13	0
30	0	59017	0	29811	1046	0
31	9	2599	0	1325	78	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	10	0	0	1	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	94	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	1	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5938	0	0	160	0
38	1	51	0	0	1	0
38	2	37	0	0	1	0
38	3	72	0	0	4	0
38	9	145	0	0	9	0
38	A	117	0	0	8	0
38	B	139	0	0	16	0
38	C	165	0	0	10	0
38	D	48	0	0	5	0
38	E	49	0	0	1	0
38	F	25	0	0	1	0
38	G	18	0	0	1	0
38	H	71	0	0	5	0
38	I	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	J	55	0	0	1	0
38	K	55	0	0	2	0
38	L	79	0	0	8	0
38	M	138	0	0	3	0
38	N	58	0	0	6	0
38	O	40	0	0	0	0
38	P	61	0	0	1	0
38	Q	49	0	0	2	0
38	R	78	0	0	2	0
38	S	32	0	0	3	0
38	T	36	0	0	3	0
38	U	28	0	0	2	0
38	V	13	0	0	2	0
38	W	68	0	0	5	0
38	X	24	0	0	3	0
38	Y	97	0	0	8	0
38	Z	29	0	0	3	0
All	All	99119	0	59911	1801	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1801) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.97	1.41
30:0:2537:G:H5''	30:0:2538:A:H5''	1.17	1.14
30:0:871:G:C8	30:0:871:G:H5'	1.83	1.14
30:0:1205:U:H2'	30:0:1206:U:H5''	1.27	1.12
30:0:1160:G:H5'	30:0:1161:A:H5'	1.13	1.11
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.30	1.11
15:O:3:THR:HG22	30:0:656:G:H5'	1.26	1.10
14:N:37:ARG:NH1	31:9:6:C:H5''	1.67	1.09
30:0:2102:G:H21	30:0:2103:A:H2'	0.97	1.09
30:0:1160:G:C5'	30:0:1161:A:H5'	1.84	1.07
30:0:871:G:H8	30:0:871:G:H5'	1.12	1.07
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07
30:0:1165:G:H1'	30:0:1174:A:H1'	1.34	1.07
30:0:1189:A:H3'	38:0:7701:HOH:O	1.56	1.04
9:I:130:LEU:HD21	30:0:1167:G:H4'	1.40	1.04
30:0:542:A:H5'	30:0:542:A:H8	1.24	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:82:THR:HG23	30:0:1242:A:H5'	1.37	1.02
31:9:56:A:H2'	31:9:57:A:H5''	1.42	1.01
30:0:1160:G:H5'	30:0:1161:A:C5'	1.91	1.01
30:0:1166:A:H61	30:0:1180:U:H3	1.04	1.01
3:C:236:THR:HG22	3:C:239:ALA:H	1.22	1.01
30:0:2748:G:OP1	30:0:2749:U:H5''	1.58	1.00
31:9:76:G:H3'	31:9:77:A:H5''	1.41	1.00
13:M:171:ARG:HD3	30:0:156:C:H5''	1.39	0.98
30:0:2100:A:H5'	38:0:7413:HOH:O	1.63	0.98
30:0:870:G:H2'	30:0:871:G:H5''	1.42	0.98
22:V:1:THR:HB	30:0:93:C:H5''	1.43	0.97
30:0:282:C:O2'	30:0:283:U:H5'	1.64	0.96
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.11	0.96
30:0:1372:A:H3'	38:0:7215:HOH:O	1.65	0.95
30:0:1625:U:H4'	38:0:4678:HOH:O	1.67	0.95
30:0:2102:G:H1'	30:0:2103:A:C8	2.02	0.95
30:0:2541:U:H5'	30:0:2541:U:C6	2.00	0.95
30:0:2102:G:N2	30:0:2103:A:H2'	1.82	0.95
30:0:2588:OMG:H5''	38:0:7509:HOH:O	1.64	0.94
16:P:115:SER:H	16:P:118:GLN:HE21	1.09	0.94
30:0:2717:C:C2'	30:0:2718:C:H5''	1.98	0.94
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.48	0.93
30:0:2710:U:H1'	38:0:7642:HOH:O	1.66	0.93
11:K:10:GLN:H	11:K:10:GLN:HE21	1.05	0.93
30:0:2491:G:H1'	38:0:6895:HOH:O	1.68	0.93
38:B:9058:HOH:O	30:0:2672:C:H1'	1.67	0.92
30:0:1116:U:H3	30:0:1246:A:H62	1.16	0.92
30:0:1205:U:C2'	30:0:1206:U:H5''	1.99	0.92
30:0:2896:A:H5''	38:0:6127:HOH:O	1.70	0.92
30:0:2103:A:H62	30:0:2538:A:H8	1.16	0.91
30:0:2851:G:C2'	30:0:2852:A:H5'	2.01	0.91
30:0:1878:G:H1'	38:0:6149:HOH:O	1.71	0.91
30:0:1290:G:H3'	38:0:5188:HOH:O	1.70	0.90
30:0:1701:A:H4'	30:0:1702:U:H5''	1.54	0.90
30:0:2748:G:H5'	38:0:7565:HOH:O	1.71	0.90
30:0:2406:U:H1'	38:0:6728:HOH:O	1.71	0.90
30:0:2506:A:O2'	30:0:2507:G:H8	1.55	0.90
30:0:2851:G:H2'	30:0:2852:A:H5'	1.54	0.89
30:0:1118:A:H3'	30:0:1118:A:H8	1.36	0.88
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.55	0.88
30:0:1184:C:H1'	38:0:7491:HOH:O	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.88
30:0:2812:A:H2	30:0:2814:A:H62	1.06	0.88
30:0:2541:U:H5'	30:0:2541:U:H6	1.34	0.88
30:0:2717:C:H2'	30:0:2718:C:H5''	1.54	0.88
30:0:1300:G:H1'	38:0:4694:HOH:O	1.72	0.88
30:0:2637:A:H5'	38:0:9280:HOH:O	1.73	0.87
30:0:871:G:H8	30:0:871:G:C5'	1.88	0.87
28:2:41:HIS:H	28:2:45:ASN:HD22	1.22	0.87
1:A:211:LYS:HG2	1:A:212:PRO:HD2	1.55	0.87
30:0:1118:A:H3'	30:0:1118:A:C8	2.09	0.86
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.40	0.86
30:0:2537:G:C5'	30:0:2538:A:H5''	2.03	0.86
30:0:256:C:H5''	38:0:5505:HOH:O	1.77	0.85
2:B:238:ASN:HD22	2:B:240:GLY:H	1.19	0.85
30:0:506:G:H22	30:0:509:A:C5'	1.89	0.85
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.19	0.85
30:0:1119:G:N2	30:0:1246:A:C2	2.43	0.85
30:0:545:G:H8	30:0:545:G:H5'	1.41	0.85
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.41	0.85
30:0:2004:U:H2'	30:0:2004:U:O2	1.76	0.85
30:0:1426:C:H2'	38:0:9601:HOH:O	1.76	0.84
30:0:1183:C:N4	30:0:1184:C:H41	1.75	0.84
30:0:2586:U:H3	30:0:2592:G:H22	1.24	0.84
8:H:30:LYS:H	8:H:62:HIS:HD2	1.26	0.84
15:O:3:THR:CG2	30:0:656:G:H5'	2.08	0.84
31:9:23:U:O2'	31:9:24:U:H4'	1.78	0.84
15:O:57:THR:HB	15:O:111:VAL:HG23	1.60	0.83
30:0:1632:A:H2'	30:0:1633:C:H5'	1.60	0.83
30:0:1750:C:H4'	38:0:7509:HOH:O	1.76	0.83
30:0:559:U:H5'	30:0:559:U:H6	1.42	0.83
30:0:2505:G:O2'	30:0:2506:A:H5'	1.79	0.83
30:0:1165:G:O3'	30:0:1174:A:H4'	1.78	0.82
30:0:2783:A:H3'	38:0:5253:HOH:O	1.78	0.82
30:0:1615:A:H5'	38:0:4198:HOH:O	1.76	0.82
30:0:1666:C:O2'	30:0:1667:A:H5''	1.78	0.82
30:0:960:G:H3'	30:0:960:G:N3	1.94	0.82
11:K:39:GLY:HA2	38:0:5242:HOH:O	1.79	0.82
14:N:113:SER:HB2	38:N:8854:HOH:O	1.78	0.82
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.15	0.82
30:0:1116:U:HO2'	30:0:1118:A:H2	0.82	0.82
30:0:544:G:H2'	30:0:545:G:H5''	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2506:A:HO2'	30:0:2507:G:H8	0.82	0.81
30:0:558:C:C2'	30:0:559:U:H5''	2.10	0.81
22:V:1:THR:HG23	22:V:2:VAL:H	1.43	0.81
30:0:558:C:O2'	30:0:559:U:H5''	1.81	0.81
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.28	0.81
30:0:1667:A:H8	30:0:1667:A:H5'	1.45	0.81
30:0:1183:C:H2'	38:0:6274:HOH:O	1.79	0.81
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.95	0.81
30:0:2005:G:H3'	30:0:2005:G:OP2	1.81	0.81
30:0:1632:A:C2'	30:0:1633:C:H5'	2.10	0.81
30:0:69:A:H5'	30:0:69:A:C8	2.16	0.81
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.16	0.80
30:0:870:G:C2'	30:0:871:G:H5''	2.09	0.80
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.62	0.80
4:D:172:VAL:HG12	4:D:173:GLU:H	1.47	0.80
30:0:272:A:H3'	38:0:7553:HOH:O	1.81	0.80
30:0:282:C:H1'	30:0:368:C:N4	1.97	0.80
31:9:56:A:C2'	31:9:57:A:H5''	2.12	0.80
30:0:1474:C:H6	30:0:1474:C:H5'	1.47	0.79
30:0:1189:A:H1'	30:0:1209:C:O4'	1.82	0.79
27:1:25:LYS:HD2	28:2:49:GLU:H	1.48	0.79
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.64	0.79
30:0:1973:A:H5'	30:0:1973:A:H8	1.46	0.79
30:0:558:C:H2'	30:0:559:U:C5'	2.13	0.79
30:0:2100:A:H1'	38:0:5670:HOH:O	1.83	0.79
2:B:206:THR:HG21	30:0:2716:G:H5''	1.65	0.79
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.64	0.79
1:A:199:HIS:HD2	1:A:201:PHE:H	1.28	0.79
30:0:1634:G:H3'	38:0:3910:HOH:O	1.82	0.78
31:9:29:C:H2'	31:9:30:C:H5'	1.65	0.78
30:0:1118:A:H62	30:0:1244:U:H3	1.31	0.78
2:B:211:THR:HG23	30:0:2840:A:OP1	1.82	0.78
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.12	0.78
30:0:381:G:H5''	38:0:4335:HOH:O	1.82	0.78
30:0:1279:U:O2	30:0:1279:U:H2'	1.83	0.78
30:0:2524:G:N2	30:0:2526:C:H41	1.82	0.78
31:9:39:U:H1'	31:9:44:A:H61	1.46	0.78
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.14	0.78
30:0:1377:C:H6	30:0:1377:C:H5'	1.48	0.77
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.67	0.77
30:0:69:A:H5'	30:0:69:A:H8	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:SER:OG	30:0:2101:A:H2'	1.85	0.77
23:W:21:LEU:HD22	23:W:26:ILE:HD13	1.67	0.77
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.67	0.77
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.66	0.77
30:0:2852:A:H5''	38:0:5255:HOH:O	1.85	0.77
30:0:877:G:H5'	30:0:878:G:OP1	1.84	0.77
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.50	0.76
28:2:20:ARG:HG3	28:2:39:ARG:HH21	1.49	0.76
30:0:1175:G:H1'	30:0:1193:A:H2'	1.65	0.76
30:0:2765:C:H4'	38:0:5545:HOH:O	1.85	0.76
30:0:1730:G:H5''	30:0:1731:C:H6	1.51	0.76
30:0:2769:C:O2'	30:0:2770:G:H5'	1.86	0.76
30:0:1700:C:H5''	30:0:1701:A:OP2	1.86	0.76
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.51	0.76
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.67	0.76
30:0:2537:G:H5''	30:0:2538:A:C5'	2.10	0.75
30:0:1603:A:H5'	30:0:1605:G:O4'	1.86	0.75
30:0:2769:C:C2'	30:0:2770:G:H5'	2.17	0.75
31:9:39:U:H1'	31:9:44:A:N6	2.01	0.75
30:0:1165:G:H21	30:0:1173:A:H5''	1.52	0.75
30:0:2502:C:C2'	30:0:2503:A:H5'	2.17	0.75
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.69	0.75
30:0:506:G:H22	30:0:509:A:H5''	1.50	0.75
6:F:91:VAL:HG12	6:F:92:GLY:H	1.51	0.75
30:0:1116:U:O2'	30:0:1118:A:H2	1.66	0.75
21:U:14:GLU:O	21:U:17:THR:HB	1.87	0.75
1:A:48:ASP:HB3	38:A:9069:HOH:O	1.87	0.74
30:0:2524:G:H21	30:0:2526:C:H41	1.31	0.74
30:0:1206:U:H6	30:0:1206:U:H5'	1.52	0.74
31:9:2:U:H4'	38:9:9099:HOH:O	1.88	0.74
14:N:144:GLY:O	14:N:147:ILE:HG22	1.87	0.74
23:W:88:THR:HB	38:W:6679:HOH:O	1.88	0.74
4:D:154:LYS:HD2	4:D:154:LYS:H	1.53	0.74
30:0:1552:G:N2	30:0:1634:G:H1'	2.03	0.74
30:0:1666:C:H2'	30:0:1667:A:H5'	1.69	0.74
18:R:128:ARG:NH2	30:0:2054:A:N3	2.36	0.74
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.68	0.74
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.68	0.74
30:0:1701:A:H4'	30:0:1702:U:C5'	2.17	0.74
30:0:541:C:C2'	30:0:542:A:H5''	2.17	0.74
30:0:541:C:H2'	30:0:542:A:C5'	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:396:U:H1'	38:0:7649:HOH:O	1.87	0.73
30:0:871:G:C8	30:0:871:G:C5'	2.64	0.73
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.69	0.73
18:R:39:THR:HG22	18:R:42:GLU:H	1.53	0.73
30:0:1209:C:H2'	30:0:1210:G:H8	1.53	0.73
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.69	0.73
30:0:2438:G:H5'	38:0:6199:HOH:O	1.87	0.73
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.71	0.73
4:D:58:VAL:HB	4:D:62:ASP:HB3	1.69	0.73
13:M:171:ARG:CD	30:0:156:C:H5''	2.17	0.73
30:0:558:C:H2'	30:0:559:U:H5'	1.71	0.73
31:9:14:G:H5'	31:9:14:G:H8	1.53	0.73
30:0:1201:C:H5''	38:0:6263:HOH:O	1.87	0.73
30:0:542:A:H5'	30:0:542:A:C8	2.15	0.73
30:0:1165:G:C1'	30:0:1174:A:H1'	2.17	0.73
29:3:48:ASN:HD21	30:0:2468:A:H61	1.37	0.73
30:0:1166:A:N6	30:0:1180:U:H3	1.85	0.72
30:0:2502:C:H2'	30:0:2503:A:H5'	1.71	0.72
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.71	0.72
30:0:2769:C:H2'	30:0:2770:G:O4'	1.88	0.72
30:0:1476:A:O2'	30:0:1477:C:H5'	1.89	0.72
30:0:2812:A:C2	30:0:2814:A:N6	2.54	0.72
30:0:119:A:H2'	30:0:120:A:H5''	1.71	0.72
30:0:1119:G:H22	30:0:1246:A:H2	1.37	0.72
30:0:1165:G:H1'	30:0:1174:A:C1'	2.15	0.72
30:0:1730:G:H5''	30:0:1731:C:C6	2.23	0.72
30:0:2718:C:H6	30:0:2718:C:H5'	1.54	0.72
30:0:544:G:C2'	30:0:545:G:H5''	2.19	0.72
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.37	0.72
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.02	0.71
30:0:138:U:H5''	30:0:139:C:OP2	1.90	0.71
30:0:2908:A:H2'	30:0:2909:G:O4'	1.90	0.71
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.72	0.71
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.71	0.71
30:0:2635:A:O2'	30:0:2636:C:H5'	1.91	0.71
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.70	0.71
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.73	0.71
3:C:139:VAL:HG13	38:C:8641:HOH:O	1.89	0.71
30:0:506:G:H22	30:0:509:A:H5'	1.55	0.71
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.21	0.71
30:0:848:C:H5'	38:0:7298:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2747:C:O3'	30:0:2748:G:H4'	1.90	0.71
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.26	0.71
30:0:1878:G:O2'	30:0:1879:U:C6	2.44	0.71
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.90	0.70
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.72	0.70
30:0:2106:C:H5'	30:0:2284:G:H21	1.55	0.70
30:0:2487:C:H5	38:0:4903:HOH:O	1.74	0.70
30:0:2507:G:H2'	30:0:2510:C:H42	1.57	0.70
30:0:272:A:H5'	30:0:273:G:OP2	1.91	0.70
30:0:2578:G:H5'	30:0:2578:G:H8	1.56	0.70
30:0:282:C:C2'	30:0:283:U:H5'	2.21	0.70
30:0:1058:A:H2'	30:0:1060:C:H5''	1.73	0.70
30:0:1730:G:H5'	30:0:1731:C:C5	2.27	0.70
18:R:29:LYS:HD3	30:0:524:A:H5''	1.73	0.70
30:0:1724:U:H5''	38:0:3745:HOH:O	1.92	0.70
30:0:462:A:H2'	38:0:4898:HOH:O	1.91	0.70
30:0:1278:A:O2'	30:0:1279:U:H3'	1.92	0.69
31:9:49:G:H5''	38:9:9086:HOH:O	1.91	0.69
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.74	0.69
30:0:1165:G:H21	30:0:1173:A:C5'	2.04	0.69
30:0:280:C:H2'	30:0:281:U:O4'	1.90	0.69
30:0:1380:U:O4	30:0:2748:G:H1'	1.92	0.69
30:0:1299:G:H5'	38:0:4092:HOH:O	1.92	0.69
30:0:1666:C:C2'	30:0:1667:A:H5''	2.22	0.69
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.69
30:0:1666:C:H2'	30:0:1667:A:C5'	2.22	0.69
30:0:2748:G:C8	30:0:2748:G:H5'	2.28	0.69
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.41	0.69
18:R:39:THR:HG23	18:R:107:GLU:O	1.92	0.69
30:0:2064:U:H5'	30:0:2652:U:H4'	1.75	0.69
30:0:2421:G:H4'	38:0:4795:HOH:O	1.92	0.69
30:0:2541:U:H3'	38:0:9415:HOH:O	1.93	0.69
30:0:2717:C:O2'	30:0:2718:C:H5''	1.91	0.69
30:0:681:G:N3	30:0:681:G:H5'	2.08	0.69
30:0:282:C:H1'	30:0:368:C:H42	1.58	0.69
30:0:292:G:H2'	30:0:358:G:N2	2.08	0.69
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.74	0.69
9:I:108:HIS:H	9:I:109:PRO:HD2	1.56	0.69
30:0:2533:C:H5'	30:0:2533:C:H6	1.57	0.69
1:A:199:HIS:CD2	1:A:201:PHE:H	2.09	0.69
2:B:238:ASN:HD22	2:B:240:GLY:N	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1505:U:H1'	38:0:7611:HOH:O	1.92	0.68
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.07	0.68
30:0:2524:G:H21	30:0:2526:C:N4	1.90	0.68
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.75	0.68
31:9:13:A:O2'	31:9:14:G:H5''	1.92	0.68
3:C:1:MET:HG2	3:C:2:GLN:H	1.59	0.68
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.90	0.68
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.94	0.68
30:0:2102:G:H2'	38:0:7788:HOH:O	1.93	0.68
30:0:558:C:C2'	30:0:559:U:C5'	2.72	0.68
8:H:168:VAL:HG13	38:H:214:HOH:O	1.93	0.68
30:0:2896:A:N3	30:0:2896:A:H2'	2.08	0.68
28:2:28:LYS:O	30:0:87:C:H2'	1.93	0.68
14:N:7:LYS:HE3	17:Q:21:ARG:O	1.92	0.68
30:0:1118:A:C8	30:0:1118:A:C3'	2.73	0.67
30:0:2420:G:O2'	30:0:2421:G:H5'	1.94	0.67
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.76	0.67
30:0:2291:A:C8	30:0:2309:C:H5'	2.29	0.67
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.75	0.67
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.59	0.67
1:A:51:ARG:HB2	38:A:9069:HOH:O	1.94	0.67
14:N:160:SER:HB3	31:9:51:A:H5'	1.77	0.67
25:Y:235:GLU:H	25:Y:235:GLU:CD	1.96	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.27	0.67
6:F:96:ALA:HA	38:F:3111:HOH:O	1.94	0.67
30:0:1377:C:H5'	30:0:1377:C:C6	2.29	0.67
30:0:2661:U:H3	30:0:2812:A:H62	1.42	0.67
30:0:2505:G:C2'	30:0:2506:A:H5'	2.25	0.67
30:0:2878:U:H2'	30:0:2879:A:O4'	1.94	0.67
30:0:1641:A:H2'	30:0:1642:A:H5'	1.77	0.67
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.29	0.67
12:L:18:HIS:HD2	30:0:902:G:N7	1.93	0.67
28:2:49:GLU:HB2	38:2:131:HOH:O	1.93	0.67
14:N:160:SER:CB	31:9:51:A:H5'	2.25	0.67
12:L:136:ALA:HB3	38:L:8867:HOH:O	1.95	0.67
10:J:131:THR:HG22	10:J:134:GLU:H	1.61	0.66
14:N:37:ARG:NH1	31:9:6:C:C5'	2.53	0.66
18:R:150:PRO:O	18:R:150:PRO:CG	2.42	0.66
25:Y:200:THR:HG22	25:Y:201:GLU:HG3	1.77	0.66
30:0:182:G:H5'	38:0:5177:HOH:O	1.96	0.66
30:0:1603:A:H5''	30:0:1605:G:H5'	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2004:U:O2	30:0:2004:U:C2'	2.43	0.66
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.77	0.66
30:0:541:C:H2'	30:0:542:A:H5''	1.78	0.66
27:1:16:HIS:HD2	30:0:470:U:O2'	1.78	0.66
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.78	0.66
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.33	0.66
30:0:1730:G:C5'	30:0:1731:C:C6	2.79	0.66
30:0:2426:G:H1'	38:0:6120:HOH:O	1.95	0.65
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.77	0.65
23:W:26:ILE:HB	38:W:5420:HOH:O	1.96	0.65
30:0:256:C:H2'	30:0:257:G:O4'	1.96	0.65
30:0:1187:U:H5''	38:0:6214:HOH:O	1.96	0.65
30:0:1119:G:N2	30:0:1246:A:H2	1.94	0.65
30:0:545:G:C8	30:0:545:G:H5'	2.30	0.65
2:B:211:THR:HG21	38:0:7480:HOH:O	1.96	0.65
30:0:2032:U:H2'	30:0:2033:G:C5'	2.26	0.65
30:0:299:U:H5'	38:0:7361:HOH:O	1.96	0.65
30:0:567:U:H5''	38:0:6432:HOH:O	1.96	0.65
30:0:1878:G:HO2'	30:0:1879:U:H6	1.41	0.65
30:0:2524:G:H21	30:0:2526:C:H5	1.44	0.65
24:X:61:ARG:HH11	24:X:65:ASN:HB3	1.62	0.65
2:B:51:VAL:CG1	2:B:53:LEU:HD13	2.26	0.65
12:L:140:VAL:HB	38:L:8851:HOH:O	1.96	0.65
15:O:32:ARG:HH21	15:O:35:LYS:NZ	1.94	0.65
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.89	0.65
30:0:125:U:H2'	38:0:3780:HOH:O	1.97	0.64
31:9:24:U:H3'	31:9:25:G:H5'	1.79	0.64
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.80	0.64
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.97	0.64
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.78	0.64
30:0:1166:A:H1'	30:0:1192:A:N3	2.13	0.64
30:0:1187:U:H1'	30:0:1189:A:H2	1.62	0.64
30:0:1166:A:H1'	30:0:1192:A:C2	2.31	0.64
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.79	0.64
3:C:174:ILE:CD1	30:0:338:C:H4'	2.28	0.64
17:Q:25:PRO:HB2	38:9:9078:HOH:O	1.98	0.64
