



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:55 PM GMT

PDB ID : 1YIT
Title : Crystal Structure Of Virginiamycin M and S Bound To The 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-13
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

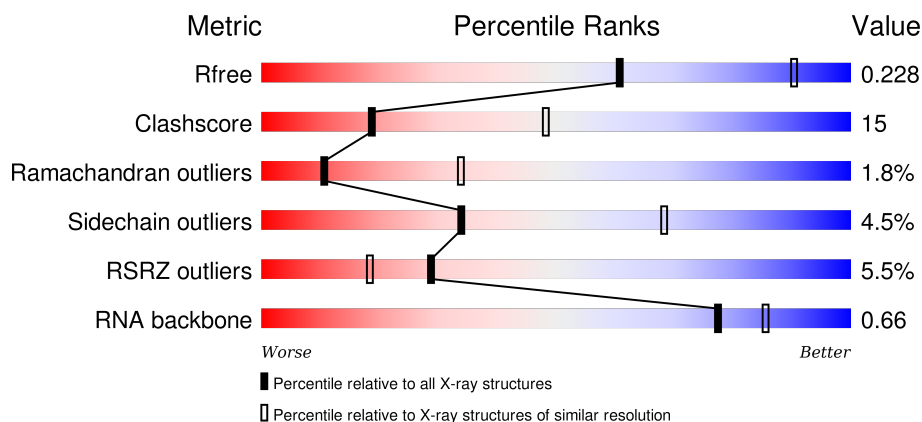
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>59%</div> <div>30%</div> <div>5%</div> <div>6%</div> </div>
2	1	57	<div> <div>67%</div> <div>32%</div> <div>.</div> </div>
3	2	50	<div> <div>16%</div> <div>44%</div> <div>48%</div> <div>8%</div> </div>
4	3	92	<div> <div>12%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
5	8	7	
6	9	122	
7	A	240	
8	B	338	
9	C	246	
10	D	177	
11	E	178	
12	F	120	
13	G	348	
14	H	177	
15	I	162	
16	J	145	
17	K	132	
18	L	165	
19	M	195	
20	N	187	
21	O	116	
22	P	149	
23	Q	96	
24	R	155	
25	S	85	
26	T	120	
27	U	66	
28	V	71	
29	W	154	

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Mol	Chain	Length	Quality of chain
30	X	92	
31	Y	241	
32	Z	83	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8002	-	-	-	X
33	MG	0	8003	-	-	-	X
33	MG	0	8004	-	-	-	X
33	MG	0	8006	-	-	-	X
33	MG	0	8008	-	-	-	X
33	MG	0	8010	-	-	-	X
33	MG	0	8012	-	-	-	X
33	MG	0	8013	-	-	-	X
33	MG	0	8015	-	-	-	X
33	MG	0	8017	-	-	-	X
33	MG	0	8018	-	-	-	X
33	MG	0	8019	-	-	-	X
33	MG	0	8020	-	-	-	X
33	MG	0	8032	-	-	-	X
33	MG	0	8035	-	-	-	X
33	MG	0	8038	-	-	-	X
33	MG	0	8044	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8049	-	-	-	X
33	MG	0	8052	-	-	-	X
33	MG	0	8053	-	-	-	X
33	MG	0	8054	-	-	-	X
33	MG	0	8058	-	-	-	X
33	MG	0	8060	-	-	-	X
33	MG	0	8071	-	-	-	X
33	MG	0	8072	-	-	-	X
33	MG	0	8077	-	-	-	X
33	MG	0	8080	-	-	-	X
33	MG	0	8084	-	-	-	X
33	MG	0	8091	-	-	-	X
33	MG	0	8096	-	-	-	X
33	MG	0	8109	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8111	-	-	-	X
33	MG	0	8117	-	-	-	X
33	MG	A	8065	-	-	-	X
33	MG	B	8055	-	-	-	X
33	MG	B	8056	-	-	-	X
33	MG	K	8069	-	-	-	X
33	MG	Y	8108	-	-	-	X
34	K	0	8402	-	-	-	X
35	NA	0	8502	-	-	-	X
35	NA	0	8503	-	-	-	X
35	NA	0	8505	-	-	-	X
35	NA	0	8510	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8523	-	-	-	X
35	NA	0	8525	-	-	-	X
35	NA	0	8526	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8531	-	-	-	X
35	NA	0	8532	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8566	-	-	-	X
35	NA	0	8570	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	0	8572	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	0	8575	-	-	-	X
35	NA	0	8576	-	-	-	X
35	NA	0	8577	-	-	-	X
35	NA	9	8582	-	-	-	X
35	NA	A	8545	-	-	-	X
35	NA	L	8579	-	-	-	X
35	NA	M	8547	-	-	-	X
35	NA	R	8585	-	-	-	X
36	CL	0	8815	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	VIR	0	9000	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 91326 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	MODIFIED RESIDUE	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 protein called 50S RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 5 is a protein called VIRGINIAMYCIN S1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	8	7	Total	C	N	O	0	0	0
			60	43	7	10			

- Molecule 6 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L2P.

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

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L3P.

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

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L4E.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L5P.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L6P.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L7AE.

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

- Molecule 13 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L13P.

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

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	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 18 is a protein called 50S RIBOSOMAL PROTEIN L15P.

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

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	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 20 is a protein called 50S RIBOSOMAL PROTEIN L18P.

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

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L18E.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L19E.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L21E.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L22P.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L23P.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24P.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L24E.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29P.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30P.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31E.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32E.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	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 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	109	Total	Mg	0	0
			109	109		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	A	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	3	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	1	Total	K	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	73	Total Na 73 73	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	A	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	L	1	Total Na 1 1	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).

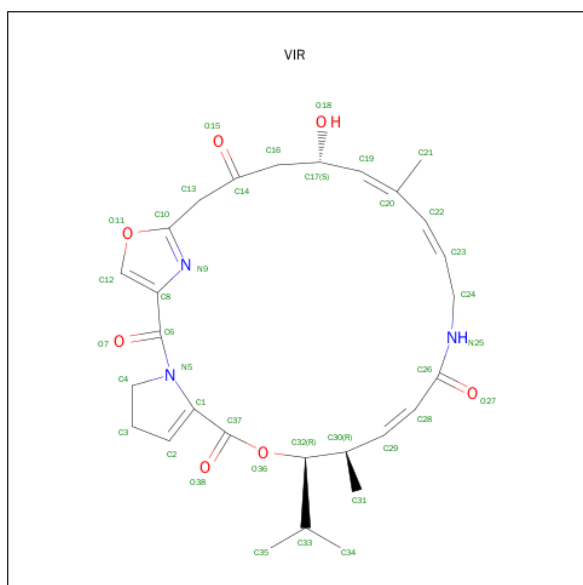
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0

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

- Molecule 37 is VIRGINIAMYCIN M1 (three-letter code: VIR) (formula: $C_{28}H_{35}N_3O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	1	Total C N O 38 28 3 7	0	0

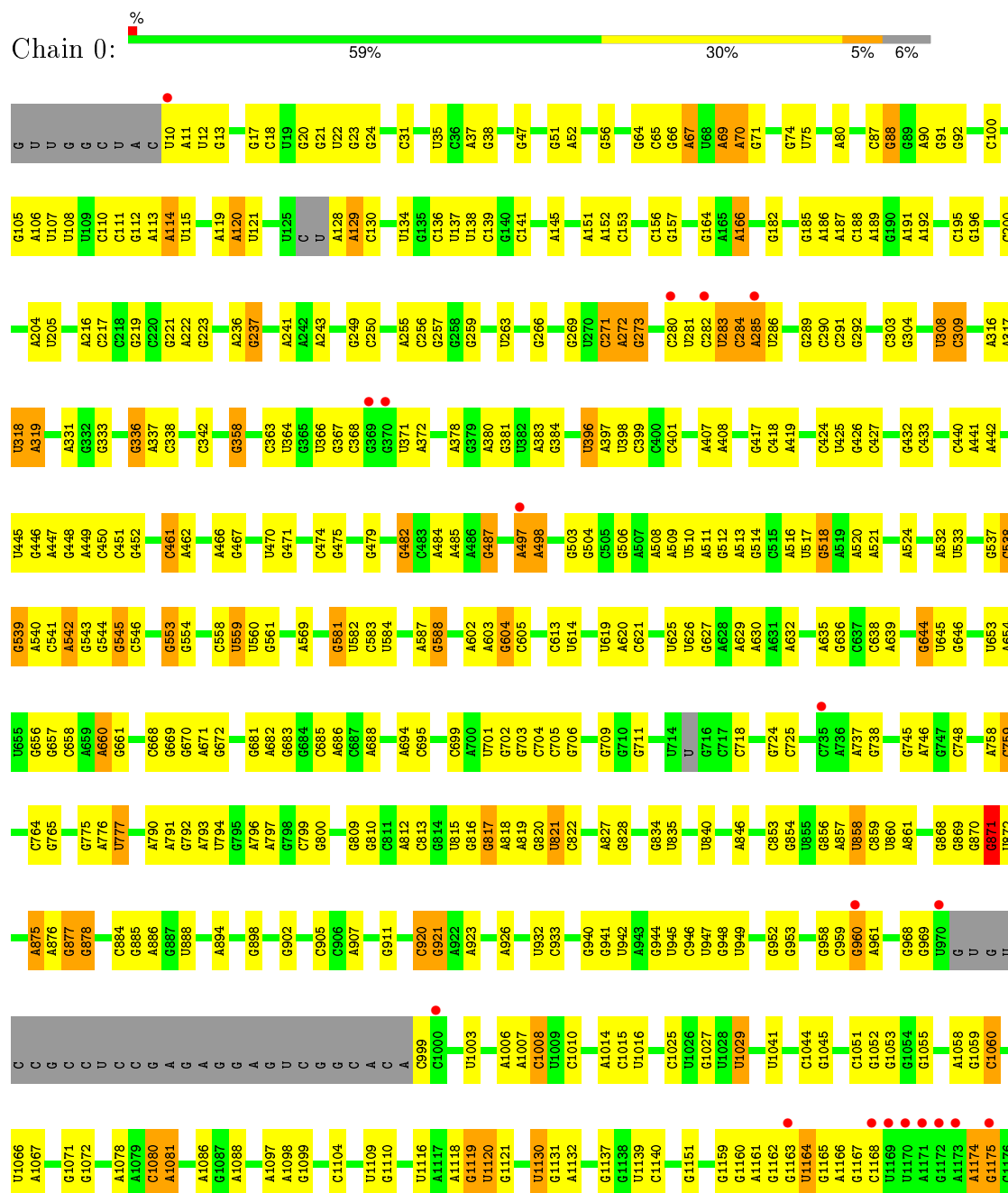
- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

