



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:26 am GMT

PDB ID : 1YHQ
Title : Crystal Structure Of Azithromycin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-10
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

<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 : trunk28620
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) : recalc28949

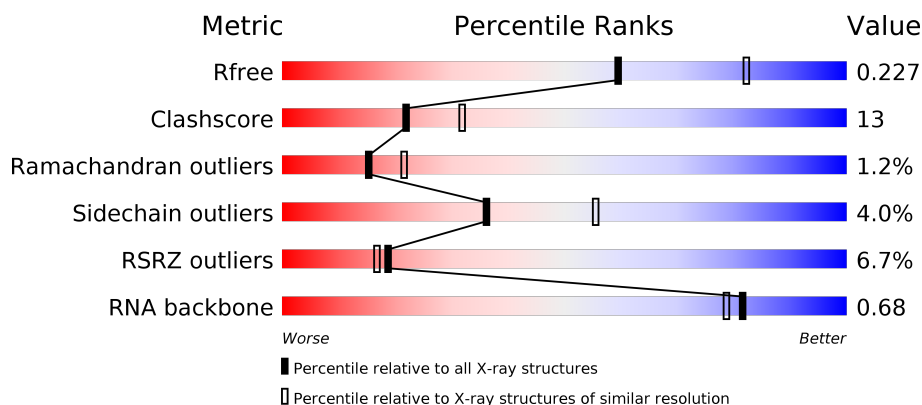
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)
RNA backbone	2435	1034 (2.86-1.94)

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	0	2922	<div> <div>3%</div> <div>65%</div> <div>24%</div> <div>6%</div> </div>
2	9	122	<div> <div>5%</div> <div>60%</div> <div>30%</div> <div>10%</div> </div>
3	A	240	<div> <div>5%</div> <div>63%</div> <div>30%</div> <div>5%</div> </div>
4	B	338	<div> <div>3%</div> <div>60%</div> <div>36%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	
31	3	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8517	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8523	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8534	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	R	8575	-	-	-	X
36	CL	M	8818	-	-	-	X
37	SR	0	8903	-	-	-	X
37	SR	0	8969	-	-	-	X
37	SR	0	8992	-	-	-	X
37	SR	A	8929	-	-	-	X
37	SR	B	8987	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99116 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 RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10873	19053	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	MODIFIED RESIDUE	GB 55229667
0	2099	A	G	ENGINEERED	GB 55229667
0	2587	OMU	U	MODIFIED RESIDUE	GB 55229667
0	2588	OMG	G	MODIFIED RESIDUE	GB 55229667
0	2619	UR3	U	MODIFIED RESIDUE	GB 55229667
0	2621	PSU	U	MODIFIED RESIDUE	GB 55229667

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

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

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

- Molecule 5 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

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

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

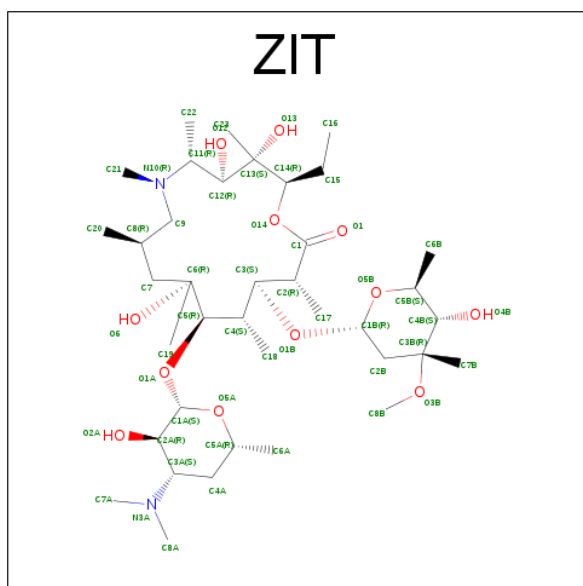
- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is AZITHROMYCIN (three-letter code: ZIT) (formula: $C_{38}H_{72}N_2O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	0	1	Total	C	N	O	0	0
			52	38	2	12		

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	86	Total	Mg	0	0
			86	86		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	2	Total K 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	65	Total Na 65 65	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	9	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	Y	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	94	Total 94	Sr 94	0	0
37	1	2	Total 2	Sr 2	0	0
37	H	1	Total 1	Sr 1	0	0
37	B	2	Total 2	Sr 2	0	0
37	3	1	Total 1	Sr 1	0	0
37	A	3	Total 3	Sr 3	0	0
37	R	1	Total 1	Sr 1	0	0
37	9	2	Total 2	Sr 2	0	0
37	S	1	Total 1	Sr 1	0	0
37	F	1	Total 1	Sr 1	0	0

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total 1	Cd 1	0	0
38	Z	1	Total 1	Cd 1	0	0
38	1	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	3	1	Total 1	Cd 1	0	0
38	U	1	Total 1	Cd 1	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5845	Total 5845	O 5845	0	0
39	9	145	Total 145	O 145	0	0
39	A	118	Total 118	O 118	0	0
39	B	151	Total 151	O 151	0	0
39	C	176	Total 176	O 176	0	0
39	D	49	Total 49	O 49	0	0
39	E	40	Total 40	O 40	0	0
39	F	26	Total 26	O 26	0	0
39	G	18	Total 18	O 18	0	0
39	H	72	Total 72	O 72	0	0
39	I	8	Total 8	O 8	0	0
39	J	59	Total 59	O 59	0	0
39	K	58	Total 58	O 58	0	0
39	L	72	Total 72	O 72	0	0
39	M	124	Total 124	O 124	0	0
39	N	61	Total 61	O 61	0	0
39	O	38	Total 38	O 38	0	0

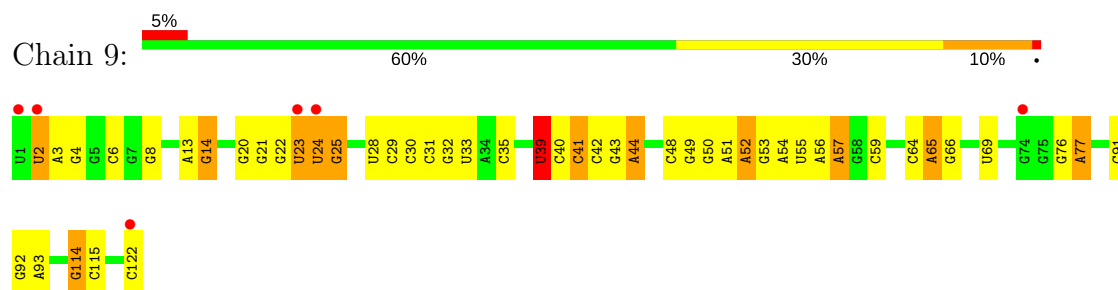
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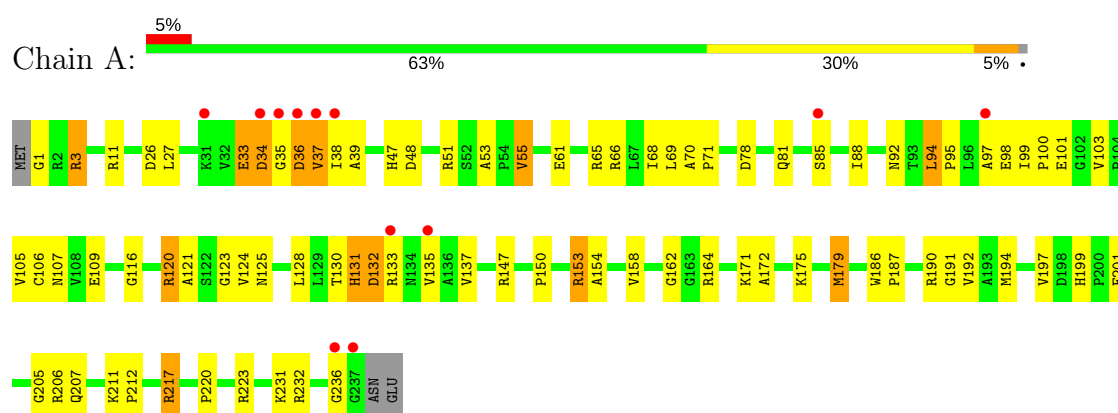
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	P	66	Total 66	O 66	0	0
39	Q	53	Total 53	O 53	0	0
39	R	87	Total 87	O 87	0	0
39	S	32	Total 32	O 32	0	0
39	T	41	Total 41	O 41	0	0
39	U	28	Total 28	O 28	0	0
39	V	12	Total 12	O 12	0	0
39	W	68	Total 68	O 68	0	0
39	X	24	Total 24	O 24	0	0
39	Y	95	Total 95	O 95	0	0
39	Z	32	Total 32	O 32	0	0
39	1	50	Total 50	O 50	0	0
39	2	44	Total 44	O 44	0	0
39	3	71	Total 71	O 71	0	0

G2884	C2780	A2649	U2527	U2435	C2309	A	G	G2014	G1753	U1625	G1452	G1300	C1196
G2781	U2761	U2652	C2533	G2442	C2313	C	A	A2015	A1754	A1626	G1458	U1304	G1197
A2783	G2782	A2653	C2534	C2443	G2317	A	U	G1926	A1755	G1627	A1458	C1305	A1199
C2787	A2783	U2661	G2537	U2444	G2317	U	G	C2031	C1762	A1630	A1470	U1306	C1201
U2791	C2787	A2664	C2541	U2445	C2317	A	C	U2032	C1766	A1634	C1474	A1307	C1202
A2792	U2791	A	C2542	G2453	A2321	A	A	U2034	U1766	A1641	C1477	U1314	G1203
C2793	C2792	U	C2543	A2456	A2326	U	C	C2036	C1768	A1642	C1477	U1314	C1204
G2794	G2793	G2667	G2544	U2457	C2326	A	U	G2044	C1769	A1642	G1484	A1328	U1205
U2796	U2795	G2670	C2547	G2462	G2336	C	U	A2054	G1773	A1653	G1497	U1333	A1206
A2800	C2796	U2671	C2548	G2465	G2337	U	A	G2054	U1777	U1654	G1497	C1334	C1207
U2800	U2800	U2672	C2552	A2466	G2338	A	G	U2064	C1777	A1656	U1500	C1335	C1209
G2807	U2807	U2673	A2553	A2467	A	C	U	G2072	A1778	A1657	U1503	C1342	G1210
C2809	C2808	C2676	C2559	A2468	C	C	G	G2073	A1779	A1658	U1504	C1343	C1212
G2810	U2809	A	U2563	C2472	A	U	A	A2081	G1786	G1665	A1504	G1216	G1216
A2811	C2810	G	C2564	C2476	A	U	A	G2074	C1787	C1666	U1505	G1217	U1218
A2812	A2811	G	C2565	C2477	C	C	G	A2091	C1798	U1668	U1506	U1219	U1219
A2813	A2812	A	G2570	C2478	C2346	U	U	G2090	G1809	U1677	U1524	C1360	C1229
G2814	C2813	A2694	G2578	U2478	G2344	U	G	G2091	U1678	A1678	A1526	A1230	A1230
A2815	U2814	G2697	U2578	A2479	A2345	A	U	A2096	U1679	C1679	A1527	G1363	C1234
C2816	C2815	G2698	C2578	C2483	A2346	C	C	A2097	A1682	U1528	A1528	C1366	U1234
G2817	A2816	G2712	U2586	A2484	A2361	U	A	C2098	U1683	A1529	G1529	G1235	G1235
C2818	C2817	G2716	U2587	A2485	A2362	C	G	G2101	A1684	C1535	G1535	U1236	U1236
A2819	C2818	C2717	C2588	A2486	A2363	A	A	G2102	A1685	C1536	C1536	A1372	U1237
C2820	U2819	G2718	U2589	A2488	A2364	G	G	A2103	U1686	G1555	G1555	C1377	C1238
G2825	C2820	A2719	U2590	G2489	A2369	U	U	C2104	C1687	U1840	G1559	G1378	C1239
U2827	G2825	C2720	C2591	A2490	A2372	C	C	G2110	C1692	A1845	U1561	C1384	A1242
G2828	C2827	U2721	G2592	U2491	U2372	C	A	U1972	G1697	U1846	C1562	U1244	C1243
C2831	A2830	G2723	C2601	U2492	C2373	C	C	A1973	U1700	C1853	C1564	A1393	G1245
U2840	C2831	G2724	G2602	C2493	G2379	U	U	G1976	C1700	C1856	C1564	C1394	A1246
A2841	U2840	G2725	U2607	C2498	A2382	C	C	U1977	U1701	A1857	A1573	G1398	U1249
G2842	C2841	U2726	C2608	U2499	A2387	C	C	A1978	U1702	C1857	C1574	A1399	C1250
G2851	U2842	G2740	U2613	C2502	A2401	U	U	G1980	A1717	A1407	C1574	A1406	C1251
A2852	C2851	A2741	G2613	A2503	C2403	A	A	U1985	U1722	U1408	G1589	A1407	A1252
G2862	G2852	G2747	C2626	G2505	A2412	G	G	U1992	G1723	C1593	G1593	U1408	C1253
C2863	U2862	U2748	G2627	A2506	G2413	C	C	U1996	U1724	C1594	C1594	G1417	G1268
U2864	C2863	G2750	C2630	C2507	A2414	G	G	A1997	C1725	C1594	C1594	G1417	G1269
G2865	U2864	C2751	U2631	A2509	A2415	C	C	U2003	G1730	C1597	C1597	U1418	U1279
U2866	C2865	G2754	G2632	C2510	G2416	A	A	U2004	G1731	U1596	U1596	U1419	A1278
G2867	U2866	G2755	A2633	C2511	G2417	C	C	G2005	A1732	A1597	A1597	C1420	U1287
C2868	G2867	U2756	G2634	C2515	U2419	C	C	U2008	G1877	A1598	A1598	A1426	C1288
G2869	U2868	C2762	A2635	G2516	G2420	C	C	G	U1879	A1604	A1604	C1439	G1290
C2876	C2869	A2768	G2636	U2422	G2421	A	A	U	C1882	G1740	G1604	A1291	A1291
G2877	U2876	C2769	A2637	G2422	A2291	C	C	C	G1882	U1741	G1605	U1440	G1295
U2878	C2877	G2770	G2638	G2426	A2300	C	C	U2011	G1902	A1742	A1615	A1442	G1299
A2879	U2878	C2771	G2642	C2427	A2301	A	A	G	U1903	A1919			
C2883	G2882	G2779	G2643	G2428	A2302	C	C	C	A1919				

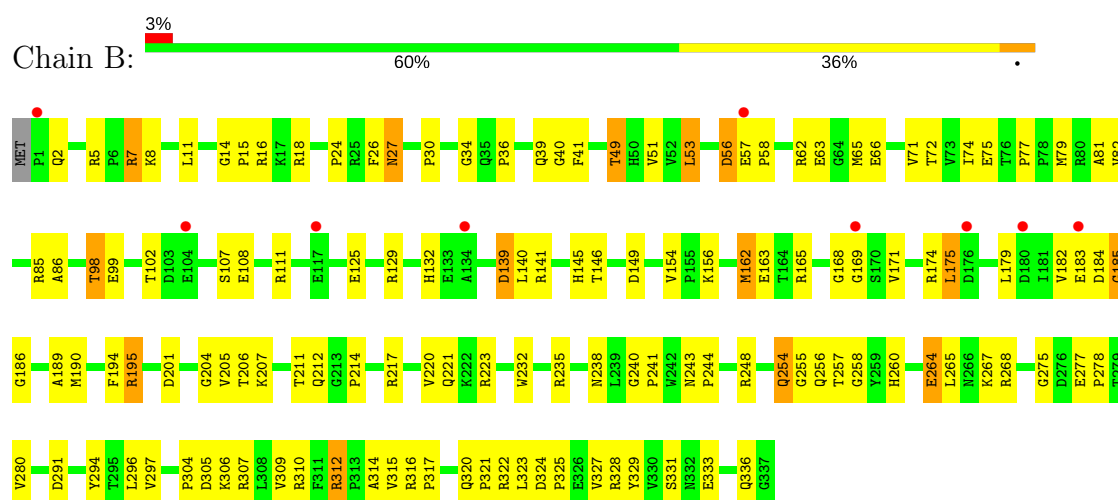
- Molecule 2: 5S Ribosomal RNA



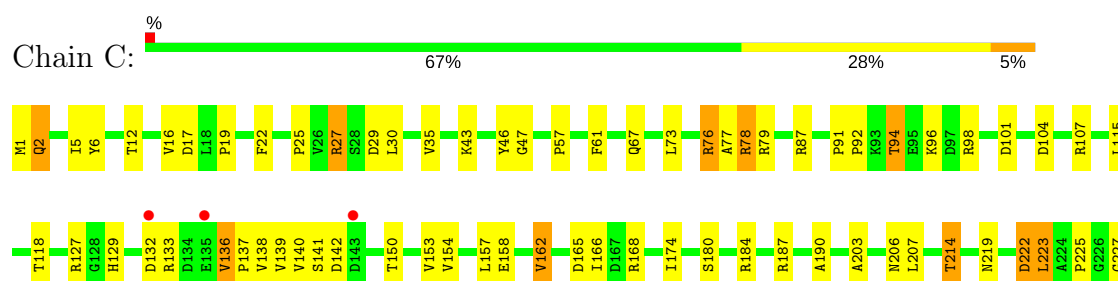
- Molecule 3: 50S ribosomal protein L2P

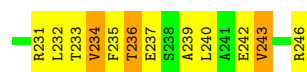


- Molecule 4: 50S ribosomal protein L3P

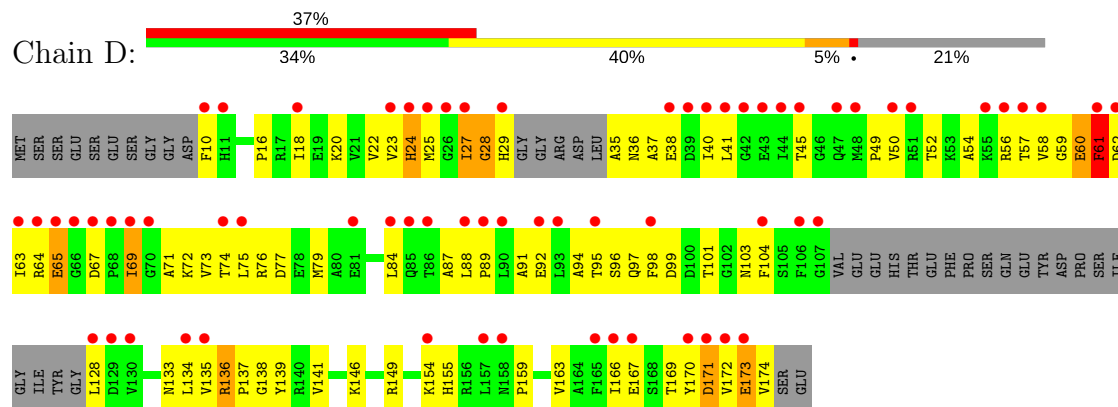


- Molecule 5: 50S ribosomal protein L4E

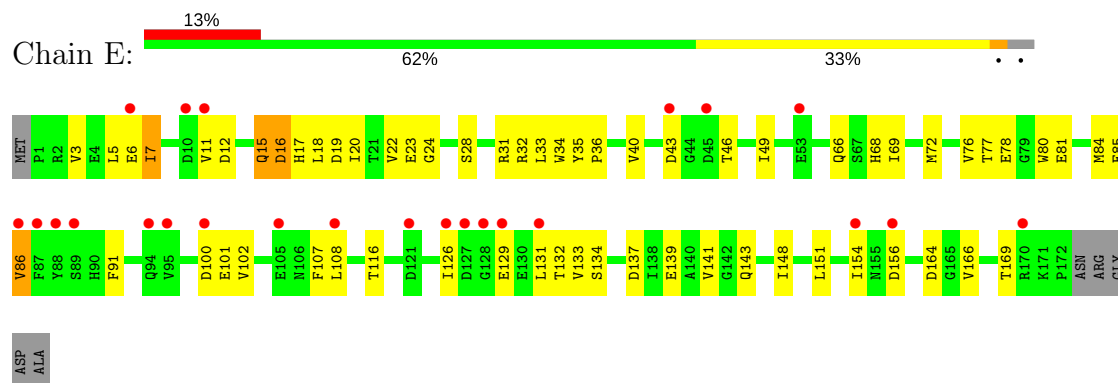




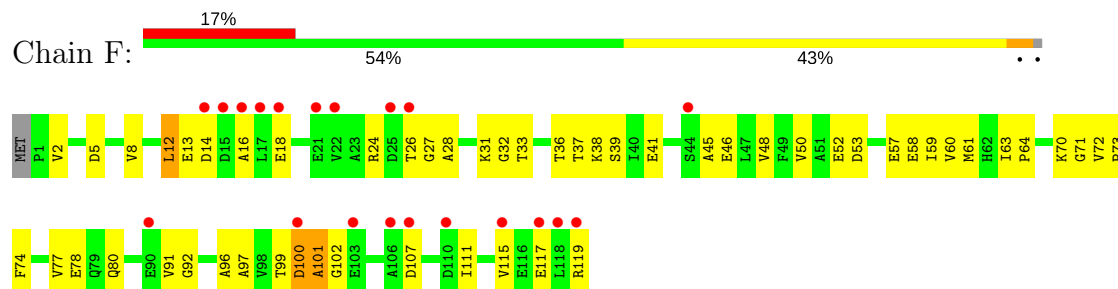
• Molecule 6: 50S ribosomal protein L5P



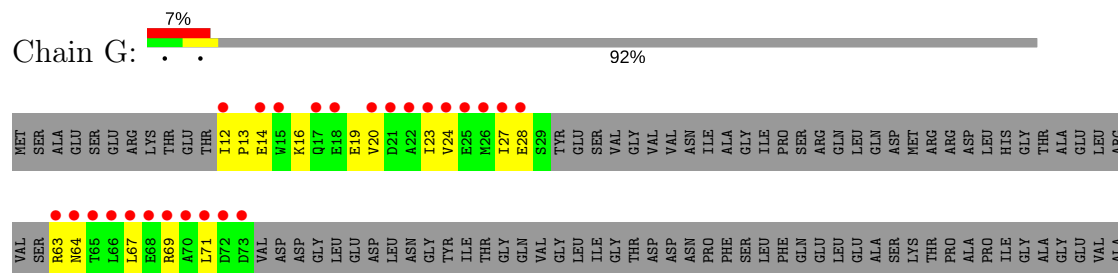
• Molecule 7: 50S ribosomal protein L6P

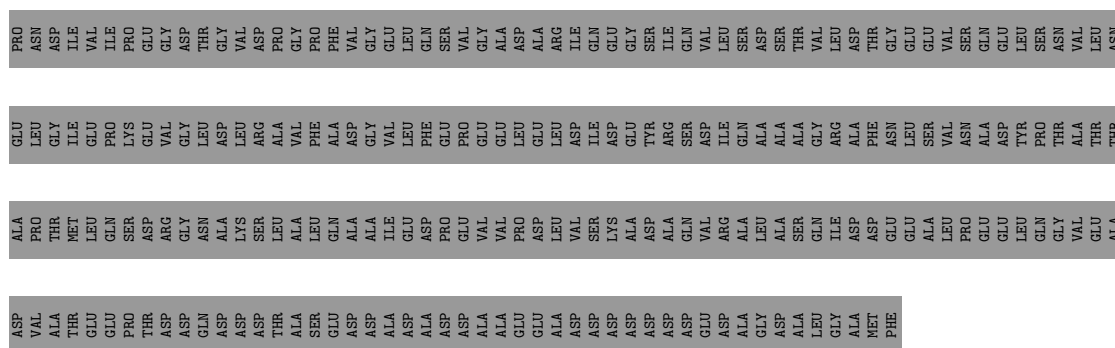


• Molecule 8: 50S ribosomal protein L7AE

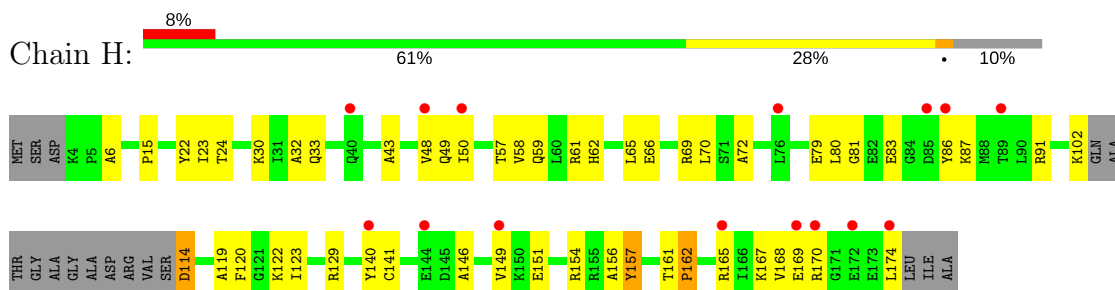


• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

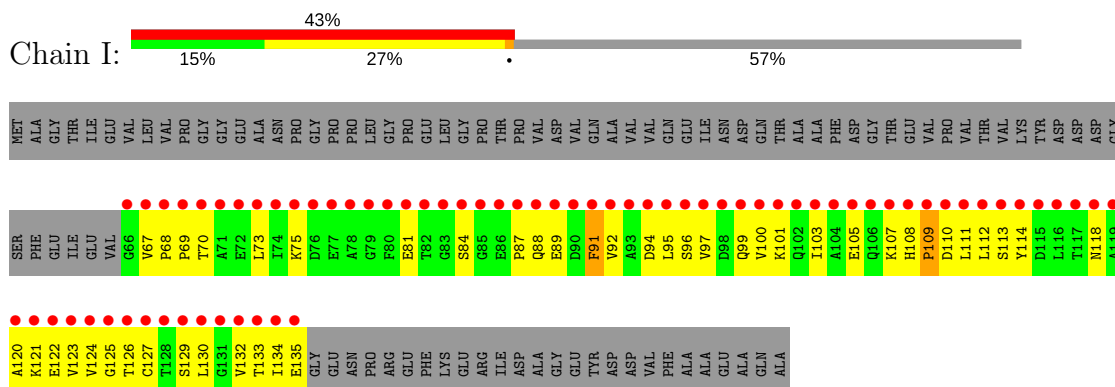




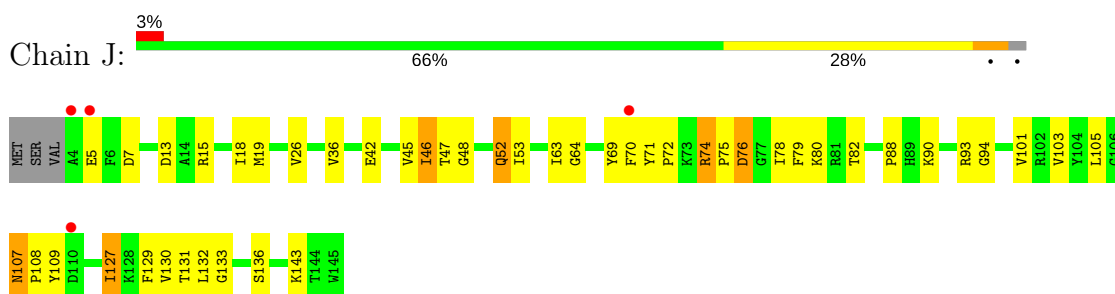
- Molecule 10: 50S RIBOSOMAL PROTEIN L10E



- Molecule 11: 50S RIBOSOMAL PROTEIN L11P

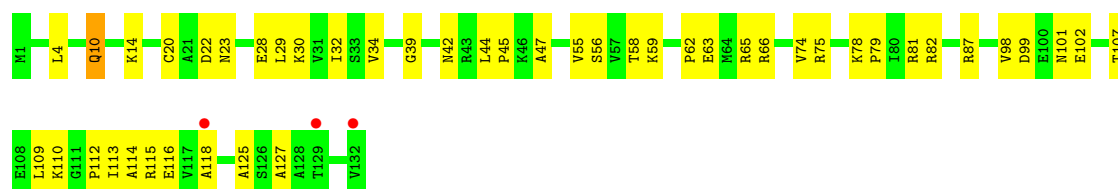


- Molecule 12: 50S ribosomal protein L13P

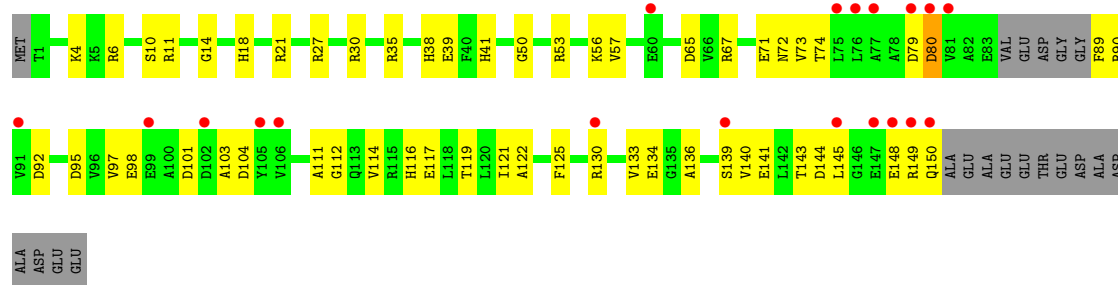


- Molecule 13: 50S ribosomal protein L14P

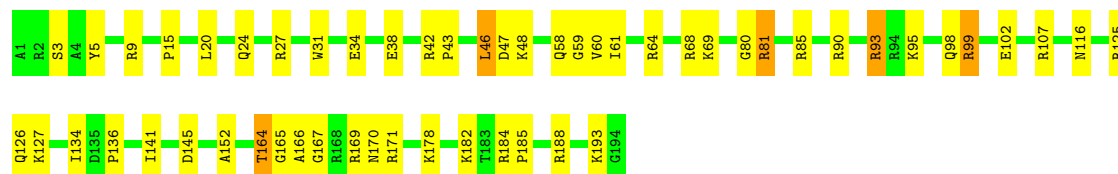




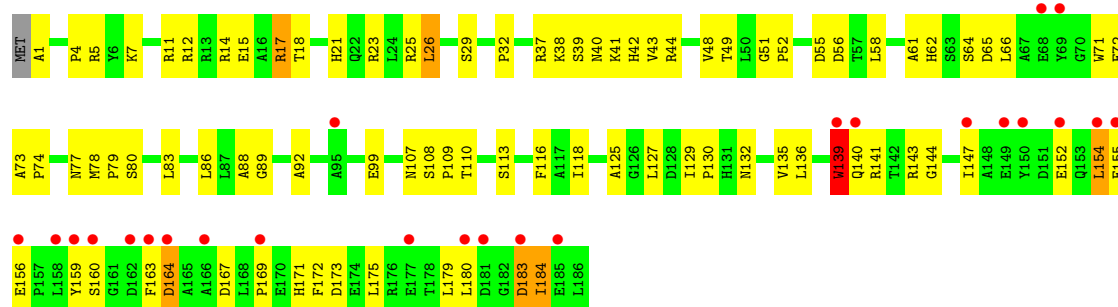
• Molecule 14: 50S ribosomal protein L15P