30:0:1451:C:H5'	30:0:1505:U:C5	2.33	0.64
30:0:196:G:H2'	38:0:6681:HOH:O	1.98	0.64
30:0:271:C:H41	30:0:378:A:H2	1.46	0.64
30:0:1187:U:HO2'	30:0:1188:A:H8	1.44	0.64
30:0:2539:U:H3'	38:0:9174:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:76:ASP:HA	38:J:5907:HOH:O	1.97	0.64
27:1:10:LYS:HG3	38:1:2979:HOH:O	1.98	0.64
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.78	0.64
20:T:9:LYS:HD3	38:0:3770:HOH:O	1.97	0.64
24:X:61:ARG:NH1	24:X:65:ASN:HB3	2.12	0.64
30:0:541:C:H2'	30:0:542:A:H5'	1.78	0.64
8:H:59:GLN:HE22	8:H:96:GLN:HG2	1.62	0.64
30:0:380:A:H2'	38:0:7253:HOH:O	1.97	0.63
31:9:54:A:H2	38:9:9062:HOH:O	1.80	0.63
3:C:2:GLN:HB3	38:C:8580:HOH:O	1.97	0.63
18:R:98:ASN:HD21	30:0:500:G:H21	1.46	0.63
23:W:80:ASP:O	23:W:84:VAL:HG23	1.97	0.63
6:F:91:VAL:HG12	6:F:92:GLY:N	2.13	0.63
30:0:1187:U:O2'	30:0:1188:A:H8	1.80	0.63
30:0:1666:C:C2'	30:0:1667:A:C5'	2.77	0.63
27:1:20:ARG:HG2	30:0:111:C:O2'	1.98	0.63
2:B:179:LEU:O	2:B:183:GLU:HG2	1.99	0.63
30:0:1919:A:H4'	38:0:4866:HOH:O	1.98	0.63
30:0:283:U:H5	30:0:284:C:N3	1.97	0.63
30:0:1207:A:OP2	30:0:1207:A:H8	1.81	0.63
30:0:1878:G:O2'	30:0:1879:U:H6	1.82	0.63
18:R:117:HIS:HD2	30:0:20:G:H21	1.46	0.63
24:X:25:ARG:HD2	38:X:5356:HOH:O	1.98	0.63
30:0:2670:G:O2'	30:0:2671:U:H5'	1.99	0.63
30:0:2908:A:C2'	30:0:2909:G:H5'	2.29	0.63
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.99	0.63
16:P:115:SER:H	16:P:118:GLN:NE2	1.90	0.63
30:0:441:A:H1'	30:0:442:A:N7	2.13	0.62
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.81	0.62
30:0:1835:U:C5	30:0:1840:A:N7	2.62	0.62
31:9:1:U:H5''	31:9:3:A:OP1	1.99	0.62
30:0:1681:G:H5''	30:0:1682:A:H5'	1.80	0.62
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.81	0.62
25:Y:169:ARG:HD2	30:0:1328:A:OP1	2.00	0.62
30:0:2537:G:H3'	38:0:3125:HOH:O	1.98	0.62
1:A:211:LYS:O	30:0:1943:C:H4'	1.99	0.62
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.29	0.62
30:0:2112:A:H2'	30:0:2113:G:C8	2.33	0.62
30:0:1359:U:C6	30:0:2537:G:N2	2.67	0.62
30:0:42:C:H1'	38:0:4687:HOH:O	1.98	0.62
7:G:12:ILE:HG23	38:0:5483:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.82	0.62
2:B:214:PRO:HD2	38:B:8953:HOH:O	2.00	0.62
11:K:10:GLN:N	11:K:10:GLN:HE21	1.88	0.62
22:V:5:VAL:HG23	38:V:2271:HOH:O	1.99	0.62
4:D:57:THR:HG23	4:D:63:ILE:HA	1.80	0.62
15:O:3:THR:HG22	30:0:656:G:C5'	2.16	0.62
30:0:1205:U:H2'	30:0:1206:U:C5'	2.18	0.62
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.30	0.62
23:W:65:VAL:HA	23:W:68:THR:HG22	1.81	0.62
1:A:125:ASN:HB3	1:A:158:VAL:HG12	1.81	0.62
23:W:125:HIS:HD2	23:W:127:GLY:H	1.48	0.62
30:0:1167:G:H2'	30:0:1168:C:O4'	1.99	0.61
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.81	0.61
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.40	0.61
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.82	0.61
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.82	0.61
30:0:1183:C:H5	30:0:1192:A:OP1	1.83	0.61
3:C:236:THR:HG22	3:C:239:ALA:N	2.05	0.61
31:9:92:G:H2'	31:9:93:A:C8	2.35	0.61
30:0:2607:U:H4'	38:0:9446:HOH:O	1.99	0.61
4:D:103:ASN:ND2	4:D:134:LEU:H	1.98	0.61
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.98	0.61
30:0:1200:A:H3'	38:0:5785:HOH:O	2.00	0.61
30:0:2748:G:H8	38:0:7565:HOH:O	1.84	0.61
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.31	0.61
12:L:6:ARG:HD3	30:0:1299:G:O6	2.00	0.61
30:0:1973:A:H5'	30:0:1973:A:C8	2.33	0.61
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.65	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.30	0.61
5:E:68:HIS:O	5:E:72:MET:HG3	2.00	0.61
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.81	0.61
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.81	0.61
30:0:1187:U:O2'	30:0:1188:A:C8	2.54	0.60
30:0:558:C:H2'	30:0:559:U:H5''	1.77	0.60
3:C:140:VAL:HB	38:C:8644:HOH:O	2.00	0.60
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.00	0.60
17:Q:95:GLU:HA	30:0:949:U:H4'	1.82	0.60
30:0:204:A:C2'	30:0:205:U:H5'	2.31	0.60
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.60
1:A:3:ARG:HD3	30:0:870:G:OP2	2.01	0.60
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.15	0.60
31:9:54:A:O2'	31:9:55:U:H5'	2.01	0.60
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.83	0.60
2:B:254:GLN:HG2	2:B:255:GLY:N	2.16	0.60
14:N:80:SER:HB2	38:N:8834:HOH:O	2.01	0.60
30:0:1189:A:H1'	30:0:1209:C:C1'	2.31	0.60
30:0:1679:C:H5'	38:0:9330:HOH:O	2.02	0.60
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.83	0.60
13:M:164:THR:HG22	13:M:166:ALA:H	1.66	0.60
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.83	0.60
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.67	0.60
13:M:83:SER:HB3	38:0:4395:HOH:O	2.01	0.60
23:W:21:LEU:CD2	23:W:48:VAL:HG11	2.29	0.60
30:0:1342:C:C2'	30:0:1343:C:H5'	2.32	0.60
30:0:254:C:O2	30:0:254:C:H2'	2.01	0.60
4:D:25:MET:SD	4:D:40:ILE:HD11	2.42	0.60
13:M:82:ARG:HD2	38:0:9124:HOH:O	2.01	0.60
25:Y:141:THR:HG23	38:Y:8888:HOH:O	2.00	0.60
30:0:1189:A:O2'	30:0:1208:C:H2'	2.02	0.60
12:L:104:ASP:HB2	38:L:8857:HOH:O	2.00	0.60
30:0:1476:A:N7	38:0:5190:HOH:O	2.32	0.60
30:0:1528:A:H2'	30:0:1529:G:O4'	2.02	0.60
30:0:1667:A:C8	30:0:1667:A:H5'	2.33	0.60
30:0:1766:U:O2	30:0:1778:A:H5'	2.02	0.60
2:B:145:HIS:HD2	2:B:146:THR:O	1.85	0.60
30:0:2769:C:H2'	30:0:2770:G:C5'	2.32	0.59
15:O:32:ARG:HD3	15:O:32:ARG:O	2.02	0.59
23:W:125:HIS:CD2	23:W:127:GLY:H	2.20	0.59
30:0:1632:A:C3'	30:0:1633:C:H5'	2.33	0.59
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.37	0.59
14:N:179:LEU:HA	14:N:184:ILE:HD12	1.84	0.59
30:0:2825:C:H4'	30:0:2826:G:O5'	2.02	0.59
14:N:11:ARG:HD3	31:9:114:G:O6	2.02	0.59
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.84	0.59
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.84	0.59
30:0:1116:U:O2'	30:0:1118:A:C2	2.47	0.59
30:0:1342:C:O2'	30:0:1343:C:H5'	2.01	0.59
30:0:2073:G:OP2	30:0:2490:A:H5'	2.03	0.59
38:Z:8718:HOH:O	30:0:819:A:H5''	2.01	0.59
12:L:30:ARG:HD3	30:0:164:G:H4'	1.85	0.59
30:0:2626:C:H2'	30:0:2627:G:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:81:LYS:HG2	38:0:9547:HOH:O	2.02	0.59
20:T:112:LEU:HD23	20:T:119:ALA:HB3	1.84	0.59
28:2:10:ARG:NH2	30:0:121:U:OP2	2.32	0.59
30:0:2239:C:H2'	30:0:2240:U:H6	1.67	0.59
17:Q:45:PRO:O	30:0:2365:G:H4'	2.03	0.59
11:K:32:ILE:HD11	11:K:56:SER:HB2	1.84	0.59
30:0:1278:A:H4'	30:0:1279:U:C4	2.37	0.59
30:0:407:A:H3'	38:0:4474:HOH:O	2.03	0.59
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.85	0.59
3:C:214:THR:HB	38:0:9688:HOH:O	2.02	0.59
4:D:57:THR:HA	38:D:5728:HOH:O	2.01	0.59
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.84	0.59
30:0:1862:C:H1'	38:0:7245:HOH:O	2.01	0.59
30:0:291:C:H2'	30:0:292:G:O4'	2.03	0.59
30:0:960:G:C3'	30:0:960:G:N3	2.66	0.59
20:T:26:THR:HA	20:T:39:ASN:HB3	1.85	0.59
30:0:2239:C:H2'	30:0:2240:U:C6	2.38	0.59
30:0:834:G:H4'	30:0:835:U:OP2	2.03	0.59
3:C:174:ILE:HD11	30:0:338:C:H4'	1.85	0.59
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.85	0.59
30:0:1182:C:H1'	30:0:1192:A:C8	2.38	0.59
30:0:1819:G:H2'	30:0:1820:G:H4'	1.85	0.59
30:0:2372:A:H2'	30:0:2373:U:C6	2.38	0.59
30:0:603:A:H4'	30:0:604:G:O5'	2.03	0.59
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.68	0.59
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.68	0.59
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.84	0.58
30:0:1218:U:H2'	30:0:1219:U:C6	2.38	0.58
30:0:2102:G:H21	30:0:2103:A:C2'	1.91	0.58
30:0:2894:C:O2'	30:0:2895:C:H5'	2.02	0.58
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.84	0.58
30:0:1118:A:H8	30:0:1119:G:H5''	1.68	0.58
30:0:2089:A:O2'	30:0:2090:G:H5'	2.03	0.58
30:0:396:U:O2'	30:0:418:C:H4'	2.03	0.58
30:0:1165:G:N2	30:0:1173:A:C5'	2.67	0.58
30:0:200:C:H2'	38:0:3459:HOH:O	2.03	0.58
30:0:2453:G:H5''	38:0:4736:HOH:O	2.04	0.58
2:B:16:ARG:NH1	38:B:9042:HOH:O	2.35	0.58
3:C:202:THR:HG22	30:0:328:U:O4'	2.04	0.58
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.85	0.58
2:B:162:MET:CE	2:B:310:ARG:HD3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:55:LYS:HG2	16:P:56:GLY:N	2.19	0.58
20:T:1:SER:HB2	30:0:447:A:P	2.44	0.58
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.19	0.58
12:L:39:GLU:OE2	30:0:926:A:H5'	2.02	0.58
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.01	0.58
14:N:162:ASP:HA	38:N:8831:HOH:O	2.03	0.58
30:0:541:C:C2'	30:0:542:A:C5'	2.80	0.58
30:0:999:C:C2'	30:0:1000:C:H5'	2.34	0.58
30:0:1595:G:O2'	30:0:1596:U:H5'	2.04	0.58
30:0:2541:U:C6	30:0:2541:U:C5'	2.82	0.58
2:B:298:LYS:HG2	38:0:5545:HOH:O	2.04	0.58
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.19	0.57
30:0:12:U:H2'	30:0:13:G:H5'	1.86	0.57
30:0:1730:G:C5'	30:0:1731:C:C5	2.86	0.57
2:B:17:LYS:O	2:B:260:HIS:HD2	1.87	0.57
30:0:130:C:H5'	38:0:5234:HOH:O	2.02	0.57
30:0:2102:G:H1'	30:0:2103:A:H8	1.65	0.57
4:D:103:ASN:HD22	4:D:134:LEU:H	1.50	0.57
22:V:55:ARG:O	22:V:59:ILE:HG12	2.05	0.57
23:W:44:MET:CE	30:0:944:G:H21	2.16	0.57
30:0:1667:A:H2'	30:0:1668:U:H6	1.70	0.57
30:0:2032:U:H2'	30:0:2033:G:H5'	1.86	0.57
20:T:1:SER:HB2	30:0:447:A:OP2	2.05	0.57
30:0:951:A:C2'	30:0:952:G:H5'	2.34	0.57
28:2:36:ASN:HB3	28:2:39:ARG:HG3	1.86	0.57
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.39	0.57
30:0:2320:U:H4'	30:0:2321:A:O4'	2.05	0.57
19:S:57:THR:HG22	19:S:58:MET:N	2.20	0.57
22:V:1:THR:CB	30:0:93:C:H5''	2.28	0.57
15:O:32:ARG:NE	15:O:35:LYS:HD2	2.16	0.57
30:0:1044:C:H3'	30:0:1045:G:H5''	1.86	0.57
30:0:1355:A:H2'	38:0:4139:HOH:O	2.05	0.57
31:9:2:U:OP2	31:9:3:A:H5'	2.05	0.57
30:0:2717:C:H2'	30:0:2718:C:C5'	2.30	0.57
30:0:59:A:H5'	38:0:4347:HOH:O	2.05	0.57
11:K:29:LEU:HB3	11:K:55:VAL:HG21	1.85	0.57
30:0:1878:G:H4'	38:0:4133:HOH:O	2.05	0.57
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.39	0.57
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.87	0.57
30:0:1201:C:H2'	30:0:1202:A:H5'	1.86	0.57
30:0:2541:U:H6	30:0:2541:U:C5'	2.11	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2827:A:H2'	30:0:2828:G:O4'	2.05	0.57
31:9:24:U:H3'	31:9:25:G:C5'	2.35	0.57
4:D:58:VAL:HG12	4:D:60:GLU:HG2	1.87	0.57
10:J:63:ILE:HD11	30:0:1236:A:C8	2.40	0.57
30:0:1174:A:C5	30:0:1201:C:H4'	2.39	0.56
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.40	0.56
3:C:236:THR:HG21	38:C:8570:HOH:O	2.04	0.56
6:F:58:GLU:HG3	6:F:61:MET:HE1	1.87	0.56
26:Z:34:SER:HB3	30:0:797:A:H4'	1.86	0.56
30:0:2912:C:H3'	38:0:6403:HOH:O	2.03	0.56
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.41	0.56
10:J:19:MET:CE	10:J:132:LEU:HD11	2.35	0.56
30:0:1165:G:N2	30:0:1173:A:H5''	2.17	0.56
24:X:30:MET:HG2	30:0:1384:C:H5'	1.85	0.56
30:0:2316:G:H4'	38:0:6120:HOH:O	2.05	0.56
30:0:2361:A:H2'	30:0:2362:A:C8	2.40	0.56
30:0:2866:U:H4'	30:0:2867:G:H5'	1.87	0.56
5:E:15:GLN:HG3	5:E:20:ILE:HG12	1.88	0.56
21:U:49:LEU:HG	38:U:3805:HOH:O	2.05	0.56
30:0:1474:C:C6	30:0:1474:C:H5'	2.34	0.56
30:0:1838:U:O2'	30:0:2644:C:H5'	2.05	0.56
29:3:61:PRO:HG2	38:0:7581:HOH:O	2.04	0.56
29:3:73:GLU:HB3	38:3:9055:HOH:O	2.04	0.56
38:Z:8706:HOH:O	30:0:1886:A:H4'	2.05	0.56
30:0:2697:A:H2'	30:0:2698:G:O4'	2.06	0.56
30:0:2851:G:O2'	30:0:2852:A:H5'	2.04	0.56
30:0:432:G:O2'	30:0:433:C:H5'	2.06	0.56
29:3:70:ARG:HG2	38:3:9067:HOH:O	2.05	0.56
18:R:9:ASP:O	18:R:13:THR:HG22	2.06	0.56
30:0:1921:A:C6	30:0:1922:A:C2	2.93	0.56
30:0:2032:U:O2'	30:0:2033:G:H5''	2.05	0.56
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.21	0.56
30:0:2712:G:H5'	38:0:5242:HOH:O	2.03	0.56
31:9:1:U:O3'	31:9:3:A:H5''	2.05	0.56
30:0:1527:A:H1'	30:0:1528:A:C8	2.41	0.56
30:0:1667:A:H2'	30:0:1668:U:C6	2.41	0.56
30:0:349:U:O2'	30:0:350:G:H5'	2.06	0.56
30:0:1819:G:H5'	38:0:4724:HOH:O	2.04	0.56
30:0:2524:G:N2	30:0:2526:C:H5	2.04	0.56
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.70	0.56
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:4:PRO:HG3	31:9:69:U:OP1	2.06	0.56
30:0:1166:A:P	30:0:1174:A:H4'	2.46	0.56
30:0:204:A:H2'	30:0:205:U:H5'	1.86	0.56
5:E:3:VAL:CG2	5:E:49:ILE:HB	2.35	0.56
10:J:82:THR:HG23	30:0:1242:A:C5'	2.25	0.56
24:X:22:ASN:ND2	30:0:2726:U:O2'	2.39	0.56
30:0:602:A:O2'	30:0:605:C:H4'	2.05	0.56
3:C:115:LEU:O	3:C:118:THR:HB	2.06	0.56
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.88	0.56
18:R:99:ALA:HB1	18:R:109:MET:CE	2.34	0.56
18:R:150:PRO:CG	18:R:150:PRO:CB	2.82	0.56
30:0:2100:A:C8	30:0:2538:A:C2	2.94	0.55
3:C:214:THR:HG23	38:C:8628:HOH:O	2.05	0.55
30:0:2645:U:O2'	30:0:2646:G:P	2.65	0.55
31:9:76:G:C3'	31:9:77:A:H5''	2.27	0.55
1:A:211:LYS:CG	1:A:212:PRO:HD2	2.32	0.55
30:0:1477:C:H5'	30:0:1868:G:H5'	1.87	0.55
30:0:2101:A:O4'	30:0:2537:G:H1'	2.05	0.55
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.06	0.55
30:0:1279:U:O2	30:0:1279:U:C2'	2.53	0.55
30:0:1477:C:H5'	30:0:1868:G:C5'	2.36	0.55
13:M:69:LYS:O	13:M:73:ARG:NH2	2.39	0.55
30:0:1044:C:H5	38:0:6631:HOH:O	1.90	0.55
31:9:52:A:O2'	31:9:53:G:H5'	2.06	0.55
31:9:7:G:H5'	38:9:9096:HOH:O	2.06	0.55
5:E:143:GLN:NE2	30:0:2779:G:H21	2.05	0.55
13:M:76:ARG:HG3	13:M:88:VAL:HG21	1.89	0.55
30:0:1972:U:H2'	30:0:1973:A:C5'	2.36	0.55
30:0:2415:A:H2'	30:0:2416:G:H5'	1.87	0.55
30:0:271:C:C2	30:0:273:G:O4'	2.60	0.55
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.87	0.55
6:F:118:LEU:O	6:F:119:ARG:HB3	2.07	0.55
12:L:143:THR:HG22	12:L:144:ASP:N	2.22	0.55
14:N:110:THR:HB	14:N:113:SER:OG	2.07	0.55
26:Z:51:ALA:HA	38:Z:8715:HOH:O	2.05	0.55
30:0:1191:A:H2	30:0:1206:U:H3	1.55	0.55
30:0:1406:A:H4'	30:0:1407:A:H5''	1.87	0.55
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.71	0.55
31:9:3:A:H2'	38:9:9042:HOH:O	2.05	0.55
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.87	0.55
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:101:LYS:O	9:I:105:GLU:HG3	2.07	0.55
30:0:999:C:O2'	30:0:1000:C:H5'	2.07	0.55
9:I:129:SER:HB3	30:0:1192:A:H61	1.72	0.55
30:0:1946:C:H2'	30:0:1971:G:C8	2.41	0.55
10:J:70:PHE:HD1	30:0:2676:C:H4'	1.71	0.55
14:N:37:ARG:NH1	31:9:6:C:OP1	2.37	0.55
3:C:79:ARG:O	3:C:87:ARG:HG2	2.06	0.55
13:M:9:ARG:HD2	30:0:380:A:OP2	2.07	0.55
30:0:2718:C:H5'	30:0:2718:C:C6	2.40	0.55
30:0:2908:A:H2'	30:0:2909:G:C4'	2.37	0.55
3:C:184:ARG:NH2	30:0:450:C:OP1	2.34	0.55
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.71	0.55
26:Z:40:ALA:HA	30:0:1773:G:C8	2.41	0.54
27:1:16:HIS:HE1	30:0:775:G:OP1	1.90	0.54
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.70	0.54
25:Y:133:HIS:HD2	38:Y:8882:HOH:O	1.90	0.54
30:0:2323:G:H5''	38:0:4795:HOH:O	2.05	0.54
30:0:271:C:H4'	30:0:272:A:OP1	2.08	0.54
31:9:42:C:H5'	31:9:43:G:OP2	2.07	0.54
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.90	0.54
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.35	0.54
11:K:81:ARG:HD3	11:K:87:ARG:CZ	2.37	0.54
30:0:1118:A:C8	30:0:1119:G:H5''	2.42	0.54
30:0:1730:G:H5'	30:0:1731:C:H5	1.70	0.54
15:O:37:ARG:HD2	30:0:656:G:OP2	2.08	0.54
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.36	0.54
2:B:297:VAL:HB	38:B:9030:HOH:O	2.08	0.54
30:0:2769:C:H2'	30:0:2770:G:H5'	1.89	0.54
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.88	0.54
30:0:952:G:N3	30:0:2302:A:H2'	2.22	0.54
30:0:249:G:O2'	30:0:250:C:H5'	2.08	0.54
30:0:482:G:H4'	30:0:508:A:N1	2.22	0.54
30:0:541:C:O2'	30:0:542:A:H5''	2.07	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.06	0.54
30:0:1183:C:H42	30:0:1184:C:H41	1.51	0.54
30:0:1350:U:H4'	38:0:5141:HOH:O	2.06	0.54
30:0:2681:A:H4'	30:0:2682:C:H5'	1.90	0.54
31:9:52:A:H2'	31:9:53:G:O4'	2.06	0.54
30:0:2032:U:C2'	30:0:2033:G:H5''	2.38	0.54
23:W:21:LEU:O	23:W:26:ILE:HG23	2.08	0.54
30:0:1175:G:H1'	30:0:1193:A:C2'	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:37:ARG:NE	38:N:8832:HOH:O	2.36	0.54
15:O:24:ALA:HB3	30:0:710:G:OP1	2.07	0.54
20:T:49:GLU:HB3	20:T:59:GLU:HG2	1.90	0.54
23:W:48:VAL:HG12	23:W:48:VAL:O	2.07	0.54
30:0:1206:U:H2'	30:0:1207:A:O4'	2.06	0.54
3:C:43:LYS:HG2	30:0:449:A:N7	2.23	0.54
13:M:80:GLY:O	13:M:81:ARG:HD2	2.08	0.54
23:W:130:HIS:O	23:W:136:GLY:HA3	2.08	0.54
30:0:1878:G:C1'	38:0:6149:HOH:O	2.40	0.54
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.38	0.54
27:1:17:THR:HG21	30:0:120:A:C6	2.43	0.53
1:A:17:ARG:HD2	38:A:9013:HOH:O	2.08	0.53
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.89	0.53
4:D:135:VAL:HG22	4:D:136:ARG:H	1.73	0.53
8:H:30:LYS:N	8:H:62:HIS:HD2	2.02	0.53
13:M:59:GLY:HA3	13:M:141:ILE:HD12	1.89	0.53
23:W:38:THR:HB	38:W:5390:HOH:O	2.08	0.53
30:0:2102:G:N3	30:0:2103:A:C8	2.75	0.53
15:O:39:THR:O	15:O:115:ARG:NH2	2.41	0.53
25:Y:186:ARG:HG2	25:Y:186:ARG:HH11	1.72	0.53
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.08	0.53
27:1:9:GLY:HA2	30:0:1687:C:O2	2.09	0.53
30:0:2104:C:O2	30:0:2485:A:N1	2.41	0.53
30:0:2506:A:O2'	30:0:2507:G:C8	2.42	0.53
30:0:2506:A:N6	30:0:2511:A:O2'	2.40	0.53
2:B:125:GLU:O	2:B:129:ARG:HG3	2.08	0.53
4:D:169:THR:HG22	4:D:170:TYR:HD1	1.72	0.53
30:0:2766:A:H5'	38:0:9572:HOH:O	2.06	0.53
30:0:368:C:H2'	30:0:369:G:H5'	1.91	0.53
10:J:19:MET:HE2	10:J:132:LEU:HD11	1.90	0.53
31:9:39:U:C2'	31:9:40:C:OP1	2.56	0.53
3:C:64:GLY:O	30:0:2100:A:H4'	2.08	0.53
38:B:9058:HOH:O	30:0:2818:A:H2	1.92	0.53
30:0:307:G:H3'	38:0:6710:HOH:O	2.06	0.53