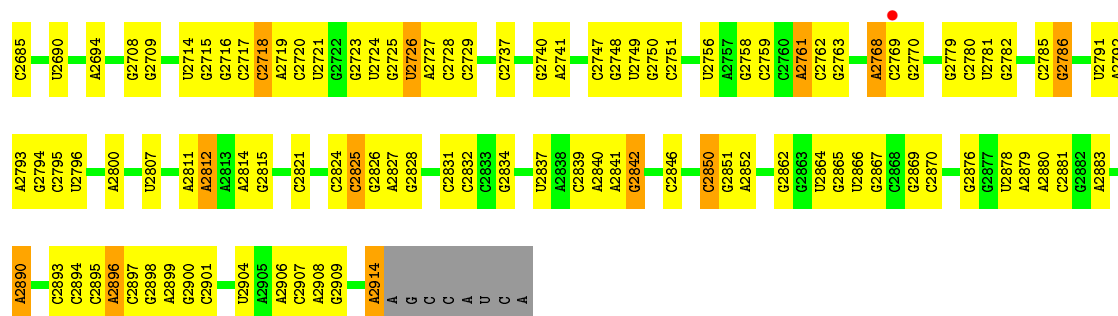
3 Residue-property plots

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

• Molecule 1: 23S RIBOSOMAL RNA

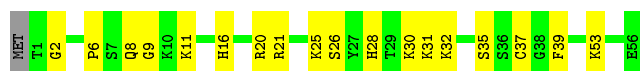


C2594	G2270	G2211	G2270	A1919	A1821	G1723	A1807	U1503	G1376	C1268	A1177
U2595	G2271	U2012	A2011	C1920	A1822	U1724	C1617	A1504	C1377	G1269	U1180
A2596	G2272	G2013	G2013	A1921	U1825	C1725	U1625	U1505	U1380	C1273	A1181
U2597	U2276	U2028	U2028	G1925	C1826	G1730	A1626	U1506	G1384	A1278	C1182
A2598	U2277	C2029	C2029	G1926	A1829	U1731	U1631	U1514	C1385	U1279	C1183
U2599	C2281	A2030	A2030	A1927	C1830	A1732	A1630	C1515	U1285	U1186	C1184
A2600	U2282	G2031	G2031	C1928	C1831	U1733	A1631	U1516	U1286	U1187	U1186
G2601	G2281	G2032	G2032	G1929	C1834	C1735	A1632	U1524	A1287	U1188	U1188
A2602	U2282	U2033	U2033	A1930	U1835	C1736	C1633	G1525	C1392	U1288	U1189
G2603	A2291	G2034	G2034	A1931	C1836	U1741	U1634	A1526	A1393	U1289	U1190
U2604	A2300	C2035	C2035	G1932	A1839	A1742	U1635	A1527	C1394	G1290	A1191
A2605	A2301	G2036	G2036	G1933	A1840	A1743	G1636	A1528	G1398	U1291	U1192
G2606	A2302	U2037	U2037	A1934	C1841	U1744	A1637	G1529	A1399	U1292	A1193
U2607	C2309	A2038	A2038	C1940	A1842	U1745	A1641	U1530	U1407	U1293	U1198
C2608	G2313	G2044	G2044	A1941	A1845	G1751	A1642	G1535	U1408	A1294	A1199
U2609	G2314	G2045	G2045	A1942	U1846	C1752	C1643	C1536	U1298	G1295	U1205
G2610	G2315	A2046	A2046	C1943	A1847	U1753	C1644	U1544	U1418	U1304	U1206
A2611	G2316	G2047	G2047	G1944	G1848	A1754	U1645	C1545	U1419	C1305	U1207
U2612	C2317	A2048	A2048	G1945	U1850	G1756	C1652	U1555	C1420	U1306	C1208
G2613	U2320	U2049	U2049	G1946	G1851	C1762	U1653	G1556	U1421	A1307	C1209
C2614	A2321	G2050	G2050	A1947	A1852	U1763	U1654	G1557	U1422	U1308	U1210
U2615	G2322	A2051	A2051	G1948	C1853	U1764	A1655	C1558	C1423	U1311	G1211
G2616	C2323	G2052	G2052	G1949	G1854	U1765	A1656	U1561	G1430	U1312	G1212
A2617	U2324	U2053	U2053	A1950	C1855	U1766	A1657	C1564	U1441	U1313	G1213
U2618	G2325	A2054	A2054	G1951	G1856	U1767	A1658	U1565	U1442	G1315	G1214
C2619	C2326	G2055	G2055	G1952	C1857	C1768	U1659	C1572	U1446	G1316	A1215
G2620	U2327	U2056	U2056	A1953	C1858	U1769	A1660	A1573	A1450	G1321	G1216
A2621	G2328	A2057	A2057	A1954	G1859	U1770	C1661	A1574	C1451	G1322	C1229
U2622	U2329	G2058	G2058	A1955	C1860	U1771	A1662	G1576	U1461	G1325	U1234
G2623	C2330	A2059	A2059	A1956	G1861	U1772	A1663	U1577	C1462	G1235	G1235
A2624	U2331	G2060	G2060	C1957	C1862	G1773	U1664	C1578	U1463	A1236	U1236
U2625	G2332	U2061	U2061	G1958	G1863	U1774	U1665	C1579	C1464	U1237	U1237
C2626	U2333	A2062	A2062	A1959	C1864	G1775	C1666	A1580	U1333	C1238	C1238
G2627	C2334	G2063	G2063	A1960	G1865	U1776	C1667	U1587	C1334	G1239	G1239
U2628	U2335	U2064	U2064	A1961	C1866	U1777	C1668	G1588	C1471	A1242	A1242
A2629	G2336	A2065	A2065	A1962	G1867	U1778	C1669	G1589	U1472	G1340	U1243
U2630	U2337	G2066	G2066	A1963	C1868	U1779	C1670	C1592	U1473	C1243	U1244
G2631	C2338	U2067	U2067	A1964	G1869	A1778	A1671	C1593	C1474	C1245	A1245
A2632	U2339	A2068	A2068	A1965	C1870	A1779	U1672	C1594	C1477	A1246	A1246
U2633	G2340	G2069	G2069	C1966	A1871	U1780	G1706	C1595	U1483	U1249	U1249
C2634	U2341	U2070	U2070	A1967	C1872	U1781	G1707	U1596	G1484	C1250	C1250
G2635	A2342	A2071	A2071	A1968	G1873	U1782	G1708	A1597	U1346	C1251	C1251
A2636	G2343	G2072	G2072	A1969	C1874	U1783	U1709	A1598	G1351	U1352	U1352
U2637	U2344	U2073	U2073	A1970	G1875	U1784	A1710	U1599	A1353	C1353	C1353
C2638	C2345	A2074	A2074	A1971	C1876	U1785	G1711	G1600	A1494	U1266	U1266
U2639	G2346	G2075	G2075	A1972	G1877	U1786	A1712	A1603	C1495	C1267	C1267
G2640	U2347	U2076	U2076	A1973	C1878	U1787	A1713	G1604	A1496	U1500	U1500
A2641	C2348	A2077	A2077	A1974	U1879	U1788	A1714	A1605	U1497	U1501	U1501
U2642	U2349	G2078	G2078	A1975	C1880	U1789	A1715	A1606	U1498	U1502	U1502
C2643	G2350	U2079	U2079	A1976	G1881	G1790	A1716	A1607	U1499	U1503	U1503
G2644	U2351	A2080	A2080	A1977	C1882	U1791	A1717	A1608	U1500	U1504	U1504
U2645	C2352	G2081	G2081	A1978	G1884	U1792	A1718	A1609	U1501	U1505	U1505
A2646	U2353	U2082	U2082	A1979	C1885	U1793	A1719	A1610	U1502	U1506	U1506
G2647	G2354	A2083	A2083	A1980	G1886	U1794	A1720	A1611	U1503	U1507	U1507
U2648	C2355	G2084	G2084	A1981	C1887	U1795	A1721	A1612	U1504	U1508	U1508
C2649	U2356	U2085	U2085	A1982	G1888	U1796	A1722	A1613	U1505	U1509	U1509
G2650	G2357	A2086	A2086	A1983	C1889	U1797	A1723	A1614	U1506	U1510	U1510
A2651	C2358	G2087	G2087	A1984	G1890	U1798	A1724	A1615	U1507	U1511	U1511
U2652	U2359	U2088	U2088	A1985	C1891	U1799	A1725	A1616	U1508	U1512	U1512
G2653	G2360	A2089	A2089	A1986	G1892	U1800	A1726	A1617	U1509	U1513	U1513
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U2657	U2364	G2093	G2093	A1990	G1896	U1804	A1730	A1621	U1513	U1517	U1517
A2658	C2365	U2094	U2094	A1991	C1897	U1805	A1731	A1622	U1514	U1518	U1518
G2659	G2366	A2095	A2095	A1992	G1898	U1806	A1732	A1623	U1515	U1519	U1519
U2660	U2367	G2096	G2096	A1993	C1899	U1807	A1733	A1624	U1516	U1520	U1520
C2661	C2368	U2097	U2097	A1994	G1899	U1808	A1734	A1625	U1517	U1521	U1521
G2662	G2369	A2098	A2098	A1995	C1900	U1809	A1735	A1626	U1518	U1522	U1522
U2663	U2370	G2099	G2099	A1996	G1901	U1810	A1736	A1627	U1519	U1523	U1523
A2664	C2371	U2100	U2100	A1997	C1902	U1811	A1737	A1628	U1520	U1524	U1524
G2665	G2372	A2101	A2101	A1998	G1903	U1812	A1738	A1629	U1521	U1525	U1525
U2666	U2373	G2102	G2102	A1999	C1904	U1813	A1739	A1630	U1522	U1526	U1526
C2667	C2374	A2103	A2103	A2000	U1905	U1814	A1740	A1631	U1523	U1527	U1527
G2668	G2375	C2104	C2104	G1974	G1911	U1815	A1741	A1632	U1524	U1528	U1528
U2669	U2376	U2105	U2105	A1978	C1912	U1816	A1742	A1633	U1525	U1529	U1529
G2670	C2377	C2106	C2106	G1979	G1913	U1817	A1743	A1634	U1526	U1530	U1530
U2671	A2378	A2107	A2107	A1980	C1914	U1818	A1744	A1635	U1527	U1531	U1531
C2672	G2379	G2111	G2111	A1981	G1915	U1819	A1745	A1636	U1528	U1532	U1532
U2673	U2380	A2112	A2112	A1982	C1916	U1820	A1746	A1637	U1529	U1533	U1533
G2674	C2381	G2113	G2113	A1983	G1917	U1821	A1747	A1638	U1530	U1534	U1534
A2675	G2382	C2114	C2114	A1984	C1918	U1822	A1748	A1639	U1531	U1535	U1535
U2676	U2383	U2115	U2115	A1985	G1919	U1823	A1749	A1640	U1532	U1536	U1536
C2677	C2384	G2116	G2116	A1986	C1920	U1824	A1750	A1641	U1533	U1537	U1537
G2678	G2385	A2117	A2117	A1987	G1921	U1825	A1751	A1642	U1534	U1538	U1538
U2679	U2386	U2118	U2118	A1988	C1922	U1826	A1752	A1643	U1535	U1539	U1539
A2680	C2387	G2119	G2119	A1989	G1923	U1827	A1753	A1644	U1536	U1540	U1540
G2681	G2388	A2119	A2119	A1990	C1924	U1828	A1754	A1645	U1537	U1541	U1541
U2682	U2389	U2120	U2120	A1991	G1925	U1829	A1755	A1646	U1538	U1542	U1542
C2683	C2390	G2121	G2121	A1992	C1926	U1830	A1756	A1647	U1539	U1543	U1543
G2684	U2391	A2121	A2121	A1993	G1927	U1831	A1757	A1648	U1540	U1544	U1544
U2685	G2392	U2122	U2122	A1994	C1928	U1832	A1758	A1649	U1541	U1545	U1545
A2686	C2393	G2123	G2123	A1995	G1929	U1833	A1759	A1650	U1542	U1546	U1546
G2687	U2394	A2123	A2123	A1996	C1930	U1834	A1760	A1651	U1543	U1547	U1547
U2688	C2395	U2124	U2124	A1997	G1931	U1835	A1761	A1652	U1544	U1548	U1548
C2689	G2396	G2125	G2125	A1998	C1932	U1836	A1762	A1653	U1545	U1549	U1549
G2690	U2397	A2124	A2124	A1999	G1933	U1837	A1763	A1654	U1546	U1550	U1550
U2691	C2398	U2125	U2125	A2000	C1934	U1838	A1764	A1655	U1547	U1551	U1551
A2692	G2399	G2126	G2126	A2001	G1935	U1839	A1765	A1656	U1548	U1552	U1552
G2693	U2399	A2126	A2126	A2002	C1936	U1840	A1766	A1657	U1549	U1553	U1553
U2694	C2400	U2127	U2127	A2003	G1937	U1841	A1767	A1658	U1550	U1554	U1554
C2695	G2401	G2128	G2128	A2004	C1938	U1842	A1768	A1659	U1551	U1555	U1555
G2696	U2402	A2128	A2128	A2005	G1939	U1843	A1769	A1660	U1552	U1556	U1556
U2697	C2403	U2129	U2129	A2006	C1940	U1844	A1770	A1661	U1553	U1557	U1557
A2698	G2404										



• Molecule 2: 50S RIBOSOMAL PROTEIN L37E

Chain 1: 67% 32%



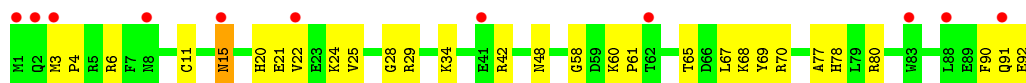
• Molecule 3: 50S RIBOSOMAL PROTEIN L39E