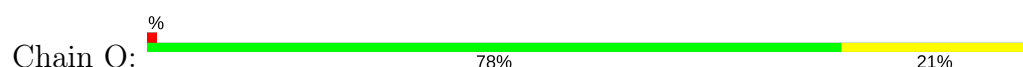
• Molecule 15: 50S Ribosomal Protein L15E



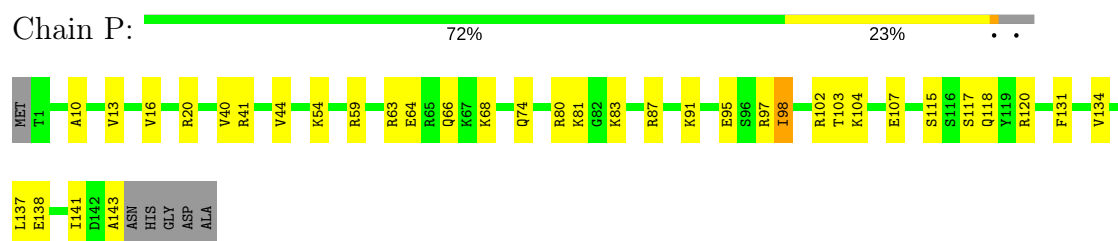
• Molecule 16: 50S ribosomal protein L18P



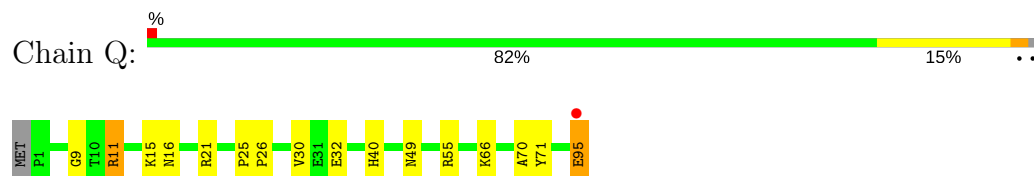
• Molecule 17: 50S ribosomal protein L18e



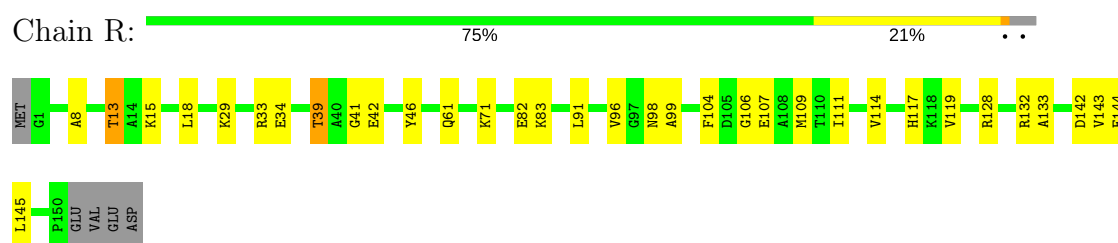
- Molecule 18: 50S ribosomal protein L19E



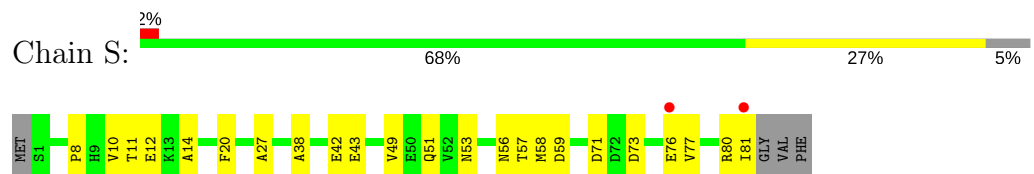
- Molecule 19: 50S ribosomal protein L21e



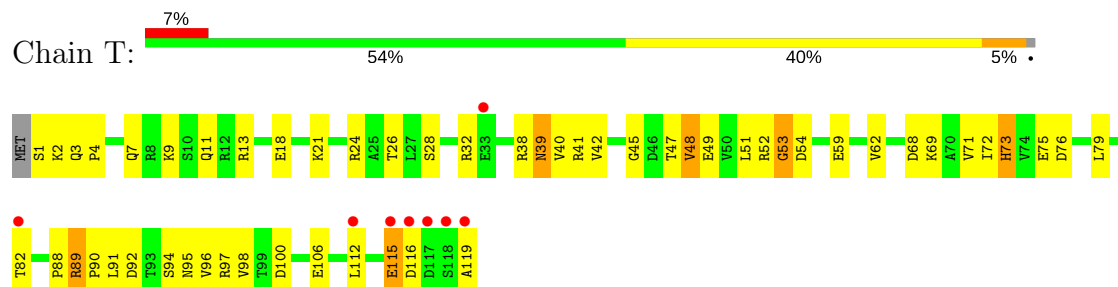
- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P

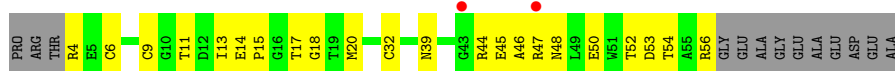


- Molecule 22: 50S ribosomal protein L24P

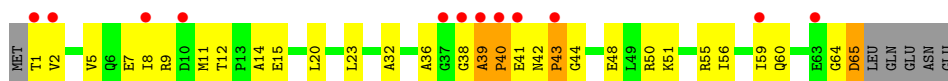


- Molecule 23: 50S ribosomal protein L24E





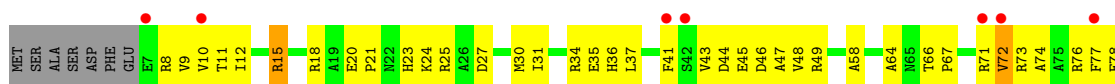
• Molecule 24: 50S ribosomal protein L29P



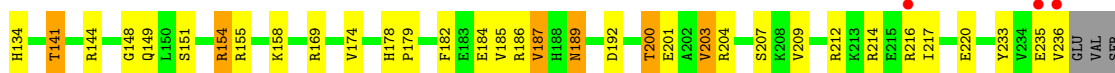
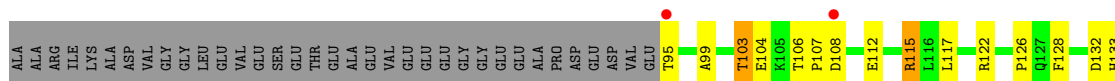
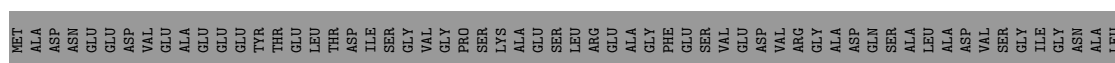
• Molecule 25: 50S ribosomal protein L30P



• Molecule 26: 50S ribosomal protein L31e



• Molecule 27: 50S ribosomal protein L32E



• Molecule 28: 50S ribosomal protein L37Ae





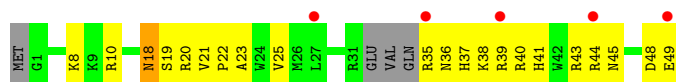
- Molecule 29: 50S ribosomal protein L37e

Chain 1: 70% 28%



- Molecule 30: 50S ribosomal protein L39e

Chain 2: 10% 50% 40% 8%



- Molecule 31: 50S ribosomal protein L44E

Chain 3: 2% 68% 32%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.08Å 298.91Å 574.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.40 49.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (29.96-2.40) 90.2 (49.82-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.229 0.190 , 0.227	Depositor DCC
R_{free} test set	6150 reflections (0.98%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.8	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	0.95	EDS
Total number of atoms	99116	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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, ZIT, 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	0	0.35	0/65957	0.69	25/102867 (0.0%)
2	9	0.32	0/2904	0.70	1/4526 (0.0%)
3	A	0.33	0/1786	0.66	0/2408
4	B	0.31	0/2690	0.64	0/3652
5	C	0.37	0/1884	0.64	0/2551
6	D	0.29	0/1111	0.53	0/1498
7	E	0.31	0/1382	0.57	0/1880
8	F	0.31	0/901	0.55	0/1224
9	G	0.27	0/241	0.47	0/324
10	H	0.35	0/1302	0.65	0/1743
11	I	0.28	0/526	0.48	0/716
12	J	0.34	0/1136	0.59	0/1530
13	K	0.33	0/1001	0.65	0/1347
14	L	0.32	0/1130	0.64	0/1509
15	M	0.33	0/1582	0.61	0/2117
16	N	0.28	0/1474	0.60	0/1999
17	O	0.32	0/874	0.59	0/1181
18	P	0.32	0/1147	0.53	0/1528
19	Q	0.34	0/749	0.69	0/1005
20	R	0.34	0/1172	0.64	0/1578
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.30	0/958	0.62	0/1289
23	U	0.32	0/417	0.53	0/562
24	V	0.29	0/502	0.53	0/675
25	W	0.33	0/1219	0.62	0/1655
26	X	0.31	0/664	0.56	0/895
27	Y	0.34	0/1146	0.62	0/1536
28	Z	0.34	0/589	0.64	0/787
29	1	0.40	0/438	0.64	0/578
30	2	0.33	0/401	0.55	0/529
31	3	0.36	0/771	0.58	0/1024
All	All	0.34	0/98702	0.67	27/147588 (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
1	0	0	53
2	9	0	2
All	All	0	55

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1942	A	C5'-C4'-C3'	8.34	129.34	116.00
1	0	871	G	C5'-C4'-O4'	-7.87	99.66	109.10
2	9	39	U	N1-C1'-C2'	6.90	122.97	114.00
1	0	1979	G	C2'-C3'-O3'	6.61	124.27	113.70
1	0	1504	A	C1'-O4'-C4'	-6.48	104.71	109.90
1	0	2316	G	C5'-C4'-C3'	-6.23	106.04	116.00
1	0	1559	A	C2'-C3'-O3'	6.21	123.64	113.70
1	0	1819	G	C5'-C4'-C3'	6.18	125.89	116.00
1	0	1592	G	N9-C1'-C2'	6.17	122.02	114.00
1	0	206	G	C5'-C4'-C3'	-6.11	106.22	116.00
1	0	2291	A	N9-C1'-C2'	6.06	121.88	114.00
1	0	2726	U	N1-C1'-C2'	5.79	121.53	114.00
1	0	2313	C	C5'-C4'-O4'	5.77	116.03	109.10
1	0	2467	A	C1'-O4'-C4'	-5.72	105.32	109.90
1	0	1120	U	C5'-C4'-C3'	-5.62	107.02	116.00
1	0	777	U	O4'-C1'-N1	5.49	112.59	108.20
1	0	1504	A	N9-C1'-C2'	5.42	121.05	114.00
21	S	27	ALA	N-CA-C	-5.38	96.48	111.00
1	0	1942	A	C4'-C3'-C2'	-5.37	97.23	102.60
1	0	1819	G	C1'-O4'-C4'	-5.32	105.65	109.90
1	0	1829	A	N9-C1'-C2'	-5.31	106.16	112.00
1	0	841	A	C1'-O4'-C4'	-5.29	105.67	109.90
1	0	1452	G	C5'-C4'-C3'	-5.17	107.72	116.00
1	0	2607	U	N1-C1'-C2'	5.14	120.68	114.00
1	0	69	A	C5'-C4'-O4'	-5.13	102.95	109.10
1	0	2313	C	C5'-C4'-C3'	5.08	124.13	116.00
1	0	129	A	C2'-C3'-O3'	5.05	121.78	113.70

