



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:38 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 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/ValidationPDFNotes.html>

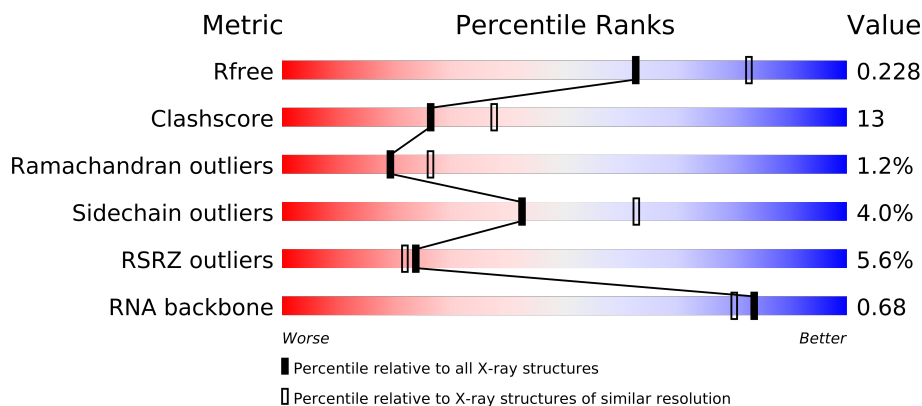
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)
RNA backbone	1838	1029 (3.00-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	0	2922	
2	9	122	
3	A	240	
4	B	338	
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	

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

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8030	-	X
33	MG	0	8037	-	X
33	MG	0	8063	-	X
33	MG	0	8068	-	X
33	MG	0	8071	-	X
33	MG	0	8073	-	X
33	MG	0	8081	-	X
33	MG	0	8085	-	X
33	MG	0	8089	-	X
35	NA	0	8505	-	X
35	NA	0	8506	-	X
35	NA	0	8508	-	X
35	NA	0	8509	-	X
35	NA	0	8514	-	X
35	NA	0	8516	-	X
35	NA	0	8517	-	X
35	NA	0	8521	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	0	8522	-	X
35	NA	0	8524	-	X
35	NA	0	8525	-	X
35	NA	0	8528	-	X
35	NA	0	8536	-	X
35	NA	0	8542	-	X
35	NA	0	8547	-	X
35	NA	0	8549	-	X
35	NA	0	8550	-	X
35	NA	0	8551	-	X
35	NA	0	8552	-	X
35	NA	0	8553	-	X
35	NA	0	8554	-	X
35	NA	0	8555	-	X
35	NA	0	8556	-	X
35	NA	0	8560	-	X
35	NA	0	8561	-	X
35	NA	0	8562	-	X
35	NA	0	8563	-	X
35	NA	0	8564	-	X
35	NA	0	8565	-	X
35	NA	0	8567	-	X
35	NA	0	8568	-	X
35	NA	0	8571	-	X
35	NA	0	8574	-	X
35	NA	9	8572	-	X
35	NA	R	8575	-	X
36	CL	0	8822	-	X
37	SR	0	8903	-	X
37	SR	0	8905	-	X
37	SR	0	8919	-	X
37	SR	0	8955	-	X
37	SR	0	8957	-	X
37	SR	0	8962	-	X
37	SR	0	8969	-	X
37	SR	0	8974	-	X
37	SR	0	8976	-	X
37	SR	0	8979	-	X
37	SR	0	8982	-	X
37	SR	0	8986	-	X
37	SR	0	8989	-	X
37	SR	0	8992	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
37	SR	0	8994	-	X
37	SR	0	8996	-	X
37	SR	0	8997	-	X
37	SR	0	9000	-	X
37	SR	0	9001	-	X
37	SR	0	9002	-	X
37	SR	0	9004	-	X
37	SR	0	9006	-	X
37	SR	0	9007	-	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 hydrogen and 0 are deuterium.

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			

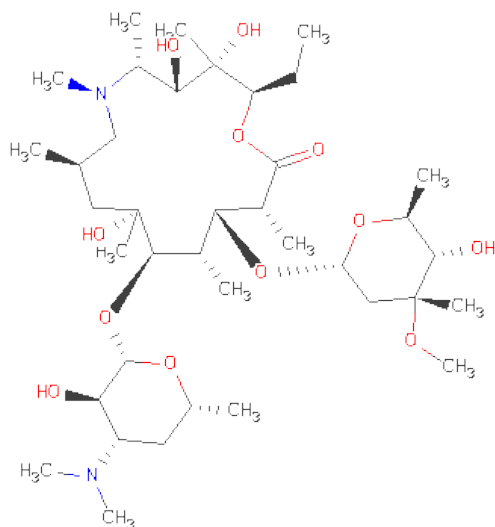
- Molecule 30 is a protein called 50S ribosomal protein L39e.

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	Cd	0	0
			1	1		
38	U	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

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

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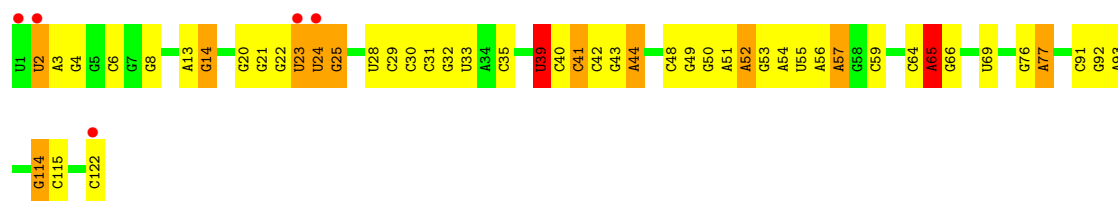
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	P	66	Total 66	O 66	0	0
39	Q	53	Total 53	O 53	0	0
39	R	87	Total 87	O 87	0	0
39	S	32	Total 32	O 32	0	0
39	T	41	Total 41	O 41	0	0
39	U	28	Total 28	O 28	0	0
39	V	12	Total 12	O 12	0	0
39	W	68	Total 68	O 68	0	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

C2867	U2756	G2634	G2516	G2421	U2590	C	G	G2005	U1740	A1603	A1427	C1289	A1191
C2868	A2761	A2635	A2521	U2422	A2291	C	U	U2008	U1741	G1604	A1439	G1290	A1192
G2869	C2762	C2636	G2524	G2426	A2300	A	C	A2011	A1742	G1605	U1440	A1291	A1193
G2876	A2768	G2638	G2525	G2427	A2301	C	C	G2012	G1752	A1615	G1441	G1295	G1195
G2877	C2769	C2637	G2526	G2428	A2302	C	C	G2013	C1753	U1625	A1442	G1299	G1196
U2878	G2770	G2642	U2527	U2435	C2309	A	C	G2014	A1754	A1626	G1452	G1300	G1197
A2879		G2643	G2533	U2442	C2313	C	U	U2016	G1755	A1627	U1458	U1304	U1198
		G2644	G2534	U2443	G2316	G	G	C2031	A1756	A1630	A1470	U1305	C1201
		U2661	G2535	U2444	C2317	A	C	G2032	G1757	A1634	G1474	U1306	A1202
		G2662	G2536	U2445	U2320	A	A	U2034	G1758	A1642	C1477	U1307	G1203
		G2663	G2537	U2446	A2321	A	G	C2036	C1759	A1644	U1477	A1308	C1204
		U2664	G2538	G2453	C2326	U	C	G2044	G1773	A1653	G1484	U1314	U1205
		A	U2541	A2456	C2327	U	C	A2054	G1774	U1654	U1497	A1328	U1206
		U	G2543	U2457	G2336	U	U	U2064	G1777	G1655	G1497	U1329	C1208
		G2667	G2544	G2462	G2337	A	G	G2072	A1778	U1656	U1500	U1333	C1209
		G2670	C2547	A2465	G2338	C	G	A2081	A1779	A1657	U1503	C1334	G1210
		G2671	G2548	A2466	A	C	U	G2089	G1950	A1658	U1504	C1335	G1211
		G2672	C2549	A2467	C	C	C	G2090	G1951	A1666	A1504	C1342	G1212
		U2673	A	A2468	C	C	A	A2096	U	A1667	U1505	C1343	G1216
			C		C	C	G	A2097	A	U1668	U1506	U1218	U1219
			G		A	U	G	A2098	C	C1786	U1507	G1351	
			A		G	U	C	G2099	C	C1787	U1508	A1352	
			A		A	C	U	A2099	U	C1788	U1509	A1353	
			A		A	C	U	A2099	U	C1789	U1510	G1354	
			A		A	C	U	A2099	U	C1790	U1511	C1355	
			A		A	C	U	A2099	U	C1791	U1512	C1356	
			A		A	C	U	A2099	U	C1792	U1513	C1357	
			A		A	C	U	A2099	U	C1793	U1514	C1358	
			A		A	C	U	A2099	U	C1794	U1515	C1359	
			A		A	C	U	A2099	U	C1795	U1516	C1360	
			A		A	C	U	A2099	U	C1796	U1517	C1361	
			A		A	C	U	A2099	U	C1797	U1518	C1362	
			A		A	C	U	A2099	U	C1798	U1519	C1363	
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			A		A	C	U	A2099	U	C1800	U1521	C1365	
			A		A	C	U	A2099	U	C1801	U1522	C1366	
			A		A	C	U	A2099	U	C1802	U1523	C1367	
			A		A	C	U	A2099	U	C1803	U1524	C1368	
			A		A	C	U	A2099	U	C1804	U1525	C1369	
			A		A	C	U	A2099	U	C1805	U1526	C1370	
			A		A	C	U	A2099	U	C1806	U1527	C1371	
			A		A	C	U	A2099	U	C1807	U1528	C1372	
			A		A	C	U	A2099	U	C1808	U1529	C1373	
			A		A	C	U	A2099	U	C1809	U1530	C1374	
			A		A	C	U	A2099	U	C1810	U1531	C1375	
			A		A	C	U	A2099	U	C1811	U1532	C1376	
			A		A	C	U	A2099	U	C1812	U1533	C1377	
			A		A	C	U	A2099	U	C1813	U1534	C1378	
			A		A	C	U	A2099	U	C1814	U1535	C1379	
			A		A	C	U	A2099	U	C1815	U1536	C1380	
			A		A	C	U	A2099	U	C1816	U1537	C1381	
			A		A	C	U	A2099	U	C1817	U1538	C1382	
			A		A	C	U	A2099	U	C1818	U1539	C1383	
			A		A	C	U	A2099	U	C1819	U1540	C1384	
			A		A	C	U	A2099	U	C1820	U1541	C1385	
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			A		A	C	U	A2099	U	C1822	U1543	C1387	
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			A		A	C	U	A2099	U	C1896	U1617	C1461	
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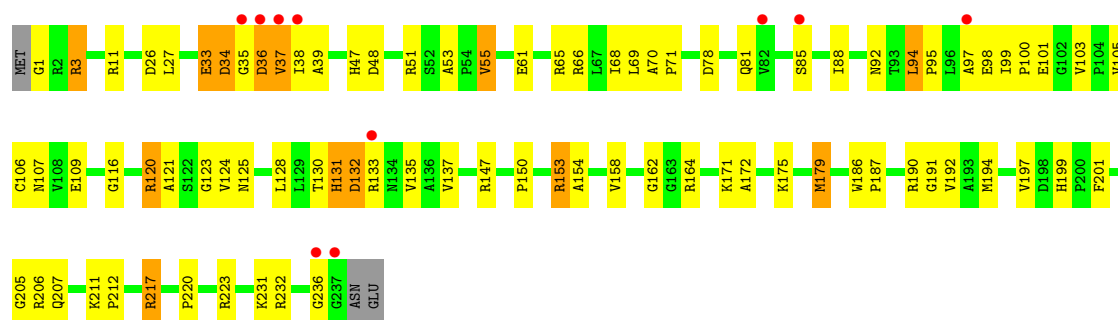
- Molecule 2: 5S Ribosomal RNA

Chain 9:



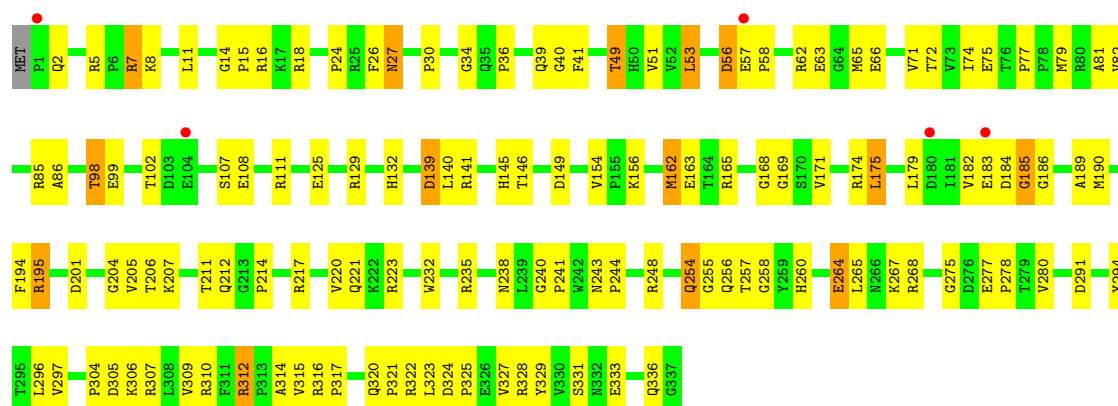
- Molecule 3: 50S ribosomal protein L2P

Chain A:



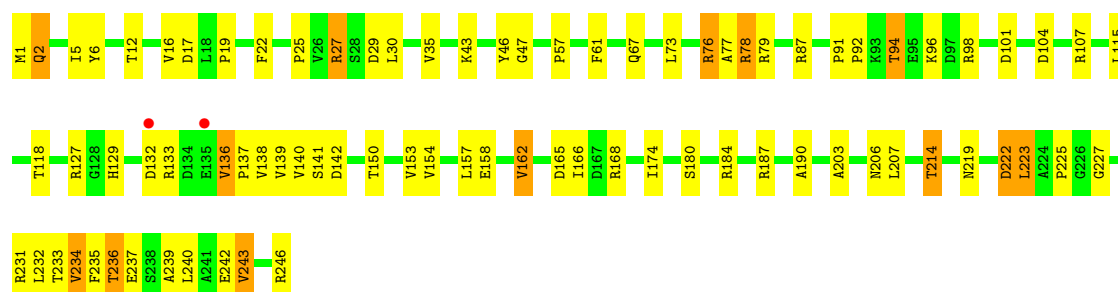
- Molecule 4: 50S ribosomal protein L3P

Chain B:

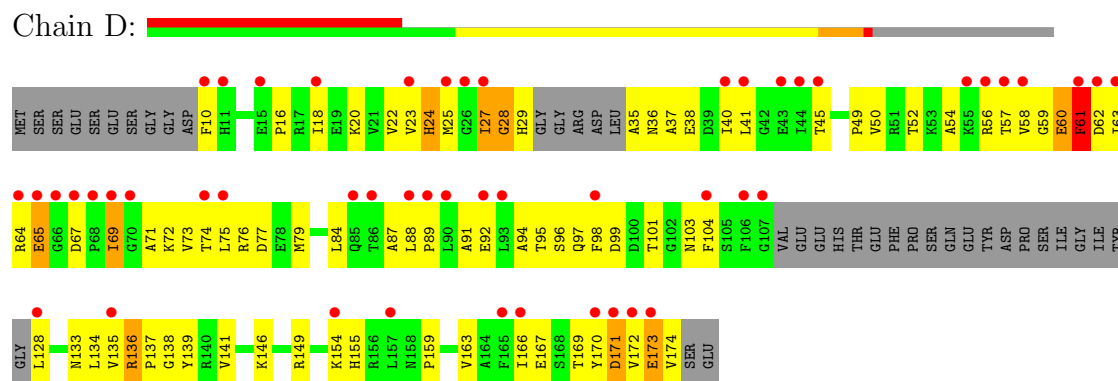


- Molecule 5: 50S ribosomal protein L4E

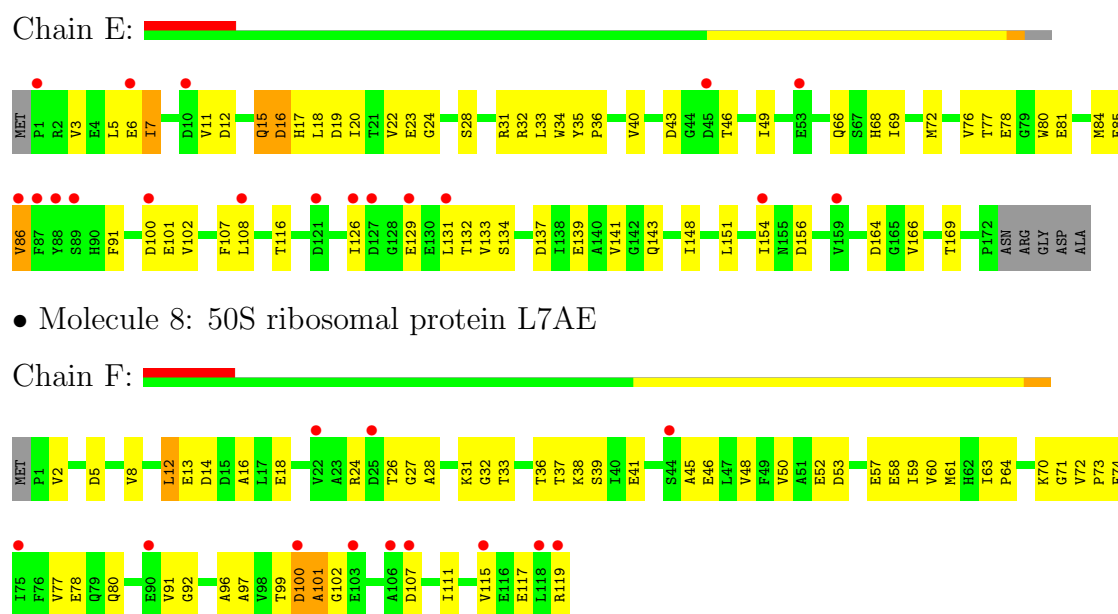
Chain C:



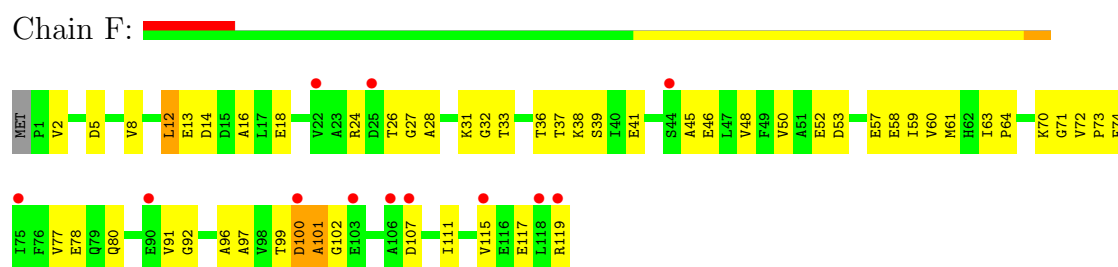
- Molecule 6: 50S ribosomal protein L5P



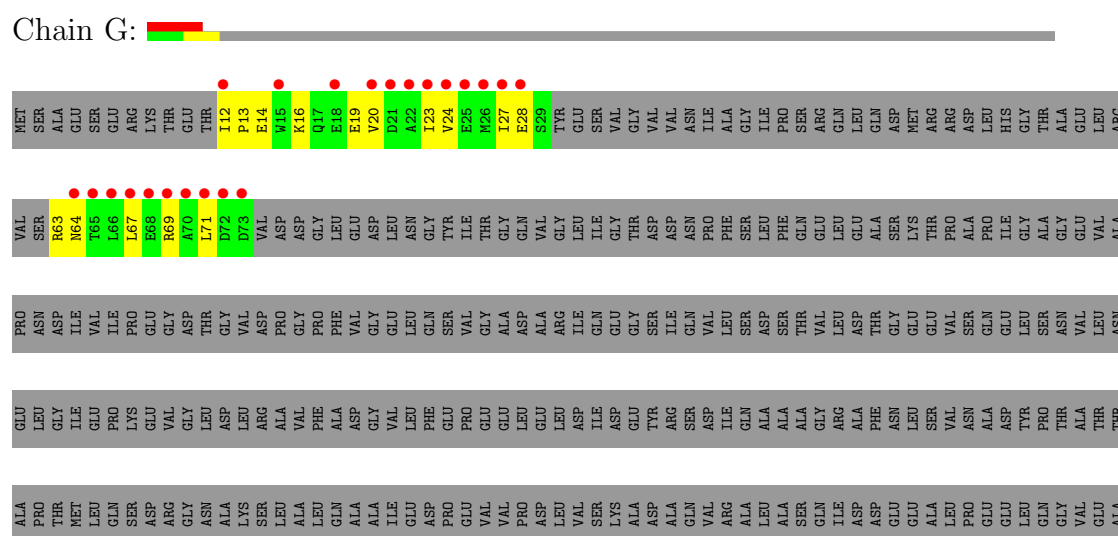
- Molecule 7: 50S ribosomal protein L6P



- Molecule 8: 50S ribosomal protein L7AE



- Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



ASP	VAL	ALA	THR	GLU	PRO	THR	ASP	ASP	GLN	ASP	ASP	THR	ALA	SER	GLU	ASP	ALA	ALA	ASP	ALA	ALA	GLU	GLU	ALA	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLU	ALA	GLY	ASP	ALA	LEU	GLY	ALA	GLY	ASP	THR
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- Molecule 10: 50S RIBOSOMAL PROTEIN L10E

Chain H:

[illegible]

- Molecule 11: 50S RIBOSOMAL PROTEIN L11P

Chain I: 

[illegible]

- Molecule 12: 50S ribosomal protein L13P

Chain J:

M107	P108 Y109	I127	K128 F129	V130 T131 L132 G133	S136	K143 T144	#145													
MET	SER	VAL	A4	F6 D7	D13 A14 R15	I18 M19	V26	V36	E42	V45 I46 T47 G48	Q52	I53	I63 G64	Y69 F70 Y71 <i>P72</i>	<i>K73</i> R74 P75 <i>G77</i> I78 F79 K80 R81	T82	P88 H89	K90	R93 G94	V101 R102 V103 Y104 L105

- Molecule 13: 50S ribosomal protein L14P

Chain K:

E108	L109	K110	G111	P112	I113	A114	R115	E116	V117	A118	A125	S126	A127	V132	E133	L134	K135	G136	P137	I138	A139	R140	E141	V142	A143	A144	R145	E146	V147	A148	A149	R150	E151	V152	A153	A154	R155	E156	V157	A158	A159	R160	E161	V162	A163	A164	R165	E166	V167	A168	A169	R170	E171	V172	A173	A174	R175	E176	V177	A178	A179	R180	E181	V182	A183	A184	R185	E186	V187	A188	A189	R190	E191	V192	A193	A194	R195	E196	V197	A198	A199	R200	E201	V202	A203	A204	R205	E206	V207	A208	A209	R210	E211	V212	A213	A214	R215	E216	V217	A218	A219	R220	E221	V222	A223	A224	R225	E226	V227	A228	A229	R230	E231	V232	A233	A234	R235	E236	V237	A238	A239	R240	E241	V242	A243	A244	R245	E246	V247	A248	A249	R250	E251	V252	A253	A254	R255	E256	V257	A258	A259	R260	E261	V262	A263	A264	R265	E266	V267	A268	A269	R270	E271	V272	A273	A274	R275	E276	V277	A278	A279	R280	E281	V282	A283	A284	R285	E286	V287	A288	A289	R290	E291	V292	A293	A294	R295	E296	V297	A298	A299	R300	E301	V302	A303	A304	R305	E306	V307	A308	A309	R310	E311	V312	A313	A314	R315	E316	V317	A318	A319	R320	E321	V322	A323	A324	R325	E326	V327	A328	A329	R330	E331	V332	A333	A334	R335	E336	V337	A338	A339	R340	E341	V342	A343	A344	R345	E346	V347	A348	A349	R350	E351	V352	A353	A354	R355	E356	V357	A358	A359	R360	E361	V362	A363	A364	R365	E366	V367	A368	A369	R370	E371	V372	A373	A374	R375	E376	V377	A378	A379	R380	E381	V382	A383	A384	R385	E386	V387	A388	A389	R390	E391	V392	A393	A394	R395	E396	V397	A398	A399	R400	E401	V402	A403	A404	R405	E406	V407	A408	A409	R410	E411	V412	A413	A414	R415	E416	V417	A418	A419	R420	E421	V422	A423	A424	R425	E426	V427	A428	A429	R430	E431	V432	A433	A434	R435	E436	V437	A438	A439	R440	E441	V442	A443	A444	R445	E446	V447	A448	A449	R450	E451	V452	A453	A454	R455	E456	V457	A458	A459	R460	E461	V462	A463	A464	R465	E466	V467	A468	A469	R470	E471	V472	A473	A474	R475	E476	V477	A478	A479	R480	E481	V482	A483	A484	R485	E486	V487	A488	A489	R490	E491	V492	A493	A494	R495	E496	V497	A498	A499	R500	E501	V502	A503	A504	R505	E506	V507	A508	A509	R510	E511	V512	A513	A514	R515	E516	V517	A518	A519	R520	E521	V522	A523	A524	R525	E526	V527	A528	A529	R530	E531	V532	A533	A534	R535	E536	V537	A538	A539	R540	E541	V542	A543	A544	R545	E546	V547	A548	A549	R550	E551	V552	A553	A554	R555	E556	V557	A558	A559	R560	E561	V562	A563	A564	R565	E566	V567	A568	A569	R570	E571	V572	A573	A574	R575	E576	V577	A578	A579	R580	E581	V582	A583	A584	R585	E586	V587	A588	A589	R590	E591	V592	A593	A594	R595	E596	V597	A598	A599	R600	E601	V602	A603	A604	R605	E606	V607	A608	A609	R610	E611	V612	A613	A614	R615	E616	V617	A618	A619	R620	E621	V622	A623	A624	R625	E626	V627	A628	A62
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- Molecule 14: 50S ribosomal protein L15P

Chain L:

[illegible]



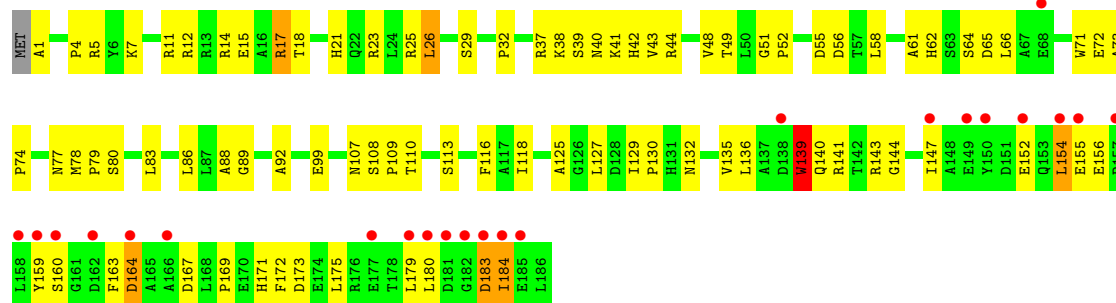
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



• Molecule 16: 50S ribosomal protein L18P

Chain N:



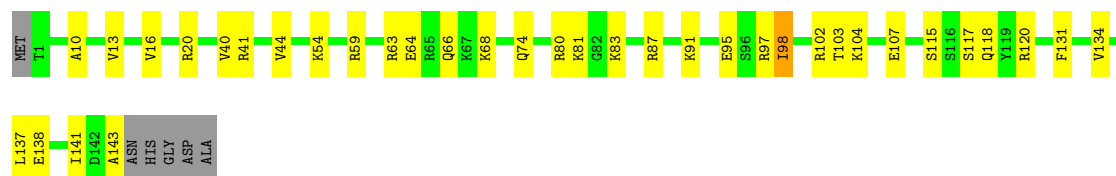
• Molecule 17: 50S ribosomal protein L18e

Chain O:



• Molecule 18: 50S ribosomal protein L19E

Chain P:



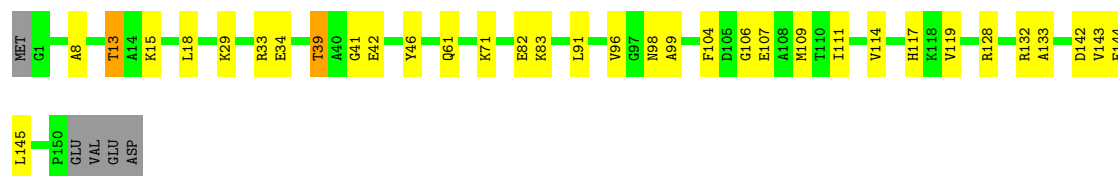
• Molecule 19: 50S ribosomal protein L21e

Chain Q:



- Molecule 20: 50S ribosomal protein L22P

Chain R:



- Molecule 21: 50S ribosomal protein L23P

Chain S:



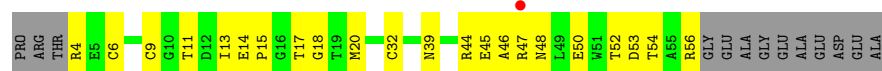
- Molecule 22: 50S ribosomal protein L24P

Chain T:



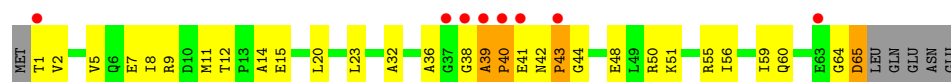
- Molecule 23: 50S ribosomal protein L24E

Chain U:



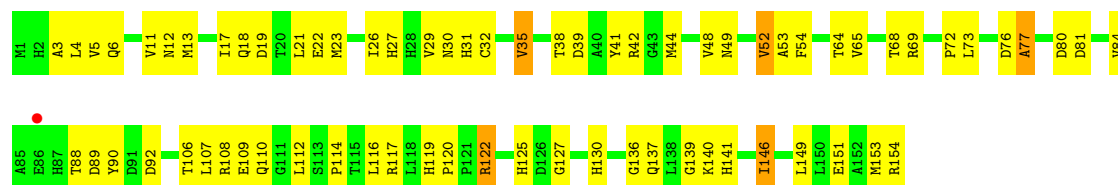
- Molecule 24: 50S ribosomal protein L29P

Chain V:



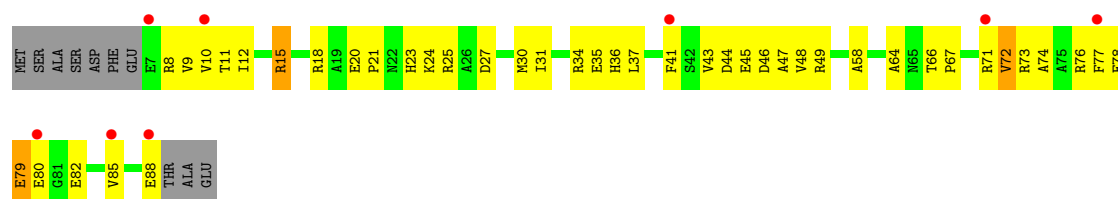
- Molecule 25: 50S ribosomal protein L30P

Chain W:



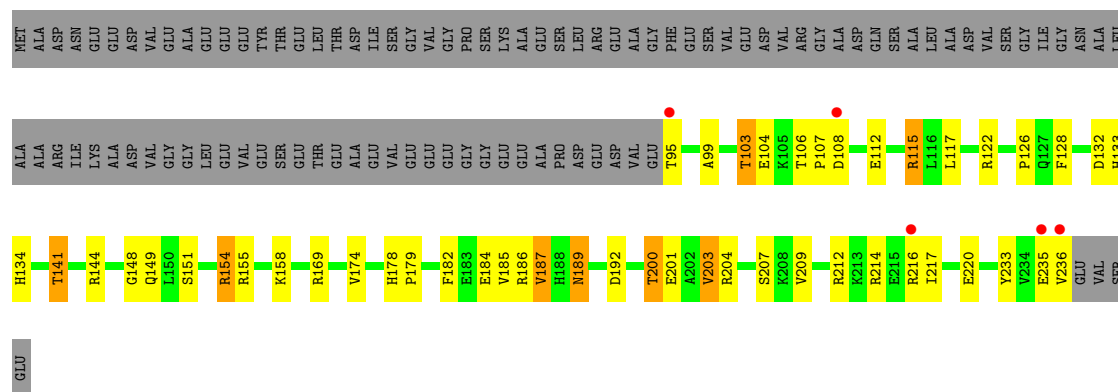
- Molecule 26: 50S ribosomal protein L31e

Chain X:



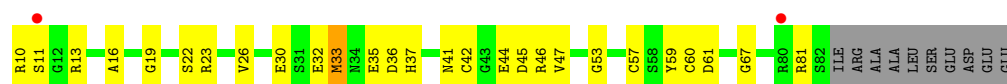
- Molecule 27: 50S ribosomal protein L32E

Chain Y:



- Molecule 28: 50S ribosomal protein L37Ae

Chain Z:



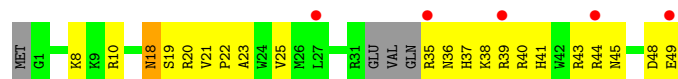
- Molecule 29: 50S ribosomal protein L37e

Chain 1:



- Molecule 30: 50S ribosomal protein L39e

Chain 2:



- Molecule 31: 50S ribosomal protein L44E

Chain 3:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.08Å 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) 90.1 (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 0.191 , 0.228	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)	0.35 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 634402 reflections	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	R	1149	0	1122	41	0
21	S	641	0	605	20	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	1	2	0	0	0	0
37	3	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	X	24	0	0	8	0
39	Y	95	0	0	13	0
39	Z	32	0	0	2	0
All	All	99116	0	59987	2007	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (2007) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
15:M:164:THR:HG22	15:M:167:GLY:H	1.32	0.95
2:9:56:A:H2'	2:9:57:A:H5''	1.46	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
16:N:144:GLY:O	16:N:147:ILE:HG22	1.68	0.92
12:J:19:MET:HE3	12:J:132:LEU:HD21	1.50	0.92
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.69	0.92
25:W:88:THR:HB	39:W:6679:HOH:O	1.70	0.92
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.50	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	Distance(Å)	Clash(Å)
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.91
4:B:162:MET:HE2	4:B:310:ARG:HD3	1.51	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
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.73	0.89
4:B:238:ASN:HD22	4:B:240:GLY:H	1.18	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
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.38	0.88
3:A:35:GLY:O	3:A:36:ASP:HB3	1.71	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
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.57	0.86
24:V:1:THR:HG23	24:V:2:VAL:H	1.40	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
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
1:0:282:C:H1'	1:0:368:C:N4	1.92	0.84
10:H:170:ARG:HD2	39:H:8989:HOH:O	1.78	0.84
13:K:10:GLN:H	13:K:10:GLN:HE21	0.88	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:O: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
1:O:1116:U:HO2'	1:O:1118:A:H2	0.83	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:O:1667:A:H8	1:O:1667:A:H5'	1.41	0.83
1:O:1701:A:H4'	1:O:1702:U:H5''	1.60	0.83
1:O:1041:U:H5'	39:L:8881:HOH:O	1.77	0.82
1:O:506:G:H22	1:O: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:O:1474:C:H6	1:O:1474:C:H5'	1.43	0.82
1:O:541:C:C2'	1:O: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:O: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
11:I:73:LEU:HD12	11:I:107:LYS:HZ2	1.46	0.81
3:A:153:ARG:HH11	3:A:153:ARG:HB2	1.45	0.81
1:O:2890:A:H1'	23:U:56:ARG:NH2	1.96	0.80
1:O:1973:A:H5'	1:O:1973:A:H8	1.45	0.80
28:Z:10:ARG:HA	39:Z:8714:HOH:O	1.79	0.80
39:9:9098:HOH:O	16:N:23:ARG:HD3	1.80	0.80
1:O:2054:A:N3	20:R:128:ARG:NH2	2.30	0.80
1:O:2840:A:OP1	4:B:211:THR:HG23	1.82	0.80
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.96	0.79
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.46	0.79
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.63	0.79
1:O: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:O:2586:U:H3	1:O:2592:G:H22	1.28	0.78
1:O:2488:A:H61	1:O: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:O:1116:U:O2'	1:O:1118:A:H2	1.65	0.78
8:F:91:VAL:HG12	8:F:92:GLY:N	1.98	0.78
29:1:25:LYS:HD2	30:2:49:GLU:H	1.46	0.78
14:L:133:VAL:HA	39:L:8865:HOH:O	1.84	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:2506:A:O2'	1:O:2507:G:H8	1.68	0.76
1:O:1116:U:H3	1:O:1246:A:H62	1.33	0.76
7:E:100:ASP:HB2	39:E:2789:HOH:O	1.85	0.76
5:C:236:THR:CG2	5:C:239:ALA:H	1.95	0.76
1:O:1878:G:H1'	39:O:6568:HOH:O	1.85	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:871:G:H8	1:O:871:G:C5'	1.99	0.76
8:F:91:VAL:HG12	8:F:92:GLY:H	1.48	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
1:O:544:G:H2'	1:O:545:G:H5''	1.67	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
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
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.16	0.75
4:B:62:ARG:HA	4:B:65:MET:HE2	1.68	0.75
4:B:201:ASP:HB2	4:B:312:ARG:HD2	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
21:S:57:THR:HG22	21:S:59:ASP:N	2.01	0.74
3:A:199:HIS:CD2	3:A:201:PHE:H	2.04	0.74
1:O:236:A:H4'	1:O:237:G:H5'	1.69	0.74
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.68	0.74
5:C:140:VAL:HB	39:C:8656:HOH:O	1.88	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:506:G:H22	1:0:509:A:C5'	2.01	0.74
1:0:545:G:H8	1:0:545:G:H5'	1.51	0.74
5:C:139:VAL:HG13	39:C:8653:HOH:O	1.86	0.74
2:9:56:A:C2'	2:9:57:A:H5''	2.18	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
1:0:1183:C:H2'	39:0:6690:HOH:O	1.87	0.74
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.70	0.74
4:B:16:ARG:NH1	39:B:9084:HOH:O	2.20	0.74
1:0:1372:A:H3'	39:0:7622:HOH:O	1.88	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
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
1:0:1819:G:H2'	1:0:1820:G:H4'	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
4:B:221:GLN:HE22	13:K:42:ASN:HD22	1.33	0.72
1:0:2908:A:H2'	1:0:2909:G:O4'	1.89	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
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.69	0.72
1:0:450:C:OP1	5:C:184:ARG:NH2	2.22	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
25:W:125:HIS:HD2	25:W:127:GLY:H	1.36	0.72
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.71	0.72
1:0:2896:A:H5''	39:0:6546:HOH:O	1.89	0.71
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.21	0.71
8:F:96:ALA:HA	39:F:3111:HOH:O	1.89	0.71
17:O:32:ARG:HD3	17:O:32:ARG:O	1.90	0.71
1:0:962:C:H1'	16:N:5:ARG:NH1	2.05	0.71
2:9:29:C:H2'	2:9:30:C:H5'	1.73	0.71
1:0:1603:A:H5'	1:0:1605:G:O4'	1.91	0.71
21:S:43:GLU:HB3	39:S:8990:HOH:O	1.90	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.21	0.71
1:0:1666:C:O2'	1:0:1667:A:H5''	1.91	0.71
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
1:0:481: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
39:0:4698:HOH:O	30:2:38:LYS:HE3	1.90	0.70
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.73	0.70
1:0:877:G:H5'	1:0:878:G:OP1	1.92	0.70
4:B:275:GLY:O	4:B:291:ASP:HA	1.91	0.70
3:A:164:ARG:NE	39:A:9050:HOH:O	2.24	0.70
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.74	0.70
2:9:39:U:H1'	2:9:44:A:H61	1.55	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
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.73	0.70
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.73	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
1:0:1184:C:H1'	39:0:7891:HOH:O	1.90	0.70
1:0:541:C:H2'	1:0:542:A:C5'	2.21	0.70
12:J:45:VAL:HG23	12:J:130:VAL:O	1.91	0.70
1:0:244:C:OP2	8:F:38:LYS:HE3	1.91	0.70
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.72	0.70
6:D:128:LEU:HB2	39:D:6007:HOH:O	1.90	0.70
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.20	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
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
20:R:39:THR:HG23	20:R:107:GLU:O	1.93	0.69
1:0:2748:G:H2'	39:0:7963:HOH:O	1.91	0.69
8:F:58:GLU:OE1	15:M:27:ARG:NH2	2.25	0.69
2:9:6:C:OP1	16:N:37:ARG:NH1	2.25	0.69
1:0:796:A:HO2'	28:Z:10:ARG:N	1.91	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2780:C:H1'	7:E:143:GLN:HE21	1.58	0.69
1:0:1593:C:OP1	18:P:117:SER:HB3	1.93	0.69
1:0:2533:C:H5'	1:0:2533:C:H6	1.58	0.69
16:N:80:SER:HB2	39:N:8835:HOH:O	1.92	0.69
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.28	0.69
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.28	0.69
1:0:1118:A:C8	1:0:1118:A:H3'	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
14:L:148:GLU:HA	39:L:8864:HOH:O	1.93	0.68
4:B:58:PRO:HA	4:B:63:GLU:OE1	1.92	0.68
4:B:190:MET:HE2	4:B:194:PHE:HD1	1.59	0.68
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.76	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
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.25	0.67
24:V:12:THR:HG22	24:V:15:GLU:CG	2.24	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
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.07	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
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
5:C:1:MET:HG2	5:C:2:GLN:N	2.10	0.67
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.76	0.67
15:M:164:THR:HG22	15:M:167:GLY:N	2.09	0.66
1:0:338:C:H4'	5:C:174:ILE:CD1	2.25	0.66
1:0:1679:C:H5'	39:0:9811:HOH:O	1.95	0.66
1:0:794:U:H3	1:0:819:A:H61	1.42	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1667:A:C8	1:0:1667:A:H5'	2.29	0.66
25:W:13:MET:CE	25:W:17:ILE:HG22	2.24	0.66
1:0:558:C:C2'	1:0:559:U:H5''	2.26	0.66
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.11	0.66
5:C:2:GLN:HB3	39:C:8589:HOH:O	1.96	0.66
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.61	0.66
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.61	0.66
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.96	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
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.61	0.65
1:0:2851:G:O2'	1:0:2852:A:H5'	1.96	0.65
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.27	0.65
39:O:5438:HOH:O	15:M:125:ARG:HD3	1.96	0.65
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.79	0.65
4:B:185:GLY:HA2	39:B:9103:HOH:O	1.96	0.65
25:W:21:LEU:HD21	25:W:48:VAL:CG1	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
1:0:1163:G:H5'	11:I:110:ASP:O	1.97	0.65
25:W:13:MET:HE1	25:W:18:GLN:HA	1.78	0.65
16:N:132:ASN:O	16:N:135:VAL:HG12	1.97	0.65
1:0:513:A:N3	39:O:4140:HOH:O	2.29	0.65
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
1:0:2505:G:O2'	1:0:2506:A:H5'	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
10:H:114:ASP:HB2	39:H:8996:HOH:O	1.96	0.65
5:C:236:THR:HA	39:C:8656:HOH:O	1.96	0.65
1:0:1183:C:N4	1:0:1184:C:H41	1.95	0.65
1:0:871:G:C8	1:0:871:G:C5'	2.74	0.64
1:0:282:C:O2'	1:0:283:U:H5'	1.96	0.64
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.12	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:W:80:ASP:O	25:W:84:VAL:HG23	1.97	0.64
20:R:99:ALA:HB1	20:R:109:MET:CE	2.26	0.64
1:O:797:A:C4'	28:Z:10:ARG:N	2.61	0.64
29:1:42:SER:HB2	39:1:8957:HOH:O	1.97	0.64
1:O:2004:U:H4'	39:0:5759:HOH:O	1.96	0.64
1:O:470:U:O2'	29:1:16:HIS:HD2	1.80	0.64
1:O:2783:A:H3'	39:0:5684:HOH:O	1.96	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
2:9:39:U:H1'	2:9:44:A:N6	2.11	0.64
1:O:1165:G:H4'	1:O:1174:A:O2'	1.97	0.64
14:L:143:THR:HG22	14:L:144:ASP:N	2.12	0.64
1:O:1684:A:H1'	30:2:43:ARG:HH22	1.62	0.64
25:W:151:GLU:O	25:W:154:ARG:HB2	1.98	0.64
39:0:5912:HOH:O	9:G:12:ILE:HG23	1.98	0.64
1:O:2827:A:H2'	1:O:2828:G:O4'	1.98	0.64
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.44	0.64
25:W:149:LEU:HG	25:W:153:MET:HE2	1.80	0.64
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.77	0.64
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.45	0.64
26:X:9:VAL:HG13	26:X:88:GLU:OE1	1.97	0.64
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.78	0.64
1:O:544:G:C2'	1:O:545:G:H5''	2.27	0.64
1:O:1189:A:H3'	39:0:8185:HOH:O	1.97	0.64
18:P:115:SER:N	18:P:118:GLN:HE21	1.88	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
1:O:1641:A:H2'	1:O:1642:A:H5'	1.79	0.64
3:A:33:GLU:CD	3:A:33:GLU:H	2.01	0.64
1:O:2721:U:H4'	13:K:87:ARG:HG3	1.80	0.64
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.27	0.64
27:Y:144:ARG:NH1	39:Y:8875:HOH:O	2.26	0.64
4:B:305:ASP:O	4:B:306:LYS:HB2	1.98	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
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.79	0.63
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.79	0.63
11:I:100:VAL:HG11	11:I:124:VAL:HG22	1.80	0.63
1:O:396:U:H1'	39:0:8134:HOH:O	1.99	0.63
39:0:7310:HOH:O	15:M:178:LYS:HB2	1.97	0.63
28:Z:13:ARG:NH1	39:Z:8719:HOH:O	2.30	0.63
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.64	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
2:9:6:C:C5'	16:N:37:ARG:NH1	2.57	0.63
2:9:14:G:H5'	2:9:14:G:C8	2.32	0.63
7:E:69:ILE:HA	7:E:72:MET:HE3	1.80	0.63
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.80	0.63
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.80	0.63
13:K:98:VAL:HG11	13:K:102:GLU:HA	1.78	0.63
1:0:1209:C:H2'	1:0:1210:G:H8	1.64	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
23:U:17:THR:HG22	23:U:18:GLY:N	2.14	0.63
7:E:69:ILE:HA	7:E:72:MET:CE	2.29	0.63
25:W:65:VAL:HA	25:W:68:THR:HG22	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
25:W:84:VAL:HG12	39:W:6679:HOH:O	1.98	0.62
10:H:49:GLN:HG3	10:H:140:TYR:CE2	2.34	0.62
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.98	0.62
8:F:38:LYS:NZ	15:M:3:SER:HA	2.15	0.62
1:0:2426:G:H1'	39:0:6539:HOH:O	1.99	0.62
11:I:101:LYS:O	11:I:105:GLU:HG3	1.99	0.62
7:E:68:HIS:O	7:E:72:MET: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
23:U:14:GLU:O	23:U:17:THR:HB	2.00	0.62
1:0:2578:G:H5'	1:0:2578:G:H8	1.64	0.62
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.81	0.62
25:W:4:LEU:O	25:W:32:CYS:HA	1.99	0.62
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.65	0.62
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.30	0.62
6:D:99:ASP:HB3	6:D:103:ASN:H	1.64	0.62
24:V:64:GLY:O	24:V:65:ASP:HB2	2.00	0.62
1:0:1377:C:H6	1:0:1377:C:H5'	1.65	0.62
11:I:108:HIS:N	11:I:109:PRO:HD2	2.14	0.62
3:A:194:MET:CE	3:A:199:HIS:HB2	2.29	0.61
1:0:2533:C:C6	1:0:2533:C:H5'	2.34	0.61
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.32	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:V:39:ALA:N	24:V:40:PRO:HD2	2.16	0.61
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.65	0.61
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.80	0.61
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.99	0.61
1:0:656:G:H5'	17:O:3:THR:CG2	2.30	0.61
1:0:558:C:H2'	1:0:559:U:C5'	2.30	0.61
1:0:2420:G:O2'	1:0:2421:G:H5'	2.00	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
1:0:1819:G:H5'	39:0:5176:HOH:O	2.01	0.61
5:C:236:THR:H	5:C:239:ALA:HB3	1.64	0.61
4:B:307:ARG:HD2	39:B:9123:HOH:O	2.00	0.61
1:0:1189:A:H1'	1:0:1209:C:C1'	2.30	0.61
6:D:91:ALA:HB1	39:D:5198:HOH:O	2.00	0.61
1:0:2414:A:H2'	1:0:2415:A:C8	2.36	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
1:0:2769:C:C2'	1:0:2770:G:H5'	2.31	0.61
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.34	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
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.82	0.61
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.82	0.61
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.83	0.61
27:Y:144:ARG:NH2	39:Y:8910:HOH:O	2.33	0.61
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.81	0.61
16:N:169:PRO:O	16:N:172:PHE:HB3	2.00	0.61
5:C:162:VAL:HG22	5:C:232:LEU:HD21	1.83	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
1:0:1058:A:H2'	1:0:1060:C:H5'	1.82	0.61
14:L:79:ASP:HB3	39:L:8850:HOH:O	2.01	0.61
1:0:709:G:O2'	17:O:25:VAL:HG12	2.00	0.61
29:1:10:LYS:HG3	39:1:8979:HOH:O	2.00	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
18:P:115:SER:H	18:P:118:GLN:NE2	1.89	0.60
1:0:2718:C:H6	1:0:2718:C:H5'	1.67	0.60
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.29	0.60
3:A:88:ILE:HG22	3:A:88:ILE:O	2.00	0.60
1:0:757:C:OP1	14:L:27:ARG:HD2	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.83	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
12:J:103:VAL:HG12	39:J:5907:HOH:O	2.01	0.60
4:B:145:HIS:HD2	4:B:146:THR:O	1.84	0.60
31:3:55:VAL:HG22	39:3:8937:HOH:O	2.01	0.60
1:0:2064:U:H5'	1:0:2652:U:H4'	1.83	0.60
4:B:102:THR:CG2	4:B:182:VAL:HG12	2.31	0.60
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.82	0.60
22:T:7:GLN:O	22:T:11:GLN:HG3	2.02	0.60
1:0:69:A:H5'	1:0:69:A:C8	2.36	0.60
1:0:1701:A:H5''	1:0:1702:U:H3'	1.82	0.60
20:R:39:THR:HG22	20:R:42:GLU:H	1.65	0.60
1:0:90:A:H2'	1:0:91:G:O4'	2.02	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
6:D:25:MET:HE3	6:D:37:ALA:CB	2.23	0.60
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.82	0.60
14:L:145:LEU:O	14:L:148:GLU:HG3	2.02	0.60
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.67	0.60
39:O:3045:HOH:O	25:W:119:HIS:HE1	1.84	0.60
15:M:60:VAL:C	15:M:61:ILE:HD12	2.22	0.60
1:0:2005:G:H3'	1:0:2005:G:OP2	2.02	0.60
4:B:254:GLN:HG2	4:B:255:GLY:N	2.16	0.60
31:3:17:HIS:O	31:3:18:GLN:HG3	2.02	0.60
3:A:36:ASP:O	3:A:38:ILE:N	2.27	0.59
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
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
27:Y:122:ARG:NH2	39:Y:8834:HOH:O	2.35	0.59
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.62	0.59
11:I:105:GLU:HA	11:I:108:HIS:NE2	2.18	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
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.83	0.59
16:N:37:ARG:NE	39:N:8832:HOH:O	2.35	0.59
4:B:51:VAL:HG23	4:B:329:TYR:O	2.00	0.59
1:0:121:U:OP2	30:2:10:ARG:NH2	2.31	0.59
6:D:65:GLU:HA	39:D:6752:HOH:O	2.03	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:I:129:SER:O	11:I:130:LEU:HD23	2.02	0.59
1:0:474:C:O3'	5:C:73:LEU:HD21	2.02	0.59
14:L:80:ASP:HB2	14:L:90:ARG:O	2.03	0.59
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.02	0.59
8:F:91:VAL:CG1	8:F:92:GLY:H	2.15	0.59
20:R:39:THR:HB	20:R:42:GLU:CG	2.32	0.59
6:D:159:PRO:O	6:D:163:VAL:HG23	2.02	0.59
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.84	0.59
3:A:191:GLY:HA2	3:A:194:MET:CE	2.33	0.59
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.01	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
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.84	0.59
31:3:62:THR:HB	39:3:8977:HOH:O	2.01	0.59
6:D:136:ARG:HB2	39:D:7597:HOH:O	2.03	0.59
1:0:316:A:H5'	22:T:54:ASP:OD2	2.03	0.59
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.32	0.59
31:3:6:ARG:NH1	31:3:21:GLU:HG3	2.17	0.59
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.59
4:B:102:THR:HG23	4:B:182:VAL:HG12	1.84	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
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.85	0.58
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
2:9:114:G:O6	16:N:11:ARG:HD3	2.03	0.58
15:M:107:ARG:NH1	39:M:8876:HOH:O	2.35	0.58
7:E:11:VAL:HG12	7:E:12:ASP:N	2.18	0.58
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.66	0.58
2:9:13:A:O2'	2:9:14:G:H5''	2.03	0.58
39:0:5912:HOH:O	9:G:12:ILE:HA	2.02	0.58
5:C:98:ARG:NH1	39:C:8561:HOH:O	2.34	0.58
1:0:603:A:H5''	1:0:604:G:OP1	2.02	0.58
7:E:166:VAL:HG12	39:E:3134:HOH:O	2.02	0.58
5:C:27:ARG:HG3	5:C:29:ASP:OD1	2.02	0.58
3:A:131:HIS:O	3:A:132:ASP:HB2	2.02	0.58
1:0:164:G:H4'	14:L:30:ARG:HD3	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.69	0.58
1:0:1528:A:H2'	1:0:1529:G:O4'	2.02	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
24:V:12:THR:HG23	24:V:14:ALA:H	1.68	0.58
1:0:1166:A:H61	1:0:1180:U:H3	1.51	0.58
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.68	0.58
1:0:1118:A:H62	1:0:1244:U:H3	1.52	0.58
8:F:91:VAL:CG1	8:F:92:GLY:N	2.67	0.58
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.33	0.58
25:W:125:HIS:CD2	25:W:127:GLY:H	2.20	0.58
3:A:164:ARG:CZ	39:A:9050:HOH:O	2.51	0.58
1:0:2779:G:H21	7:E:143:GLN:NE2	2.02	0.58
6:D:50:VAL:O	6:D:71:ALA:HA	2.04	0.58
14:L:72:ASN:HB2	39:L:8872:HOH:O	2.03	0.58
3:A:55:VAL:HG22	3:A:68:ILE:O	2.04	0.58
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.33	0.58
1:0:125:U:H2'	39:0:4245:HOH:O	2.03	0.58
1:0:1730:G:H5'	1:0:1731:C:C5	2.38	0.58
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.34	0.58
1:0:2717:C:O2'	1:0:2718:C:H5''	2.02	0.58
1:0:558:C:H2'	1:0:559:U:H5''	1.85	0.58
1:0:396:U:O2'	1:0:418:C:H4'	2.04	0.58
7:E:35:TYR:HA	12:J:127:ILE:HD12	1.86	0.58
25:W:130:HIS:O	25:W:136:GLY:HA3	2.04	0.58
6:D:154:LYS:H	6:D:154:LYS:CD	2.06	0.57
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.86	0.57
6:D:95:THR:OG1	6:D:174:VAL:HG22	2.04	0.57
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.04	0.57
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.04	0.57
1:0:299:U:H5'	39:0:7766:HOH:O	2.03	0.57
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.04	0.57
39:0:7854:HOH:O	22:T:9:LYS:HB2	2.03	0.57
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.03	0.57
25:W:38:THR:HG22	25:W:39:ASP:N	2.20	0.57
39:9:9062:HOH:O	16:N:41:LYS:HD3	2.05	0.57
14:L:133:VAL:HB	39:L:8849:HOH:O	2.03	0.57
1:0:119:A:H2'	1:0:120:A:H5''	1.87	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
1:0:1634:G:H3'	39:0:4370:HOH:O	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:N:11:ARG:NH2	39:N:8817:HOH:O	2.38	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
1:0:1615:A:H5'	39:0:4655:HOH:O	2.03	0.57
1:0:588:G:O6	25:W:154:ARG:NH1	2.37	0.57
5:C:107:ARG:NH1	39:C:8637:HOH:O	2.37	0.57
2:9:92:G:H2'	2:9:93:A:C8	2.40	0.57
2:9:39:U:HO2'	2:9:42:C:H5	1.52	0.57
1:0:1175:G:H1'	1:0:1193:A:H2'	1.86	0.57
11:I:124:VAL:O	11:I:124:VAL:HG12	2.05	0.57
39:0:7881:HOH:O	4:B:211:THR:HG21	2.04	0.57
14:L:148:GLU:HB2	39:L:8877:HOH:O	2.03	0.57
1:0:2320:U:H4'	1:0:2321:A:O4'	2.05	0.57
6:D:58:VAL:CG1	6:D:60:GLU:HG2	2.33	0.57
5:C:233:THR:HG22	5:C:234:VAL:N	2.18	0.57
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.85	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
3:A:33:GLU:O	3:A:34:ASP:HB2	2.04	0.57
10:H:48:VAL:HA	10:H:170:ARG:O	2.04	0.57
1:0:1205:U:H2'	1:0:1206:U:C5'	2.34	0.57
8:F:101:ALA:HA	39:F:5413:HOH: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
12:J:19:MET:CE	12:J:132:LEU:HD11	2.35	0.56
4:B:307:ARG:NH1	4:B:307:ARG:HG3	2.11	0.56
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.07	0.56
6:D:135:VAL:HG22	6:D:136:ARG:H	1.70	0.56
4:B:254:GLN:HG3	39:B:9000:HOH:O	2.05	0.56
1:0:1164:U:OP1	11:I:69:PRO:HA	2.05	0.56
1:0:263:U:O4'	8:F:59:ILE:HD13	2.05	0.56
1:0:681:G:N3	1:0:681:G:H5'	2.20	0.56
39:C:8563:HOH:O	17:O:3:THR:HG21	2.05	0.56
1:0:545:G:C8	1:0:545:G:H5'	2.37	0.56
20:R:29:LYS:HD3	39:R:8944:HOH:O	2.05	0.56
1:0:949: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
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
4:B:62:ARG:HA	4:B:65:MET:HE3	1.88	0.56
2:9:91:C:H2'	2:9:92:G:O4'	2.05	0.56
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.40	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.71	0.56
1:0:1299:G:O6	14:L:6:ARG:HD3	2.05	0.56
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.71	0.56
9:G:12:ILE:N	9:G:13:PRO:HD3	2.21	0.56
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.04	0.56
1:0:272:A:H5'	1:0:273:G:OP2	2.06	0.56
11:I:113:SER:HB2	11:I:118:ASN:HB2	1.88	0.56
10:H:30:LYS:N	10:H:62:HIS:HD2	2.00	0.56
1:0:1786:C:OP1	18:P:74:GLN:HG2	2.05	0.56
1:0:2820:A:OP1	4:B:98:THR:HG22	2.06	0.56
1:0:1086:A:C6	25:W:11:VAL:HG11	2.40	0.56
4:B:85:ARG:NH1	39:B:9104:HOH:O	2.38	0.56
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.37	0.56
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.87	0.56
22:T:71:VAL:HG12	22:T:72:ILE:N	2.21	0.56
1:0:797:A:H4'	28:Z:10:ARG:N	2.21	0.56
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.87	0.56
5:C:132:ASP:HB3	39:C:8567:HOH:O	2.06	0.56
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.36	0.56
14:L:73:VAL:HG23	14:L:74:THR:H	1.70	0.56
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.88	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:21:LEU:HB3	25:W:26:ILE:HG12	1.87	0.55
1:0:1835:U:C5	1:0:1840:A:N7	2.65	0.55
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.37	0.55
12:J:107:ASN:C	12:J:107:ASN:HD22	2.09	0.55
27:Y:144:ARG:CZ	39:Y:8910:HOH:O	2.54	0.55
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.35	0.55
17:O:73:ASP:HA	17:O:92:VAL:O	2.06	0.55
4:B:280:VAL:HG13	4:B:333:GLU:O	2.05	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
1:0:1234:U:N3	4:B:244:PRO:HB3	2.21	0.55
8:F:99:THR:HA	39:F:3461:HOH:O	2.05	0.55
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.87	0.55
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.87	0.55
16:N:58:LEU:N	16:N:58:LEU:HD12	2.20	0.55
1:0:1182:C:H1'	1:0:1192:A:H8	1.72	0.55
1:0:1120:U:H5''	1:0:1120:U:C6	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:417:G:P	39:0:7848:HOH:O	2.64	0.55
1:0:20:G:H21	20:R:117:HIS:HD2	1.53	0.55
29:1:25:LYS:CD	30:2:49:GLU:H	2.18	0.55
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.41	0.55
1:0:2346:C:O5'	1:0:2346:C:H6	1.89	0.55
1:0:1363:G:OP1	5:C:76:ARG:NH2	2.39	0.55
1:0:380:A:OP2	15:M:9:ARG:HD2	2.07	0.55
2:9:2:U:OP2	2:9:3:A:H5'	2.07	0.55
1:0:447:A:P	22:T:1:SER:HB2	2.45	0.55
16:N:147:ILE:HD12	39:N:8845:HOH:O	2.06	0.55
39:0:4235:HOH:O	22:T:9:LYS:HD3	2.06	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
2:9:28:U:H5''	16:N:40:ASN:ND2	2.22	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
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
39:0:9846:HOH:O	29:1:1:THR:HA	2.06	0.55
6:D:154:LYS:HD2	6:D:154:LYS:N	2.08	0.55
25:W:139:GLY:O	25:W:141:HIS:HD2	1.88	0.55
1:0:319:A:H4'	1:0:338:C:C4	2.42	0.55
1:0:1384:C:H5'	26:X:30:MET:HG2	1.87	0.55
1:0:645:U:OP2	14:L:4:LYS:HE2	2.06	0.55
39:0:5193:HOH:O	16:N:21:HIS:HD2	1.90	0.55
13:K:82:ARG:NH2	13:K:115:ARG:HG2	2.22	0.55
11:I:120:ALA:O	11:I:124:VAL:HG23	2.06	0.55
1:0:1116:U:O2'	1:0:1118:A:C2	2.47	0.55
1:0:447:A:OP2	22:T:1:SER:HB2	2.07	0.55
22:T:26:THR:HA	22:T:39:ASN:HB3	1.88	0.55
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.42	0.55
1:0:316:A:N3	1:0:336:G:O2'	2.40	0.55
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.72	0.55
1:0:93:C:H5''	24:V:1:THR:CB	2.37	0.55
30:2:48:ASP:O	30:2:49:GLU:HB2	2.07	0.55
24:V:42:ASN:O	24:V:44:GLY:N	2.40	0.55
10:H:69:ARG:HD3	39:H:9031:HOH:O	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
2:9:51:A:H5'	16:N:160:SER:HB3	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.88	0.55
5:C:115:LEU:O	5:C:118:THR:HB	2.06	0.54
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.37	0.54
4:B:79:MET:HE1	39:B:9094:HOH:O	2.06	0.54
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
27:Y:133:HIS:HD2	39:Y:8880:HOH:O	1.90	0.54
1:O:2036:C:O4'	13:K:44:LEU:HG	2.07	0.54
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.42	0.54
5:C:16:VAL:HG12	5:C:17:ASP:H	1.71	0.54
1:O:69:A:H5'	1:O:69:A:H8	1.72	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
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.88	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
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
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
5:C:214:THR:HG23	39:C:8643:HOH:O	2.07	0.54
1:O:1677:U:OP2	30:2:8:LYS:NZ	2.40	0.54
1:O:1278:A:H4'	1:O:1279:U:C4	2.43	0.54
4:B:66:GLU:OE1	4:B:328:ARG:HD2	2.07	0.54
1:O:1205:U:H2'	1:O:1206:U:H5"	1.89	0.54
18:P:103:THR:O	18:P:107:GLU:HG3	2.07	0.54
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.88	0.54
5:C:79:ARG:O	5:C:87:ARG:HG2	2.08	0.54
7:E:31:ARG:NH1	39:E:5919:HOH:O	2.40	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
1:O:1625:U:H4'	39:O:5132:HOH:O	2.07	0.54
13:K:55:VAL:HG12	13:K:56:SER:N	2.22	0.54
1:O:2769:C:H2'	1:O:2770:G:H5'	1.89	0.54
25:W:108:ARG:HE	25:W:114:PRO:CG	2.20	0.54