Chain 2: 16% 44% 48% 8%



• Molecule 4: 50S RIBOSOMAL PROTEIN L44E

Chain 3: 12% 68% 30%



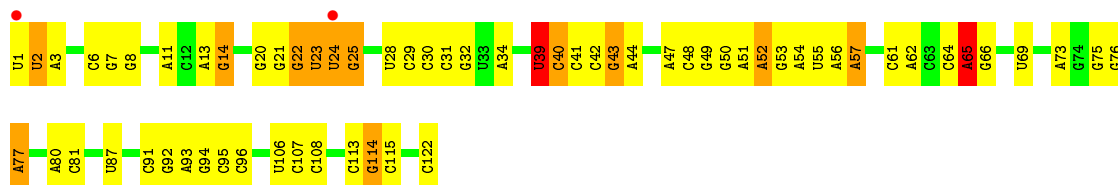
• Molecule 5: VIRGINIAMYCIN S1

Chain 8: 86% 14%



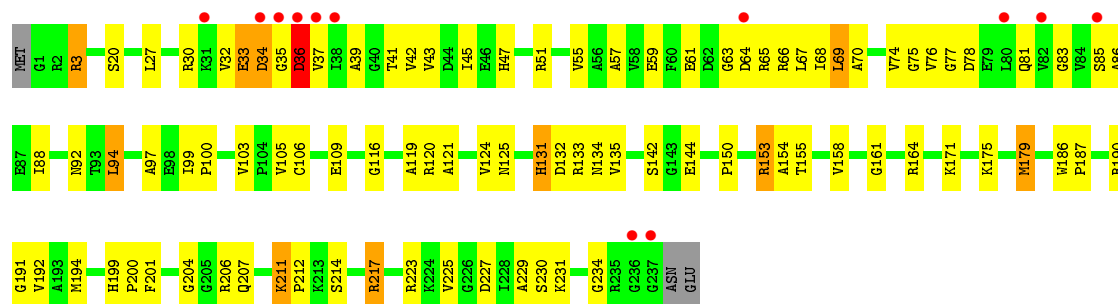
• Molecule 6: 5S RIBOSOMAL RNA

Chain 9: 2% 48% 41% 10%

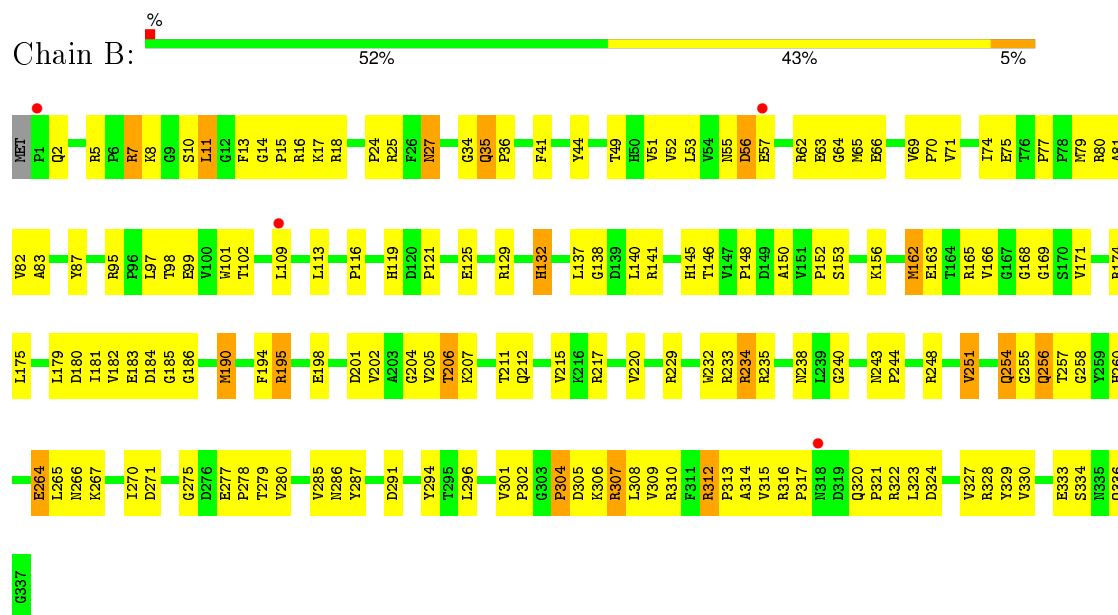


• Molecule 7: 50S RIBOSOMAL PROTEIN L2P

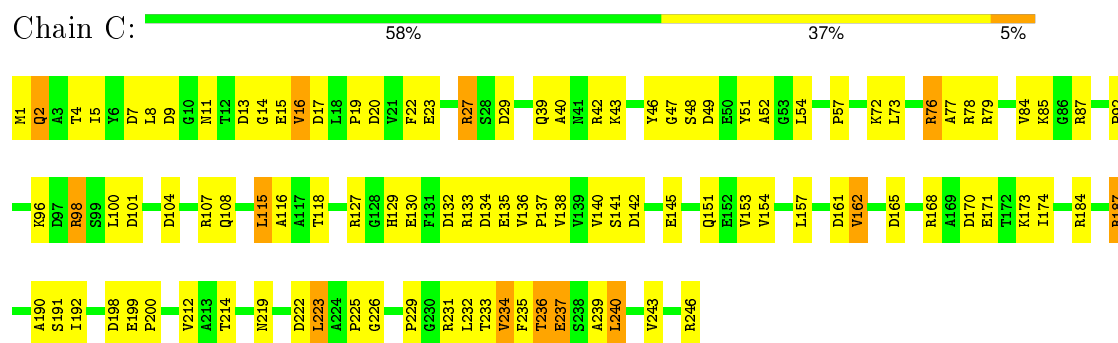
Chain A: 5% 60% 35%



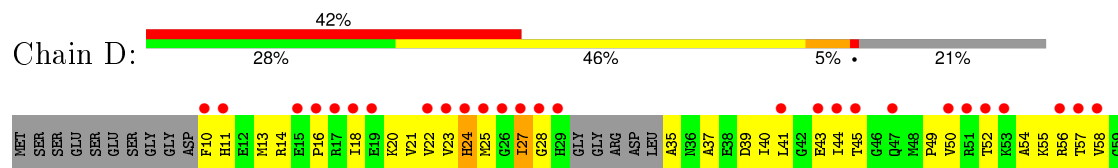
• Molecule 8: 50S RIBOSOMAL PROTEIN L3P

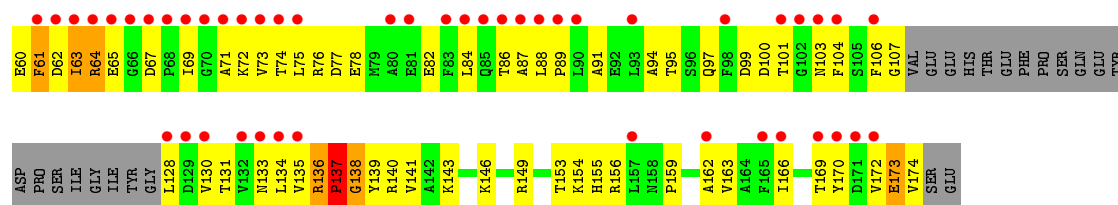


• Molecule 9: 50S RIBOSOMAL PROTEIN L4E

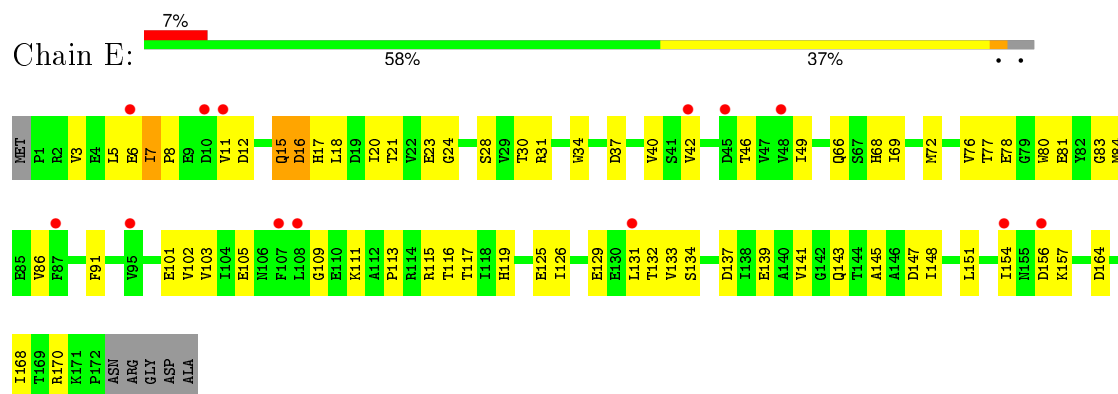


• Molecule 10: 50S RIBOSOMAL PROTEIN L5P

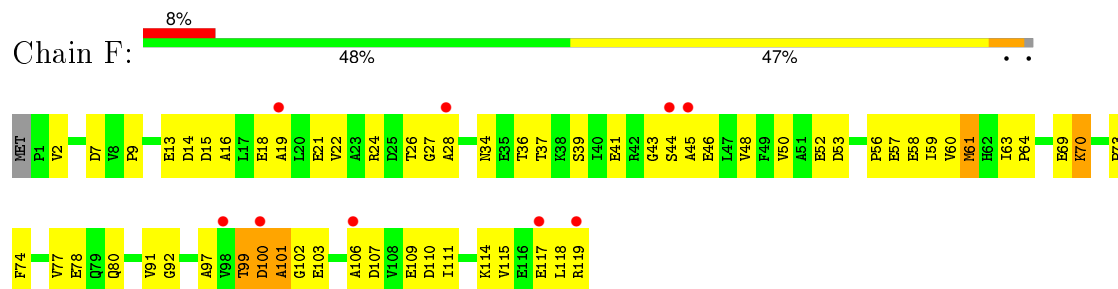




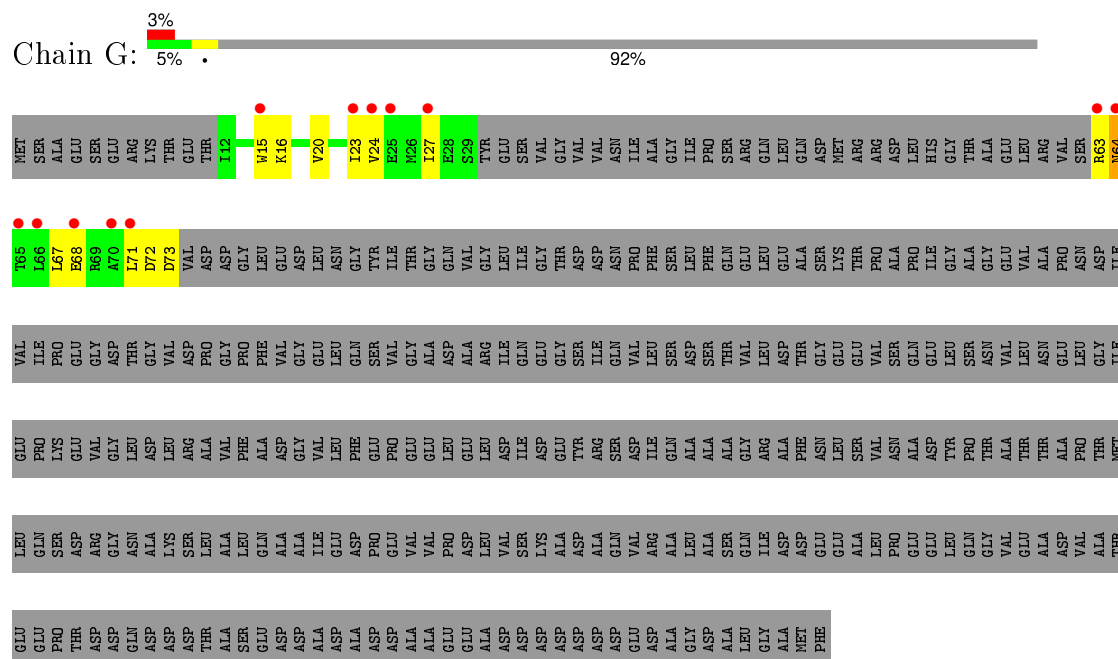
- Molecule 11: 50S RIBOSOMAL PROTEIN L6P



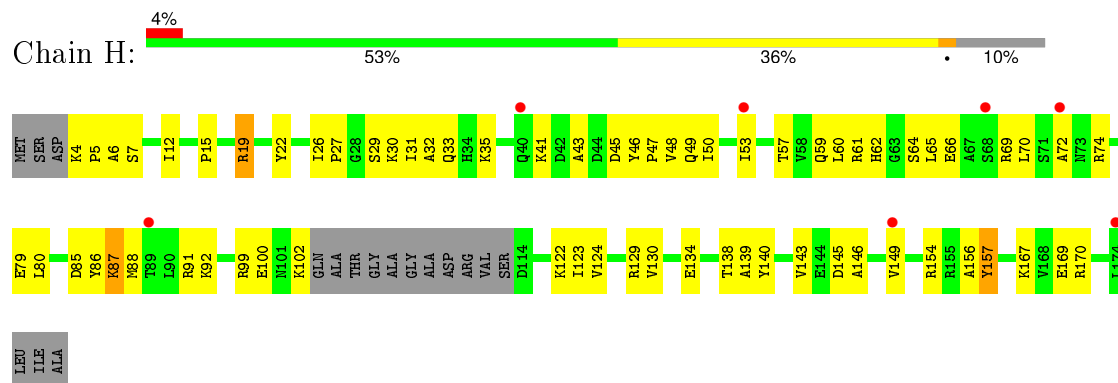
- Molecule 12: 50S RIBOSOMAL PROTEIN L7AE



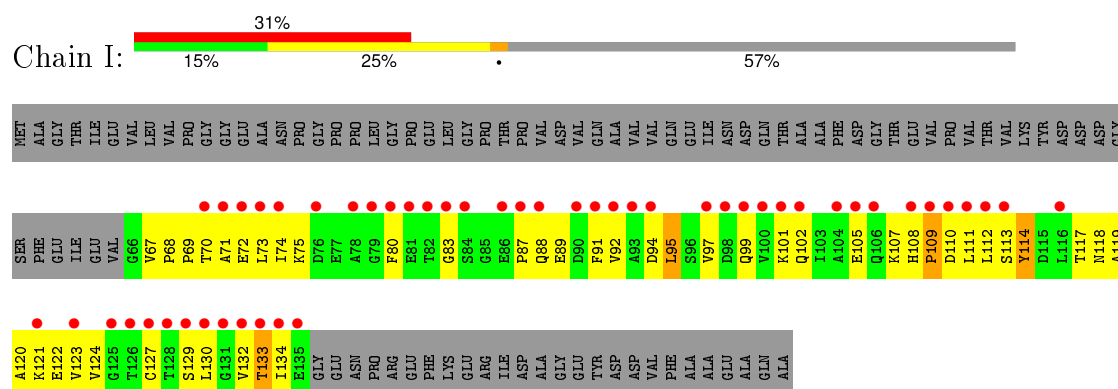
• Molecule 13: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



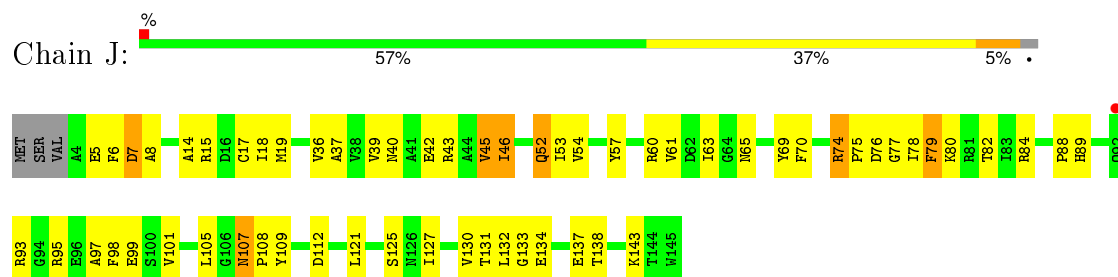
- Molecule 14: 50S RIBOSOMAL PROTEIN L10E



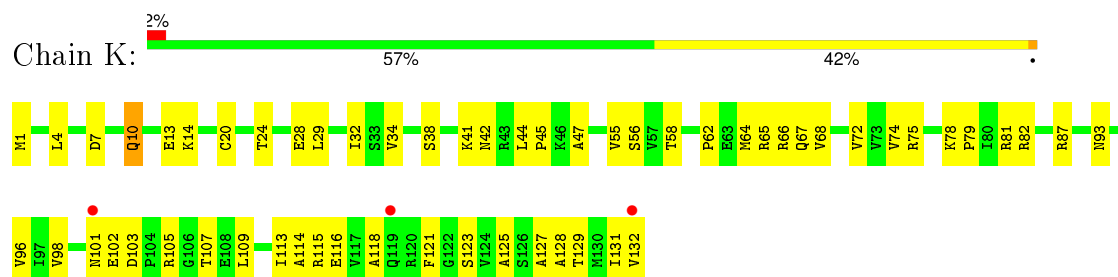
● Molecule 15: 50S RIBOSOMAL PROTEIN L11P



- Molecule 16: 50S RIBOSOMAL PROTEIN L13P

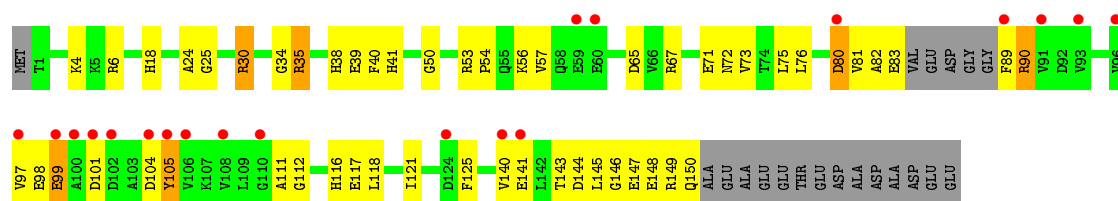


● Molecule 17: 50S RIBOSOMAL PROTEIN L14P



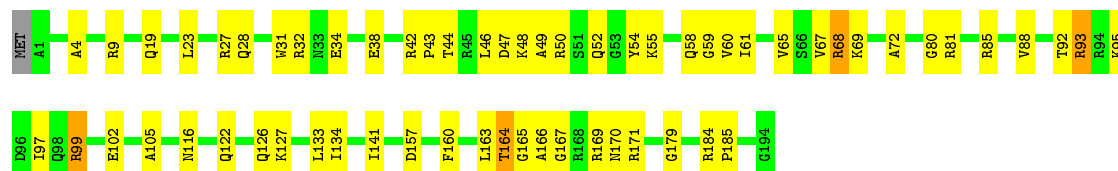
- Molecule 18: 50S RIBOSOMAL PROTEIN L15P





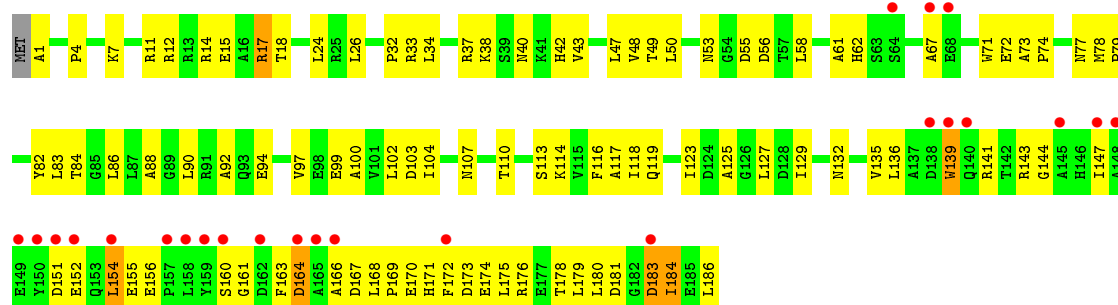
• Molecule 19: 50S RIBOSOMAL PROTEIN L15E

Chain M: 68% 29% ..



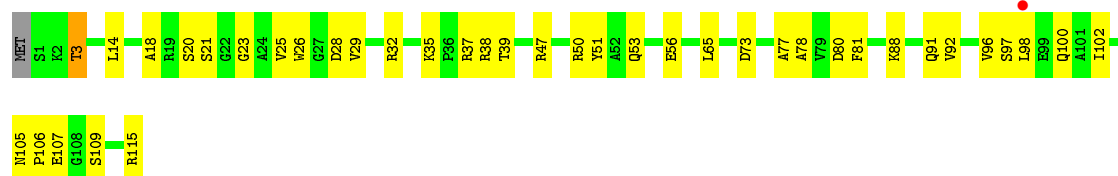
• Molecule 20: 50S RIBOSOMAL PROTEIN L18P

Chain N: 13% 47% 49% ..



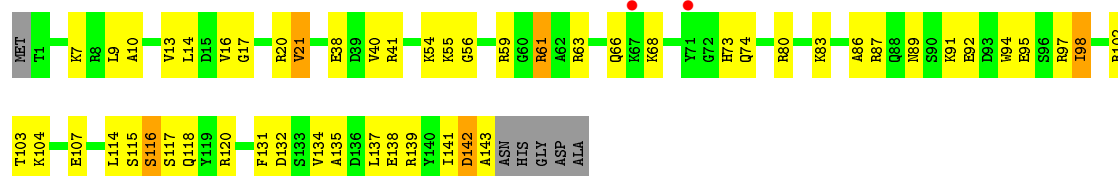
• Molecule 21: 50S RIBOSOMAL PROTEIN L18E

Chain O: % 66% 33% ..

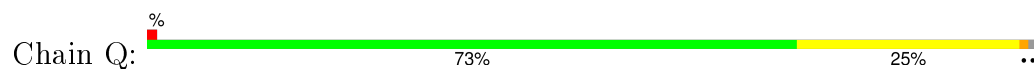


• Molecule 22: 50S RIBOSOMAL PROTEIN L19E

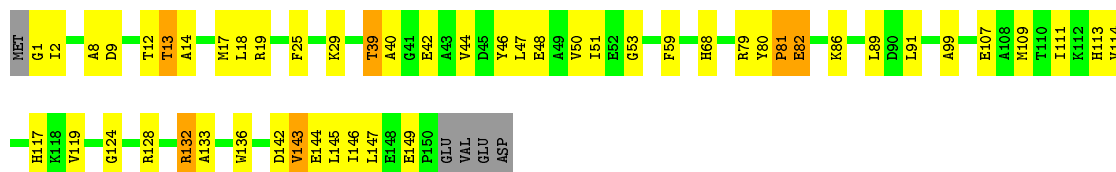
Chain P: % 60% 32% ..