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.90	0.53
14:N:29:SER:HB3	30:0:2415:A:O2'	2.08	0.53
30:0:1741:U:O2'	30:0:2723:G:H4'	2.09	0.53
30:0:821:U:H2'	30:0:822:C:H6	1.73	0.53
8:H:66:GLU:HA	38:H:234:HOH:O	2.09	0.53
20:T:19:ARG:HD3	20:T:67:LEU:O	2.09	0.53
23:W:38:THR:HG22	23:W:39:ASP:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.91	0.53
30:0:2591:C:H2'	30:0:2592:G:O4'	2.09	0.53
30:0:2795:C:O2'	30:0:2796:U:H5'	2.09	0.53
13:M:178:LYS:HB2	38:0:6901:HOH:O	2.08	0.53
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.23	0.53
1:A:210:GLY:N	38:A:9052:HOH:O	2.40	0.53
23:W:5:VAL:HG11	23:W:153:MET:HE3	1.91	0.53
24:X:23:HIS:CD2	24:X:24:LYS:HG3	2.44	0.53
30:0:151:A:H2'	30:0:152:A:O4'	2.09	0.53
30:0:2112:A:H2'	30:0:2113:G:H8	1.72	0.53
30:0:2505:G:H2'	30:0:2506:A:H5'	1.91	0.53
30:0:2735:U:H2'	30:0:2736:U:C6	2.44	0.53
30:0:347:A:H2'	30:0:348:C:O4'	2.08	0.53
30:0:407:A:H5'	38:0:6054:HOH:O	2.09	0.53
30:0:1972:U:H2'	30:0:1973:A:H5'	1.91	0.52
30:0:2379:G:N7	30:0:2408:A:N1	2.57	0.52
30:0:2505:G:HO2'	30:0:2506:A:H5'	1.73	0.52
30:0:644:G:N3	30:0:644:G:H5'	2.24	0.52
12:L:41:HIS:HD2	30:0:926:A:O2'	1.91	0.52
28:2:20:ARG:HG3	28:2:39:ARG:NH2	2.23	0.52
30:0:2515:C:C2'	30:0:2516:G:H5'	2.39	0.52
30:0:2563:U:H2'	30:0:2565:C:O5'	2.09	0.52
12:L:133:VAL:HA	38:L:8867:HOH:O	2.10	0.52
23:W:119:HIS:HE1	38:0:9563:HOH:O	1.91	0.52
25:Y:204:ARG:HH22	30:0:553:G:P	2.32	0.52
30:0:559:U:C5'	30:0:559:U:H6	2.19	0.52
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.08	0.52
11:K:41:LYS:HE3	38:0:6239:HOH:O	2.08	0.52
13:M:164:THR:HG22	13:M:165:GLY:N	2.24	0.52
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.91	0.52
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.52
30:0:136:C:H2'	30:0:137:U:O4'	2.10	0.52
30:0:485:A:N3	30:0:487:G:H5''	2.24	0.52
30:0:920:C:H4'	30:0:921:G:C2	2.45	0.52
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.07	0.52
30:0:2346:C:O5'	30:0:2346:C:H6	1.92	0.52
30:0:958:G:O2'	30:0:959:C:H5'	2.10	0.52
1:A:192:VAL:HB	38:0:5683:HOH:O	2.09	0.52
2:B:53:LEU:HD11	2:B:327:VAL:HG22	1.92	0.52
4:D:50:VAL:HG13	31:9:41:C:O4'	2.10	0.52
7:G:64:ASN:N	7:G:64:ASN:HD22	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:4:PRO:HD2	38:0:6797:HOH:O	2.09	0.52
30:0:137:U:H2'	30:0:139:C:C5	2.44	0.52
30:0:2820:A:H2'	30:0:2821:C:C6	2.44	0.52
31:9:92:G:H2'	31:9:93:A:H8	1.74	0.52
2:B:229:ARG:HD2	38:0:9115:HOH:O	2.09	0.52
10:J:52:GLN:NE2	30:0:1119:G:H8	2.07	0.52
11:K:29:LEU:HB3	11:K:55:VAL:CG2	2.40	0.52
12:L:41:HIS:CD2	30:0:926:A:O2'	2.63	0.52
14:N:132:ASN:O	14:N:135:VAL:HG12	2.10	0.52
30:0:1878:G:O2'	30:0:1879:U:P	2.68	0.52
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.24	0.52
13:M:82:ARG:HB3	38:0:7854:HOH:O	2.09	0.52
14:N:11:ARG:NH1	31:9:8:G:O6	2.42	0.52
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.39	0.52
20:T:38:ARG:HH21	30:0:306:A:P	2.33	0.52
30:0:1160:G:H5'	30:0:1161:A:C4'	2.40	0.52
30:0:2070:G:H2'	30:0:2072:G:OP1	2.10	0.52
30:0:95:A:H5''	30:0:97:G:O4'	2.10	0.52
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.92	0.52
2:B:268:ARG:NH2	2:B:325:PRO:HG3	2.23	0.52
2:B:53:LEU:HD12	2:B:327:VAL:HA	1.90	0.52
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.90	0.52
30:0:1724:U:H4'	38:0:4582:HOH:O	2.09	0.52
30:0:1778:A:H2'	30:0:1779:A:H5'	1.92	0.52
30:0:2072:G:C6	30:0:2533:C:H1'	2.45	0.52
29:3:84:ARG:NE	38:3:9045:HOH:O	2.43	0.52
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.73	0.52
30:0:790:A:H1'	30:0:1710:A:H2'	1.92	0.52
30:0:2531:U:O2'	30:0:2532:A:H5'	2.10	0.52
30:0:255:A:H2'	30:0:256:C:C6	2.45	0.52
2:B:27:ASN:HD21	30:0:2807:U:P	2.32	0.52
30:0:544:G:H2'	30:0:545:G:C5'	2.37	0.52
2:B:178:ALA:O	2:B:182:VAL:HG23	2.10	0.52
26:Z:42:TYR:HA	30:0:1829:A:N6	2.25	0.52
30:0:1164:U:O2	30:0:1166:A:H4'	2.09	0.51
30:0:2252:A:C5	30:0:2253:G:H1'	2.43	0.51
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.55	0.51
23:W:151:GLU:O	23:W:154:ARG:HB2	2.10	0.51
30:0:343:C:O2'	30:0:344:C:H5'	2.09	0.51
30:0:389:G:H5''	38:0:6487:HOH:O	2.10	0.51
27:1:25:LYS:HD2	28:2:49:GLU:N	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:91:GLN:O	29:3:92:GLU:HB2	2.10	0.51
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.46	0.51
13:M:69:LYS:HG3	13:M:127:LYS:HG3	1.91	0.51
25:Y:144:ARG:NE	38:Y:8913:HOH:O	2.43	0.51
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.76	0.51
30:0:1209:C:H2'	30:0:1210:G:C8	2.41	0.51
30:0:2883:A:H2'	30:0:2884:G:O4'	2.10	0.51
30:0:564:G:H1'	38:0:6341:HOH:O	2.10	0.51
31:9:20:G:O2'	31:9:21:G:H5'	2.10	0.51
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.92	0.51
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.10	0.51
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.74	0.51
4:D:49:PRO:HB3	4:D:73:VAL:HG22	1.93	0.51
21:U:37:GLU:HB3	38:U:408:HOH:O	2.09	0.51
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.45	0.51
30:0:542:A:H2'	30:0:543:G:O4'	2.11	0.51
30:0:661:G:C5	30:0:686:A:C2	2.99	0.51
30:0:1506:U:H5'	30:0:1506:U:H6	1.75	0.51
30:0:1909:A:N1	30:0:2128:G:H1'	2.25	0.51
30:0:856:G:C8	38:0:5452:HOH:O	2.54	0.51
3:C:87:ARG:NH2	30:0:894:A:N1	2.58	0.51
1:A:206:ARG:HD3	1:A:206:ARG:H	1.75	0.51
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.17	0.51
9:I:114:TYR:CE1	30:0:1186:C:H5''	2.45	0.51
24:X:43:VAL:HG12	24:X:44:ASP:N	2.25	0.51
25:Y:174:VAL:HG22	25:Y:177:LYS:HD2	1.92	0.51
30:0:2251:G:H2'	30:0:2252:A:C8	2.46	0.51
6:F:58:GLU:HA	6:F:61:MET:HE2	1.93	0.51
12:L:90:ARG:NH2	12:L:121:ILE:HD11	2.25	0.51
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.58	0.51
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.73	0.51
30:0:1067:A:H5'	38:0:4364:HOH:O	2.10	0.51
30:0:2510:C:H5'	30:0:2511:A:OP2	2.11	0.51
30:0:2908:A:H2'	30:0:2909:G:H5'	1.92	0.51
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.08	0.51
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.92	0.51
2:B:190:MET:HE2	2:B:194:PHE:HD1	1.76	0.51
30:0:1947:G:N2	30:0:1966:U:C2	2.79	0.51
30:0:2414:A:H2'	30:0:2415:A:C8	2.46	0.51
30:0:282:C:O2'	30:0:283:U:C5'	2.48	0.51
30:0:1218:U:H2'	30:0:1219:U:H6	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:18:ASN:ND2	28:2:40:ARG:H	2.08	0.51
2:B:294:TYR:HE2	38:B:9074:HOH:O	1.94	0.51
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.11	0.51
23:W:139:GLY:O	23:W:141:HIS:HD2	1.93	0.51
26:Z:35:SER:CB	26:Z:47:ARG:HB2	2.39	0.51
30:0:101:C:H2'	30:0:102:A:C8	2.46	0.51
30:0:1182:C:H4'	30:0:1192:A:N7	2.26	0.51
16:P:1:THR:O	30:0:1396:C:H1'	2.10	0.51
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.46	0.51
31:9:108:C:H2'	31:9:109:G:C8	2.46	0.51
3:C:153:VAL:O	3:C:157:LEU:HG	2.11	0.51
8:H:31:ILE:HG23	38:H:234:HOH:O	2.11	0.51
22:V:39:ALA:N	22:V:40:PRO:HD2	2.26	0.51
30:0:1196:C:H2'	30:0:1197:G:H5'	1.93	0.50
30:0:1739:G:H1'	30:0:2726:U:O4	2.11	0.50
30:0:440:C:H2'	30:0:441:A:C8	2.46	0.50
1:A:223:ARG:NH1	38:A:8987:HOH:O	2.44	0.50
10:J:39:VAL:HG21	10:J:107:ASN:ND2	2.25	0.50
30:0:1745:G:H22	30:0:2033:G:H5'	1.76	0.50
30:0:2515:C:H2'	30:0:2516:G:H5'	1.93	0.50
3:C:93:LYS:O	3:C:98:ARG:NH2	2.44	0.50
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.76	0.50
30:0:1948:G:H2'	30:0:1949:G:O4'	2.11	0.50
30:0:2908:A:H2'	30:0:2909:G:C5'	2.40	0.50
30:0:407:A:H2'	30:0:408:A:C8	2.47	0.50
30:0:441:A:H8	30:0:441:A:O5'	1.94	0.50
31:9:51:A:H8	31:9:51:A:OP2	1.94	0.50
11:K:10:GLN:H	11:K:10:GLN:NE2	1.90	0.50
30:0:1060:C:H6	30:0:1060:C:H5'	1.76	0.50
10:J:86:MET:HE2	30:0:1241:G:H2'	1.93	0.50
30:0:2769:C:C2'	30:0:2770:G:C5'	2.87	0.50
30:0:522:U:O2'	30:0:1366:C:H5'	2.12	0.50
5:E:145:ALA:HB1	5:E:168:ILE:CD1	2.41	0.50
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.12	0.50
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.98	0.50
30:0:1149:U:H5''	30:0:1151:G:O4'	2.11	0.50
30:0:2032:U:H2'	30:0:2033:G:H5''	1.91	0.50
30:0:2265:U:H2'	30:0:2266:A:C8	2.47	0.50
30:0:532:A:H3'	38:0:9472:HOH:O	2.11	0.50
31:9:49:G:H2'	31:9:50:G:O4'	2.12	0.50
14:N:160:SER:HB2	31:9:51:A:H5'	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.12	0.50
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.69	0.50
23:W:119:HIS:HD2	23:W:120:PRO:O	1.95	0.50
30:0:1314:U:H5''	30:0:1316:G:O4'	2.11	0.50
30:0:2756:U:O2	30:0:2896:A:H2	1.95	0.50
30:0:612:U:H2'	30:0:613:C:C6	2.47	0.50
30:0:830:G:O2'	30:0:831:U:H5'	2.12	0.50
8:H:48:VAL:HA	8:H:170:ARG:O	2.12	0.50
16:P:73:HIS:HE1	30:0:1789:G:O6	1.95	0.50
30:0:2252:A:H2'	30:0:2253:G:O4'	2.12	0.50
30:0:2587:OMU:HM23	30:0:2589:U:C6	2.47	0.50
30:0:497:A:H5''	38:0:3610:HOH:O	2.11	0.50
30:0:585:C:H5''	38:0:4886:HOH:O	2.10	0.50
30:0:920:C:H5''	30:0:921:G:O5'	2.11	0.50
31:9:49:G:O2'	31:9:50:G:H5'	2.12	0.50
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.10	0.50
24:X:78:GLU:HB3	38:X:5564:HOH:O	2.12	0.50
25:Y:144:ARG:NH1	38:Y:8875:HOH:O	2.44	0.50
30:0:1193:A:C2	30:0:1194:A:N6	2.80	0.50
30:0:1131:G:C6	30:0:1230:A:C4	2.99	0.50
30:0:2649:A:H5'	30:0:2649:A:C8	2.47	0.50
30:0:2649:A:H5'	30:0:2649:A:H8	1.77	0.50
27:1:1:THR:HA	38:0:9363:HOH:O	2.11	0.50
2:B:321:PRO:HA	38:B:9081:HOH:O	2.11	0.50
5:E:20:ILE:HD11	5:E:40:VAL:CG1	2.41	0.50
12:L:145:LEU:O	12:L:148:GLU:HG3	2.12	0.50
30:0:861:A:H4'	30:0:1697:G:H4'	1.94	0.50
30:0:282:C:C2'	30:0:283:U:C5'	2.89	0.50
5:E:81:GLU:HG2	5:E:134:SER:CB	2.42	0.50
8:H:48:VAL:HG13	38:H:214:HOH:O	2.11	0.50
13:M:188:ARG:HD3	30:0:155:C:OP2	2.11	0.50
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.47	0.50
30:0:1422:U:H2'	30:0:1423:C:C6	2.47	0.49
13:M:75:ARG:HH11	30:0:1864:C:H5	1.58	0.49
30:0:69:A:H8	30:0:69:A:C5'	2.23	0.49
30:0:834:G:H3'	30:0:835:U:H4'	1.94	0.49
30:0:2032:U:C2'	30:0:2033:G:C5'	2.89	0.49
12:L:143:THR:HG22	12:L:144:ASP:H	1.75	0.49
30:0:1168:C:H5	38:0:7521:HOH:O	1.94	0.49
30:0:603:A:H5''	30:0:604:G:OP1	2.11	0.49
31:9:64:C:C2'	31:9:65:A:H5'	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ALA:O	1:A:124:VAL:HG22	2.11	0.49
9:I:120:ALA:O	9:I:124:VAL:HG23	2.11	0.49
18:R:29:LYS:NZ	38:R:8943:HOH:O	2.46	0.49
25:Y:165:GLU:HB3	38:0:6729:HOH:O	2.12	0.49
30:0:1044:C:H5''	38:0:9029:HOH:O	2.12	0.49
30:0:1159:G:H1	30:0:1208:C:H42	1.58	0.49
30:0:1207:A:C8	30:0:1208:C:C5	3.00	0.49
31:9:105:A:H2'	31:9:106:U:H5'	1.94	0.49
30:0:912:A:C4	30:0:1294:A:C2	3.01	0.49
28:2:42:TRP:HB3	30:0:1418:U:OP1	2.12	0.49
30:0:1834:C:H2'	30:0:1840:A:N6	2.27	0.49
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.45	0.49
2:B:280:VAL:HG13	2:B:333:GLU:O	2.12	0.49
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.94	0.49
11:K:66:ARG:HH22	30:0:1994:A:P	2.35	0.49
12:L:41:HIS:HE1	38:0:9778:HOH:O	1.95	0.49
30:0:1163:G:N2	30:0:1184:C:C4	2.81	0.49
27:1:28:HIS:HE1	30:0:776:A:OP1	1.95	0.49
28:2:41:HIS:HD2	28:2:44:ARG:H	1.60	0.49
3:C:1:MET:HG2	3:C:2:GLN:N	2.25	0.49
25:Y:146:PRO:O	25:Y:154:ARG:HG3	2.13	0.49
30:0:1865:A:C2	38:0:3075:HOH:O	2.55	0.49
2:B:36:PRO:HG3	2:B:169:GLY:H	1.76	0.49
3:C:77:ALA:O	3:C:78:ARG:HD3	2.12	0.49
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.43	0.49
6:F:58:GLU:HA	6:F:61:MET:CE	2.42	0.49
13:M:59:GLY:HA3	13:M:141:ILE:CD1	2.42	0.49
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.12	0.49
30:0:1562:C:N4	38:0:5891:HOH:O	2.45	0.49
30:0:1761:U:H2'	30:0:1762:C:C6	2.47	0.49
1:A:175:LYS:HG3	30:0:1847:A:OP1	2.13	0.49
30:0:1909:A:H2'	30:0:1910:A:C8	2.47	0.49
5:E:101:GLU:HB3	5:E:117:THR:HA	1.94	0.49
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.48	0.49
14:N:41:LYS:HD3	38:9:9059:HOH:O	2.12	0.49
30:0:1414:A:H2'	30:0:1415:G:O4'	2.12	0.49
30:0:2587:OMU:H6	30:0:2587:OMU:O5'	2.12	0.49
30:0:304:G:H1'	30:0:347:A:N6	2.27	0.49
30:0:426:G:H2'	30:0:427:C:O4'	2.12	0.49
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.94	0.49
2:B:87:TYR:HD1	38:B:9004:HOH:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:59:VAL:HG23	15:O:111:VAL:HG22	1.94	0.49
30:O:1196:C:C2'	30:O:1197:G:H5'	2.42	0.49
30:O:1755:A:H2'	30:O:1756:G:O4'	2.13	0.49
11:K:66:ARG:HD2	30:O:1992:U:OP2	2.13	0.49
18:R:117:HIS:CD2	30:O:20:G:H21	2.30	0.49
29:3:60:LYS:HE2	30:O:2428:G:N7	2.27	0.49
27:1:20:ARG:HH21	30:O:120:A:H5'	1.77	0.49
2:B:256:GLN:HG2	38:B:9080:HOH:O	2.11	0.49
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.95	0.49
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.42	0.49
30:O:1166:A:C6	30:O:1181:A:C2	3.01	0.48
30:O:1321:A:H2'	30:O:1322:G:C8	2.48	0.48
30:O:696:C:O2'	30:O:697:G:H5'	2.13	0.48
27:1:28:HIS:CD2	27:1:31:LYS:H	2.31	0.48
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.04	0.48
2:B:41:PHE:HB3	2:B:190:MET:CE	2.43	0.48
12:L:6:ARG:NH2	38:L:8843:HOH:O	2.45	0.48
14:N:169:PRO:O	14:N:172:PHE:HB3	2.13	0.48
20:T:54:ASP:OD2	30:O:316:A:H5'	2.13	0.48
23:W:4:LEU:O	23:W:32:CYS:HA	2.13	0.48
30:O:2512:U:H4'	30:O:2514:U:O4	2.13	0.48
30:O:2637:A:C5'	38:O:4944:HOH:O	2.61	0.48
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.95	0.48
2:B:248:ARG:NH2	30:O:2549:C:H1'	2.28	0.48
2:B:258:GLY:H	2:B:260:HIS:CE1	2.30	0.48
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.95	0.48
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.94	0.48
25:Y:132:ASP:OD2	30:O:621:C:H5'	2.13	0.48
3:C:173:LYS:HE3	30:O:1311:G:O6	2.13	0.48
30:O:221:G:H5''	38:O:5772:HOH:O	2.13	0.48
30:O:635:A:H2'	30:O:636:G:H5''	1.95	0.48
30:O:820:G:O2'	30:O:856:G:H4'	2.13	0.48
10:J:88:PRO:O	10:J:94:GLY:HA3	2.13	0.48
11:K:49:LEU:CD2	11:K:80:ILE:HD13	2.43	0.48
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.45	0.48
13:M:107:ARG:NH2	30:O:181:G:H4'	2.27	0.48
30:O:1185:U:H2'	30:O:1186:C:C6	2.48	0.48
30:O:120:A:H2'	30:O:120:A:N3	2.28	0.48
30:O:625:U:H5''	30:O:1044:C:N4	2.28	0.48
14:N:147:ILE:HD12	38:9:9086:HOH:O	2.13	0.48
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:55:SER:O	26:Z:59:GLU:HG3	2.14	0.48
10:J:75:PRO:HD3	10:J:136:SER:OG	2.12	0.48
10:J:52:GLN:HE22	30:0:1119:G:H8	1.62	0.48
30:0:1205:U:C3'	30:0:1206:U:H5''	2.43	0.48
30:0:1205:U:H5	38:0:4455:HOH:O	1.97	0.48
30:0:1353:C:H6	30:0:1353:C:H5'	1.78	0.48
30:0:2134:G:C6	30:0:2258:A:C8	3.02	0.48
30:0:2506:A:H1'	38:0:3761:HOH:O	2.13	0.48
30:0:856:G:H2'	38:0:5452:HOH:O	2.13	0.48
6:F:91:VAL:HG11	30:0:262:A:OP2	2.14	0.48
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.43	0.48
30:0:1298:U:H2'	30:0:1299:G:C8	2.48	0.48
30:0:1790:C:H2'	30:0:1791:U:C6	2.49	0.48
30:0:1972:U:C2'	30:0:1973:A:H5''	2.44	0.48
30:0:316:A:N3	30:0:336:G:O2'	2.42	0.48
30:0:447:A:O2'	30:0:448:G:H5'	2.14	0.48
30:0:627:G:H2'	30:0:2071:C:C4	2.48	0.48
2:B:254:GLN:HG3	38:B:8960:HOH:O	2.13	0.48
2:B:305:ASP:O	2:B:306:LYS:HB2	2.14	0.48
30:0:10:U:H6	30:0:10:U:H3'	1.79	0.48
30:0:1117:A:C2	30:0:1244:U:C2	3.01	0.48
30:0:152:A:O2'	30:0:153:C:H5'	2.13	0.48
30:0:1559:A:H4'	38:0:5891:HOH:O	2.13	0.48
30:0:1632:A:H2'	30:0:1633:C:C5'	2.38	0.48
30:0:1838:U:H1'	30:0:2644:C:H5'	1.96	0.48
30:0:1902:G:H2'	30:0:1903:U:O4'	2.14	0.48
30:0:2101:A:H1'	30:0:2537:G:O4'	2.14	0.48
1:A:36:ASP:O	1:A:38:ILE:N	2.38	0.48
3:C:233:THR:HG22	3:C:234:VAL:N	2.28	0.48
30:0:1081:A:H5''	38:0:3162:HOH:O	2.14	0.48
30:0:697:G:H4'	30:0:730:G:O3'	2.14	0.48
6:F:111:ILE:O	6:F:115:VAL:HG23	2.14	0.48
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.48
25:Y:145:LYS:HE2	38:Y:8907:HOH:O	2.14	0.48
30:0:1194:A:C2	30:0:1206:U:H1'	2.48	0.48
30:0:1535:G:H2'	30:0:1536:C:C6	2.49	0.48
30:0:1555:G:H4'	30:0:1630:A:H2	1.79	0.48
30:0:2809:G:H2'	30:0:2810:G:O4'	2.14	0.48
30:0:1181:A:N1	30:0:1192:A:O2'	2.41	0.47
30:0:1333:U:H2'	30:0:1334:C:C6	2.49	0.47
30:0:1524:U:HO2'	30:0:1525:G:P	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:5:LYS:HD2	30:0:1675:C:H5''	1.96	0.47
30:0:2238:A:C2	30:0:2239:C:C6	3.02	0.47
30:0:821:U:H2'	30:0:822:C:C6	2.49	0.47
30:0:960:G:N3	30:0:960:G:C2'	2.76	0.47
2:B:102:THR:HG21	2:B:182:VAL:O	2.14	0.47
3:C:246:ARG:NE	38:C:8616:HOH:O	2.38	0.47
12:L:30:ARG:HD2	38:0:9024:HOH:O	2.14	0.47
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.28	0.47
13:M:64:ARG:HD2	38:M:8887:HOH:O	2.15	0.47
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.43	0.47
23:W:154:ARG:NH1	30:0:588:G:O6	2.47	0.47
30:0:23:G:C6	30:0:24:G:N1	2.83	0.47
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.14	0.47
12:L:73:VAL:HG23	12:L:74:THR:H	1.79	0.47
14:N:155:GLU:O	14:N:156:GLU:HG3	2.14	0.47
19:S:76:GLU:HB3	38:S:7263:HOH:O	2.13	0.47
1:A:237:GLY:HA3	30:0:1939:U:H5''	1.95	0.47
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.30	0.47
14:N:114:LYS:O	14:N:118:ILE:HG13	2.14	0.47
30:0:999:C:H2'	30:0:1000:C:H5'	1.95	0.47
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.96	0.47
30:0:1132:A:N6	30:0:1229:C:H2'	2.30	0.47
30:0:1182:C:C1'	30:0:1192:A:C8	2.97	0.47
30:0:1656:A:H2'	30:0:1657:A:O4'	2.15	0.47
30:0:2001:G:O2'	30:0:2002:C:H5'	2.14	0.47
30:0:2102:G:H3'	38:0:3643:HOH:O	2.14	0.47
15:O:25:VAL:HG13	30:0:710:G:H5'	1.97	0.47
27:1:28:HIS:HD2	27:1:30:LYS:H	1.61	0.47
31:9:50:G:H2'	31:9:51:A:C8	2.48	0.47
3:C:242:GLU:HB2	38:C:8578:HOH:O	2.14	0.47
25:Y:155:ARG:NH1	38:Y:8857:HOH:O	2.47	0.47
25:Y:216:ARG:HD2	38:Y:8869:HOH:O	2.12	0.47
30:0:1406:A:H4'	30:0:1407:A:C5'	2.45	0.47
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.48	0.47
7:G:23:ILE:O	7:G:27:ILE:HG13	2.14	0.47