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1237	U	Sidechain
1	0	1342	C	Sidechain
1	0	1417	G	Sidechain
1	0	1458	A	Sidechain
1	0	1592	G	Sidechain
1	0	1653	A	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1985	U	Sidechain
1	0	221	G	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	246	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2681	A	Sidechain
1	0	270	U	Sidechain
1	0	2842	G	Sidechain
1	0	324	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	417	G	Sidechain
1	0	460	A	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	792	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	881	C	Sidechain
1	0	888	U	Sidechain
1	0	893	C	Sidechain
2	9	39	U	Sidechain
2	9	65	A	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	0	59020	0	29808	686	0
2	9	2599	0	1325	53	0
3	A	1753	0	1766	109	0
4	B	2625	0	2533	125	0
5	C	1859	0	1816	97	0
6	D	1094	0	1085	91	0
7	E	1357	0	1266	55	0
8	F	890	0	843	51	0
9	G	240	0	231	18	0
10	H	1282	0	1292	53	0
11	I	519	0	500	47	0
12	J	1120	0	1098	58	0
13	K	992	0	1031	56	0
14	L	1118	0	1076	52	0
15	M	1558	0	1566	63	0
16	N	1445	0	1401	100	0
17	O	865	0	873	30	0
18	P	1136	0	1123	34	0
19	Q	735	0	728	14	0
20	R	1149	0	1122	41	0
21	S	641	0	605	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	950	0	923	51	0
23	U	410	0	364	24	0
24	V	499	0	511	35	0
25	W	1196	0	1137	88	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	58	0
28	Z	578	0	539	19	0
29	1	431	0	426	22	0
30	2	396	0	413	25	0
31	3	755	0	728	24	0
32	0	52	0	72	0	0
33	0	86	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	65	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	94	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	9	2	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5845	0	0	120	0
39	1	50	0	0	2	0
39	2	44	0	0	3	0
39	3	71	0	0	5	0
39	9	145	0	0	4	0
39	A	118	0	0	19	0
39	B	151	0	0	25	0
39	C	176	0	0	24	0
39	D	49	0	0	19	0
39	E	40	0	0	5	0
39	F	26	0	0	7	0
39	G	18	0	0	2	0
39	H	72	0	0	12	0
39	I	8	0	0	2	0
39	J	59	0	0	2	0
39	K	58	0	0	7	0
39	L	72	0	0	15	0
39	M	124	0	0	8	0
39	N	61	0	0	12	0
39	O	38	0	0	6	0
39	P	66	0	0	4	0
39	Q	53	0	0	4	0
39	R	87	0	0	7	0
39	S	32	0	0	3	0
39	T	41	0	0	4	0
39	U	28	0	0	3	0
39	V	12	0	0	2	0
39	W	68	0	0	7	0
39	X	24	0	0	8	0
39	Y	95	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	Z	32	0	0	2	0
All	All	99116	0	59987	2007	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (2007) 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)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.18	1.10
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.32	1.09
5:C:236:THR:HG22	5:C:239:ALA:H	1.10	1.06
6:D:25:MET:HE3	6:D:37:ALA:HB1	1.34	1.04
1:0:1242:A:H5'	12:J:82:THR:HG23	1.39	1.04
2:9:6:C:H5''	16:N:37:ARG:NH1	1.74	1.03
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.41	1.01
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.45	0.99
1:0:156:C:H5''	15:M:171:ARG:HD3	1.43	0.99
18:P:115:SER:H	18:P:118:GLN:HE21	1.09	0.99
6:D:154:LYS:HD2	6:D:154:LYS:H	1.27	0.98
1:0:871:G:C8	1:0:871:G:H5'	1.97	0.98
5:C:78:ARG:HG3	5:C:78:ARG:HH11	1.28	0.97
2:9:76:G:H3'	2:9:77:A:H5''	1.47	0.95
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.46	0.95
2:9:56:A:H2'	2:9:57:A:H5''	1.46	0.95
15:M:164:THR:HG22	15:M:167:GLY:H	1.32	0.95
4:B:140:LEU:HA	39:B:9048:HOH:O	1.65	0.95
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.82	0.94
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.07	0.94
4:B:86:ALA:HA	39:B:9048:HOH:O	1.68	0.93
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.50	0.93
1:0:871:G:H8	1:0:871:G:H5'	1.30	0.93
12:J:19:MET:HE3	12:J:132:LEU:HD21	1.50	0.92
16:N:144:GLY:O	16:N:147:ILE:HG22	1.68	0.92
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.69	0.92
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.50	0.92
25:W:88:THR:HB	39:W:6679:HOH:O	1.70	0.92
1:0:541:C:H2'	1:0:542:A:H5''	1.52	0.92
30:2:41:HIS:H	30:2:45:ASN:HD22	1.12	0.91
13:K:10:GLN:H	13:K:10:GLN:NE2	1.67	0.91
6:D:57:THR:HG23	6:D:63:ILE:HA	1.52	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:162:MET:HE2	4:B:310:ARG:HD3	1.51	0.91
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.91
1:0:542:A:H5'	1:0:542:A:H8	1.34	0.91
21:S:57:THR:HG22	21:S:59:ASP:H	1.36	0.90
1:0:870:G:H2'	1:0:871:G:H5''	1.51	0.90
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.51	0.90
1:0:2717:C:C2'	1:0:2718:C:H5''	2.02	0.90
13:K:10:GLN:N	13:K:10:GLN:HE21	1.70	0.89
1:0:2717:C:H2'	1:0:2718:C:H5''	1.54	0.89
4:B:238:ASN:HD22	4:B:240:GLY:H	1.18	0.89
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.73	0.89
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.53	0.89
1:0:2812:A:H2	1:0:2814:A:H62	1.19	0.89
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.36	0.88
6:D:28:GLY:HA2	6:D:69:ILE:HG23	1.56	0.88
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.88	0.88
3:A:35:GLY:O	3:A:36:ASP:HB3	1.71	0.88
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.38	0.88
1:0:1160:G:C5'	1:0:1161:A:H5'	2.03	0.88
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.54	0.88
1:0:1160:G:H5'	1:0:1161:A:C5'	2.04	0.87
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.54	0.87
25:W:122:ARG:NH2	25:W:154:ARG:HB3	1.90	0.87
1:0:2506:A:HO2'	1:0:2507:G:H8	0.89	0.87
2:9:6:C:H5''	16:N:37:ARG:HH12	1.37	0.87
10:H:49:GLN:HE21	10:H:140:TYR:HE2	1.21	0.87
1:0:1835:U:H5	1:0:1840:A:N7	1.73	0.86
24:V:1:THR:HG23	24:V:2:VAL:H	1.40	0.86
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.57	0.86
11:I:127:CYS:HB3	11:I:132:VAL:HB	1.58	0.86
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.04	0.85
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.75	0.85
1:0:960:G:H4'	39:0:7859:HOH:O	1.75	0.85
18:P:115:SER:OG	18:P:118:GLN:HG3	1.77	0.85
31:3:65:THR:HG22	31:3:67:LEU:HG	1.59	0.85
3:A:199:HIS:HD2	3:A:201:PHE:H	1.23	0.85
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.39	0.84
1:0:282:C:H1'	1:0:368:C:N4	1.92	0.84
5:C:236:THR:HG22	5:C:239:ALA:N	1.92	0.84
25:W:137:GLN:HE21	25:W:141:HIS:CE1	1.95	0.84
10:H:170:ARG:HD2	39:H:8989:HOH:O	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:10:GLN:H	13:K:10:GLN:HE21	0.88	0.84
1:0:1116:U:HO2'	1:0:1118:A:H2	0.83	0.83
1:0:2716:G:H5''	4:B:206:THR:HG21	1.60	0.83
8:F:58:GLU:HA	8:F:61:MET:HE2	1.58	0.83
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.41	0.83
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.60	0.83
3:A:192:VAL:HG22	39:A:9095:HOH:O	1.77	0.83
17:O:42:GLU:HB2	39:O:2176:HOH:O	1.78	0.83
1:0:1667:A:H8	1:0:1667:A:H5'	1.41	0.83
1:0:1701:A:H4'	1:0:1702:U:H5''	1.60	0.83
1:0:1041:U:H5'	39:L:8881:HOH:O	1.77	0.82
1:0:506:G:H22	1:0:509:A:H5''	1.42	0.82
3:A:211:LYS:HB2	39:A:9081:HOH:O	1.78	0.82
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.60	0.82
1:0:1474:C:H6	1:0:1474:C:H5'	1.43	0.82
1:0:541:C:C2'	1:0:542:A:H5''	2.09	0.81
11:I:97:VAL:HG12	11:I:101:LYS:HE3	1.59	0.81
16:N:113:SER:HB2	39:N:8856:HOH:O	1.78	0.81
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.46	0.81
1:0:1300:G:H1'	39:O:5149:HOH:O	1.79	0.81
27:Y:187:VAL:HG23	39:Y:8869:HOH:O	1.79	0.81
3:A:153:ARG:HH11	3:A:153:ARG:HB2	1.45	0.81
11:I:73:LEU:HD12	11:I:107:LYS:HZ2	1.46	0.81
1:0:2890:A:H1'	23:U:56:ARG:NH2	1.96	0.80
1:0:1973:A:H5'	1:0:1973:A:H8	1.45	0.80
39:9:9098:HOH:O	16:N:23:ARG:HD3	1.80	0.80
28:Z:10:ARG:HA	39:Z:8714:HOH:O	1.79	0.80
1:0:2054:A:N3	20:R:128:ARG:NH2	2.30	0.80
1:0:2840:A:OP1	4:B:211:THR:HG23	1.82	0.80
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.46	0.79
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.96	0.79
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.63	0.79
1:0:656:G:H5'	17:O:3:THR:HG22	1.64	0.79
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.65	0.79
1:0:2586:U:H3	1:0:2592:G:H22	1.28	0.78
1:0:2488:A:H61	1:0:2534:C:H42	1.32	0.78
3:A:192:VAL:HB	39:A:9056:HOH:O	1.82	0.78
5:C:1:MET:HG2	5:C:2:GLN:H	1.46	0.78
5:C:242:GLU:HG3	39:C:8586:HOH:O	1.84	0.78
1:0:1116:U:O2'	1:0:1118:A:H2	1.65	0.78
29:1:25:LYS:HD2	30:2:49:GLU:H	1.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:91:VAL:HG12	8:F:92:GLY:N	1.98	0.78
14:L:133:VAL:HA	39:L:8865:HOH:O	1.84	0.78
11:I:73:LEU:HD12	11:I:107:LYS:NZ	1.97	0.78
25:W:88:THR:HG23	25:W:110:GLN:NE2	1.97	0.78
10:H:59:GLN:HE21	10:H:129:ARG:HE	1.30	0.77
3:A:51:ARG:HB2	39:A:9068:HOH:O	1.83	0.77
12:J:76:ASP:HA	39:J:5907:HOH:O	1.85	0.77
4:B:62:ARG:HA	4:B:65:MET:CE	2.15	0.77
4:B:179:LEU:O	4:B:183:GLU:HG2	1.84	0.77
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.20	0.77
39:O:5298:HOH:O	12:J:47:THR:HB	1.84	0.77
24:V:42:ASN:HB3	39:V:7247:HOH:O	1.85	0.77
1:O:1116:U:H3	1:O:1246:A:H62	1.33	0.76
1:O:2506:A:O2'	1:O:2507:G:H8	1.68	0.76
7:E:100:ASP:HB2	39:E:2789:HOH:O	1.85	0.76
1:O:1878:G:H1'	39:O:6568:HOH:O	1.85	0.76
5:C:236:THR:CG2	5:C:239:ALA:H	1.95	0.76
1:O:381:G:H5''	39:O:4785:HOH:O	1.84	0.76
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.15	0.76
1:O:544:G:H2'	1:O:545:G:H5''	1.67	0.76
1:O:871:G:H8	1:O:871:G:C5'	1.99	0.76
2:9:14:G:H5'	2:9:14:G:H8	1.51	0.76
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.67	0.76
8:F:91:VAL:HG12	8:F:92:GLY:H	1.48	0.76
10:H:30:LYS:H	10:H:62:HIS:HD2	1.31	0.76
1:O:559:U:H5'	1:O:559:U:H6	1.51	0.76
10:H:59:GLN:NE2	10:H:129:ARG:HE	1.83	0.75
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.16	0.75
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.83	0.75
20:R:39:THR:HB	20:R:42:GLU:HG3	1.68	0.75
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.68	0.75
4:B:62:ARG:HA	4:B:65:MET:HE2	1.68	0.75
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.67	0.75
3:A:194:MET:HE1	3:A:199:HIS:HB2	1.68	0.75
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.69	0.75
27:Y:212:ARG:HD2	39:Y:8899:HOH:O	1.86	0.75
1:O:870:G:C2'	1:O:871:G:H5''	2.17	0.74
4:B:162:MET:CE	4:B:310:ARG:HD3	2.17	0.74
1:O:1206:U:H6	1:O:1206:U:H5'	1.52	0.74
1:O:236:A:H4'	1:O:237:G:H5'	1.69	0.74
3:A:199:HIS:CD2	3:A:201:PHE:H	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.68	0.74
21:S:57:THR:HG22	21:S:59:ASP:N	2.01	0.74
1:0:506:G:H22	1:0:509:A:C5'	2.01	0.74
5:C:140:VAL:HB	39:C:8656:HOH:O	1.88	0.74
1:0:545:G:H8	1:0:545:G:H5'	1.51	0.74
2:9:56:A:C2'	2:9:57:A:H5''	2.18	0.74
5:C:139:VAL:HG13	39:C:8653:HOH:O	1.86	0.74
1:0:1183:C:H2'	39:0:6690:HOH:O	1.87	0.74
3:A:36:ASP:OD2	3:A:85:SER:HB2	1.88	0.74
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.70	0.74
1:0:1372:A:H3'	39:0:7622:HOH:O	1.88	0.74
4:B:16:ARG:NH1	39:B:9084:HOH:O	2.20	0.74
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.70	0.74
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.88	0.73
5:C:236:THR:HG21	39:C:8579:HOH:O	1.85	0.73
6:D:25:MET:HE1	6:D:41:LEU:HG	1.69	0.73
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.18	0.73
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.70	0.73
1:0:1819:G:H2'	1:0:1820:G:H4'	1.71	0.73
3:A:48:ASP:HB3	39:A:9068:HOH:O	1.89	0.73
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.71	0.73
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.92	0.73
1:0:93:C:H5''	24:V:1:THR:HB	1.69	0.73
39:0:6936:HOH:O	27:Y:141:THR:HG23	1.86	0.73
1:0:2908:A:H2'	1:0:2909:G:O4'	1.89	0.72
4:B:221:GLN:HE22	13:K:42:ASN:HD22	1.33	0.72
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.71	0.72
12:J:107:ASN:ND2	12:J:109:TYR:H	1.86	0.72
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.72	0.72
1:0:2570:G:H5''	39:0:5371:HOH:O	1.88	0.72
1:0:2291:A:C8	1:0:2309:C:H5'	2.25	0.72
1:0:450:C:OP1	5:C:184:ARG:NH2	2.22	0.72
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.69	0.72
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.04	0.72
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.72	0.72
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.71	0.72
25:W:125:HIS:HD2	25:W:127:GLY:H	1.36	0.72
1:0:2896:A:H5''	39:0:6546:HOH:O	1.89	0.71
8:F:96:ALA:HA	39:F:3111:HOH:O	1.89	0.71
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.21	0.71
17:O:32:ARG:HD3	17:O:32:ARG:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:962:C:H1'	16:N:5:ARG:NH1	2.05	0.71
1:0:1603:A:H5'	1:0:1605:G:O4'	1.91	0.71
2:9:29:C:H2'	2:9:30:C:H5'	1.73	0.71
21:S:43:GLU:HB3	39:S:8990:HOH:O	1.90	0.71
1:0:1666:C:O2'	1:0:1667:A:H5''	1.91	0.71
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.21	0.71
1:0:481:U:H5''	39:0:6102:HOH:O	1.91	0.70
1:0:111:C:O2'	29:1:20:ARG:HG2	1.92	0.70
3:A:223:ARG:HG3	39:A:9064:HOH:O	1.91	0.70
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.73	0.70
1:0:877:G:H5'	1:0:878:G:OP1	1.92	0.70
39:0:4698:HOH:O	30:2:38:LYS:HE3	1.90	0.70
4:B:275:GLY:O	4:B:291:ASP:HA	1.91	0.70
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.73	0.70
2:9:39:U:H1'	2:9:44:A:H61	1.55	0.70
3:A:164:ARG:NE	39:A:9050:HOH:O	2.24	0.70
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.73	0.70
16:N:164:ASP:CG	16:N:167:ASP:HA	2.11	0.70
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.73	0.70
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.74	0.70
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.73	0.70
1:0:1184:C:H1'	39:0:7891:HOH:O	1.90	0.70
1:0:542:A:H5'	1:0:542:A:C8	2.23	0.70
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.74	0.70
1:0:541:C:H2'	1:0:542:A:C5'	2.21	0.70
1:0:244:C:OP2	8:F:38:LYS:HE3	1.91	0.70
12:J:45:VAL:HG23	12:J:130:VAL:O	1.91	0.70
6:D:128:LEU:HB2	39:D:6007:HOH:O	1.90	0.70
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.72	0.70
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.91	0.70
12:J:74:ARG:CB	12:J:74:ARG:HH11	2.05	0.70
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.06	0.70
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.20	0.70
1:0:2635:A:O2'	1:0:2636:C:H5'	1.92	0.70
8:F:13:GLU:OE2	8:F:78:GLU:HG2	1.90	0.70
2:9:49:G:H5''	39:N:8845:HOH:O	1.92	0.69
4:B:238:ASN:HD22	4:B:240:GLY:N	1.90	0.69
1:0:281:U:H2'	1:0:282:C:O4'	1.91	0.69
10:H:102:LYS:HD3	10:H:122:LYS:HD3	1.74	0.69
10:H:32:ALA:HB3	10:H:69:ARG:HH12	1.55	0.69
1:0:1701:A:H5'	39:0:6730:HOH:O	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2748:G:H2'	39:0:7963:HOH:O	1.91	0.69
20:R:39:THR:HG23	20:R:107:GLU:O	1.93	0.69
8:F:58:GLU:OE1	15:M:27:ARG:NH2	2.25	0.69
1:0:2533:C:H5'	1:0:2533:C:H6	1.58	0.69
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.58	0.69
2:9:6:C:OP1	16:N:37:ARG:NH1	2.25	0.69
1:0:1593:C:OP1	18:P:117:SER:HB3	1.93	0.69
1:0:796:A:HO2'	28:Z:10:ARG:N	1.91	0.69
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.28	0.69
16:N:80:SER:HB2	39:N:8835:HOH:O	1.92	0.69
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.28	0.69
1:0:1118:A:H3'	1:0:1118:A:C8	2.28	0.68
1:0:1118:A:H3'	1:0:1118:A:H8	1.58	0.68
1:0:2468:A:H61	31:3:48:ASN:HD21	1.40	0.68
1:0:1666:C:H2'	1:0:1667:A:H5'	1.75	0.68
4:B:58:PRO:HA	4:B:63:GLU:OE1	1.92	0.68
14:L:148:GLU:HA	39:L:8864:HOH:O	1.93	0.68
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.76	0.68
4:B:190:MET:HE2	4:B:194:PHE:HD1	1.59	0.68
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.29	0.68
6:D:146:LYS:NZ	16:N:107:ASN:HD21	1.92	0.68
8:F:2:VAL:HG22	8:F:57:GLU:OE1	1.94	0.68
10:H:6:ALA:HA	10:H:61:ARG:HH12	1.58	0.68
16:N:17:ARG:HB3	16:N:17:ARG:HH11	1.57	0.68
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.01	0.67
1:0:1119:G:N2	1:0:1246:A:C2	2.58	0.67
1:0:272:A:H3'	39:0:7953:HOH:O	1.93	0.67
24:V:12:THR:HG22	24:V:15:GLU:CG	2.24	0.67
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.25	0.67
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.07	0.67
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.76	0.67
1:0:657:G:OP1	5:C:27:ARG:NH2	2.27	0.67
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.30	0.67
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.95	0.67
1:0:1701:A:H4'	1:0:1702:U:C5'	2.25	0.67
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.74	0.67
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.07	0.67
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.24	0.67
10:H:6:ALA:HA	10:H:61:ARG:NH1	2.09	0.67
27:Y:115:ARG:NE	39:Y:8853:HOH:O	2.27	0.67
27:Y:185:VAL:HG12	39:Y:8869:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.76	0.67
5:C:1:MET:HG2	5:C:2:GLN:N	2.10	0.67
1:O:338:C:H4'	5:C:174:ILE:CD1	2.25	0.66
15:M:164:THR:HG22	15:M:167:GLY:N	2.09	0.66
1:O:1679:C:H5'	39:O:9811:HOH:O	1.95	0.66
1:O:794:U:H3	1:O:819:A:H61	1.42	0.66
1:O:1667:A:C8	1:O:1667:A:H5'	2.29	0.66
25:W:13:MET:CE	25:W:17:ILE:HG22	2.24	0.66
1:O:558:C:C2'	1:O:559:U:H5''	2.26	0.66
1:O:1328:A:OP1	27:Y:169:ARG:HD2	1.96	0.66
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.61	0.66
5:C:2:GLN:HB3	39:C:8589:HOH:O	1.96	0.66
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.11	0.66
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.61	0.66
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.24	0.66
27:Y:144:ARG:NE	39:Y:8910:HOH:O	2.27	0.66
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.76	0.66
14:L:136:ALA:HB3	39:L:8865:HOH:O	1.96	0.66
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.78	0.66
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.26	0.66
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.78	0.65
7:E:15:GLN:HG2	7:E:19:ASP:O	1.96	0.65
39:O:7208:HOH:O	16:N:4:PRO:HD2	1.95	0.65
10:H:83:GLU:HA	39:H:9037:HOH:O	1.96	0.65
1:O:2851:G:O2'	1:O:2852:A:H5'	1.96	0.65
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.61	0.65
4:B:185:GLY:HA2	39:B:9103:HOH:O	1.96	0.65
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.79	0.65
39:O:5438:HOH:O	15:M:125:ARG:HD3	1.96	0.65
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.27	0.65
6:D:166:ILE:HB	39:D:6326:HOH:O	1.97	0.65
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.61	0.65
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.27	0.65
1:O:513:A:N3	39:O:4140:HOH:O	2.29	0.65
1:O:1163:G:H5'	11:I:110:ASP:O	1.97	0.65
16:N:132:ASN:O	16:N:135:VAL:HG12	1.97	0.65
25:W:13:MET:HE1	25:W:18:GLN:HA	1.78	0.65
1:O:2505:G:O2'	1:O:2506:A:H5'	1.96	0.65
10:H:114:ASP:HB2	39:H:8996:HOH:O	1.96	0.65
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.42	0.65
18:P:91:LYS:O	18:P:95:GLU:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:88:THR:HG22	25:W:89:ASP:H	1.59	0.65
25:W:88:THR:HG22	25:W:89:ASP:N	2.11	0.65
1:0:1183:C:N4	1:0:1184:C:H41	1.95	0.65
5:C:236:THR:HA	39:C:8656:HOH:O	1.96	0.65
1:0:282:C:O2'	1:0:283:U:H5'	1.96	0.64
1:0:871:G:C8	1:0:871:G:C5'	2.74	0.64
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.12	0.64
1:0:2004:U:H4'	39:0:5759:HOH:O	1.96	0.64
1:0:2783:A:H3'	39:0:5684:HOH:O	1.96	0.64
1:0:470:U:O2'	29:1:16:HIS:HD2	1.80	0.64
29:1:42:SER:HB2	39:1:8957:HOH:O	1.97	0.64
20:R:99:ALA:HB1	20:R:109:MET:CE	2.26	0.64
25:W:80:ASP:O	25:W:84:VAL:HG23	1.97	0.64
1:0:797:A:C4'	28:Z:10:ARG:N	2.61	0.64
6:D:25:MET:SD	6:D:40:ILE:HD11	2.37	0.64
39:0:6115:HOH:O	22:T:68:ASP:HB2	1.98	0.64
1:0:1165:G:H4'	1:0:1174:A:O2'	1.97	0.64
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.62	0.64
2:9:39:U:H1'	2:9:44:A:N6	2.11	0.64
14:L:143:THR:HG22	14:L:144:ASP:N	2.12	0.64
1:0:2827:A:H2'	1:0:2828:G:O4'	1.98	0.64
39:0:5912:HOH:O	9:G:12:ILE:HG23	1.98	0.64
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.44	0.64
25:W:151:GLU:O	25:W:154:ARG:HB2	1.98	0.64
25:W:149:LEU:HG	25:W:153:MET:HE2	1.80	0.64
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.45	0.64
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.78	0.64
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.77	0.64
26:X:9:VAL:HG13	26:X:88:GLU:OE1	1.97	0.64
1:0:1189:A:H3'	39:0:8185:HOH:O	1.97	0.64
1:0:544:G:C2'	1:0:545:G:H5''	2.27	0.64
1:0:1641:A:H2'	1:0:1642:A:H5'	1.79	0.64
6:D:170:TYR:O	6:D:171:ASP:HB3	1.98	0.64
9:G:20:VAL:O	9:G:24:VAL:HG23	1.98	0.64
18:P:115:SER:N	18:P:118:GLN:HE21	1.88	0.64
3:A:33:GLU:CD	3:A:33:GLU:H	2.01	0.64
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.27	0.64
4:B:305:ASP:O	4:B:306:LYS:HB2	1.98	0.64
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.80	0.64
24:V:39:ALA:C	24:V:41:GLU:H	1.99	0.64
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:144:ARG:NH1	39:Y:8875:HOH:O	2.26	0.64
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.79	0.63
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.79	0.63
11:I:100:VAL:HG11	11:I:124:VAL:HG22	1.80	0.63
1:0:396:U:H1'	39:0:8134:HOH:O	1.99	0.63
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.80	0.63
39:0:7310:HOH:O	15:M:178:LYS:HB2	1.97	0.63
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.64	0.63
28:Z:13:ARG:NH1	39:Z:8719:HOH:O	2.30	0.63
1:0:2816:A:H2'	39:0:8430:HOH:O	1.97	0.63
3:A:153:ARG:CB	3:A:153:ARG:HH11	2.12	0.63
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.80	0.63
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.79	0.63
2:9:14:G:H5'	2:9:14:G:C8	2.32	0.63
2:9:6:C:C5'	16:N:37:ARG:NH1	2.57	0.63
7:E:69:ILE:HA	7:E:72:MET:HE3	1.80	0.63
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.80	0.63
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.80	0.63
1:0:1209:C:H2'	1:0:1210:G:H8	1.64	0.63
13:K:98:VAL:HG11	13:K:102:GLU:HA	1.78	0.63
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.81	0.63
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.80	0.63
1:0:2781:U:H1'	7:E:139:GLU:OE2	1.99	0.63
1:0:500:G:H21	20:R:98:ASN:HD21	1.45	0.63
7:E:69:ILE:HA	7:E:72:MET:CE	2.29	0.63
23:U:17:THR:HG22	23:U:18:GLY:N	2.14	0.63
25:W:65:VAL:HA	25:W:68:THR:HG22	1.80	0.63
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.98	0.62
10:H:49:GLN:HG3	10:H:140:TYR:CE2	2.34	0.62
25:W:84:VAL:HG12	39:W:6679:HOH:O	1.98	0.62
1:0:2426:G:H1'	39:0:6539:HOH:O	1.99	0.62
8:F:38:LYS:NZ	15:M:3:SER:HA	2.15	0.62
7:E:68:HIS:O	7:E:72:MET:HG3	1.99	0.62
11:I:101:LYS:O	11:I:105:GLU:HG3	1.99	0.62
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.81	0.62
4:B:41:PHE:HA	4:B:79:MET:HE2	1.82	0.62
3:A:179:MET:HG2	3:A:186:TRP:CB	2.30	0.62
1:0:2578:G:H5'	1:0:2578:G:H8	1.64	0.62
23:U:14:GLU:O	23:U:17:THR:HB	2.00	0.62
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.65	0.62
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:4:LEU:O	25:W:32:CYS:HA	1.99	0.62
1:0:1377:C:H6	1:0:1377:C:H5'	1.65	0.62
6:D:99:ASP:HB3	6:D:103:ASN:H	1.64	0.62
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.30	0.62
24:V:64:GLY:O	24:V:65:ASP:HB2	2.00	0.62
11:I:108:HIS:N	11:I:109:PRO:HD2	2.14	0.62
1:0:2533:C:C6	1:0:2533:C:H5'	2.34	0.61
3:A:194:MET:CE	3:A:199:HIS:HB2	2.29	0.61
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.32	0.61
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.65	0.61
24:V:39:ALA:N	24:V:40:PRO:HD2	2.16	0.61
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.80	0.61
1:0:2420:G:O2'	1:0:2421:G:H5'	2.00	0.61
1:0:558:C:H2'	1:0:559:U:C5'	2.30	0.61
1:0:656:G:H5'	17:O:3:THR:CG2	2.30	0.61
5:C:25:PRO:HG2	39:C:8522:HOH:O	1.99	0.61
22:T:53:GLY:HA3	39:T:6384:HOH:O	2.00	0.61
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.99	0.61
1:0:1819:G:H5'	39:O:5176:HOH:O	2.01	0.61
1:0:1189:A:H1'	1:0:1209:C:C1'	2.30	0.61
4:B:307:ARG:HD2	39:B:9123:HOH:O	2.00	0.61
5:C:236:THR:H	5:C:239:ALA:HB3	1.64	0.61
6:D:91:ALA:HB1	39:D:5198:HOH:O	2.00	0.61
1:0:1168:C:H4'	39:I:5128:HOH:O	2.00	0.61
1:0:1441:G:O2'	1:0:1442:A:H5'	2.00	0.61
1:0:2414:A:H2'	1:0:2415:A:C8	2.36	0.61
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.34	0.61
1:0:2769:C:C2'	1:0:2770:G:H5'	2.31	0.61
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.82	0.61
10:H:167:LYS:HE2	10:H:169:GLU:OE1	2.01	0.61
12:J:74:ARG:O	12:J:78:ILE:HG12	2.00	0.61
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.81	0.61
5:C:162:VAL:HG22	5:C:232:LEU:HD21	1.83	0.61
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.83	0.61
16:N:169:PRO:O	16:N:172:PHE:HB3	2.00	0.61
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.82	0.61
27:Y:144:ARG:NH2	39:Y:8910:HOH:O	2.33	0.61
1:0:1058:A:H2'	1:0:1060:C:H5''	1.82	0.61
1:0:1189:A:H1'	1:0:1209:C:H1'	1.83	0.61
1:0:259:G:H21	15:M:58:GLN:NE2	1.99	0.61
1:0:709:G:O2'	17:O:25:VAL:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:10:LYS:HG3	39:1:8979:HOH:O	2.00	0.61
14:L:79:ASP:HB3	39:L:8850:HOH:O	2.01	0.61
4:B:312:ARG:HB2	39:B:9118:HOH:O	2.00	0.60
29:1:25:LYS:HD2	30:2:49:GLU:N	2.15	0.60
4:B:8:LYS:HG3	4:B:220:VAL:HG12	1.83	0.60
1:0:2718:C:H6	1:0:2718:C:H5'	1.67	0.60
1:0:757:C:OP1	14:L:27:ARG:HD2	2.01	0.60
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.83	0.60
3:A:88:ILE:HG22	3:A:88:ILE:O	2.00	0.60
18:P:115:SER:H	18:P:118:GLN:NE2	1.89	0.60
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.29	0.60
1:0:1119:G:H8	12:J:52:GLN:HE22	1.48	0.60
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.65	0.60
17:O:87:THR:O	17:O:91:GLN:HG3	2.02	0.60
1:0:2064:U:H5'	1:0:2652:U:H4'	1.83	0.60
31:3:55:VAL:HG22	39:3:8937:HOH:O	2.01	0.60
4:B:102:THR:CG2	4:B:182:VAL:HG12	2.31	0.60
4:B:145:HIS:HD2	4:B:146:THR:O	1.84	0.60
12:J:103:VAL:HG12	39:J:5907:HOH:O	2.01	0.60
1:0:69:A:H5'	1:0:69:A:C8	2.36	0.60
22:T:7:GLN:O	22:T:11:GLN:HG3	2.02	0.60
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.82	0.60
1:0:1701:A:H5''	1:0:1702:U:H3'	1.82	0.60
1:0:90:A:H2'	1:0:91:G:O4'	2.02	0.60
20:R:39:THR:HG22	20:R:42:GLU:H	1.65	0.60
8:F:37:THR:O	8:F:41:GLU:HG3	2.02	0.60
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.01	0.60
1:0:2005:G:H3'	1:0:2005:G:OP2	2.02	0.60
6:D:25:MET:HE3	6:D:37:ALA:CB	2.23	0.60
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.67	0.60
14:L:145:LEU:O	14:L:148:GLU:HG3	2.02	0.60
15:M:60:VAL:C	15:M:61:ILE:HD12	2.22	0.60
39:O:3045:HOH:O	25:W:119:HIS:HE1	1.84	0.60
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.82	0.60
31:3:17:HIS:O	31:3:18:GLN:HG3	2.02	0.60
4:B:254:GLN:HG2	4:B:255:GLY:N	2.16	0.60
1:0:2507:G:H2'	1:0:2510:C:H42	1.66	0.59
1:0:2768:A:H2'	1:0:2769:C:O4'	2.02	0.59
3:A:36:ASP:O	3:A:38:ILE:N	2.27	0.59
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.36	0.59
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:122:ARG:NH2	39:Y:8834:HOH:O	2.35	0.59
11:I:105:GLU:HA	11:I:108:HIS:NE2	2.18	0.59
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.62	0.59
24:V:38:GLY:C	24:V:40:PRO:HD2	2.22	0.59
2:9:44:A:O4'	6:D:76:ARG:NE	2.35	0.59
1:0:2866:U:C4	23:U:50:GLU:HB3	2.37	0.59
1:0:121:U:OP2	30:2:10:ARG:NH2	2.31	0.59
4:B:51:VAL:HG23	4:B:329:TYR:O	2.00	0.59
1:0:474:C:O3'	5:C:73:LEU:HD21	2.02	0.59
6:D:65:GLU:HA	39:D:6752:HOH:O	2.03	0.59
11:I:129:SER:O	11:I:130:LEU:HD23	2.02	0.59
14:L:80:ASP:HB2	14:L:90:ARG:O	2.03	0.59
16:N:37:ARG:NE	39:N:8832:HOH:O	2.35	0.59
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.02	0.59
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.83	0.59
6:D:159:PRO:O	6:D:163:VAL:HG23	2.02	0.59
8:F:91:VAL:CG1	8:F:92:GLY:H	2.15	0.59
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.84	0.59
20:R:39:THR:HB	20:R:42:GLU:CG	2.32	0.59
1:0:1474:C:C6	1:0:1474:C:H5'	2.32	0.59
1:0:558:C:O2'	1:0:559:U:H5''	2.02	0.59
31:3:62:THR:HB	39:3:8977:HOH:O	2.01	0.59
3:A:191:GLY:HA2	3:A:194:MET:CE	2.33	0.59
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.84	0.59
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.01	0.59
1:0:316:A:H5'	22:T:54:ASP:OD2	2.03	0.59
31:3:6:ARG:NH1	31:3:21:GLU:HG3	2.17	0.59
6:D:136:ARG:HB2	39:D:7597:HOH:O	2.03	0.59
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.32	0.59
4:B:102:THR:HG23	4:B:182:VAL:HG12	1.84	0.59
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.59
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.17	0.59
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.37	0.59
26:X:43:VAL:HG22	26:X:76:ARG:NH1	2.18	0.59
1:0:1080:C:H4'	1:0:1081:A:OP1	2.02	0.58
17:O:39:THR:O	17:O:115:ARG:NH2	2.36	0.58
9:G:23:ILE:O	9:G:27:ILE:HG13	2.03	0.58
1:0:2717:C:H2'	1:0:2718:C:C5'	2.30	0.58
2:9:114:G:O6	16:N:11:ARG:HD3	2.03	0.58
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.85	0.58
7:E:11:VAL:HG12	7:E:12:ASP:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:70:THR:OG1	11:I:107:LYS:HE2	2.03	0.58
12:J:131:THR:HG22	12:J:133:GLY:N	2.18	0.58
15:M:107:ARG:NH1	39:M:8876:HOH:O	2.35	0.58
1:O:603:A:H5''	1:O:604:G:OP1	2.02	0.58
2:9:13:A:O2'	2:9:14:G:H5''	2.03	0.58
5:C:98:ARG:NH1	39:C:8561:HOH:O	2.34	0.58
7:E:166:VAL:HG12	39:E:3134:HOH:O	2.02	0.58
39:O:5912:HOH:O	9:G:12:ILE:HA	2.02	0.58
1:O:1119:G:H2'	12:J:52:GLN:HE22	1.66	0.58
1:O:1528:A:H2'	1:O:1529:G:O4'	2.02	0.58
3:A:131:HIS:O	3:A:132:ASP:HB2	2.02	0.58
5:C:27:ARG:HG3	5:C:29:ASP:OD1	2.02	0.58
1:O:164:G:H4'	14:L:30:ARG:HD3	1.86	0.58
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.69	0.58
6:D:54:ALA:CB	6:D:69:ILE:HD12	2.32	0.58
12:J:47:THR:HG22	12:J:48:GLY:N	2.19	0.58
26:X:25:ARG:HD3	26:X:64:ALA:O	2.04	0.58
1:O:1166:A:H61	1:O:1180:U:H3	1.51	0.58
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.68	0.58
24:V:12:THR:HG23	24:V:14:ALA:H	1.68	0.58
1:O:1118:A:H62	1:O:1244:U:H3	1.52	0.58
1:O:2779:G:H21	7:E:143:GLN:NE2	2.02	0.58
3:A:164:ARG:CZ	39:A:9050:HOH:O	2.51	0.58
3:A:55:VAL:HG22	3:A:68:ILE:O	2.04	0.58
6:D:50:VAL:O	6:D:71:ALA:HA	2.04	0.58
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.33	0.58
8:F:91:VAL:CG1	8:F:92:GLY:N	2.67	0.58
14:L:72:ASN:HB2	39:L:8872:HOH:O	2.03	0.58
25:W:125:HIS:CD2	25:W:127:GLY:H	2.20	0.58
1:O:125:U:H2'	39:O:4245:HOH:O	2.03	0.58
1:O:1730:G:H5'	1:O:1731:C:C5	2.38	0.58
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.33	0.58
1:O:2717:C:O2'	1:O:2718:C:H5''	2.02	0.58
1:O:396:U:O2'	1:O:418:C:H4'	2.04	0.58
1:O:558:C:H2'	1:O:559:U:H5''	1.85	0.58
7:E:35:TYR:HA	12:J:127:ILE:HD12	1.86	0.58
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.34	0.58
25:W:130:HIS:O	25:W:136:GLY:HA3	2.04	0.58
1:O:299:U:H5'	39:O:7766:HOH:O	2.03	0.57
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.04	0.57
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:154:LYS:H	6:D:154:LYS:CD	2.06	0.57
6:D:95:THR:OG1	6:D:174:VAL:HG22	2.04	0.57
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.86	0.57
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.04	0.57
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.03	0.57
39:9:9062:HOH:O	16:N:41:LYS:HD3	2.05	0.57
39:0:7854:HOH:O	22:T:9:LYS:HB2	2.03	0.57
25:W:38:THR:HG22	25:W:39:ASP:N	2.20	0.57
1:0:119:A:H2'	1:0:120:A:H5''	1.87	0.57
1:0:1634:G:H3'	39:0:4370:HOH:O	2.04	0.57
1:0:1766:U:O2	1:0:1778:A:H5'	2.04	0.57
1:0:2346:C:O2'	6:D:52:THR:HG21	2.04	0.57
14:L:133:VAL:HB	39:L:8849:HOH:O	2.03	0.57
1:0:1615:A:H5'	39:0:4655:HOH:O	2.03	0.57
2:9:20:G:O2'	2:9:21:G:H5'	2.04	0.57
8:F:31:LYS:HE3	39:F:2623:HOH:O	2.04	0.57
16:N:11:ARG:NH2	39:N:8817:HOH:O	2.38	0.57
1:0:588:G:O6	25:W:154:ARG:NH1	2.37	0.57
2:9:92:G:H2'	2:9:93:A:C8	2.40	0.57
5:C:107:ARG:NH1	39:C:8637:HOH:O	2.37	0.57
1:0:1175:G:H1'	1:0:1193:A:H2'	1.86	0.57
2:9:39:U:HO2'	2:9:42:C:H5	1.52	0.57
1:0:2320:U:H4'	1:0:2321:A:O4'	2.05	0.57
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.85	0.57
39:0:7881:HOH:O	4:B:211:THR:HG21	2.04	0.57
5:C:233:THR:HG22	5:C:234:VAL:N	2.18	0.57
6:D:58:VAL:CG1	6:D:60:GLU:HG2	2.33	0.57
11:I:124:VAL:O	11:I:124:VAL:HG12	2.05	0.57
14:L:148:GLU:HB2	39:L:8877:HOH:O	2.03	0.57
26:X:80:GLU:HB3	39:X:5564:HOH:O	2.04	0.57
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.70	0.57
1:0:1205:U:H2'	1:0:1206:U:C5'	2.34	0.57
3:A:33:GLU:O	3:A:34:ASP:HB2	2.04	0.57
8:F:101:ALA:HA	39:F:5413:HOH:O	2.04	0.57
10:H:48:VAL:HA	10:H:170:ARG:O	2.04	0.57
1:0:280:C:H2'	1:0:281:U:O4'	2.05	0.57
4:B:214:PRO:HD2	39:B:8990:HOH:O	2.05	0.57
4:B:307:ARG:NH1	4:B:307:ARG:HG3	2.11	0.56
6:D:135:VAL:HG22	6:D:136:ARG:H	1.70	0.56
12:J:19:MET:CE	12:J:132:LEU:HD11	2.35	0.56
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.07	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1164:U:OP1	11:I:69:PRO:HA	2.05	0.56
1:O:263:U:O4'	8:F:59:ILE:HD13	2.05	0.56
1:O:681:G:N3	1:O:681:G:H5'	2.20	0.56
4:B:254:GLN:HG3	39:B:9000:HOH:O	2.05	0.56
1:O:545:G:C8	1:O:545:G:H5'	2.37	0.56
1:O:949:U:O2'	19:Q:40:HIS:HE1	1.89	0.56
10:H:23:ILE:HG23	10:H:123:ILE:HD11	1.88	0.56
20:R:29:LYS:HD3	39:R:8944:HOH:O	2.05	0.56
4:B:125:GLU:O	4:B:129:ARG:HG3	2.05	0.56
5:C:246:ARG:NH1	39:C:8575:HOH:O	2.38	0.56
39:C:8563:HOH:O	17:O:3:THR:HG21	2.05	0.56
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.40	0.56
2:9:91:C:H2'	2:9:92:G:O4'	2.05	0.56