• Molecule 23: 50S RIBOSOMAL PROTEIN L21E



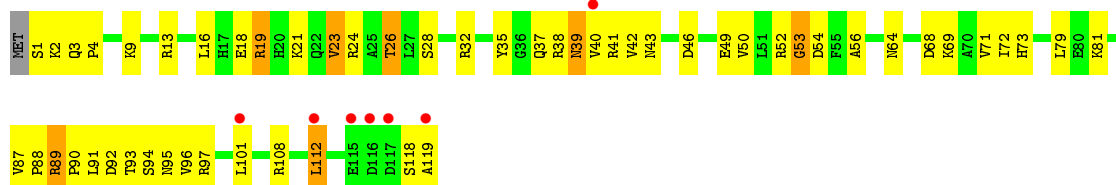
• Molecule 24: 50S RIBOSOMAL PROTEIN L22P



• Molecule 25: 50S RIBOSOMAL PROTEIN L23P



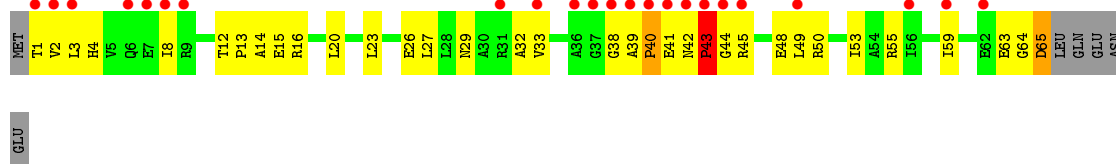
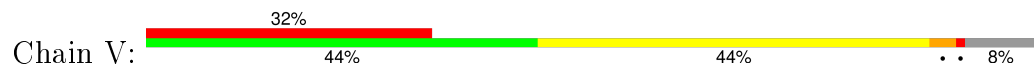
• Molecule 26: 50S RIBOSOMAL PROTEIN L24P



• Molecule 27: 50S RIBOSOMAL PROTEIN L24E

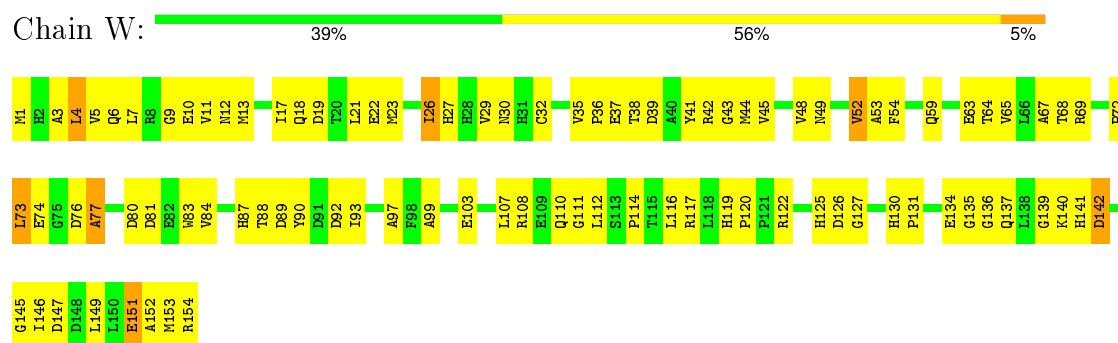


• Molecule 28: 50S RIBOSOMAL PROTEIN L29P



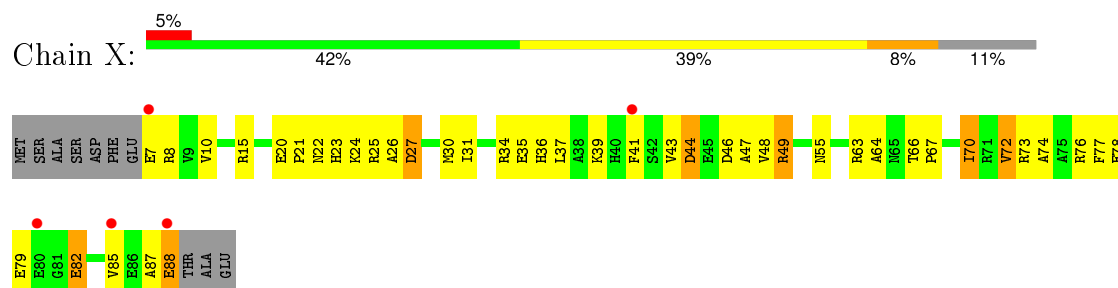
• Molecule 29: 50S RIBOSOMAL PROTEIN L30P

Chain W:



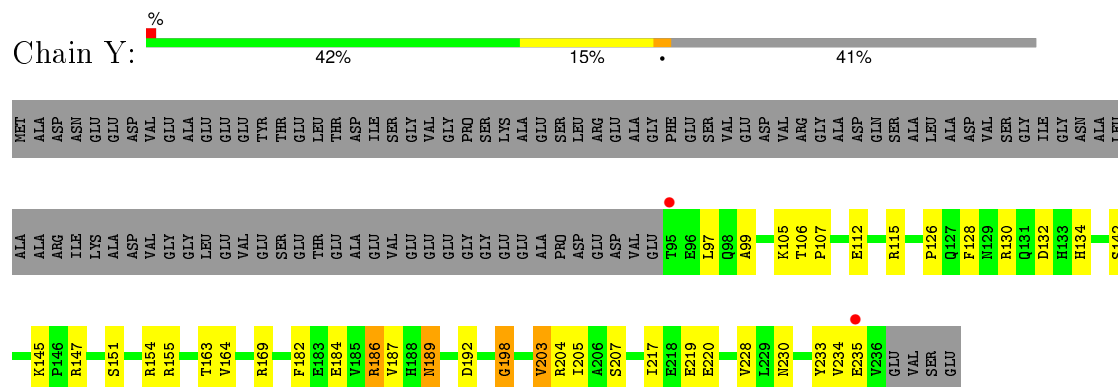
- Molecule 30: 50S RIBOSOMAL PROTEIN L31E

Chain X:



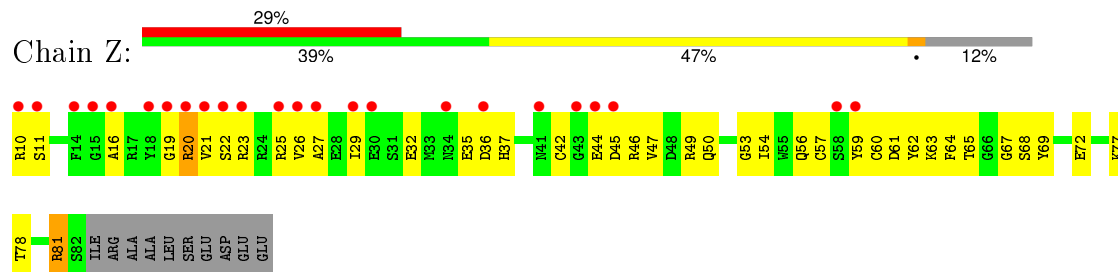
- Molecule 31: 50S RIBOSOMAL PROTEIN L32E

Chain Y:



- Molecule 32: 50S RIBOSOMAL PROTEIN L37AE

Chain Z:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.58 Å 299.76 Å 573.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.80 49.90 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.99-2.80) 93.7 (49.90-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.81 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.175 , 0.221 0.209 , 0.228	Depositor DCC
R_{free} test set	4114 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 418145 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	91326	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, DBB, CD, VIR, 1MA, UR3, OMU, 004, MHV, MEA, MHW, 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	0.37	0/65958	0.69	12/102869 (0.0%)
2	1	0.41	0/438	0.62	0/578
3	2	0.34	0/401	0.53	0/529
4	3	0.35	0/771	0.55	0/1024
5	8	1.13	0/13	1.01	0/15
6	9	0.33	0/2904	0.69	1/4526 (0.0%)
7	A	0.32	0/1786	0.64	0/2408
8	B	0.33	0/2690	0.64	0/3652
9	C	0.36	0/1884	0.63	0/2551
10	D	0.31	0/1111	0.53	0/1498
11	E	0.33	0/1382	0.58	0/1880
12	F	0.31	0/901	0.56	0/1224
13	G	0.29	0/241	0.47	0/324
14	H	0.34	0/1302	0.64	0/1743
15	I	0.29	0/526	0.55	0/716
16	J	0.37	0/1136	0.63	0/1530
17	K	0.34	0/1001	0.68	0/1347
18	L	0.32	0/1130	0.62	0/1509
19	M	0.33	0/1582	0.61	0/2117
20	N	0.29	0/1474	0.60	0/1999
21	O	0.33	0/874	0.59	0/1181
22	P	0.32	0/1147	0.54	0/1528
23	Q	0.36	0/749	0.69	0/1005
24	R	0.35	0/1172	0.64	0/1578
25	S	0.33	0/648	0.58	0/875
26	T	0.32	0/958	0.63	0/1289
27	U	0.33	0/417	0.58	0/562
28	V	0.28	0/502	0.58	0/675
29	W	0.35	0/1219	0.65	0/1655
30	X	0.34	0/664	0.59	0/895
31	Y	0.34	0/1146	0.65	0/1536
32	Z	0.32	0/589	0.59	0/787

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98716	0.67	13/147605 (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	38
6	9	0	4
All	All	0	42

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1942	A	C5'-C4'-C3'	7.56	128.09	116.00
1	0	871	G	C5'-C4'-O4'	-6.96	100.74	109.10
1	0	1504	A	C1'-O4'-C4'	-6.20	104.94	109.90
6	9	39	U	N1-C1'-C2'	6.08	121.90	114.00
1	0	2467	A	C1'-O4'-C4'	-5.61	105.42	109.90
1	0	2291	A	N9-C1'-C2'	5.59	121.27	114.00
1	0	1120	U	C5'-C4'-C3'	-5.49	107.22	116.00
1	0	1819	G	C5'-C4'-C3'	5.48	124.77	116.00
1	0	1504	A	N9-C1'-C2'	5.41	121.03	114.00
1	0	1971	G	N9-C1'-C2'	5.29	120.88	114.00
1	0	2526	C	N1-C1'-C2'	5.24	120.81	114.00
1	0	2313	C	C5'-C4'-O4'	5.11	115.24	109.10
1	0	2726	U	N1-C1'-C2'	5.09	120.62	114.00