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.96	0.47
17:Q:75:ILE:HD13	17:Q:84:ILE:HD11	1.95	0.47
30:0:1165:G:N2	30:0:1173:A:H5'	2.30	0.47
30:0:1477:C:H2'	30:0:1478:U:C6	2.50	0.47
30:0:2616:G:N3	30:0:2616:G:H2'	2.28	0.47
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:538:C:H5''	30:0:539:G:C8	2.48	0.47
31:9:65:A:N6	31:9:112:U:C6	2.82	0.47
3:C:127:ARG:HD3	3:C:129:HIS:CE1	2.50	0.47
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.80	0.47
20:T:79:LEU:HG	20:T:89:ARG:HB2	1.96	0.47
23:W:5:VAL:HG11	23:W:153:MET:CE	2.44	0.47
26:Z:46:SER:O	26:Z:50:VAL:HG23	2.14	0.47
30:0:1178:G:C6	30:0:1179:C:N4	2.83	0.47
30:0:1925:G:O2'	30:0:1926:G:H5'	2.15	0.47
4:D:52:THR:HG21	30:0:2346:C:O2'	2.14	0.47
30:0:2502:C:H2'	30:0:2503:A:C5'	2.42	0.47
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.45	0.47
17:Q:32:GLU:HA	17:Q:71:TYR:OH	2.15	0.47
23:W:11:VAL:HG11	30:0:1086:A:C6	2.49	0.47
30:0:1181:A:H2'	30:0:1182:C:H5'	1.95	0.47
30:0:1193:A:H2	30:0:1194:A:N6	2.13	0.47
30:0:2456:A:H2'	30:0:2457:U:C6	2.50	0.47
30:0:2541:U:H5''	38:0:5423:HOH:O	2.14	0.47
30:0:10:U:O4	30:0:532:A:OP2	2.32	0.47
30:0:561:G:O2'	30:0:562:A:H5'	2.15	0.47
30:0:999:C:H2'	30:0:1000:C:C5'	2.45	0.47
28:2:38:LYS:HE3	38:0:4243:HOH:O	2.15	0.47
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.45	0.47
10:J:39:VAL:HG22	10:J:107:ASN:HA	1.95	0.47
12:L:91:VAL:HG13	12:L:120:LEU:HD23	1.96	0.47
25:Y:148:GLY:HA3	30:0:622:G:P	2.55	0.47
30:0:1252:A:H2'	30:0:1253:C:O4'	2.15	0.47
30:0:1985:U:C2	30:0:1996:U:O4'	2.68	0.47
30:0:280:C:O2'	30:0:281:U:H5'	2.15	0.47
30:0:1014:A:H5''	31:9:101:G:O2'	2.15	0.47
10:J:107:ASN:HD22	10:J:109:TYR:H	1.63	0.47
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.40	0.47
10:J:52:GLN:NE2	30:0:1119:G:H2'	2.30	0.47
9:I:114:TYR:HE1	30:0:1186:C:H5''	1.78	0.47
30:0:1496:A:H2'	30:0:1497:G:O4'	2.15	0.47
30:0:2828:G:O2'	30:0:2829:G:H5'	2.14	0.47
31:9:95:C:O2'	31:9:96:C:H5'	2.15	0.47
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.15	0.47
30:0:1163:G:N1	30:0:1184:C:N4	2.63	0.46
30:0:64:G:H2'	30:0:65:C:O4'	2.15	0.46
27:1:25:LYS:CD	28:2:49:GLU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:20:VAL:O	7:G:24:VAL:HG23	2.15	0.46
20:T:49:GLU:CB	20:T:59:GLU:HG2	2.46	0.46
30:0:1120:U:H5''	30:0:1120:U:C6	2.51	0.46
30:0:1160:G:H5''	30:0:1161:A:H5'	1.87	0.46
30:0:1735:C:O2'	30:0:1736:A:H5'	2.14	0.46
30:0:2247:C:H2'	30:0:2248:C:H6	1.81	0.46
31:9:60:C:O2'	31:9:61:C:H5'	2.15	0.46
2:B:258:GLY:HA2	38:0:4025:HOH:O	2.15	0.46
8:H:30:LYS:H	8:H:62:HIS:CD2	2.17	0.46
10:J:45:VAL:CG2	10:J:129:PHE:HD1	2.29	0.46
14:N:37:ARG:HH11	31:9:6:C:P	2.37	0.46
16:P:16:VAL:HG12	16:P:17:GLY:N	2.30	0.46
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.28	0.46
30:0:1592:G:O2'	30:0:1593:C:O5'	2.34	0.46
2:B:282:GLY:O	30:0:2898:G:H1'	2.15	0.46
5:E:126:ILE:HB	5:E:131:LEU:HD23	1.97	0.46
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.96	0.46
10:J:45:VAL:CG2	10:J:129:PHE:CD1	2.98	0.46
13:M:77:HIS:HD2	13:M:79:ALA:O	1.98	0.46
30:0:1120:U:H5'	30:0:1121:G:OP2	2.16	0.46
30:0:1164:U:C2	30:0:1166:A:H4'	2.50	0.46
30:0:1192:A:H3'	30:0:1193:A:H5'	1.98	0.46
30:0:1518:A:H2'	30:0:1519:U:C6	2.50	0.46
30:0:1942:A:H3'	38:0:7372:HOH:O	2.15	0.46
30:0:2241:C:O2'	30:0:2242:U:H5'	2.15	0.46
30:0:2372:A:H2'	30:0:2373:U:H6	1.80	0.46
30:0:2515:C:H2'	30:0:2516:G:C5'	2.46	0.46
30:0:690:G:H4'	30:0:741:C:O2	2.16	0.46
13:M:68:ARG:NH2	13:M:73:ARG:HD3	2.30	0.46
16:P:40:VAL:O	16:P:44:VAL:HG23	2.16	0.46
30:0:2004:U:H5''	30:0:2005:G:C8	2.50	0.46
30:0:255:A:C5	30:0:256:C:C4	3.03	0.46
30:0:703:G:O2'	30:0:704:C:H5'	2.16	0.46
27:1:48:TYR:HE2	38:0:9317:HOH:O	1.99	0.46
1:A:211:LYS:HB3	38:0:7455:HOH:O	2.15	0.46
1:A:71:PRO:HD2	1:A:74:VAL:HG21	1.98	0.46
2:B:307:ARG:HD2	38:B:9077:HOH:O	2.15	0.46
6:F:37:THR:O	6:F:41:GLU:HG3	2.15	0.46
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.97	0.46
30:0:1203:G:O2'	30:0:1204:C:H5'	2.16	0.46
30:0:2356:A:H5'	38:0:5662:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2507:G:H2'	30:0:2510:C:N4	2.27	0.46
30:0:2103:A:N6	30:0:2538:A:H8	1.97	0.46
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.45	0.46
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.97	0.46
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.84	0.46
38:Q:2875:HOH:O	30:0:2392:C:H4'	2.15	0.46
30:0:816:G:C6	30:0:817:G:N1	2.84	0.46
1:A:11:ARG:HD3	38:0:9224:HOH:O	2.15	0.46
2:B:148:PRO:HD2	38:B:9005:HOH:O	2.15	0.46
6:F:107:ASP:O	6:F:111:ILE:HG13	2.16	0.46
30:0:1211:G:H2'	30:0:1212:C:H6	1.81	0.46
30:0:1819:G:H2'	30:0:1820:G:C4'	2.45	0.46
30:0:2072:G:H3'	30:0:2073:G:C5'	2.46	0.46
12:L:32:ASP:HB3	30:0:222:A:H5''	1.97	0.46
30:0:2351:C:H2'	30:0:2352:G:O4'	2.16	0.46
30:0:2587:OMU:CM2	30:0:2589:U:C6	2.99	0.46
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.98	0.46
10:J:80:LYS:HE2	10:J:98:PHE:CE1	2.51	0.46
18:R:3:SER:HB2	30:0:20:G:O3'	2.16	0.46
21:U:33:SER:O	21:U:37:GLU:HG3	2.15	0.46
30:0:1014:A:H2'	30:0:1015:C:H5'	1.97	0.46
30:0:1484:G:H3'	38:0:7841:HOH:O	2.16	0.46
30:0:1524:U:OP1	30:0:1524:U:H4'	2.16	0.46
30:0:1615:A:H4'	38:0:5912:HOH:O	2.16	0.46
30:0:1641:A:C2'	30:0:1642:A:H5'	2.45	0.46
30:0:1851:G:O2'	30:0:1852:A:H5'	2.16	0.46
30:0:1996:U:O2'	30:0:1997:A:H5'	2.16	0.46
17:Q:67:GLN:NE2	30:0:2403:C:O2	2.47	0.46
31:9:22:G:H5'	31:9:23:U:OP1	2.16	0.46
1:A:105:VAL:HG11	1:A:154:ALA:CB	2.46	0.46
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.98	0.46
13:M:75:ARG:NH1	30:0:1864:C:H5	2.14	0.46
30:0:2839:C:H2'	30:0:2840:A:H5''	1.98	0.46
30:0:407:A:H8	38:0:4474:HOH:O	1.99	0.46
30:0:830:G:H2'	30:0:831:U:C6	2.51	0.46
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.78	0.46
12:L:97:VAL:HG12	12:L:98:GLU:O	2.16	0.46
13:M:79:ALA:HB3	13:M:81:ARG:NH1	2.31	0.46
13:M:82:ARG:HA	38:M:8836:HOH:O	2.16	0.46
23:W:149:LEU:HG	23:W:153:MET:HE2	1.98	0.46
30:0:1175:G:H8	30:0:1193:A:HO2'	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2282:U:H4'	30:0:2309:C:C5	2.51	0.45
30:0:2421:G:H2'	38:0:4096:HOH:O	2.16	0.45
2:B:316:ARG:HB2	30:0:2768:A:C8	2.51	0.45
30:0:666:A:H2'	30:0:667:C:O4'	2.16	0.45
4:D:76:ARG:CZ	31:9:44:A:H1'	2.46	0.45
3:C:180:SER:HB2	38:C:8638:HOH:O	2.15	0.45
4:D:36:ASN:HB3	38:D:7502:HOH:O	2.15	0.45
30:0:2506:A:H2'	30:0:2506:A:O5'	2.16	0.45
30:0:2748:G:C5'	30:0:2748:G:C8	2.98	0.45
30:0:664:U:O4	30:0:681:G:H5''	2.16	0.45
2:B:13:PHE:HB2	2:B:16:ARG:NH1	2.31	0.45
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.98	0.45
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.98	0.45
15:O:96:VAL:HG13	15:O:100:GLN:HB2	1.98	0.45
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.16	0.45
30:0:1008:C:H2'	30:0:1009:U:C6	2.51	0.45
30:0:1185:U:H5'	38:0:7491:HOH:O	2.15	0.45
30:0:1948:G:H2'	30:0:1949:G:H8	1.80	0.45
30:0:2314:G:C2'	30:0:2315:C:H5'	2.47	0.45
30:0:2906:A:H5'	30:0:2907:C:O4'	2.17	0.45
29:3:42:ARG:NH1	30:0:396:U:H5'	2.31	0.45
30:0:560:U:C2	30:0:561:G:C8	3.04	0.45
4:D:37:ALA:HA	38:D:5583:HOH:O	2.16	0.45
5:E:126:ILE:HB	5:E:131:LEU:CD2	2.46	0.45
5:E:1:PRO:HG2	5:E:59:MET:SD	2.57	0.45
11:K:114:ALA:HB3	11:K:117:VAL:HG23	1.97	0.45
15:O:32:ARG:HH21	15:O:35:LYS:HZ3	1.62	0.45
19:S:67:ARG:HD3	38:S:3430:HOH:O	2.17	0.45
30:0:1021:G:O2'	30:0:1022:A:H5'	2.17	0.45
30:0:1335:C:H2'	30:0:1336:U:C6	2.51	0.45
30:0:1739:G:O2'	30:0:1740:U:H5'	2.16	0.45
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.15	0.45
30:0:2679:G:H2'	30:0:2681:A:OP2	2.17	0.45
30:0:24:G:N2	30:0:518:G:H1'	2.31	0.45
27:1:28:HIS:HD2	27:1:31:LYS:H	1.64	0.45
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.51	0.45
31:9:59:C:H2'	31:9:60:C:C6	2.52	0.45
3:C:150:THR:HA	3:C:203:ALA:O	2.17	0.45
9:I:129:SER:HB3	30:0:1192:A:N6	2.31	0.45
24:X:22:ASN:O	24:X:64:ALA:HA	2.17	0.45
30:0:1163:G:H2'	30:0:1164:U:C5	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1236:A:H2'	30:0:1237:U:O4'	2.16	0.45
30:0:1119:G:C5	30:0:1243:C:C4	3.04	0.45
30:0:806:A:H2'	30:0:807:A:O4'	2.16	0.45
31:9:29:C:H2'	31:9:30:C:C5'	2.43	0.45
31:9:76:G:H3'	31:9:77:A:C5'	2.30	0.45
1:A:125:ASN:CB	1:A:158:VAL:HG12	2.44	0.45
30:0:2502:C:O2'	30:0:2503:A:H5'	2.17	0.45
30:0:2831:C:H2'	30:0:2832:C:H5'	1.99	0.45
2:B:212:GLN:HA	30:0:1733:A:H4'	1.98	0.45
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.98	0.45
30:0:1182:C:H1'	30:0:1192:A:H8	1.82	0.45
30:0:2238:A:O2'	30:0:2239:C:H5'	2.17	0.45
30:0:2493:C:H2'	30:0:2493:C:O2	2.16	0.45
30:0:2508:C:H2'	30:0:2509:A:O5'	2.17	0.45
30:0:407:A:O2'	30:0:408:A:H5'	2.17	0.45
30:0:95:A:O5'	30:0:97:G:H5'	2.17	0.45
30:0:969:G:H1	30:0:999:C:N4	2.15	0.45
1:A:186:TRP:CG	1:A:187:PRO:HA	2.52	0.45
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.98	0.45
14:N:108:SER:HA	14:N:109:PRO:HD3	1.76	0.45
20:T:52:ARG:O	30:0:317:A:OP1	2.33	0.45
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.52	0.45
23:W:3:ALA:O	23:W:54:PHE:HA	2.16	0.45
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.52	0.45
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.37	0.45
30:0:1391:G:H2'	30:0:1392:A:H5'	1.99	0.45
30:0:1419:U:H2'	30:0:1685:A:C2	2.51	0.45
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.97	0.45
9:I:108:HIS:N	9:I:109:PRO:HD2	2.29	0.45
13:M:164:THR:CG2	13:M:165:GLY:N	2.80	0.45
21:U:52:THR:HG22	21:U:55:ALA:H	1.81	0.45
30:0:1714:C:O2'	30:0:1715:C:H5'	2.17	0.45
30:0:2429:A:H2'	30:0:2430:A:C8	2.52	0.45
1:A:165:THR:HG22	38:A:9083:HOH:O	2.17	0.45
3:C:218:VAL:N	38:C:8616:HOH:O	2.48	0.45
3:C:236:THR:HA	38:C:8644:HOH:O	2.16	0.45
5:E:6:GLU:HA	5:E:46:THR:HG22	1.99	0.45
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.52	0.45
21:U:52:THR:CG2	21:U:54:THR:HB	2.47	0.45
30:0:1759:A:N3	30:0:1818:C:H2'	2.32	0.45
30:0:195:C:H5"	38:0:5427:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2102:G:H1'	30:0:2103:A:N7	2.29	0.45
30:0:2509:A:OP2	30:0:2510:C:H5	2.00	0.45
30:0:2096:A:N7	30:0:2539:U:C4	2.84	0.45
4:D:23:VAL:HG11	4:D:83:PHE:CZ	2.52	0.45
17:Q:49:ASN:HB2	38:Q:5227:HOH:O	2.17	0.45
38:K:7438:HOH:O	21:U:20:MET:HE1	2.16	0.45
30:0:1198:U:C6	30:0:1200:A:OP2	2.70	0.44
30:0:1588:G:C5	30:0:1589:G:C6	3.05	0.44
30:0:2775:A:C6	30:0:2799:A:C8	3.04	0.44
30:0:368:C:C2'	30:0:369:G:H5'	2.46	0.44
2:B:235:ARG:HD3	30:0:2091:G:O3'	2.16	0.44
16:P:68:LYS:HE2	30:0:1787:C:OP1	2.17	0.44
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.37	0.44
30:0:2038:A:O2'	30:0:2039:A:H5'	2.16	0.44
30:0:2072:G:P	38:0:3107:HOH:O	2.76	0.44
30:0:2425:A:H5'	30:0:2426:G:OP2	2.18	0.44
30:0:2819:C:H2'	30:0:2820:A:C8	2.53	0.44
30:0:638:C:H2'	30:0:639:A:C8	2.52	0.44
31:9:105:A:C2'	31:9:106:U:H5'	2.46	0.44
14:N:37:ARG:HD2	31:9:6:C:OP1	2.16	0.44
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.99	0.44
4:D:173:GLU:HA	38:D:6326:HOH:O	2.17	0.44
8:H:33:GLN:H	8:H:69:ARG:NH1	2.15	0.44
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.17	0.44
30:0:1334:C:O2'	30:0:1335:C:H5'	2.17	0.44
30:0:1592:G:O2'	30:0:1593:C:O4'	2.27	0.44
30:0:2064:U:H5'	30:0:2652:U:O3'	2.17	0.44
30:0:2506:A:O2'	30:0:2507:G:P	2.75	0.44
30:0:286:U:H2'	30:0:287:C:C6	2.52	0.44
30:0:699:C:H2'	30:0:744:G:O4'	2.16	0.44
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.99	0.44
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.98	0.44
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.44
30:0:2896:A:C2'	30:0:2896:A:N3	2.78	0.44
20:T:52:ARG:HD2	30:0:317:A:H5''	1.98	0.44
30:0:319:A:H4'	30:0:338:C:C4	2.53	0.44
30:0:557:C:C2	30:0:601:G:N2	2.85	0.44
30:0:750:A:H2'	30:0:751:U:C6	2.53	0.44
30:0:876:A:N3	30:0:876:A:H2'	2.33	0.44
11:K:20:CYS:HB2	11:K:29:LEU:HG	2.00	0.44
14:N:171:HIS:CE1	38:N:8860:HOH:O	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2090:G:H2'	30:0:2091:G:C8	2.53	0.44
31:9:74:G:C6	31:9:75:G:N7	2.85	0.44
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.17	0.44
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.16	0.44
20:T:77:VAL:HG11	20:T:91:LEU:HD11	1.98	0.44
23:W:115:THR:HG23	38:W:5420:HOH:O	2.16	0.44
25:Y:144:ARG:NH2	38:Y:8913:HOH:O	2.51	0.44
30:0:1182:C:O2'	30:0:1192:A:H8	1.99	0.44
30:0:1588:G:C6	30:0:1589:G:N1	2.86	0.44
30:0:1790:C:H2'	30:0:1791:U:H6	1.83	0.44
30:0:1819:G:H2'	30:0:1820:G:C5'	2.48	0.44
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.17	0.44
30:0:2505:G:H2'	30:0:2506:A:C5'	2.48	0.44
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.33	0.44
31:9:65:A:C2'	31:9:66:G:OP2	2.65	0.44
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.17	0.44
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.47	0.44
20:T:2:LYS:HG2	30:0:447:A:OP1	2.17	0.44
30:0:1183:C:H41	30:0:1192:A:P	2.41	0.44
30:0:1471:A:H5'	38:0:3202:HOH:O	2.17	0.44
30:0:366:U:H2'	30:0:367:G:O4'	2.17	0.44
4:D:135:VAL:HG22	4:D:136:ARG:N	2.32	0.44
14:N:71:TRP:HB2	38:N:8837:HOH:O	2.17	0.44
23:W:88:THR:HG22	23:W:89:ASP:N	2.32	0.44
30:0:1121:G:H4'	38:0:5565:HOH:O	2.17	0.44
30:0:1367:A:H2'	30:0:1368:U:O4'	2.18	0.44
30:0:1603:A:C5'	30:0:1605:G:O4'	2.59	0.44
30:0:496:G:H3'	38:0:7689:HOH:O	2.18	0.44
33:0:8813:CL:CL	38:0:4694:HOH:O	2.58	0.44
31:9:1:U:O3'	31:9:3:A:C5'	2.66	0.44
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.17	0.44
14:N:119:GLN:O	14:N:123:ILE:HG13	2.18	0.44
22:V:12:THR:HG22	22:V:15:GLU:CG	2.48	0.44
23:W:52:VAL:HG13	23:W:53:ALA:N	2.32	0.44
25:Y:151:SER:HB3	25:Y:154:ARG:HB2	1.99	0.44
30:0:101:C:H2'	30:0:102:A:H8	1.83	0.44
30:0:1304:U:H2'	30:0:1305:C:C6	2.53	0.44
30:0:1883:U:H5'	30:0:2012:U:OP2	2.18	0.44
30:0:1996:U:H6	30:0:2586:U:O2	2.00	0.44
30:0:2611:U:O2'	30:0:2614:C:OP2	2.32	0.44
30:0:816:G:H5'	30:0:1598:A:H4'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:17:THR:HG21	30:0:120:A:C5	2.52	0.44
2:B:75:GLU:C	2:B:77:PRO:HD3	2.38	0.44
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.76	0.44
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.44
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.01	0.44
30:0:1210:G:O2'	30:0:1211:G:H5'	2.17	0.43
30:0:1211:G:O2'	30:0:1212:C:H5'	2.18	0.43
30:0:2105:C:H2'	30:0:2106:C:C6	2.53	0.43
30:0:59:A:C5'	38:0:4347:HOH:O	2.64	0.43
3:C:49:ASP:HB3	3:C:52:ALA:HB2	1.99	0.43
11:K:75:ARG:HD3	11:K:112:PRO:O	2.18	0.43
13:M:95:LYS:HG2	13:M:99:ARG:HB3	2.00	0.43
14:N:116:PHE:HB3	14:N:136:LEU:HD23	2.00	0.43
20:T:97:ARG:NH2	30:0:308:U:H5'	2.32	0.43
19:S:8:PRO:HD2	22:V:32:ALA:HA	2.00	0.43
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.99	0.43
30:0:1257:C:H2'	30:0:1258:G:O4'	2.19	0.43
30:0:177:A:H2'	30:0:178:U:O4'	2.18	0.43
30:0:2369:A:C8	30:0:2371:G:C6	3.06	0.43
12:L:50:GLY:C	30:0:2453:G:H4'	2.38	0.43
30:0:2617:G:N3	30:0:2617:G:H2'	2.32	0.43
30:0:2756:U:N3	30:0:2896:A:C2	2.76	0.43
30:0:445:U:H1'	38:0:7361:HOH:O	2.18	0.43
30:0:523:C:H2'	30:0:524:A:C8	2.53	0.43
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.83	0.43
12:L:21:ARG:N	38:L:8826:HOH:O	2.51	0.43
14:N:36:ALA:HB1	14:N:118:ILE:HD12	2.01	0.43
30:0:1736:A:H1'	38:0:7607:HOH:O	2.18	0.43
30:0:776:A:H1'	30:0:779:U:O4	2.19	0.43
30:0:951:A:H2'	30:0:952:G:H5'	1.99	0.43
31:9:39:U:HO2'	31:9:42:C:H5	1.59	0.43
8:H:59:GLN:NE2	8:H:96:GLN:HG2	2.30	0.43
10:J:132:LEU:HA	10:J:132:LEU:HD23	1.80	0.43
20:T:62:VAL:N	38:T:3851:HOH:O	2.52	0.43
25:Y:208:LYS:O	30:0:1313:A:H5'	2.18	0.43
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.83	0.43
30:0:1849:G:H1'	30:0:2011:A:N1	2.34	0.43
30:0:2099:A:N6	30:0:2100:A:N6	2.66	0.43
30:0:305:A:C5	30:0:329:A:C2	3.06	0.43
30:0:542:A:C5'	30:0:542:A:C8	2.96	0.43
2:B:62:ARG:HA	2:B:65:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:VAL:HG12	2:B:82:VAL:O	2.18	0.43
3:C:118:THR:CG2	3:C:137:PRO:HB3	2.48	0.43
5:E:159:VAL:O	5:E:163:GLN:HG2	2.18	0.43
11:K:74:VAL:HG13	11:K:113:ILE:HG23	2.00	0.43
30:0:1015:C:H2'	30:0:1016:U:H6	1.84	0.43
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.43
30:0:1787:C:H4'	30:0:2883:A:O4'	2.19	0.43
30:0:1940:C:H4'	38:0:7372:HOH:O	2.17	0.43
30:0:2004:U:H2'	30:0:2005:G:OP1	2.18	0.43
30:0:38:G:N2	38:0:7361:HOH:O	2.50	0.43
30:0:887:G:H2'	30:0:888:U:C6	2.53	0.43
30:0:960:G:C2'	30:0:961:A:OP2	2.66	0.43
29:3:3:MET:CG	29:3:4:PRO:HD2	2.49	0.43
31:9:96:C:H2'	31:9:97:U:C6	2.54	0.43
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.31	0.43
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.48	0.43
23:W:108:ARG:NH2	23:W:114:PRO:HG2	2.31	0.43
30:0:1183:C:H42	30:0:1184:C:N4	2.16	0.43
30:0:1377:C:C5'	30:0:1377:C:H6	2.24	0.43
30:0:1871:U:O4'	30:0:1873:G:C8	2.72	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.97	0.43
30:0:2329:C:O2'	30:0:2330:U:H5'	2.17	0.43
30:0:39:G:H2'	30:0:40:C:O4'	2.19	0.43
30:0:708:A:H2'	30:0:709:G:O4'	2.18	0.43
3:C:104:ASP:HA	3:C:107:ARG:HH12	1.83	0.43
3:C:104:ASP:HA	3:C:107:ARG:NH1	2.34	0.43
21:U:20:MET:CG	21:U:28:THR:HG23	2.48	0.43
30:0:1179:C:H2'	30:0:1180:U:H6	1.83	0.43
30:0:1682:A:H2'	38:0:9811:HOH:O	2.19	0.43
30:0:2004:U:H4'	38:0:5331:HOH:O	2.19	0.43
30:0:2460:A:C2	30:0:2461:U:C2	3.06	0.43
30:0:31:C:H4'	38:0:7452:HOH:O	2.19	0.43
31:9:12:C:H5'	31:9:70:U:O4'	2.18	0.43
1:A:82:VAL:HG13	1:A:93:THR:HB	2.00	0.43
2:B:286:ASN:O	2:B:306:LYS:HE3	2.18	0.43
22:V:43:PRO:O	22:V:46:ILE:HG22	2.18	0.43