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	2.06	0.54
10:H:79:GLU:O	10:H:80:LEU:HD23	2.08	0.54
1:O:2894:C:O2'	1:O:2895:C:H5'	2.08	0.54
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.43	0.54
1:O:1189:A:H1'	1:O:1209:C:O4'	2.08	0.54
7:E:7:ILE:HD11	7:E:11:VAL:C	2.29	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
26:X:25:ARG:HD2	39:X:3861:HOH:O	2.07	0.54
5:C:104:ASP:HA	5:C:107:ARG:HH12	1.71	0.54
1:O: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
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
1:O:2862:G:H4'	4:B:336:GLN:O	2.07	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
5:C:2:GLN:HB3	39:C:8535:HOH:O	2.08	0.53
4:B:329:TYR:CE2	23:U:15:PRO:HG2	2.43	0.53
6:D:23:VAL:HG22	6:D:73:VAL:HB	1.89	0.53
1:O:338:C:H4'	5:C:174:ILE:HD11	1.89	0.53
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.22	0.53
39:O:3028:HOH:O	18:P:81:LYS:HG2	2.07	0.53
1:O:902:G:N7	14:L:18:HIS:HD2	2.06	0.53
1:O:2878:U:H2'	1:O:2879:A:O4'	2.08	0.53
2:9:29:C:C2'	2:9:30:C:H5'	2.38	0.53
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:485:A:N3	1:O:487:G:H5"	2.23	0.53
1:O:200:C:H2'	39:O:3929:HOH:O	2.07	0.53
1:O:1314:U:H2'	39:O:6326:HOH:O	2.07	0.53
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.48	0.53
3:A:121:ALA:O	3:A:124:VAL:HG22	2.07	0.53
11:I:94:ASP:OD1	11:I:133:THR:HB	2.09	0.53
25:W:149:LEU:HG	25:W:153:MET:CE	2.38	0.53
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.09	0.53
1:O:538:C:OP2	27:Y:134:HIS:HE1	1.91	0.53
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.38	0.53
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.91	0.53
1:O:2670:G:O2'	1:O:2671:U:H5'	2.08	0.53
4:B:82:VAL:HG12	4:B:82:VAL:O	2.07	0.53
24:V:1:THR:HG23	24:V:2:VAL:N	2.19	0.53
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.38	0.53
1:O:1268:C:O2'	27:Y:169:ARG:HB2	2.08	0.53
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.07	0.53
39:O:7836:HOH:O	22:T:2:LYS:HE2	2.07	0.53
30:2:23:ALA:HB3	39:2:6863:HOH:O	2.08	0.53
1:O:1594:C:OP2	18:P:120:ARG:HD2	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:N:154:LEU:O	16:N:155:GLU:HB3	2.08	0.53
26:X:8:ARG:NH1	39:X:2479:HOH:O	2.40	0.53
1:0:10:U:O4	1:0:532:A:OP2	2.26	0.53
30:2:41:HIS:HD2	30:2:44:ARG:H	1.56	0.53
1:0:905:C:OP1	27:Y:144:ARG:NH1	2.42	0.53
30:2:39:ARG:HG2	39:2:3143:HOH:O	2.09	0.53
22:T:69:LYS:O	22:T:71:VAL:HG23	2.08	0.53
6:D:65:GLU:HG3	39:D:6752:HOH:O	2.07	0.53
3:A:66:ARG:HH11	3:A:66:ARG:HB2	1.74	0.53
1:0:2243:C:H5''	39:0:4230:HOH:O	2.09	0.53
1:0:536:A:H3'	39:0:5504:HOH:O	2.09	0.53
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.90	0.53
2:9:69:U:OP1	16:N:4:PRO:HG3	2.09	0.53
23:U:52:THR:HG22	23:U:54:THR:N	2.23	0.53
1:0:156:C:H5''	15:M:171:ARG:CD	2.29	0.53
1:0:1972:U:C2'	1:0:1973:A:H5''	2.39	0.53
4:B:321:PRO:HA	39:B:9127:HOH:O	2.09	0.53
1:0:1187:U:O2'	1:0:1189:A:H2	1.92	0.53
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.91	0.53
6:D:24:HIS:HB2	6:D:72:LYS:CB	2.39	0.53
8:F:38:LYS:HZ3	15:M:3:SER:HA	1.74	0.53
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.42	0.53
1:0:1201:C:H5''	39:0:6679:HOH:O	2.09	0.53
1:0:2419:U:H5''	1:0:2420:G:H5'	1.90	0.53
26:X:43:VAL:HG12	26:X:44:ASP:N	2.24	0.53
5:C:107:ARG:NE	39:C:8661:HOH:O	2.20	0.53
10:H:165:ARG:HD2	39:H:9034:HOH:O	2.08	0.53
1:0:2812:A:C2	1:0:2814:A:N6	2.68	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
5:C:118:THR:O	5:C:136:VAL:HG13	2.08	0.52
1:0:2817:G:P	39:0:8430:HOH:O	2.67	0.52
17:O:25:VAL:HG23	17:O:26:TRP:N	2.23	0.52
1:0:820:G:O2'	1:0:856:G:H4'	2.09	0.52
12:J:80:LYS:HE3	12:J:101:VAL:O	2.08	0.52
16:N:32:PRO:HD2	16:N:99:GLU:O	2.09	0.52
1:0:2712:G:H5'	39:K:4183:HOH:O	2.09	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
1:0:2044:G:OP1	26:X:23:HIS:HE1	1.92	0.52
21:S:81:ILE:HG23	39:S:8984:HOH:O	2.10	0.52
1:0:1162:G:H1'	11:I:112:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:265:LEU:HD21	4:B:316:ARG:HD3	1.91	0.52
1:0:870:G:OP2	3:A:3:ARG:HD3	2.09	0.52
1:0:1119:G:H22	1:0:1246:A:H2	1.51	0.52
5:C:162:VAL:CG2	5:C:232:LEU:HD21	2.40	0.52
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.90	0.52
11:I:96:SER:H	11:I:99:GLN:NE2	2.07	0.52
7:E:154:ILE:HG13	7:E:156:ASP:OD1	2.10	0.52
11:I:87:PRO:C	11:I:89:GLU:H	2.12	0.52
1:0:1120:U:H5'	1:0:1121:G:OP2	2.08	0.52
21:S:77:VAL:O	21:S:80:ARG:HG2	2.09	0.52
14:L:101:ASP:C	14:L:103:ALA:H	2.13	0.52
1:0:711:G:H1'	39:0:7530:HOH:O	2.09	0.52
1:0:2491:G:H1'	39:0:7304:HOH:O	2.09	0.52
1:0:1972:U:H2'	1:0:1973:A:C5'	2.39	0.52
3:A:53:ALA:HB3	39:A:9068:HOH:O	2.10	0.52
17:O:32:ARG:HH21	17:O:35:LYS:NZ	2.07	0.52
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.39	0.52
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.24	0.52
1:0:564:G:H1'	39:0:6756:HOH:O	2.08	0.52
26:X:34:ARG:NH1	26:X:48:VAL:O	2.36	0.52
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.92	0.52
1:0:1666:C:H2'	1:0:1667:A:C5'	2.38	0.52
11:I:108:HIS:N	11:I:109:PRO:CD	2.72	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
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.91	0.52
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.90	0.52
39:0:6731:HOH:O	27:Y:158:LYS:HD3	2.10	0.52
14:L:67:ARG:O	14:L:71:GLU:HG3	2.10	0.52
30:2:41:HIS:H	30:2:45:ASN:ND2	1.95	0.52
1:0:31:C:H4'	39:0:7854:HOH:O	2.10	0.52
1:0:1119:G:H8	12:J:52:GLN:NE2	2.08	0.52
17:O:26:TRP:N	39:O:3062:HOH:O	2.42	0.52
1:0:1730:G:C5'	1:0:1731:C:C6	2.93	0.52
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.56	0.52
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.35	0.52
11:I:133:THR:HG22	11:I:134:ILE:N	2.24	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
1:0:949: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:O:449:A:N7	5:C:43:LYS:HG2	2.25	0.52
7:E:15:GLN:NE2	7:E:40:VAL:O	2.43	0.52
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.92	0.52
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.71	0.52
1:O:1700:C:H5''	1:O:1701:A:OP2	2.09	0.52
10:H:62:HIS:HA	10:H:65:LEU:HD23	1.92	0.52
5:C:27:ARG:HG2	5:C:30:LEU:HD12	1.91	0.52
25:W:5:VAL:HG11	25:W:153:MET:HE3	1.92	0.52
16:N:49:THR:CG2	16:N:58:LEU:HD11	2.40	0.52
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.45	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
9:G:64:ASN:HD22	9:G:64:ASN:N	2.08	0.52
27:Y:187:VAL:HB	27:Y:203:VAL:HG22	1.92	0.51
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
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
23:U:9:CYS:HA	23:U:52:THR:HG23	1.92	0.51
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.41	0.51
20:R:106:GLY:HA2	20:R:109:MET:CE	2.41	0.51
1:O:653:U:H2'	1:O:654:A:C8	2.44	0.51
1:O:2643:G:H5''	39:O:4401:HOH:O	2.09	0.51
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.74	0.51
1:O:2289:G:H21	1:O:2291:A:H2	1.54	0.51
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.92	0.51
1:O:775:G:OP1	29:1:16:HIS:HE1	1.94	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
3:A:105:VAL:HG12	3:A:106:CYS:N	2.24	0.51
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.25	0.51
4:B:72:THR:HB	39:B:9073:HOH:O	2.10	0.51
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.91	0.51
16:N:152:GLU:C	16:N:154:LEU:H	2.14	0.51
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.11	0.51
22:T:115:GLU:HG3	22:T:116:ASP:N	2.25	0.51
1:O:1242:A:C5'	12:J:82:THR:HG23	2.27	0.51
1:O:2661:U:H3	1:O:2812:A:H62	1.59	0.51
6:D:136:ARG:HD2	6:D:155:HIS:O	2.10	0.51
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.75	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:136:C:H2'	1:0:137:U:O4'	2.10	0.51
3:A:97:ALA:HB2	3:A:150:PRO:HB2	1.93	0.51
6:D:58:VAL:HB	6:D:62:ASP:HB3	1.93	0.51
1:0:1947:G:H2'	1:0:1948:G:H8	1.75	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
1:0:2748:G:H5'	39:0:7963:HOH:O	2.11	0.51
1:0:1159:G:H1	1:0:1208:C:H42	1.58	0.51
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.40	0.51
16:N:154:LEU:HG	16:N:155:GLU:H	1.76	0.51
1:0:2795:C:O2'	1:0:2796:U:H5'	2.10	0.51
5:C:166:ILE:CD1	5:C:207:LEU:HD13	2.41	0.51
1:0:123:U:H5'	39:0:7091:HOH:O	2.10	0.51
2:9:54:A:O2'	2:9:55:U:H5'	2.10	0.51
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.93	0.51
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.44	0.51
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.91	0.51
1:0:1595:G:O2'	1:0:1596:U:H5'	2.11	0.51
28:Z:26:VAL:O	28:Z:30:GLU:HG3	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
1:0:1351:G:OP1	5:C:96:LYS:NZ	2.37	0.51
8:F:58:GLU:CD	15:M:27:ARG:HH22	2.14	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
1:0:262:A:OP2	8:F:91:VAL:HG11	2.10	0.51
5:C:136:VAL:HG22	5:C:137:PRO:HA	1.93	0.51
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.09	0.51
1:0:392:U:O2'	15:M:182:LYS:HE2	2.11	0.51
5:C:61:PHE:HB3	39:C:8650:HOH:O	2.10	0.51
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.91	0.51
1:0:2073:G:OP2	1:0:2490:A:H5'	2.11	0.51
16:N:116:PHE:HB3	16:N:136:LEU:HD23	1.93	0.51
1:0:2301:A:H5''	1:0:2302:A:H5'	1.93	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
1:0:92:G:H4'	24:V:44:GLY:HA3	1.93	0.50
12:J:131:THR:HG22	12:J:133:GLY:H	1.76	0.50
4:B:297:VAL:HB	39:B:9073:HOH:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.11	0.50
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.92	0.50
1:0:2456:A:H5'	39:0:6149:HOH:O	2.10	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
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.23	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
30:2:20:ARG:HG3	30:2:21:VAL:H	1.77	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
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.40	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
25:W:122:ARG:NH2	39:W:5817:HOH:O	2.44	0.50
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.41	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
1:0:1289:C:O2'	1:0:1290:G:H5'	2.11	0.50
7:E:108:LEU:HD11	7:E:164:ASP:HB2	1.94	0.50
1:0:1118:A:C8	1:0:1118:A:C3'	2.90	0.50
10:H:30:LYS:H	10:H:62:HIS:CD2	2.21	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
24:V:64:GLY:O	24:V:65:ASP:CB	2.59	0.50
1:0:1181:A:C2'	1:0:1182:C:H5'	2.42	0.50
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.92	0.50
17:O:78:ALA:C	17:O:98:LEU:HD13	2.32	0.50
1:0:1250:C:O2'	1:0:1251:C:H5'	2.12	0.50
1:0:1299:G:H5'	39:0:4547:HOH:O	2.12	0.50
6:D:103:ASN:ND2	6:D:134:LEU:H	2.08	0.50
1:0:2769:C:H2'	1:0:2770:G:C5'	2.41	0.50
1:0:2638:G:H1'	39:0:8261:HOH:O	2.11	0.50
25:W:48:VAL:CG1	25:W:48:VAL:O	2.60	0.50
1:0:1666:C:C2'	1:0:1667:A:C5'	2.89	0.50
1:0:1163:G:H5''	11:I:110:ASP:HB3	1.94	0.50
39:0:3115:HOH:O	8:F:38:LYS:HE2	2.11	0.50
39:0:8211:HOH:O	5:C:94:THR:HG21	2.12	0.50
14:L:89:PHE:N	39:L:8863:HOH:O	2.45	0.50
5:C:77:ALA:O	5:C:78:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:Y:187:VAL:HG22	27:Y:192:ASP:CB	2.42	0.50
1:O:2756:U:H3	1:O:2896:A:H2	1.50	0.50
39:O:3724:HOH:O	11:I:87:PRO:HD3	2.11	0.50
39:O:9515:HOH:O	14:L:30:ARG:HD2	2.10	0.50
8:F:46:GLU:OE1	8:F:100:ASP:HA	2.12	0.50
3:A:65:ARG:C	3:A:66:ARG:HG3	2.32	0.50
21:S:81:ILE:HG12	39:S:8984:HOH:O	2.11	0.50
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.52	0.49
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.11	0.49
25:W:38:THR:HG22	39:W:3580:HOH:O	2.11	0.49
5:C:246:ARG:NE	39:C:8630:HOH:O	2.26	0.49
13:K:115:ARG:HG3	13:K:116:GLU:N	2.26	0.49
2:9:64:C:C2'	2:9:65:A:H5'	2.41	0.49
11:I:126:THR:O	11:I:126:THR:HG22	2.11	0.49
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.25	0.49
8:F:58:GLU:HG3	8:F:61:MET:HE1	1.94	0.49
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.47	0.49
9:G:16:LYS:O	9:G:20:VAL:HG23	2.13	0.49
1:O:1377:C:H5'	1:O:1377:C:C6	2.45	0.49
1:O:2415:A:H2'	1:O:2416:G:H5'	1.93	0.49
1:O:776:A:OP1	29:1:28:HIS:HE1	1.95	0.49
30:2:20:ARG:CG	30:2:21:VAL:N	2.76	0.49
1:O:2363:G:O3'	19:Q:11:ARG:NH1	2.45	0.49
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.76	0.49
25:W:26:ILE:O	25:W:26:ILE:HG13	2.12	0.49
1:O:2812:A:H1'	39:O:6244:HOH:O	2.12	0.49
13:K:55:VAL:CG1	13:K:56:SER:N	2.75	0.49
10:H:43:ALA:HB1	10:H:140:TYR:CE2	2.47	0.49
26:X:9:VAL:HG13	26:X:88:GLU:CD	2.32	0.49
3:A:192:VAL:HG13	39:A:9022:HOH:O	2.12	0.49
10:H:6:ALA:CA	10:H:61:ARG:HH12	2.22	0.49
6:D:23:VAL:O	6:D:23:VAL:HG23	2.13	0.49
4:B:74:ILE:HG13	39:B:9073:HOH:O	2.12	0.49
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.93	0.49
1:O:1200:A:H3'	39:O:6208:HOH:O	2.13	0.49
1:O:2791:U:H1'	1:O:2792:A:H5''	1.94	0.49
4:B:149:ASP:HB2	39:B:9049:HOH:O	2.13	0.49
1:O:2825:C:H4'	1:O:2826:G:O5'	2.12	0.49
1:O:343:C:O2'	1:O:344:C:H5'	2.11	0.49
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.48	0.49
27:Y:209:VAL:HG12	27:Y:214:ARG:HG3	1.94	0.49
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1306:U:OP1	5:C:184:ARG:HD2	2.13	0.49
31:3:48:ASN:ND2	31:3:50:GLY:H	2.10	0.49
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.94	0.49
5:C:133:ARG:NH1	39:C:8616:HOH:O	2.45	0.49
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.12	0.49
4:B:223:ARG:HG3	4:B:232:TRP:O	2.11	0.49
6:D:29:HIS:HB2	39:D:2768:HOH:O	2.11	0.49
4:B:49:THR:HG21	4:B:331:SER:O	2.13	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
3:A:1:GLY:HA2	3:A:197:VAL:HG23	1.95	0.49
16:N:147:ILE:HB	39:N:8845:HOH:O	2.12	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
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
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.95	0.49
1:0:899:C:H5'	39:0:3690:HOH:O	2.11	0.49
1:0:638:C:H2'	1:0:639:A:C8	2.47	0.49
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.45	0.49
25:W:65:VAL:HA	25:W:68:THR:CG2	2.42	0.49
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.48	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
8:F:16:ALA:HA	8:F:111:ILE:HD13	1.94	0.49
5:C:19:PRO:HG2	5:C:22:PHE:CE1	2.48	0.49
6:D:18:ILE:HG12	6:D:134:LEU:CD2	2.43	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
22:T:62:VAL:HB	39:T:3851:HOH:O	2.13	0.49
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.95	0.49
3:A:34:ASP:OD1	3:A:35:GLY:N	2.39	0.49
10:H:61:ARG:HG3	10:H:61:ARG:HH11	1.77	0.49
4:B:102:THR:HG21	4:B:182:VAL:O	2.13	0.49
1:0:793:A:H5''	18:P:83:LYS:HG2	1.95	0.49
1:0:1426:C:H2'	39:0:3083:HOH:O	2.11	0.49
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.28	0.49
15:M:99:ARG:HE	15:M:170:ASN:HD22	1.59	0.49
14:L:130:ARG:HA	39:L:8849:HOH:O	2.12	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
3:A:81:GLN:HG3	3:A:92:ASN:HD21	1.77	0.49
1:0:2697:A:H2'	1:0:2698:G:O4'	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	2.13	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
1:0:602: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
1:0:291:C:H2'	1:0:292:G:O4'	2.13	0.49
12:J:130:VAL:HG12	12:J:131:THR:N	2.28	0.48
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.47	0.48
15:M:58:GLN:HG3	39:M:8905:HOH:O	2.11	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
1:0:2667:G:H1'	1:0:2914:A:N3	2.27	0.48
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
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.95	0.48
27:Y:216:ARG:HD2	39:Y:8868:HOH:O	2.13	0.48
24:V:12:THR:HG23	24:V:14:ALA:N	2.28	0.48
29:1:28:HIS:HD2	29:1:30:LYS:H	1.60	0.48
1:0:2672:C:H1'	39:B:9104:HOH:O	2.12	0.48
20:R:132:ARG:HG2	20:R:133:ALA:N	2.28	0.48
1:0:666:A:H2'	1:0:667:C:O4'	2.14	0.48
1:0:138:U:H5''	1:0:139:C:OP2	2.14	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
6:D:35:ALA:N	39:D:5576:HOH:O	2.46	0.48
15:M:164:THR:HG23	15:M:165:GLY:N	2.26	0.48
12:J:19:MET:HE3	12:J:132:LEU:CD2	2.34	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
1:0:656:G:C5'	17:O:3:THR:HG22	2.40	0.48
1:0:1942:A:H3'	39:0:7777:HOH:O	2.13	0.48
1:0:1741:U:H5'	1:0:1742:A:OP1	2.13	0.48
1:0:1477:C:H5'	1:0:1868:G:C5'	2.43	0.48
1:0:304:G:H1'	1:0:347:A:N6	2.28	0.48
7:E:85:GLU:HG3	7:E:169:THR:OG1	2.13	0.48
25:W:48:VAL:HG12	25:W:48:VAL:O	2.13	0.48
24:V:23:LEU:HD12	24:V:56:ILE:HD12	1.95	0.48
1:0:2769:C:O2'	1:0:2770:G:H5'	2.13	0.48
1:0:2064:U:H5'	1:0:2652:U:O3'	2.13	0.48
1:0:1166:A:H1'	1:0:1192:A:C2	2.48	0.48
1:0:1120:U:H6	1:0:1120:U:H5''	1.78	0.48
1:0:57:C:H5''	39:0:7195:HOH:O	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.95	0.48
1:0:462:A:H2'	39:0:5343:HOH:O	2.14	0.48
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.12	0.48
25:W:139:GLY:O	25:W:141:HIS:CD2	2.65	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
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
1:0:1053:G:OP1	10:H:15:PRO:HG3	2.13	0.48
5:C:168:ARG:NH2	5:C:190:ALA:O	2.47	0.48
12:J:13:ASP:OD1	12:J:15:ARG:HB3	2.14	0.48
5:C:180:SER:HB2	39:C:8651:HOH:O	2.13	0.48
6:D:149:ARG:NH2	39:D:3066:HOH:O	2.45	0.48
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.95	0.48
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.13	0.48
1:0:447:A:OP1	22:T:2:LYS:HG2	2.13	0.48
22:T:40:VAL:HG22	22:T:41:ARG:N	2.29	0.48
1:0:292:G:H2'	1:0:358:G:N2	2.29	0.48
27:Y:149:GLN:NE2	39:Y:8900:HOH:O	2.41	0.48
1:0:1427:A:H61	1:0:1440:U:H1'	1.79	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
1:0:377:C:H5	39:0:3795:HOH:O	1.97	0.48
6:D:37:ALA:O	6:D:40:ILE:HG12	2.13	0.48
21:S:57:THR:CG2	21:S:58:MET:N	2.76	0.48
1:0:1874:U:H2'	3:A:120:ARG:HG3	1.96	0.48
1:0:1878:G:O2'	1:0:1879:U:OP2	2.31	0.48
1:0:1185:U:H2'	1:0:1186:C:C6	2.49	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
3:A:36:ASP:HB2	3:A:85:SER:H	1.79	0.48
39:0:5740:HOH:O	25:W:122:ARG:NH2	2.46	0.48
4:B:195:ARG:HD2	4:B:324:ASP:OD1	2.13	0.48
2:9:8:G:O6	16:N:11:ARG:NH1	2.46	0.48
7:E:80:TRP:O	7:E:134:SER:HA	2.13	0.48
23:U:52:THR:CG2	23:U:54:THR:HB	2.44	0.48
6:D:75:LEU:HD22	6:D:79:MET:HB3	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.14	0.48
1:0:814:G:H4'	39:0:3620:HOH:O	2.12	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
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.77	0.48
1:0:1132:A:N6	1:0:1229:C:H2'	2.29	0.48
39:0:7437:HOH:O	19:Q:9:GLY:HA2	2.13	0.48
18:P:97:ARG:HD2	39:P:162:HOH:O	2.13	0.48
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.44	0.48
1:0:644:G:N3	1:0:644:G:H5'	2.29	0.48
6:D:40:ILE:HG13	6:D:41:LEU:N	2.29	0.47
2:9:49:G:H2'	2:9:50:G:O4'	2.14	0.47
24:V:39:ALA:O	24:V:41:GLU:N	2.47	0.47
7:E:101:GLU:HB2	7:E:116:THR:O	2.13	0.47
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.95	0.47
1:0:1527:A:H1'	1:0:1528:A:C8	2.48	0.47
5:C:104:ASP:HA	5:C:107:ARG:NH1	2.29	0.47
39:0:7978:HOH:O	31:3:60:LYS:HG3	2.13	0.47
1:0:2456:A:H2'	1:0:2457:U:C6	2.49	0.47
18:P:104:LYS:HE2	18:P:138:GLU:OE2	2.14	0.47
10:H:169:GLU:C	39:H:8993:HOH:O	2.51	0.47
1:0:1882:C:OP1	3:A:192:VAL:HG23	2.14	0.47
11:I:105:GLU:HA	11:I:108:HIS:CE1	2.49	0.47
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.96	0.47
1:0:1878:G:O2'	1:0:1879:U:C6	2.63	0.47
1:0:1819:G:H2'	1:0:1820:G:C4'	2.41	0.47
13:K:125:ALA:C	13:K:127:ALA:H	2.17	0.47
1:0:1730:G:C5'	1:0:1731:C:H6	2.27	0.47
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.62	0.47
1:0:1014:A:H2'	1:0:1015:C:H5'	1.95	0.47
1:0:951:A:C2'	1:0:952:G:H5'	2.44	0.47
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.14	0.47
1:0:2809:G:H2'	1:0:2810:G:O4'	2.15	0.47
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.13	0.47
24:V:44:GLY:O	24:V:48:GLU:HG2	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
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.95	0.47
5:C:142:ASP:OD1	5:C:236:THR:HG23	2.14	0.47
3:A:220:PRO:HD2	3:A:223:ARG:HD3	1.96	0.47
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.14	0.47
27:Y:187:VAL:HG22	27:Y:192:ASP:HB2	1.95	0.47
25:W:5:VAL:HG11	25:W:153:MET:CE	2.44	0.47
1:0:1641:A:C2'	1:0:1642:A:H5'	2.44	0.47
1:0:1441:G:H1'	39:0:8267:HOH:O	2.15	0.47
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.49	0.47
16:N:65:ASP:HB3	39:N:8821:HOH:O	2.14	0.47
6:D:24:HIS:HB2	6:D:72:LYS:HB3	1.97	0.47
1:0:2787:C:H5	39:0:5098:HOH:O	1.96	0.47
3:A:130:THR:HB	3:A:137:VAL:HB	1.95	0.47
1:0:1056:U:H2'	1:0:1057:A:O4'	2.13	0.47
1:0:1926:G:H2'	1:0:1927:A:C8	2.49	0.47
1:0:1342:C:O2'	1:0:1343:C:H5'	2.14	0.47
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.44	0.47
1:0:185:G:H4'	1:0:186:A:H4'	1.96	0.47
1:0:1667:A:H2'	1:0:1668:U:C6	2.50	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
1:0:1167:G:H2'	1:0:1168:C:O4'	2.15	0.47
23:U:44:ARG:HB3	39:U:3805:HOH:O	2.15	0.47
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.49	0.47
1:0:2133:U:H4'	1:0:2134:G:H5'	1.95	0.47
15:M:98:GLN:O	15:M:102:GLU:HG3	2.14	0.47
4:B:205:VAL:O	4:B:307:ARG:NE	2.46	0.47
1:0:282:C:H1'	1:0:368:C:H42	1.79	0.47
1:0:1943:C:O4'	3:A:212:PRO:HA	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
17:O:23:GLY:C	39:O:3062:HOH:O	2.52	0.47
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.97	0.47
6:D:172:VAL:HG12	6:D:173:GLU:N	2.29	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
1:0:1086:A:N6	25:W:11:VAL:HG11	2.30	0.47
1:0:553:G:P	27:Y:204:ARG:HH22	2.37	0.47
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.14	0.47
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.97	0.47
16:N:171:HIS:CE1	39:N:8863:HOH:O	2.68	0.47
26:X:78:GLU:HG2	26:X:79:GLU:H	1.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:737:A:H2'	1:0:738:G:O4'	2.15	0.47
1:0:2251:G:H2'	1:0:2252:A:C8	2.50	0.47
15:M:169:ARG:NH1	39:M:8871:HOH:O	2.47	0.47
1:0:1291:A:H2	39:0:5743:HOH:O	1.97	0.47
6:D:35:ALA:C	6:D:37:ALA:H	2.18	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
11:I:67:VAL:HG13	11:I:68:PRO:HD2	1.97	0.47
4:B:81:ALA:O	4:B:186:GLY:HA3	2.14	0.47
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.97	0.47
25:W:125:HIS:HE1	39:W:3071:HOH:O	1.97	0.47
1:0:1593:C:OP1	18:P:117:SER:CB	2.63	0.47
1:0:2672:C:O2'	1:0:2673:U:H5'	2.15	0.47
2:9:51:A:H5'	16:N:160:SER:CB	2.45	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
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.96	0.47
1:0:285:A:H2'	1:0:286:U:O4'	2.15	0.47
1:0:2505:G:C2'	1:0:2506:A:H5'	2.44	0.47
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.97	0.47
39:0:6693:HOH:O	23:U:56:ARG:HD3	2.15	0.47
1:0:2591:C:H2'	1:0:2592:G:O4'	2.15	0.47
5:C:118:THR:CG2	5:C:137:PRO:HB3	2.44	0.47
1:0:1159:G:H21	1:0:1189:A:H8	1.63	0.47
11:I:75:LYS:HD3	11:I:81:GLU:O	2.15	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
1:0:157:G:H4'	15:M:95:LYS:HE2	1.97	0.47
5:C:12:THR:HB	39:C:8646:HOH:O	2.14	0.47
1:0:1506:U:H6	1:0:1506:U:H5'	1.80	0.47
5:C:142:ASP:OD1	5:C:237:GLU:HB3	2.15	0.46
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.34	0.46
4:B:238:ASN:ND2	4:B:240:GLY:H	2.00	0.46
1:0:2506:A:O2'	1:0:2507:G:O5'	2.34	0.46
1:0:2507:G:H2'	1:0:2510:C:N4	2.30	0.46
1:0:2769:C:H2'	1:0:2770:G:O4'	2.15	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
10:H:119:ALA:O	10:H:120:PHE:C	2.54	0.46
1:0:1130:U:H2'	1:0:1131:G:O4'	2.15	0.46
1:0:255:A:H2'	1:0:256:C:C6	2.50	0.46
1:0:12:U:H2'	1:0:13:G:H5'	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1535:G:H2'	1:0:1536:C:C6	2.50	0.46
13:K:113:ILE:HG22	13:K:114:ALA:N	2.29	0.46
1:0:1666:C:C2'	1:0:1667:A:H5''	2.44	0.46
1:0:1185:U:OP1	11:I:121:LYS:HD3	2.15	0.46
1:0:2851:G:C2'	1:0:2852:A:H5'	2.45	0.46
7:E:81:GLU:HG2	7:E:134:SER:CB	2.45	0.46
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.48	0.46
4:B:241:PRO:HD2	39:B:9125:HOH:O	2.15	0.46
5:C:236:THR:HG22	5:C:239:ALA:CB	2.46	0.46
15:M:167:GLY:O	15:M:171:ARG:HG3	2.15	0.46
1:0:2716:G:H5''	4:B:206:THR:CG2	2.41	0.46
14:L:114:VAL:HG11	39:L:8865:HOH:O	2.14	0.46
26:X:76:ARG:O	26:X:77:PHE:HB3	2.15	0.46
3:A:109:GLU:HG2	3:A:116:GLY:H	1.81	0.46
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.63	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
1:0:317:A:H4'	39:O:4251:HOH:O	2.16	0.46
1:0:2807:U:P	4:B:27:ASN:HD21	2.39	0.46
1:0:2265:U:H2'	1:0:2266:A:C8	2.51	0.46
21:S:38:ALA:O	21:S:42:GLU:HG3	2.16	0.46
5:C:153:VAL:O	5:C:157:LEU:HG	2.16	0.46
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.15	0.46
5:C:140:VAL:HG12	5:C:141:SER:N	2.31	0.46
2:9:6:C:C5'	16:N:37:ARG:HH12	2.19	0.46
14:L:143:THR:HG22	14:L:144:ASP:H	1.76	0.46
1:0:1500:U:P	18:P:41:ARG:HH22	2.38	0.46
15:M:166:ALA:HA	15:M:169:ARG:NH1	2.30	0.46
1:0:1211:G:O2'	1:0:1212:C:H5'	2.15	0.46
1:0:1687:C:O2	29:1:9:GLY:HA2	2.16	0.46
14:L:21:ARG:N	39:L:8826:HOH:O	2.47	0.46
1:0:1333:U:H2'	1:0:1334:C:C6	2.51	0.46
1:0:1172:G:H1'	39:O:5430:HOH:O	2.15	0.46
20:R:82:GLU:HG3	20:R:83:LYS:N	2.30	0.46
22:T:71:VAL:HG13	22:T:91:LEU:O	2.15	0.46
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.97	0.46
25:W:38:THR:HG22	25:W:39:ASP:H	1.80	0.46
1:0:2526:C:O2'	1:0:2527:U:H5'	2.16	0.46
1:0:2256:G:H2'	1:0:2257:G:C5'	2.46	0.46
1:0:426:G:H2'	1:0:427:C:O4'	2.16	0.46
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:H:49:GLN:HG3	10:H:140:TYR:CD2	2.51	0.46
3:A:51:ARG:NH1	3:A:120:ARG:O	2.49	0.46
1:O:1419:U:H2'	1:O:1685:A:C2	2.51	0.46
7:E:34:TRP:O	12:J:127:ILE:HD11	2.15	0.46
1:O:894:A:C2	5:C:87:ARG:NH2	2.83	0.46
20:R:39:THR:HG22	20:R:41:GLY:N	2.30	0.46
1:O:1603:A:H5''	1:O:1605:G:H5'	1.96	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
1:O:1279:U:O2	1:O:1279:U:H2'	2.15	0.46
1:O:317:A:H5''	22:T:52:ARG:HD2	1.98	0.46
1:O:484:A:N1	1:O:506:G:H4'	2.31	0.46
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.66	0.46
1:O:470:U:O2'	29:1:16:HIS:CD2	2.65	0.46
17:O:26:TRP:HB2	39:O:3062:HOH:O	2.15	0.46
1:O:1625:U:H5''	39:O:6473:HOH:O	2.16	0.46
1:O:2300:A:H4'	1:O:2301:A:O5'	2.16	0.46
5:C:19:PRO:HG2	5:C:22:PHE:CD1	2.51	0.46
1:O:1025:C:H5'	25:W:23:MET:O	2.16	0.46
1:O:1497:G:H4'	1:O:1627:G:O2'	2.16	0.46
1:O:2626:C:H2'	1:O:2627:G:C8	2.51	0.46
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.15	0.46
1:O:2911:C:H2'	1:O:2912:C:C6	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
11:I:94:ASP:O	11:I:95:LEU:HD23	2.16	0.46
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.31	0.46
14:L:73:VAL:HG23	14:L:74:THR:N	2.30	0.46
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.64	0.46
1:O:2256:G:H2'	1:O:2257:G:H5'	1.98	0.46
14:L:97:VAL:HG12	14:L:98:GLU:O	2.16	0.46
1:O:1044:C:H5''	39:O:9520:HOH:O	2.15	0.46
1:O:420:U:H2'	1:O:421:C:C6	2.51	0.46
1:O:1295:G:H5''	14:L:14:GLY:O	2.16	0.46
15:M:47:ASP:CG	15:M:48:LYS:N	2.69	0.46
1:O:1717:A:H5''	18:P:54:LYS:HB2	1.97	0.46
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
1:O:2720:C:O2	13:K:87:ARG:NH2	2.50	0.45
7:E:31:ARG:NH1	7:E:68:HIS:CG	2.84	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:81:GLN:HB2	3:A:92:ASN:HD22	1.81	0.45
1:0:2502:C:H2'	1:0:2503:A:H5'	1.98	0.45
1:0:2266:A:OP2	15:M:90:ARG:NH2	2.49	0.45
6:D:101:THR:HG22	39:D:7400:HOH:O	2.15	0.45
4:B:14:GLY:HA2	4:B:15:PRO:C	2.36	0.45
2:9:49:G:O2'	2:9:50:G:H5'	2.16	0.45
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.31	0.45
1:0:875:A:C2	3:A:194:MET:SD	3.10	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
1:0:1741:U:O2'	1:0:2723:G:H4'	2.16	0.45
4:B:24:PRO:HG3	4:B:204:GLY:HA2	1.98	0.45
24:V:7:GLU:O	24:V:11:MET:HG3	2.16	0.45
1:0:629:A:H2'	1:0:630:A:O4'	2.16	0.45
23:U:47:ARG:HG2	39:U:4381:HOH:O	2.15	0.45
11:I:134:ILE:HG22	11:I:135:GLU:N	2.31	0.45
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.47	0.45
1:0:2421:G:H3'	1:0:2422:U:H5''	1.98	0.45