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain
1	0	1417	G	Sidechain
1	0	1430	G	Sidechain
1	0	1681	G	Sidechain
1	0	1829	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1835	U	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1972	U	Sidechain
1	0	1979	G	Sidechain
1	0	22	U	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	462	A	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	521	A	Sidechain
1	0	619	U	Sidechain
1	0	817	G	Sidechain
1	0	818	A	Sidechain
1	0	888	U	Sidechain
6	9	39	U	Sidechain
6	9	65	A	Sidechain
6	9	87	U	Sidechain
6	9	94	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29810	865	0
2	1	431	0	426	23	0
3	2	396	0	413	22	0
4	3	755	0	728	22	0
5	8	60	0	46	1	0
6	9	2599	0	1325	70	0
7	A	1753	0	1766	125	0
8	B	2625	0	2533	156	0
9	C	1859	0	1816	108	0
10	D	1094	0	1085	90	0
11	E	1357	0	1266	64	0
12	F	890	0	843	51	0
13	G	240	0	231	17	0
14	H	1282	0	1292	74	0
15	I	519	0	500	52	0
16	J	1120	0	1098	68	0
17	K	992	0	1031	62	0
18	L	1118	0	1076	47	0
19	M	1558	0	1566	60	0
20	N	1445	0	1401	105	0
21	O	865	0	873	29	0
22	P	1136	0	1123	54	0
23	Q	735	0	729	22	0
24	R	1149	0	1122	56	0
25	S	641	0	605	24	0
26	T	950	0	923	53	0
27	U	410	0	364	26	0
28	V	499	0	511	37	0
29	W	1196	0	1137	109	0
30	X	654	0	653	42	0
31	Y	1130	0	1133	43	0
32	Z	578	0	540	42	0
33	0	109	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	2	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	1	0	0	0	0
35	0	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	9	2	0	0	0	0
35	A	1	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	L	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	1	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	38	0	34	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
All	All	91326	0	59999	2318	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (2318) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:656:G:H5'	21:O:3:THR:HG22	1.23	1.16
1:0:871:G:H8	1:0:871:G:H5'	1.13	1.14
9:C:236:THR:HG22	9:C:239:ALA:H	1.13	1.07
1:0:871:G:C8	1:0:871:G:H5'	1.92	1.04
1:0:21:G:H5'	24:R:2:ILE:HA	1.40	1.04
6:9:6:C:H5''	20:N:37:ARG:HH12	1.19	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1242:A:H5'	16:J:82:THR:HG23	1.41	1.03
1:0:56:G:H5''	28:V:50:ARG:HH12	1.20	1.03
26:T:71:VAL:HG11	26:T:90:PRO:HB3	1.37	1.02
1:0:156:C:H5''	19:M:171:ARG:HD3	1.37	1.01
1:0:870:G:H2'	1:0:871:G:H5''	1.42	1.01
31:Y:187:VAL:HG23	31:Y:192:ASP:HB2	1.42	1.01
14:H:59:GLN:HE21	14:H:129:ARG:HE	1.08	0.99
10:D:25:MET:HE3	10:D:37:ALA:HB1	1.42	0.98
10:D:154:LYS:H	10:D:154:LYS:HD2	1.26	0.98
32:Z:46:ARG:HD2	32:Z:59:TYR:HB2	1.47	0.97
1:0:1751:G:H2'	1:0:1752:G:H5''	1.44	0.96
6:9:6:C:H5''	20:N:37:ARG:NH1	1.78	0.96
29:W:72:PRO:HG2	29:W:77:ALA:HB3	1.48	0.95
1:0:1119:G:H2'	16:J:52:GLN:NE2	1.80	0.95
6:9:76:G:H3'	6:9:77:A:H5''	1.47	0.95
17:K:10:GLN:H	17:K:10:GLN:NE2	1.65	0.94
10:D:57:THR:HG23	10:D:63:ILE:HA	1.49	0.94
7:A:211:LYS:HB3	7:A:212:PRO:HD2	1.50	0.93
6:9:56:A:H2'	6:9:57:A:H5''	1.48	0.93
1:0:2717:C:H2'	1:0:2718:C:H5''	1.51	0.93
16:J:74:ARG:HB3	16:J:74:ARG:HH11	1.34	0.93
15:I:127:CYS:HB3	15:I:132:VAL:HB	1.50	0.93
8:B:62:ARG:HA	8:B:65:MET:HE3	1.50	0.92
26:T:9:LYS:HE3	26:T:13:ARG:NH1	1.84	0.92
1:0:545:G:H8	1:0:545:G:H5'	1.34	0.92
8:B:320:GLN:HE21	8:B:321:PRO:HD2	1.34	0.92
4:3:60:LYS:HG3	4:3:61:PRO:HD2	1.51	0.91
22:P:115:SER:H	22:P:118:GLN:HE21	0.91	0.91
1:0:2890:A:H1'	27:U:56:ARG:NH2	1.85	0.91
22:P:59:ARG:HH22	22:P:66:GLN:HE22	0.95	0.91
9:C:127:ARG:NH2	9:C:225:PRO:HG2	1.85	0.91
9:C:78:ARG:HG3	9:C:78:ARG:HH11	1.32	0.91
1:0:1116:U:HO2'	1:0:1118:A:H2	0.91	0.91
29:W:137:GLN:HE21	29:W:141:HIS:HE1	1.15	0.90
30:X:37:LEU:HD13	30:X:85:VAL:HG21	1.53	0.90
1:0:2506:A:HO2'	1:0:2507:G:H8	1.15	0.90
1:0:1187:U:HO2'	1:0:1189:A:H2	1.14	0.90
7:A:35:GLY:O	7:A:36:ASP:HB3	1.71	0.90
1:0:1119:G:H2'	16:J:52:GLN:HE22	1.30	0.90
1:0:1160:G:H5'	1:0:1161:A:H5'	1.54	0.90
17:K:10:GLN:N	17:K:10:GLN:HE21	1.69	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:115:SER:N	22:P:118:GLN:HE21	1.71	0.89
1:0:1474:C:H6	1:0:1474:C:H5'	1.37	0.89
4:3:25:VAL:HG22	4:3:68:LYS:HG3	1.54	0.89
1:0:2586:U:H3	1:0:2592:G:H22	1.16	0.89
17:K:10:GLN:H	17:K:10:GLN:HE21	0.89	0.88
9:C:1:MET:HG2	9:C:2:GLN:H	1.37	0.88
1:0:870:G:C2'	1:0:871:G:H5''	2.04	0.87
8:B:179:LEU:O	8:B:183:GLU:HG2	1.75	0.87
1:0:541:C:H2'	1:0:542:A:H5''	1.56	0.87
10:D:63:ILE:HG13	10:D:64:ARG:H	1.38	0.87
22:P:59:ARG:NH2	22:P:66:GLN:HE22	1.73	0.87
7:A:100:PRO:HG2	7:A:103:VAL:HG21	1.55	0.87
17:K:98:VAL:CG1	17:K:102:GLU:HA	2.05	0.86
29:W:13:MET:HE2	29:W:18:GLN:HA	1.56	0.86
1:0:2533:C:H5'	1:0:2533:C:H6	1.40	0.86
8:B:41:PHE:HB3	8:B:190:MET:HE3	1.57	0.85
14:H:59:GLN:NE2	14:H:129:ARG:HE	1.74	0.85
14:H:32:ALA:HB3	14:H:69:ARG:HH12	1.40	0.85
1:0:282:C:H1'	1:0:368:C:N4	1.92	0.85
1:0:2717:C:C2'	1:0:2718:C:H5''	2.06	0.85
29:W:6:GLN:HB2	29:W:26:ILE:HD12	1.59	0.84
1:0:2756:U:H3	1:0:2896:A:H2	1.25	0.84
16:J:93:ARG:HH11	16:J:93:ARG:HB3	1.41	0.84
19:M:102:GLU:OE1	19:M:164:THR:HG21	1.76	0.84
1:0:1835:U:H5	1:0:1840:A:N7	1.74	0.84
1:0:1593:C:H5'	22:P:116:SER:O	1.77	0.84
7:A:88:ILE:HD13	7:A:100:PRO:HD3	1.57	0.83
24:R:18:LEU:HB2	24:R:143:VAL:HG13	1.60	0.83
14:H:102:LYS:HD3	14:H:122:LYS:HD3	1.60	0.83
25:S:57:THR:HG22	25:S:59:ASP:H	1.44	0.83
29:W:4:LEU:HD23	29:W:54:PHE:HB3	1.59	0.83
1:0:656:G:H5'	21:O:3:THR:CG2	2.07	0.83
20:N:164:ASP:OD1	20:N:167:ASP:HA	1.78	0.83
1:0:559:U:H5'	1:0:559:U:H6	1.43	0.83
1:0:1450:C:H4'	1:0:1451:C:OP2	1.79	0.82
12:F:91:VAL:HG12	12:F:92:GLY:N	1.94	0.82
21:O:14:LEU:HD23	21:O:102:ILE:HD11	1.60	0.82
8:B:55:ASN:HB3	8:B:63:GLU:HA	1.60	0.82
22:P:115:SER:H	22:P:118:GLN:NE2	1.75	0.82
22:P:59:ARG:HH22	22:P:66:GLN:NE2	1.78	0.82
1:0:1118:A:H3'	1:0:1118:A:H8	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:101:LEU:HD13	26:T:112:LEU:HD11	1.63	0.81
28:V:12:THR:HG22	28:V:15:GLU:HG3	1.61	0.81
9:C:236:THR:HG22	9:C:239:ALA:N	1.94	0.81
8:B:201:ASP:HB2	8:B:312:ARG:HD2	1.63	0.81
1:0:1118:A:H3'	1:0:1118:A:C8	2.16	0.81
1:0:1666:C:O2'	1:0:1667:A:H5''	1.81	0.80
31:Y:187:VAL:HG23	31:Y:192:ASP:CB	2.11	0.80
7:A:153:ARG:HH11	7:A:153:ARG:HB2	1.45	0.80
1:0:1164:U:H3	1:0:1192:A:H2	1.29	0.80
1:0:2768:A:H2'	1:0:2769:C:O4'	1.82	0.80
32:Z:37:HIS:HB2	32:Z:47:VAL:HB	1.64	0.80
30:X:76:ARG:HH11	30:X:76:ARG:HG3	1.45	0.80
8:B:304:PRO:HD2	8:B:307:ARG:HD2	1.64	0.80
1:0:1667:A:H8	1:0:1667:A:H5'	1.46	0.80
1:0:1701:A:H4'	1:0:1702:U:H5''	1.63	0.80
1:0:56:G:H5''	28:V:50:ARG:NH1	1.95	0.80
14:H:41:LYS:HE2	14:H:45:ASP:HB3	1.64	0.79
20:N:7:LYS:HE3	23:Q:21:ARG:O	1.83	0.79
8:B:320:GLN:NE2	8:B:321:PRO:HD2	1.96	0.79
1:0:2291:A:C8	1:0:2309:C:H5'	2.18	0.79
17:K:29:LEU:HB3	17:K:55:VAL:HG11	1.64	0.79
8:B:162:MET:HE3	8:B:308:LEU:HD21	1.64	0.79
10:D:28:GLY:HA2	10:D:69:ILE:HG23	1.65	0.79
29:W:81:ASP:OD1	29:W:92:ASP:HB2	1.82	0.78
20:N:48:VAL:CG1	20:N:55:ASP:HB3	2.14	0.78
19:M:99:ARG:HD2	19:M:167:GLY:HA2	1.63	0.78
8:B:18:ARG:HG3	8:B:256:GLN:HG3	1.65	0.78
16:J:19:MET:HE1	16:J:132:LEU:HD21	1.66	0.78
17:K:118:ALA:HA	17:K:125:ALA:HB2	1.64	0.78
1:0:541:C:C2'	1:0:542:A:H5''	2.14	0.78
13:G:68:GLU:O	13:G:72:ASP:HB2	1.83	0.78
7:A:36:ASP:OD2	7:A:85:SER:HB2	1.83	0.78
1:0:877:G:H5'	1:0:878:G:OP1	1.84	0.78
12:F:91:VAL:HG12	12:F:92:GLY:H	1.47	0.77
1:0:2812:A:H2	1:0:2814:A:H62	1.32	0.77
2:1:25:LYS:HD2	3:2:49:GLU:H	1.50	0.77
6:9:48:C:H4'	20:N:141:ARG:HH21	1.50	0.77
29:W:21:LEU:HD22	29:W:26:ILE:CD1	2.15	0.77
10:D:58:VAL:HB	10:D:62:ASP:HB3	1.67	0.76
1:0:1160:G:C5'	1:0:1161:A:H5'	2.14	0.76
30:X:72:VAL:HG22	30:X:85:VAL:HG12	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:75:PRO:HG2	16:J:105:LEU:HD21	1.67	0.76
1:O:2679:G:H2'	1:O:2681:A:OP2	1.86	0.76
20:N:132:ASN:O	20:N:135:VAL:HG12	1.86	0.76
17:K:98:VAL:HG11	17:K:102:GLU:HA	1.68	0.75
1:O:1684:A:H1'	3:2:43:ARG:HH22	1.51	0.75
1:O:1205:U:H2'	1:O:1206:U:H5''	1.67	0.75
9:C:98:ARG:HH11	9:C:98:ARG:HG2	1.51	0.75
9:C:76:ARG:HB3	9:C:76:ARG:NH1	2.01	0.75
1:O:1116:U:H3	1:O:1246:A:H62	1.33	0.75
1:O:1206:U:H6	1:O:1206:U:H5'	1.51	0.75
1:O:542:A:H5'	1:O:542:A:H8	1.52	0.75
8:B:238:ASN:HD22	8:B:240:GLY:H	1.34	0.75
1:O:1205:U:H2'	1:O:1206:U:C5'	2.17	0.74
12:F:63:ILE:HB	12:F:64:PRO:HD3	1.67	0.74
2:1:8:GLN:HE22	2:1:11:LYS:NZ	1.84	0.74
1:O:871:G:H8	1:O:871:G:C5'	1.98	0.74
1:O:21:G:C5'	24:R:2:ILE:HA	2.16	0.74
1:O:2716:G:H5''	8:B:206:THR:HG21	1.68	0.74
1:O:541:C:H2'	1:O:542:A:C5'	2.17	0.74
29:W:21:LEU:HD21	29:W:48:VAL:HG11	1.70	0.74
8:B:162:MET:HG3	8:B:310:ARG:HD3	1.69	0.74
6:9:14:G:H5'	6:9:14:G:H8	1.51	0.74
6:9:56:A:C2'	6:9:57:A:H5''	2.18	0.74
24:R:14:ALA:HB3	24:R:147:LEU:HB2	1.70	0.74
1:O:506:G:H22	1:O:509:A:C5'	2.00	0.73
8:B:258:GLY:H	8:B:260:HIS:CE1	2.06	0.73
8:B:264:GLU:HG2	8:B:267:LYS:HE2	1.68	0.73
1:O:545:G:C8	1:O:545:G:H5'	2.21	0.73
1:O:2908:A:H2'	1:O:2909:G:O4'	1.87	0.73
12:F:2:VAL:HG22	12:F:57:GLU:OE1	1.88	0.73
1:O:450:C:OP1	9:C:184:ARG:NH2	2.22	0.73
12:F:34:ASN:HA	19:M:4:ALA:HB2	1.70	0.73
14:H:12:ILE:HG23	14:H:129:ARG:CZ	2.19	0.73
9:C:78:ARG:HG3	9:C:78:ARG:NH1	2.01	0.73
1:O:1603:A:H5'	1:O:1605:G:O4'	1.89	0.73
7:A:191:GLY:HA2	7:A:194:MET:CE	2.19	0.73
1:O:1474:C:C6	1:O:1474:C:H5'	2.23	0.73
1:O:2502:C:H2'	1:O:2503:A:H5'	1.70	0.73
20:N:47:LEU:HD11	20:N:127:LEU:HD21	1.71	0.73
17:K:74:VAL:CG1	17:K:113:ILE:HG12	2.19	0.73
1:O:2578:G:H5'	1:O:2578:G:H8	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:88:THR:HG22	29:W:89:ASP:H	1.52	0.72
1:0:2533:C:C6	1:0:2533:C:H5'	2.23	0.72
30:X:30:MET:HE1	30:X:55:ASN:HA	1.72	0.72
20:N:169:PRO:O	20:N:172:PHE:HB3	1.90	0.72
1:0:272:A:H5'	1:0:273:G:OP2	1.88	0.72
1:0:2837:U:H1'	8:B:307:ARG:HH12	1.53	0.72
6:9:114:G:O6	20:N:11:ARG:HD3	1.89	0.72
29:W:65:VAL:HA	29:W:68:THR:HG22	1.72	0.72
1:0:2506:A:O2'	1:0:2507:G:H8	1.72	0.71
7:A:81:GLN:HB2	7:A:92:ASN:ND2	2.05	0.71
1:0:111:C:O2'	2:1:20:ARG:HG2	1.90	0.71
6:9:73:A:H61	6:9:108:C:H42	1.38	0.71
1:0:447:A:OP1	26:T:2:LYS:HG2	1.89	0.71
19:M:164:THR:HG22	19:M:167:GLY:H	1.55	0.71