24:X:80:GLU:HB3	38:X:5564:HOH:O	2.18	0.43
30:0:1280:A:H3'	30:0:1280:A:P	2.58	0.43
30:0:1588:G:C6	30:0:1589:G:C6	3.06	0.43
30:0:2252:A:H2'	30:0:2253:G:H5'	1.99	0.43
30:0:2321:A:C5	30:0:2323:G:C8	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2569:A:H2'	30:0:2570:G:O4'	2.19	0.43
30:0:767:A:H2	30:0:2110:G:N3	2.16	0.43
1:A:164:ARG:NE	38:A:9053:HOH:O	2.47	0.43
1:A:33:GLU:CD	1:A:33:GLU:H	2.22	0.43
3:C:54:LEU:HD23	3:C:79:ARG:HG3	2.01	0.43
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.01	0.43
12:L:59:GLU:HB3	38:L:8857:HOH:O	2.17	0.43
12:L:72:ASN:HB2	38:L:8876:HOH:O	2.19	0.43
14:N:26:LEU:HD13	30:0:2415:A:N3	2.33	0.43
9:I:86:GLU:CG	30:0:1180:U:H4'	2.43	0.43
30:0:2704:C:H2'	30:0:2705:U:O4'	2.19	0.43
30:0:2791:U:H1'	30:0:2792:A:H5''	2.00	0.43
15:O:25:VAL:HG12	30:0:709:G:O2'	2.19	0.43
30:0:883:U:H3'	30:0:883:U:O2	2.19	0.43
31:9:114:G:H2'	31:9:115:C:C6	2.54	0.43
31:9:45:A:C5	31:9:46:C:C4	3.06	0.43
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.54	0.43
3:C:140:VAL:HG12	3:C:141:SER:N	2.33	0.43
5:E:11:VAL:HG12	5:E:12:ASP:N	2.33	0.43
15:O:96:VAL:CG1	15:O:100:GLN:HB2	2.49	0.43
30:0:1482:A:O2'	30:0:1483:C:H5'	2.19	0.43
30:0:2456:A:H2'	30:0:2457:U:H6	1.84	0.43
30:0:2523:U:O2'	30:0:2524:G:H5'	2.19	0.43
30:0:2787:C:H5	38:0:4644:HOH:O	2.02	0.43
30:0:398:U:H2'	30:0:399:C:C6	2.54	0.43
4:D:25:MET:HE1	4:D:37:ALA:O	2.19	0.43
12:L:121:ILE:HG12	12:L:141:GLU:HB2	2.01	0.43
17:Q:9:GLY:HA2	38:0:7028:HOH:O	2.19	0.43
2:B:333:GLU:HB2	21:U:14:GLU:OE2	2.18	0.43
30:0:1188:A:H62	30:0:1189:A:N6	2.17	0.42
30:0:1503:U:H2'	30:0:1504:A:O4'	2.19	0.42
30:0:2344:G:N3	30:0:2344:G:H2'	2.34	0.42
30:0:2505:G:C2'	30:0:2506:A:C5'	2.94	0.42
30:0:2893:C:O2'	30:0:2894:C:H5'	2.19	0.42
30:0:523:C:H2'	30:0:524:A:H8	1.83	0.42
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.48	0.42
2:B:198:GLU:HA	38:B:9081:HOH:O	2.18	0.42
8:H:91:ARG:HG2	8:H:91:ARG:H	1.69	0.42
9:I:133:THR:HG22	9:I:134:ILE:N	2.34	0.42
11:K:115:ARG:HG3	11:K:116:GLU:N	2.34	0.42
13:M:24:GLN:HA	13:M:24:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:18:LEU:HB2	18:R:143:VAL:HG13	2.01	0.42
18:R:96:VAL:HG13	18:R:106:GLY:HA3	2.00	0.42
23:W:38:THR:HG22	23:W:39:ASP:H	1.83	0.42
30:0:1213:C:O2'	30:0:1214:G:H5'	2.19	0.42
30:0:1249:U:H2'	30:0:1250:C:C6	2.54	0.42
30:0:1279:U:C5'	30:0:1280:A:OP2	2.68	0.42
30:0:1659:A:H2'	30:0:1660:G:O4'	2.18	0.42
30:0:1934:A:C8	30:0:1935:C:C5	3.07	0.42
30:0:2316:G:OP1	30:0:2317:C:H1'	2.19	0.42
30:0:2588:OMG:HM23	30:0:2617:G:C2	2.54	0.42
30:0:69:A:C8	30:0:69:A:C5'	2.96	0.42
30:0:951:A:O2'	30:0:952:G:H5'	2.20	0.42
28:2:40:ARG:HG3	28:2:45:ASN:HB2	2.00	0.42
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.84	0.42
2:B:16:ARG:NH2	38:B:8982:HOH:O	2.49	0.42
30:0:1163:G:H2'	30:0:1164:U:H5	1.84	0.42
30:0:1522:A:H2'	30:0:1523:G:H5'	2.01	0.42
30:0:2486:A:H3'	38:0:4903:HOH:O	2.18	0.42
30:0:2536:C:HO2'	30:0:2537:G:P	2.42	0.42
30:0:660:A:H4'	30:0:661:G:O5'	2.20	0.42
14:N:37:ARG:HH11	31:9:6:C:H5"	1.71	0.42
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.01	0.42
4:D:172:VAL:HG12	4:D:173:GLU:N	2.23	0.42
14:N:115:VAL:HG13	38:9:9105:HOH:O	2.19	0.42
22:V:1:THR:HG23	22:V:2:VAL:N	2.24	0.42
30:0:128:A:H3'	30:0:128:A:C8	2.55	0.42
30:0:2254:G:O2'	30:0:2255:A:H5'	2.19	0.42
30:0:2540:G:N2	38:0:9380:HOH:O	2.52	0.42
30:0:2829:G:O2'	30:0:2830:U:H5'	2.20	0.42
23:W:44:MET:HE2	30:0:944:G:H21	1.83	0.42
4:D:99:ASP:HB3	4:D:103:ASN:H	1.84	0.42
5:E:145:ALA:HB1	5:E:168:ILE:HD11	2.02	0.42
13:M:179:GLY:O	30:0:399:C:H5'	2.19	0.42
16:P:13:VAL:HG11	16:P:40:VAL:HG12	2.00	0.42
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.54	0.42
30:0:1099:G:H2'	30:0:1100:G:O4'	2.20	0.42
30:0:1183:C:C6	30:0:1192:A:N7	2.87	0.42
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.20	0.42
30:0:1552:G:N2	30:0:1634:G:C1'	2.80	0.42
30:0:1701:A:H4'	30:0:1702:U:O5'	2.20	0.42
30:0:2637:A:H5"	38:0:4944:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:867:A:H2	30:0:880:C:O2	2.03	0.42
2:B:124:ALA:O	2:B:128:ILE:HG13	2.19	0.42
3:C:236:THR:H	3:C:239:ALA:HB3	1.85	0.42
5:E:101:GLU:HA	5:E:118:ILE:HG13	2.01	0.42
15:O:44:ASN:OD1	15:O:67:SER:HB2	2.20	0.42
16:P:115:SER:OG	16:P:118:GLN:HG3	2.20	0.42
23:W:88:THR:HG22	23:W:90:TYR:CD1	2.51	0.42
30:0:1342:C:H2'	30:0:1343:C:H5'	2.02	0.42
30:0:1972:U:H2'	30:0:1973:A:H5''	1.99	0.42
30:0:1842:A:C4	30:0:1979:G:C6	3.06	0.42
30:0:2645:U:OP2	30:0:2645:U:C6	2.72	0.42
30:0:807:A:N1	30:0:808:A:C2	2.88	0.42
2:B:244:PRO:HB3	30:0:1234:U:N3	2.35	0.42
3:C:168:ARG:NH2	3:C:190:ALA:O	2.53	0.42
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.45	0.42
26:Z:56:GLU:O	26:Z:61:HIS:HE1	2.03	0.42
30:0:1042:U:O2'	30:0:1043:C:H5'	2.19	0.42
30:0:138:U:OP2	30:0:139:C:H5	2.02	0.42
30:0:1520:G:H2'	30:0:1521:C:C6	2.54	0.42
30:0:1380:U:C4	30:0:2748:G:H1'	2.54	0.42
30:0:812:A:H2'	30:0:813:C:C6	2.54	0.42
3:C:87:ARG:NH2	30:0:894:A:C2	2.88	0.42
5:E:84:MET:HE1	5:E:148:ILE:HD12	2.02	0.42
7:G:63:ARG:N	38:G:2569:HOH:O	2.52	0.42
17:Q:11:ARG:HB2	38:0:7028:HOH:O	2.20	0.42
18:R:106:GLY:HA2	18:R:109:MET:HE3	2.02	0.42
18:R:92:LEU:HD23	18:R:145:LEU:HD21	2.02	0.42
19:S:33:SER:O	19:S:37:VAL:HG23	2.19	0.42
30:0:1066:U:H2'	30:0:1067:A:C8	2.54	0.42
30:0:1167:G:N2	30:0:1180:U:C2	2.88	0.42
30:0:1201:C:C2'	30:0:1202:A:H5'	2.49	0.42
30:0:1367:A:H2'	30:0:1368:U:H5'	2.02	0.42
13:M:84:LYS:HG3	30:0:171:C:OP2	2.20	0.42
38:A:9042:HOH:O	30:0:2271:G:H5'	2.20	0.42
30:0:2356:A:H2'	30:0:2357:G:O4'	2.19	0.42
30:0:2419:U:H5''	30:0:2420:G:H5'	2.02	0.42
30:0:2504:A:H2'	30:0:2505:G:O4'	2.20	0.42
30:0:451:C:O2'	30:0:452:G:H5'	2.19	0.42
31:9:108:C:H2'	31:9:109:G:H8	1.82	0.42
6:F:91:VAL:CG1	6:F:92:GLY:N	2.83	0.42
8:H:61:ARG:HG3	8:H:61:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:18:LEU:HD12	18:R:143:VAL:HG11	2.01	0.42
25:Y:107:PRO:HD3	25:Y:182:PHE:CE1	2.55	0.42
30:0:1335:C:H2'	30:0:1336:U:H6	1.85	0.42
30:0:1626:A:H2'	30:0:1627:G:O4'	2.20	0.42
30:0:1926:G:H2'	30:0:1927:A:C8	2.54	0.42
30:0:2699:A:H2'	30:0:2700:G:O4'	2.19	0.42
30:0:629:A:H2'	30:0:630:A:O4'	2.20	0.42
30:0:90:A:H2'	30:0:91:G:O4'	2.19	0.42
31:9:80:A:C2	31:9:103:A:C4	3.08	0.42
31:9:38:A:H2	31:9:43:G:H5''	1.84	0.42
12:L:10:SER:O	12:L:11:ARG:HB3	2.19	0.42
13:M:68:ARG:HD3	13:M:68:ARG:O	2.19	0.42
19:S:43:GLU:HB3	38:S:7106:HOH:O	2.18	0.42
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	2.02	0.42
30:0:1055:G:N7	38:0:4091:HOH:O	2.51	0.42
30:0:1103:C:C2	30:0:1241:G:N2	2.88	0.42
30:0:1181:A:C2'	30:0:1182:C:H5'	2.49	0.42
30:0:1189:A:H1'	30:0:1209:C:H1'	2.02	0.42
16:P:37:ARG:HD2	30:0:1501:A:OP2	2.20	0.42
30:0:2326:C:H4'	30:0:2412:G:C4'	2.50	0.42
30:0:2757:A:H2'	30:0:2758:G:O4'	2.20	0.42
27:I:16:HIS:CD2	30:0:470:U:O2'	2.67	0.42
30:0:734:U:O2'	30:0:737:A:N6	2.53	0.42
31:9:107:C:O2'	31:9:108:C:H5'	2.20	0.42
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.31	0.42
8:H:36:MET:SD	8:H:69:ARG:HD2	2.60	0.42
14:N:13:ARG:HA	14:N:13:ARG:HD2	1.89	0.42
15:O:32:ARG:HH21	15:O:35:LYS:HZ2	1.68	0.42
15:O:87:THR:O	15:O:91:GLN:HG3	2.19	0.42
30:0:1183:C:N3	30:0:1184:C:C5	2.88	0.41
30:0:1298:U:H2'	30:0:1299:G:H8	1.85	0.41
30:0:1309:U:O2'	30:0:1310:U:H5'	2.20	0.41
30:0:2099:A:N6	30:0:2100:A:H61	2.17	0.41
30:0:2281:C:C2'	30:0:2282:U:H5'	2.49	0.41
30:0:2776:A:H2'	30:0:2777:G:O4'	2.19	0.41
30:0:506:G:N2	30:0:509:A:H5''	2.27	0.41
31:9:49:G:C2'	31:9:50:G:H5'	2.50	0.41
5:E:84:MET:HG2	5:E:168:ILE:HD13	2.02	0.41
9:I:86:GLU:HA	9:I:87:PRO:HD2	1.94	0.41
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.55	0.41
30:0:1006:A:N1	30:0:2311:A:H1'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1183:C:C5	30:0:1192:A:C8	3.08	0.41
30:0:1367:A:C2'	30:0:1368:U:H5'	2.51	0.41
30:0:1641:A:C8	30:0:1702:U:O4	2.73	0.41
30:0:2011:A:H4'	30:0:2012:U:O5'	2.20	0.41
30:0:607:G:H2'	30:0:608:A:O4'	2.21	0.41
31:9:40:C:H2'	31:9:41:C:OP1	2.20	0.41
3:C:76:ARG:HH22	30:0:1363:G:P	2.42	0.41
10:J:88:PRO:HD3	30:0:1104:C:H4'	2.01	0.41
11:K:101:ASN:O	11:K:102:GLU:HB2	2.20	0.41
16:P:16:VAL:CG1	16:P:17:GLY:N	2.83	0.41
30:0:1878:G:O2'	30:0:1879:U:OP2	2.38	0.41
30:0:1980:U:O2'	30:0:1981:A:H5'	2.20	0.41
30:0:2089:A:C2'	30:0:2090:G:H5'	2.50	0.41
30:0:537:G:O4'	30:0:538:C:C5	2.73	0.41
30:0:876:A:N3	30:0:876:A:C2'	2.83	0.41
31:9:31:C:C2	31:9:50:G:N2	2.89	0.41
2:B:243:ASN:HA	2:B:244:PRO:C	2.39	0.41
11:K:81:ARG:HB2	11:K:87:ARG:HH11	1.84	0.41
12:L:56:LYS:HE3	30:0:2443:C:H1'	2.02	0.41
21:U:17:THR:CG2	21:U:18:GLY:N	2.83	0.41
30:0:1116:U:H3	30:0:1246:A:N6	1.98	0.41
30:0:1552:G:C6	30:0:1553:C:C4	3.08	0.41
30:0:1657:A:H2'	30:0:1658:A:C8	2.55	0.41
30:0:254:C:C2'	30:0:254:C:O2	2.64	0.41
30:0:581:G:O2'	30:0:582:U:H5'	2.21	0.41
30:0:696:C:C2'	30:0:697:G:H5'	2.51	0.41
29:3:73:GLU:HB2	38:3:9023:HOH:O	2.20	0.41
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.55	0.41
6:F:99:THR:HG23	6:F:99:THR:O	2.20	0.41
25:Y:117:LEU:HB2	25:Y:174:VAL:HG21	2.01	0.41
25:Y:174:VAL:CG2	25:Y:177:LYS:HD2	2.50	0.41
8:H:174:LEU:HD21	30:0:1220:U:H4'	2.03	0.41
30:0:1406:A:H5'	30:0:1407:A:C8	2.56	0.41
30:0:1948:G:H2'	30:0:1949:G:C8	2.55	0.41
30:0:1971:G:H5'	38:0:7098:HOH:O	2.20	0.41
30:0:236:A:H8	30:0:236:A:OP1	2.03	0.41
30:0:2667:G:H1'	30:0:2914:A:N3	2.36	0.41
30:0:80:A:H4'	30:0:81:G:O5'	2.21	0.41
30:0:969:G:H1	30:0:999:C:H42	1.67	0.41
14:N:44:ARG:NH1	31:9:4:G:H21	2.18	0.41
31:9:64:C:H2'	31:9:65:A:H5'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:PRO:HD2	3:C:240:LEU:HD11	2.03	0.41
5:E:143:GLN:OE1	30:0:2796:U:H1'	2.21	0.41
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.55	0.41
22:V:7:GLU:O	22:V:11:MET:HG3	2.20	0.41
30:0:1211:G:H2'	30:0:1212:C:C6	2.56	0.41
30:0:1116:U:C2	30:0:1246:A:N6	2.88	0.41
30:0:204:A:O2'	30:0:205:U:H5'	2.20	0.41
30:0:2094:G:O6	30:0:2649:A:H2	2.04	0.41
30:0:2823:G:H4'	30:0:2827:A:O4'	2.20	0.41
30:0:2864:U:O2'	30:0:2865:G:H5'	2.20	0.41
30:0:484:A:N1	30:0:506:G:H4'	2.35	0.41
30:0:559:U:H5'	30:0:559:U:C6	2.34	0.41
30:0:612:U:H2'	30:0:613:C:H6	1.86	0.41
13:M:79:ALA:HB1	30:0:770:C:OP1	2.21	0.41
2:B:254:GLN:NE2	38:B:9014:HOH:O	2.52	0.41
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.87	0.41
3:C:5:ILE:HD11	3:C:16:VAL:HG13	2.03	0.41
17:Q:30:VAL:O	17:Q:30:VAL:HG12	2.20	0.41
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.20	0.41
20:T:40:VAL:HG22	20:T:41:ARG:N	2.35	0.41
21:U:6:CYS:HB2	21:U:32:CYS:HB3	2.03	0.41
23:W:146:ILE:HA	23:W:146:ILE:HD13	1.83	0.41
30:0:1523:G:C6	30:0:1524:U:O4	2.74	0.41
30:0:2506:A:C2'	30:0:2506:A:O5'	2.68	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.21	0.41
30:0:2644:C:O2'	30:0:2645:U:O5'	2.37	0.41
30:0:466:A:H2'	30:0:467:G:O4'	2.20	0.41
30:0:503:G:H2'	30:0:504:G:H8	1.84	0.41
30:0:69:A:C8	30:0:69:A:C3'	3.04	0.41
30:0:1131:G:H4'	31:9:91:C:O4'	2.20	0.41
1:A:211:LYS:CB	38:0:7455:HOH:O	2.69	0.41
4:D:138:GLY:N	38:D:7597:HOH:O	2.53	0.41
13:M:137:ASN:ND2	30:0:145:A:H4'	2.36	0.41
13:M:68:ARG:HG3	13:M:73:ARG:HE	1.84	0.41
14:N:32:PRO:HD2	14:N:99:GLU:O	2.21	0.41
17:Q:75:ILE:CD1	17:Q:84:ILE:HD11	2.51	0.41
18:R:114:VAL:HA	18:R:144:GLU:O	2.21	0.41
20:T:27:LEU:HD23	20:T:98:VAL:HB	2.02	0.41
30:0:1046:G:N3	30:0:1082:A:H2	2.19	0.41
30:0:2388:C:H2'	30:0:2389:U:O4'	2.21	0.41
30:0:2597:U:H2'	30:0:2598:U:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2826:G:C5	30:0:2913:A:C6	3.08	0.41
5:E:133:VAL:HG12	5:E:141:VAL:HG13	2.02	0.41
10:J:107:ASN:HD22	10:J:107:ASN:C	2.24	0.41
12:L:4:LYS:HE2	30:0:645:U:OP2	2.20	0.41
16:P:55:LYS:CG	16:P:56:GLY:N	2.84	0.41
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.89	0.41
30:0:1076:G:C2	30:0:1084:C:C2	3.09	0.41
30:0:1206:U:C5'	30:0:1206:U:H6	2.28	0.41
18:R:64:SER:OG	30:0:1369:A:H4'	2.21	0.41
30:0:1592:G:H2'	30:0:1593:C:C6	2.56	0.41
30:0:2061:C:C2'	30:0:2062:A:H5'	2.51	0.41
30:0:2455:A:H2'	30:0:2456:A:O4'	2.20	0.41
2:B:81:ALA:HB1	2:B:142:LEU:HD13	2.03	0.41
8:H:98:LEU:HD11	8:H:127:ALA:HB2	2.02	0.41
13:M:102:GLU:OE1	13:M:164:THR:HG21	2.20	0.41
14:N:23:ARG:O	14:N:27:LEU:HG	2.21	0.41
30:0:1165:G:H3'	30:0:1166:A:C5'	2.50	0.41
30:0:1441:G:O2'	30:0:1442:A:H5'	2.21	0.41
30:0:2453:G:H5'	38:0:4702:HOH:O	2.21	0.41
30:0:2526:C:H5''	38:0:7627:HOH:O	2.20	0.41
30:0:2644:C:HO2'	30:0:2645:U:P	2.44	0.41
30:0:243:A:H61	30:0:269:G:H1'	1.86	0.41
30:0:757:C:H2'	30:0:758:A:C8	2.56	0.41
2:B:87:TYR:O	2:B:138:GLY:N	2.47	0.41
3:C:118:THR:O	3:C:136:VAL:HG13	2.20	0.41
4:D:154:LYS:HD2	4:D:154:LYS:N	2.30	0.41
6:F:21:GLU:O	6:F:24:ARG:HG2	2.21	0.41
8:H:50:ILE:HG21	38:H:231:HOH:O	2.21	0.41
13:M:91:ILE:HG23	38:M:8953:HOH:O	2.20	0.41
30:0:1484:G:H2'	38:0:9110:HOH:O	2.20	0.41
30:0:1768:C:H2'	30:0:1769:C:O4'	2.21	0.41
30:0:1816:C:H2'	30:0:1817:U:O4'	2.21	0.41
30:0:2588:OMG:HM23	30:0:2617:G:N2	2.36	0.41
30:0:2645:U:H6	30:0:2645:U:H2'	1.62	0.41
15:O:25:VAL:HG13	30:0:709:G:O3'	2.20	0.41
4:D:167:GLU:C	4:D:169:THR:H	2.24	0.41
7:G:67:LEU:O	7:G:71:LEU:HG	2.21	0.41
19:S:57:THR:HG22	19:S:58:MET:H	1.84	0.41
22:V:1:THR:CG2	22:V:2:VAL:H	2.21	0.41
30:0:12:U:C2'	30:0:13:G:H5'	2.49	0.40
30:0:1400:C:H1'	38:0:4150:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2748:G:P	30:0:2749:U:H5''	2.59	0.40
5:E:143:GLN:HE22	30:0:2779:G:H21	1.67	0.40
30:0:2831:C:C2'	30:0:2832:C:H5'	2.51	0.40
30:0:304:G:H1'	30:0:347:A:H61	1.86	0.40
30:0:336:G:H5''	38:0:3737:HOH:O	2.21	0.40
30:0:553:G:O4'	30:0:1325:G:H5'	2.21	0.40
3:C:185:LYS:HD3	3:C:186:TYR:CE1	2.56	0.40
4:D:40:ILE:HG13	4:D:41:LEU:N	2.36	0.40
11:K:118:ALA:HA	11:K:125:ALA:HB2	2.03	0.40
15:O:53:GLN:HG2	15:O:56:GLU:OE1	2.21	0.40
18:R:9:ASP:HA	18:R:10:PRO:HD2	1.94	0.40
18:R:132:ARG:NH2	38:R:8983:HOH:O	2.54	0.40
30:0:1573:A:H2'	30:0:1574:C:O4'	2.21	0.40
1:A:212:PRO:HA	30:0:1943:C:O4'	2.21	0.40
30:0:2102:G:C2	30:0:2103:A:C4	3.10	0.40
30:0:2332:A:H5'	30:0:2333:G:OP2	2.20	0.40
30:0:669:G:O2'	30:0:670:G:H5'	2.21	0.40
30:0:787:G:O2'	30:0:788:A:H5'	2.20	0.40
29:3:38:ARG:HB3	29:3:42:ARG:HH12	1.85	0.40
1:A:36:ASP:C	1:A:38:ILE:H	2.21	0.40
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.89	0.40
9:I:87:PRO:C	9:I:89:GLU:H	2.23	0.40
12:L:6:ARG:NH1	30:0:1299:G:N7	2.69	0.40
15:O:77:ALA:HA	15:O:96:VAL:O	2.20	0.40
20:T:2:LYS:HE2	38:0:7433:HOH:O	2.21	0.40
30:0:1339:G:C6	30:0:1340:G:N1	2.89	0.40
30:0:1624:A:H4'	30:0:1625:U:H5'	2.03	0.40
30:0:2250:G:H2'	30:0:2251:G:O4'	2.20	0.40
30:0:2328:U:C4	30:0:2329:C:C5	3.09	0.40
30:0:2712:G:P	38:0:5242:HOH:O	2.80	0.40
30:0:2819:C:H2'	30:0:2820:A:H8	1.87	0.40
2:B:16:ARG:NE	38:B:8982:HOH:O	2.46	0.40
6:F:30:LYS:HD3	6:F:30:LYS:HA	1.88	0.40
25:Y:186:ARG:HG2	25:Y:186:ARG:NH1	2.35	0.40
23:W:23:MET:O	30:0:1025:C:H5'	2.21	0.40
30:0:907:A:H4'	30:0:1328:A:C2	2.57	0.40
30:0:1398:G:H2'	30:0:1399:A:C8	2.56	0.40
30:0:1524:U:H3'	38:0:5355:HOH:O	2.21	0.40
30:0:1476:A:H1'	30:0:1867:G:O2'	2.21	0.40
30:0:2135:A:O4'	30:0:2243:C:N4	2.55	0.40
30:0:2482:G:H4'	30:0:2483:A:C5'	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2578:G:C8	30:0:2578:G:H5'	2.44	0.40
30:0:297:U:H2'	30:0:298:C:C6	2.55	0.40
30:0:412:C:H2'	30:0:413:G:O4'	2.21	0.40
30:0:482:G:O4'	30:0:511:A:C2	2.74	0.40
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.51	0.40
3:C:84:VAL:O	3:C:85:LYS:HB2	2.22	0.40
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.92	0.40
6:F:57:GLU:O	6:F:61:MET:HG3	2.21	0.40
10:J:90:LYS:HB2	33:J:8802:CL:CL	2.57	0.40
16:P:115:SER:HB2	38:P:4299:HOH:O	2.21	0.40
30:0:1345:A:H2'	30:0:1346:U:C6	2.55	0.40
30:0:1511:U:O2'	30:0:1512:G:H5'	2.21	0.40
30:0:1589:G:N2	30:0:1605:G:H1'	2.35	0.40
30:0:2102:G:HO2'	30:0:2103:A:P	2.44	0.40
30:0:420:U:H2'	30:0:421:C:C6	2.57	0.40
30:0:483:C:C4	30:0:484:A:C6	3.10	0.40
30:0:968:G:C2	30:0:1001:U:O2	2.75	0.40
1:A:1:GLY:HA2	1:A:197:VAL:HG23	2.04	0.40
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.88	0.40
16:P:83:LYS:HG2	30:0:793:A:H5''	2.03	0.40
18:R:104:PHE:HB3	18:R:109:MET:HE1	2.04	0.40
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.87	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%)	209 (89%)	24 (10%)	2 (1%)	20	34
2	B	335/338 (99%)	315 (94%)	18 (5%)	2 (1%)	28	46
3	C	244/246 (99%)	233 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	134/177 (76%)	111 (83%)	20 (15%)	3 (2%)	8	11
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	20	34
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	149 (96%)	7 (4%)	0	100	100
9	I	68/162 (42%)	55 (81%)	12 (18%)	1 (2%)	12	20
10	J	140/145 (97%)	133 (95%)	5 (4%)	2 (1%)	13	22
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	8	12
13	M	192/196 (98%)	183 (95%)	9 (5%)	0	100	100
14	N	184/187 (98%)	171 (93%)	8 (4%)	5 (3%)	6	8
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	77 (98%)	2 (2%)	0	100	100
20	T	117/120 (98%)	113 (97%)	3 (3%)	1 (1%)	20	34
21	U	51/67 (76%)	49 (96%)	2 (4%)	0	100	100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100	100
23	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
24	X	80/92 (87%)	76 (95%)	2 (2%)	2 (2%)	6	9
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	63 (89%)	7 (10%)	1 (1%)	13	22
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	17	28
All	All	3705/4472 (83%)	3486 (94%)	195 (5%)	24 (1%)	28	46