4:B:62:ARG:HA	4:B:65:MET:HE3	1.88	0.56
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.71	0.56
1:O:1299:G:O6	14:L:6:ARG:HD3	2.05	0.56
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.04	0.56
9:G:12:ILE:N	9:G:13:PRO:HD3	2.21	0.56
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.71	0.56
1:O:272:A:H5'	1:O:273:G:OP2	2.06	0.56
11:I:113:SER:HB2	11:I:118:ASN:HB2	1.88	0.56
1:O:1786:C:OP1	18:P:74:GLN:HG2	2.05	0.56
4:B:85:ARG:NH1	39:B:9104:HOH:O	2.38	0.56
1:O:2820:A:OP1	4:B:98:THR:HG22	2.06	0.56
10:H:30:LYS:N	10:H:62:HIS:HD2	2.00	0.56
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.37	0.56
1:O:1086:A:C6	25:W:11:VAL:HG11	2.40	0.56
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.87	0.56
1:O:797:A:H4'	28:Z:10:ARG:N	2.21	0.56
5:C:132:ASP:HB3	39:C:8567:HOH:O	2.06	0.56
14:L:73:VAL:HG23	14:L:74:THR:H	1.70	0.56
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.87	0.56
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.36	0.56
22:T:71:VAL:HG12	22:T:72:ILE:N	2.21	0.56
3:A:153:ARG:NH1	3:A:153:ARG:HB2	2.17	0.56
16:N:17:ARG:NH1	16:N:17:ARG:HB3	2.21	0.56
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.36	0.56
22:T:28:SER:O	22:T:32:ARG:HG3	2.06	0.56
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.88	0.56
1:O:1835:U:C5	1:O:1840:A:N7	2.65	0.55
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.37	0.55
4:B:280:VAL:HG13	4:B:333:GLU:O	2.05	0.55
12:J:107:ASN:C	12:J:107:ASN:HD22	2.09	0.55
17:O:73:ASP:HA	17:O:92:VAL:O	2.06	0.55
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.87	0.55
27:Y:144:ARG:CZ	39:Y:8910:HOH:O	2.54	0.55
1:0:1234:U:N3	4:B:244:PRO:HB3	2.21	0.55
1:0:960:G:H2'	1:0:960:G:N3	2.22	0.55
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.86	0.55
8:F:99:THR:HA	39:F:3461:HOH:O	2.05	0.55
1:0:1120:U:H5''	1:0:1120:U:C6	2.41	0.55
1:0:1182:C:H1'	1:0:1192:A:H8	1.72	0.55
1:0:417:G:P	39:0:7848:HOH:O	2.64	0.55
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.87	0.55
16:N:58:LEU:N	16:N:58:LEU:HD12	2.20	0.55
1:0:20:G:H21	20:R:117:HIS:HD2	1.53	0.55
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.87	0.55
1:0:2346:C:O5'	1:0:2346:C:H6	1.89	0.55
1:0:380:A:OP2	15:M:9:ARG:HD2	2.07	0.55
29:1:25:LYS:CD	30:2:49:GLU:H	2.18	0.55
2:9:2:U:OP2	2:9:3:A:H5'	2.07	0.55
1:0:1363:G:OP1	5:C:76:ARG:NH2	2.39	0.55
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.41	0.55
1:0:447:A:P	22:T:1:SER:HB2	2.45	0.55
11:I:97:VAL:O	11:I:101:LYS:HG3	2.06	0.55
12:J:107:ASN:HD22	12:J:109:TYR:H	1.53	0.55
16:N:147:ILE:HD12	39:N:8845:HOH:O	2.06	0.55
2:9:28:U:H5''	16:N:40:ASN:ND2	2.22	0.55
39:0:4235:HOH:O	22:T:9:LYS:HD3	2.06	0.55
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.89	0.55
27:Y:155:ARG:NH1	39:Y:8855:HOH:O	2.39	0.55
1:0:1972:U:H2'	1:0:1973:A:H5''	1.88	0.55
1:0:1973:A:H5'	1:0:1973:A:C8	2.33	0.55
39:0:9846:HOH:O	29:1:1:THR:HA	2.06	0.55
3:A:69:LEU:HD23	3:A:107:ASN:HB2	1.87	0.55
26:X:25:ARG:HG2	39:X:5356:HOH:O	2.07	0.55
1:0:1384:C:H5'	26:X:30:MET:HG2	1.87	0.55
1:0:319:A:H4'	1:0:338:C:C4	2.42	0.55
6:D:154:LYS:HD2	6:D:154:LYS:N	2.08	0.55
13:K:82:ARG:NH2	13:K:115:ARG:HG2	2.22	0.55
1:0:645:U:OP2	14:L:4:LYS:HE2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:5193:HOH:O	16:N:21:HIS:HD2	1.90	0.55
25:W:139:GLY:O	25:W:141:HIS:HD2	1.88	0.55
1:O:1116:U:O2'	1:O:1118:A:C2	2.47	0.55
1:O:447:A:OP2	22:T:1:SER:HB2	2.07	0.55
11:I:120:ALA:O	11:I:124:VAL:HG23	2.06	0.55
22:T:26:THR:HA	22:T:39:ASN:HB3	1.88	0.55
1:O:316:A:N3	1:O:336:G:O2'	2.40	0.55
1:O:2694:A:H4'	7:E:91:PHE:CE1	2.42	0.55
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.72	0.55
30:2:48:ASP:O	30:2:49:GLU:HB2	2.07	0.55
2:9:33:U:H2'	39:9:9068:HOH:O	2.07	0.55
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.89	0.55
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.88	0.55
10:H:69:ARG:HD3	39:H:9031:HOH:O	2.07	0.55
2:9:51:A:H5'	16:N:160:SER:HB3	1.88	0.55
1:O:93:C:H5''	24:V:1:THR:CB	2.37	0.55
24:V:42:ASN:O	24:V:44:GLY:N	2.40	0.55
1:O:475:G:H5'	5:C:73:LEU:HD23	1.88	0.54
2:9:23:U:O2'	2:9:24:U:H4'	2.07	0.54
4:B:79:MET:HE1	39:B:9094:HOH:O	2.06	0.54
5:C:115:LEU:O	5:C:118:THR:HB	2.06	0.54
1:O:2036:C:O4'	13:K:44:LEU:HG	2.07	0.54
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.37	0.54
27:Y:133:HIS:HD2	39:Y:8880:HOH:O	1.90	0.54
1:O:69:A:H5'	1:O:69:A:H8	1.72	0.54
5:C:16:VAL:HG12	5:C:17:ASP:H	1.71	0.54
2:9:41:C:O4'	6:D:50:VAL:HG22	2.06	0.54
39:O:7121:HOH:O	22:T:38:ARG:NH1	2.39	0.54
24:V:55:ARG:O	24:V:59:ILE:HG12	2.08	0.54
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.42	0.54
1:O:1201:C:H2'	1:O:1202:A:H5'	1.88	0.54
1:O:2676:C:H4'	12:J:70:PHE:HE1	1.72	0.54
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.88	0.54
16:N:183:ASP:O	16:N:184:ILE:O	2.25	0.54
20:R:132:ARG:CZ	39:R:8991:HOH:O	2.55	0.54
1:O:1278:A:H4'	1:O:1279:U:C4	2.43	0.54
1:O:1677:U:OP2	30:2:8:LYS:NZ	2.40	0.54
5:C:214:THR:HG23	39:C:8643:HOH:O	2.07	0.54
7:E:36:PRO:HD3	12:J:127:ILE:HD12	1.89	0.54
26:X:31:ILE:O	26:X:35:GLU:HG3	2.08	0.54
4:B:66:GLU:OE1	4:B:328:ARG:HD2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1205:U:H2'	1:0:1206:U:H5''	1.89	0.54
5:C:79:ARG:O	5:C:87:ARG:HG2	2.08	0.54
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.88	0.54
18:P:103:THR:O	18:P:107:GLU:HG3	2.07	0.54
1:0:1625:U:H4'	39:0:5132:HOH:O	2.07	0.54
3:A:94:LEU:N	3:A:94:LEU:HD23	2.23	0.54
5:C:129:HIS:HD2	5:C:165:ASP:OD2	1.90	0.54
7:E:31:ARG:NH1	39:E:5919:HOH:O	2.40	0.54
1:0:2769:C:H2'	1:0:2770:G:H5'	1.89	0.54
1:0:2894:C:O2'	1:0:2895:C:H5'	2.08	0.54
10:H:79:GLU:O	10:H:80:LEU:HD23	2.08	0.54
13:K:55:VAL:HG12	13:K:56:SER:N	2.22	0.54
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	2.06	0.54
25:W:108:ARG:HE	25:W:114:PRO:CG	2.20	0.54
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.43	0.54
1:0:1189:A:H1'	1:0:1209:C:O4'	2.08	0.54
1:0:1853:C:OP1	3:A:231:LYS:HG3	2.08	0.54
4:B:56:ASP:OD1	4:B:322:ARG:HB3	2.08	0.54
5:C:104:ASP:HA	5:C:107:ARG:HH12	1.71	0.54
7:E:7:ILE:HD11	7:E:11:VAL:C	2.29	0.54
26:X:25:ARG:HD2	39:X:3861:HOH:O	2.07	0.54
1:0:2862:G:H4'	4:B:336:GLN:O	2.07	0.54
3:A:179:MET:HA	3:A:179:MET:CE	2.38	0.54
6:D:58:VAL:HG12	6:D:60:GLU:HG2	1.89	0.54
8:F:14:ASP:O	8:F:18:GLU:HG3	2.08	0.54
13:K:66:ARG:HD3	39:K:2777:HOH:O	2.07	0.54
15:M:80:GLY:O	15:M:81:ARG:HD3	2.08	0.54
1:0:2878:U:H2'	1:0:2879:A:O4'	2.08	0.53
1:0:338:C:H4'	5:C:174:ILE:HD11	1.89	0.53
5:C:2:GLN:HB3	39:C:8535:HOH:O	2.08	0.53
6:D:23:VAL:HG22	6:D:73:VAL:HB	1.89	0.53
1:0:902:G:N7	14:L:18:HIS:HD2	2.06	0.53
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.22	0.53
39:0:3028:HOH:O	18:P:81:LYS:HG2	2.07	0.53
4:B:329:TYR:CE2	23:U:15:PRO:HG2	2.43	0.53
1:0:1314:U:H2'	39:0:6326:HOH:O	2.07	0.53
1:0:200:C:H2'	39:0:3929:HOH:O	2.07	0.53
1:0:485:A:N3	1:0:487:G:H5''	2.23	0.53
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.48	0.53
2:9:29:C:C2'	2:9:30:C:H5'	2.38	0.53
3:A:121:ALA:O	3:A:124:VAL:HG22	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:163:VAL:HA	39:D:6326:HOH:O	2.06	0.53
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.89	0.53
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.23	0.53
1:O:2670:G:O2'	1:O:2671:U:H5'	2.08	0.53
1:O:538:C:OP2	27:Y:134:HIS:HE1	1.91	0.53
4:B:82:VAL:HG12	4:B:82:VAL:O	2.07	0.53
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.38	0.53
11:I:94:ASP:OD1	11:I:133:THR:HB	2.09	0.53
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.91	0.53
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.09	0.53
25:W:149:LEU:HG	25:W:153:MET:CE	2.38	0.53
1:O:10:U:O4	1:O:532:A:OP2	2.26	0.53
30:2:23:ALA:HB3	39:2:6863:HOH:O	2.08	0.53
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.07	0.53
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.38	0.53
16:N:154:LEU:O	16:N:155:GLU:HB3	2.08	0.53
1:O:1594:C:OP2	18:P:120:ARG:HD2	2.08	0.53
39:O:7836:HOH:O	22:T:2:LYS:HE2	2.07	0.53
24:V:1:THR:HG23	24:V:2:VAL:N	2.19	0.53
26:X:8:ARG:NH1	39:X:2479:HOH:O	2.40	0.53
1:O:1268:C:O2'	27:Y:169:ARG:HB2	2.08	0.53
30:2:39:ARG:HG2	39:2:3143:HOH:O	2.09	0.53
30:2:41:HIS:HD2	30:2:44:ARG:H	1.56	0.53
1:O:905:C:OP1	27:Y:144:ARG:NH1	2.42	0.53
3:A:66:ARG:HH11	3:A:66:ARG:HB2	1.74	0.53
6:D:65:GLU:HG3	39:D:6752:HOH:O	2.07	0.53
22:T:69:LYS:O	22:T:71:VAL:HG23	2.08	0.53
1:O:2243:C:H5''	39:O:4230:HOH:O	2.09	0.53
1:O:536:A:H3'	39:O:5504:HOH:O	2.09	0.53
2:9:69:U:OP1	16:N:4:PRO:HG3	2.09	0.53
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.90	0.53
23:U:52:THR:HG22	23:U:54:THR:N	2.23	0.53
1:O:1187:U:O2'	1:O:1189:A:H2	1.92	0.53
1:O:156:C:H5''	15:M:171:ARG:CD	2.29	0.53
1:O:1972:U:C2'	1:O:1973:A:H5''	2.39	0.53
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.91	0.53
4:B:321:PRO:HA	39:B:9127:HOH:O	2.09	0.53
6:D:24:HIS:HB2	6:D:72:LYS:CB	2.39	0.53
1:O:1201:C:H5''	39:O:6679:HOH:O	2.09	0.53
1:O:2419:U:H5''	1:O:2420:G:H5'	1.90	0.53
5:C:107:ARG:NE	39:C:8661:HOH:O	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:38:LYS:HZ3	15:M:3:SER:HA	1.74	0.53
10:H:165:ARG:HD2	39:H:9034:HOH:O	2.08	0.53
26:X:43:VAL:HG12	26:X:44:ASP:N	2.24	0.53
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.42	0.53
1:O:2812:A:C2	1:O:2814:A:N6	2.68	0.52
1:O:2817:G:P	39:O:8430:HOH:O	2.67	0.52
1:O:820:G:O2'	1:O:856:G:H4'	2.09	0.52
5:C:118:THR:O	5:C:136:VAL:HG13	2.08	0.52
12:J:80:LYS:HE3	12:J:101:VAL:O	2.08	0.52
14:L:134:GLU:HG3	39:L:8849:HOH:O	2.08	0.52
2:9:14:G:O2'	16:N:1:ALA:HB2	2.08	0.52
16:N:32:PRO:HD2	16:N:99:GLU:O	2.09	0.52
17:O:25:VAL:HG23	17:O:26:TRP:N	2.23	0.52
1:O:1162:G:H1'	11:I:112:LEU:HD11	1.91	0.52
1:O:2044:G:OP1	26:X:23:HIS:HE1	1.92	0.52
1:O:2712:G:H5'	39:K:4183:HOH:O	2.09	0.52
21:S:81:ILE:HG23	39:S:8984:HOH:O	2.10	0.52
25:W:64:THR:O	25:W:68:THR:HG22	2.09	0.52
26:X:18:ARG:NH1	39:X:4132:HOH:O	2.40	0.52
4:B:265:LEU:HD21	4:B:316:ARG:HD3	1.91	0.52
1:O:1119:G:H22	1:O:1246:A:H2	1.51	0.52
1:O:870:G:OP2	3:A:3:ARG:HD3	2.09	0.52
5:C:162:VAL:CG2	5:C:232:LEU:HD21	2.40	0.52
7:E:154:ILE:HG13	7:E:156:ASP:OD1	2.10	0.52
11:I:96:SER:H	11:I:99:GLN:NE2	2.07	0.52
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.90	0.52
1:O:1120:U:H5'	1:O:1121:G:OP2	2.08	0.52
1:O:2491:G:H1'	39:O:7304:HOH:O	2.09	0.52
1:O:711:G:H1'	39:O:7530:HOH:O	2.09	0.52
11:I:87:PRO:C	11:I:89:GLU:H	2.12	0.52
14:L:101:ASP:C	14:L:103:ALA:H	2.13	0.52
21:S:77:VAL:O	21:S:80:ARG:HG2	2.09	0.52
1:O:1972:U:H2'	1:O:1973:A:C5'	2.39	0.52
1:O:564:G:H1'	39:O:6756:HOH:O	2.08	0.52
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.92	0.52
3:A:53:ALA:HB3	39:A:9068:HOH:O	2.10	0.52
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.39	0.52
17:O:32:ARG:HH21	17:O:35:LYS:NZ	2.07	0.52
26:X:34:ARG:NH1	26:X:48:VAL:O	2.36	0.52
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.24	0.52
1:O:1666:C:H2'	1:O:1667:A:C5'	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.91	0.52
11:I:108:HIS:N	11:I:109:PRO:CD	2.72	0.52
14:L:67:ARG:O	14:L:71:GLU:HG3	2.10	0.52
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.90	0.52
23:U:17:THR:CG2	23:U:18:GLY:N	2.73	0.52
24:V:56:ILE:O	24:V:60:GLN:HG3	2.10	0.52
39:O:6731:HOH:O	27:Y:158:LYS:HD3	2.10	0.52
1:O:1119:G:H8	12:J:52:GLN:NE2	2.08	0.52
1:O:1730:G:C5'	1:O:1731:C:C6	2.93	0.52
1:O:31:C:H4'	39:O:7854:HOH:O	2.10	0.52
30:2:41:HIS:H	30:2:45:ASN:ND2	1.95	0.52
17:O:26:TRP:N	39:O:3062:HOH:O	2.42	0.52
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.56	0.52
1:O:449:A:N7	5:C:43:LYS:HG2	2.25	0.52
1:O:949:U:H4'	19:Q:95:GLU:HA	1.90	0.52
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.24	0.52
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.92	0.52
6:D:135:VAL:HG22	6:D:136:ARG:N	2.25	0.52
8:F:27:GLY:HA3	8:F:101:ALA:O	2.10	0.52
11:I:133:THR:HG22	11:I:134:ILE:N	2.24	0.52
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.35	0.52
1:O:1700:C:H5''	1:O:1701:A:OP2	2.09	0.52
1:O:407:A:H5'	39:O:6477:HOH:O	2.10	0.52
3:A:37:VAL:HG13	39:A:9072:HOH:O	2.10	0.52
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.45	0.52
5:C:27:ARG:HG2	5:C:30:LEU:HD12	1.91	0.52
7:E:15:GLN:NE2	7:E:40:VAL:O	2.43	0.52
9:G:64:ASN:N	9:G:64:ASN:HD22	2.08	0.52
10:H:62:HIS:HA	10:H:65:LEU:HD23	1.92	0.52
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.92	0.52
16:N:49:THR:CG2	16:N:58:LEU:HD11	2.40	0.52
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.71	0.52
25:W:5:VAL:HG11	25:W:153:MET:HE3	1.92	0.52
1:O:1730:G:H5''	1:O:1731:C:H6	1.74	0.51
3:A:232:ARG:NH2	3:A:236:GLY:O	2.34	0.51
10:H:174:LEU:HA	39:H:9021:HOH:O	2.10	0.51
27:Y:187:VAL:HB	27:Y:203:VAL:HG22	1.92	0.51
12:J:75:PRO:HD3	12:J:136:SER:OG	2.09	0.51
39:O:6168:HOH:O	13:K:87:ARG:CZ	2.57	0.51
16:N:110:THR:HB	16:N:113:SER:OG	2.11	0.51
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:9:CYS:HA	23:U:52:THR:HG23	1.92	0.51
1:0:2643:G:H5''	39:0:4401:HOH:O	2.09	0.51
1:0:653:U:H2'	1:0:654:A:C8	2.44	0.51
20:R:106:GLY:HA2	20:R:109:MET:CE	2.41	0.51
1:0:2289:G:H21	1:0:2291:A:H2	1.54	0.51
1:0:775:G:OP1	29:1:16:HIS:HE1	1.94	0.51
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.74	0.51
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.92	0.51
3:A:105:VAL:HG12	3:A:106:CYS:N	2.24	0.51
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.91	0.51
4:B:72:THR:HB	39:B:9073:HOH:O	2.10	0.51
6:D:25:MET:CE	6:D:41:LEU:HG	2.39	0.51
11:I:97:VAL:CG1	11:I:101:LYS:HE3	2.35	0.51
16:N:152:GLU:C	16:N:154:LEU:H	2.14	0.51
22:T:115:GLU:HG3	22:T:116:ASP:N	2.25	0.51
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.11	0.51
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.25	0.51
1:0:136:C:H2'	1:0:137:U:O4'	2.10	0.51
1:0:1947:G:H2'	1:0:1948:G:H8	1.75	0.51
1:0:2661:U:H3	1:0:2812:A:H62	1.59	0.51
1:0:834:G:H4'	1:0:835:U:OP2	2.11	0.51
2:9:35:C:H5''	39:9:9078:HOH:O	2.09	0.51
3:A:109:GLU:HG2	3:A:116:GLY:N	2.26	0.51
3:A:97:ALA:HB2	3:A:150:PRO:HB2	1.93	0.51
6:D:136:ARG:HD2	6:D:155:HIS:O	2.10	0.51
6:D:58:VAL:HB	6:D:62:ASP:HB3	1.93	0.51
1:0:1242:A:C5'	12:J:82:THR:HG23	2.27	0.51
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.75	0.51
1:0:1159:G:H1	1:0:1208:C:H42	1.58	0.51
1:0:123:U:H5'	39:0:7091:HOH:O	2.10	0.51
1:0:2748:G:H5'	39:0:7963:HOH:O	2.11	0.51
1:0:2795:C:O2'	1:0:2796:U:H5'	2.10	0.51
2:9:54:A:O2'	2:9:55:U:H5'	2.10	0.51
5:C:166:ILE:CD1	5:C:207:LEU:HD13	2.41	0.51
16:N:154:LEU:HG	16:N:155:GLU:H	1.76	0.51
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.40	0.51
1:0:1351:G:OP1	5:C:96:LYS:NZ	2.37	0.51
1:0:1595:G:O2'	1:0:1596:U:H5'	2.11	0.51
1:0:162:C:H2'	1:0:163:U:H5'	1.93	0.51
1:0:2563:U:H2'	1:0:2565:C:O5'	2.11	0.51
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.91	0.51
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.44	0.51
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.11	0.51
1:0:1118:A:H8	1:0:1119:G:H5''	1.76	0.51
1:0:474:C:O3'	5:C:73:LEU:CD2	2.59	0.51
10:H:50:ILE:HG21	39:H:9028:HOH:O	2.11	0.51
11:I:84:SER:HB3	11:I:92:VAL:CG2	2.41	0.51
8:F:58:GLU:CD	15:M:27:ARG:HH22	2.14	0.51
1:0:2301:A:H5''	1:0:2302:A:H5'	1.93	0.51
1:0:2073:G:OP2	1:0:2490:A:H5'	2.11	0.51
1:0:392:U:O2'	15:M:182:LYS:HE2	2.11	0.51
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.91	0.51
5:C:136:VAL:HG22	5:C:137:PRO:HA	1.93	0.51
5:C:61:PHE:HB3	39:C:8650:HOH:O	2.10	0.51
1:0:262:A:OP2	8:F:91:VAL:HG11	2.10	0.51
16:N:116:PHE:HB3	16:N:136:LEU:HD23	1.93	0.51
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.09	0.51
23:U:4:ARG:HH11	23:U:4:ARG:HG2	1.74	0.51
1:0:1244:U:H2'	12:J:47:THR:HG21	1.92	0.50
1:0:2456:A:H5'	39:0:6149:HOH:O	2.10	0.50
1:0:92:G:H4'	24:V:44:GLY:HA3	1.93	0.50
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.11	0.50
2:9:64:C:H2'	2:9:65:A:H5'	1.93	0.50
4:B:258:GLY:H	4:B:260:HIS:CE1	2.29	0.50
4:B:297:VAL:HB	39:B:9073:HOH:O	2.11	0.50
12:J:131:THR:HG22	12:J:133:GLY:H	1.76	0.50
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.92	0.50
30:2:20:ARG:HG3	30:2:21:VAL:H	1.77	0.50
2:9:48:C:H4'	16:N:141:ARG:HH21	1.76	0.50
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.08	0.50
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.23	0.50
1:0:2502:C:C2'	1:0:2503:A:H5'	2.40	0.50
1:0:2472:C:O2'	1:0:2634:G:H4'	2.11	0.50
2:9:76:G:C3'	2:9:77:A:H5''	2.31	0.50
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.10	0.50
20:R:132:ARG:NH2	39:R:8991:HOH:O	2.45	0.50
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.40	0.50
1:0:1289:C:O2'	1:0:1290:G:H5'	2.11	0.50
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.12	0.50
1:0:2089:A:O2'	1:0:2090:G:H5'	2.11	0.50
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:108:LEU:HD11	7:E:164:ASP:HB2	1.94	0.50
25:W:122:ARG:NH2	39:W:5817:HOH:O	2.44	0.50
1:0:1118:A:C8	1:0:1118:A:C3'	2.90	0.50
1:0:1181:A:C2'	1:0:1182:C:H5'	2.42	0.50
1:0:1250:C:O2'	1:0:1251:C:H5'	2.12	0.50
1:0:558:C:H2'	1:0:559:U:H5'	1.93	0.50
4:B:51:VAL:HG21	4:B:327:VAL:HG13	1.92	0.50
6:D:23:VAL:CG2	6:D:73:VAL:HB	2.41	0.50
10:H:30:LYS:H	10:H:62:HIS:CD2	2.21	0.50
17:O:78:ALA:C	17:O:98:LEU:HD13	2.32	0.50
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.92	0.50
24:V:64:GLY:O	24:V:65:ASP:CB	2.59	0.50
1:0:1299:G:H5'	39:0:4547:HOH:O	2.12	0.50
1:0:2638:G:H1'	39:0:8261:HOH:O	2.11	0.50
1:0:2769:C:H2'	1:0:2770:G:C5'	2.41	0.50
6:D:103:ASN:ND2	6:D:134:LEU:H	2.08	0.50
1:0:1666:C:C2'	1:0:1667:A:C5'	2.89	0.50
39:0:8211:HOH:O	5:C:94:THR:HG21	2.12	0.50
39:0:3115:HOH:O	8:F:38:LYS:HE2	2.11	0.50
1:0:1163:G:H5''	11:I:110:ASP:HB3	1.94	0.50
14:L:89:PHE:N	39:L:8863:HOH:O	2.45	0.50
25:W:48:VAL:CG1	25:W:48:VAL:O	2.60	0.50
1:0:2756:U:H3	1:0:2896:A:H2	1.50	0.50
3:A:65:ARG:C	3:A:66:ARG:HG3	2.32	0.50
5:C:77:ALA:O	5:C:78:ARG:HG3	2.11	0.50
8:F:46:GLU:OE1	8:F:100:ASP:HA	2.12	0.50
39:0:3724:HOH:O	11:I:87:PRO:HD3	2.11	0.50
39:0:9515:HOH:O	14:L:30:ARG:HD2	2.10	0.50
21:S:81:ILE:HG12	39:S:8984:HOH:O	2.11	0.50
27:Y:187:VAL:HG22	27:Y:192:ASP:CB	2.42	0.50
2:9:64:C:C2'	2:9:65:A:H5'	2.41	0.49
5:C:246:ARG:NE	39:C:8630:HOH:O	2.26	0.49
11:I:126:THR:O	11:I:126:THR:HG22	2.11	0.49
13:K:115:ARG:HG3	13:K:116:GLU:N	2.26	0.49
25:W:38:THR:HG22	39:W:3580:HOH:O	2.11	0.49
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.11	0.49
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.52	0.49
1:0:1377:C:H5'	1:0:1377:C:C6	2.45	0.49
1:0:2363:G:O3'	19:Q:11:ARG:NH1	2.45	0.49
1:0:2415:A:H2'	1:0:2416:G:H5'	1.93	0.49
1:0:776:A:OP1	29:1:28:HIS:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:20:ARG:CG	30:2:21:VAL:N	2.76	0.49
8:F:58:GLU:HG3	8:F:61:MET:HE1	1.94	0.49
9:G:16:LYS:O	9:G:20:VAL:HG23	2.13	0.49
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.76	0.49
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.25	0.49
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.47	0.49
1:0:1200:A:H3'	39:0:6208:HOH:O	2.13	0.49
1:0:2791:U:H1'	1:0:2792:A:H5''	1.94	0.49
1:0:2812:A:H1'	39:0:6244:HOH:O	2.12	0.49
1:0:2825:C:H4'	1:0:2826:G:O5'	2.12	0.49
1:0:343:C:O2'	1:0:344:C:H5'	2.11	0.49
3:A:192:VAL:HG13	39:A:9022:HOH:O	2.12	0.49
4:B:149:ASP:HB2	39:B:9049:HOH:O	2.13	0.49
4:B:74:ILE:HG13	39:B:9073:HOH:O	2.12	0.49
6:D:23:VAL:O	6:D:23:VAL:HG23	2.13	0.49
10:H:43:ALA:HB1	10:H:140:TYR:CE2	2.47	0.49
10:H:6:ALA:CA	10:H:61:ARG:HH12	2.22	0.49
13:K:55:VAL:CG1	13:K:56:SER:N	2.75	0.49
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.48	0.49
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.93	0.49
25:W:26:ILE:O	25:W:26:ILE:HG13	2.12	0.49
26:X:9:VAL:HG13	26:X:88:GLU:CD	2.32	0.49
27:Y:209:VAL:HG12	27:Y:214:ARG:HG3	1.94	0.49
1:0:1306:U:OP1	5:C:184:ARG:HD2	2.13	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
31:3:48:ASN:ND2	31:3:50:GLY:H	2.10	0.49
3:A:1:GLY:HA2	3:A:197:VAL:HG23	1.95	0.49
4:B:223:ARG:HG3	4:B:232:TRP:O	2.11	0.49
4:B:49:THR:HG21	4:B:331:SER:O	2.13	0.49
5:C:133:ARG:NH1	39:C:8616:HOH:O	2.45	0.49
6:D:29:HIS:HB2	39:D:2768:HOH:O	2.11	0.49
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.12	0.49
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.94	0.49
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.42	0.49
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.45	0.49
1:0:638:C:H2'	1:0:639:A:C8	2.47	0.49
1:0:899:C:H5'	39:0:3690:HOH:O	2.11	0.49
1:0:2270:G:C4'	3:A:223:ARG:HH12	2.18	0.49
6:D:104:PHE:CE2	6:D:166:ILE:HD13	2.47	0.49
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.95	0.49
16:N:147:ILE:HB	39:N:8845:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.48	0.49
25:W:31:HIS:HB3	39:W:5420:HOH:O	2.12	0.49
30:2:35:ARG:HB2	39:2:2691:HOH:O	2.11	0.49
4:B:268:ARG:NH2	4:B:325:PRO:HG3	2.28	0.49
5:C:19:PRO:HG2	5:C:22:PHE:CE1	2.48	0.49
8:F:16:ALA:HA	8:F:111:ILE:HD13	1.94	0.49
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.48	0.49
25:W:65:VAL:HA	25:W:68:THR:CG2	2.42	0.49
1:0:1181:A:H2'	1:0:1182:C:H5'	1.94	0.49
1:0:1778:A:H2'	1:0:1779:A:H5'	1.95	0.49
6:D:18:ILE:HG12	6:D:134:LEU:CD2	2.43	0.49
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.95	0.49
22:T:62:VAL:HB	39:T:3851:HOH:O	2.13	0.49
1:0:1426:C:H2'	39:0:3083:HOH:O	2.11	0.49
3:A:34:ASP:OD1	3:A:35:GLY:N	2.39	0.49
4:B:102:THR:HG21	4:B:182:VAL:O	2.13	0.49
10:H:61:ARG:HG3	10:H:61:ARG:HH11	1.77	0.49
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.28	0.49
1:0:793:A:H5''	18:P:83:LYS:HG2	1.95	0.49
1:0:1205:U:C2'	1:0:1206:U:H5''	2.43	0.49
1:0:2521:A:OP2	10:H:6:ALA:HB3	2.13	0.49
1:0:2697:A:H2'	1:0:2698:G:O4'	2.13	0.49
3:A:81:GLN:HG3	3:A:92:ASN:HD21	1.77	0.49
14:L:130:ARG:HA	39:L:8849:HOH:O	2.12	0.49
15:M:99:ARG:HE	15:M:170:ASN:HD22	1.59	0.49
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	2.13	0.49
1:0:291:C:H2'	1:0:292:G:O4'	2.13	0.49
1:0:602:A:O2'	1:0:605:C:H4'	2.12	0.49
31:3:56:PRO:N	39:3:8976:HOH:O	2.45	0.49
1:0:475:G:C5'	5:C:73:LEU:HD23	2.43	0.49
13:K:22:ASP:O	13:K:110:LYS:HE3	2.13	0.49
1:0:1525:G:H5'	1:0:1526:A:OP2	2.13	0.48
1:0:1996:U:O2'	1:0:1997:A:H5'	2.13	0.48
1:0:2667:G:H1'	1:0:2914:A:N3	2.27	0.48
2:9:92:G:H2'	2:9:93:A:H8	1.78	0.48
6:D:36:ASN:HA	39:D:7500:HOH:O	2.12	0.48
12:J:130:VAL:HG12	12:J:131:THR:N	2.28	0.48
15:M:58:GLN:HG3	39:M:8905:HOH:O	2.11	0.48
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.47	0.48
27:Y:216:ARG:HD2	39:Y:8868:HOH:O	2.13	0.48
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:138:U:H5''	1:0:139:C:OP2	2.14	0.48
1:0:2672:C:H1'	39:B:9104:HOH:O	2.12	0.48
1:0:666:A:H2'	1:0:667:C:O4'	2.14	0.48
29:1:28:HIS:HD2	29:1:30:LYS:H	1.60	0.48
39:0:7653:HOH:O	3:A:11:ARG:HA	2.13	0.48
8:F:36:THR:HG23	8:F:97:ALA:HB2	1.94	0.48
20:R:132:ARG:HG2	20:R:133:ALA:N	2.28	0.48
24:V:12:THR:HG23	24:V:14:ALA:N	2.28	0.48
1:0:1477:C:H5'	1:0:1868:G:C5'	2.43	0.48
1:0:1741:U:H5'	1:0:1742:A:OP1	2.13	0.48
1:0:1942:A:H3'	39:0:7777:HOH:O	2.13	0.48
1:0:304:G:H1'	1:0:347:A:N6	2.28	0.48
6:D:35:ALA:N	39:D:5576:HOH:O	2.46	0.48
7:E:85:GLU:HG3	7:E:169:THR:OG1	2.13	0.48
12:J:19:MET:HE3	12:J:132:LEU:CD2	2.34	0.48
15:M:164:THR:HG23	15:M:165:GLY:N	2.26	0.48
1:0:656:G:C5'	17:O:3:THR:HG22	2.40	0.48
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.46	0.48
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.11	0.48
1:0:1120:U:H6	1:0:1120:U:H5''	1.78	0.48
1:0:1166:A:H1'	1:0:1192:A:C2	2.48	0.48
1:0:2064:U:H5'	1:0:2652:U:O3'	2.13	0.48
1:0:2769:C:O2'	1:0:2770:G:H5'	2.13	0.48
1:0:462:A:H2'	39:0:5343:HOH:O	2.14	0.48
1:0:57:C:H5''	39:0:7195:HOH:O	2.12	0.48
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.95	0.48
24:V:23:LEU:HD12	24:V:56:ILE:HD12	1.95	0.48
25:W:48:VAL:HG12	25:W:48:VAL:O	2.13	0.48
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.12	0.48
1:0:558:C:C2'	1:0:559:U:C5'	2.90	0.48
10:H:66:GLU:HA	39:H:9031:HOH:O	2.13	0.48
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.94	0.48
25:W:139:GLY:O	25:W:141:HIS:CD2	2.65	0.48
1:0:1053:G:OP1	10:H:15:PRO:HG3	2.13	0.48
5:C:180:SER:HB2	39:C:8651:HOH:O	2.13	0.48
5:C:168:ARG:NH2	5:C:190:ALA:O	2.47	0.48
2:9:30:C:OP1	6:D:137:PRO:O	2.31	0.48
6:D:155:HIS:NE2	39:D:7597:HOH:O	2.31	0.48
7:E:133:VAL:HG12	7:E:141:VAL:HG13	1.96	0.48
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.96	0.48
10:H:141:CYS:HB2	39:H:8994:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:13:ASP:OD1	12:J:15:ARG:HB3	2.14	0.48
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.95	0.48
1:0:1427:A:H61	1:0:1440:U:H1'	1.79	0.48
1:0:292:G:H2'	1:0:358:G:N2	2.29	0.48
1:0:377:C:H5	39:0:3795:HOH:O	1.97	0.48
1:0:447:A:OP1	22:T:2:LYS:HG2	2.13	0.48
6:D:149:ARG:NH2	39:D:3066:HOH:O	2.45	0.48
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.13	0.48
8:F:26:THR:HG21	8:F:102:GLY:C	2.34	0.48
15:M:64:ARG:HD2	39:M:8884:HOH:O	2.14	0.48
22:T:40:VAL:HG22	22:T:41:ARG:N	2.29	0.48
27:Y:149:GLN:NE2	39:Y:8900:HOH:O	2.41	0.48
1:0:1185:U:H2'	1:0:1186:C:C6	2.49	0.48
1:0:1878:G:O2'	1:0:1879:U:OP2	2.31	0.48
1:0:1874:U:H2'	3:A:120:ARG:HG3	1.96	0.48
6:D:37:ALA:O	6:D:40:ILE:HG12	2.13	0.48
1:0:2036:C:C1'	13:K:44:LEU:HG	2.43	0.48
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.14	0.48
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.14	0.48
21:S:57:THR:CG2	21:S:58:MET:N	2.76	0.48
1:0:814:G:H4'	39:0:3620:HOH:O	2.12	0.48
3:A:36:ASP:HB2	3:A:85:SER:H	1.79	0.48
4:B:195:ARG:HD2	4:B:324:ASP:OD1	2.13	0.48
6:D:75:LEU:HD22	6:D:79:MET:HB3	1.96	0.48
7:E:80:TRP:O	7:E:134:SER:HA	2.13	0.48
2:9:8:G:O6	16:N:11:ARG:NH1	2.46	0.48
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.14	0.48
23:U:52:THR:CG2	23:U:54:THR:HB	2.44	0.48
39:0:5740:HOH:O	25:W:122:ARG:NH2	2.46	0.48
1:0:1132:A:N6	1:0:1229:C:H2'	2.29	0.48
1:0:644:G:N3	1:0:644:G:H5'	2.29	0.48
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.44	0.48
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.42	0.48
13:K:30:LYS:O	13:K:55:VAL:HG13	2.14	0.48
1:0:654:A:OP2	17:O:38:ARG:HD3	2.14	0.48
18:P:97:ARG:HD2	39:P:162:HOH:O	2.13	0.48
39:0:7437:HOH:O	19:Q:9:GLY:HA2	2.13	0.48
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.77	0.48
1:0:1527:A:H1'	1:0:1528:A:C8	2.48	0.47
1:0:2456:A:H2'	1:0:2457:U:C6	2.49	0.47
39:0:7978:HOH:O	31:3:60:LYS:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:49:G:H2'	2:9:50:G:O4'	2.14	0.47
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.95	0.47
5:C:104:ASP:HA	5:C:107:ARG:NH1	2.29	0.47
6:D:40:ILE:HG13	6:D:41:LEU:N	2.29	0.47
7:E:101:GLU:HB2	7:E:116:THR:O	2.13	0.47
18:P:104:LYS:HE2	18:P:138:GLU:OE2	2.14	0.47
24:V:39:ALA:O	24:V:41:GLU:N	2.47	0.47
1:0:1014:A:H2'	1:0:1015:C:H5'	1.95	0.47
1:0:1730:G:C5'	1:0:1731:C:H6	2.27	0.47
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.14	0.47
1:0:1819:G:H2'	1:0:1820:G:C4'	2.41	0.47
1:0:1878:G:O2'	1:0:1879:U:C6	2.63	0.47
1:0:1882:C:OP1	3:A:192:VAL:HG23	2.14	0.47
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.13	0.47
1:0:2809:G:H2'	1:0:2810:G:O4'	2.15	0.47
1:0:951:A:C2'	1:0:952:G:H5'	2.44	0.47
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.96	0.47
10:H:169:GLU:C	39:H:8993:HOH:O	2.51	0.47
11:I:105:GLU:HA	11:I:108:HIS:CE1	2.49	0.47
13:K:125:ALA:C	13:K:127:ALA:H	2.17	0.47
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.62	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.47
1:0:396:U:OP2	31:3:38:ARG:HD2	2.15	0.47
31:3:3:MET:O	31:3:90:PHE:HA	2.14	0.47
4:B:71:VAL:HG11	4:B:296:LEU:HD22	1.96	0.47
13:K:63:GLU:HG2	39:K:6344:HOH:O	2.14	0.47
39:K:1387:HOH:O	23:U:20:MET:HE3	2.14	0.47
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.95	0.47
24:V:44:GLY:O	24:V:48:GLU:HG2	2.14	0.47
1:0:1056:U:H2'	1:0:1057:A:O4'	2.13	0.47
1:0:1441:G:H1'	39:0:8267:HOH:O	2.15	0.47
1:0:1641:A:C2'	1:0:1642:A:H5'	2.44	0.47
1:0:2787:C:H5	39:0:5098:HOH:O	1.96	0.47
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.49	0.47
3:A:130:THR:HB	3:A:137:VAL:HB	1.95	0.47
3:A:220:PRO:HD2	3:A:223:ARG:HD3	1.96	0.47
5:C:142:ASP:OD1	5:C:236:THR:HG23	2.14	0.47
6:D:24:HIS:HB2	6:D:72:LYS:HB3	1.97	0.47
16:N:65:ASP:HB3	39:N:8821:HOH:O	2.14	0.47
25:W:5:VAL:HG11	25:W:153:MET:CE	2.44	0.47
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:187:VAL:HG22	27:Y:192:ASP:HB2	1.95	0.47
1:0:1342:C:O2'	1:0:1343:C:H5'	2.14	0.47
1:0:185:G:H4'	1:0:186:A:H4'	1.96	0.47
1:0:1926:G:H2'	1:0:1927:A:C8	2.49	0.47
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.44	0.47
1:0:1167:G:H2'	1:0:1168:C:O4'	2.15	0.47
1:0:1667:A:H2'	1:0:1668:U:C6	2.50	0.47
1:0:2133:U:H4'	1:0:2134:G:H5'	1.95	0.47
1:0:2896:A:N3	1:0:2896:A:H2'	2.29	0.47
6:D:170:TYR:O	6:D:171:ASP:CB	2.61	0.47
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.49	0.47
23:U:44:ARG:HB3	39:U:3805:HOH:O	2.15	0.47
1:0:1206:U:H2'	1:0:1207:A:O4'	2.15	0.47
1:0:1419:U:H5'	1:0:1420:C:OP2	2.14	0.47
1:0:1943:C:O4'	3:A:212:PRO:HA	2.15	0.47
1:0:737:A:H2'	1:0:738:G:O4'	2.15	0.47
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.61	0.47
4:B:85:ARG:HB2	4:B:99:GLU:HG2	1.95	0.47
6:D:172:VAL:HG12	6:D:173:GLU:N	2.29	0.47
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.97	0.47
16:N:171:HIS:CE1	39:N:8863:HOH:O	2.68	0.47
17:O:23:GLY:C	39:O:3062:HOH:O	2.52	0.47
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.97	0.47
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.14	0.47
26:X:78:GLU:HG2	26:X:79:GLU:H	1.79	0.47
1:0:553:G:P	27:Y:204:ARG:HH22	2.37	0.47
1:0:1086:A:N6	25:W:11:VAL:HG11	2.30	0.47
1:0:1291:A:H2	39:O:5743:HOH:O	1.97	0.47
1:0:2251:G:H2'	1:0:2252:A:C8	2.50	0.47
1:0:282:C:H1'	1:0:368:C:H42	1.79	0.47
4:B:205:VAL:O	4:B:307:ARG:NE	2.46	0.47
15:M:98:GLN:O	15:M:102:GLU:HG3	2.14	0.47
15:M:169:ARG:NH1	39:M:8871:HOH:O	2.47	0.47
4:B:81:ALA:O	4:B:186:GLY:HA3	2.14	0.47
6:D:35:ALA:C	6:D:37:ALA:H	2.18	0.47
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.97	0.47
11:I:67:VAL:HG13	11:I:68:PRO:HD2	1.97	0.47
11:I:87:PRO:O	11:I:89:GLU:HG3	2.15	0.47
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.80	0.47
1:0:1593:C:OP1	18:P:117:SER:CB	2.63	0.47
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2672:C:O2'	1:0:2673:U:H5'	2.15	0.47
1:0:285:A:H2'	1:0:286:U:O4'	2.15	0.47
1:0:553:G:OP2	27:Y:204:ARG:NH2	2.47	0.47
6:D:92:GLU:HB2	39:D:3862:HOH:O	2.14	0.47
2:9:51:A:H5'	16:N:160:SER:CB	2.45	0.47
25:W:125:HIS:HE1	39:W:3071:HOH:O	1.97	0.47
1:0:1159:G:H21	1:0:1189:A:H8	1.63	0.47
1:0:1506:U:H6	1:0:1506:U:H5'	1.80	0.47
1:0:157:G:H4'	15:M:95:LYS:HE2	1.97	0.47
1:0:2505:G:C2'	1:0:2506:A:H5'	2.44	0.47
1:0:2591:C:H2'	1:0:2592:G:O4'	2.15	0.47
5:C:12:THR:HB	39:C:8646:HOH:O	2.14	0.47
5:C:118:THR:CG2	5:C:137:PRO:HB3	2.44	0.47
9:G:14:GLU:HB3	39:G:4173:HOH:O	2.14	0.47
10:H:161:THR:HB	10:H:162:PRO:HD3	1.97	0.47
11:I:75:LYS:HD3	11:I:81:GLU:O	2.15	0.47
39:O:6693:HOH:O	23:U:56:ARG:HD3	2.15	0.47
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.97	0.47
1:0:1130:U:H2'	1:0:1131:G:O4'	2.15	0.46
1:0:12:U:H2'	1:0:13:G:H5'	1.97	0.46
1:0:1535:G:H2'	1:0:1536:C:C6	2.50	0.46
1:0:2507:G:H2'	1:0:2510:C:N4	2.30	0.46
1:0:2506:A:O2'	1:0:2507:G:O5'	2.34	0.46
1:0:255:A:H2'	1:0:256:C:C6	2.50	0.46
1:0:2769:C:H2'	1:0:2770:G:O4'	2.15	0.46
4:B:238:ASN:ND2	4:B:240:GLY:H	2.00	0.46
5:C:142:ASP:OD1	5:C:237:GLU:HB3	2.15	0.46
10:H:119:ALA:O	10:H:120:PHE:C	2.54	0.46
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.15	0.46
16:N:152:GLU:HA	16:N:152:GLU:OE1	2.15	0.46
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.34	0.46
1:0:1666:C:C2'	1:0:1667:A:H5''	2.44	0.46
1:0:2851:G:C2'	1:0:2852:A:H5'	2.45	0.46
4:B:241:PRO:HD2	39:B:9125:HOH:O	2.15	0.46
7:E:81:GLU:HG2	7:E:134:SER:CB	2.45	0.46
1:0:1185:U:OP1	11:I:121:LYS:HD3	2.15	0.46
13:K:113:ILE:HG22	13:K:114:ALA:N	2.29	0.46
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.48	0.46
1:0:2716:G:H5''	4:B:206:THR:CG2	2.41	0.46
3:A:109:GLU:HG2	3:A:116:GLY:H	1.81	0.46
5:C:236:THR:HG22	5:C:239:ALA:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:114:VAL:HG11	39:L:8865:HOH:O	2.14	0.46
15:M:167:GLY:O	15:M:171:ARG:HG3	2.15	0.46
26:X:76:ARG:O	26:X:77:PHE:HB3	2.15	0.46
1:O:2265:U:H2'	1:O:2266:A:C8	2.51	0.46
1:O:2807:U:P	4:B:27:ASN:HD21	2.39	0.46
1:O:317:A:H4'	39:O:4251:HOH:O	2.16	0.46
5:C:153:VAL:O	5:C:157:LEU:HG	2.16	0.46
6:D:94:ALA:HA	6:D:174:VAL:O	2.15	0.46
16:N:179:LEU:HA	16:N:184:ILE:HD12	1.97	0.46
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.98	0.46
21:S:38:ALA:O	21:S:42:GLU:HG3	2.16	0.46
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.63	0.46
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.15	0.46
1:O:1172:G:H1'	39:O:5430:HOH:O	2.15	0.46
1:O:1211:G:O2'	1:O:1212:C:H5'	2.15	0.46