1:0:2415:A:O2'	16:N:29:SER:HB3	2.17	0.45
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.97	0.45
14:L:57:VAL:O	14:L:57:VAL:HG12	2.17	0.45
20:R:119:VAL:HG12	20:R:119:VAL:O	2.16	0.45
39:0:6804:HOH:O	3:A:205:GLY:HA3	2.16	0.45
4:B:294:TYR:HE2	39:B:9120:HOH:O	1.98	0.45
6:D:27:ILE:HD11	6:D:37:ALA:HB3	1.99	0.45
1:0:1589:G:N2	1:0:1605:G:H1'	2.31	0.45
1:0:2781:U:H2'	1:0:2782:G:H5'	1.99	0.45
6:D:59:GLY:O	6:D:61:PHE:N	2.47	0.45
16:N:37:ARG:CZ	39:N:8832:HOH:O	2.64	0.45
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.40	0.45
1:0:1205:U:H2'	1:0:1206:U:H5'	1.99	0.45
2:9:28:U:H2'	2:9:29:C:C6	2.52	0.45
9:G:27:ILE:HD13	9:G:71:LEU:HD23	1.98	0.45
3:A:132:ASP:OD1	3:A:133:ARG:N	2.48	0.45
15:M:81:ARG:HG3	15:M:85:ARG:HB2	1.98	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
7:E:6:GLU:HA	7:E:46:THR:HG22	1.98	0.45
2:9:52:A:H2'	2:9:53:G:O4'	2.17	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
3:A:128:LEU:HG	39:A:9038:HOH:O	2.15	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
27:Y:174:VAL:HG12	27:Y:174:VAL:O	2.17	0.45
1:0:2112:A:H2'	1:0:2113:G:C8	2.52	0.45
14:L:119:THR:HG23	14:L:139:SER:OG	2.17	0.45
15:M:99:ARG:HE	15:M:170:ASN:ND2	2.15	0.45
6:D:63:ILE:HG13	6:D:64:ARG:N	2.32	0.45
4:B:304:PRO:HD2	4:B:307:ARG:NE	2.32	0.45
1:0:558:C:H5'	39:0:5710:HOH:O	2.16	0.45
4:B:305:ASP:O	4:B:306:LYS:CB	2.62	0.45
1:0:2421:G:H3'	1:0:2422:U:C5'	2.47	0.45
1:0:2064:U:H4'	1:0:2653:A:OP1	2.16	0.45
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.82	0.45
1:0:820:G:C6	3:A:171:LYS:HB2	2.52	0.45
10:H:50:ILE:HD12	10:H:149:VAL:CG1	2.47	0.45
1:0:2032:U:H5'	39:0:4980:HOH:O	2.16	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
6:D:96:SER:C	6:D:98:PHE:H	2.20	0.45
1:0:2717:C:OP1	4:B:207:LYS:HG3	2.17	0.45
1:0:1878:G:O2'	1:0:1879:U:P	2.75	0.45
7:E:3:VAL:CG2	7:E:49:ILE:HB	2.42	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
14:L:10:SER:O	14:L:11:ARG:HB3	2.17	0.45
1:0:1979:G:H2'	39:0:3782:HOH:O	2.16	0.45
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.46	0.45
1:0:932:U:H2'	1:0:933:C:C6	2.52	0.45
1:0:1163:G:N2	39:0:5189:HOH:O	2.49	0.45
1:0:2756:U:N3	1:0:2896:A:C2	2.75	0.45
10:H:33:GLN:H	10:H:69:ARG:HH11	1.65	0.45
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.52	0.45
5:C:107:ARG:NH2	39:C:8661:HOH:O	2.47	0.45
20:R:29:LYS:HD3	39:R:8937:HOH:O	2.17	0.45
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.47	0.45
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.99	0.45
2:9:24:U:H3'	2:9:25:G:H5'	1.98	0.45
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.98	0.45
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.99	0.45
1:0:1406:A:H4'	1:0:1407:A:H5''	1.98	0.45
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.99	0.45
1:0:2649:A:H5'	1:0:2649:A:H8	1.81	0.45
15:M:99:ARG:HH21	15:M:170:ASN:ND2	2.11	0.45
1:0:1943:C:H4'	3:A:211:LYS:O	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:D:76:ARG:O	6:D:77:ASP:HB2	2.17	0.45
5:C:27:ARG:HG2	5:C:30:LEU:CD1	2.46	0.45
1:O:2852:A:H5''	39:O:5686:HOH:O	2.17	0.45
1:O:1174:A:C5	1:O:1201:C:H4'	2.52	0.45
9:G:67:LEU:O	9:G:71:LEU:HG	2.16	0.45
7:E:18:LEU:HD13	7:E:34:TRP:CG	2.52	0.45
1:O:1947:G:H2'	1:O:1948:G:C8	2.51	0.45
1:O:951:A:O2'	1:O:952:G:H5'	2.17	0.45
39:K:7438:HOH:O	23:U:20:MET:HE1	2.16	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
6:D:27:ILE:HD11	6:D:37:ALA:CB	2.47	0.45
1:O:1592:G:O2'	1:O:1593:C:O4'	2.33	0.45
1:O:1060:C:H6	1:O:1060:C:H5'	1.82	0.45
4:B:5:ARG:NH1	4:B:8:LYS:HE2	2.32	0.45
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.47	0.45
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.98	0.45
10:H:149:VAL:HG13	39:H:9028:HOH:O	2.16	0.45
30:2:18:ASN:HD21	30:2:40:ARG:H	1.65	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
9:G:69:ARG:NH1	39:G:3513:HOH:O	2.50	0.45
7:E:116:THR:CG2	7:E:151:LEU:HD22	2.45	0.44
7:E:11:VAL:HG13	7:E:23:GLU:O	2.17	0.44
4:B:82:VAL:CG1	4:B:82:VAL:O	2.65	0.44
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.47	0.44
5:C:35:VAL:HG21	5:C:227:GLY:HA2	1.98	0.44
1:O:2361:A:H5''	39:O:9501:HOH:O	2.17	0.44
1:O:1007:A:H2'	10:H:22:TYR:CZ	2.52	0.44
1:O:1654:U:H2'	3:A:47:HIS:HD2	1.82	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
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
16:N:108:SER:HA	16:N:109:PRO:HD3	1.80	0.44
1:O:960:G:N3	1:O:960:G:C2'	2.80	0.44
25:W:52:VAL:HG22	25:W:53:ALA:H	1.82	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
1:O:380:A:H2'	39:O:7660:HOH:O	2.16	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:2256:G:C2'	1:0:2257:G:H5'	2.47	0.44
1:0:1755:A:H2'	1:0:1756:G:O4'	2.17	0.44
5:C:150:THR:HA	5:C:203:ALA:O	2.17	0.44
1:0:1555:G:H4'	1:0:1630:A:H2	1.82	0.44
1:0:2003:U:H4'	1:0:2004:U:H5	1.82	0.44
25:W:38:THR:HB	39:W:5390:HOH:O	2.17	0.44
1:0:524:A:C5'	20:R:29:LYS:HE2	2.47	0.44
1:0:204:A:C2'	1:0:205:U:H5'	2.48	0.44
4:B:217:ARG:HG3	4:B:257:THR:CG2	2.48	0.44
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.50	0.44
1:0:488:U:H2'	39:0:4480:HOH:O	2.17	0.44
1:0:308:U:C4	1:0:342:C:H1'	2.52	0.44
25:W:41:TYR:HA	25:W:44:MET:HE3	1.99	0.44
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.32	0.44
6:D:167:GLU:C	6:D:169:THR:H	2.21	0.44
6:D:35:ALA:C	6:D:37:ALA:N	2.71	0.44
2:9:50:G:H5''	16:N:159:TYR:HE1	1.83	0.44
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.30	0.44
1:0:2756:U:N3	1:0:2896:A:H2	2.13	0.44
16:N:15:GLU:HB2	16:N:17:ARG:HG3	1.98	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
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.52	0.44
7:E:84:MET:HE1	7:E:148:ILE:HD12	2.00	0.44
17:O:98:LEU:O	17:O:102:ILE:HG13	2.17	0.44
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.53	0.44
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.53	0.44
1:0:2104:C:O2	1:0:2485:A:N1	2.51	0.44
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.98	0.44
31:3:91:GLN:O	31:3:92:GLU:HB2	2.17	0.44
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.72	0.44
1:0:1882:C:O2'	1:0:2012:U:OP2	2.33	0.44
3:A:153:ARG:HD3	39:A:8995:HOH:O	2.16	0.44
1:0:559:U:H2'	1:0:560:U:O4'	2.17	0.44
6:D:146:LYS:NZ	16:N:107:ASN:ND2	2.64	0.44
25:W:11:VAL:O	25:W:12:ASN:HB2	2.16	0.44
16:N:154:LEU:O	16:N:155:GLU:CB	2.66	0.44
1:0:1131:G:C6	1:0:1230:A:C4	3.06	0.44
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.33	0.44
1:0:1137:G:H1'	39:0:4354:HOH:O	2.17	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	Distance(Å)	Clash(Å)
10:H:81:GLY:C	10:H:83:GLU:H	2.21	0.44
8:F:46:GLU:N	39:F:3461:HOH:O	2.51	0.44
3:A:81:GLN:H	3:A:92:ASN:ND2	2.16	0.44
1:0:2642:G:H2'	1:0:2643:G:O4'	2.18	0.44
1:0:138:U:OP2	1:0:139:C:H5	2.00	0.44
1:0:1044:C:H3'	1:0:1045:G:H5''	1.99	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
1:0:2793:A:H2'	1:0:2794:G:H5'	1.99	0.44
6:D:64:ARG:HG2	6:D:67:ASP:HB3	2.00	0.44
26:X:25:ARG:CG	39:X:5356:HOH:O	2.65	0.44
1:0:1307:A:H2'	1:0:1308:A:C8	2.53	0.44
21:S:11:THR:H	21:S:14:ALA:HB3	1.81	0.44
12:J:90:LYS:HB2	36:J:8802:CL:CL	2.54	0.44
7:E:132:THR:HB	39:E:2227:HOH:O	2.17	0.44
12:J:19:MET:HE2	12:J:132:LEU:HD11	1.99	0.43
1:0:1119:G:C8	12:J:52:GLN:NE2	2.86	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
9:G:19:GLU:O	9:G:23:ILE:HG13	2.18	0.43
1:0:1181:A:N1	1:0:1192:A:O2'	2.50	0.43
1:0:2524:G:H21	1:0:2526:C:N4	2.16	0.43
27:Y:95:THR:N	27:Y:236:VAL:O	2.51	0.43
1:0:1946:C:H2'	1:0:1971:G:C8	2.53	0.43
4:B:108:GLU:HB3	4:B:111:ARG:HD2	2.00	0.43
3:A:223:ARG:NE	39:A:9037:HOH:O	2.51	0.43
1:0:559:U:H5'	1:0:559:U:C6	2.41	0.43
4:B:51:VAL:HG23	4:B:327:VAL:HG13	1.98	0.43
27:Y:115:ARG:HH11	27:Y:115:ARG:HB3	1.83	0.43
1:0:392:U:C5'	15:M:193:LYS:HB3	2.49	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
1:0:1252:A:H2'	1:0:1253:C:O4'	2.19	0.43
1:0:1733:A:H4'	4:B:212:GLN:HA	1.99	0.43
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.19	0.43
1:0:1119:G:C6	1:0:1244:U:C5	3.06	0.43
12:J:107:ASN:HD22	12:J:108:PRO:N	2.16	0.43
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.18	0.43
1:0:1730:G:H5'	1:0:1731:C:H5	1.81	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
13:K:113:ILE:CG2	13:K:114:ALA:N	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:542:A:H2'	1:0:543:G:O4'	2.18	0.43
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.49	0.43
11:I:67:VAL:CG1	11:I:68:PRO:HD2	2.48	0.43
1:0:2526:C:H5'	1:0:2526:C:C6	2.53	0.43
20:R:119:VAL:CG1	20:R:119:VAL:O	2.65	0.43
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.81	0.43
1:0:517:U:H1'	39:0:7997:HOH:O	2.18	0.43
1:0:2115:U:H2'	1:0:2116:U:C6	2.53	0.43
10:H:57:THR:O	10:H:58:VAL:HG13	2.19	0.43
21:S:20:PHE:CD2	21:S:20:PHE:N	2.85	0.43
12:J:45:VAL:HG22	12:J:46:ILE:N	2.33	0.43
31:3:70:ARG:CG	31:3:77:ALA:HB2	2.47	0.43
1:0:2090:G:H2'	1:0:2091:G:C8	2.53	0.43
14:L:122:ALA:HB3	14:L:125:PHE:CZ	2.54	0.43
1:0:920:C:H5'	1:0:921:G:C4	2.53	0.43
16:N:73:ALA:N	39:N:8863:HOH:O	2.48	0.43
1:0:284:C:H4'	1:0:285:A:H8	1.83	0.43
1:0:2649:A:C8	1:0:2649:A:H5'	2.54	0.43
1:0:2326:C:H4'	1:0:2412:G:C4'	2.49	0.43
1:0:790:A:H2'	1:0:791:A:O4'	2.18	0.43
22:T:71:VAL:CG1	22:T:72:ILE:N	2.81	0.43
16:N:77:ASN:OD1	16:N:80:SER:HB2	2.18	0.43
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.54	0.43
1:0:2819:C:H2'	1:0:2820:A:C8	2.53	0.43
13:K:28:GLU:HG2	13:K:58:THR:HB	2.00	0.43
1:0:2868:C:H2'	1:0:2869:G:O4'	2.19	0.43
1:0:1484:G:H2'	39:0:9594:HOH:O	2.17	0.43
25:W:29:VAL:O	25:W:30:ASN:HB2	2.18	0.43
1:0:130:C:H5'	39:0:5666:HOH:O	2.18	0.43
7:E:77:THR:OG1	7:E:78:GLU:N	2.51	0.43
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.18	0.43
3:A:39:ALA:O	3:A:61:GLU:HG3	2.18	0.43
1:0:2121:G:O2'	1:0:2122:C:H5'	2.19	0.43
4:B:175:LEU:O	4:B:175:LEU:HD23	2.19	0.43
1:0:189:A:OP1	15:M:171:ARG:NH2	2.51	0.43
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.53	0.43
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.84	0.43
1:0:920:C:H4'	1:0:921:G:C2	2.54	0.43
1:0:622:G:P	27:Y:148:GLY:HA3	2.58	0.43
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.19	0.43
13:K:75:ARG:HD3	13:K:112:PRO:O	2.19	0.43
15:M:164:THR:CG2	15:M:165:GLY:N	2.82	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:D:149:ARG:HH12	16:N:15:GLU:HA	1.84	0.43
1:0:512:G:O3'	1:0:513:A:H8	2.02	0.43
1:0:137:U:OP1	1:0:259:G:O2'	2.35	0.43
3:A:125:ASN:CB	3:A:158:VAL:HG12	2.49	0.43
1:0:2256:G:O2'	1:0:2257:G:H5'	2.19	0.43
1:0:2031:C:H2'	1:0:2032:U:O4'	2.19	0.43
20:R:15:LYS:HE3	39:R:8984:HOH:O	2.18	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.54	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
4:B:40:GLY:HA3	39:B:9118:HOH:O	2.19	0.43
4:B:53:LEU:HD11	4:B:327:VAL:HG22	2.01	0.43
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.54	0.43
1:0:1853:C:O2'	3:A:217:ARG:NH2	2.52	0.43
13:K:66:ARG:HH11	13:K:66:ARG:HG2	1.84	0.43
5:C:166:ILE:HD11	5:C:207:LEU:HD13	2.01	0.43
1:0:2133:U:H4'	1:0:2134:G:C5'	2.48	0.43
1:0:2326:C:H4'	1:0:2412:G:H4'	2.01	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
7:E:86:VAL:CG1	7:E:129:GLU:HA	2.49	0.43
1:0:2403:C:OP1	19:Q:49:ASN:HB3	2.19	0.43
15:M:99:ARG:CD	15:M:167:GLY:HA2	2.49	0.43
21:S:57:THR:HG22	21:S:59:ASP:HB2	2.01	0.43
8:F:60:VAL:HG12	8:F:60:VAL:O	2.19	0.43
1:0:1185:U:H5'	39:0:7891:HOH:O	2.18	0.43
1:0:1158:G:O2'	1:0:1159:G: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
1:0:2103:A:O2'	1:0:2104:C:H5'	2.19	0.43
19:Q:55:ARG:HD2	39:Q:2875:HOH:O	2.19	0.43
22:T:18:GLU:O	22:T:21:LYS:HG2	2.19	0.43
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
1:0:2316:G:H4'	39:0:6539:HOH:O	2.18	0.42
1:0:2768:A:O2'	1:0:2769:C:H5'	2.19	0.42
1:0:263:U:C2	8:F:59:ILE:CD1	3.02	0.42
1:0:524:A:H5'	20:R:29:LYS:HE2	2.01	0.42
8:F:111:ILE:O	8:F:115:VAL:HG23	2.18	0.42
7:E:22:VAL:O	7:E:28:SER:HA	2.19	0.42
1:0:1768:C:H2'	1:0:1769:C:O4'	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:56:G:H5''	24:V:50:ARG:NH1	2.33	0.42
1:0:1218:U:H2'	1:0:1219:U:C6	2.53	0.42
11:I:123:VAL:C	11:I:125:GLY:H	2.22	0.42
11:I:88:GLN:HA	11:I:91:PHE:HE2	1.84	0.42
1:0:451:C:O2'	1:0:452:G:H5'	2.19	0.42
6:D:37:ALA:HA	39:D:5583:HOH:O	2.19	0.42
1:0:567:U:H5''	39:0:5740:HOH:O	2.19	0.42
3:A:107:ASN:OD1	3:A:120:ARG:HD2	2.19	0.42
18:P:59:ARG:HD3	39:P:191: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
1:0:1202:A:H2'	1:0:1203:G:O4'	2.19	0.42
3:A:37:VAL:HG22	39:A:9059:HOH:O	2.19	0.42
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.19	0.42
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.49	0.42
3:A:135:VAL:N	39:A:9058:HOH:O	2.51	0.42
18:P:64:GLU:HG2	39:P:167:HOH:O	2.18	0.42
1:0:2630:G:O6	3:A:206:ARG:NH2	2.49	0.42
1:0:241:A:C2	1:0:378:A:H4'	2.54	0.42
16:N:37:ARG:NH2	39:N:8832:HOH:O	2.52	0.42
1:0:1439:C:OP1	30:2:41:HIS:HE1	2.03	0.42
1:0:2718:C:H5'	1:0:2718:C:C6	2.51	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
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
1:0:1573:A:H2'	1:0:1574:C:O4'	2.19	0.42
15:M:15:PRO:HA	15:M:20:LEU:HD23	2.01	0.42
1:0:1846:U:O2'	3:A:172:ALA:HB2	2.19	0.42
1:0:1287:A:O4'	25:W:117:ARG:HD3	2.20	0.42
39:0:6168:HOH:O	13:K:87:ARG:NE	2.52	0.42
5:C:246:ARG:NH2	39:C:8630:HOH:O	2.46	0.42
1:0:1948:G:H2'	1:0:1949:G:O4'	2.20	0.42
7:E:107:PHE:CZ	7:E:108:LEU:HD13	2.54	0.42
1:0:903:U:OP2	14:L:11:ARG:NH1	2.50	0.42
1:0:926:A:O2'	14:L:41:HIS:HD2	2.01	0.42
1:0:1029:U:H5'	1:0:1031:G:N7	2.34	0.42
1:0:1562:C:N4	39:0:6317:HOH:O	2.34	0.42
1:0:2353:A:H4'	1:0:2354:A:O5'	2.18	0.42
3:A:175:LYS:HE2	39:A:9040:HOH:O	2.19	0.42
1:0:1066:U:H2'	1:0:1067:A:C8	2.54	0.42
20:R:104:PHE:HB2	20:R:109:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:B:162:MET:HG3	4:B:310:ARG:HD3	2.01	0.42
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.43	0.42
10:H:66:GLU:O	10:H:70:LEU:HB2	2.20	0.42
1:0:1845:A:O3'	3:A:187:PRO:HB2	2.19	0.42
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.54	0.42
4:B:139:ASP:HB2	39:B:8998:HOH:O	2.18	0.42
5:C:133:ARG:NE	5:C:138:VAL:HG22	2.34	0.42
3:A:217:ARG:CG	3:A:217:ARG:HH11	2.33	0.42
1:0:392:U:H5''	15:M:193:LYS:HB3	2.01	0.42
1:0:1940:C:H4'	39:0:7777:HOH:O	2.18	0.42
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.55	0.42
1:0:669:G:O2'	1:0:670:G:H5'	2.19	0.42
15:M:152:ALA:HB1	39:M:8934:HOH:O	2.20	0.42
1:0:2478:U:O2'	1:0:2479:A:H5'	2.19	0.42
1:0:646:G:H2'	1:0:647:U:C6	2.54	0.42
21:S:57:THR:CG2	21:S:59:ASP:HB2	2.50	0.42
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.53	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
26:X:41:PHE:O	26:X:43:VAL:HG23	2.19	0.42
4:B:243:ASN:HA	4:B:244:PRO:C	2.39	0.42
8:F:99:THR:O	8:F:99:THR:HG23	2.20	0.42
9:G:64:ASN:N	9:G:64:ASN:ND2	2.68	0.42
23:U:13:ILE:HG12	23:U:32:CYS:HB3	2.00	0.42
1:0:1925:G:O2'	1:0:1926:G:H5'	2.20	0.42
1:0:1626:A:H2'	1:0:1627:G:O4'	2.19	0.42
1:0:1406:A:H4'	1:0:1407:A:C5'	2.50	0.42
12:J:26:VAL:HG13	12:J:36:VAL:HG11	2.01	0.42
7:E:43:ASP:HA	39:E:5864:HOH:O	2.18	0.42
14:L:92:ASP:HB3	14:L:95:ASP:OD2	2.19	0.42
2:9:59:C:H6	2:9:59:C:O5'	2.02	0.42
6:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.65	0.42
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.55	0.42
21:S:56:ASN:O	30:2:8:LYS:NZ	2.47	0.42
25:W:107:LEU:O	25:W:112:LEU:HB2	2.18	0.42
1:0:2442:G:H3'	39:0:7065:HOH:O	2.19	0.42
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.54	0.42
1:0:2754:G:H2'	1:0:2755:G:O4'	2.19	0.42
22:T:47:THR:HB	22:T:100:ASP:HB3	2.02	0.42
14:L:6:ARG:NH2	39:L:8842:HOH:O	2.47	0.42
1:0:962:C:H1'	16:N:5:ARG:HH12	1.79	0.42
24:V:60:GLN:O	24:V:65:ASP:N	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
28:Z:30:GLU:HA	28:Z:33:MET:HE3	2.01	0.42
25:W:19:ASP:O	25:W:23:MET:HG3	2.20	0.42
1:O:926:A:O2'	14:L:41:HIS:CD2	2.73	0.42
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.54	0.42
13:K:23:ASN:HD21	13:K:107:THR:HB	1.83	0.42
17:O:41:ALA:HA	39:O:5104:HOH:O	2.19	0.42
1:O:1902:G:H2'	1:O:1903:U:O4'	2.20	0.42
1:O:2401:A:H2'	1:O:2402:A:C8	2.55	0.42
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.35	0.42
5:C:78:ARG:CG	5:C:78:ARG:NH1	2.74	0.42
2:9:42:C:O2	6:D:76:ARG:NH1	2.53	0.42
1:O:2578:G:C8	1:O:2578:G:H5'	2.51	0.42
16:N:140:GLN:O	16:N:143:ARG:HB2	2.19	0.42
25:W:76:ASP:O	25:W:77:ALA:C	2.57	0.42
6:D:60:GLU:O	6:D:61:PHE:C	2.57	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
27:Y:117:LEU:HD12	27:Y:174:VAL:HG11	2.02	0.42
3:A:135:VAL:HG11	3:A:147:ARG:NH1	2.35	0.42
22:T:96:VAL:HG13	22:T:97:ARG:N	2.35	0.42
5:C:219:ASN:O	5:C:222:ASP:OD1	2.37	0.42
5:C:219:ASN:N	5:C:222:ASP:OD1	2.52	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
12:J:46:ILE:HD11	12:J:53:ILE:HG23	2.01	0.42
1:O:1684:A:O2'	1:O:1685:A:H5''	2.19	0.42
1:O:1209:C:H2'	1:O:1210:G:C8	2.51	0.42
18:P:10:ALA:CA	18:P:13:VAL:HG12	2.46	0.42
3:A:97:ALA:C	3:A:131:HIS:HE2	2.22	0.42
7:E:24:GLY:HA3	7:E:76:VAL:HB	2.02	0.42
15:M:145:ASP:HA	39:M:8909:HOH:O	2.19	0.42
1:O:214:U:H5'	39:O:6586:HOH:O	2.19	0.42
8:F:24:ARG:NH2	39:F:6800:HOH:O	2.48	0.42
16:N:64:SER:C	16:N:66:LEU:H	2.22	0.42
4:B:248:ARG:NH2	39:B:8993:HOH:O	2.50	0.42
15:M:5:TYR:HE2	15:M:46:LEU:HD13	1.84	0.42
11:I:109:PRO:HG2	11:I:110:ASP:H	1.84	0.41
3:A:105:VAL:CG1	3:A:106:CYS:N	2.82	0.41
9:G:24:VAL:O	9:G:28:GLU:HB2	2.19	0.41
5:C:138:VAL:O	5:C:234:VAL:HA	2.20	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	Distance(Å)	Clash(Å)
1:0:304:G:H1'	1:0:347:A:H61	1.85	0.41
21:S:42:GLU:HG2	21:S:49:VAL:HG23	2.01	0.41
1:0:1754:A:H2'	1:0:1755:A:O4'	2.20	0.41
3:A:206:ARG:NH1	39:A:8979:HOH:O	2.53	0.41
1:0:482:G:H4'	1:0:508:A:N1	2.35	0.41
4:B:132:HIS:CE1	4:B:171:VAL:HG21	2.55	0.41
15:M:99:ARG:NH2	15:M:170:ASN:HD22	2.15	0.41
5:C:127:ARG:HG2	5:C:127:ARG:HH11	1.84	0.41
25:W:146:ILE:HA	25:W:146:ILE:HD13	1.89	0.41
18:P:63:ARG:NH2	39:P:191:HOH:O	2.51	0.41
1:0:2756:U:C2	1:0:2896:A:H2	2.37	0.41
1:0:1197:G:N2	39:0:6679:HOH:O	2.52	0.41
5:C:246:ARG:HB3	5:C:246:ARG:NH1	2.35	0.41
1:0:2503:A:OP1	10:H:154:ARG:NH2	2.47	0.41
10:H:154:ARG:HA	10:H:157:TYR:CE2	2.55	0.41
1:0:2252:A:C5	1:0:2253:G:H1'	2.54	0.41
20:R:114:VAL:HG13	20:R:114:VAL:O	2.20	0.41
10:H:72:ALA:HB2	10:H:156:ALA:HB2	2.02	0.41
1:0:1762:C:H4'	39:0:5120:HOH:O	2.21	0.41
1:0:2336:G:H1'	39:D:5675:HOH:O	2.19	0.41
1:0:1236:A:C8	12:J:63:ILE:HD11	2.55	0.41
1:0:2453:G:H4'	14:L:50:GLY:C	2.40	0.41
1:0:383:A:H2'	1:0:384:G:O4'	2.20	0.41
3:A:211:LYS:HD2	39:A:9081:HOH:O	2.21	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
11:I:129:SER:N	39:I:7330:HOH:O	2.47	0.41
1:0:1730:G:H5''	1:0:1731:C:C6	2.54	0.41
10:H:24:THR:O	10:H:123:ILE:HD12	2.20	0.41
16:N:154:LEU:HG	16:N:155:GLU:N	2.35	0.41
10:H:146:ALA:O	10:H:149:VAL:HG12	2.20	0.41
1:0:1657:A:H2'	1:0:1658:A:C8	2.55	0.41
1:0:2726:U:O2	1:0:2749:U:O5'	2.38	0.41
1:0:1980:U:O2	1:0:2008:U:H4'	2.20	0.41
4:B:189:ALA:HB1	39:B:9033:HOH:O	2.19	0.41
1:0:1118:A:C8	1:0:1119:G:H5''	2.54	0.41
5:C:118:THR:HG22	5:C:137:PRO:HB3	2.03	0.41
8:F:38:LYS:HZ1	15:M:3:SER:HA	1.85	0.41
7:E:81:GLU:HA	7:E:133:VAL:O	2.20	0.41
26:X:66:THR:CG2	26:X:67:PRO:HD2	2.48	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1181:A:H2'	1:0:1182:C:C5'	2.50	0.41
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.90	0.41
1:0:827:A:H2'	1:0:828:G:O4'	2.19	0.41
3:A:194:MET:CE	3:A:199:HIS:CB	2.98	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
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.19	0.41
11:I:87:PRO:HB3	11:I:129:SER:C	2.41	0.41
8:F:28:ALA:CB	8:F:99:THR:HG23	2.50	0.41
15:M:169:ARG:NH2	39:M:8852:HOH:O	2.47	0.41
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.56	0.41
1:0:1739:G:O2'	1:0:1740:U:H5'	2.20	0.41
11:I:111:LEU:HD22	11:I:122:GLU:OE1	2.21	0.41
1:0:2241:C:O2'	1:0:2242:U:H5'	2.20	0.41
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.40	0.41
16:N:39:SER:HB3	16:N:42:HIS:H	1.86	0.41
6:D:10:PHE:N	39:D:7345:HOH:O	2.53	0.41
10:H:86:TYR:C	10:H:86:TYR:CD1	2.93	0.41
24:V:12:THR:CG2	24:V:15:GLU:H	2.34	0.41
4:B:57:GLU:HA	4:B:58:PRO:HD2	1.96	0.41
6:D:173:GLU:O	6:D:174:VAL:C	2.59	0.41
30:2:19:SER:O	30:2:36:ASN:ND2	2.54	0.41
1:0:660:A:H4'	1:0:661:G:O5'	2.20	0.41
4:B:75:GLU:C	4:B:77:PRO:HD3	2.41	0.41
1:0:329:A:OP2	5:C:206:ASN:HB2	2.20	0.41
1:0:88:G:H2'	1:0:89:G:C8	2.55	0.41
1:0:2543:G:H2'	1:0:2544:G:O4'	2.20	0.41
1:0:702:G:O2'	1:0:703:G:H5'	2.21	0.41
1:0:249:G:O2'	1:0:250:C:H5'	2.21	0.41
5:C:154:VAL:O	5:C:158:GLU:HG3	2.21	0.41
10:H:151:GLU:HA	10:H:151:GLU:OE1	2.21	0.41
7:E:16:ASP:O	7:E:17:HIS:HB2	2.19	0.41
10:H:49:GLN:OE1	10:H:169:GLU:HB3	2.21	0.41
1:0:2054:A:H2	20:R:128:ARG:HH22	1.56	0.41
11:I:87:PRO:C	11:I:89:GLU:N	2.74	0.41
5:C:57:PRO:HG2	5:C:73:LEU:HD13	2.02	0.41
15:M:134:ILE:O	15:M:136:PRO:HD3	2.21	0.41
26:X:20:GLU:CD	26:X:21:PRO:HD2	2.41	0.41
1:0:1596:U:H2'	1:0:1598:A:OP2	2.20	0.41
22:T:41:ARG:NH1	22:T:42:VAL:O	2.53	0.41
1:0:256:C:H2'	1:0:257:G:O4'	2.21	0.41
4:B:14:GLY:HA3	39:B:9076:HOH:O	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:L:38:HIS:CD2	14:L:39:GLU:HG3	2.55	0.41
1:0:2724:U:H2'	1:0:2725:G:O4'	2.20	0.41
1:0:1352:A:H4'	1:0:1353:C:OP2	2.20	0.41
12:J:64:GLY:HA3	36:J:8821:CL:CL	2.58	0.41
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.82	0.41
1:0:2498:C:O2'	1:0:2499:U:H5'	2.20	0.41
11:I:103:ILE:HG22	11:I:103:ILE:O	2.20	0.41
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.30	0.41
1:0:1165:G:H1'	1:0:1174:A:H1'	2.03	0.41
8:F:5:ASP:O	8:F:119:ARG:NH1	2.53	0.41
1:0:95:A:H5''	1:0:97:G:O4'	2.21	0.41
1:0:2906:A:H5'	1:0:2907:C:O4'	2.21	0.41
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.03	0.41
1:0:23:G:C6	1:0:24:G:N1	2.89	0.41
22:T:106:GLU:HG3	39:T:4913:HOH:O	2.21	0.41
26:X:74:ALA:HB1	26:X:85:VAL:HG22	2.03	0.41
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.48	0.41
12:J:75:PRO:HB3	12:J:132:LEU:HB3	2.02	0.41
3:A:36:ASP:CB	3:A:85:SER:H	2.34	0.41
39:O:5740:HOH:O	25:W:122:ARG:CZ	2.68	0.41
16:N:49:THR:HG22	16:N:56:ASP:CB	2.49	0.41
6:D:170:TYR:CD1	6:D:170:TYR:N	2.89	0.41
15:M:61:ILE:N	15:M:61:ILE:HD12	2.35	0.41
6:D:173:GLU:HG3	6:D:174:VAL:N	2.35	0.41
8:F:33:THR:HG21	8:F:59:ILE:O	2.20	0.41
29:1:28:HIS:O	29:1:32:LYS:N	2.47	0.41
1:0:553:G:O2'	27:Y:179:PRO:HG3	2.21	0.41
26:X:23:HIS:CD2	26:X:24:LYS:HG3	2.56	0.41
17:O:14:LEU:HG	17:O:102:ILE:HD11	2.03	0.41
13:K:28:GLU:OE2	13:K:58:THR:HG21	2.20	0.41
1:0:2089:A:C2'	1:0:2090:G:H5'	2.51	0.41
15:M:69:LYS:HG3	15:M:126:GLN:CA	2.51	0.41
22:T:48:VAL:CG2	22:T:96:VAL:HG13	2.51	0.41
15:M:46:LEU:HG	39:M:8917:HOH:O	2.19	0.41
26:X:10:VAL:HG12	26:X:11:THR:N	2.35	0.41
1:0:2883:A:H2'	1:0:2884:G:O4'	2.21	0.41
1:0:2515:C:H2'	1:0:2516:G:O4'	2.20	0.41
20:R:33:ARG:NH1	39:R:8947:HOH:O	2.37	0.41
1:0:1976:G:O2'	1:0:1977:U:H5'	2.21	0.41
1:0:2559:C:H4'	39:O:7688:HOH:O	2.20	0.41
1:0:522:U:O2'	1:0:1366:C:H5'	2.20	0.41
1:0:2740:G:H2'	1:0:2741:A:O4'	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:4:G:H21	16:N:44:ARG:NH1	2.19	0.41
1:0:366:U:H2'	1:0:367: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
39:0:4461:HOH:O	22:T:82:THR:HA	2.21	0.41
1:0:958:G:H2'	1:0:959:C:C6	2.55	0.41
1:0:222:A:H2'	1:0:223:G:O4'	2.20	0.41
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.91	0.41
1:0:1098:A:H2'	1:0:1099:G:O4'	2.21	0.41
20:R:96:VAL:HG13	20:R:106:GLY:HA3	2.03	0.41
4:B:26:PHE:CE1	4:B:310:ARG:HB3	2.56	0.41
1:0:1299:G:N2	39:0:5149:HOH:O	2.54	0.41
6:D:49:PRO:HB3	39:D:5828:HOH:O	2.21	0.41
26:X:43:VAL:HG12	26:X:47:ALA:HB3	2.02	0.41
1:0:2428:G:N7	31:3:60:LYS:NZ	2.67	0.41
24:V:51:LYS:O	24:V:55:ARG:HG3	2.21	0.41
14:L:67:ARG:HG2	14:L:67:ARG:HH11	1.86	0.41
3:A:81:GLN:CB	3:A:92:ASN:ND2	2.84	0.41
1:0:1249:U:H2'	1:0:1250:C:C6	2.56	0.41
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.50	0.41
1:0:155:C:OP2	15:M:188:ARG:HD3	2.20	0.41
1:0:612:U:H2'	1:0:613:C:C6	2.56	0.41
1:0:2015:A:H2'	1:0:2016:U:O4'	2.20	0.41
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
10:H:61:ARG:HG3	10:H:61:ARG:NH1	2.36	0.40
1:0:1268:C:O2'	1:0:1269:G:H5'	2.20	0.40
1:0:1328:A:C8	27:Y:169:ARG:HD3	2.56	0.40
6:D:99:ASP:N	6:D:103:ASN:O	2.30	0.40
3:A:179:MET:HG2	3:A:186:TRP:HB2	2.01	0.40
1:0:447:A:O2'	1:0:448:G:H5'	2.22	0.40
22:T:48:VAL:HG23	22:T:98:VAL:HA	2.03	0.40
1:0:213:G:O2'	1:0:214:U:OP2	2.40	0.40
18:P:40:VAL:O	18:P:44:VAL:HG23	2.21	0.40
1:0:1773:G:C8	28:Z:16:ALA:HA	2.55	0.40
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.36	0.40
1:0:2382:A:H5'	39:3:8962:HOH:O	2.21	0.40
5:C:236:THR:C	39:C:8653:HOH:O	2.60	0.40
4:B:310:ARG:HD2	39:B:9057:HOH:O	2.20	0.40
1:0:655:U:O2'	17:O:3:THR:HB	2.21	0.40
12:J:46:ILE:HD11	12:J:53:ILE:CG2	2.51	0.40
10:H:6:ALA:CB	10:H:61:ARG:HH12	2.33	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:G:12:ILE:N	9:G:13:PRO:CD	2.84	0.40
4:B:254:GLN:NE2	39:B:9058:HOH:O	2.54	0.40
29:1:37:CYS:SG	29:1:39:PHE:HB2	2.61	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
30:2:18:ASN:ND2	30:2:40:ARG:H	2.19	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
1:0:1072:G:OP2	27:Y:154:ARG:NH2	2.54	0.40
24:V:8:ILE:HG21	24:V:59:ILE:HG13	2.02	0.40
1:0:1398:G:H2'	1:0:1399:A:C8	2.56	0.40
16:N:129:ILE:HA	16:N:130:PRO:HD3	1.98	0.40
1:0:1304:U:H2'	1:0:1305:C:C6	2.56	0.40
8:F:52:GLU:HG3	8:F:77:VAL:O	2.21	0.40
1:0:59:A:H5'	39:0:4798:HOH:O	2.20	0.40
16:N:51:GLY:HA2	16:N:52:PRO:HD3	1.94	0.40
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.53	0.40
4:B:62:ARG:HG2	4:B:65:MET:HE3	2.03	0.40
1:0:1186:C:H4'	11:I:114:TYR:HE1	1.87	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
16:N:86:LEU:HD12	16:N:125:ALA:HB2	2.04	0.40
8:F:107:ASP:O	8:F:111:ILE:HG13	2.21	0.40
16:N:72:GLU:H	16:N:171:HIS:CE1	2.39	0.40
1:0:1020:A:H1'	39:Q:6976:HOH:O	2.22	0.40
1:0:861:A:H4'	1:0:1697:G:H4'	2.03	0.40
1:0:2445:U:H2'	1:0:2446:G:C8	2.56	0.40
13:K:99:ASP:OD1	13:K:101:ASN:N	2.53	0.40
39:0:4832:HOH:O	3:A:212:PRO:HB2	2.20	0.40
7:E:69:ILE:HA	7:E:72:MET:HE2	2.01	0.40
2:9:114:G:H2'	2:9:115:C:C6	2.57	0.40
10:H:33:GLN:H	10:H:69:ARG:NH1	2.19	0.40
16:N:38:LYS:HB2	16:N:38:LYS:HE3	1.80	0.40
5:C:6:TYR:HE1	5:C:133:ARG:HH22	1.68	0.40
1:0:820:G:C5	3:A:171:LYS:HB2	2.57	0.40
1:0:212:A:O4'	1:0:214:U:C6	2.75	0.40
14:L:149:ARG:O	14:L:150:GLN:HB2	2.21	0.40
1:0:1039:G:H2'	1:0:1040:A:O4'	2.22	0.40
2:9:31:C:H2'	2:9:32:G:O4'	2.22	0.40
1:0:2435:U:OP1	31:3:28:GLY:HA3	2.20	0.40
1:0:2900:G:H2'	1:0:2901:C:O4'	2.22	0.40
1:0:1829:A:H2'	1:0:1830:C:H5'	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:278:A:H2'	1:0:279:C:O4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	218 (93%)	13 (6%)	4 (2%)	14	17
4	B	335/338 (99%)	314 (94%)	14 (4%)	7 (2%)	11	12
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%)	8	8
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%)	7	6
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	16	22
13	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
14	L	141/165 (86%)	124 (88%)	16 (11%)	1 (1%)	30	43
15	M	192/194 (99%)	181 (94%)	11 (6%)	0	100	100
16	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	8	7
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%)	25	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
24	V	63/71 (89%)	58 (92%)	2 (3%)	3 (5%)	4	2
25	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	18	24
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%)	4	3
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	40 (95%)	1 (2%)	1 (2%)	9	9
31	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
All	All	3705/4436 (84%)	3437 (93%)	223 (6%)	45 (1%)	19	26