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
10	J	5	GLU

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	170 (95%)	9 (5%)	28	49
2	B	282/283 (100%)	268 (95%)	14 (5%)	28	49
3	C	193/193 (100%)	178 (92%)	15 (8%)	15	26
4	D	117/148 (79%)	112 (96%)	5 (4%)	33	56
5	E	152/156 (97%)	147 (97%)	5 (3%)	43	68
6	F	93/94 (99%)	92 (99%)	1 (1%)	78	91
7	G	27/282 (10%)	26 (96%)	1 (4%)	39	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	134/145 (92%)	129 (96%)	5 (4%)	39	63
9	I	58/130 (45%)	58 (100%)	0	100	100
10	J	118/121 (98%)	111 (94%)	7 (6%)	23	39
11	K	106/106 (100%)	103 (97%)	3 (3%)	49	74
12	L	113/127 (89%)	109 (96%)	4 (4%)	41	65
13	M	158/160 (99%)	152 (96%)	6 (4%)	38	62
14	N	149/150 (99%)	145 (97%)	4 (3%)	50	75
15	O	93/94 (99%)	88 (95%)	5 (5%)	26	44
16	P	113/117 (97%)	110 (97%)	3 (3%)	50	75
17	Q	79/80 (99%)	76 (96%)	3 (4%)	38	62
18	R	117/122 (96%)	115 (98%)	2 (2%)	66	85
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	98 (93%)	7 (7%)	19	33
21	U	44/53 (83%)	43 (98%)	1 (2%)	56	79
22	V	51/57 (90%)	50 (98%)	1 (2%)	60	82
23	W	130/130 (100%)	124 (95%)	6 (5%)	31	52
24	X	66/74 (89%)	61 (92%)	5 (8%)	15	27
25	Y	120/196 (61%)	110 (92%)	10 (8%)	13	23
26	Z	60/94 (64%)	58 (97%)	2 (3%)	43	68
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	42 (100%)	0	100	100
29	3	79/79 (100%)	76 (96%)	3 (4%)	38	62
All	All	3095/3646 (85%)	2968 (96%)	127 (4%)	35	58

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	68	ILE
1	A	69	LEU
1	A	94	LEU
1	A	131	HIS
1	A	147	ARG
1	A	184	THR

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Mol	Chain	Res	Type
1	A	206	ARG
1	A	217	ARG
2	B	2	GLN
2	B	5	ARG
2	B	11	LEU
2	B	27	ASN
2	B	51	VAL
2	B	53	LEU
2	B	98	THR
2	B	162	MET
2	B	175	LEU
2	B	190	MET
2	B	254	GLN
2	B	265	LEU
2	B	279	THR
2	B	312	ARG
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	94	THR
3	C	101	ASP
3	C	115	LEU
3	C	136	VAL
3	C	187	ARG
3	C	211	ASP
3	C	214	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	243	VAL
4	D	24	HIS
4	D	36	ASN
4	D	39	ASP
4	D	50	VAL
4	D	149	ARG
5	E	7	ILE
5	E	86	VAL
5	E	102	VAL
5	E	132	THR
5	E	154	ILE
6	F	12	LEU

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Mol	Chain	Res	Type
7	G	73	ASP
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	173	GLU
10	J	39	VAL
10	J	46	ILE
10	J	52	GLN
10	J	70	PHE
10	J	79	PHE
10	J	107	ASN
10	J	131	THR
11	K	4	LEU
11	K	10	GLN
11	K	55	VAL
12	L	32	ASP
12	L	35	ARG
12	L	43	HIS
12	L	140	VAL
13	M	46	LEU
13	M	68	ARG
13	M	82	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
14	N	26	LEU
14	N	49	THR
14	N	135	VAL
14	N	163	PHE
15	O	3	THR
15	O	25	VAL
15	O	38	ARG
15	O	43	VAL
15	O	111	VAL
16	P	21	VAL
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	16	ASN
17	Q	95	GLU
18	R	39	THR

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Mol	Chain	Res	Type
18	R	82	GLU
20	T	39	ASN
20	T	48	VAL
20	T	71	VAL
20	T	73	HIS
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
21	U	17	THR
22	V	65	ASP
23	W	26	ILE
23	W	52	VAL
23	W	76	ASP
23	W	78	ASP
23	W	142	ASP
23	W	146	ILE
24	X	27	ASP
24	X	72	VAL
24	X	79	GLU
24	X	80	GLU
24	X	82	GLU
25	Y	103	THR
25	Y	108	ASP
25	Y	141	THR
25	Y	163	THR
25	Y	172	THR
25	Y	174	VAL
25	Y	189	ASN
25	Y	200	THR
25	Y	203	VAL
25	Y	235	GLU
26	Z	65	ASN
26	Z	68	GLU
29	3	18	GLN
29	3	56	PRO
29	3	92	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS

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Mol	Chain	Res	Type
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	103	ASN
4	D	133	ASN
5	E	106	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	73	ASN
10	J	25	GLN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	58	GLN
13	M	77	HIS
13	M	137	ASN
13	M	170	ASN
14	N	21	HIS
14	N	107	ASN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS

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Mol	Chain	Res	Type
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
19	S	44	GLN
19	S	51	GLN
19	S	53	ASN
20	T	37	GLN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	60	GLN
23	W	87	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	22	ASN
24	X	23	HIS
25	Y	133	HIS
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	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	15	ASN
29	3	48	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	28 (1%)
31	9	121/122 (99%)	17 (14%)	3 (2%)
All	All	2866/3045 (94%)	259 (9%)	31 (1%)

All (259) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	131	A
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	185	G
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	200	C
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	368	C
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A

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Mol	Chain	Res	Type
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	702	G
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	868	G
30	0	869	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U

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Mol	Chain	Res	Type
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G
30	0	1088	A
30	0	1100	G
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1151	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1207	A
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1280	A
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1357	A
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U

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Mol	Chain	Res	Type
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1562	C
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1633	C
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	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	1943	C
30	0	1971	G
30	0	1973	A
30	0	1979	G
30	0	1996	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G

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Mol	Chain	Res	Type
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2100	A
30	0	2101	A
30	0	2102	G
30	0	2103	A
30	0	2110	G
30	0	2238	A
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2320	U
30	0	2321	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2467	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2539	U
30	0	2540	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U

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Mol	Chain	Res	Type
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2611	U
30	0	2613	G
30	0	2644	C
30	0	2645	U
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2727	A
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	39	U
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A

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Mol	Chain	Res	Type
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	603	A
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1506	U
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1856	C
30	0	1942	A
30	0	1979	G
30	0	2313	C
30	0	2467	A
30	0	2541	U
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2748	G
30	0	2791	U
31	9	43	G
31	9	55	U
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMU	0	2587	30	14,22,23	1.00	1 (7%)	18,31,34	3.65	2 (11%)
30	OMG	0	2588	30	18,26,27	1.09	1 (5%)	22,38,41	2.46	5 (22%)
30	UR3	0	2619	30	14,22,23	0.72	0	16,32,35	0.73	0
30	PSU	0	2621	30	16,21,22	1.76	3 (18%)	20,30,33	6.10	5 (25%)
30	1MA	0	628	30,35	16,25,26	0.98	1 (6%)	13,37,40	1.16	1 (7%)