1:O:1333:U:H2'	1:O:1334:C:C6	2.51	0.46
1:O:1500:U:P	18:P:41:ARG:HH22	2.38	0.46
1:O:1687:C:O2	29:1:9:GLY:HA2	2.16	0.46
5:C:140:VAL:HG12	5:C:141:SER:N	2.31	0.46
14:L:143:THR:HG22	14:L:144:ASP:H	1.76	0.46
14:L:21:ARG:N	39:L:8826:HOH:O	2.47	0.46
15:M:166:ALA:HA	15:M:169:ARG:NH1	2.30	0.46
2:9:6:C:C5'	16:N:37:ARG:HH12	2.19	0.46
20:R:82:GLU:HG3	20:R:83:LYS:N	2.30	0.46
1:O:2256:G:H2'	1:O:2257:G:C5'	2.46	0.46
1:O:2526:C:O2'	1:O:2527:U:H5'	2.16	0.46
1:O:426:G:H2'	1:O:427:C:O4'	2.16	0.46
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.97	0.46
22:T:71:VAL:HG13	22:T:91:LEU:O	2.15	0.46
25:W:38:THR:HG22	25:W:39:ASP:H	1.80	0.46
1:O:1419:U:H2'	1:O:1685:A:C2	2.51	0.46
3:A:51:ARG:NH1	3:A:120:ARG:O	2.49	0.46
1:O:894:A:C2	5:C:87:ARG:NH2	2.83	0.46
7:E:34:TRP:O	12:J:127:ILE:HD11	2.15	0.46
10:H:49:GLN:HG3	10:H:140:TYR:CD2	2.51	0.46
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.46	0.46
1:O:1279:U:O2	1:O:1279:U:H2'	2.15	0.46
1:O:1603:A:H5''	1:O:1605:G:H5'	1.96	0.46
1:O:317:A:H5''	22:T:52:ARG:HD2	1.98	0.46
1:O:475:G:OP1	5:C:73:LEU:HD22	2.16	0.46
8:F:46:GLU:O	8:F:73:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:39:THR:HG22	20:R:41:GLY:N	2.30	0.46
1:0:1497:G:H4'	1:0:1627:G:O2'	2.16	0.46
1:0:1625:U:H5''	39:0:6473:HOH:O	2.16	0.46
1:0:2300:A:H4'	1:0:2301:A:O5'	2.16	0.46
1:0:2626:C:H2'	1:0:2627:G:C8	2.51	0.46
1:0:2911:C:H2'	1:0:2912:C:C6	2.51	0.46
1:0:470:U:O2'	29:1:16:HIS:CD2	2.65	0.46
1:0:484:A:N1	1:0:506:G:H4'	2.31	0.46
5:C:19:PRO:HG2	5:C:22:PHE:CD1	2.51	0.46
12:J:88:PRO:O	12:J:94:GLY:HA3	2.16	0.46
15:M:69:LYS:HG2	15:M:127:LYS:HG3	1.98	0.46
17:O:26:TRP:HB2	39:O:3062:HOH:O	2.15	0.46
1:0:1025:C:H5'	25:W:23:MET:O	2.16	0.46
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.15	0.46
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.66	0.46
1:0:1044:C:H5''	39:0:9520:HOH:O	2.15	0.46
1:0:1295:G:H5''	14:L:14:GLY:O	2.16	0.46
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.97	0.46
1:0:2256:G:H2'	1:0:2257:G:H5'	1.98	0.46
1:0:420:U:H2'	1:0:421:C:C6	2.51	0.46
11:I:94:ASP:O	11:I:95:LEU:HD23	2.16	0.46
14:L:73:VAL:HG23	14:L:74:THR:N	2.30	0.46
14:L:97:VAL:HG12	14:L:98:GLU:O	2.16	0.46
15:M:47:ASP:CG	15:M:48:LYS:N	2.69	0.46
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.64	0.46
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.31	0.46
1:0:2266:A:OP2	15:M:90:ARG:NH2	2.49	0.45
1:0:2502:C:H2'	1:0:2503:A:H5'	1.98	0.45
1:0:2720:C:O2	13:K:87:ARG:NH2	2.50	0.45
3:A:81:GLN:HB2	3:A:92:ASN:HD22	1.81	0.45
4:B:14:GLY:HA2	4:B:15:PRO:C	2.36	0.45
6:D:101:THR:HG22	39:D:7400:HOH:O	2.15	0.45
7:E:31:ARG:NH1	7:E:68:HIS:CG	2.84	0.45
11:I:124:VAL:HG13	11:I:134:ILE:HD11	1.99	0.45
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.49	0.45
14:L:145:LEU:O	14:L:145:LEU:HD23	2.16	0.45
25:W:38:THR:O	25:W:42:ARG:HB2	2.15	0.45
1:0:1741:U:O2'	1:0:2723:G:H4'	2.16	0.45
1:0:629:A:H2'	1:0:630:A:O4'	2.16	0.45
2:9:49:G:O2'	2:9:50:G:H5'	2.16	0.45
1:0:875:A:C2	3:A:194:MET:SD	3.10	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:24:PRO:HG3	4:B:204:GLY:HA2	1.98	0.45
5:C:118:THR:HG23	39:C:8504:HOH:O	2.15	0.45
22:T:32:ARG:HH12	22:T:38:ARG:HH12	1.64	0.45
23:U:47:ARG:HG2	39:U:4381:HOH:O	2.15	0.45
24:V:7:GLU:O	24:V:11:MET:HG3	2.16	0.45
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.31	0.45
1:O:2415:A:O2'	16:N:29:SER:HB3	2.17	0.45
1:O:2421:G:H3'	1:O:2422:U:H5''	1.98	0.45
39:O:6804:HOH:O	3:A:205:GLY:HA3	2.16	0.45
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.47	0.45
4:B:294:TYR:HE2	39:B:9120:HOH:O	1.98	0.45
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.97	0.45
11:I:134:ILE:HG22	11:I:135:GLU:N	2.31	0.45
14:L:57:VAL:HG12	14:L:57:VAL:O	2.17	0.45
20:R:119:VAL:HG12	20:R:119:VAL:O	2.16	0.45
1:O:1589:G:N2	1:O:1605:G:H1'	2.31	0.45
1:O:2781:U:H2'	1:O:2782:G:H5'	1.99	0.45
6:D:27:ILE:HD11	6:D:37:ALA:HB3	1.99	0.45
6:D:59:GLY:O	6:D:61:PHE:N	2.47	0.45
1:O:1205:U:H2'	1:O:1206:U:H5'	1.99	0.45
1:O:2112:A:H2'	1:O:2113:G:C8	2.52	0.45
2:9:28:U:H2'	2:9:29:C:C6	2.52	0.45
2:9:52:A:H2'	2:9:53:G:O4'	2.17	0.45
3:A:128:LEU:HG	39:A:9038:HOH:O	2.15	0.45
3:A:132:ASP:OD1	3:A:133:ARG:N	2.48	0.45
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.99	0.45
4:B:277:GLU:N	4:B:278:PRO:HD2	2.31	0.45
7:E:6:GLU:HA	7:E:46:THR:HG22	1.98	0.45
9:G:27:ILE:HD13	9:G:71:LEU:HD23	1.98	0.45
14:L:119:THR:HG23	14:L:139:SER:OG	2.17	0.45
15:M:81:ARG:HG3	15:M:85:ARG:HB2	1.98	0.45
16:N:37:ARG:CZ	39:N:8832:HOH:O	2.64	0.45
19:Q:11:ARG:NH1	39:Q:5620:HOH:O	2.49	0.45
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.37	0.45
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.40	0.45
27:Y:174:VAL:HG12	27:Y:174:VAL:O	2.17	0.45
1:O:2032:U:H5'	39:O:4980:HOH:O	2.16	0.45
1:O:2421:G:H3'	1:O:2422:U:C5'	2.47	0.45
1:O:2064:U:H4'	1:O:2653:A:OP1	2.16	0.45
1:O:558:C:H5'	39:O:5710:HOH:O	2.16	0.45
1:O:820:G:C6	3:A:171:LYS:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.82	0.45
4:B:304:PRO:HD2	4:B:307:ARG:NE	2.32	0.45
4:B:305:ASP:O	4:B:306:LYS:CB	2.62	0.45
6:D:63:ILE:HG13	6:D:64:ARG:N	2.32	0.45
6:D:96:SER:C	6:D:98:PHE:H	2.20	0.45
10:H:50:ILE:HD12	10:H:149:VAL:CG1	2.47	0.45
15:M:99:ARG:HE	15:M:170:ASN:ND2	2.15	0.45
17:O:21:SER:OG	17:O:106:PRO:HB2	2.17	0.45
20:R:114:VAL:HA	20:R:144:GLU:O	2.16	0.45
1:O:1878:G:O2'	1:O:1879:U:P	2.75	0.45
1:O:1979:G:H2'	39:O:3782:HOH:O	2.16	0.45
1:O:932:U:H2'	1:O:933:C:C6	2.52	0.45
1:O:2717:C:OP1	4:B:207:LYS:HG3	2.17	0.45
7:E:3:VAL:CG2	7:E:49:ILE:HB	2.42	0.45
14:L:10:SER:O	14:L:11:ARG:HB3	2.17	0.45
14:L:143:THR:CG2	14:L:144:ASP:N	2.77	0.45
16:N:72:GLU:H	16:N:171:HIS:HE1	1.65	0.45
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.46	0.45
1:O:1163:G:N2	39:O:5189:HOH:O	2.49	0.45
1:O:1406:A:H4'	1:O:1407:A:H5''	1.98	0.45
1:O:2649:A:H5'	1:O:2649:A:H8	1.81	0.45
1:O:2756:U:N3	1:O:2896:A:C2	2.75	0.45
2:9:24:U:H3'	2:9:25:G:H5'	1.98	0.45
5:C:107:ARG:NH2	39:C:8661:HOH:O	2.47	0.45
10:H:33:GLN:H	10:H:69:ARG:HH11	1.65	0.45
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.99	0.45
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.99	0.45
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.98	0.45
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.52	0.45
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.47	0.45
20:R:29:LYS:HD3	39:R:8937:HOH:O	2.17	0.45
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.99	0.45
1:O:1174:A:C5	1:O:1201:C:H4'	2.52	0.45
1:O:1947:G:H2'	1:O:1948:G:C8	2.51	0.45
1:O:2852:A:H5''	39:O:5686:HOH:O	2.17	0.45
1:O:951:A:O2'	1:O:952:G:H5'	2.17	0.45
31:3:30:GLN:NE2	39:3:8980:HOH:O	2.45	0.45
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.81	0.45
1:O:1943:C:H4'	3:A:211:LYS:O	2.16	0.45
5:C:27:ARG:HG2	5:C:30:LEU:CD1	2.46	0.45
6:D:76:ARG:O	6:D:77:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:18:LEU:HD13	7:E:34:TRP:CG	2.52	0.45
9:G:67:LEU:O	9:G:71:LEU:HG	2.16	0.45
15:M:99:ARG:HH21	15:M:170:ASN:ND2	2.11	0.45
39:K:7438:HOH:O	23:U:20:MET:HE1	2.16	0.45
1:O:1060:C:H6	1:O:1060:C:H5'	1.82	0.45
1:O:1592:G:O2'	1:O:1593:C:O4'	2.33	0.45
30:2:18:ASN:HD21	30:2:40:ARG:H	1.65	0.45
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.47	0.45
4:B:5:ARG:NH1	4:B:8:LYS:HE2	2.32	0.45
6:D:27:ILE:HD11	6:D:37:ALA:CB	2.47	0.45
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.98	0.45
9:G:69:ARG:NH1	39:G:3513:HOH:O	2.50	0.45
10:H:149:VAL:HG13	39:H:9028:HOH:O	2.16	0.45
18:P:134:VAL:O	18:P:137:LEU:HB3	2.18	0.45
18:P:141:ILE:C	18:P:143:ALA:H	2.19	0.45
1:O:2361:A:H5''	39:O:9501:HOH:O	2.17	0.44
1:O:1654:U:H2'	3:A:47:HIS:HD2	1.82	0.44
4:B:82:VAL:CG1	4:B:82:VAL:O	2.65	0.44
5:C:35:VAL:HG21	5:C:227:GLY:HA2	1.98	0.44
7:E:11:VAL:HG13	7:E:23:GLU:O	2.17	0.44
7:E:116:THR:CG2	7:E:151:LEU:HD22	2.45	0.44
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.47	0.44
1:O:1007:A:H2'	10:H:22:TYR:CZ	2.52	0.44
1:O:2866:U:H4'	1:O:2867:G:H5'	1.98	0.44
1:O:969:G:H1	1:O:999:C:H42	1.65	0.44
3:A:192:VAL:HG12	3:A:207:GLN:CB	2.47	0.44
14:L:143:THR:HG21	39:L:8833:HOH:O	2.18	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.80	0.44
1:O:1555:G:H4'	1:O:1630:A:H2	1.82	0.44
1:O:1755:A:H2'	1:O:1756:G:O4'	2.17	0.44
1:O:2256:G:C2'	1:O:2257:G:H5'	2.47	0.44
1:O:380:A:H2'	39:O:7660:HOH:O	2.16	0.44
1:O:960:G:C2'	1:O:960:G:N3	2.80	0.44
5:C:150:THR:HA	5:C:203:ALA:O	2.17	0.44
5:C:16:VAL:HG12	5:C:17:ASP:N	2.31	0.44
1:O:1150:A:C2	9:G:20:VAL:HG21	2.52	0.44
16:N:154:LEU:C	16:N:156:GLU:H	2.20	0.44
23:U:9:CYS:O	23:U:52:THR:HG23	2.16	0.44
25:W:52:VAL:HG22	25:W:53:ALA:H	1.82	0.44
1:O:2003:U:H4'	1:O:2004:U:H5	1.82	0.44
1:O:204:A:C2'	1:O:205:U:H5'	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:524:A:C5'	20:R:29:LYS:HE2	2.47	0.44
25:W:38:THR:HB	39:W:5390:HOH:O	2.17	0.44
1:0:308:U:C4	1:0:342:C:H1'	2.52	0.44
1:0:488:U:H2'	39:0:4480:HOH:O	2.17	0.44
4:B:217:ARG:HG3	4:B:257:THR:CG2	2.48	0.44
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.32	0.44
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.50	0.44
6:D:167:GLU:C	6:D:169:THR:H	2.21	0.44
25:W:41:TYR:HA	25:W:44:MET:HE3	1.99	0.44
1:0:2104:C:O2	1:0:2485:A:N1	2.51	0.44
1:0:2756:U:N3	1:0:2896:A:H2	2.13	0.44
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.52	0.44
31:3:91:GLN:O	31:3:92:GLU:HB2	2.17	0.44
2:9:50:G:H5''	16:N:159:TYR:HE1	1.83	0.44
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.53	0.44
4:B:41:PHE:HA	4:B:79:MET:CE	2.46	0.44
5:C:46:TYR:CE2	5:C:98:ARG:NH1	2.86	0.44
6:D:35:ALA:C	6:D:37:ALA:N	2.71	0.44
7:E:84:MET:HE1	7:E:148:ILE:HD12	2.00	0.44
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.30	0.44
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.98	0.44
16:N:15:GLU:HB2	16:N:17:ARG:HG3	1.98	0.44
17:O:98:LEU:O	17:O:102:ILE:HG13	2.17	0.44
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.53	0.44
1:0:1131:G:C6	1:0:1230:A:C4	3.06	0.44
1:0:1137:G:H1'	39:0:4354:HOH:O	2.17	0.44
1:0:1882:C:O2'	1:0:2012:U:OP2	2.33	0.44
1:0:559:U:H2'	1:0:560:U:O4'	2.17	0.44
3:A:153:ARG:HD3	39:A:8995:HOH:O	2.16	0.44
6:D:146:LYS:NZ	16:N:107:ASN:ND2	2.64	0.44
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.33	0.44
16:N:154:LEU:O	16:N:155:GLU:CB	2.66	0.44
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.72	0.44
25:W:11:VAL:O	25:W:12:ASN:HB2	2.16	0.44
1:0:1044:C:H3'	1:0:1045:G:H5''	1.99	0.44
1:0:138:U:OP2	1:0:139:C:H5	2.00	0.44
1:0:2642:G:H2'	1:0:2643:G:O4'	2.18	0.44
1:0:2793:A:H2'	1:0:2794:G:H5'	1.99	0.44
3:A:81:GLN:H	3:A:92:ASN:ND2	2.16	0.44
2:9:57:A:C8	6:D:141:VAL:HG21	2.53	0.44
6:D:49:PRO:HA	6:D:73:VAL:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:46:GLU:N	39:F:3461:HOH:O	2.51	0.44
10:H:81:GLY:C	10:H:83:GLU:H	2.21	0.44
22:T:75:GLU:O	22:T:76:ASP:HB2	2.18	0.44
22:T:79:LEU:HG	22:T:89:ARG:HB2	1.98	0.44
1:0:1307:A:H2'	1:0:1308:A:C8	2.53	0.44
6:D:64:ARG:HG2	6:D:67:ASP:HB3	2.00	0.44
7:E:132:THR:HB	39:E:2227:HOH:O	2.17	0.44
12:J:90:LYS:HB2	36:J:8802:CL:CL	2.54	0.44
21:S:11:THR:H	21:S:14:ALA:HB3	1.81	0.44
26:X:25:ARG:CG	39:X:5356:HOH:O	2.65	0.44
1:0:1119:G:C8	12:J:52:GLN:NE2	2.86	0.43
1:0:1181:A:N1	1:0:1192:A:O2'	2.50	0.43
1:0:1946:C:H2'	1:0:1971:G:C8	2.53	0.43
1:0:2524:G:H21	1:0:2526:C:N4	2.16	0.43
4:B:108:GLU:HB3	4:B:111:ARG:HD2	2.00	0.43
9:G:19:GLU:O	9:G:23:ILE:HG13	2.18	0.43
12:J:19:MET:HE2	12:J:132:LEU:HD11	1.99	0.43
23:U:17:THR:HG21	39:U:3194:HOH:O	2.17	0.43
25:W:119:HIS:HD2	25:W:120:PRO:O	2.01	0.43
27:Y:95:THR:N	27:Y:236:VAL:O	2.51	0.43
1:0:1252:A:H2'	1:0:1253:C:O4'	2.19	0.43
1:0:1393:A:H2'	1:0:1394:C:C6	2.53	0.43
1:0:432:G:O2'	1:0:433:C:H5'	2.18	0.43
1:0:559:U:H5'	1:0:559:U:C6	2.41	0.43
3:A:223:ARG:NE	39:A:9037:HOH:O	2.51	0.43
4:B:51:VAL:HG23	4:B:327:VAL:HG13	1.98	0.43
1:0:392:U:C5'	15:M:193:LYS:HB3	2.49	0.43
27:Y:115:ARG:HH11	27:Y:115:ARG:HB3	1.83	0.43
1:0:1119:G:C6	1:0:1244:U:C5	3.06	0.43
1:0:1730:G:H5'	1:0:1731:C:H5	1.81	0.43
1:0:1733:A:H4'	4:B:212:GLN:HA	1.99	0.43
1:0:2864:U:O2'	1:0:2865:G:H5'	2.18	0.43
10:H:168:VAL:HG13	39:H:9009:HOH:O	2.17	0.43
12:J:107:ASN:HD22	12:J:108:PRO:N	2.16	0.43
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.19	0.43
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.18	0.43
1:0:2115:U:H2'	1:0:2116:U:C6	2.53	0.43
1:0:2526:C:H5'	1:0:2526:C:C6	2.53	0.43
1:0:517:U:H1'	39:0:7997:HOH:O	2.18	0.43
1:0:542:A:H2'	1:0:543:G:O4'	2.18	0.43
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:57:THR:O	10:H:58:VAL:HG13	2.19	0.43
11:I:67:VAL:CG1	11:I:68:PRO:HD2	2.48	0.43
13:K:113:ILE:CG2	13:K:114:ALA:N	2.81	0.43
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.49	0.43
20:R:119:VAL:CG1	20:R:119:VAL:O	2.65	0.43
21:S:20:PHE:CD2	21:S:20:PHE:N	2.85	0.43
1:0:2090:G:H2'	1:0:2091:G:C8	2.53	0.43
1:0:2326:C:H4'	1:0:2412:G:C4'	2.49	0.43
1:0:2649:A:C8	1:0:2649:A:H5'	2.54	0.43
1:0:284:C:H4'	1:0:285:A:H8	1.83	0.43
1:0:790:A:H2'	1:0:791:A:O4'	2.18	0.43
1:0:920:C:H5'	1:0:921:G:C4	2.53	0.43
31:3:70:ARG:CG	31:3:77:ALA:HB2	2.47	0.43
12:J:45:VAL:HG22	12:J:46:ILE:N	2.33	0.43
14:L:122:ALA:HB3	14:L:125:PHE:CZ	2.54	0.43
16:N:73:ALA:N	39:N:8863:HOH:O	2.48	0.43
1:0:130:C:H5'	39:0:5666:HOH:O	2.18	0.43
1:0:1484:G:H2'	39:0:9594:HOH:O	2.17	0.43
1:0:2121:G:O2'	1:0:2122:C:H5'	2.19	0.43
1:0:2819:C:H2'	1:0:2820:A:C8	2.53	0.43
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.18	0.43
1:0:2868:C:H2'	1:0:2869:G:O4'	2.19	0.43
3:A:39:ALA:O	3:A:61:GLU:HG3	2.18	0.43
4:B:175:LEU:O	4:B:175:LEU:HD23	2.19	0.43
7:E:77:THR:OG1	7:E:78:GLU:N	2.51	0.43
13:K:28:GLU:HG2	13:K:58:THR:HB	2.00	0.43
16:N:77:ASN:OD1	16:N:80:SER:HB2	2.18	0.43
22:T:71:VAL:CG1	22:T:72:ILE:N	2.81	0.43
25:W:29:VAL:O	25:W:30:ASN:HB2	2.18	0.43
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.54	0.43
1:0:189:A:OP1	15:M:171:ARG:NH2	2.51	0.43
1:0:622:G:P	27:Y:148:GLY:HA3	2.58	0.43
1:0:920:C:H4'	1:0:921:G:C2	2.54	0.43
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.84	0.43
13:K:75:ARG:HD3	13:K:112:PRO:O	2.19	0.43
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.53	0.43
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.19	0.43
1:0:137:U:OP1	1:0:259:G:O2'	2.35	0.43
1:0:2031:C:H2'	1:0:2032:U:O4'	2.19	0.43
1:0:2256:G:O2'	1:0:2257:G:H5'	2.19	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:512:G:O3'	1:0:513:A:H8	2.02	0.43
3:A:125:ASN:CB	3:A:158:VAL:HG12	2.49	0.43
8:F:117:GLU:C	8:F:119:ARG:H	2.22	0.43
8:F:70:LYS:C	8:F:72:VAL:H	2.21	0.43
15:M:164:THR:CG2	15:M:165:GLY:N	2.82	0.43
6:D:149:ARG:HH12	16:N:15:GLU:HA	1.84	0.43
20:R:15:LYS:HE3	39:R:8984:HOH:O	2.18	0.43
1:0:1853:C:O2'	3:A:217:ARG:NH2	2.52	0.43
1:0:2133:U:H4'	1:0:2134:G:C5'	2.48	0.43
1:0:2403:C:OP1	19:Q:49:ASN:HB3	2.19	0.43
1:0:2326:C:H4'	1:0:2412:G:H4'	2.01	0.43
4:B:40:GLY:HA3	39:B:9118:HOH:O	2.19	0.43
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.54	0.43
4:B:53:LEU:HD11	4:B:327:VAL:HG22	2.01	0.43
5:C:166:ILE:HD11	5:C:207:LEU:HD13	2.01	0.43
7:E:86:VAL:CG1	7:E:129:GLU:HA	2.49	0.43
13:K:66:ARG:HH11	13:K:66:ARG:HG2	1.84	0.43
16:N:89:GLY:O	16:N:92:ALA:HB3	2.18	0.43
1:0:1335:C:OP2	27:Y:207:SER:HB3	2.18	0.43
1:0:1158:G:O2'	1:0:1159:G:H5'	2.19	0.43
1:0:1185:U:H5'	39:0:7891:HOH:O	2.18	0.43
1:0:2103:A:O2'	1:0:2104:C:H5'	2.19	0.43
3:A:186:TRP:CG	3:A:187:PRO:HA	2.54	0.43
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.49	0.43
6:D:20:LYS:HA	6:D:75:LEU:O	2.19	0.43
8:F:60:VAL:HG12	8:F:60:VAL:O	2.19	0.43
15:M:99:ARG:CD	15:M:167:GLY:HA2	2.49	0.43
19:Q:55:ARG:HD2	39:Q:2875:HOH:O	2.19	0.43
21:S:57:THR:HG22	21:S:59:ASP:HB2	2.01	0.43
22:T:18:GLU:O	22:T:21:LYS:HG2	2.19	0.43
1:0:1218:U:H2'	1:0:1219:U:C6	2.53	0.42
1:0:1768:C:H2'	1:0:1769:C:O4'	2.19	0.42
1:0:2316:G:H4'	39:0:6539:HOH:O	2.18	0.42
1:0:263:U:C2	8:F:59:ILE:CD1	3.02	0.42
1:0:2768:A:O2'	1:0:2769:C:H5'	2.19	0.42
1:0:451:C:O2'	1:0:452:G:H5'	2.19	0.42
2:9:56:A:C3'	2:9:57:A:H5''	2.48	0.42
7:E:15:GLN:HG3	7:E:20:ILE:HG12	2.00	0.42
7:E:22:VAL:O	7:E:28:SER:HA	2.19	0.42
8:F:111:ILE:O	8:F:115:VAL:HG23	2.18	0.42
11:I:123:VAL:C	11:I:125:GLY:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:88:GLN:HA	11:I:91:PHE:HE2	1.84	0.42
1:O:524:A:H5'	20:R:29:LYS:HE2	2.01	0.42
1:O:56:G:H5''	24:V:50:ARG:NH1	2.33	0.42
1:O:1202:A:H2'	1:O:1203:G:O4'	2.19	0.42
1:O:2630:G:O6	3:A:206:ARG:NH2	2.49	0.42
1:O:241:A:C2	1:O:378:A:H4'	2.54	0.42
1:O:567:U:H5''	39:O:5740:HOH:O	2.19	0.42
3:A:107:ASN:OD1	3:A:120:ARG:HD2	2.19	0.42
3:A:135:VAL:N	39:A:9058:HOH:O	2.51	0.42
3:A:37:VAL:HG22	39:A:9059:HOH:O	2.19	0.42
6:D:37:ALA:HA	39:D:5583:HOH:O	2.19	0.42
8:F:32:GLY:N	39:F:3111:HOH:O	2.52	0.42
17:O:32:ARG:HH21	17:O:35:LYS:HD2	1.84	0.42
18:P:59:ARG:HD3	39:P:191:HOH:O	2.19	0.42
18:P:64:GLU:HG2	39:P:167:HOH:O	2.18	0.42
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.49	0.42
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.19	0.42
1:O:1287:A:O4'	25:W:117:ARG:HD3	2.20	0.42
1:O:1439:C:OP1	30:2:41:HIS:HE1	2.03	0.42
1:O:1573:A:H2'	1:O:1574:C:O4'	2.19	0.42
1:O:1846:U:O2'	3:A:172:ALA:HB2	2.19	0.42
1:O:2718:C:H5'	1:O:2718:C:C6	2.51	0.42
15:M:15:PRO:HA	15:M:20:LEU:HD23	2.01	0.42
16:N:37:ARG:NH2	39:N:8832:HOH:O	2.52	0.42
20:R:61:GLN:NE2	39:R:8944:HOH:O	2.53	0.42
25:W:35:VAL:HG23	25:W:41:TYR:CD2	2.54	0.42
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.42
26:X:43:VAL:HG12	26:X:44:ASP:H	1.84	0.42
1:O:1029:U:H5'	1:O:1031:G:N7	2.34	0.42
1:O:1066:U:H2'	1:O:1067:A:C8	2.54	0.42
1:O:1562:C:N4	39:O:6317:HOH:O	2.34	0.42
1:O:1948:G:H2'	1:O:1949:G:O4'	2.20	0.42
1:O:2353:A:H4'	1:O:2354:A:O5'	2.18	0.42
1:O:903:U:OP2	14:L:11:ARG:NH1	2.50	0.42
1:O:926:A:O2'	14:L:41:HIS:HD2	2.01	0.42
3:A:175:LYS:HE2	39:A:9040:HOH:O	2.19	0.42
5:C:246:ARG:NH2	39:C:8630:HOH:O	2.46	0.42
7:E:107:PHE:CZ	7:E:108:LEU:HD13	2.54	0.42
39:O:6168:HOH:O	13:K:87:ARG:NE	2.52	0.42
1:O:1940:C:H4'	39:O:7777:HOH:O	2.18	0.42
1:O:2478:U:O2'	1:O:2479:A:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:646:G:H2'	1:0:647:U:C6	2.54	0.42
1:0:669:G:O2'	1:0:670:G:H5'	2.19	0.42
1:0:1845:A:O3'	3:A:187:PRO:HB2	2.19	0.42
3:A:217:ARG:HH11	3:A:217:ARG:CG	2.33	0.42
4:B:139:ASP:HB2	39:B:8998:HOH:O	2.18	0.42
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.43	0.42
4:B:162:MET:HG3	4:B:310:ARG:HD3	2.01	0.42
5:C:133:ARG:NE	5:C:138:VAL:HG22	2.34	0.42
10:H:66:GLU:O	10:H:70:LEU:HB2	2.20	0.42
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.54	0.42
15:M:152:ALA:HB1	39:M:8934:HOH:O	2.20	0.42
1:0:392:U:H5''	15:M:193:LYS:HB3	2.01	0.42
20:R:104:PHE:HB2	20:R:109:MET:HE1	2.01	0.42
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.55	0.42
1:0:1406:A:H4'	1:0:1407:A:C5'	2.50	0.42
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.53	0.42
1:0:1626:A:H2'	1:0:1627:G:O4'	2.19	0.42
1:0:1925:G:O2'	1:0:1926:G:H5'	2.20	0.42
1:0:2781:U:C2'	1:0:2782:G:H5'	2.49	0.42
31:3:20:HIS:HA	31:3:70:ARG:O	2.19	0.42
2:9:59:C:H6	2:9:59:C:O5'	2.02	0.42
4:B:243:ASN:HA	4:B:244:PRO:C	2.39	0.42
7:E:43:ASP:HA	39:E:5864:HOH:O	2.18	0.42
8:F:99:THR:HG23	8:F:99:THR:O	2.20	0.42
9:G:64:ASN:N	9:G:64:ASN:ND2	2.68	0.42
12:J:26:VAL:HG13	12:J:36:VAL:HG11	2.01	0.42
14:L:92:ASP:HB3	14:L:95:ASP:OD2	2.19	0.42
21:S:57:THR:CG2	21:S:59:ASP:HB2	2.50	0.42
23:U:13:ILE:HG12	23:U:32:CYS:HB3	2.00	0.42
26:X:41:PHE:O	26:X:43:VAL:HG23	2.19	0.42
1:0:2442:G:H3'	39:0:7065:HOH:O	2.19	0.42
1:0:2754:G:H2'	1:0:2755:G:O4'	2.19	0.42
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.55	0.42
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.54	0.42
6:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.65	0.42
21:S:56:ASN:O	30:2:8:LYS:NZ	2.47	0.42
22:T:47:THR:HB	22:T:100:ASP:HB3	2.02	0.42
25:W:107:LEU:O	25:W:112:LEU:HB2	2.18	0.42
1:0:1902:G:H2'	1:0:1903:U:O4'	2.20	0.42
1:0:2401:A:H2'	1:0:2402:A:C8	2.55	0.42
1:0:962:C:H1'	16:N:5:ARG:HH12	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:23:ASN:HD21	13:K:107:THR:HB	1.83	0.42
1:O:926:A:O2'	14:L:41:HIS:CD2	2.73	0.42
14:L:6:ARG:NH2	39:L:8842:HOH:O	2.47	0.42
17:O:41:ALA:HA	39:O:5104:HOH:O	2.19	0.42
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.35	0.42
24:V:60:GLN:O	24:V:65:ASP:N	2.52	0.42
25:W:19:ASP:O	25:W:23:MET:HG3	2.20	0.42
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.54	0.42
28:Z:30:GLU:HA	28:Z:33:MET:HE3	2.01	0.42
1:O:1162:G:H1'	11:I:112:LEU:CD1	2.49	0.42
1:O:2072:G:H3'	1:O:2073:G:C5'	2.50	0.42
1:O:2578:G:C8	1:O:2578:G:H5'	2.51	0.42
1:O:441:A:H1'	1:O:442:A:N7	2.35	0.42
1:O:635:A:H2'	1:O:636:G:H5''	2.01	0.42
2:9:42:C:O2	6:D:76:ARG:NH1	2.53	0.42
3:A:135:VAL:HG11	3:A:147:ARG:NH1	2.35	0.42
5:C:219:ASN:N	5:C:222:ASP:OD1	2.52	0.42
5:C:219:ASN:O	5:C:222:ASP:OD1	2.37	0.42
5:C:78:ARG:CG	5:C:78:ARG:NH1	2.74	0.42
6:D:60:GLU:O	6:D:61:PHE:C	2.57	0.42
16:N:140:GLN:O	16:N:143:ARG:HB2	2.19	0.42
22:T:96:VAL:HG13	22:T:97:ARG:N	2.35	0.42
25:W:76:ASP:O	25:W:77:ALA:C	2.57	0.42
27:Y:117:LEU:HD12	27:Y:174:VAL:HG11	2.02	0.42
1:O:1209:C:H2'	1:O:1210:G:C8	2.51	0.42
1:O:1684:A:O2'	1:O:1685:A:H5''	2.19	0.42
1:O:214:U:H5'	39:O:6586:HOH:O	2.19	0.42
3:A:97:ALA:C	3:A:131:HIS:HE2	2.22	0.42
4:B:248:ARG:NH2	39:B:8993:HOH:O	2.50	0.42
7:E:24:GLY:HA3	7:E:76:VAL:HB	2.02	0.42
8:F:24:ARG:NH2	39:F:6800:HOH:O	2.48	0.42
12:J:46:ILE:HD11	12:J:53:ILE:HG23	2.01	0.42
15:M:145:ASP:HA	39:M:8909:HOH:O	2.19	0.42
15:M:5:TYR:HE2	15:M:46:LEU:HD13	1.84	0.42
16:N:64:SER:C	16:N:66:LEU:H	2.22	0.42
18:P:10:ALA:CA	18:P:13:VAL:HG12	2.46	0.42
1:O:1754:A:H2'	1:O:1755:A:O4'	2.20	0.41
1:O:304:G:H1'	1:O:347:A:H61	1.85	0.41
1:O:482:G:H4'	1:O:508:A:N1	2.35	0.41
1:O:776:A:H1'	1:O:779:U:O4	2.20	0.41
30:2:36:ASN:HB3	30:2:39:ARG:HG3	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:105:VAL:CG1	3:A:106:CYS:N	2.82	0.41
3:A:206:ARG:NH1	39:A:8979:HOH:O	2.53	0.41
4:B:132:HIS:CE1	4:B:171:VAL:HG21	2.55	0.41
5:C:138:VAL:O	5:C:234:VAL:HA	2.20	0.41
9:G:24:VAL:O	9:G:28:GLU:HB2	2.19	0.41
11:I:109:PRO:HG2	11:I:110:ASP:H	1.84	0.41
21:S:42:GLU:HG2	21:S:49:VAL:HG23	2.01	0.41
1:0:1197:G:N2	39:0:6679:HOH:O	2.52	0.41
1:0:1236:A:C8	12:J:63:ILE:HD11	2.55	0.41
1:0:1762:C:H4'	39:0:5120:HOH:O	2.21	0.41
1:0:2252:A:C5	1:0:2253:G:H1'	2.54	0.41
1:0:2336:G:H1'	39:D:5675:HOH:O	2.19	0.41
1:0:2453:G:H4'	14:L:50:GLY:C	2.40	0.41
1:0:2503:A:OP1	10:H:154:ARG:NH2	2.47	0.41
1:0:2756:U:C2	1:0:2896:A:H2	2.37	0.41
1:0:383:A:H2'	1:0:384:G:O4'	2.20	0.41
5:C:127:ARG:HG2	5:C:127:ARG:HH11	1.84	0.41
5:C:246:ARG:HB3	5:C:246:ARG:NH1	2.35	0.41
10:H:154:ARG:HA	10:H:157:TYR:CE2	2.55	0.41
10:H:72:ALA:HB2	10:H:156:ALA:HB2	2.02	0.41
15:M:99:ARG:NH2	15:M:170:ASN:HD22	2.15	0.41
18:P:63:ARG:NH2	39:P:191:HOH:O	2.51	0.41
20:R:114:VAL:HG13	20:R:114:VAL:O	2.20	0.41
25:W:146:ILE:HA	25:W:146:ILE:HD13	1.89	0.41
1:0:1657:A:H2'	1:0:1658:A:C8	2.55	0.41
1:0:1730:G:H5''	1:0:1731:C:C6	2.54	0.41
1:0:1980:U:O2	1:0:2008:U:H4'	2.20	0.41
1:0:2726:U:O2	1:0:2749:U:O5'	2.38	0.41
3:A:211:LYS:HD2	39:A:9081:HOH:O	2.21	0.41
4:B:189:ALA:HB1	39:B:9033:HOH:O	2.19	0.41
10:H:24:THR:O	10:H:123:ILE:HD12	2.20	0.41
10:H:146:ALA:O	10:H:149:VAL:HG12	2.20	0.41
11:I:129:SER:N	39:I:7330:HOH:O	2.47	0.41
12:J:42:GLU:O	12:J:131:THR:HG23	2.19	0.41
6:D:146:LYS:HZ1	16:N:107:ASN:HD21	1.64	0.41
16:N:154:LEU:HG	16:N:155:GLU:N	2.35	0.41
1:0:1118:A:C8	1:0:1119:G:H5''	2.54	0.41
1:0:1181:A:H2'	1:0:1182:C:C5'	2.50	0.41
1:0:2415:A:N3	16:N:26:LEU:HD13	2.36	0.41
1:0:2547:C:OP2	4:B:5:ARG:NH1	2.53	0.41
1:0:827:A:H2'	1:0:828:G:O4'	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:118:THR:HG22	5:C:137:PRO:HB3	2.03	0.41
7:E:81:GLU:HA	7:E:133:VAL:O	2.20	0.41
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.90	0.41
8:F:38:LYS:HZ1	15:M:3:SER:HA	1.85	0.41
26:X:66:THR:CG2	26:X:67:PRO:HD2	2.48	0.41
1:O:1739:G:O2'	1:O:1740:U:H5'	2.20	0.41
1:O:2241:C:O2'	1:O:2242:U:H5'	2.20	0.41
3:A:194:MET:CE	3:A:199:HIS:CB	2.98	0.41
1:O:1654:U:H2'	3:A:47:HIS:CD2	2.56	0.41
6:D:10:PHE:N	39:D:7345:HOH:O	2.53	0.41
8:F:28:ALA:CB	8:F:99:THR:HG23	2.50	0.41
10:H:86:TYR:C	10:H:86:TYR:CD1	2.93	0.41
11:I:111:LEU:HD22	11:I:122:GLU:OE1	2.21	0.41
11:I:87:PRO:HB3	11:I:129:SER:C	2.41	0.41
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.40	0.41
15:M:169:ARG:NH2	39:M:8852:HOH:O	2.47	0.41
1:O:2416:G:O2'	16:N:25:ARG:HG2	2.19	0.41
16:N:39:SER:HB3	16:N:42:HIS:H	1.86	0.41
20:R:18:LEU:HG	20:R:91:LEU:HD13	2.03	0.41
21:S:51:GLN:NE2	21:S:53:ASN:HD21	2.13	0.41
1:O:249:G:O2'	1:O:250:C:H5'	2.21	0.41
1:O:2543:G:H2'	1:O:2544:G:O4'	2.20	0.41
1:O:329:A:OP2	5:C:206:ASN:HB2	2.20	0.41
1:O:660:A:H4'	1:O:661:G:O5'	2.20	0.41
1:O:702:G:O2'	1:O:703:G:H5'	2.21	0.41
1:O:88:G:H2'	1:O:89:G:C8	2.55	0.41
30:2:19:SER:O	30:2:36:ASN:ND2	2.54	0.41
4:B:57:GLU:HA	4:B:58:PRO:HD2	1.96	0.41
4:B:75:GLU:C	4:B:77:PRO:HD3	2.41	0.41
5:C:154:VAL:O	5:C:158:GLU:HG3	2.21	0.41
6:D:173:GLU:O	6:D:174:VAL:C	2.59	0.41
7:E:16:ASP:O	7:E:17:HIS:HB2	2.19	0.41
10:H:151:GLU:HA	10:H:151:GLU:OE1	2.21	0.41
24:V:12:THR:CG2	24:V:15:GLU:H	2.34	0.41
1:O:1352:A:H4'	1:O:1353:C:OP2	2.20	0.41
1:O:1596:U:H2'	1:O:1598:A:OP2	2.20	0.41
1:O:2498:C:O2'	1:O:2499:U:H5'	2.20	0.41
1:O:256:C:H2'	1:O:257:G:O4'	2.21	0.41
1:O:2724:U:H2'	1:O:2725:G:O4'	2.20	0.41
4:B:14:GLY:HA3	39:B:9076:HOH:O	2.21	0.41
5:C:57:PRO:HG2	5:C:73:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:49:GLN:OE1	10:H:169:GLU:HB3	2.21	0.41
11:I:103:ILE:HG22	11:I:103:ILE:O	2.20	0.41
11:I:87:PRO:C	11:I:89:GLU:N	2.74	0.41
12:J:64:GLY:HA3	36:J:8821:CL:CL	2.58	0.41
14:L:38:HIS:CD2	14:L:39:GLU:HG3	2.55	0.41
15:M:134:ILE:O	15:M:136:PRO:HD3	2.21	0.41
1:0:2054:A:H2	20:R:128:ARG:HH22	1.56	0.41
22:T:41:ARG:NH1	22:T:42:VAL:O	2.53	0.41
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.82	0.41
26:X:20:GLU:CD	26:X:21:PRO:HD2	2.41	0.41
1:0:1165:G:H1'	1:0:1174:A:H1'	2.03	0.41
1:0:23:G:C6	1:0:24:G:N1	2.89	0.41
1:0:2906:A:H5'	1:0:2907:C:O4'	2.21	0.41
1:0:95:A:H5''	1:0:97:G:O4'	2.21	0.41
8:F:5:ASP:O	8:F:119:ARG:NH1	2.53	0.41
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.03	0.41
22:T:106:GLU:HG3	39:T:4913:HOH:O	2.21	0.41
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.30	0.41
1:0:1976:G:O2'	1:0:1977:U:H5'	2.21	0.41
1:0:2515:C:H2'	1:0:2516:G:O4'	2.20	0.41
1:0:2559:C:H4'	39:0:7688:HOH:O	2.20	0.41
1:0:2740:G:H2'	1:0:2741:A:O4'	2.21	0.41
1:0:2883:A:H2'	1:0:2884:G:O4'	2.21	0.41
1:0:366:U:H2'	1:0:367:G:O4'	2.20	0.41
1:0:522:U:O2'	1:0:1366:C:H5'	2.20	0.41
1:0:553:G:O2'	27:Y:179:PRO:HG3	2.21	0.41
3:A:36:ASP:CB	3:A:85:SER:H	2.34	0.41
8:F:33:THR:HG21	8:F:59:ILE:O	2.20	0.41
13:K:28:GLU:OE2	13:K:58:THR:HG21	2.20	0.41
15:M:46:LEU:HG	39:M:8917:HOH:O	2.19	0.41
2:9:4:G:H21	16:N:44:ARG:NH1	2.19	0.41
16:N:49:THR:HG22	16:N:56:ASP:CB	2.49	0.41
20:R:33:ARG:NH1	39:R:8947:HOH:O	2.37	0.41
26:X:10:VAL:HG12	26:X:11:THR:N	2.35	0.41
26:X:23:HIS:CD2	26:X:24:LYS:HG3	2.56	0.41
1:0:1098:A:H2'	1:0:1099:G:O4'	2.21	0.41
1:0:2089:A:C2'	1:0:2090:G:H5'	2.51	0.41
1:0:222:A:H2'	1:0:223:G:O4'	2.20	0.41
1:0:2884:G:H5'	39:0:4600:HOH:O	2.20	0.41
1:0:64:G:H2'	1:0:65:C:O4'	2.21	0.41
1:0:958:G:H2'	1:0:959:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:28:HIS:O	29:1:32:LYS:N	2.47	0.41
6:D:170:TYR:N	6:D:170:TYR:CD1	2.89	0.41
6:D:173:GLU:HG3	6:D:174:VAL:N	2.35	0.41
12:J:75:PRO:HB3	12:J:132:LEU:HB3	2.02	0.41
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.48	0.41
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.91	0.41
15:M:61:ILE:N	15:M:61:ILE:HD12	2.35	0.41
15:M:69:LYS:HG3	15:M:126:GLN:CA	2.51	0.41
17:O:14:LEU:HG	17:O:102:ILE:HD11	2.03	0.41
39:O:4461:HOH:O	22:T:82:THR:HA	2.21	0.41
22:T:48:VAL:CG2	22:T:96:VAL:HG13	2.51	0.41
39:O:5740:HOH:O	25:W:122:ARG:CZ	2.68	0.41
26:X:74:ALA:HB1	26:X:85:VAL:HG22	2.03	0.41
1:O:1249:U:H2'	1:O:1250:C:C6	2.56	0.41
1:O:1299:G:N2	39:O:5149:HOH:O	2.54	0.41
1:O:2015:A:H2'	1:O:2016:U:O4'	2.20	0.41
1:O:2428:G:N7	31:3:60:LYS:NZ	2.67	0.41
1:O:612:U:H2'	1:O:613:C:C6	2.56	0.41
3:A:81:GLN:CB	3:A:92:ASN:ND2	2.84	0.41
4:B:26:PHE:CE1	4:B:310:ARG:HB3	2.56	0.41
6:D:49:PRO:HB3	39:D:5828:HOH:O	2.21	0.41
14:L:67:ARG:HG2	14:L:67:ARG:HH11	1.86	0.41
1:O:155:C:OP2	15:M:188:ARG:HD3	2.20	0.41
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.50	0.41
20:R:96:VAL:HG13	20:R:106:GLY:HA3	2.03	0.41
24:V:51:LYS:O	24:V:55:ARG:HG3	2.21	0.41
26:X:43:VAL:HG12	26:X:47:ALA:HB3	2.02	0.41
1:O:1268:C:O2'	1:O:1269:G:H5'	2.20	0.40
1:O:1328:A:C8	27:Y:169:ARG:HD3	2.56	0.40
1:O:213:G:O2'	1:O:214:U:OP2	2.40	0.40
1:O:2382:A:H5'	39:3:8962:HOH:O	2.21	0.40
1:O:447:A:O2'	1:O:448:G:H5'	2.22	0.40
3:A:179:MET:HG2	3:A:186:TRP:HB2	2.01	0.40
6:D:99:ASP:N	6:D:103:ASN:O	2.30	0.40
10:H:61:ARG:HG3	10:H:61:ARG:NH1	2.36	0.40
11:I:95:LEU:HG	11:I:132:VAL:CG1	2.51	0.40
13:K:98:VAL:HG13	13:K:102:GLU:CA	2.46	0.40
18:P:40:VAL:O	18:P:44:VAL:HG23	2.21	0.40
22:T:48:VAL:HG23	22:T:98:VAL:HA	2.03	0.40
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.36	0.40
1:O:1773:G:C8	28:Z:16:ALA:HA	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:655:U:O2'	17:O:3:THR:HB	2.21	0.40
29:1:37:CYS:SG	29:1:39:PHE:HB2	2.61	0.40
30:2:18:ASN:ND2	30:2:40:ARG:H	2.19	0.40
4:B:254:GLN:NE2	39:B:9058:HOH:O	2.54	0.40
4:B:310:ARG:HD2	39:B:9057:HOH:O	2.20	0.40
5:C:236:THR:C	39:C:8653:HOH:O	2.60	0.40
7:E:32:ARG:O	7:E:33:LEU:HD23	2.21	0.40
8:F:8:VAL:HG13	8:F:12:LEU:HD13	2.02	0.40
9:G:12:ILE:N	9:G:13:PRO:CD	2.84	0.40
10:H:6:ALA:CB	10:H:61:ARG:HH12	2.33	0.40
12:J:46:ILE:HD11	12:J:53:ILE:CG2	2.51	0.40
22:T:45:GLY:C	39:T:3851:HOH:O	2.59	0.40
22:T:49:GLU:OE2	22:T:51:LEU:HD21	2.21	0.40
1:O:1072:G:OP2	27:Y:154:ARG:NH2	2.54	0.40
1:O:1304:U:H2'	1:O:1305:C:C6	2.56	0.40
1:O:1398:G:H2'	1:O:1399:A:C8	2.56	0.40
1:O:59:A:H5'	39:O:4798:HOH:O	2.20	0.40
8:F:52:GLU:HG3	8:F:77:VAL:O	2.21	0.40
16:N:129:ILE:HA	16:N:130:PRO:HD3	1.98	0.40
16:N:51:GLY:HA2	16:N:52:PRO:HD3	1.94	0.40
24:V:8:ILE:HG21	24:V:59:ILE:HG13	2.02	0.40
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.53	0.40
1:O:1020:A:H1'	39:Q:6976:HOH:O	2.22	0.40
1:O:1186:C:H4'	11:I:114:TYR:HE1	1.87	0.40
1:O:861:A:H4'	1:O:1697:G:H4'	2.03	0.40
1:O:2445:U:H2'	1:O:2446:G:C8	2.56	0.40
4:B:62:ARG:HG2	4:B:65:MET:HE3	2.03	0.40
6:D:138:GLY:N	39:D:7597:HOH:O	2.29	0.40
6:D:38:GLU:HB3	6:D:49:PRO:HG3	2.02	0.40
8:F:107:ASP:O	8:F:111:ILE:HG13	2.21	0.40
13:K:99:ASP:OD1	13:K:101:ASN:N	2.53	0.40
16:N:86:LEU:HD12	16:N:125:ALA:HB2	2.04	0.40
16:N:72:GLU:H	16:N:171:HIS:CE1	2.39	0.40
1:O:1039:G:H2'	1:O:1040:A:O4'	2.22	0.40
1:O:1829:A:H2'	1:O:1830:C:H5'	2.04	0.40
1:O:212:A:O4'	1:O:214:U:C6	2.75	0.40
1:O:2435:U:OP1	31:3:28:GLY:HA3	2.20	0.40
1:O:278:A:H2'	1:O:279:C:O4'	2.21	0.40
1:O:2900:G:H2'	1:O:2901:C:O4'	2.22	0.40
2:9:114:G:H2'	2:9:115:C:C6	2.57	0.40
2:9:31:C:H2'	2:9:32:G:O4'	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:820:G:C5	3:A:171:LYS:HB2	2.57	0.40
39:O:4832:HOH:O	3:A:212:PRO:HB2	2.20	0.40
5:C:6:TYR:HE1	5:C:133:ARG:HH22	1.68	0.40
7:E:69:ILE:HA	7:E:72:MET:HE2	2.01	0.40
10:H:33:GLN:H	10:H:69:ARG:NH1	2.19	0.40
14:L:149:ARG:O	14:L:150:GLN:HB2	2.21	0.40
16:N:38:LYS:HE3	16:N:38:LYS:HB2	1.80	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	
3	A	235/240 (98%)	218 (93%)	13 (6%)	4 (2%)	11	13
4	B	335/338 (99%)	314 (94%)	14 (4%)	7 (2%)	8	9
5	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
6	D	134/177 (76%)	103 (77%)	20 (15%)	11 (8%)	1	0
7	E	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
8	F	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	6	6
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/177 (88%)	143 (92%)	13 (8%)	0	100	100
11	I	68/162 (42%)	49 (72%)	17 (25%)	2 (3%)	5	5
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	13	18
13	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
14	L	141/165 (86%)	124 (88%)	16 (11%)	1 (1%)	25	37
15	M	192/194 (99%)	181 (94%)	11 (6%)	0	100	100
16	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	6	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
18	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
19	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
22	T	117/120 (98%)	111 (95%)	5 (4%)	1 (1%)	20	29
23	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
24	V	63/71 (89%)	58 (92%)	2 (3%)	3 (5%)	2	1
25	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	14	19
26	X	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	61 (86%)	7 (10%)	3 (4%)	3	2
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	40 (95%)	1 (2%)	1 (2%)	7	7
31	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
All	All	3705/4436 (84%)	3437 (93%)	223 (6%)	45 (1%)	15	21