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
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

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Mol	Chain	Res	Type
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%)	23	35
4	B	282/283 (100%)	268 (95%)	14 (5%)	34	51
5	C	193/193 (100%)	175 (91%)	18 (9%)	13	19
6	D	117/148 (79%)	113 (97%)	4 (3%)	49	70
7	E	152/156 (97%)	147 (97%)	5 (3%)	50	71
8	F	93/94 (99%)	92 (99%)	1 (1%)	84	94
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	134/145 (92%)	129 (96%)	5 (4%)	45	66
11	I	58/130 (45%)	58 (100%)	0	100	100
12	J	118/121 (98%)	110 (93%)	8 (7%)	22	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	K	106/106 (100%)	105 (99%)	1 (1%)	87	96
14	L	113/127 (89%)	110 (97%)	3 (3%)	57	78
15	M	158/158 (100%)	151 (96%)	7 (4%)	39	58
16	N	149/150 (99%)	145 (97%)	4 (3%)	57	78
17	O	93/94 (99%)	91 (98%)	2 (2%)	64	83
18	P	113/117 (97%)	112 (99%)	1 (1%)	87	96
19	Q	79/80 (99%)	76 (96%)	3 (4%)	44	65
20	R	117/122 (96%)	115 (98%)	2 (2%)	73	89
21	S	71/74 (96%)	69 (97%)	2 (3%)	56	77
22	T	105/106 (99%)	100 (95%)	5 (5%)	35	53
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	43	64
25	W	130/130 (100%)	125 (96%)	5 (4%)	44	65
26	X	66/74 (89%)	59 (89%)	7 (11%)	10	14
27	Y	120/196 (61%)	111 (92%)	9 (8%)	19	29
28	Z	60/68 (88%)	58 (97%)	2 (3%)	50	71
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	61	81
31	3	79/79 (100%)	79 (100%)	0	100	100
All	All	3095/3618 (86%)	2972 (96%)	123 (4%)	42	63