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	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.50	1.47	1.52
30	0	2621	PSU	C2-N1	2.52	1.43	1.38
30	0	2587	OMU	C4-N3	2.71	1.38	1.33
30	0	628	1MA	C6-N6	2.80	1.33	1.27
30	0	2621	PSU	C4-N3	2.86	1.38	1.33
30	0	2588	OMG	C6-N1	3.47	1.39	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-19.35	114.49	128.40
30	0	2621	PSU	C5-C4-N3	-12.84	114.90	125.43
30	0	2588	OMG	C5-C6-N1	-8.38	111.55	123.48
30	0	628	1MA	C2-N3-C4	-3.66	110.79	116.41
30	0	2587	OMU	C5-C4-N3	-3.58	114.57	123.12
30	0	2588	OMG	C2-N3-C4	-2.68	112.03	115.16
30	0	2588	OMG	N3-C2-N1	-2.44	123.89	127.46
30	0	2621	PSU	C5-C1'-C2'	-2.33	111.52	115.55
30	0	2588	OMG	C6-C5-C4	-2.13	118.72	120.84
30	0	2621	PSU	C6-N1-C2	2.94	120.06	115.36
30	0	2588	OMG	C6-N1-C2	6.32	125.15	116.06
30	0	2621	PSU	C4-N3-C2	13.37	126.86	115.16
30	0	2587	OMU	C4-N3-C2	14.91	126.94	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	0.52	19 (8%) 13 13	20, 40, 77, 100	0
2	B	337/338 (99%)	0.34	8 (2%) 59 62	21, 44, 73, 83	0
3	C	246/246 (100%)	0.37	9 (3%) 42 45	17, 36, 60, 73	0
4	D	140/177 (79%)	2.33	71 (50%) 0 0	48, 89, 116, 126	0
5	E	172/178 (96%)	0.60	11 (6%) 20 21	34, 59, 79, 85	0
6	F	119/120 (99%)	1.31	31 (26%) 1 0	34, 61, 91, 105	0
7	G	29/348 (8%)	2.64	17 (58%) 0 0	70, 87, 96, 98	0
8	H	160/177 (90%)	0.96	26 (16%) 2 2	32, 50, 85, 91	0
9	I	70/162 (43%)	6.43	68 (97%) 0 0	124, 138, 156, 156	0
10	J	142/145 (97%)	0.17	3 (2%) 64 67	27, 41, 63, 89	0
11	K	132/132 (100%)	0.08	2 (1%) 74 76	23, 39, 63, 72	0
12	L	145/165 (87%)	1.08	22 (15%) 2 2	18, 55, 103, 118	0
13	M	194/196 (98%)	0.43	15 (7%) 14 15	23, 34, 54, 59	0
14	N	186/187 (99%)	1.15	37 (19%) 1 1	34, 52, 104, 112	0
15	O	115/116 (99%)	0.31	1 (0%) 84 86	31, 45, 61, 69	0
16	P	143/149 (95%)	0.10	1 (0%) 87 89	28, 43, 56, 68	0
17	Q	95/96 (98%)	0.16	0 100 100	29, 37, 55, 66	0
18	R	150/155 (96%)	0.20	1 (0%) 87 89	23, 36, 57, 71	0
19	S	81/85 (95%)	0.73	11 (13%) 3 3	33, 48, 70, 81	0
20	T	119/120 (99%)	0.63	8 (6%) 19 20	29, 46, 74, 101	0
21	U	53/67 (79%)	0.63	3 (5%) 24 26	33, 46, 65, 74	0
22	V	65/71 (91%)	2.37	25 (38%) 0 0	41, 63, 106, 113	0
23	W	154/154 (100%)	0.30	2 (1%) 77 79	26, 42, 59, 71	0
24	X	82/92 (89%)	0.57	5 (6%) 22 23	34, 49, 77, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.10	5 (3%) 44 48	19, 34, 58, 80	0
26	Z	73/116 (62%)	1.43	21 (28%) 1 0	36, 55, 72, 89	0
27	1	56/57 (98%)	0.43	0 100 100	18, 24, 34, 41	0
28	2	46/50 (92%)	0.54	2 (4%) 36 39	25, 49, 74, 86	0
29	3	92/92 (100%)	0.44	3 (3%) 47 51	27, 45, 60, 74	0
30	0	2749/2923 (94%)	-0.14	104 (3%) 41 44	14, 35, 77, 154	0
31	9	122/122 (100%)	-0.05	5 (4%) 38 41	29, 54, 76, 138	0
All	All	6646/7517 (88%)	0.36	536 (8%) 13 13	14, 41, 89, 156	0

All (536) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	63	ILE	17.7
22	V	1	THR	16.7
22	V	39	ALA	15.0
9	I	91	PHE	14.0
9	I	74	ILE	11.6
30	0	2101	A	11.6
14	N	166	ALA	11.3
9	I	132	VAL	11.2
9	I	128	THR	11.0
9	I	70	THR	10.9
22	V	40	PRO	10.8
9	I	108	HIS	10.8
9	I	100	VAL	10.5
9	I	104	ALA	10.2
9	I	80	PHE	10.2
9	I	88	GLN	9.8
9	I	103	ILE	9.7
9	I	116	LEU	9.6
9	I	97	VAL	9.5
4	D	10	PHE	9.0
20	T	119	ALA	8.8
4	D	57	THR	8.7
7	G	23	ILE	8.6
9	I	72	GLU	8.5
9	I	111	LEU	8.5
9	I	120	ALA	8.4
9	I	127	CYS	8.4
1	A	37	VAL	8.4

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Mol	Chain	Res	Type	RSRZ
9	I	82	THR	8.3
9	I	133	THR	8.2
30	0	2537	G	8.1
9	I	66	GLY	8.1
26	Z	35	SER	8.0
4	D	61	PHE	7.9
30	0	2102	G	7.8
19	S	81	ILE	7.8
1	A	35	GLY	7.7
9	I	71	ALA	7.6
9	I	113	SER	7.6
30	0	1951	G	7.5
9	I	92	VAL	7.5
9	I	121	LYS	7.5
9	I	73	LEU	7.4
9	I	69	PRO	7.2
9	I	98	ASP	7.2
9	I	106	GLN	7.2
30	0	2103	A	7.2
9	I	117	THR	7.2
30	0	1177	A	7.2
9	I	83	GLY	7.0
26	Z	46	SER	7.0
1	A	237	GLY	7.0
20	T	118	SER	6.9
9	I	112	LEU	6.9
9	I	109	PRO	6.8
30	0	1202	A	6.6
12	L	75	LEU	6.6
9	I	76	ASP	6.6
9	I	118	ASN	6.5
30	0	1163	G	6.5
9	I	122	GLU	6.5
26	Z	45	VAL	6.4
30	0	1172	G	6.3
9	I	123	VAL	6.2
9	I	90	ASP	6.2
7	G	24	VAL	6.1
30	0	1198	U	6.1
9	I	81	GLU	6.1
4	D	64	ARG	6.1
31	9	1	U	6.1

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Mol	Chain	Res	Type	RSRZ
30	0	1948	G	6.0
4	D	90	LEU	6.0
24	X	88	GLU	5.9
9	I	78	ALA	5.9
30	0	1199	A	5.8
30	0	1965	C	5.8
22	V	38	GLY	5.8
4	D	11	HIS	5.8
30	0	2100	A	5.8
1	A	31	LYS	5.8
20	T	117	ASP	5.8
30	0	1164	U	5.8
9	I	94	ASP	5.7
30	0	2538	A	5.7
14	N	160	SER	5.7
9	I	86	GLU	5.6
30	0	2769	C	5.6
9	I	131	GLY	5.6
9	I	130	LEU	5.5
28	2	49	GLU	5.5
14	N	163	PHE	5.5
9	I	102	GLN	5.4
4	D	166	ILE	5.4
26	Z	49	ARG	5.4
30	0	2540	G	5.3
26	Z	34	SER	5.2
9	I	101	LYS	5.2
9	I	105	GLU	5.2
13	M	79	ALA	5.2
4	D	93	LEU	5.2
20	T	116	ASP	5.1
13	M	75	ARG	5.0
30	0	1192	A	5.0
30	0	1173	A	5.0
22	V	2	VAL	5.0
9	I	99	GLN	4.9
9	I	129	SER	4.9
1	A	85	SER	4.9
30	0	1179	C	4.9
30	0	272	A	4.8
4	D	92	GLU	4.7
22	V	46	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
30	0	1966	U	4.7
19	S	77	VAL	4.7
4	D	170	TYR	4.7
30	0	2539	U	4.7
30	0	1171	A	4.7
26	Z	55	SER	4.6
4	D	134	LEU	4.6
7	G	26	MET	4.6
5	E	45	ASP	4.6
5	E	100	ASP	4.6
30	0	1200	A	4.6
8	H	141	CYS	4.6
9	I	110	ASP	4.6
30	0	2237	G	4.5
6	F	117	GLU	4.5
13	M	71	SER	4.5
30	0	282	C	4.5
14	N	165	ALA	4.5
30	0	970	U	4.5
30	0	1170	U	4.5
30	0	1176	C	4.5
6	F	25	ASP	4.4
9	I	89	GLU	4.4
11	K	118	ALA	4.4
30	0	10	U	4.4
30	0	2645	U	4.4
30	0	1175	G	4.4
9	I	93	ALA	4.4
6	F	110	ASP	4.4
30	0	1180	U	4.3
31	9	23	U	4.3
13	M	70	GLY	4.3
12	L	91	VAL	4.3
9	I	114	TYR	4.3
6	F	22	VAL	4.2
30	0	514	G	4.2
9	I	125	GLY	4.2
7	G	69	ARG	4.2
22	V	45	ARG	4.2
26	Z	58	ASN	4.2
14	N	164	ASP	4.2
30	0	1189	A	4.2

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Mol	Chain	Res	Type	RSRZ
30	0	1525	G	4.2
4	D	40	ILE	4.2
8	H	81	GLY	4.1
4	D	69	ILE	4.1
12	L	99	GLU	4.1
4	D	73	VAL	4.1
19	S	78	ALA	4.1
30	0	1178	G	4.1
31	9	24	U	4.1
13	M	194	GLY	4.1
26	Z	48	ARG	4.1
14	N	81	ALA	4.1
8	H	174	LEU	4.0
4	D	157	LEU	4.0
30	0	1950	G	4.0
1	A	36	ASP	4.0
4	D	104	PHE	4.0
8	H	86	TYR	4.0
7	G	71	LEU	4.0
30	0	1181	A	4.0
22	V	27	LEU	4.0
8	H	40	GLN	4.0
12	L	77	ALA	4.0
30	0	999	C	3.9
30	0	1208	C	3.9
5	E	6	GLU	3.9
6	F	12	LEU	3.9
22	V	35	ALA	3.9
30	0	2004	U	3.9
9	I	107	LYS	3.9
12	L	97	VAL	3.9
30	0	1162	G	3.9
13	M	74	LYS	3.9
13	M	80	GLY	3.8
26	Z	60	ASP	3.8
22	V	37	GLY	3.8
30	0	1184	C	3.8
12	L	150	GLN	3.8
30	0	1190	G	3.8
6	F	106	ALA	3.8
30	0	1196	C	3.8
4	D	130	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
9	I	87	PRO	3.8
4	D	56	ARG	3.8
30	0	1967	U	3.8
4	D	66	GLY	3.7
4	D	62	ASP	3.7
6	F	16	ALA	3.7
26	Z	38	PHE	3.7
6	F	26	THR	3.7
4	D	160	ALA	3.7
1	A	38	ILE	3.7
12	L	60	GLU	3.7
4	D	77	ASP	3.7
30	0	1947	G	3.7
22	V	42	ASN	3.7
30	0	1169	U	3.6
14	N	175	LEU	3.6
4	D	135	VAL	3.6
5	E	87	PHE	3.6
12	L	80	ASP	3.6
9	I	124	VAL	3.6
9	I	126	THR	3.6
10	J	70	PHE	3.6
14	N	147	ILE	3.6
26	Z	43	GLY	3.6
4	D	85	GLN	3.6
9	I	119	ALA	3.6
31	9	2	U	3.6
14	N	139	TRP	3.6
14	N	159	TYR	3.6
1	A	134	ASN	3.6
8	H	73	ASN	3.6
4	D	81	GLU	3.6
9	I	115	ASP	3.6
24	X	80	GLU	3.6
30	0	1197	G	3.6
9	I	79	GLY	3.6
4	D	23	VAL	3.6
14	N	155	GLU	3.5
30	0	2238	A	3.5
19	S	76	GLU	3.5
21	U	47	ARG	3.5
4	D	86	THR	3.5

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Mol	Chain	Res	Type	RSRZ
7	G	25	GLU	3.5
4	D	91	ALA	3.5
30	0	283	U	3.5
9	I	95	LEU	3.5
30	0	1201	C	3.5
16	P	143	ALA	3.5
30	0	1165	G	3.5
14	N	172	PHE	3.4
4	D	18	ILE	3.4
30	0	2637	A	3.4
7	G	21	ASP	3.4
4	D	107	GLY	3.4
7	G	22	ALA	3.4
14	N	145	ALA	3.4
7	G	73	ASP	3.4
6	F	107	ASP	3.3
22	V	31	ARG	3.3
8	H	70	LEU	3.3
4	D	99	ASP	3.3
30	0	1166	A	3.3
30	0	1174	A	3.3
30	0	138	U	3.3
30	0	1203	G	3.3
14	N	183	ASP	3.3
22	V	28	LEU	3.3
26	Z	36	GLY	3.3
13	M	87	GLY	3.3
1	A	97	ALA	3.2
26	Z	104	ARG	3.2
30	0	284	C	3.2
2	B	183	GLU	3.2
4	D	53	LYS	3.2
12	L	147	GLU	3.2
9	I	67	VAL	3.2
12	L	93	VAL	3.2
1	A	99	ILE	3.2
8	H	149	VAL	3.2
15	O	23	GLY	3.2
4	D	68	PRO	3.2
14	N	70	GLY	3.2
4	D	162	ALA	3.2
6	F	23	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
8	H	77	ILE	3.2
30	0	1964	U	3.2
4	D	74	THR	3.1
26	Z	42	TYR	3.1
3	C	135	GLU	3.1
9	I	68	PRO	3.1
19	S	80	ARG	3.1
22	V	32	ALA	3.1
4	D	95	THR	3.1
30	0	1168	C	3.1
7	G	66	LEU	3.1
22	V	44	GLY	3.1
14	N	152	GLU	3.1
30	0	1183	C	3.1
22	V	36	ALA	3.1
4	D	172	VAL	3.1
13	M	76	ARG	3.0
2	B	57	GLU	3.0
4	D	165	PHE	3.0
14	N	68	GLU	3.0
8	H	69	ARG	3.0
13	M	78	LYS	3.0
14	N	180	LEU	3.0
7	G	68	GLU	3.0
14	N	97	VAL	3.0
9	I	75	LYS	3.0
2	B	168	GLY	3.0
30	0	960	G	3.0
30	0	1625	U	3.0
4	D	84	LEU	3.0
8	H	80	LEU	3.0
28	2	35	ARG	3.0
1	A	34	ASP	2.9
24	X	85	VAL	2.9
3	C	63	SER	2.9
4	D	17	ARG	2.9
30	0	280	C	2.9
30	0	2508	C	2.9
1	A	236	GLY	2.9
6	F	72	VAL	2.9
24	X	77	PHE	2.9
30	0	1185	U	2.9

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Mol	Chain	Res	Type	RSRZ
7	G	72	ASP	2.9
8	H	85	ASP	2.9
30	0	1188	A	2.9
8	H	38	ARG	2.9
12	L	81	VAL	2.9
14	N	154	LEU	2.9
14	N	153	GLN	2.8
1	A	203	GLY	2.8
19	S	1	SER	2.8
4	D	21	VAL	2.8
14	N	184	ILE	2.8
30	0	1182	C	2.8
4	D	171	ASP	2.8
2	B	117	GLU	2.8
4	D	51	ARG	2.8
12	L	102	ASP	2.8
13	M	86	GLN	2.8
30	0	1157	C	2.8
5	E	10	ASP	2.8
8	H	50	ILE	2.8
4	D	132	VAL	2.7
30	0	1929	G	2.7
30	0	2748	G	2.7
6	F	18	GLU	2.7
6	F	49	PHE	2.7
4	D	88	LEU	2.7
25	Y	234	VAL	2.7
5	E	118	ILE	2.7
23	W	93	ILE	2.7
14	N	134	ASP	2.7
30	0	1161	A	2.7
3	C	244	ALA	2.7
22	V	59	ILE	2.7
4	D	173	GLU	2.7
22	V	43	PRO	2.7
1	A	86	ALA	2.7
13	M	1	ALA	2.7
30	0	1206	U	2.7
7	G	67	LEU	2.7
26	Z	56	GLU	2.7
8	H	27	PRO	2.7
29	3	57	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
26	Z	57	MET	2.7
6	F	10	ALA	2.7
6	F	45	ALA	2.7
30	0	969	G	2.7
6	F	100	ASP	2.7
26	Z	44	ARG	2.6
8	H	89	THR	2.6
4	D	22	VAL	2.6
12	L	78	ALA	2.6
30	0	1194	A	2.6
30	0	2511	A	2.6
4	D	38	GLU	2.6
24	X	7	GLU	2.6
12	L	57	VAL	2.6
4	D	128	LEU	2.6
6	F	111	ILE	2.6
7	G	12	ILE	2.6
2	B	118	ASP	2.6
4	D	94	ALA	2.6
4	D	142	ALA	2.6
14	N	148	ALA	2.6
30	0	1187	U	2.6
12	L	121	ILE	2.6
30	0	1949	G	2.6
8	H	35	LYS	2.6
30	0	1000	C	2.6
1	A	64	ASP	2.6
20	T	112	LEU	2.6
30	0	365	G	2.6
30	0	1167	G	2.6
30	0	1195	G	2.6
6	F	99	THR	2.5
22	V	25	THR	2.5
25	Y	236	VAL	2.5
8	H	114	ASP	2.5
9	I	85	GLY	2.5
25	Y	98	GLN	2.5
4	D	129	ASP	2.5
19	S	79	SER	2.5
11	K	27	ARG	2.5
22	V	41	GLU	2.5
8	H	76	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
30	0	285	A	2.5
9	I	84	SER	2.5
6	F	14	ASP	2.5
5	E	169	THR	2.5
7	G	20	VAL	2.5
30	0	1526	A	2.5
14	N	138	ASP	2.5
6	F	24	ARG	2.4
26	Z	47	ARG	2.4
30	0	2768	A	2.4
4	D	52	THR	2.4
8	H	78	LYS	2.4
12	L	130	ARG	2.4
8	H	48	VAL	2.4
19	S	20	PHE	2.4
25	Y	235	GLU	2.4
30	0	1186	C	2.4
2	B	100	VAL	2.4
10	J	5	GLU	2.4
26	Z	51	ALA	2.4
1	A	133	ARG	2.4
30	0	2890	A	2.4
19	S	2	TRP	2.4
14	N	179	LEU	2.4
22	V	34	GLN	2.4
4	D	167	GLU	2.4
8	H	172	GLU	2.4
20	T	115	GLU	2.4
14	N	182	GLY	2.3
4	D	44	ILE	2.3
4	D	106	PHE	2.3
8	H	146	ALA	2.3
5	E	42	VAL	2.3
4	D	89	PRO	2.3
6	F	95	ALA	2.3
7	G	70	ALA	2.3
3	C	62	GLY	2.3
4	D	26	GLY	2.3
6	F	114	LYS	2.3
1	A	135	VAL	2.3
14	N	88	ALA	2.3
20	T	82	THR	2.3