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	LEU
3	A	37	VAL
6	D	171	ASP
8	F	101	ALA
12	J	5	GLU
14	L	80	ASP
16	N	154	LEU
16	N	183	ASP
16	N	184	ILE
24	V	43	PRO
28	Z	81	ARG
4	B	139	ASP
6	D	27	ILE
6	D	56	ARG
6	D	65	GLU
6	D	173	GLU
12	J	143	LYS

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Mol	Chain	Res	Type
22	T	53	GLY
25	W	77	ALA
28	Z	42	CYS
3	A	34	ASP
4	B	34	GLY
4	B	169	GLY
4	B	185	GLY
6	D	61	PHE
6	D	97	GLN
11	I	91	PHE
16	N	164	ASP
6	D	16	PRO
6	D	60	GLU
8	F	100	ASP
16	N	139	TRP
4	B	2	GLN
4	B	107	SER
4	B	184	ASP
6	D	28	GLY
25	W	49	ASN
28	Z	41	ASN
30	2	37	HIS
3	A	132	ASP
8	F	71	GLY
11	I	109	PRO
24	V	40	PRO
6	D	69	ILE
24	V	39	ALA

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	
3	A	179/182 (98%)	167 (93%)	12 (7%)	19	30
4	B	282/283 (100%)	268 (95%)	14 (5%)	28	45
5	C	193/193 (100%)	175 (91%)	18 (9%)	10	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	D	117/148 (79%)	113 (97%)	4 (3%)	42	63
7	E	152/156 (97%)	147 (97%)	5 (3%)	43	64
8	F	93/94 (99%)	92 (99%)	1 (1%)	78	90
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	134/145 (92%)	129 (96%)	5 (4%)	39	59
11	I	58/130 (45%)	58 (100%)	0	100	100
12	J	118/121 (98%)	110 (93%)	8 (7%)	18	29
13	K	106/106 (100%)	105 (99%)	1 (1%)	82	92
14	L	113/127 (89%)	110 (97%)	3 (3%)	50	71
15	M	158/158 (100%)	151 (96%)	7 (4%)	33	51
16	N	149/150 (99%)	145 (97%)	4 (3%)	50	71
17	O	93/94 (99%)	91 (98%)	2 (2%)	57	76
18	P	113/117 (97%)	112 (99%)	1 (1%)	82	92
19	Q	79/80 (99%)	76 (96%)	3 (4%)	38	58
20	R	117/122 (96%)	115 (98%)	2 (2%)	66	82
21	S	71/74 (96%)	69 (97%)	2 (3%)	49	70
22	T	105/106 (99%)	100 (95%)	5 (5%)	30	47
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	37	56
25	W	130/130 (100%)	125 (96%)	5 (4%)	38	58
26	X	66/74 (89%)	59 (89%)	7 (11%)	8	11
27	Y	120/196 (61%)	111 (92%)	9 (8%)	16	24
28	Z	60/68 (88%)	58 (97%)	2 (3%)	43	64
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	54	74
31	3	79/79 (100%)	79 (100%)	0	100	100
All	All	3095/3618 (86%)	2972 (96%)	123 (4%)	36	55