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

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	34 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	2866/3044 (94%)	242 (8%)	35 (1%)

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A

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Mol	Chain	Res	Type
1	0	129	A
1	0	169	A
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1232	A
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2103	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2538	A
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2791	U
2	9	65	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMU	0	2587	1	20,22,23	0.76	1 (5%)	24,31,34	0.77	0
1	OMG	0	2588	1	24,26,27	0.82	0	32,38,41	5.10	3 (9%)
1	UR3	0	2619	1	20,22,23	0.79	1 (5%)	23,32,35	0.85	0
1	PSU	0	2621	1	19,21,22	1.12	2 (10%)	23,30,33	0.99	1 (4%)
1	1MA	0	628	1	23,25,26	0.82	0	32,37,40	1.00	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/8/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/10/27/28	0/1/3/3
1	UR3	0	2619	1	-	0/6/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/8/25/26	0/2/2/2
1	1MA	0	628	1	-	1/8/25/26	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	3.13	1.43	1.37
1	0	2621	PSU	C6-N1	2.36	1.34	1.32
1	0	2587	OMU	P-OP1	2.20	1.49	1.46
1	0	2619	UR3	P-OP1	2.15	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-C5-N7	-28.26	130.34	134.14
1	0	2588	OMG	C6-N1-C2	3.33	125.33	119.51
1	0	628	1MA	C2-N3-C4	-3.17	110.81	116.23
1	0	2588	OMG	C2-N3-C4	-2.29	111.88	115.09
1	0	2621	PSU	C5-C4-N3	-2.20	114.85	118.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1.30	5 (9%)	83,83,83	1.13	5 (6%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	ZIT	C22-C11	3.40	1.58	1.52
32	0	9500	ZIT	C13-C14	2.88	1.60	1.54
32	0	9500	ZIT	O13-C13	2.39	1.48	1.44
32	0	9500	ZIT	C13-C12	2.07	1.61	1.55
32	0	9500	ZIT	C6-C5	2.03	1.60	1.55

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9500	ZIT	C12-C11-N10	-4.07	105.83	110.02
32	0	9500	ZIT	C9-N10-C11	-2.93	106.97	112.06
32	0	9500	ZIT	C7-C8-C9	2.62	116.14	112.24
32	0	9500	ZIT	C4A-C3A-C2A	-2.25	106.90	110.12
32	0	9500	ZIT	O6-C6-C7	2.05	113.87	108.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2754/2922 (94%)	-0.22	91 (3%) 44 42	15, 38, 82, 157	0
2	9	122/122 (100%)	0.11	5 (4%) 35 33	32, 58, 80, 139	0
3	A	237/240 (98%)	0.07	10 (4%) 35 32	19, 40, 75, 96	0
4	B	337/338 (99%)	0.05	5 (1%) 70 69	21, 47, 73, 84	0
5	C	246/246 (100%)	-0.21	2 (0%) 83 82	17, 36, 60, 69	0
6	D	140/177 (79%)	1.77	50 (35%) 1 0	51, 88, 114, 122	0
7	E	172/178 (96%)	0.73	18 (10%) 7 6	39, 61, 80, 84	0
8	F	119/120 (99%)	0.66	12 (10%) 7 7	38, 62, 88, 103	0
9	G	29/348 (8%)	2.56	22 (75%) 0 0	71, 87, 93, 95	0
10	H	160/177 (90%)	0.28	10 (6%) 19 18	31, 50, 83, 91	0
11	I	70/162 (43%)	6.09	70 (100%) 0 0	122, 135, 154, 155	0
12	J	142/145 (97%)	0.00	3 (2%) 60 58	29, 44, 65, 88	0
13	K	132/132 (100%)	-0.23	1 (0%) 83 82	24, 43, 65, 77	0
14	L	145/165 (87%)	0.46	19 (13%) 4 4	18, 56, 101, 115	0
15	M	194/194 (100%)	-0.18	0 100 100	21, 33, 49, 56	0
16	N	186/187 (99%)	0.60	23 (12%) 5 4	34, 55, 102, 112	0
17	O	115/116 (99%)	-0.03	1 (0%) 81 81	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%)	-0.14	1 (1%) 77 77	30, 37, 54, 68	0
20	R	150/155 (96%)	-0.24	0 100 100	25, 38, 58, 66	0
21	S	81/85 (95%)	0.08	3 (3%) 39 38	34, 50, 71, 81	0
22	T	119/120 (99%)	0.32	5 (4%) 35 32	29, 47, 76, 103	0
23	U	53/66 (80%)	0.17	1 (1%) 64 61	35, 48, 66, 78	0
24	V	65/71 (91%)	1.14	8 (12%) 5 4	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%)	-0.12	1 (0%) 86 86	29, 43, 58, 69	0
26	X	82/92 (89%)	0.51	8 (9%) 8 7	37, 50, 78, 94	0
27	Y	142/241 (58%)	0.02	5 (3%) 42 40	21, 36, 59, 80	0
28	Z	73/83 (87%)	0.01	2 (2%) 52 49	35, 51, 68, 86	0
29	1	56/57 (98%)	-0.62	0 100 100	18, 24, 32, 43	0
30	2	46/50 (92%)	0.43	5 (10%) 6 6	26, 51, 75, 89	0
31	3	92/92 (100%)	0.12	1 (1%) 77 77	26, 48, 62, 77	0
All	All	6651/7480 (88%)	0.09	382 (5%) 24 21	15, 43, 89, 157	0

All (382) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	I	74	ILE	14.7
11	I	66	GLY	13.7
11	I	128	THR	13.6
11	I	91	PHE	13.2
11	I	88	GLN	12.8
11	I	71	ALA	12.4
24	V	1	THR	10.9
2	9	1	U	10.7
11	I	132	VAL	10.4
11	I	80	PHE	10.2
6	D	63	ILE	10.0
24	V	39	ALA	9.8
11	I	70	THR	9.5
11	I	97	VAL	8.9
11	I	111	LEU	8.5
11	I	104	ALA	8.4
24	V	40	PRO	8.2
11	I	72	GLU	8.2
6	D	10	PHE	8.2
16	N	166	ALA	8.0
11	I	106	GLN	8.0
11	I	103	ILE	7.7
11	I	131	GLY	7.6
1	0	1172	G	7.4
11	I	93	ALA	7.4
11	I	92	VAL	7.4
11	I	84	SER	7.4
11	I	86	GLU	7.2

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Mol	Chain	Res	Type	RSRZ
11	I	127	CYS	7.2
1	0	1199	A	7.1
3	A	37	VAL	7.1
11	I	100	VAL	7.1
1	0	1951	G	6.8
1	0	2237	G	6.7
1	0	1198	U	6.7
11	I	108	HIS	6.6
11	I	109	PRO	6.5
11	I	76	ASP	6.5
11	I	82	THR	6.5
11	I	129	SER	6.4
6	D	170	TYR	6.4
11	I	133	THR	6.3
11	I	113	SER	6.1
11	I	99	GLN	6.1
1	0	1169	U	6.1
1	0	1181	A	6.0
11	I	79	GLY	5.9
1	0	1177	A	5.9
26	X	88	GLU	5.9
10	H	174	LEU	5.9
11	I	124	VAL	5.8
11	I	78	ALA	5.8
11	I	116	LEU	5.8
6	D	69	ILE	5.7
1	0	960	G	5.6
11	I	89	GLU	5.6
6	D	57	THR	5.5
11	I	83	GLY	5.4
1	0	1173	A	5.3
1	0	1192	A	5.3
11	I	102	GLN	5.3
1	0	1168	C	5.3
1	0	999	C	5.2
11	I	73	LEU	5.2
11	I	68	PRO	5.2
6	D	26	GLY	5.1
1	0	1202	A	5.0
3	A	237	GLY	5.0
11	I	118	ASN	5.0
24	V	38	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
11	I	94	ASP	5.0
11	I	112	LEU	5.0
11	I	98	ASP	5.0
9	G	27	ILE	4.9
6	D	61	PHE	4.9
11	I	130	LEU	4.8
1	0	1948	G	4.8
1	0	1950	G	4.7
2	9	2	U	4.7
11	I	67	VAL	4.7
6	D	66	GLY	4.6
1	0	1182	C	4.6
14	L	80	ASP	4.5
22	T	116	ASP	4.5
2	9	24	U	4.5
11	I	87	PRO	4.4
11	I	114	TYR	4.4
6	D	11	HIS	4.3
1	0	1200	A	4.3
1	0	1178	G	4.3
1	0	1176	C	4.3
6	D	90	LEU	4.3
6	D	64	ARG	4.3
9	G	23	ILE	4.2
11	I	120	ALA	4.2
1	0	735	C	4.2
1	0	2004	U	4.2
6	D	44	ILE	4.2
1	0	2344	G	4.2
11	I	121	LYS	4.1
11	I	69	PRO	4.1
1	0	2238	A	4.1
1	0	970	U	4.1
9	G	71	LEU	4.1
6	D	85	GLN	4.1
11	I	81	GLU	4.1
9	G	24	VAL	4.1
6	D	93	LEU	4.0
1	0	1163	G	4.0
1	0	1171	A	4.0
1	0	1525	G	4.0
24	V	43	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
11	I	95	LEU	4.0
1	0	2637	A	3.9
14	L	60	GLU	3.9
14	L	81	VAL	3.9
1	0	284	C	3.8
11	I	117	THR	3.8
27	Y	95	THR	3.8
1	0	1180	U	3.8
11	I	110	ASP	3.8
26	X	85	VAL	3.8
7	E	45	ASP	3.8
6	D	27	ILE	3.8
26	X	80	GLU	3.7
30	2	49	GLU	3.7
6	D	166	ILE	3.7
9	G	72	ASP	3.7
16	N	181	ASP	3.7
11	I	75	LYS	3.7
9	G	20	VAL	3.7
1	0	2508	C	3.7
9	G	26	MET	3.7
11	I	134	ILE	3.7
22	T	117	ASP	3.7
8	F	119	ARG	3.6
16	N	158	LEU	3.6
1	0	1179	C	3.6
6	D	88	LEU	3.6
21	S	81	ILE	3.6
1	0	282	C	3.6
1	0	1203	G	3.6
1	0	1170	U	3.6
7	E	127	ASP	3.5
6	D	68	PRO	3.5
1	0	497	A	3.5
1	0	1197	G	3.5
6	D	172	VAL	3.5
16	N	152	GLU	3.5
6	D	56	ARG	3.4
11	I	90	ASP	3.4
27	Y	235	GLU	3.4
1	0	1204	C	3.4
1	0	1949	G	3.4

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Mol	Chain	Res	Type	RSRZ
6	D	40	ILE	3.4
1	0	1167	G	3.4
10	H	169	GLU	3.4
11	I	119	ALA	3.4
26	X	7	GLU	3.4
9	G	69	ARG	3.4
7	E	10	ASP	3.3
24	V	41	GLU	3.3
7	E	100	ASP	3.3
11	I	85	GLY	3.3
16	N	183	ASP	3.3
1	0	1165	G	3.3
22	T	119	ALA	3.3
2	9	23	U	3.3
1	0	138	U	3.2
9	G	65	THR	3.2
4	B	1	PRO	3.2
1	0	1625	U	3.2
10	H	40	GLN	3.2
9	G	73	ASP	3.2
16	N	155	GLU	3.2
23	U	47	ARG	3.2
2	9	122	C	3.2
1	0	1279	U	3.2
1	0	10	U	3.2
1	0	2769	C	3.1
1	0	285	A	3.1
8	F	106	ALA	3.1
11	I	107	LYS	3.1
14	L	150	GLN	3.1
6	D	106	PHE	3.1
11	I	125	GLY	3.1
7	E	87	PHE	3.1
22	T	118	SER	3.1
6	D	62	ASP	3.1
6	D	58	VAL	3.1
1	0	272	A	3.1
14	L	148	GLU	3.0
27	Y	108	ASP	3.0
11	I	126	THR	3.0
1	0	1000	C	3.0
22	T	115	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
9	G	66	LEU	3.0
10	H	172	GLU	3.0
14	L	149	ARG	3.0
14	L	105	TYR	3.0
30	2	39	ARG	3.0
6	D	92	GLU	3.0
30	2	35	ARG	3.0
6	D	75	LEU	2.9
1	0	1947	G	2.9
1	0	1183	C	2.9
7	E	126	ILE	2.9
8	F	118	LEU	2.9
1	0	1964	U	2.9
1	0	1162	G	2.9
4	B	183	GLU	2.9
1	0	128	A	2.9
19	Q	95	GLU	2.9
11	I	96	SER	2.9
11	I	105	GLU	2.9
1	0	280	C	2.9
16	N	177	GLU	2.9
1	0	1190	G	2.8
11	I	135	GLU	2.8
16	N	185	GLU	2.8
11	I	115	ASP	2.8
3	A	236	GLY	2.8
1	0	969	G	2.8
4	B	57	GLU	2.8
6	D	86	THR	2.8
6	D	89	PRO	2.8
3	A	35	GLY	2.8
11	I	77	GLU	2.8
6	D	18	ILE	2.8
6	D	173	GLU	2.8
1	0	1196	C	2.8
6	D	165	PHE	2.8
5	C	135	GLU	2.7
31	3	92	GLU	2.7
16	N	162	ASP	2.7
6	D	104	PHE	2.7
16	N	150	TYR	2.7
7	E	6	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	A	133	ARG	2.7
3	A	85	SER	2.7
14	L	77	ALA	2.7
7	E	154	ILE	2.7
27	Y	236	VAL	2.7
6	D	157	LEU	2.7
14	L	147	GLU	2.7
1	0	1175	G	2.6
14	L	75	LEU	2.6
6	D	55	LYS	2.6
3	A	38	ILE	2.6
1	0	2239	C	2.6
1	0	283	U	2.6
27	Y	216	ARG	2.6
13	K	132	VAL	2.6
6	D	65	GLU	2.6
12	J	70	PHE	2.6
16	N	179	LEU	2.6
1	0	514	G	2.6
30	2	27	LEU	2.6
1	0	1174	A	2.6
1	0	1965	C	2.6
7	E	159	VAL	2.6
16	N	159	TYR	2.6
24	V	37	GLY	2.5
9	G	28	GLU	2.5
12	J	5	GLU	2.5
7	E	86	VAL	2.5
11	I	101	LYS	2.5
1	0	2664	A	2.5
6	D	23	VAL	2.5
24	V	63	GLU	2.5
9	G	21	ASP	2.5
6	D	154	LYS	2.5
28	Z	11	SER	2.5
8	F	90	GLU	2.5
1	0	1193	A	2.5
1	0	2345	A	2.5
1	0	1186	C	2.5
9	G	67	LEU	2.5
16	N	180	LEU	2.5
1	0	1967	U	2.5

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Mol	Chain	Res	Type	RSRZ
1	0	362	G	2.5
3	A	36	ASP	2.5
7	E	88	TYR	2.4
11	I	123	VAL	2.4
26	X	71	ARG	2.4
6	D	43	GLU	2.4
8	F	103	GLU	2.4
10	H	165	ARG	2.4
1	0	372	A	2.4
5	C	132	ASP	2.4
16	N	154	LEU	2.4
3	A	97	ALA	2.4
16	N	182	GLY	2.4
6	D	171	ASP	2.4
1	0	1164	U	2.4
6	D	107	GLY	2.4
10	H	86	TYR	2.4
1	0	1201	C	2.4
1	0	1195	G	2.4
21	S	20	PHE	2.4
10	H	144	GLU	2.4
9	G	70	ALA	2.4
1	0	1191	A	2.4
8	F	107	ASP	2.4
8	F	25	ASP	2.4
8	F	22	VAL	2.4
9	G	15	TRP	2.4
10	H	170	ARG	2.3
16	N	68	GLU	2.3
6	D	45	THR	2.3
12	J	4	ALA	2.3
14	L	82	ALA	2.3
14	L	101	ASP	2.3
1	0	1184	C	2.3
6	D	98	PHE	2.3
6	D	70	GLY	2.3
9	G	18	GLU	2.3
7	E	108	LEU	2.3
7	E	131	LEU	2.3
26	X	41	PHE	2.3
6	D	15	GLU	2.3
6	D	25	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	0	370	G	2.2
7	E	89	SER	2.2
14	L	91	VAL	2.2
4	B	104	GLU	2.2
9	G	68	GLU	2.2
14	L	99	GLU	2.2
10	H	85	ASP	2.2
8	F	100	ASP	2.2
16	N	164	ASP	2.2
7	E	1	PRO	2.2
7	E	53	GLU	2.2
7	E	129	GLU	2.2
4	B	180	ASP	2.2
7	E	121	ASP	2.2
16	N	138	ASP	2.2
10	H	76	LEU	2.2
28	Z	80	ARG	2.2
6	D	135	VAL	2.2
1	0	2914	A	2.2
8	F	75	ILE	2.2
9	G	22	ALA	2.2
6	D	74	THR	2.1
8	F	44	SER	2.1
16	N	149	GLU	2.1
21	S	76	GLU	2.1
9	G	12	ILE	2.1
16	N	184	ILE	2.1
6	D	128	LEU	2.1
9	G	25	GLU	2.1
25	W	86	GLU	2.1
1	0	1526	A	2.1
14	L	139	SER	2.1
16	N	160	SER	2.1
26	X	77	PHE	2.1
1	0	736	A	2.1
1	0	1527	A	2.1
6	D	67	ASP	2.1
14	L	145	LEU	2.1
1	0	1966	U	2.1
3	A	82	VAL	2.1
14	L	106	VAL	2.1
1	0	87	C	2.1

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Mol	Chain	Res	Type	RSRZ
1	0	2909	G	2.1
6	D	41	LEU	2.1
14	L	89	PHE	2.1
9	G	64	ASN	2.1
1	0	1166	A	2.1
1	0	2511	A	2.1
14	L	102	ASP	2.1
1	0	1929	G	2.0
30	2	44	ARG	2.0
11	I	122	GLU	2.0
16	N	157	PRO	2.0
8	F	115	VAL	2.0
26	X	10	VAL	2.0
1	0	716	G	2.0
1	0	2507	G	2.0
16	N	147	ILE	2.0
17	O	23	GLY	2.0
1	0	371	U	2.0