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Mol	Chain	Res	Type	RSRZ
30	0	370	G	2.3
12	L	79	ASP	2.3
4	D	43	GLU	2.3
4	D	48	MET	2.3
30	0	281	U	2.3
9	I	77	GLU	2.3
4	D	54	ALA	2.3
30	0	271	C	2.3
31	9	122	C	2.3
1	A	153	ARG	2.2
30	0	1970	G	2.2
13	M	88	VAL	2.2
5	E	156	ASP	2.2
12	L	106	VAL	2.2
22	V	26	GLU	2.2
6	F	119	ARG	2.2
12	L	149	ARG	2.2
14	N	177	GLU	2.2
30	0	1279	U	2.2
9	I	134	ILE	2.2
21	U	55	ALA	2.2
21	U	54	THR	2.2
30	0	2289	G	2.2
29	3	92	GLU	2.2
29	3	22	VAL	2.2
4	D	80	ALA	2.2
6	F	28	ALA	2.2
22	V	18	ALA	2.2
30	0	497	A	2.2
3	C	143	ASP	2.2
22	V	65	ASP	2.2
4	D	75	LEU	2.2
8	H	165	ARG	2.2
8	H	66	GLU	2.2
6	F	98	VAL	2.2
5	E	43	ASP	2.2
14	N	156	GLU	2.2
19	S	45	TYR	2.1
10	J	4	ALA	2.1
14	N	137	ALA	2.1
25	Y	216	ARG	2.1
14	N	170	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
12	L	142	LEU	2.1
13	M	85	ARG	2.1
20	T	35	TYR	2.1
23	W	76	ASP	2.1
18	R	150	PRO	2.1
12	L	76	LEU	2.1
14	N	158	LEU	2.1
4	D	25	MET	2.1
4	D	133	ASN	2.1
1	A	158	VAL	2.1
4	D	87	ALA	2.1
6	F	76	PHE	2.1
2	B	33	ASP	2.1
6	F	43	GLY	2.1
3	C	139	VAL	2.1
6	F	101	ALA	2.1
14	N	71	TRP	2.1
3	C	126	ASP	2.1
30	0	735	C	2.1
2	B	35	GLN	2.1
3	C	68	ALA	2.1
7	G	65	THR	2.1
30	0	1524	U	2.1
4	D	24	HIS	2.1
26	Z	59	GLU	2.1
14	N	84	THR	2.1
12	L	89	PHE	2.1
4	D	37	ALA	2.0
22	V	30	ALA	2.0
6	F	19	ALA	2.0
4	D	101	THR	2.0
13	M	77	HIS	2.0
30	0	1527	A	2.0
6	F	11	ASP	2.0
8	H	83	GLU	2.0
4	D	154	LYS	2.0
19	S	21	GLN	2.0
14	N	161	GLY	2.0
26	Z	105	ARG	2.0
5	E	20	ILE	2.0
30	0	2747	C	2.0
3	C	61	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
6	F	105	ASP	2.0
30	0	1919	A	2.0
30	0	2506	A	2.0
14	N	140	GLN	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
30	1MA	0	628	23/24	0.97	0.19	-	20,23,25,25	0
30	UR3	0	2619	21/22	0.96	0.15	-	43,48,52,56	0
30	OMU	0	2587	21/22	0.98	0.14	-	23,27,29,29	0
30	OMG	0	2588	24/25	0.97	0.14	-	23,29,30,31	0
30	PSU	0	2621	20/21	0.97	0.16	-	29,31,42,42	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	8555	1/1	0.91	0.92	73.30	59,59,59,59	0
32	MG	0	8065	1/1	0.87	0.98	72.81	68,68,68,68	0
35	NA	0	8562	1/1	0.42	0.58	43.94	61,61,61,61	0
35	NA	0	8569	1/1	0.84	0.53	41.78	61,61,61,61	0
35	NA	0	8521	1/1	0.90	0.53	38.59	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	8987	1/1	0.73	0.67	22.97	199,199,199,199	0
35	NA	0	8553	1/1	0.88	0.34	20.34	61,61,61,61	0
32	MG	0	8006	1/1	0.99	0.32	19.26	1,1,1,1	0
35	NA	0	8563	1/1	0.90	0.51	18.79	64,64,64,64	0
35	NA	0	8575	1/1	0.56	0.54	16.43	78,78,78,78	0
35	NA	0	8542	1/1	0.85	0.40	15.64	44,44,44,44	0
32	MG	0	8085	1/1	0.79	0.21	12.51	90,90,90,90	0
35	NA	0	8547	1/1	0.93	0.28	12.07	49,49,49,49	0
35	NA	0	8504	1/1	0.85	0.28	11.28	34,34,34,34	0
35	NA	0	8559	1/1	0.83	0.26	10.68	67,67,67,67	0
32	MG	0	8044	1/1	0.75	0.23	10.25	62,62,62,62	0
34	SR	0	8910	1/1	0.99	0.24	9.88	60,60,60,60	0
34	SR	0	8918	1/1	0.99	0.22	8.39	45,45,45,45	0
35	NA	0	8528	1/1	0.95	0.25	8.35	67,67,67,67	0
35	NA	0	8558	1/1	0.93	0.29	8.23	39,39,39,39	0
32	MG	0	8028	1/1	0.99	0.29	7.74	1,1,1,1	0
32	MG	0	8012	1/1	0.99	0.24	7.70	4,4,4,4	0
32	MG	0	8009	1/1	0.97	0.32	7.21	1,1,1,1	0
32	MG	0	8041	1/1	0.91	0.26	7.17	52,52,52,52	0
32	MG	0	8047	1/1	0.84	0.33	5.99	66,66,66,66	0
32	MG	0	8015	1/1	0.93	0.20	5.98	50,50,50,50	0
35	NA	0	8517	1/1	0.88	0.43	5.97	68,68,68,68	0
35	NA	0	8523	1/1	0.94	0.21	5.11	48,48,48,48	0
35	NA	0	8508	1/1	0.91	0.19	4.85	36,36,36,36	0
32	MG	0	8062	1/1	0.92	0.29	4.84	46,46,46,46	0
32	MG	0	8004	1/1	0.98	0.20	4.73	13,13,13,13	0
33	CL	B	8819	1/1	0.95	0.26	4.41	57,57,57,57	0
35	NA	0	8530	1/1	0.95	0.22	4.31	41,41,41,41	0
32	MG	A	8051	1/1	0.94	0.34	4.19	51,51,51,51	0
35	NA	0	8512	1/1	0.82	0.63	3.78	63,63,63,63	0
35	NA	0	8520	1/1	0.93	0.24	3.67	49,49,49,49	0
32	MG	0	8008	1/1	0.95	0.19	3.54	27,27,27,27	0
32	MG	0	8014	1/1	0.97	0.18	3.16	23,23,23,23	0
32	MG	0	8020	1/1	0.94	0.18	3.14	22,22,22,22	0
35	NA	0	8564	1/1	0.86	0.16	2.97	49,49,49,49	0
32	MG	0	8001	1/1	0.94	0.20	2.94	9,9,9,9	0
35	NA	0	8513	1/1	0.95	0.21	2.35	32,32,32,32	0
35	NA	C	8503	1/1	0.95	0.26	2.06	19,19,19,19	0
32	MG	0	8070	1/1	0.85	0.17	1.79	50,50,50,50	0
35	NA	0	8527	1/1	0.96	0.18	1.40	35,35,35,35	0
37	K	0	8401	1/1	0.69	0.44	1.39	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	8947	1/1	0.98	0.21	1.18	73,73,73,73	0
37	K	0	8402	1/1	0.90	0.26	1.15	77,77,77,77	0
32	MG	0	8011	1/1	0.95	0.23	0.98	26,26,26,26	0
35	NA	0	8533	1/1	0.91	0.19	0.91	57,57,57,57	0
35	NA	0	8534	1/1	0.82	0.36	0.91	56,56,56,56	0
32	MG	0	8067	1/1	0.72	0.38	0.89	55,55,55,55	0
35	NA	M	8539	1/1	0.88	0.18	0.73	34,34,34,34	0
36	CD	Z	8703	1/1	0.99	0.20	0.60	67,67,67,67	0
35	NA	0	8556	1/1	0.89	0.26	0.56	38,38,38,38	0
34	SR	0	8985	1/1	0.94	0.19	0.46	98,98,98,98	0
35	NA	0	8515	1/1	0.97	0.20	0.39	28,28,28,28	0
33	CL	J	8821	1/1	0.97	0.22	0.29	52,52,52,52	0
34	SR	0	8972	1/1	0.93	0.17	0.25	121,121,121,121	0
32	MG	0	8084	1/1	0.86	0.17	0.08	59,59,59,59	0
36	CD	U	8701	1/1	0.99	0.17	-0.18	62,62,62,62	0
32	MG	0	8058	1/1	0.98	0.16	-0.46	3,3,3,3	0
34	SR	0	8995	1/1	0.93	0.17	-0.48	94,94,94,94	0
34	SR	0	8981	1/1	0.92	0.15	-0.51	115,115,115,115	0
35	NA	0	8571	1/1	0.90	0.12	-0.52	83,83,83,83	0
35	NA	J	8538	1/1	0.90	0.15	-0.63	47,47,47,47	0
34	SR	R	8912	1/1	1.00	0.15	-0.68	55,55,55,55	0
33	CL	0	8812	1/1	0.99	0.14	-0.74	43,43,43,43	0
34	SR	0	8975	1/1	0.94	0.14	-0.76	114,114,114,114	0
32	MG	0	8013	1/1	0.88	0.14	-0.81	41,41,41,41	0
32	MG	0	8003	1/1	0.95	0.15	-0.89	24,24,24,24	0
32	MG	0	8021	1/1	0.98	0.12	-0.93	24,24,24,24	0
36	CD	1	8702	1/1	0.99	0.13	-1.14	54,54,54,54	0
34	SR	A	8929	1/1	0.97	0.11	-1.30	78,78,78,78	0
32	MG	0	8087	1/1	0.97	0.15	-1.31	33,33,33,33	0
34	SR	1	8913	1/1	0.99	0.15	-1.32	32,32,32,32	0
33	CL	M	8818	1/1	0.99	0.14	-1.32	22,22,22,22	0
34	SR	A	8930	1/1	0.99	0.12	-1.37	57,57,57,57	0
34	SR	0	8942	1/1	0.98	0.12	-1.38	55,55,55,55	0
32	MG	T	8057	1/1	0.95	0.15	-1.39	32,32,32,32	0
34	SR	0	8969	1/1	0.89	0.16	-1.40	115,115,115,115	0
35	NA	9	8572	1/1	0.88	0.12	-1.62	66,66,66,66	0
33	CL	O	8808	1/1	0.97	0.10	-1.75	52,52,52,52	0
36	CD	3	8704	1/1	1.00	0.14	-1.75	63,63,63,63	0
35	NA	Q	8540	1/1	0.96	0.09	-1.75	39,39,39,39	0
35	NA	0	8568	1/1	0.97	0.16	-1.79	33,33,33,33	0
32	MG	Y	8086	1/1	0.93	0.13	-1.80	30,30,30,30	0
35	NA	0	8550	1/1	0.96	0.17	-1.87	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8043	1/1	0.93	0.12	-1.89	51,51,51,51	0
32	MG	0	8053	1/1	0.98	0.12	-1.90	45,45,45,45	0
34	SR	F	9005	1/1	0.98	0.11	-1.94	77,77,77,77	0
33	CL	0	8816	1/1	0.94	0.12	-2.00	49,49,49,49	0
35	NA	0	8557	1/1	0.85	0.10	-2.03	63,63,63,63	0
33	CL	3	8804	1/1	0.97	0.09	-2.50	48,48,48,48	0
34	SR	0	8970	1/1	0.95	0.12	-2.53	73,73,73,73	0
35	NA	T	8537	1/1	0.91	0.09	-2.61	26,26,26,26	0
34	SR	0	8943	1/1	0.99	0.08	-2.67	49,49,49,49	0
34	SR	0	8959	1/1	0.84	0.10	-2.77	129,129,129,129	0
32	MG	0	8075	1/1	0.89	0.11	-2.95	37,37,37,37	0
35	NA	0	8519	1/1	0.99	0.14	-3.10	29,29,29,29	0
34	SR	0	8935	1/1	1.00	0.09	-3.11	54,54,54,54	0
32	MG	0	8034	1/1	0.98	0.11	-3.37	25,25,25,25	0
32	MG	0	8052	1/1	0.91	0.10	-3.39	29,29,29,29	0
32	MG	0	8025	1/1	0.86	0.12	-3.41	40,40,40,40	0
32	MG	0	8002	1/1	0.92	0.16	-3.79	33,33,33,33	0
34	SR	0	8945	1/1	0.96	0.10	-3.79	71,71,71,71	0
34	SR	0	8992	1/1	0.91	0.09	-4.02	108,108,108,108	0
33	CL	0	8805	1/1	0.99	0.10	-4.26	39,39,39,39	0
35	NA	0	8565	1/1	0.94	0.09	-4.78	39,39,39,39	0
34	SR	0	8978	1/1	0.98	0.10	-5.37	47,47,47,47	0
34	SR	0	8964	1/1	0.98	0.09	-5.42	76,76,76,76	0
34	SR	0	8936	1/1	0.99	0.12	-5.84	44,44,44,44	0
34	SR	0	8948	1/1	0.98	0.10	-6.01	57,57,57,57	0
32	MG	0	8088	1/1	0.90	0.09	-6.24	25,25,25,25	0
34	SR	3	8932	1/1	0.99	0.08	-6.43	65,65,65,65	0
34	SR	0	8904	1/1	0.99	0.08	-9.63	20,20,20,20	0
35	NA	0	8535	1/1	0.90	0.30	-	55,55,55,55	0
35	NA	0	8574	1/1	0.95	0.31	-	47,47,47,47	0
34	SR	S	8961	1/1	0.93	0.10	-	98,98,98,98	0
34	SR	0	8901	1/1	1.00	0.17	-	35,35,35,35	0
34	SR	0	8919	1/1	0.85	0.19	-	167,167,167,167	0
35	NA	0	8505	1/1	0.94	0.22	-	37,37,37,37	0
32	MG	0	8033	1/1	0.96	0.10	-	45,45,45,45	0
34	SR	0	8925	1/1	0.99	0.13	-	55,55,55,55	0
32	MG	0	8083	1/1	0.97	0.07	-	35,35,35,35	0
35	NA	0	8501	1/1	0.97	0.16	-	30,30,30,30	0
34	SR	0	8949	1/1	0.93	0.50	-	184,184,184,184	0
34	SR	0	8933	1/1	0.97	0.06	-	54,54,54,54	0
34	SR	0	8971	1/1	0.41	0.14	-	153,153,153,153	0
34	SR	0	8922	1/1	0.86	0.54	-	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	8956	1/1	0.93	0.10	-	111,111,111,111	0
34	SR	0	8915	1/1	0.98	0.11	-	58,58,58,58	0
34	SR	0	8907	1/1	0.98	0.20	-	50,50,50,50	0
32	MG	0	8035	1/1	0.90	0.10	-	63,63,63,63	0
32	MG	0	8090	1/1	0.89	0.10	-	51,51,51,51	0
34	SR	0	8931	1/1	0.99	0.11	-	61,61,61,61	0
34	SR	0	9004	1/1	0.42	0.68	-	182,182,182,182	0
32	MG	0	8076	1/1	0.82	0.22	-	52,52,52,52	0
32	MG	0	8010	1/1	0.81	0.30	-	69,69,69,69	0
34	SR	9	8980	1/1	0.74	0.14	-	144,144,144,144	0
35	NA	0	8566	1/1	0.96	0.41	-	37,37,37,37	0
32	MG	0	8093	1/1	0.97	0.17	-	29,29,29,29	0
32	MG	0	8071	1/1	0.83	0.23	-	73,73,73,73	0
32	MG	0	8018	1/1	0.89	0.28	-	13,13,13,13	0
34	SR	0	8991	1/1	0.75	0.25	-	171,171,171,171	0
32	MG	0	8023	1/1	0.99	0.12	-	30,30,30,30	0
34	SR	0	8965	1/1	0.97	0.12	-	80,80,80,80	0
32	MG	0	8092	1/1	0.95	0.11	-	53,53,53,53	0
35	NA	0	8525	1/1	0.80	0.20	-	57,57,57,57	0
32	MG	0	8078	1/1	0.88	0.25	-	52,52,52,52	0
35	NA	0	8570	1/1	0.94	0.18	-	35,35,35,35	0
35	NA	0	8526	1/1	0.79	0.12	-	43,43,43,43	0
35	NA	0	8541	1/1	0.98	0.24	-	33,33,33,33	0
32	MG	0	8066	1/1	0.89	0.33	-	67,67,67,67	0
35	NA	0	8506	1/1	0.95	0.14	-	44,44,44,44	0
32	MG	0	8068	1/1	0.87	0.17	-	50,50,50,50	0
34	SR	0	8906	1/1	0.99	0.20	-	50,50,50,50	0
33	CL	R	8806	1/1	0.98	0.16	-	28,28,28,28	0
34	SR	0	8962	1/1	0.71	1.21	-	165,165,165,165	0
34	SR	0	8903	1/1	0.99	0.18	-	36,36,36,36	0
34	SR	A	8977	1/1	0.97	0.13	-	88,88,88,88	0
34	SR	0	9008	1/1	0.97	0.14	-	59,59,59,59	0
35	NA	9	8543	1/1	0.71	0.16	-	60,60,60,60	0
34	SR	0	9000	1/1	0.93	0.16	-	125,125,125,125	0
34	SR	0	8998	1/1	0.92	0.14	-	99,99,99,99	0
32	MG	0	8039	1/1	0.93	0.33	-	42,42,42,42	0
34	SR	0	8974	1/1	0.95	0.34	-	119,119,119,119	0
34	SR	0	8937	1/1	1.00	0.16	-	53,53,53,53	0
34	SR	3	8999	1/1	0.99	0.10	-	63,63,63,63	0
34	SR	0	8997	1/1	0.97	0.22	-	115,115,115,115	0
32	MG	0	8061	1/1	0.98	0.22	-	17,17,17,17	0
34	SR	0	8934	1/1	0.99	0.11	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	8916	1/1	0.99	0.11	-	45,45,45,45	0
32	MG	0	8072	1/1	0.90	0.15	-	36,36,36,36	0
34	SR	0	8958	1/1	0.97	0.10	-	57,57,57,57	0
32	MG	0	8027	1/1	0.93	0.09	-	36,36,36,36	0
35	NA	0	8522	1/1	0.90	0.20	-	52,52,52,52	0
34	SR	0	8938	1/1	0.88	0.19	-	102,102,102,102	0
34	SR	0	8953	1/1	0.98	0.07	-	76,76,76,76	0
32	MG	0	8081	1/1	0.80	0.30	-	65,65,65,65	0
32	MG	0	8059	1/1	0.88	0.09	-	31,31,31,31	0
35	NA	0	8549	1/1	0.89	0.43	-	73,73,73,73	0
33	CL	J	8802	1/1	0.92	0.13	-	49,49,49,49	0
35	NA	0	8546	1/1	0.95	0.41	-	51,51,51,51	0
32	MG	0	8005	1/1	0.98	0.15	-	29,29,29,29	0
34	SR	0	8982	1/1	0.95	0.15	-	116,116,116,116	0
33	CL	0	8822	1/1	0.92	0.11	-	46,46,46,46	0
34	SR	0	8905	1/1	1.00	0.25	-	43,43,43,43	0
32	MG	0	8049	1/1	0.82	0.41	-	78,78,78,78	0
34	SR	0	8966	1/1	0.98	0.10	-	68,68,68,68	0
34	SR	0	8979	1/1	0.06	0.20	-	193,193,193,193	0
32	MG	0	8055	1/1	0.98	0.27	-	12,12,12,12	0
34	SR	0	8993	1/1	0.89	0.08	-	154,154,154,154	0
34	SR	0	8960	1/1	0.94	0.09	-	100,100,100,100	0
32	MG	0	8029	1/1	0.93	0.12	-	35,35,35,35	0
32	MG	0	8017	1/1	0.78	0.41	-	67,67,67,67	0
32	MG	0	8030	1/1	0.96	0.28	-	51,51,51,51	0
35	NA	0	8531	1/1	0.97	0.10	-	17,17,17,17	0
32	MG	0	8019	1/1	0.98	0.26	-	18,18,18,18	0
33	CL	0	8803	1/1	0.98	0.14	-	38,38,38,38	0
32	MG	0	8016	1/1	0.92	0.31	-	75,75,75,75	0
34	SR	0	8927	1/1	0.99	0.17	-	58,58,58,58	0
33	CL	0	8817	1/1	0.99	0.08	-	33,33,33,33	0
34	SR	1	8952	1/1	1.00	0.15	-	47,47,47,47	0
34	SR	0	8946	1/1	0.97	0.18	-	75,75,75,75	0
32	MG	0	8036	1/1	0.97	0.16	-	37,37,37,37	0
34	SR	0	8988	1/1	0.94	0.11	-	110,110,110,110	0
34	SR	0	8996	1/1	0.94	0.29	-	173,173,173,173	0
34	SR	0	8983	1/1	0.47	0.22	-	151,151,151,151	0
32	MG	0	8091	1/1	0.93	0.11	-	50,50,50,50	0
35	NA	0	8529	1/1	0.98	0.10	-	29,29,29,29	0
34	SR	0	8990	1/1	0.85	0.13	-	132,132,132,132	0
32	MG	0	8022	1/1	0.97	0.15	-	7,7,7,7	0
34	SR	0	8994	1/1	0.48	0.51	-	173,173,173,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8573	1/1	0.88	0.19	-	69,69,69,69	0
34	SR	0	8926	1/1	0.99	0.16	-	69,69,69,69	0
33	CL	J	8801	1/1	0.98	0.10	-	42,42,42,42	0
34	SR	0	8911	1/1	0.98	0.11	-	48,48,48,48	0
34	SR	0	8928	1/1	0.97	0.09	-	67,67,67,67	0
34	SR	0	8921	1/1	0.99	0.15	-	46,46,46,46	0
34	SR	0	8940	1/1	0.98	0.11	-	62,62,62,62	0
35	NA	0	8514	1/1	0.94	0.19	-	34,34,34,34	0
34	SR	9	8968	1/1	0.88	0.14	-	96,96,96,96	0
34	SR	0	9007	1/1	0.48	1.11	-	178,178,178,178	0
32	MG	0	8046	1/1	0.99	0.16	-	1,1,1,1	0
32	MG	0	8045	1/1	0.94	0.20	-	40,40,40,40	0
35	NA	S	8510	1/1	0.94	0.07	-	32,32,32,32	0
32	MG	0	8024	1/1	0.95	0.14	-	45,45,45,45	0
35	NA	0	8516	1/1	0.77	0.38	-	50,50,50,50	0
32	MG	0	8037	1/1	0.78	0.35	-	77,77,77,77	0
35	NA	0	8545	1/1	0.93	0.30	-	40,40,40,40	0
34	SR	B	8950	1/1	0.98	0.14	-	83,83,83,83	0
33	CL	0	8815	1/1	0.99	0.12	-	38,38,38,38	0
34	SR	0	8984	1/1	0.98	0.09	-	75,75,75,75	0
34	SR	0	8920	1/1	0.99	0.07	-	63,63,63,63	0
35	NA	0	8548	1/1	0.98	0.30	-	41,41,41,41	0
33	CL	0	8811	1/1	0.92	0.17	-	54,54,54,54	0
32	MG	0	8077	1/1	0.95	0.14	-	34,34,34,34	0
35	NA	0	8552	1/1	0.94	0.29	-	51,51,51,51	0
34	SR	0	8986	1/1	0.93	0.17	-	136,136,136,136	0
35	NA	0	8536	1/1	0.80	0.17	-	62,62,62,62	0
35	NA	0	8551	1/1	0.96	0.17	-	40,40,40,40	0
34	SR	0	8923	1/1	0.99	0.10	-	54,54,54,54	0
32	MG	0	8080	1/1	0.89	0.13	-	54,54,54,54	0
32	MG	0	8007	1/1	0.89	0.29	-	53,53,53,53	0
32	MG	0	8040	1/1	0.43	0.55	-	81,81,81,81	0
34	SR	0	8939	1/1	0.97	0.10	-	62,62,62,62	0
32	MG	0	8089	1/1	0.88	0.20	-	48,48,48,48	0
35	NA	0	8518	1/1	0.68	0.63	-	81,81,81,81	0
34	SR	0	8908	1/1	0.99	0.15	-	46,46,46,46	0
35	NA	0	8509	1/1	0.91	0.26	-	60,60,60,60	0
35	NA	0	8502	1/1	0.97	0.30	-	52,52,52,52	0
35	NA	0	8561	1/1	0.93	0.39	-	67,67,67,67	0
32	MG	K	8054	1/1	0.97	0.14	-	20,20,20,20	0
32	MG	0	8082	1/1	0.61	0.49	-	63,63,63,63	0
34	SR	0	8976	1/1	0.92	0.29	-	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8544	1/1	0.97	0.14	-	53,53,53,53	0
35	NA	0	8524	1/1	0.99	0.16	-	27,27,27,27	0
34	SR	0	8924	1/1	0.99	0.12	-	50,50,50,50	0
32	MG	0	8073	1/1	0.89	0.31	-	72,72,72,72	0
33	CL	N	8807	1/1	0.97	0.11	-	43,43,43,43	0
32	MG	0	8038	1/1	0.56	0.40	-	80,80,80,80	0
32	MG	0	8032	1/1	0.96	0.21	-	42,42,42,42	0
33	CL	L	8810	1/1	0.97	0.14	-	43,43,43,43	0
33	CL	0	8813	1/1	0.97	0.10	-	34,34,34,34	0
33	CL	A	8809	1/1	0.94	0.14	-	51,51,51,51	0
34	SR	0	9002	1/1	0.85	0.17	-	141,141,141,141	0
34	SR	0	8955	1/1	0.82	0.21	-	140,140,140,140	0
35	NA	0	8567	1/1	0.84	0.53	-	59,59,59,59	0
34	SR	0	8951	1/1	0.94	0.07	-	99,99,99,99	0
33	CL	0	8814	1/1	0.98	0.14	-	35,35,35,35	0
34	SR	0	9001	1/1	0.89	0.05	-	142,142,142,142	0
34	SR	0	8973	1/1	0.98	0.13	-	79,79,79,79	0
32	MG	0	8026	1/1	0.91	0.11	-	44,44,44,44	0
34	SR	0	8989	1/1	0.88	0.24	-	149,149,149,149	0
32	MG	0	8060	1/1	0.95	0.13	-	41,41,41,41	0
32	MG	0	8056	1/1	0.83	0.21	-	66,66,66,66	0
35	NA	0	8511	1/1	0.93	0.25	-	61,61,61,61	0
34	SR	0	9006	1/1	0.20	0.59	-	199,199,199,199	0
34	SR	0	8909	1/1	0.99	0.14	-	44,44,44,44	0
34	SR	0	8954	1/1	0.98	0.12	-	60,60,60,60	0
32	MG	0	8079	1/1	0.88	0.31	-	52,52,52,52	0
34	SR	0	8957	1/1	0.83	0.33	-	149,149,149,149	0
36	CD	O	8705	1/1	0.96	0.05	-	88,88,88,88	0
34	SR	0	8914	1/1	0.98	0.21	-	67,67,67,67	0
32	MG	0	8050	1/1	0.85	0.50	-	63,63,63,63	0
32	MG	0	8048	1/1	0.80	0.27	-	55,55,55,55	0
35	NA	R	8532	1/1	0.73	0.13	-	32,32,32,32	0
35	NA	0	8554	1/1	0.87	0.47	-	55,55,55,55	0
34	SR	0	8941	1/1	0.98	0.14	-	60,60,60,60	0
35	NA	0	8560	1/1	0.92	0.30	-	67,67,67,67	0
33	CL	Y	8820	1/1	0.99	0.09	-	27,27,27,27	0
32	MG	9	8074	1/1	0.96	0.28	-	42,42,42,42	0
34	SR	0	8967	1/1	0.97	0.10	-	86,86,86,86	0
34	SR	0	8944	1/1	0.91	0.16	-	117,117,117,117	0
34	SR	0	8963	1/1	0.92	0.13	-	135,135,135,135	0
32	MG	0	8064	1/1	0.96	0.20	-	54,54,54,54	0
34	SR	9	9003	1/1	0.92	0.06	-	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8507	1/1	0.97	0.22	-	19,19,19,19	0
32	MG	0	8031	1/1	0.92	0.09	-	39,39,39,39	0
32	MG	B	8042	1/1	0.86	0.26	-	75,75,75,75	0
32	MG	0	8063	1/1	0.89	0.32	-	74,74,74,74	0
34	SR	0	8902	1/1	0.80	0.57	-	112,112,112,112	0
32	MG	0	8069	1/1	0.90	0.27	-	75,75,75,75	0
34	SR	0	8917	1/1	0.99	0.14	-	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.