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	26	ASP

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Mol	Chain	Res	Type
3	A	33	GLU
3	A	36	ASP
3	A	55	VAL
3	A	78	ASP
3	A	94	LEU
3	A	120	ARG
3	A	131	HIS
3	A	153	ARG
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	49	THR
4	B	53	LEU
4	B	56	ASP
4	B	98	THR
4	B	162	MET
4	B	174	ARG
4	B	175	LEU
4	B	195	ARG
4	B	254	GLN
4	B	264	GLU
4	B	312	ARG
5	C	2	GLN
5	C	27	ARG
5	C	67	GLN
5	C	76	ARG
5	C	78	ARG
5	C	91	PRO
5	C	94	THR
5	C	101	ASP
5	C	136	VAL
5	C	162	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	240	LEU
5	C	243	VAL

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Mol	Chain	Res	Type
6	D	24	HIS
6	D	61	PHE
6	D	133	ASN
6	D	136	ARG
7	E	7	ILE
7	E	15	GLN
7	E	16	ASP
7	E	86	VAL
7	E	102	VAL
8	F	12	LEU
10	H	87	LYS
10	H	91	ARG
10	H	114	ASP
10	H	157	TYR
10	H	162	PRO
12	J	7	ASP
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	76	ASP
12	J	79	PHE
12	J	107	ASN
12	J	127	ILE
13	K	10	GLN
14	L	35	ARG
14	L	104	ASP
14	L	117	GLU
15	M	46	LEU
15	M	68	ARG
15	M	81	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
15	M	164	THR
16	N	17	ARG
16	N	26	LEU
16	N	127	LEU
16	N	139	TRP
17	O	3	THR
17	O	111	VAL
18	P	98	ILE
19	Q	11	ARG

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Mol	Chain	Res	Type
19	Q	16	ASN
19	Q	95	GLU
20	R	13	THR
20	R	39	THR
21	S	12	GLU
21	S	71	ASP
22	T	39	ASN
22	T	48	VAL
22	T	73	HIS
22	T	89	ARG
22	T	115	GLU
24	V	43	PRO
24	V	65	ASP
25	W	35	VAL
25	W	52	VAL
25	W	73	LEU
25	W	122	ARG
25	W	146	ILE
26	X	15	ARG
26	X	27	ASP
26	X	46	ASP
26	X	49	ARG
26	X	72	VAL
26	X	79	GLU
26	X	82	GLU
27	Y	103	THR
27	Y	115	ARG
27	Y	141	THR
27	Y	154	ARG
27	Y	187	VAL
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	220	GLU
28	Z	33	MET
28	Z	44	GLU
30	2	18	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	92	ASN

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Mol	Chain	Res	Type
3	A	199	HIS
4	B	27	ASN
4	B	145	HIS
4	B	191	ASN
4	B	221	GLN
4	B	238	ASN
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	129	HIS
6	D	47	GLN
6	D	97	GLN
6	D	103	ASN
6	D	133	ASN
7	E	15	GLN
7	E	90	HIS
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
9	G	17	GLN
9	G	64	ASN
10	H	34	HIS
10	H	59	GLN
10	H	62	HIS
10	H	73	ASN
11	I	88	GLN
11	I	99	GLN
12	J	25	GLN
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	137	ASN
15	M	170	ASN

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Mol	Chain	Res	Type
16	N	40	ASN
16	N	93	GLN
16	N	107	ASN
16	N	153	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
21	S	25	GLN
21	S	51	GLN
22	T	39	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	27	HIS
25	W	28	HIS
25	W	59	GLN
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	23	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	15	ASN

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Mol	Chain	Res	Type
31	3	30	GLN
31	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	226 (8%)	0
2	9	121/122 (99%)	16 (13%)	0
All	All	2866/3044 (94%)	242 (8%)	0

All (242) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	170	U
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	C
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C

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Mol	Chain	Res	Type
1	0	318	U
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	846	A
1	0	868	G
1	0	869	G
1	0	871	G

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Mol	Chain	Res	Type
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C

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Mol	Chain	Res	Type
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1562	C
1	0	1564	C
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1857	A
1	0	1879	U
1	0	1919	A

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Mol	Chain	Res	Type
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2104	C
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G

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Mol	Chain	Res	Type
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2649	A
1	0	2664	A
1	0	2676	C
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	2	U
2	9	14	G
2	9	22	G
2	9	23	U
2	9	24	U
2	9	25	G
2	9	40	C
2	9	41	C
2	9	43	G
2	9	44	A
2	9	52	A
2	9	57	A

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Mol	Chain	Res	Type
2	9	66	G
2	9	77	A
2	9	114	G
2	9	122	C

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	OMU	0	2587	1	14,22,23	1.01	1 (7%)	18,31,34	3.68	2 (11%)
1	OMG	0	2588	1	18,26,27	1.06	1 (5%)	22,38,41	2.49	4 (18%)
1	UR3	0	2619	1	14,22,23	0.76	0	16,32,35	0.74	0
1	PSU	0	2621	1	16,21,22	1.57	3 (18%)	20,30,33	6.08	4 (20%)
1	1MA	0	628	1	16,25,26	1.05	1 (6%)	13,37,40	1.17	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
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	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)
1	0	2621	PSU	C5-C1'	-4.72	1.48	1.52
1	0	2587	OMU	C4-N3	2.60	1.37	1.33
1	0	2621	PSU	C2-N1	2.65	1.43	1.38
1	0	2621	PSU	C4-N3	2.72	1.38	1.33
1	0	628	1MA	C6-N6	2.82	1.33	1.27
1	0	2588	OMG	C6-N1	3.33	1.39	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-19.09	114.67	128.40
1	0	2621	PSU	C5-C4-N3	-12.90	114.85	125.43
1	0	2588	OMG	C5-C6-N1	-8.46	111.44	123.48
1	0	628	1MA	C2-N3-C4	-3.65	110.81	116.41
1	0	2587	OMU	C5-C4-N3	-3.47	114.84	123.12
1	0	2588	OMG	C2-N3-C4	-2.81	111.88	115.16
1	0	2588	OMG	N3-C2-N1	-2.39	123.97	127.46
1	0	2621	PSU	C6-N1-C2	2.93	120.04	115.36
1	0	2588	OMG	C6-N1-C2	6.44	125.33	116.06
1	0	2621	PSU	C4-N3-C2	13.76	127.19	115.16
1	0	2587	OMU	C4-N3-C2	15.04	127.05	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 are monoatomic - leaving 1 for Mogul analysis.

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
32	ZIT	0	9500	-	54,54,54	1.35	7 (12%)	81,83,83	1.06	4 (4%)

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
32	ZIT	0	9500	-	-	0/72/107/107	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	ZIT	O5A-C1A	2.02	1.46	1.41
32	0	9500	ZIT	O6-C6	2.04	1.48	1.44
32	0	9500	ZIT	C13-C12	2.22	1.61	1.55
32	0	9500	ZIT	C6-C5	2.31	1.60	1.55
32	0	9500	ZIT	O13-C13	2.58	1.48	1.44
32	0	9500	ZIT	C13-C14	3.03	1.60	1.54
32	0	9500	ZIT	C22-C11	3.26	1.58	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9500	ZIT	C9-N10-C11	-2.96	106.97	112.26
32	0	9500	ZIT	C4A-C3A-C2A	-2.24	106.90	110.07
32	0	9500	ZIT	O6-C6-C7	2.08	113.87	108.37
32	0	9500	ZIT	C7-C8-C9	2.66	116.14	112.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.46	92 (3%) 47 45	15, 38, 82, 157	0
2	9	122/122 (100%)	-0.12	6 (4%) 30 29	32, 58, 80, 139	0
3	A	237/240 (98%)	0.24	12 (5%) 29 27	19, 40, 75, 96	0
4	B	337/338 (99%)	0.18	9 (2%) 55 52	21, 47, 73, 84	0
5	C	246/246 (100%)	-0.14	3 (1%) 79 77	17, 36, 60, 69	0
6	D	140/177 (79%)	2.12	66 (47%) 0 0	51, 88, 114, 122	0
7	E	172/178 (96%)	0.86	24 (13%) 3 3	39, 61, 80, 84	0
8	F	119/120 (99%)	0.80	20 (16%) 2 1	38, 62, 88, 103	0
9	G	29/348 (8%)	3.20	25 (86%) 0 0	71, 87, 93, 95	0
10	H	160/177 (90%)	0.43	15 (9%) 9 8	31, 50, 83, 91	0
11	I	70/162 (43%)	6.91	70 (100%) 0 0	122, 135, 154, 155	0
12	J	142/145 (97%)	0.06	4 (2%) 53 51	29, 44, 65, 88	0
13	K	132/132 (100%)	-0.10	3 (2%) 61 58	24, 43, 65, 77	0
14	L	145/165 (87%)	0.59	19 (13%) 4 3	18, 56, 101, 115	0
15	M	194/194 (100%)	0.02	0 100 100	21, 33, 49, 56	0
16	N	186/187 (99%)	0.72	25 (13%) 4 3	34, 55, 102, 112	0
17	O	115/116 (99%)	0.03	1 (0%) 84 82	30, 45, 61, 69	0
18	P	143/149 (95%)	-0.05	0 100 100	30, 44, 57, 68	0
19	Q	95/96 (98%)	-0.04	1 (1%) 80 79	30, 37, 54, 68	0
20	R	150/155 (96%)	-0.15	0 100 100	25, 38, 58, 66	0
21	S	81/85 (95%)	0.11	2 (2%) 58 55	34, 50, 71, 81	0
22	T	119/120 (99%)	0.40	8 (6%) 19 17	29, 47, 76, 103	0
23	U	53/66 (80%)	0.28	2 (3%) 41 40	35, 48, 66, 78	0
24	V	65/71 (91%)	1.45	12 (18%) 1 1	43, 62, 107, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.03	1 (0%) 89 87	29, 43, 58, 69	0
26	X	82/92 (89%)	0.54	10 (12%) 5 4	37, 50, 78, 94	0
27	Y	142/241 (58%)	0.13	5 (3%) 44 43	21, 36, 59, 80	0
28	Z	73/83 (87%)	0.06	2 (2%) 55 52	35, 51, 68, 86	0
29	1	56/57 (98%)	-0.44	0 100 100	18, 24, 32, 43	0
30	2	46/50 (92%)	0.48	5 (10%) 6 5	26, 51, 75, 89	0
31	3	92/92 (100%)	0.22	2 (2%) 62 59	26, 48, 62, 77	0
All	All	6646/7480 (88%)	0.06	444 (6%) 19 17	15, 43, 89, 157	0

All (444) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	I	74	ILE	15.4
11	I	91	PHE	15.2
11	I	66	GLY	14.4
11	I	128	THR	14.2
11	I	88	GLN	13.8
11	I	71	ALA	13.4
24	V	1	THR	13.2
11	I	80	PHE	12.6
2	9	1	U	11.4
11	I	132	VAL	11.3
6	D	63	ILE	11.3
11	I	97	VAL	11.0
11	I	100	VAL	10.6
11	I	104	ALA	9.9
6	D	10	PHE	9.7
11	I	131	GLY	9.3
11	I	70	THR	9.1
16	N	166	ALA	9.0
24	V	39	ALA	8.9
11	I	92	VAL	8.9
11	I	86	GLU	8.8
11	I	93	ALA	8.4
11	I	103	ILE	8.3
11	I	111	LEU	8.1
11	I	108	HIS	8.1
11	I	127	CYS	7.9
1	0	1198	U	7.8
3	A	37	VAL	7.7

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Mol	Chain	Res	Type	RSRZ
11	I	78	ALA	7.6
11	I	84	SER	7.6
11	I	116	LEU	7.6
11	I	83	GLY	7.5
11	I	113	SER	7.5
11	I	109	PRO	7.4
24	V	40	PRO	7.4
11	I	82	THR	7.3
11	I	106	GLN	7.2
11	I	72	GLU	7.0
11	I	76	ASP	7.0
11	I	99	GLN	6.9
6	D	61	PHE	6.8
11	I	79	GLY	6.8
11	I	112	LEU	6.5
1	0	1177	A	6.5
11	I	118	ASN	6.4
26	X	88	GLU	6.4
6	D	57	THR	6.4
1	0	1951	G	6.4
11	I	89	GLU	6.3
6	D	170	TYR	6.2
11	I	98	ASP	6.1
1	0	2237	G	6.1
1	0	1172	G	6.1
11	I	87	PRO	6.1
9	G	23	ILE	5.9
11	I	124	VAL	5.9
11	I	129	SER	5.9
6	D	11	HIS	5.8
10	H	174	LEU	5.8
6	D	69	ILE	5.8
11	I	133	THR	5.7
11	I	130	LEU	5.7
6	D	26	GLY	5.7
1	0	1169	U	5.7
1	0	1199	A	5.6
11	I	90	ASP	5.6
3	A	237	GLY	5.6
11	I	73	LEU	5.6
11	I	120	ALA	5.5
11	I	102	GLN	5.5

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Mol	Chain	Res	Type	RSRZ
24	V	38	GLY	5.4
1	0	1192	A	5.4
1	0	1202	A	5.4
11	I	121	LYS	5.3
6	D	64	ARG	5.3
9	G	24	VAL	5.3
11	I	117	THR	5.2
11	I	68	PRO	5.2
1	0	1181	A	5.1
6	D	90	LEU	5.0
1	0	1176	C	5.0
11	I	75	LYS	5.0
1	0	1163	G	4.9
1	0	1168	C	4.9
1	0	1178	G	4.9
11	I	81	GLU	4.9
1	0	970	U	4.8
11	I	94	ASP	4.8
11	I	67	VAL	4.8
14	L	80	ASP	4.8
1	0	1173	A	4.8
2	9	2	U	4.7
9	G	71	LEU	4.7
2	9	24	U	4.6
9	G	27	ILE	4.6
11	I	69	PRO	4.6
1	0	2238	A	4.5
21	S	81	ILE	4.5
6	D	40	ILE	4.4
1	0	1525	G	4.4
1	0	960	G	4.4
11	I	107	LYS	4.3
24	V	43	PRO	4.3
22	T	116	ASP	4.3
22	T	118	SER	4.3
1	0	1179	C	4.3
9	G	26	MET	4.3
11	I	110	ASP	4.3
22	T	119	ALA	4.3
11	I	95	LEU	4.3
9	G	66	LEU	4.2
1	0	2004	U	4.2

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Mol	Chain	Res	Type	RSRZ
7	E	127	ASP	4.2
11	I	85	GLY	4.2
9	G	20	VAL	4.1
6	D	166	ILE	4.1
11	I	119	ALA	4.1
4	B	57	GLU	4.1
1	0	1950	G	4.1
6	D	93	LEU	4.1
6	D	58	VAL	4.0
26	X	85	VAL	4.0
6	D	106	PHE	4.0
6	D	44	ILE	4.0
6	D	85	GLN	4.0
1	0	1200	A	4.0
7	E	87	PHE	4.0
1	0	1948	G	4.0
1	0	1170	U	4.0
6	D	66	GLY	4.0
7	E	45	ASP	4.0
3	A	35	GLY	4.0
8	F	119	ARG	3.9
11	I	105	GLU	3.9
11	I	125	GLY	3.9
11	I	126	THR	3.9
9	G	73	ASP	3.9
6	D	88	LEU	3.9
10	H	169	GLU	3.9
1	0	10	U	3.9
16	N	181	ASP	3.9
16	N	152	GLU	3.9
1	0	1180	U	3.8
1	0	284	C	3.8
1	0	999	C	3.8
14	L	81	VAL	3.8
9	G	72	ASP	3.8
1	0	1175	G	3.8
11	I	114	TYR	3.8
6	D	56	ARG	3.7
6	D	62	ASP	3.7
9	G	69	ARG	3.7
31	3	92	GLU	3.7
4	B	183	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
26	X	80	GLU	3.7
14	L	77	ALA	3.7
1	0	1182	C	3.7
10	H	40	GLN	3.7
1	0	735	C	3.7
6	D	68	PRO	3.7
30	2	49	GLU	3.7
6	D	92	GLU	3.6
11	I	122	GLU	3.6
27	Y	235	GLU	3.6
6	D	172	VAL	3.6
6	D	27	ILE	3.6
1	0	1171	A	3.5
9	G	21	ASP	3.5
14	L	60	GLU	3.5
6	D	86	THR	3.5
27	Y	95	THR	3.5
7	E	86	VAL	3.5
10	H	172	GLU	3.5
1	0	282	C	3.4
2	9	23	U	3.4
30	2	39	ARG	3.4
16	N	158	LEU	3.4
3	A	85	SER	3.4
11	I	115	ASP	3.4
14	L	75	LEU	3.4
19	Q	95	GLU	3.4
11	I	101	LYS	3.4
26	X	7	GLU	3.4
9	G	67	LEU	3.4
8	F	106	ALA	3.4
9	G	70	ALA	3.4
16	N	177	GLU	3.4
1	0	2344	G	3.4
14	L	149	ARG	3.3
11	I	77	GLU	3.3
7	E	10	ASP	3.3
9	G	18	GLU	3.3
1	0	1949	G	3.3
6	D	18	ILE	3.3
6	D	135	VAL	3.3
22	T	117	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
6	D	165	PHE	3.2
9	G	65	THR	3.2
1	0	285	A	3.2
6	D	41	LEU	3.2
8	F	118	LEU	3.2
1	0	1190	G	3.2
1	0	138	U	3.2
1	0	1625	U	3.2
6	D	104	PHE	3.2
5	C	135	GLU	3.2
1	0	1162	G	3.2
11	I	123	VAL	3.2
9	G	68	GLU	3.2
1	0	1167	G	3.1
1	0	2508	C	3.1
16	N	68	GLU	3.1
24	V	41	GLU	3.1
23	U	47	ARG	3.1
16	N	183	ASP	3.1
11	I	96	SER	3.1
8	F	25	ASP	3.1
3	A	133	ARG	3.1
9	G	22	ALA	3.1
6	D	107	GLY	3.1
9	G	28	GLU	3.1
3	A	36	ASP	3.1
1	0	1165	G	3.1
6	D	75	LEU	3.1
6	D	157	LEU	3.1
6	D	89	PRO	3.1
1	0	1183	C	3.1
1	0	1191	A	3.0
1	0	1964	U	3.0
1	0	2769	C	3.0
16	N	150	TYR	3.0
16	N	180	LEU	3.0
16	N	155	GLU	3.0
7	E	100	ASP	3.0
14	L	91	VAL	3.0
8	F	15	ASP	3.0
6	D	38	GLU	3.0
1	0	497	A	3.0