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

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	UR3	0	2619	21/22	0.12	0.90	29,33,35,41	0
1	1MA	0	628	23/24	0.13	0.33	22,24,25,28	0
1	OMU	0	2587	21/22	0.10	-0.96	26,28,29,32	0
1	PSU	0	2621	20/21	0.12	-1.23	22,25,33,33	0
1	OMG	0	2588	24/25	0.11	-1.26	23,27,29,30	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
37	SR	0	9006	1/1	0.87	168.33	200,200,200,200	0
37	SR	0	8996	1/1	0.54	127.59	185,185,185,185	0
35	NA	0	8549	1/1	0.52	87.66	74,74,74,74	0
37	SR	0	8997	1/1	0.43	70.79	171,171,171,171	0
37	SR	0	8955	1/1	0.33	59.40	169,169,169,169	0
35	NA	0	8555	1/1	0.38	50.73	43,43,43,43	0
35	NA	0	8561	1/1	0.47	32.75	62,62,62,62	0
35	NA	0	8542	1/1	0.32	31.97	51,51,51,51	0
37	SR	0	9007	1/1	0.24	28.93	154,154,154,154	0
33	MG	0	8073	1/1	0.15	24.27	76,76,76,76	0
37	SR	0	8976	1/1	0.23	22.54	159,159,159,159	0
35	NA	0	8565	1/1	0.25	22.33	46,46,46,46	0
35	NA	0	8552	1/1	0.29	19.82	48,48,48,48	0
37	SR	0	8957	1/1	0.32	19.09	176,176,176,176	0
35	NA	9	8572	1/1	0.36	18.56	59,59,59,59	0
35	NA	0	8564	1/1	0.39	16.91	55,55,55,55	0
37	SR	0	8994	1/1	0.31	16.62	168,168,168,168	0
35	NA	0	8556	1/1	0.47	16.31	37,37,37,37	0
35	NA	0	8525	1/1	0.18	16.22	65,65,65,65	0
33	MG	0	8089	1/1	0.24	15.98	37,37,37,37	0
33	MG	0	8037	1/1	0.20	15.91	77,77,77,77	0
33	MG	0	8071	1/1	0.27	15.79	54,54,54,54	0
35	NA	0	8551	1/1	0.25	15.57	39,39,39,39	0
33	MG	0	8030	1/1	0.19	15.52	48,48,48,48	0
35	NA	0	8528	1/1	0.21	13.12	32,32,32,32	0
35	NA	0	8554	1/1	0.24	13.04	52,52,52,52	0
37	SR	B	8987	1/1	0.43	12.92	189,189,189,189	0
35	NA	0	8574	1/1	0.35	12.73	48,48,48,48	0
35	NA	0	8516	1/1	0.16	12.72	44,44,44,44	0
35	NA	0	8506	1/1	0.23	12.58	50,50,50,50	0
36	CL	0	8822	1/1	0.16	12.25	48,48,48,48	0
35	NA	0	8521	1/1	0.25	11.23	55,55,55,55	0
35	NA	0	8550	1/1	0.21	10.44	41,41,41,41	0
35	NA	0	8517	1/1	0.15	10.20	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8563	1/1	0.27	9.73	56,56,56,56	0
35	NA	0	8567	1/1	0.21	9.53	53,53,53,53	0
37	SR	0	8979	1/1	0.31	9.40	184,184,184,184	0
37	SR	0	8974	1/1	0.24	9.19	159,159,159,159	0
37	SR	0	8969	1/1	0.22	9.00	115,115,115,115	0
35	NA	0	8522	1/1	0.23	8.80	46,46,46,46	0
35	NA	0	8560	1/1	0.37	8.63	54,54,54,54	0
35	NA	0	8524	1/1	0.19	8.61	31,31,31,31	0
37	SR	0	8982	1/1	0.18	8.45	152,152,152,152	0
35	NA	0	8509	1/1	0.14	8.26	47,47,47,47	0
33	MG	0	8063	1/1	0.15	8.11	71,71,71,71	0
33	MG	0	8081	1/1	0.17	7.26	55,55,55,55	0
37	SR	0	8986	1/1	0.73	7.11	169,169,169,169	0
37	SR	0	8903	1/1	0.16	7.01	41,41,41,41	0
35	NA	0	8568	1/1	0.24	6.98	42,42,42,42	0
35	NA	0	8553	1/1	0.18	6.76	48,48,48,48	0
35	NA	0	8514	1/1	0.18	6.43	41,41,41,41	0
37	SR	0	8992	1/1	0.22	6.07	111,111,111,111	0
35	NA	0	8562	1/1	0.17	5.99	59,59,59,59	0
37	SR	0	9000	1/1	0.17	5.69	150,150,150,150	0
35	NA	0	8547	1/1	0.19	5.07	42,42,42,42	0
37	SR	0	8905	1/1	0.20	5.00	48,48,48,48	0
35	NA	0	8571	1/1	0.19	4.99	79,79,79,79	0
33	MG	0	8068	1/1	0.13	4.28	48,48,48,48	0
35	NA	0	8508	1/1	0.16	4.08	40,40,40,40	0
37	SR	0	9001	1/1	0.16	4.05	160,160,160,160	0
35	NA	0	8505	1/1	0.15	3.86	33,33,33,33	0
37	SR	0	8919	1/1	0.14	3.81	169,169,169,169	0
37	SR	0	8962	1/1	0.13	3.71	139,139,139,139	0
35	NA	R	8575	1/1	0.20	3.14	73,73,73,73	0
33	MG	0	8085	1/1	0.13	3.00	90,90,90,90	0
37	SR	A	8929	1/1	0.21	2.83	123,123,123,123	0
37	SR	0	8989	1/1	0.16	2.81	148,148,148,148	0
37	SR	0	9002	1/1	0.17	2.76	162,162,162,162	0
35	NA	0	8536	1/1	0.12	2.50	46,46,46,46	0
37	SR	0	9004	1/1	0.22	2.33	176,176,176,176	0
37	SR	0	8983	1/1	0.15	1.85	149,149,149,149	0
35	NA	0	8501	1/1	0.13	1.60	26,26,26,26	0
33	MG	0	8090	1/1	0.12	1.49	49,49,49,49	0
35	NA	0	8544	1/1	0.13	1.38	49,49,49,49	0
35	NA	0	8559	1/1	0.12	1.38	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CL	M	8818	1/1	0.19	1.32	36,36,36,36	0
33	MG	0	8056	1/1	0.14	1.23	49,49,49,49	0
37	SR	0	8991	1/1	0.13	1.17	167,167,167,167	0
35	NA	0	8557	1/1	0.15	1.15	54,54,54,54	0
37	SR	0	8998	1/1	0.13	1.11	133,133,133,133	0
37	SR	0	8922	1/1	0.12	0.99	161,161,161,161	0
35	NA	0	8569	1/1	0.13	0.97	61,61,61,61	0
33	MG	0	8082	1/1	0.17	0.72	44,44,44,44	0
33	MG	0	8017	1/1	0.15	0.69	26,26,26,26	0
33	MG	0	8069	1/1	0.17	0.68	58,58,58,58	0
35	NA	0	8523	1/1	0.12	0.57	31,31,31,31	0
35	NA	M	8539	1/1	0.15	0.56	28,28,28,28	0
35	NA	0	8546	1/1	0.20	0.54	63,63,63,63	0
35	NA	S	8510	1/1	0.16	0.47	24,24,24,24	0
33	MG	0	8018	1/1	0.12	0.39	38,38,38,38	0
35	NA	H	8518	1/1	0.18	0.39	66,66,66,66	0
33	MG	0	8047	1/1	0.12	0.27	46,46,46,46	0
33	MG	0	8008	1/1	0.13	0.26	26,26,26,26	0
35	NA	0	8530	1/1	0.13	0.15	37,37,37,37	0
37	SR	9	8980	1/1	0.13	0.15	162,162,162,162	0
33	MG	0	8038	1/1	0.13	0.00	65,65,65,65	0
32	ZIT	0	9500	52/52	0.13	-0.07	28,38,42,44	0
37	SR	0	8959	1/1	0.13	-0.14	132,132,132,132	0
36	CL	A	8809	1/1	0.16	-0.15	52,52,52,52	0
33	MG	0	8049	1/1	0.11	-0.19	64,64,64,64	0
36	CL	R	8806	1/1	0.11	-0.27	40,40,40,40	0
35	NA	0	8515	1/1	0.13	-0.30	30,30,30,30	0
35	NA	0	8535	1/1	0.15	-0.36	40,40,40,40	0
37	SR	0	8985	1/1	0.11	-0.36	104,104,104,104	0
33	MG	A	8051	1/1	0.14	-0.36	55,55,55,55	0
37	SR	0	8944	1/1	0.11	-0.40	146,146,146,146	0
33	MG	0	8022	1/1	0.13	-0.43	30,30,30,30	0
35	NA	0	8566	1/1	0.14	-0.51	44,44,44,44	0
37	SR	H	8972	1/1	0.12	-0.52	112,112,112,112	0
35	NA	0	8527	1/1	0.11	-0.52	31,31,31,31	0
37	SR	0	8933	1/1	0.10	-0.59	108,108,108,108	0
35	NA	0	8573	1/1	0.10	-0.65	55,55,55,55	0
37	SR	0	8993	1/1	0.10	-0.67	143,143,143,143	0
33	MG	0	8020	1/1	0.10	-0.73	37,37,37,37	0
37	SR	R	8912	1/1	0.11	-0.81	77,77,77,77	0
36	CL	Y	8820	1/1	0.10	-0.82	35,35,35,35	0
35	NA	0	8520	1/1	0.08	-0.86	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CL	0	8803	1/1	0.12	-0.90	41,41,41,41	0
33	MG	0	8031	1/1	0.11	-0.90	41,41,41,41	0
33	MG	0	8080	1/1	0.09	-0.95	53,53,53,53	0
34	K	0	8401	1/1	0.10	-0.96	58,58,58,58	0
37	SR	0	8947	1/1	0.09	-1.00	148,148,148,148	0
35	NA	0	8502	1/1	0.11	-1.02	43,43,43,43	0
33	MG	0	8032	1/1	0.10	-1.02	36,36,36,36	0
38	CD	U	8701	1/1	0.09	-1.03	55,55,55,55	0
37	SR	0	8975	1/1	0.10	-1.04	99,99,99,99	0
35	NA	C	8503	1/1	0.09	-1.06	29,29,29,29	0
33	MG	0	8061	1/1	0.11	-1.07	23,23,23,23	0
35	NA	0	8513	1/1	0.11	-1.10	33,33,33,33	0
35	NA	9	8543	1/1	0.19	-1.16	41,41,41,41	0
37	SR	0	8927	1/1	0.11	-1.19	133,133,133,133	0
37	SR	0	8954	1/1	0.11	-1.22	88,88,88,88	0
35	NA	0	8541	1/1	0.12	-1.23	41,41,41,41	0
33	MG	0	8009	1/1	0.12	-1.25	26,26,26,26	0
36	CL	0	8813	1/1	0.10	-1.27	45,45,45,45	0
36	CL	0	8811	1/1	0.08	-1.29	45,45,45,45	0
33	MG	0	8084	1/1	0.04	-1.34	36,36,36,36	0
36	CL	J	8821	1/1	0.10	-1.34	52,52,52,52	0
36	CL	0	8812	1/1	0.09	-1.38	39,39,39,39	0
33	MG	0	8011	1/1	0.09	-1.39	24,24,24,24	0
37	SR	0	8907	1/1	0.09	-1.39	33,33,33,33	0
37	SR	A	8977	1/1	0.08	-1.39	143,143,143,143	0
33	MG	0	8053	1/1	0.09	-1.41	58,58,58,58	0
33	MG	0	8041	1/1	0.10	-1.42	18,18,18,18	0
36	CL	O	8808	1/1	0.08	-1.43	54,54,54,54	0
37	SR	0	8981	1/1	0.10	-1.43	141,141,141,141	0
35	NA	J	8538	1/1	0.08	-1.44	48,48,48,48	0
33	MG	0	8036	1/1	0.08	-1.61	36,36,36,36	0
33	MG	0	8005	1/1	0.12	-1.64	23,23,23,23	0
33	MG	0	8058	1/1	0.08	-1.65	26,26,26,26	0
37	SR	A	8930	1/1	0.06	-1.67	82,82,82,82	0
33	MG	0	8092	1/1	0.09	-1.69	47,47,47,47	0
33	MG	A	8050	1/1	0.11	-1.70	33,33,33,33	0
35	NA	Q	8540	1/1	0.10	-1.70	39,39,39,39	0
36	CL	0	8814	1/1	0.08	-1.75	40,40,40,40	0
37	SR	0	8964	1/1	0.08	-1.76	109,109,109,109	0
36	CL	0	8816	1/1	0.09	-1.77	53,53,53,53	0
37	SR	0	8934	1/1	0.10	-1.78	116,116,116,116	0
38	CD	Z	8703	1/1	0.07	-1.89	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8512	1/1	0.09	-1.91	36,36,36,36	0
33	MG	0	8035	1/1	0.06	-1.92	52,52,52,52	0
38	CD	3	8704	1/1	0.07	-1.93	53,53,53,53	0
35	NA	0	8526	1/1	0.08	-1.94	36,36,36,36	0
35	NA	0	8529	1/1	0.07	-1.98	32,32,32,32	0
33	MG	0	8028	1/1	0.09	-1.98	19,19,19,19	0
37	SR	0	8939	1/1	0.07	-2.00	108,108,108,108	0
37	SR	0	8918	1/1	0.11	-2.06	66,66,66,66	0
35	NA	0	8533	1/1	0.08	-2.09	50,50,50,50	0
35	NA	0	8534	1/1	0.10	-2.10	29,29,29,29	0
36	CL	J	8802	1/1	0.06	-2.15	51,51,51,51	0
33	MG	T	8057	1/1	0.07	-2.17	51,51,51,51	0
35	NA	R	8532	1/1	0.07	-2.22	37,37,37,37	0
37	SR	0	8911	1/1	0.06	-2.25	65,65,65,65	0
37	SR	0	8917	1/1	0.08	-2.26	90,90,90,90	0
33	MG	0	8040	1/1	0.10	-2.34	78,78,78,78	0
37	SR	0	8940	1/1	0.04	-2.36	66,66,66,66	0
38	CD	O	8705	1/1	0.05	-2.38	58,58,58,58	0
35	NA	0	8504	1/1	0.09	-2.46	26,26,26,26	0
36	CL	J	8801	1/1	0.06	-2.49	49,49,49,49	0
35	NA	0	8548	1/1	0.09	-2.50	50,50,50,50	0
37	SR	0	8984	1/1	0.08	-2.54	98,98,98,98	0
33	MG	0	8043	1/1	0.11	-2.55	46,46,46,46	0
33	MG	0	8055	1/1	0.09	-2.57	29,29,29,29	0
33	MG	0	8062	1/1	0.08	-2.61	46,46,46,46	0
36	CL	B	8819	1/1	0.06	-2.63	46,46,46,46	0
33	MG	0	8045	1/1	0.09	-2.64	29,29,29,29	0
33	MG	0	8024	1/1	0.09	-2.66	53,53,53,53	0
36	CL	0	8805	1/1	0.07	-2.71	45,45,45,45	0
33	MG	0	8034	1/1	0.10	-2.74	35,35,35,35	0
37	SR	0	8999	1/1	0.04	-2.76	78,78,78,78	0
37	SR	F	9005	1/1	0.06	-2.81	106,106,106,106	0
37	SR	0	8943	1/1	0.08	-2.81	108,108,108,108	0
37	SR	0	8960	1/1	0.09	-2.82	128,128,128,128	0
37	SR	0	8973	1/1	0.07	-2.82	113,113,113,113	0
37	SR	0	8990	1/1	0.10	-2.83	106,106,106,106	0
34	K	0	8402	1/1	0.08	-2.90	46,46,46,46	0
37	SR	0	8908	1/1	0.07	-2.95	71,71,71,71	0
33	MG	0	8070	1/1	0.08	-2.98	36,36,36,36	0
33	MG	0	8003	1/1	0.10	-3.02	23,23,23,23	0
37	SR	0	8925	1/1	0.08	-3.05	75,75,75,75	0
37	SR	S	8961	1/1	0.09	-3.08	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	B	8042	1/1	0.07	-3.09	52,52,52,52	0
35	NA	0	8537	1/1	0.09	-3.10	32,32,32,32	0
37	SR	0	8923	1/1	0.07	-3.12	78,78,78,78	0
33	MG	0	8039	1/1	0.11	-3.16	60,60,60,60	0
37	SR	0	8970	1/1	0.08	-3.18	109,109,109,109	0
37	SR	0	8937	1/1	0.07	-3.19	94,94,94,94	0
35	NA	0	8519	1/1	0.11	-3.21	36,36,36,36	0
37	SR	0	8953	1/1	0.06	-3.26	121,121,121,121	0
37	SR	0	8936	1/1	0.08	-3.26	67,67,67,67	0
37	SR	0	8904	1/1	0.06	-3.27	34,34,34,34	0
33	MG	0	8077	1/1	0.06	-3.29	26,26,26,26	0
37	SR	0	8942	1/1	0.06	-3.34	110,110,110,110	0
37	SR	0	8924	1/1	0.12	-3.34	123,123,123,123	0
36	CL	0	8817	1/1	0.09	-3.42	46,46,46,46	0
33	MG	0	8014	1/1	0.08	-3.42	25,25,25,25	0
33	MG	0	8001	1/1	0.08	-3.49	25,25,25,25	0
33	MG	0	8066	1/1	0.09	-3.50	47,47,47,47	0
37	SR	9	9003	1/1	0.07	-3.56	141,141,141,141	0
36	CL	0	8815	1/1	0.08	-3.58	47,47,47,47	0
33	MG	0	8010	1/1	0.08	-3.58	29,29,29,29	0
33	MG	0	8065	1/1	0.06	-3.63	45,45,45,45	0
33	MG	0	8044	1/1	0.10	-3.66	40,40,40,40	0
33	MG	0	8052	1/1	0.07	-3.67	23,23,23,23	0
37	SR	3	8932	1/1	0.06	-3.69	58,58,58,58	0
37	SR	0	8956	1/1	0.07	-3.70	127,127,127,127	0
35	NA	0	8507	1/1	0.08	-3.83	27,27,27,27	0
33	MG	0	8083	1/1	0.05	-3.90	41,41,41,41	0
36	CL	L	8810	1/1	0.07	-3.92	43,43,43,43	0
38	CD	1	8702	1/1	0.04	-3.94	44,44,44,44	0
33	MG	K	8054	1/1	0.07	-3.96	34,34,34,34	0
33	MG	0	8048	1/1	0.08	-4.06	33,33,33,33	0
33	MG	0	8079	1/1	0.07	-4.08	40,40,40,40	0
33	MG	0	8075	1/1	0.06	-4.17	31,31,31,31	0
33	MG	9	8074	1/1	0.09	-4.20	64,64,64,64	0
37	SR	0	8968	1/1	0.07	-4.41	142,142,142,142	0
33	MG	0	8025	1/1	0.06	-4.49	24,24,24,24	0
33	MG	0	8012	1/1	0.05	-4.51	13,13,13,13	0
37	SR	0	8958	1/1	0.07	-4.55	83,83,83,83	0
37	SR	1	8913	1/1	0.06	-4.56	70,70,70,70	0
37	SR	0	8971	1/1	0.09	-4.60	158,158,158,158	0
36	CL	N	8807	1/1	0.09	-4.70	46,46,46,46	0
33	MG	0	8015	1/1	0.08	-4.78	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	B	8950	1/1	0.05	-5.01	90,90,90,90	0
35	NA	0	8511	1/1	0.09	-5.07	59,59,59,59	0
37	SR	0	8941	1/1	0.05	-5.12	90,90,90,90	0
37	SR	0	8915	1/1	0.05	-5.22	85,85,85,85	0
33	MG	0	8029	1/1	0.07	-5.27	40,40,40,40	0
37	SR	0	8935	1/1	0.11	-5.44	60,60,60,60	0
33	MG	0	8016	1/1	0.06	-5.51	35,35,35,35	0
37	SR	0	8914	1/1	0.08	-5.53	88,88,88,88	0
33	MG	0	8078	1/1	0.07	-5.57	40,40,40,40	0
33	MG	Y	8086	1/1	0.08	-5.79	35,35,35,35	0
33	MG	0	8007	1/1	0.08	-5.80	24,24,24,24	0
37	SR	0	8909	1/1	0.07	-5.82	70,70,70,70	0
37	SR	0	8967	1/1	0.03	-5.83	116,116,116,116	0
37	SR	0	8995	1/1	0.07	-5.89	112,112,112,112	0
33	MG	0	8093	1/1	0.07	-5.94	29,29,29,29	0
37	SR	0	8920	1/1	0.06	-5.94	96,96,96,96	0
33	MG	0	8046	1/1	0.08	-6.05	25,25,25,25	0
33	MG	0	8019	1/1	0.07	-6.09	22,22,22,22	0
33	MG	0	8023	1/1	0.06	-6.20	24,24,24,24	0
33	MG	0	8002	1/1	0.07	-6.20	27,27,27,27	0
37	SR	0	8926	1/1	0.05	-6.45	95,95,95,95	0
35	NA	0	8558	1/1	0.06	-6.55	46,46,46,46	0
33	MG	0	8033	1/1	0.06	-6.55	32,32,32,32	0
35	NA	0	8570	1/1	0.07	-6.61	35,35,35,35	0
37	SR	0	8916	1/1	0.05	-6.87	95,95,95,95	0
33	MG	0	8088	1/1	0.04	-6.96	29,29,29,29	0
33	MG	0	8006	1/1	0.06	-6.99	30,30,30,30	0
33	MG	0	8076	1/1	0.07	-7.32	28,28,28,28	0
37	SR	0	8938	1/1	0.05	-7.35	147,147,147,147	0
33	MG	0	8027	1/1	0.04	-7.36	32,32,32,32	0
37	SR	0	9008	1/1	0.06	-7.44	83,83,83,83	0
33	MG	0	8004	1/1	0.04	-7.48	22,22,22,22	0
33	MG	0	8026	1/1	0.05	-7.50	28,28,28,28	0
33	MG	0	8013	1/1	0.04	-7.62	24,24,24,24	0
37	SR	1	8952	1/1	0.05	-7.67	62,62,62,62	0
37	SR	0	8951	1/1	0.05	-7.70	137,137,137,137	0
33	MG	0	8021	1/1	0.08	-7.82	28,28,28,28	0
37	SR	0	8921	1/1	0.07	-7.91	66,66,66,66	0
36	CL	3	8804	1/1	0.04	-8.09	47,47,47,47	0
37	SR	0	8948	1/1	0.06	-8.19	69,69,69,69	0
37	SR	0	8946	1/1	0.07	-8.26	87,87,87,87	0
33	MG	0	8059	1/1	0.04	-8.45	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	8928	1/1	0.09	-8.56	112,112,112,112	0
37	SR	0	8901	1/1	0.04	-8.77	71,71,71,71	0
37	SR	0	8906	1/1	0.09	-8.81	40,40,40,40	0
37	SR	0	8978	1/1	0.04	-8.85	82,82,82,82	0
35	NA	0	8545	1/1	0.07	-8.92	29,29,29,29	0
33	MG	0	8067	1/1	0.05	-9.05	29,29,29,29	0
37	SR	0	8910	1/1	0.04	-9.18	80,80,80,80	0
37	SR	0	8945	1/1	0.04	-9.18	92,92,92,92	0
33	MG	0	8087	1/1	0.05	-9.35	26,26,26,26	0
37	SR	0	8966	1/1	0.03	-9.58	89,89,89,89	0
37	SR	0	8949	1/1	0.04	-9.67	93,93,93,93	0
33	MG	0	8060	1/1	0.06	-9.97	45,45,45,45	0
33	MG	0	8064	1/1	0.03	-10.03	34,34,34,34	0
37	SR	0	8931	1/1	0.04	-10.78	86,86,86,86	0
37	SR	0	8988	1/1	0.06	-12.50	149,149,149,149	0
33	MG	0	8072	1/1	0.06	-15.67	37,37,37,37	0
35	NA	0	8531	1/1	0.05	-23.85	29,29,29,29	0
37	SR	0	8902	1/1	0.04	-26.60	49,49,49,49	0
33	MG	0	8091	1/1	0.09	-28.00	42,42,42,42	0
37	SR	0	8965	1/1	0.05	-40.41	109,109,109,109	0
37	SR	0	8963	1/1	0.05	-93.00	103,103,103,103	0

6.5 Other polymers ⓘ

There are no such residues in this entry.