3:2:41:HIS:H	3:2:45:ASN:HD22	1.36	0.71
1:0:1751:G:C2'	1:0:1752:G:H5''	2.19	0.71
6:9:92:G:H2'	6:9:93:A:C8	2.25	0.71
7:A:36:ASP:HB2	7:A:83:GLY:HA3	1.73	0.71
1:0:2502:C:C2'	1:0:2503:A:H5'	2.21	0.71
24:R:17:MET:HE1	24:R:19:ARG:NH2	2.04	0.71
22:P:135:ALA:HB1	22:P:139:ARG:HH12	1.53	0.71
30:X:78:GLU:HG2	30:X:79:GLU:H	1.54	0.71
1:0:1160:G:H5'	1:0:1161:A:C5'	2.20	0.71
10:D:22:VAL:HG22	10:D:74:THR:HG22	1.71	0.71
6:9:75:G:H1	6:9:106:U:H3	1.35	0.71
29:W:21:LEU:HD21	29:W:48:VAL:CG1	2.20	0.71
15:I:97:VAL:HG12	15:I:101:LYS:HE3	1.73	0.71
1:0:2320:U:H4'	1:0:2321:A:O4'	1.91	0.71
1:0:236:A:H4'	1:0:237:G:H5'	1.72	0.71
1:0:470:U:O2'	2:1:16:HIS:HD2	1.74	0.71
10:D:25:MET:HE3	10:D:37:ALA:CB	2.20	0.71
9:C:76:ARG:HB3	9:C:76:ARG:HH11	1.55	0.71
9:C:115:LEU:HD13	9:C:223:LEU:HD21	1.72	0.71
1:0:1925:G:H5'	4:3:29:ARG:HH12	1.56	0.71
8:B:162:MET:CE	8:B:308:LEU:HD21	2.19	0.70
1:0:1118:A:H62	1:0:1244:U:H3	1.38	0.70
8:B:98:THR:HG22	8:B:99:GLU:H	1.56	0.70
19:M:28:GLN:O	19:M:32:ARG:HG3	1.90	0.70
29:W:137:GLN:HE21	29:W:141:HIS:CE1	2.05	0.70
28:V:12:THR:HG22	28:V:15:GLU:CG	2.20	0.70
6:9:28:U:H5''	20:N:40:ASN:ND2	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:212:GLN:HB2	8:B:257:THR:HG21	1.74	0.70
14:H:49:GLN:HE21	14:H:140:TYR:HE2	1.40	0.70
10:D:135:VAL:HG21	10:D:139:TYR:CD1	2.26	0.70
9:C:236:THR:H	9:C:239:ALA:HB3	1.57	0.70
1:O:1666:C:H2'	1:O:1667:A:H5'	1.73	0.70
17:K:74:VAL:HG11	17:K:113:ILE:HG12	1.73	0.70
16:J:93:ARG:NH1	16:J:93:ARG:HB3	2.06	0.70
9:C:235:PHE:HE2	9:C:243:VAL:HG21	1.57	0.70
24:R:8:ALA:HB1	24:R:13:THR:HG21	1.72	0.70
16:J:74:ARG:CB	16:J:74:ARG:HH11	2.03	0.70
8:B:27:ASN:H	8:B:27:ASN:HD22	1.39	0.70
24:R:39:THR:HB	24:R:42:GLU:HG3	1.74	0.69
15:I:120:ALA:O	15:I:124:VAL:HG23	1.92	0.69
1:O:338:C:H4'	9:C:174:ILE:CD1	2.22	0.69
27:U:9:CYS:HA	27:U:52:THR:HG23	1.75	0.69
6:9:2:U:OP2	6:9:3:A:H5'	1.92	0.69
1:O:1181:A:H5'	15:I:89:GLU:OE2	1.92	0.69
18:L:67:ARG:O	18:L:71:GLU:HG3	1.92	0.69
26:T:16:LEU:HA	26:T:19:ARG:HG3	1.74	0.69
29:W:88:THR:HG23	29:W:110:GLN:HB3	1.73	0.69
1:O:553:G:P	31:Y:204:ARG:HH22	2.16	0.69
29:W:6:GLN:HG2	29:W:29:VAL:HA	1.75	0.69
1:O:338:C:H4'	9:C:174:ILE:HD11	1.75	0.69
8:B:71:VAL:HG11	8:B:296:LEU:HB3	1.74	0.69
11:E:3:VAL:HG22	11:E:49:ILE:HB	1.74	0.69
1:O:1119:G:H22	1:O:1246:A:H2	1.40	0.69
1:O:2054:A:N3	24:R:128:ARG:NH2	2.40	0.69
1:O:1834:C:H2'	1:O:1840:A:N6	2.08	0.68
25:S:57:THR:HG22	25:S:59:ASP:N	2.07	0.68
22:P:115:SER:OG	22:P:118:GLN:HG3	1.94	0.68
12:F:58:GLU:HA	12:F:61:MET:HE2	1.75	0.68
1:O:69:A:H5'	1:O:69:A:C8	2.28	0.68
1:O:2346:C:O2'	10:D:52:THR:HG21	1.94	0.68
1:O:2364:A:H5''	23:Q:15:LYS:HD3	1.75	0.68
25:S:77:VAL:O	25:S:80:ARG:HG2	1.94	0.68
1:O:2690:U:O2'	11:E:111:LYS:HE3	1.94	0.68
11:E:137:ASP:OD1	11:E:139:GLU:HB2	1.93	0.68
11:E:8:PRO:HB2	11:E:11:VAL:HG23	1.74	0.68
9:C:246:ARG:NH1	9:C:246:ARG:HB3	2.07	0.68
22:P:103:THR:O	22:P:107:GLU:HG3	1.93	0.68
7:A:105:VAL:HG11	7:A:154:ALA:HB1	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:200:PRO:HG2	7:A:225:VAL:HG21	1.75	0.68
1:O:2629:C:H41	7:A:206:ARG:HH21	1.39	0.68
19:M:48:LYS:HE3	19:M:52:GLN:NE2	2.08	0.68
26:T:52:ARG:HB2	26:T:95:ASN:HB3	1.75	0.68
7:A:164:ARG:HA	32:Z:69:TYR:CE1	2.28	0.68
17:K:14:LYS:HB2	17:K:45:PRO:HG2	1.75	0.68
20:N:48:VAL:HG11	20:N:55:ASP:HB3	1.75	0.67
8:B:305:ASP:O	8:B:306:LYS:HB2	1.94	0.67
7:A:199:HIS:HD2	7:A:201:PHE:H	1.42	0.67
12:F:58:GLU:CD	19:M:27:ARG:HH22	1.97	0.67
17:K:74:VAL:HG12	17:K:75:ARG:HG3	1.76	0.67
9:C:246:ARG:HH11	9:C:246:ARG:HB3	1.57	0.67
7:A:105:VAL:HG13	7:A:155:THR:O	1.94	0.67
1:O:1116:U:O2'	1:O:1118:A:H2	1.69	0.67
1:O:1189:A:H1'	1:O:1209:C:H1'	1.76	0.67
3:2:36:ASN:HB3	3:2:39:ARG:HE	1.59	0.67
10:D:58:VAL:HG12	10:D:60:GLU:HG2	1.77	0.67
6:9:39:U:H1'	6:9:44:A:H61	1.59	0.67
24:R:111:ILE:HG23	24:R:145:LEU:HD11	1.76	0.67
1:O:1189:A:H1'	1:O:1209:C:C1'	2.23	0.67
28:V:39:ALA:N	28:V:40:PRO:HD2	2.09	0.67
1:O:1632:A:H2'	1:O:1633:C:H5'	1.77	0.67
13:G:64:ASN:N	13:G:64:ASN:HD22	1.90	0.67
24:R:99:ALA:HB1	24:R:109:MET:CE	2.23	0.67
6:9:6:C:C5'	20:N:37:ARG:NH1	2.55	0.67
11:E:37:ASP:OD1	16:J:125:SER:HB3	1.94	0.67
7:A:190:ARG:NH2	7:A:207:GLN:OE1	2.28	0.67
32:Z:78:THR:O	32:Z:81:ARG:HB2	1.95	0.67
29:W:13:MET:HE1	29:W:17:ILE:HG22	1.77	0.67
1:O:447:A:P	26:T:1:SER:HB2	2.35	0.67
11:E:81:GLU:HG2	11:E:134:SER:HB3	1.76	0.67
1:O:2769:C:O2'	1:O:2770:G:H5'	1.95	0.67
27:U:14:GLU:O	27:U:17:THR:HB	1.94	0.66
8:B:132:HIS:NE2	8:B:171:VAL:HG23	2.08	0.66
32:Z:10:ARG:HG3	32:Z:11:SER:H	1.60	0.66
21:O:47:ARG:HG3	21:O:47:ARG:HH11	1.59	0.66
30:X:44:ASP:HB3	30:X:46:ASP:OD1	1.95	0.66
6:9:29:C:H2'	6:9:30:C:H5'	1.76	0.66
8:B:314:ALA:HB3	8:B:317:PRO:HG3	1.78	0.66
1:O:657:G:OP1	9:C:27:ARG:NH2	2.28	0.66
10:D:146:LYS:NZ	20:N:107:ASN:HD21	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2769:C:C2'	1:0:2770:G:H5'	2.26	0.66
1:0:1641:A:H2'	1:0:1642:A:H5'	1.77	0.66
29:W:6:GLN:HB2	29:W:26:ILE:CD1	2.26	0.66
14:H:48:VAL:HA	14:H:170:ARG:O	1.94	0.66
26:T:71:VAL:CG1	26:T:90:PRO:HB3	2.21	0.66
1:0:1328:A:OP1	31:Y:169:ARG:HD2	1.94	0.66
1:0:1119:G:N2	1:0:1246:A:C2	2.60	0.66
1:0:506:G:H22	1:0:509:A:H5''	1.61	0.66
8:B:66:GLU:OE1	8:B:328:ARG:HD2	1.96	0.66
30:X:47:ALA:HB1	30:X:82:GLU:HB3	1.75	0.66
1:0:1819:G:H2'	1:0:1820:G:H4'	1.78	0.66
7:A:94:LEU:N	7:A:94:LEU:HD23	2.11	0.66
1:0:1183:C:N4	1:0:1184:C:H41	1.94	0.66
12:F:91:VAL:CG1	12:F:92:GLY:H	2.10	0.65
29:W:48:VAL:HG12	29:W:52:VAL:HB	1.78	0.65
7:A:217:ARG:HG2	7:A:229:ALA:HB2	1.77	0.65
9:C:142:ASP:OD1	9:C:237:GLU:HB3	1.97	0.65
8:B:56:ASP:OD1	8:B:322:ARG:HB3	1.97	0.65
29:W:21:LEU:HD22	29:W:26:ILE:HD13	1.78	0.65
3:2:41:HIS:HD2	3:2:44:ARG:H	1.45	0.65
20:N:61:ALA:HB3	20:N:88:ALA:HB2	1.78	0.65
7:A:164:ARG:HA	32:Z:69:TYR:HE1	1.62	0.65
29:W:65:VAL:HA	29:W:68:THR:CG2	2.26	0.65
20:N:17:ARG:HB3	20:N:17:ARG:HH11	1.61	0.65
9:C:115:LEU:HD21	9:C:243:VAL:HG13	1.77	0.65
1:0:69:A:H5'	1:0:69:A:H8	1.62	0.65
8:B:141:ARG:HG2	8:B:165:ARG:HA	1.78	0.65
14:H:12:ILE:O	14:H:12:ILE:HG22	1.97	0.65
6:9:29:C:O3'	10:D:138:GLY:HA2	1.97	0.65
27:U:52:THR:HG22	27:U:54:THR:H	1.61	0.65
1:0:2780:C:H1'	11:E:143:GLN:HE21	1.61	0.65
1:0:2420:G:O2'	1:0:2421:G:H5'	1.96	0.65
14:H:62:HIS:HA	14:H:65:LEU:HD23	1.79	0.65
16:J:74:ARG:O	16:J:78:ILE:HG12	1.97	0.64
6:9:13:A:O2'	6:9:14:G:H5''	1.97	0.64
10:D:50:VAL:O	10:D:71:ALA:HA	1.97	0.64
12:F:37:THR:O	12:F:41:GLU:HG3	1.98	0.64
1:0:1234:U:N3	8:B:244:PRO:HB3	2.12	0.64
1:0:1377:C:H6	1:0:1377:C:H5'	1.62	0.64
1:0:1964:U:O2	1:0:1964:U:H2'	1.97	0.64
1:0:656:G:C5'	21:O:3:THR:HG22	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:125:GLU:O	8:B:129:ARG:HG3	1.97	0.64
2:1:21:ARG:HD2	2:1:37:CYS:SG	2.37	0.64
6:9:6:C:C5'	20:N:37:ARG:HH12	2.02	0.64
20:N:34:LEU:HA	20:N:47:LEU:HD23	1.78	0.64
11:E:137:ASP:O	11:E:141:VAL:HG23	1.97	0.64
7:A:153:ARG:CB	7:A:153:ARG:HH11	2.11	0.64
13:G:27:ILE:HD13	13:G:71:LEU:HD23	1.78	0.64
31:Y:106:THR:HG23	31:Y:107:PRO:HD2	1.79	0.64
1:0:1973:A:H8	1:0:1973:A:H5'	1.61	0.64
1:0:2548:C:OP2	8:B:5:ARG:NH2	2.31	0.64
20:N:176:ARG:O	20:N:180:LEU:HD13	1.98	0.64
1:0:796:A:HO2'	32:Z:10:ARG:N	1.96	0.64
14:H:146:ALA:O	14:H:149:VAL:HG12	1.98	0.64
20:N:154:LEU:C	20:N:156:GLU:H	1.99	0.64
8:B:51:VAL:HG13	8:B:53:LEU:HD13	1.80	0.64
18:L:143:THR:HG22	18:L:144:ASP:N	2.12	0.64
7:A:121:ALA:O	7:A:124:VAL:HG22	1.98	0.64
12:F:50:VAL:HG13	12:F:60:VAL:HG11	1.80	0.64
7:A:43:VAL:HG21	7:A:59:GLU:HG3	1.79	0.64
1:0:2850:C:H6	1:0:2850:C:H5'	1.63	0.64
1:0:944:G:H21	29:W:44:MET:CE	2.11	0.63
6:9:69:U:OP1	20:N:4:PRO:HG3	1.98	0.63
10:D:63:ILE:HG13	10:D:64:ARG:N	2.11	0.63
16:J:6:PHE:HB3	16:J:109:TYR:OH	1.98	0.63
1:0:544:G:H2'	1:0:545:G:H5''	1.81	0.63
24:R:18:LEU:HD12	24:R:143:VAL:HG11	1.80	0.63
14:H:26:ILE:HA	14:H:123:ILE:HG21	1.78	0.63
19:M:60:VAL:C	19:M:61:ILE:HD12	2.19	0.63
15:I:102:GLN:HA	15:I:105:GLU:OE2	1.99	0.63
1:0:1130:U:H2'	1:0:1131:G:O4'	1.99	0.63
1:0:1058:A:H2'	1:0:1060:C:H5''	1.80	0.63
1:0:2851:G:O2'	1:0:2852:A:H5'	1.98	0.63
1:0:281:U:H2'	1:0:282:C:O4'	1.98	0.63
14:H:30:LYS:H	14:H:62:HIS:CD2	2.17	0.63
1:0:399:C:H5'	19:M:179:GLY:O	1.99	0.63
8:B:248:ARG:O	8:B:251:VAL:HG13	1.99	0.63
20:N:47:LEU:CD1	20:N:97:VAL:HG11	2.29	0.63
29:W:22:GLU:HG2	29:W:27:HIS:CD2	2.34	0.63
1:0:2036:C:O4'	17:K:44:LEU:HG	1.98	0.63
1:0:2563:U:H2'	1:0:2565:C:O5'	1.99	0.63
21:O:50:ARG:HD2	21:O:51:TYR:CE1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1118:A:H8	1:0:1119:G:H5''	1.64	0.63
27:U:52:THR:HG22	27:U:54:THR:N	2.13	0.63
29:W:38:THR:HG22	29:W:39:ASP:N	2.14	0.63
1:0:709:G:O2'	21:O:25:VAL:HG12	1.99	0.63
25:S:42:GLU:HG2	25:S:49:VAL:HG23	1.80	0.63
9:C:7:ASP:OD2	9:C:9:ASP:HB2	1.99	0.62
1:0:1187:U:O2'	1:0:1189:A:H2	1.78	0.62
8:B:132:HIS:HB2	8:B:137:LEU:HD22	1.81	0.62
13:G:23:ILE:O	13:G:27:ILE:HG13	1.98	0.62
16:J:130:VAL:HG12	16:J:131:THR:N	2.14	0.62
29:W:21:LEU:HD22	29:W:26:ILE:HD11	1.81	0.62
9:C:72:LYS:HG2	9:C:77:ALA:HA	1.81	0.62
8:B:5:ARG:HD2	8:B:8:LYS:NZ	2.15	0.62
16:J:57:TYR:O	16:J:61:VAL:HG23	1.99	0.62
29:W:13:MET:CE	29:W:17:ILE:HG22	2.29	0.62
12:F:69:GLU:O	12:F:70:LYS:HG2	2.00	0.62
30:X:43:VAL:HG12	30:X:44:ASP:N	2.14	0.62
14:H:30:LYS:H	14:H:62:HIS:HD2	1.45	0.62
6:9:14:G:H5'	6:9:14:G:C8	2.34	0.62
7:A:191:GLY:HA2	7:A:194:MET:HE2	1.82	0.62
7:A:191:GLY:HA2	7:A:194:MET:HE3	1.81	0.62
20:N:154:LEU:O	20:N:155:GLU:HB3	2.00	0.62
1:0:156:C:H5''	19:M:171:ARG:CD	2.23	0.62
2:1:8:GLN:HE22	2:1:11:LYS:HZ1	1.48	0.62
25:S:33:SER:OG	25:S:36:GLU:HG3	2.00	0.62
1:0:1053:G:OP1	14:H:15:PRO:HG3	1.99	0.62
14:H:12:ILE:HG23	14:H:129:ARG:NE	2.14	0.62
8:B:312:ARG:HD3	8:B:315:VAL:HG13	1.81	0.62
11:E:6:GLU:HA	11:E:46:THR:HG22	1.82	0.62
1:0:645:U:OP2	18:L:4:LYS:HE2	1.99	0.62
26:T:71:VAL:HG11	26:T:90:PRO:CB	2.21	0.62
10:D:54:ALA:HB2	10:D:69:ILE:HD12	1.82	0.61
7:A:76:VAL:HG23	32:Z:63:LYS:HB3	1.81	0.61
30:X:76:ARG:NH1	30:X:76:ARG:HG3	2.14	0.61
16:J:19:MET:CE	16:J:132:LEU:HD11	2.30	0.61
6:9:48:C:H4'	20:N:141:ARG:NH2	2.15	0.61
1:0:1741:U:H5'	1:0:1742:A:OP1	2.00	0.61
15:I:119:ALA:O	15:I:123:VAL:HG23	2.00	0.61