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Mol	Chain	Res	Type	RSRZ
1	0	1193	A	3.0
1	0	283	U	2.9
1	0	1184	C	2.9
14	L	147	GLU	2.9
14	L	148	GLU	2.9
8	F	22	VAL	2.9
3	A	97	ALA	2.9
1	0	272	A	2.9
1	0	1174	A	2.9
4	B	1	PRO	2.9
16	N	162	ASP	2.9
1	0	280	C	2.9
22	T	115	GLU	2.9
9	G	25	GLU	2.8
1	0	1164	U	2.8
14	L	150	GLN	2.8
22	T	82	THR	2.8
6	D	43	GLU	2.8
7	E	88	TYR	2.8
7	E	6	GLU	2.8
16	N	139	TRP	2.8
30	2	35	ARG	2.8
6	D	67	ASP	2.8
7	E	43	ASP	2.8
27	Y	108	ASP	2.8
6	D	74	THR	2.8
6	D	173	GLU	2.8
13	K	132	VAL	2.8
9	G	15	TRP	2.8
16	N	164	ASP	2.8
16	N	154	LEU	2.8
10	H	170	ARG	2.8
10	H	86	TYR	2.7
7	E	126	ILE	2.7
1	0	1197	G	2.7
2	9	122	C	2.7
27	Y	216	ARG	2.7
21	S	76	GLU	2.7
1	0	1279	U	2.7
6	D	98	PHE	2.7
7	E	121	ASP	2.7
6	D	55	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
7	E	131	LEU	2.7
1	0	1196	C	2.7
7	E	129	GLU	2.7
3	A	236	GLY	2.7
10	H	149	VAL	2.7
4	B	180	ASP	2.7
8	F	103	GLU	2.6
6	D	23	VAL	2.6
1	0	1203	G	2.6
3	A	135	VAL	2.6
6	D	171	ASP	2.6
7	E	95	VAL	2.6
9	G	17	GLN	2.6
27	Y	236	VAL	2.6
7	E	108	LEU	2.6
14	L	102	ASP	2.6
1	0	1965	C	2.6
14	L	76	LEU	2.6
1	0	1947	G	2.6
7	E	94	GLN	2.6
1	0	1186	C	2.6
1	0	2239	C	2.6
8	F	107	ASP	2.6
8	F	18	GLU	2.6
12	J	5	GLU	2.6
1	0	1204	C	2.6
24	V	59	ILE	2.5
1	0	1527	A	2.5
1	0	1208	C	2.5
6	D	65	GLU	2.5
8	F	16	ALA	2.5
14	L	105	TYR	2.5
8	F	100	ASP	2.5
26	X	77	PHE	2.5
16	N	140	GLN	2.5
12	J	4	ALA	2.5
16	N	149	GLU	2.5
1	0	1526	A	2.5
1	0	2637	A	2.5
7	E	154	ILE	2.5
3	A	34	ASP	2.5
8	F	14	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
16	N	163	PHE	2.5
1	0	1201	C	2.5
8	F	90	GLU	2.5
6	D	29	HIS	2.4
10	H	165	ARG	2.4
1	0	372	A	2.4
6	D	134	LEU	2.4
6	D	154	LYS	2.4
6	D	25	MET	2.4
1	0	1000	C	2.4
1	0	1967	U	2.4
3	A	31	LYS	2.4
13	K	118	ALA	2.4
28	Z	11	SER	2.4
14	L	99	GLU	2.4
10	H	50	ILE	2.4
16	N	147	ILE	2.4
6	D	81	GLU	2.4
16	N	160	SER	2.4
10	H	76	LEU	2.4
10	H	144	GLU	2.4
6	D	50	VAL	2.3
10	H	48	VAL	2.3
1	0	736	A	2.3
6	D	48	MET	2.3
7	E	128	GLY	2.3
1	0	362	G	2.3
1	0	1185	U	2.3
1	0	1206	U	2.3
1	0	279	C	2.3
1	0	1207	A	2.3
24	V	37	GLY	2.3
5	C	132	ASP	2.3
9	G	14	GLU	2.3
6	D	130	VAL	2.3
14	L	79	ASP	2.3
3	A	38	ILE	2.3
26	X	41	PHE	2.3
1	0	1166	A	2.3
6	D	45	THR	2.3
26	X	71	ARG	2.3
14	L	106	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
6	D	95	THR	2.3
1	0	2511	A	2.3
16	N	185	GLU	2.3
24	V	8	ILE	2.3
4	B	134	ALA	2.3
12	J	110	ASP	2.3
1	0	128	A	2.2
17	O	23	GLY	2.2
10	H	85	ASP	2.2
26	X	72	VAL	2.2
1	0	371	U	2.2
11	I	134	ILE	2.2
12	J	70	PHE	2.2
4	B	169	GLY	2.2
24	V	10	ASP	2.2
7	E	89	SER	2.2
1	0	1966	U	2.2
31	3	62	THR	2.2
11	I	135	GLU	2.2
16	N	159	TYR	2.2
1	0	1189	A	2.2
24	V	63	GLU	2.2
6	D	70	GLY	2.2
9	G	63	ARG	2.2
7	E	11	VAL	2.2
24	V	2	VAL	2.2
9	G	12	ILE	2.2
6	D	158	ASN	2.2
6	D	128	LEU	2.2
30	2	44	ARG	2.2
4	B	104	GLU	2.2
4	B	117	GLU	2.2
6	D	167	GLU	2.2
1	0	969	G	2.1
16	N	95	ALA	2.1
6	D	42	GLY	2.1
16	N	156	GLU	2.1
25	W	86	GLU	2.1
30	2	27	LEU	2.1
1	0	1188	A	2.1
8	F	44	SER	2.1
6	D	129	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
10	H	140	TYR	2.1
7	E	105	GLU	2.1
8	F	117	GLU	2.1
9	G	64	ASN	2.1
6	D	84	LEU	2.1
8	F	17	LEU	2.1
14	L	145	LEU	2.1
1	0	1665	G	2.1
2	9	74	G	2.1
6	D	24	HIS	2.1
14	L	139	SER	2.1
6	D	39	ASP	2.1
10	H	89	THR	2.1
7	E	53	GLU	2.1
28	Z	80	ARG	2.1
23	U	43	GLY	2.1
14	L	130	ARG	2.1
16	N	69	TYR	2.1
1	0	1159	G	2.1
16	N	169	PRO	2.1
26	X	10	VAL	2.1
22	T	112	LEU	2.1
8	F	21	GLU	2.1
7	E	156	ASP	2.0
13	K	129	THR	2.0
26	X	42	SER	2.0
1	0	2345	A	2.0
6	D	51	ARG	2.0
7	E	170	ARG	2.0
8	F	110	ASP	2.0
8	F	26	THR	2.0
1	0	2664	A	2.0
5	C	143	ASP	2.0
22	T	33	GLU	2.0
6	D	47	GLN	2.0
8	F	115	VAL	2.0
4	B	176	ASP	2.0
1	0	1523	G	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
1	OMU	0	2587	21/22	0.98	0.12	-	26,28,29,32	0
1	UR3	0	2619	21/22	0.98	0.13	-	29,33,35,41	0
1	PSU	0	2621	20/21	0.98	0.13	-	22,25,33,33	0
1	1MA	0	628	23/24	0.98	0.15	-	22,24,25,28	0
1	OMG	0	2588	24/25	0.98	0.12	-	23,27,29,30	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	0.82	0.49	93.70	43,43,43,43	0
35	NA	0	8542	1/1	0.85	0.43	32.60	51,51,51,51	0
35	NA	0	8563	1/1	0.84	0.39	21.85	56,56,56,56	0
35	NA	0	8565	1/1	0.89	0.29	21.02	46,46,46,46	0
37	SR	B	8987	1/1	0.14	0.48	14.67	189,189,189,189	0
35	NA	0	8553	1/1	0.93	0.23	14.40	48,48,48,48	0
37	SR	0	8969	1/1	0.97	0.25	13.74	115,115,115,115	0
35	NA	0	8550	1/1	0.92	0.21	12.73	41,41,41,41	0
35	NA	0	8564	1/1	0.86	0.37	12.07	55,55,55,55	0
35	NA	0	8517	1/1	0.94	0.21	11.56	36,36,36,36	0
35	NA	0	8562	1/1	0.72	0.27	10.20	59,59,59,59	0
35	NA	0	8560	1/1	0.98	0.36	9.84	54,54,54,54	0
35	NA	0	8521	1/1	0.87	0.24	9.60	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8571	1/1	0.55	0.25	7.35	79,79,79,79	0
37	SR	0	8903	1/1	0.99	0.17	6.41	41,41,41,41	0
35	NA	0	8528	1/1	0.98	0.20	6.38	32,32,32,32	0
35	NA	9	8572	1/1	0.89	0.29	6.06	59,59,59,59	0
37	SR	0	8992	1/1	0.97	0.22	5.02	111,111,111,111	0
35	NA	0	8568	1/1	0.91	0.24	4.60	42,42,42,42	0
35	NA	0	8535	1/1	0.94	0.26	4.20	40,40,40,40	0
37	SR	A	8929	1/1	0.68	0.25	4.05	123,123,123,123	0
35	NA	0	8547	1/1	0.94	0.19	3.81	42,42,42,42	0
35	NA	0	8559	1/1	0.92	0.15	2.69	51,51,51,51	0
35	NA	0	8527	1/1	0.95	0.17	2.49	31,31,31,31	0
35	NA	0	8534	1/1	0.95	0.15	2.43	29,29,29,29	0
35	NA	0	8523	1/1	0.93	0.16	2.29	31,31,31,31	0
35	NA	R	8575	1/1	0.90	0.21	2.22	73,73,73,73	0
36	CL	M	8818	1/1	0.97	0.23	2.16	36,36,36,36	0
37	SR	0	8991	1/1	0.79	0.15	1.94	167,167,167,167	0
35	NA	M	8539	1/1	0.95	0.18	1.60	28,28,28,28	0
35	NA	0	8530	1/1	0.97	0.16	1.53	37,37,37,37	0
35	NA	0	8556	1/1	0.94	0.22	1.31	37,37,37,37	0
35	NA	0	8552	1/1	0.96	0.14	0.98	48,48,48,48	0
35	NA	0	8515	1/1	0.97	0.17	0.48	30,30,30,30	0
35	NA	0	8508	1/1	0.92	0.13	0.20	40,40,40,40	0
37	SR	0	8959	1/1	0.86	0.17	0.19	132,132,132,132	0
37	SR	0	8975	1/1	0.94	0.13	0.08	99,99,99,99	0
33	MG	A	8051	1/1	0.97	0.17	-0.01	55,55,55,55	0
35	NA	0	8569	1/1	0.91	0.13	-0.02	61,61,61,61	0
36	CL	0	8812	1/1	0.99	0.13	-0.20	39,39,39,39	0
32	ZIT	0	9500	52/52	0.95	0.14	-0.35	28,38,42,44	0
36	CL	J	8821	1/1	0.92	0.17	-0.36	52,52,52,52	0
35	NA	Q	8540	1/1	0.98	0.17	-0.37	39,39,39,39	0
35	NA	C	8503	1/1	0.92	0.14	-0.38	29,29,29,29	0
35	NA	0	8504	1/1	0.95	0.13	-0.50	26,26,26,26	0
35	NA	0	8557	1/1	0.92	0.12	-0.57	54,54,54,54	0
37	SR	0	8993	1/1	0.69	0.10	-0.73	143,143,143,143	0
37	SR	H	8972	1/1	0.84	0.12	-0.76	112,112,112,112	0
35	NA	0	8519	1/1	0.99	0.15	-0.78	36,36,36,36	0
37	SR	R	8912	1/1	0.95	0.12	-0.79	77,77,77,77	0
33	MG	0	8047	1/1	0.98	0.13	-0.84	46,46,46,46	0
35	NA	0	8520	1/1	0.98	0.09	-0.98	50,50,50,50	0
37	SR	0	8985	1/1	0.94	0.11	-1.02	104,104,104,104	0
36	CL	0	8815	1/1	0.95	0.11	-1.04	47,47,47,47	0
35	NA	0	8512	1/1	0.97	0.11	-1.05	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8044	1/1	0.97	0.15	-1.10	40,40,40,40	0
35	NA	0	8537	1/1	0.99	0.13	-1.28	32,32,32,32	0
38	CD	U	8701	1/1	0.99	0.09	-1.35	55,55,55,55	0
37	SR	0	8947	1/1	0.83	0.10	-1.46	148,148,148,148	0
37	SR	0	8922	1/1	0.55	0.12	-1.47	161,161,161,161	0
35	NA	J	8538	1/1	0.95	0.10	-1.50	48,48,48,48	0
36	CL	O	8808	1/1	0.97	0.10	-1.52	54,54,54,54	0
37	SR	0	8981	1/1	0.94	0.11	-1.52	141,141,141,141	0
38	CD	Z	8703	1/1	0.98	0.08	-1.53	44,44,44,44	0
36	CL	0	8816	1/1	0.98	0.11	-1.57	53,53,53,53	0
33	MG	0	8009	1/1	0.98	0.13	-1.63	26,26,26,26	0
35	NA	0	8513	1/1	0.94	0.13	-1.70	33,33,33,33	0
33	MG	0	8084	1/1	0.95	0.04	-1.70	36,36,36,36	0
33	MG	0	8008	1/1	0.97	0.12	-1.77	26,26,26,26	0
33	MG	A	8050	1/1	0.96	0.13	-1.82	33,33,33,33	0
36	CL	B	8819	1/1	0.98	0.09	-1.85	46,46,46,46	0
33	MG	0	8058	1/1	0.99	0.08	-1.92	26,26,26,26	0
37	SR	0	8964	1/1	0.90	0.09	-1.92	109,109,109,109	0
37	SR	A	8930	1/1	0.96	0.05	-2.11	82,82,82,82	0
33	MG	0	8011	1/1	0.99	0.09	-2.15	24,24,24,24	0
33	MG	T	8057	1/1	0.94	0.08	-2.42	51,51,51,51	0
33	MG	0	8028	1/1	0.98	0.11	-2.45	19,19,19,19	0
38	CD	3	8704	1/1	0.99	0.07	-2.57	53,53,53,53	0
37	SR	0	8970	1/1	0.81	0.09	-2.61	109,109,109,109	0
37	SR	0	8984	1/1	0.96	0.10	-2.63	98,98,98,98	0
37	SR	0	8943	1/1	0.86	0.09	-2.67	108,108,108,108	0
37	SR	F	9005	1/1	0.91	0.05	-2.74	106,106,106,106	0
35	NA	0	8533	1/1	0.97	0.08	-2.78	50,50,50,50	0
33	MG	0	8070	1/1	0.96	0.10	-3.02	36,36,36,36	0
33	MG	0	8045	1/1	0.97	0.09	-3.08	29,29,29,29	0
33	MG	0	8003	1/1	0.97	0.11	-3.23	23,23,23,23	0
37	SR	0	8918	1/1	0.99	0.12	-3.50	66,66,66,66	0
33	MG	0	8041	1/1	0.98	0.10	-3.68	18,18,18,18	0
33	MG	0	8052	1/1	0.95	0.09	-3.72	23,23,23,23	0
37	SR	3	8932	1/1	0.99	0.07	-3.74	58,58,58,58	0
37	SR	0	8936	1/1	0.99	0.09	-3.74	67,67,67,67	0
33	MG	0	8025	1/1	0.94	0.08	-3.80	24,24,24,24	0
33	MG	Y	8086	1/1	0.97	0.11	-3.82	35,35,35,35	0
33	MG	0	8062	1/1	0.89	0.08	-3.94	46,46,46,46	0
33	MG	0	8075	1/1	0.97	0.07	-4.06	31,31,31,31	0
37	SR	0	8904	1/1	0.99	0.08	-4.23	34,34,34,34	0
33	MG	0	8065	1/1	0.95	0.07	-4.27	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CL	3	8804	1/1	0.97	0.09	-4.29	47,47,47,47	0
35	NA	0	8558	1/1	0.98	0.08	-4.53	46,46,46,46	0
33	MG	0	8014	1/1	0.99	0.09	-4.56	25,25,25,25	0
33	MG	0	8043	1/1	0.98	0.09	-4.58	46,46,46,46	0
36	CL	0	8805	1/1	0.97	0.09	-4.58	45,45,45,45	0
33	MG	0	8012	1/1	0.98	0.07	-4.59	13,13,13,13	0
33	MG	B	8042	1/1	0.97	0.05	-4.60	52,52,52,52	0
34	K	0	8402	1/1	0.99	0.09	-4.84	46,46,46,46	0
37	SR	1	8913	1/1	0.98	0.07	-4.84	70,70,70,70	0
38	CD	1	8702	1/1	0.99	0.06	-4.90	44,44,44,44	0
33	MG	0	8001	1/1	0.99	0.08	-5.57	25,25,25,25	0
33	MG	0	8034	1/1	0.98	0.08	-5.64	35,35,35,35	0
33	MG	0	8029	1/1	0.92	0.08	-5.97	40,40,40,40	0
33	MG	0	8088	1/1	0.98	0.05	-6.93	29,29,29,29	0
33	MG	0	8013	1/1	0.99	0.04	-6.97	24,24,24,24	0
33	MG	0	8040	1/1	0.93	0.09	-6.98	78,78,78,78	0
33	MG	0	8015	1/1	0.98	0.09	-7.69	31,31,31,31	0
33	MG	0	8002	1/1	0.97	0.08	-7.69	27,27,27,27	0
33	MG	0	8087	1/1	0.99	0.08	-9.06	26,26,26,26	0
33	MG	0	8006	1/1	0.99	0.06	-9.12	30,30,30,30	0
37	SR	0	8902	1/1	0.99	0.07	-9.12	49,49,49,49	0
33	MG	0	8004	1/1	0.98	0.05	-9.82	22,22,22,22	0
37	SR	0	8945	1/1	0.98	0.04	-9.98	92,92,92,92	0
37	SR	0	8910	1/1	0.96	0.04	-10.59	80,80,80,80	0
37	SR	0	8949	1/1	0.95	0.05	-11.20	93,93,93,93	0
37	SR	0	8978	1/1	0.96	0.05	-13.07	82,82,82,82	0
37	SR	0	8948	1/1	0.97	0.07	-14.93	69,69,69,69	0
37	SR	A	8977	1/1	0.89	0.07	-	143,143,143,143	0
37	SR	0	8955	1/1	0.59	0.37	-	169,169,169,169	0
33	MG	0	8007	1/1	0.97	0.10	-	24,24,24,24	0
35	NA	0	8574	1/1	0.85	0.44	-	48,48,48,48	0
35	NA	0	8511	1/1	0.96	0.11	-	59,59,59,59	0
33	MG	0	8032	1/1	0.99	0.08	-	36,36,36,36	0
33	MG	0	8053	1/1	0.93	0.09	-	58,58,58,58	0
33	MG	0	8022	1/1	0.93	0.15	-	30,30,30,30	0
33	MG	0	8021	1/1	0.97	0.09	-	28,28,28,28	0
35	NA	0	8549	1/1	0.95	0.47	-	74,74,74,74	0
33	MG	0	8079	1/1	0.89	0.08	-	40,40,40,40	0
33	MG	0	8073	1/1	0.86	0.19	-	76,76,76,76	0
35	NA	0	8551	1/1	0.93	0.20	-	39,39,39,39	0
35	NA	0	8505	1/1	0.98	0.14	-	33,33,33,33	0
37	SR	0	8958	1/1	0.96	0.07	-	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8081	1/1	0.70	0.20	-	55,55,55,55	0
37	SR	0	8960	1/1	0.73	0.09	-	128,128,128,128	0
37	SR	0	8944	1/1	0.72	0.16	-	146,146,146,146	0
33	MG	0	8072	1/1	0.97	0.09	-	37,37,37,37	0
33	MG	0	8082	1/1	0.90	0.23	-	44,44,44,44	0
37	SR	0	8920	1/1	0.95	0.08	-	96,96,96,96	0
37	SR	0	8921	1/1	0.98	0.07	-	66,66,66,66	0
37	SR	0	8927	1/1	0.80	0.12	-	133,133,133,133	0
37	SR	B	8950	1/1	0.90	0.06	-	90,90,90,90	0
35	NA	0	8570	1/1	0.97	0.09	-	35,35,35,35	0
36	CL	N	8807	1/1	0.98	0.12	-	46,46,46,46	0
33	MG	0	8061	1/1	0.97	0.12	-	23,23,23,23	0
37	SR	0	9008	1/1	0.95	0.07	-	83,83,83,83	0
33	MG	0	8019	1/1	0.96	0.07	-	22,22,22,22	0
37	SR	0	8946	1/1	0.93	0.09	-	87,87,87,87	0
36	CL	Y	8820	1/1	0.97	0.17	-	35,35,35,35	0
37	SR	0	8907	1/1	0.99	0.11	-	33,33,33,33	0
37	SR	0	8937	1/1	0.96	0.09	-	94,94,94,94	0
33	MG	0	8024	1/1	0.92	0.09	-	53,53,53,53	0
35	NA	0	8522	1/1	0.91	0.28	-	46,46,46,46	0
37	SR	0	8963	1/1	0.91	0.06	-	103,103,103,103	0
37	SR	0	8999	1/1	0.94	0.04	-	78,78,78,78	0
33	MG	0	8068	1/1	0.97	0.15	-	48,48,48,48	0
33	MG	0	8071	1/1	0.86	0.36	-	54,54,54,54	0
35	NA	S	8510	1/1	0.94	0.17	-	24,24,24,24	0
35	NA	0	8573	1/1	0.88	0.09	-	55,55,55,55	0
33	MG	0	8083	1/1	0.95	0.08	-	41,41,41,41	0
35	NA	0	8506	1/1	0.79	0.18	-	50,50,50,50	0
37	SR	0	8905	1/1	0.99	0.23	-	48,48,48,48	0
33	MG	0	8067	1/1	0.96	0.09	-	29,29,29,29	0
35	NA	0	8531	1/1	0.94	0.06	-	29,29,29,29	0
37	SR	0	9007	1/1	0.91	0.27	-	154,154,154,154	0
37	SR	0	8962	1/1	0.80	0.19	-	139,139,139,139	0
33	MG	0	8010	1/1	0.98	0.09	-	29,29,29,29	0
37	SR	0	8917	1/1	0.97	0.09	-	90,90,90,90	0
33	MG	0	8038	1/1	0.92	0.12	-	65,65,65,65	0
37	SR	0	8973	1/1	0.90	0.11	-	113,113,113,113	0
33	MG	0	8037	1/1	0.79	0.22	-	77,77,77,77	0
36	CL	0	8813	1/1	0.98	0.14	-	45,45,45,45	0
33	MG	0	8076	1/1	0.94	0.08	-	28,28,28,28	0
33	MG	0	8036	1/1	0.94	0.10	-	36,36,36,36	0
35	NA	0	8536	1/1	0.72	0.14	-	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	8911	1/1	0.97	0.08	-	65,65,65,65	0
35	NA	0	8548	1/1	0.78	0.09	-	50,50,50,50	0
33	MG	0	8048	1/1	0.99	0.07	-	33,33,33,33	0
37	SR	0	9000	1/1	0.79	0.18	-	150,150,150,150	0
33	MG	0	8077	1/1	0.96	0.08	-	26,26,26,26	0
33	MG	0	8090	1/1	0.98	0.09	-	49,49,49,49	0
33	MG	0	8018	1/1	0.99	0.13	-	38,38,38,38	0
33	MG	0	8016	1/1	0.96	0.06	-	35,35,35,35	0
33	MG	0	8023	1/1	0.98	0.06	-	24,24,24,24	0
33	MG	0	8069	1/1	0.78	0.17	-	58,58,58,58	0
37	SR	0	8956	1/1	0.92	0.06	-	127,127,127,127	0
37	SR	0	8971	1/1	0.75	0.09	-	158,158,158,158	0
35	NA	0	8561	1/1	0.87	0.55	-	62,62,62,62	0
37	SR	9	8980	1/1	0.65	0.20	-	162,162,162,162	0
37	SR	0	8990	1/1	0.93	0.10	-	106,106,106,106	0
33	MG	0	8046	1/1	0.93	0.10	-	25,25,25,25	0
36	CL	J	8802	1/1	0.97	0.09	-	51,51,51,51	0
37	SR	0	8967	1/1	0.97	0.04	-	116,116,116,116	0
37	SR	0	8938	1/1	0.97	0.05	-	147,147,147,147	0
33	MG	9	8074	1/1	0.75	0.10	-	64,64,64,64	0
35	NA	0	8554	1/1	0.76	0.31	-	52,52,52,52	0
35	NA	0	8507	1/1	0.93	0.10	-	27,27,27,27	0
33	MG	0	8093	1/1	0.94	0.09	-	29,29,29,29	0
37	SR	0	8957	1/1	0.67	0.33	-	176,176,176,176	0
37	SR	0	8979	1/1	0.49	0.29	-	184,184,184,184	0
38	CD	O	8705	1/1	0.99	0.06	-	58,58,58,58	0
37	SR	0	8995	1/1	0.95	0.07	-	112,112,112,112	0
33	MG	0	8017	1/1	0.94	0.21	-	26,26,26,26	0
37	SR	0	8906	1/1	0.99	0.10	-	40,40,40,40	0
37	SR	0	8988	1/1	0.82	0.10	-	149,149,149,149	0
33	MG	0	8027	1/1	0.95	0.04	-	32,32,32,32	0
35	NA	0	8502	1/1	0.95	0.18	-	43,43,43,43	0
37	SR	0	8909	1/1	1.00	0.08	-	70,70,70,70	0
35	NA	0	8501	1/1	0.99	0.19	-	26,26,26,26	0
37	SR	0	8982	1/1	0.91	0.19	-	152,152,152,152	0
35	NA	0	8524	1/1	0.98	0.20	-	31,31,31,31	0
37	SR	0	8931	1/1	0.96	0.06	-	86,86,86,86	0
33	MG	0	8049	1/1	0.96	0.11	-	64,64,64,64	0
36	CL	0	8814	1/1	0.97	0.11	-	40,40,40,40	0
33	MG	0	8089	1/1	0.95	0.19	-	37,37,37,37	0
36	CL	0	8811	1/1	0.97	0.11	-	45,45,45,45	0
33	MG	0	8031	1/1	0.89	0.09	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	S	8961	1/1	0.89	0.09	-	113,113,113,113	0
37	SR	0	8933	1/1	0.94	0.14	-	108,108,108,108	0
36	CL	0	8803	1/1	0.99	0.16	-	41,41,41,41	0
37	SR	0	8965	1/1	0.92	0.05	-	109,109,109,109	0
33	MG	0	8092	1/1	0.96	0.09	-	47,47,47,47	0
33	MG	0	8080	1/1	0.88	0.08	-	53,53,53,53	0
35	NA	0	8526	1/1	0.95	0.10	-	36,36,36,36	0
37	SR	0	8928	1/1	0.72	0.11	-	112,112,112,112	0
35	NA	0	8525	1/1	0.67	0.21	-	65,65,65,65	0
35	NA	0	8529	1/1	0.97	0.09	-	32,32,32,32	0
33	MG	K	8054	1/1	0.97	0.10	-	34,34,34,34	0
37	SR	0	8942	1/1	0.96	0.06	-	110,110,110,110	0
37	SR	0	8983	1/1	0.71	0.15	-	149,149,149,149	0
37	SR	0	8935	1/1	0.99	0.13	-	60,60,60,60	0
36	CL	0	8817	1/1	0.99	0.08	-	46,46,46,46	0
37	SR	1	8952	1/1	0.99	0.06	-	62,62,62,62	0
35	NA	0	8566	1/1	0.97	0.15	-	44,44,44,44	0
37	SR	0	8901	1/1	0.99	0.05	-	71,71,71,71	0
33	MG	0	8039	1/1	0.89	0.13	-	60,60,60,60	0
35	NA	0	8514	1/1	0.92	0.16	-	41,41,41,41	0
33	MG	0	8056	1/1	0.94	0.17	-	49,49,49,49	0
35	NA	0	8567	1/1	0.87	0.31	-	53,53,53,53	0
35	NA	0	8546	1/1	0.93	0.25	-	63,63,63,63	0
36	CL	A	8809	1/1	0.97	0.23	-	52,52,52,52	0
33	MG	0	8064	1/1	0.99	0.04	-	34,34,34,34	0
37	SR	0	8940	1/1	0.97	0.05	-	66,66,66,66	0
37	SR	0	8976	1/1	0.43	0.25	-	159,159,159,159	0
33	MG	0	8066	1/1	0.83	0.11	-	47,47,47,47	0
37	SR	0	8994	1/1	0.94	0.27	-	168,168,168,168	0
37	SR	0	8919	1/1	0.77	0.16	-	169,169,169,169	0
37	SR	0	9004	1/1	0.61	0.23	-	176,176,176,176	0
36	CL	L	8810	1/1	0.96	0.08	-	43,43,43,43	0
33	MG	0	8091	1/1	0.98	0.12	-	42,42,42,42	0
35	NA	0	8516	1/1	0.96	0.14	-	44,44,44,44	0
37	SR	0	8951	1/1	0.85	0.05	-	137,137,137,137	0
33	MG	0	8055	1/1	0.99	0.11	-	29,29,29,29	0
37	SR	0	8916	1/1	0.91	0.06	-	95,95,95,95	0
37	SR	0	9006	1/1	-0.01	0.99	-	200,200,200,200	0
35	NA	0	8509	1/1	0.90	0.15	-	47,47,47,47	0
37	SR	0	9002	1/1	0.63	0.17	-	162,162,162,162	0
35	NA	H	8518	1/1	0.73	0.23	-	66,66,66,66	0
37	SR	0	8989	1/1	0.87	0.18	-	148,148,148,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	8998	1/1	0.84	0.13	-	133,133,133,133	0
33	MG	0	8063	1/1	0.91	0.19	-	71,71,71,71	0
37	SR	0	8924	1/1	0.88	0.13	-	123,123,123,123	0
33	MG	0	8078	1/1	0.97	0.09	-	40,40,40,40	0
33	MG	0	8020	1/1	0.97	0.12	-	37,37,37,37	0
37	SR	0	8996	1/1	0.17	0.59	-	185,185,185,185	0
33	MG	0	8060	1/1	0.94	0.07	-	45,45,45,45	0
33	MG	0	8030	1/1	0.86	0.24	-	48,48,48,48	0
36	CL	J	8801	1/1	0.94	0.11	-	49,49,49,49	0
37	SR	0	8986	1/1	0.59	0.81	-	169,169,169,169	0
37	SR	0	8966	1/1	0.96	0.03	-	89,89,89,89	0
33	MG	0	8026	1/1	0.99	0.07	-	28,28,28,28	0
35	NA	9	8543	1/1	0.90	0.24	-	41,41,41,41	0
33	MG	0	8033	1/1	0.97	0.07	-	32,32,32,32	0
37	SR	0	8997	1/1	0.89	0.56	-	171,171,171,171	0
37	SR	0	8968	1/1	0.76	0.09	-	142,142,142,142	0
34	K	0	8401	1/1	0.93	0.11	-	58,58,58,58	0
37	SR	0	8926	1/1	0.94	0.06	-	95,95,95,95	0
37	SR	0	8908	1/1	0.97	0.09	-	71,71,71,71	0
37	SR	0	8915	1/1	0.96	0.06	-	85,85,85,85	0
35	NA	0	8544	1/1	0.89	0.20	-	49,49,49,49	0
37	SR	0	8953	1/1	0.96	0.07	-	121,121,121,121	0
37	SR	0	8941	1/1	0.93	0.05	-	90,90,90,90	0
33	MG	0	8035	1/1	0.95	0.07	-	52,52,52,52	0
37	SR	0	8925	1/1	0.99	0.06	-	75,75,75,75	0
33	MG	0	8059	1/1	0.99	0.04	-	27,27,27,27	0
33	MG	0	8085	1/1	0.73	0.12	-	90,90,90,90	0
36	CL	R	8806	1/1	0.97	0.16	-	40,40,40,40	0
35	NA	0	8545	1/1	0.99	0.13	-	29,29,29,29	0
37	SR	0	8939	1/1	0.91	0.09	-	108,108,108,108	0
36	CL	0	8822	1/1	0.98	0.15	-	48,48,48,48	0
37	SR	0	9001	1/1	0.36	0.26	-	160,160,160,160	0
37	SR	0	8923	1/1	0.98	0.08	-	78,78,78,78	0
37	SR	0	8914	1/1	0.97	0.10	-	88,88,88,88	0
33	MG	0	8005	1/1	0.98	0.10	-	23,23,23,23	0
35	NA	R	8532	1/1	0.93	0.09	-	37,37,37,37	0
37	SR	9	9003	1/1	0.90	0.08	-	141,141,141,141	0
35	NA	0	8541	1/1	0.88	0.15	-	41,41,41,41	0
37	SR	0	8934	1/1	0.96	0.12	-	116,116,116,116	0
37	SR	0	8974	1/1	0.56	0.20	-	159,159,159,159	0
37	SR	0	8954	1/1	0.95	0.11	-	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.