1:0:1299:G:O6	18:L:6:ARG:HD3	1.99	0.61
1:0:902:G:N7	18:L:18:HIS:HD2	1.98	0.61
31:Y:189:ASN:HD22	31:Y:189:ASN:C	2.04	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1835:U:C5	1:0:1840:A:N7	2.63	0.61
12:F:91:VAL:CG1	12:F:92:GLY:N	2.62	0.61
22:P:135:ALA:HB1	22:P:139:ARG:NH1	2.14	0.61
24:R:39:THR:HG23	24:R:107:GLU:O	2.01	0.61
10:D:84:LEU:HA	10:D:87:ALA:HB3	1.82	0.61
7:A:199:HIS:CD2	7:A:201:PHE:H	2.17	0.61
1:0:2414:A:H2'	1:0:2415:A:C8	2.35	0.61
18:L:143:THR:HG22	18:L:145:LEU:H	1.64	0.61
1:0:681:G:N3	1:0:681:G:H5'	2.15	0.61
1:0:871:G:C8	1:0:871:G:C5'	2.77	0.61
16:J:75:PRO:HG2	16:J:105:LEU:CD2	2.30	0.61
11:E:125:GLU:HB2	11:E:132:THR:HG23	1.82	0.61
14:H:32:ALA:HB3	14:H:69:ARG:NH1	2.14	0.61
12:F:61:MET:HB3	19:M:19:GLN:OE1	2.00	0.61
23:Q:26:PRO:O	23:Q:30:VAL:HG22	2.01	0.61
20:N:119:GLN:O	20:N:123:ILE:HG13	2.00	0.61
20:N:47:LEU:HD13	20:N:97:VAL:HG11	1.82	0.61
29:W:68:THR:HG23	29:W:69:ARG:HG2	1.83	0.61
1:0:1477:C:H5'	1:0:1868:G:C5'	2.31	0.61
1:0:2649:A:H5'	1:0:2649:A:H8	1.65	0.61
32:Z:57:CYS:SG	32:Z:59:TYR:HB3	2.41	0.60
1:0:1118:A:C8	1:0:1118:A:C3'	2.81	0.60
1:0:1168:C:H5'	15:I:83:GLY:HA3	1.83	0.60
1:0:1667:A:C8	1:0:1667:A:H5'	2.34	0.60
8:B:254:GLN:HG2	8:B:255:GLY:N	2.15	0.60
1:0:2265:U:H2'	1:0:2266:A:C8	2.36	0.60
7:A:105:VAL:CG1	7:A:154:ALA:HB1	2.30	0.60
1:0:2827:A:H2'	1:0:2828:G:O4'	2.01	0.60
18:L:73:VAL:HG11	18:L:118:LEU:HD21	1.83	0.60
16:J:107:ASN:HD21	16:J:109:TYR:HB2	1.65	0.60
10:D:63:ILE:CG1	10:D:64:ARG:H	2.10	0.60
1:0:1701:A:H4'	1:0:1702:U:C5'	2.30	0.60
1:0:1701:A:H5''	1:0:1702:U:H3'	1.83	0.60
11:E:11:VAL:HG12	11:E:12:ASP:N	2.16	0.60
13:G:16:LYS:O	13:G:20:VAL:HG23	2.01	0.60
20:N:176:ARG:HE	20:N:180:LEU:HD21	1.65	0.60
14:H:27:PRO:HD3	14:H:123:ILE:HG22	1.84	0.60
1:0:2270:G:H4'	7:A:223:ARG:HH12	1.66	0.60
24:R:82:GLU:O	24:R:86:LYS:HG3	2.01	0.60
4:3:70:ARG:HG2	4:3:77:ALA:HB2	1.82	0.60
8:B:271:ASP:HB3	8:B:296:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:12:THR:HG22	24:R:149:GLU:OE1	2.01	0.60
1:0:2468:A:H61	4:3:48:ASN:HD21	1.49	0.60
24:R:132:ARG:HG2	24:R:133:ALA:N	2.17	0.60
1:0:1080:C:H4'	1:0:1081:A:OP1	2.02	0.60
7:A:211:LYS:HB3	7:A:212:PRO:CD	2.30	0.60
22:P:115:SER:O	22:P:117:SER:N	2.31	0.60
8:B:41:PHE:HA	8:B:79:MET:HE2	1.83	0.60
29:W:88:THR:HG23	29:W:110:GLN:NE2	2.17	0.60
9:C:115:LEU:O	9:C:118:THR:HB	2.02	0.60
28:V:39:ALA:C	28:V:41:GLU:H	2.06	0.60
1:0:797:A:C4'	32:Z:10:ARG:N	2.65	0.60
8:B:62:ARG:CA	8:B:65:MET:HE3	2.29	0.60
16:J:107:ASN:ND2	16:J:109:TYR:H	1.99	0.60
1:0:1285:U:H4'	29:W:74:GLU:OE1	2.02	0.60
7:A:88:ILE:HG22	7:A:88:ILE:O	2.02	0.59
24:R:18:LEU:HD12	24:R:143:VAL:CG1	2.32	0.59
1:0:558:C:H2'	1:0:559:U:C5'	2.32	0.59
12:F:14:ASP:O	12:F:18:GLU:HG3	2.02	0.59
2:1:25:LYS:O	2:1:25:LYS:HG2	2.02	0.59
1:0:1589:G:N2	1:0:1605:G:H1'	2.16	0.59
10:D:146:LYS:NZ	20:N:107:ASN:ND2	2.49	0.59
7:A:161:GLY:O	32:Z:68:SER:HB2	2.02	0.59
1:0:259:G:H21	19:M:58:GLN:NE2	2.00	0.59
13:G:64:ASN:N	13:G:64:ASN:ND2	2.48	0.59
31:Y:151:SER:HB3	31:Y:154:ARG:HB3	1.83	0.59
17:K:62:PRO:HG3	17:K:65:ARG:NH2	2.18	0.59
22:P:134:VAL:O	22:P:137:LEU:HB3	2.02	0.59
14:H:49:GLN:HG3	14:H:140:TYR:CE2	2.37	0.59
22:P:7:LYS:HD3	22:P:21:VAL:CG2	2.32	0.59
3:2:22:PRO:HG2	3:2:25:VAL:CG2	2.32	0.59
23:Q:18:PRO:O	23:Q:21:ARG:HB2	2.03	0.59
28:V:38:GLY:C	28:V:40:PRO:HD2	2.23	0.59
1:0:407:A:H2'	1:0:408:A:C8	2.38	0.59
12:F:27:GLY:HA3	12:F:101:ALA:O	2.02	0.59
1:0:2694:A:H4'	11:E:91:PHE:HE1	1.66	0.59
29:W:21:LEU:HD13	29:W:26:ILE:HD11	1.84	0.59
11:E:133:VAL:HG12	11:E:141:VAL:HG13	1.85	0.59
29:W:73:LEU:HD22	29:W:111:GLY:HA2	1.85	0.59
22:P:61:ARG:HB2	22:P:61:ARG:HH11	1.68	0.59
11:E:116:THR:HG22	11:E:151:LEU:HD22	1.84	0.59
29:W:4:LEU:CD2	29:W:54:PHE:HB3	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:660:A:H4'	1:0:661:G:O5'	2.03	0.59
17:K:82:ARG:NH2	17:K:115:ARG:HG2	2.18	0.59
12:F:52:GLU:HG3	12:F:77:VAL:O	2.03	0.59
31:Y:189:ASN:HA	31:Y:217:ILE:HD11	1.84	0.59
10:D:23:VAL:HG23	10:D:23:VAL:O	2.03	0.59
7:A:33:GLU:OE1	7:A:33:GLU:N	2.35	0.59
1:0:2635:A:O2'	1:0:2636:C:H5'	2.03	0.59
15:I:129:SER:O	15:I:130:LEU:HD23	2.03	0.59
20:N:38:LYS:HD2	20:N:114:LYS:HE3	1.85	0.59
1:0:2408:A:H4'	4:3:15:ASN:O	2.03	0.59
19:M:134:ILE:HG23	19:M:141:ILE:HD13	1.85	0.59
16:J:39:VAL:HG12	16:J:40:ASN:ND2	2.18	0.58
1:0:1741:U:O2'	1:0:2723:G:H4'	2.03	0.58
30:X:25:ARG:HD3	30:X:64:ALA:O	2.01	0.58
12:F:19:ALA:O	12:F:22:VAL:HG22	2.02	0.58
8:B:280:VAL:HG13	8:B:333:GLU:O	2.02	0.58
8:B:275:GLY:O	8:B:291:ASP:HA	2.03	0.58
30:X:72:VAL:HG22	30:X:85:VAL:CG1	2.32	0.58
17:K:55:VAL:HG12	17:K:56:SER:N	2.19	0.58
1:0:506:G:H22	1:0:509:A:H5'	1.66	0.58
1:0:1733:A:H4'	8:B:212:GLN:HA	1.85	0.58
24:R:99:ALA:HB1	24:R:109:MET:HE3	1.83	0.58
26:T:26:THR:HA	26:T:39:ASN:HB3	1.85	0.58
19:M:164:THR:HG22	19:M:166:ALA:N	2.18	0.58
1:0:2629:C:N4	7:A:206:ARG:HH21	2.01	0.58
1:0:583:C:H2'	1:0:584:U:H6	1.67	0.58
1:0:2363:G:O2'	23:Q:11:ARG:HG3	2.03	0.58
24:R:119:VAL:HG21	24:R:142:ASP:CG	2.23	0.58
1:0:280:C:H2'	1:0:281:U:O4'	2.03	0.58
20:N:164:ASP:CG	20:N:167:ASP:HA	2.24	0.58
1:0:558:C:C2'	1:0:559:U:H5''	2.34	0.58
16:J:131:THR:HG22	16:J:134:GLU:H	1.68	0.58
20:N:100:ALA:O	20:N:129:ILE:HG23	2.03	0.58
30:X:10:VAL:HG11	30:X:36:HIS:HE1	1.69	0.58
1:0:1603:A:H5''	1:0:1605:G:H5'	1.86	0.58
1:0:2779:G:H21	11:E:143:GLN:NE2	2.01	0.58
28:V:39:ALA:N	28:V:40:PRO:CD	2.66	0.58
3:2:22:PRO:HG2	3:2:25:VAL:HG23	1.86	0.58
1:0:256:C:H2'	1:0:257:G:O4'	2.03	0.58
12:F:111:ILE:O	12:F:115:VAL:HG23	2.03	0.58
20:N:78:MET:HB2	20:N:79:PRO:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:99:ILE:O	7:A:131:HIS:HE1	1.87	0.58
16:J:107:ASN:HD22	16:J:107:ASN:C	2.05	0.58
1:O:2815:G:OP2	16:J:99:GLU:HG2	2.04	0.58
1:O:2064:U:H5'	1:O:2652:U:H4'	1.86	0.58
8:B:278:PRO:HD3	8:B:294:TYR:CE2	2.39	0.58
7:A:39:ALA:HB3	7:A:61:GLU:OE2	2.03	0.58
1:O:1118:A:C8	1:O:1119:G:H5''	2.38	0.58
9:C:1:MET:HG2	9:C:2:GLN:N	2.14	0.58
18:L:149:ARG:O	18:L:150:GLN:HB3	2.04	0.58
30:X:31:ILE:O	30:X:35:GLU:HG3	2.03	0.58
1:O:1244:U:OP1	16:J:18:ILE:HD13	2.04	0.58
20:N:97:VAL:HG12	20:N:127:LEU:HD11	1.85	0.58
1:O:1766:U:O2	1:O:1778:A:H5'	2.04	0.58
1:O:1278:A:H4'	1:O:1279:U:C4	2.39	0.58
1:O:21:G:H4'	24:R:2:ILE:HG22	1.85	0.58
3:2:36:ASN:HB3	3:2:39:ARG:NE	2.17	0.58
17:K:4:LEU:HD22	17:K:116:GLU:HB3	1.86	0.58
1:O:2676:C:H4'	16:J:70:PHE:CE1	2.39	0.58
25:S:33:SER:O	25:S:37:VAL:HG23	2.04	0.58
1:O:583:C:H2'	1:O:584:U:C6	2.39	0.58
1:O:1687:C:O2	2:1:9:GLY:HA2	2.04	0.58
15:I:73:LEU:HD12	15:I:107:LYS:HZ2	1.68	0.58
9:C:233:THR:HG22	9:C:234:VAL:H	1.69	0.58
1:O:968:G:H1'	14:H:35:LYS:HD2	1.85	0.58
26:T:50:VAL:HG12	26:T:56:ALA:HA	1.85	0.58
1:O:588:G:O6	29:W:154:ARG:NH1	2.37	0.58
16:J:52:GLN:HG3	16:J:53:ILE:N	2.19	0.57
8:B:205:VAL:O	8:B:307:ARG:NE	2.37	0.57
13:G:23:ILE:HG22	13:G:27:ILE:HD11	1.86	0.57
18:L:145:LEU:O	18:L:148:GLU:HG3	2.04	0.57
16:J:131:THR:HG22	16:J:133:GLY:N	2.19	0.57
31:Y:97:LEU:HD21	31:Y:235:GLU:OE2	2.04	0.57
9:C:77:ALA:O	9:C:78:ARG:HG3	2.04	0.57
1:O:1527:A:H1'	1:O:1528:A:C8	2.39	0.57
32:Z:72:GLU:OE1	32:Z:77:LYS:HE2	2.05	0.57
1:O:635:A:H2'	1:O:636:G:H5''	1.86	0.57
1:O:945:U:H2'	1:O:946:C:C6	2.40	0.57
28:V:49:LEU:O	28:V:53:ILE:HG13	2.04	0.57
1:O:1120:U:H5''	1:O:1120:U:C6	2.39	0.57
1:O:2824:C:H5''	1:O:2825:C:H5'	1.87	0.57
1:O:1060:C:H6	1:O:1060:C:H5'	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1771:U:H5'	32:Z:20:ARG:HH21	1.67	0.57
20:N:110:THR:HB	20:N:113:SER:OG	2.04	0.57
1:0:1555:G:H4'	1:0:1630:A:H2	1.69	0.57
6:9:54:A:O2'	6:9:55:U:H5'	2.03	0.57
24:R:111:ILE:HG23	24:R:145:LEU:CD1	2.35	0.57
7:A:94:LEU:HG	7:A:99:ILE:HD11	1.87	0.57
1:0:2721:U:H4'	17:K:87:ARG:HG3	1.86	0.57
25:S:53:ASN:N	25:S:53:ASN:HD22	2.02	0.57
10:D:23:VAL:HG21	10:D:45:THR:HG21	1.87	0.57
1:0:2505:G:O2'	1:0:2506:A:H5'	2.04	0.57
1:0:2036:C:C1'	17:K:44:LEU:HG	2.34	0.57
29:W:122:ARG:HH11	29:W:122:ARG:HG3	1.69	0.57
1:0:1162:G:H1'	15:I:112:LEU:HD11	1.87	0.57
6:9:6:C:OP1	20:N:37:ARG:NH1	2.38	0.57
29:W:21:LEU:HB3	29:W:26:ILE:HG12	1.87	0.57
8:B:55:ASN:CB	8:B:63:GLU:HA	2.33	0.57
17:K:113:ILE:HD12	17:K:128:ALA:HB2	1.87	0.57
29:W:88:THR:HG22	29:W:89:ASP:N	2.19	0.57
29:W:65:VAL:HG12	29:W:116:LEU:HD13	1.86	0.57
22:P:59:ARG:O	22:P:63:ARG:HG3	2.04	0.57
1:0:558:C:H2'	1:0:559:U:H5'	1.87	0.57
14:H:49:GLN:HG3	14:H:140:TYR:CD2	2.40	0.57
15:I:118:ASN:HA	15:I:121:LYS:HD2	1.86	0.57
1:0:2649:A:C8	1:0:2649:A:H5'	2.40	0.57
1:0:1162:G:H1'	15:I:112:LEU:CD1	2.35	0.57
15:I:71:ALA:O	15:I:75:LYS:HG3	2.04	0.57
27:U:33:SER:O	27:U:37:GLU:HG3	2.04	0.57
1:0:2795:C:O2'	1:0:2796:U:H5'	2.04	0.57
1:0:1132:A:N6	1:0:1229:C:H2'	2.20	0.57
12:F:53:ASP:OD1	12:F:80:GLN:HB2	2.05	0.57
29:W:126:ASP:HB3	29:W:135:GLY:O	2.04	0.57
15:I:108:HIS:N	15:I:109:PRO:HD2	2.20	0.56
1:0:870:G:OP2	7:A:3:ARG:HD3	2.05	0.56
1:0:544:G:C2'	1:0:545:G:H5''	2.35	0.56
8:B:217:ARG:HG3	8:B:257:THR:CG2	2.35	0.56
7:A:217:ARG:HH11	7:A:217:ARG:HG3	1.67	0.56
1:0:1972:U:H2'	1:0:1973:A:H5'	1.88	0.56
29:W:151:GLU:O	29:W:154:ARG:HB2	2.06	0.56
1:0:1393:A:H2'	1:0:1394:C:C6	2.41	0.56
9:C:151:GLN:HA	9:C:151:GLN:HE21	1.70	0.56
1:0:2840:A:OP1	8:B:211:THR:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2668:G:H2'	1:0:2669:U:C6	2.40	0.56
31:Y:126:PRO:HG2	31:Y:128:PHE:CE1	2.40	0.56
1:0:2718:C:H6	1:0:2718:C:H5'	1.70	0.56
7:A:33:GLU:O	7:A:34:ASP:HB2	2.04	0.56
29:W:4:LEU:HD22	29:W:52:VAL:HG21	1.87	0.56
20:N:152:GLU:C	20:N:154:LEU:H	2.09	0.56
21:O:73:ASP:HA	21:O:92:VAL:O	2.04	0.56
8:B:145:HIS:HD2	8:B:146:THR:O	1.86	0.56
22:P:104:LYS:HE2	22:P:138:GLU:OE1	2.04	0.56
8:B:7:ARG:HG2	8:B:7:ARG:HH11	1.70	0.56
1:0:2271:G:OP1	7:A:223:ARG:NH2	2.38	0.56
28:V:1:THR:O	28:V:4:HIS:CE1	2.59	0.56
9:C:200:PRO:HB3	9:C:212:VAL:HG23	1.88	0.56
1:0:282:C:O2'	1:0:283:U:H5'	2.06	0.56
16:J:19:MET:HE3	16:J:132:LEU:HD11	1.88	0.56
11:E:126:ILE:HB	11:E:131:LEU:CD2	2.36	0.56
6:9:42:C:O2	10:D:76:ARG:HD2	2.04	0.56
1:0:2419:U:H5''	1:0:2420:G:H5'	1.88	0.56
29:W:147:ASP:O	29:W:151:GLU:HB2	2.06	0.56
1:0:2601:A:N1	17:K:38:SER:HB2	2.20	0.56
14:H:61:ARG:HG3	14:H:61:ARG:HH11	1.71	0.56
1:0:1446:U:H2'	25:S:55:GLN:NE2	2.20	0.56
21:O:32:ARG:HD3	21:O:32:ARG:O	2.04	0.56
1:0:1666:C:H2'	1:0:1667:A:C5'	2.35	0.56
17:K:109:LEU:HD13	17:K:113:ILE:HD11	1.87	0.56
1:0:797:A:H4'	32:Z:10:ARG:N	2.21	0.56
10:D:146:LYS:HZ3	20:N:107:ASN:HD21	1.53	0.56
7:A:64:ASP:OD1	7:A:66:ARG:HD2	2.04	0.56
1:0:1735:C:OP2	8:B:234:ARG:HG3	2.06	0.56
28:V:64:GLY:O	28:V:65:ASP:HB2	2.05	0.56
1:0:694:A:H2'	1:0:695:C:H5'	1.87	0.56
1:0:538:C:OP2	31:Y:134:HIS:HE1	1.87	0.56
18:L:72:ASN:OD1	18:L:75:LEU:HD12	2.06	0.56
1:0:952:G:N3	1:0:2302:A:H2'	2.21	0.56
11:E:154:ILE:HD11	11:E:157:LYS:HB2	1.88	0.56
1:0:447:A:O2'	1:0:448:G:H5'	2.06	0.56
15:I:101:LYS:O	15:I:105:GLU:HG3	2.05	0.56
14:H:43:ALA:HB1	14:H:140:TYR:CE2	2.41	0.56
27:U:17:THR:HG22	27:U:18:GLY:N	2.21	0.56
20:N:86:LEU:HD12	20:N:125:ALA:HB2	1.88	0.56
11:E:154:ILE:HD11	11:E:157:LYS:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:168:ARG:NH2	9:C:190:ALA:O	2.39	0.56
20:N:43:VAL:HG13	20:N:118:ILE:HD11	1.88	0.56
17:K:32:ILE:HD11	17:K:56:SER:HB3	1.87	0.56
1:0:447:A:OP2	26:T:1:SER:HB2	2.05	0.56
1:0:92:G:H4'	28:V:44:GLY:HA3	1.87	0.56
22:P:13:VAL:HG21	22:P:41:ARG:HG2	1.87	0.56
1:0:737:A:H2'	1:0:738:G:O4'	2.06	0.56
9:C:127:ARG:HG2	9:C:127:ARG:HH11	1.71	0.56
1:0:1189:A:H1'	1:0:1209:C:O4'	2.06	0.56
17:K:14:LYS:CB	17:K:45:PRO:HG2	2.36	0.56
20:N:94:GLU:HG3	20:N:186:LEU:HD12	1.88	0.56
8:B:307:ARG:HB2	8:B:307:ARG:HH11	1.70	0.55
30:X:78:GLU:HG2	30:X:79:GLU:N	2.21	0.55
27:U:46:ALA:HB1	27:U:52:THR:HG21	1.88	0.55
27:U:9:CYS:CA	27:U:52:THR:HG23	2.36	0.55
8:B:314:ALA:CB	8:B:317:PRO:HG3	2.36	0.55
8:B:141:ARG:HD2	8:B:163:GLU:OE2	2.06	0.55
1:0:316:A:H5'	26:T:54:ASP:OD2	2.06	0.55
29:W:59:GLN:HE22	29:W:97:ALA:HB3	1.70	0.55
1:0:638:C:H2'	1:0:639:A:C8	2.41	0.55
1:0:558:C:O2'	1:0:559:U:H5''	2.07	0.55
15:I:118:ASN:HA	15:I:121:LYS:CD	2.37	0.55
1:0:2300:A:H4'	1:0:2301:A:O5'	2.06	0.55
11:E:21:THR:HG23	11:E:30:THR:OG1	2.06	0.55
12:F:21:GLU:O	12:F:24:ARG:HG3	2.05	0.55
1:0:90:A:H2'	1:0:91:G:O4'	2.06	0.55
1:0:1014:A:H2'	1:0:1015:C:H5'	1.88	0.55
10:D:154:LYS:H	10:D:154:LYS:CD	2.05	0.55
29:W:88:THR:HG23	29:W:110:GLN:HE21	1.70	0.55
1:0:1926:G:H2'	1:0:1927:A:C8	2.41	0.55
11:E:84:MET:HG2	11:E:168:ILE:HD13	1.88	0.55
1:0:1632:A:C2'	1:0:1633:C:H5'	2.36	0.55
8:B:329:TYR:CE2	27:U:15:PRO:HG2	2.42	0.55
20:N:38:LYS:HE2	20:N:107:ASN:HD21	1.71	0.55
12:F:46:GLU:O	12:F:73:PRO:HD2	2.06	0.55
1:0:1236:A:H2'	1:0:1237:U:O4'	2.06	0.55
32:Z:32:GLU:HA	32:Z:35:GLU:HG3	1.87	0.55
20:N:49:THR:HG22	20:N:50:LEU:N	2.21	0.55
1:0:282:C:H2'	1:0:283:U:O4'	2.07	0.55
19:M:164:THR:CG2	19:M:165:GLY:N	2.69	0.55
15:I:113:SER:HB2	15:I:118:ASN:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2081:A:H4'	16:J:69:TYR:CE1	2.41	0.55
2:1:25:LYS:HD2	3:2:49:GLU:N	2.19	0.55
1:0:470:U:O2'	2:1:16:HIS:CD2	2.59	0.55
3:2:36:ASN:HB3	3:2:39:ARG:HG3	1.88	0.55
7:A:66:ARG:HH11	7:A:66:ARG:HB2	1.71	0.55
1:0:1847:A:OP1	7:A:175:LYS:HG3	2.07	0.55
1:0:20:G:H21	24:R:117:HIS:HD2	1.54	0.55
27:U:11:THR:HG22	27:U:53:ASP:OD2	2.07	0.55
1:0:1159:G:H21	1:0:1189:A:H8	1.54	0.55
20:N:77:ASN:OD1	20:N:79:PRO:HD2	2.07	0.55
1:0:2807:U:P	8:B:27:ASN:HD21	2.30	0.55
29:W:6:GLN:CB	29:W:26:ILE:HD12	2.35	0.55
21:O:14:LEU:CD2	21:O:102:ILE:HD11	2.34	0.55
30:X:43:VAL:HG12	30:X:44:ASP:H	1.72	0.55
8:B:162:MET:HG3	8:B:310:ARG:CD	2.36	0.55
25:S:25:GLN:HG2	25:S:65:VAL:HG22	1.89	0.55
1:0:2365:G:H4'	23:Q:45:PRO:O	2.07	0.55
1:0:820:G:H5'	1:0:821:U:H5'	1.89	0.55
1:0:644:G:N3	1:0:644:G:H5'	2.22	0.55
24:R:18:LEU:HB2	24:R:143:VAL:CG1	2.33	0.55
28:V:12:THR:H	28:V:15:GLU:HB2	1.71	0.55
11:E:23:GLU:HG2	11:E:28:SER:HB2	1.89	0.55
29:W:59:GLN:NE2	29:W:97:ALA:HB3	2.22	0.55
17:K:132:VAL:HG11	27:U:22:VAL:HG22	1.88	0.55
6:9:55:U:H4'	6:9:56:A:C8	2.42	0.55
8:B:217:ARG:HE	8:B:257:THR:HG22	1.71	0.55
11:E:7:ILE:HD11	11:E:11:VAL:C	2.27	0.55
1:0:485:A:N3	1:0:487:G:H5''	2.22	0.55
1:0:2252:A:C5	1:0:2253:G:H1'	2.41	0.55
1:0:1666:C:C2'	1:0:1667:A:C5'	2.85	0.55
8:B:98:THR:HG22	8:B:99:GLU:N	2.22	0.55
4:3:11:CYS:HB2	4:3:20:HIS:CE1	2.42	0.55
8:B:74:ILE:HD13	8:B:309:VAL:HG21	1.88	0.55
22:P:98:ILE:HD12	22:P:102:ARG:NE	2.22	0.55
19:M:72:ALA:HB2	19:M:93:ARG:HG2	1.89	0.55
10:D:41:LEU:HA	10:D:44:ILE:HG22	1.88	0.54
1:0:1167:G:H4'	15:I:130:LEU:HD22	1.89	0.54
10:D:58:VAL:CG1	10:D:60:GLU:HG2	2.37	0.54
29:W:110:GLN:NE2	29:W:110:GLN:HA	2.22	0.54
27:U:14:GLU:OE1	27:U:15:PRO:HD2	2.07	0.54
2:1:21:ARG:HD2	2:1:39:PHE:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1972:U:H2'	1:0:1973:A:C5'	2.37	0.54
23:Q:94:GLN:O	23:Q:95:GLU:HB2	2.07	0.54
19:M:184:ARG:HG3	19:M:185:PRO:HA	1.89	0.54
6:9:44:A:O4'	10:D:76:ARG:NE	2.40	0.54
1:0:2737:C:OP2	22:P:61:ARG:NH2	2.37	0.54
1:0:1120:U:H6	1:0:1120:U:H5''	1.73	0.54
1:0:1657:A:H2'	1:0:1658:A:C8	2.42	0.54
32:Z:22:SER:O	32:Z:26:VAL:HG23	2.08	0.54
1:0:1007:A:H2'	14:H:22:TYR:CZ	2.42	0.54
27:U:52:THR:CG2	27:U:54:THR:HB	2.36	0.54
18:L:149:ARG:O	18:L:150:GLN:CB	2.55	0.54
31:Y:112:GLU:OE1	31:Y:112:GLU:HA	2.07	0.54
10:D:134:LEU:HD11	10:D:166:ILE:HD11	1.88	0.54
1:0:794:U:H3	1:0:819:A:H61	1.54	0.54
1:0:793:A:H5''	22:P:83:LYS:HG2	1.89	0.54
1:0:1441:G:O2'	1:0:1442:A:H5'	2.07	0.54
1:0:1164:U:OP1	15:I:69:PRO:HA	2.08	0.54
12:F:58:GLU:OE1	19:M:27:ARG:NH2	2.34	0.54
23:Q:53:HIS:CE1	23:Q:55:ARG:HG3	2.42	0.54
8:B:36:PRO:HG3	8:B:169:GLY:H	1.71	0.54
6:9:39:U:H1'	6:9:44:A:N6	2.22	0.54
16:J:42:GLU:O	16:J:131:THR:HG23	2.08	0.54
7:A:132:ASP:OD1	7:A:133:ARG:N	2.40	0.54
1:0:119:A:H2'	1:0:120:A:H5''	1.90	0.54
26:T:92:ASP:OD1	26:T:94:SER:HB3	2.08	0.54
22:P:20:ARG:NH1	22:P:54:LYS:HD3	2.22	0.54
14:H:87:LYS:NZ	14:H:87:LYS:HB2	2.22	0.54
24:R:99:ALA:CB	24:R:109:MET:HE3	2.37	0.54
19:M:134:ILE:CG2	19:M:141:ILE:HD13	2.38	0.54
1:0:2524:G:H21	1:0:2526:C:N4	2.05	0.54
1:0:2256:G:O2'	1:0:2257:G:H5'	2.07	0.54
18:L:125:PHE:CZ	18:L:140:VAL:HG13	2.42	0.54
20:N:33:ARG:NH1	20:N:103:ASP:OD2	2.33	0.54
26:T:38:ARG:HG3	26:T:38:ARG:HH11	1.71	0.54
6:9:20:G:O2'	6:9:21:G:H5'	2.07	0.54
22:P:7:LYS:HD3	22:P:21:VAL:HG21	1.89	0.54
1:0:1535:G:H2'	1:0:1536:C:C6	2.43	0.54
6:9:55:U:H4'	6:9:56:A:H8	1.72	0.54
29:W:4:LEU:HD22	29:W:52:VAL:CG2	2.38	0.54
12:F:50:VAL:CG1	12:F:60:VAL:HG11	2.37	0.54
1:0:1773:G:C8	32:Z:16:ALA:HA	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:1:THR:HG23	28:V:2:VAL:N	2.23	0.54
1:0:2526:C:O2'	1:0:2527:U:H5'	2.08	0.54
9:C:79:ARG:O	9:C:87:ARG:HG2	2.07	0.54
2:1:28:HIS:CD2	2:1:31:LYS:HG3	2.43	0.54
1:0:2831:C:H2'	1:0:2832:C:H5'	1.90	0.54
32:Z:46:ARG:O	32:Z:57:CYS:HA	2.08	0.54
6:9:42:C:H5'	6:9:43:G:OP2	2.08	0.54
24:R:145:LEU:HD12	24:R:146:ILE:H	1.73	0.54
1:0:1071:G:H4'	31:Y:154:ARG:NH2	2.23	0.54
1:0:475:G:H5'	9:C:73:LEU:HD23	1.88	0.54
1:0:1787:C:H4'	1:0:2883:A:O4'	2.08	0.54
22:P:80:ARG:HG2	22:P:87:ARG:CZ	2.38	0.54
10:D:18:ILE:HD13	10:D:84:LEU:HD12	1.89	0.53
21:O:78:ALA:C	21:O:98:LEU:HD13	2.29	0.53
7:A:36:ASP:HB2	7:A:83:GLY:CA	2.38	0.53
20:N:143:ARG:HA	20:N:172:PHE:CD2	2.43	0.53
27:U:9:CYS:HA	27:U:52:THR:CG2	2.38	0.53
20:N:43:VAL:CG1	20:N:118:ILE:HD11	2.38	0.53
1:0:2251:G:H2'	1:0:2252:A:C8	2.43	0.53
8:B:202:VAL:HG11	8:B:301:VAL:HG13	1.90	0.53
1:0:1786:C:OP1	22:P:74:GLN:HG2	2.08	0.53
1:0:2878:U:H2'	1:0:2879:A:O4'	2.07	0.53
20:N:72:GLU:H	20:N:171:HIS:CE1	2.27	0.53
1:0:1589:G:H22	1:0:1605:G:H1'	1.72	0.53
6:9:1:U:H4'	6:9:3:A:OP1	2.08	0.53
1:0:1528:A:H2'	1:0:1529:G:O4'	2.08	0.53
1:0:2433:A:H2'	1:0:2434:A:C8	2.42	0.53
15:I:88:GLN:HA	15:I:91:PHE:CE2	2.44	0.53
19:M:69:LYS:HG3	19:M:126:GLN:CA	2.38	0.53
10:D:10:PHE:CG	10:D:11:HIS:N	2.77	0.53
1:0:189:A:OP1	19:M:171:ARG:NH2	2.40	0.53
8:B:217:ARG:NE	8:B:257:THR:HG22	2.22	0.53
24:R:39:THR:HB	24:R:42:GLU:CG	2.37	0.53
20:N:170:GLU:O	20:N:174:GLU:HG3	2.09	0.53
1:0:1798:C:H4'	22:P:66:GLN:HG2	1.91	0.53
1:0:2769:C:H2'	1:0:2770:G:O4'	2.08	0.53
8:B:17:LYS:O	8:B:260:HIS:HD2	1.92	0.53
31:Y:107:PRO:HB3	31:Y:182:PHE:CD2	2.44	0.53
1:0:136:C:H2'	1:0:137:U:O4'	2.09	0.53
17:K:81:ARG:HD3	17:K:87:ARG:CZ	2.38	0.53
1:0:2521:A:OP2	14:H:6:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:88:LYS:O	21:O:91:GLN:HB2	2.08	0.53
26:T:49:GLU:OE2	26:T:97:ARG:NH1	2.39	0.53
1:O:2756:U:N3	1:O:2896:A:H2	2.02	0.53
24:R:40:ALA:O	24:R:44:VAL:HG23	2.07	0.53
28:V:55:ARG:O	28:V:59:ILE:HG12	2.09	0.53
1:O:1596:U:H2'	1:O:1598:A:OP2	2.09	0.53
27:U:6:CYS:HA	27:U:13:ILE:HD11	1.91	0.53
10:D:25:MET:SD	10:D:40:ILE:HD11	2.48	0.53
14:H:6:ALA:HA	14:H:61:ARG:NH1	2.24	0.53
25:S:14:ALA:HA	25:S:25:GLN:NE2	2.23	0.53
15:I:88:GLN:HA	15:I:91:PHE:HE2	1.74	0.53
1:O:1768:C:H2'	1:O:1769:C:O4'	2.09	0.53
10:D:49:PRO:HA	10:D:73:VAL:HG22	1.90	0.53
1:O:2578:G:C8	1:O:2578:G:H5'	2.40	0.53
8:B:52:VAL:O	8:B:53:LEU:HD12	2.09	0.53
1:O:1496:A:H5'	1:O:1572:A:H1'	1.90	0.53
20:N:42:HIS:CG	20:N:62:HIS:HE1	2.26	0.53
15:I:68:PRO:HB2	15:I:69:PRO:HD2	1.91	0.53
1:O:282:C:H1'	1:O:368:C:H42	1.74	0.53
24:R:113:HIS:O	24:R:145:LEU:HD12	2.09	0.53
20:N:73:ALA:HB1	20:N:74:PRO:CD	2.39	0.53
12:F:36:THR:HG23	12:F:97:ALA:HB2	1.90	0.53
1:O:289:G:O2'	1:O:290:C:H5'	2.09	0.53
23:Q:66:LYS:HB2	23:Q:70:ALA:O	2.09	0.53
4:3:3:MET:O	4:3:90:PHE:HA	2.09	0.53
9:C:162:VAL:HG22	9:C:232:LEU:HD21	1.89	0.53
11:E:80:TRP:O	11:E:134:SER:HA	2.09	0.53
1:O:1477:C:H5'	1:O:1868:G:H5''	1.91	0.53
12:F:107:ASP:O	12:F:111:ILE:HG13	2.09	0.53
27:U:6:CYS:HB2	27:U:32:CYS:HB3	1.90	0.53
12:F:56:PRO:HG2	19:M:43:PRO:O	2.09	0.53
17:K:62:PRO:HG3	17:K:65:ARG:HH22	1.72	0.52
1:O:396:U:O2'	1:O:418:C:H4'	2.09	0.52
19:M:34:GLU:HB3	19:M:38:GLU:HG3	1.91	0.52
17:K:103:ASP:HA	17:K:123:SER:OG	2.09	0.52
18:L:121:ILE:HG12	18:L:141:GLU:HB2	1.90	0.52
20:N:163:PHE:O	20:N:164:ASP:O	2.26	0.52
26:T:35:TYR:CG	26:T:112:LEU:HD22	2.45	0.52
30:X:41:PHE:O	30:X:43:VAL:HG23	2.10	0.52
1:O:1213:C:O2'	1:O:1214:G:H5'	2.09	0.52
7:A:51:ARG:NH1	7:A:120:ARG:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:145:GLU:OE1	9:C:198:ASP:HB2	2.09	0.52
19:M:81:ARG:HG3	19:M:85:ARG:HB2	1.90	0.52
31:Y:105:LYS:HE2	31:Y:198:GLY:O	2.10	0.52
1:0:1086:A:N6	29:W:11:VAL:HG11	2.25	0.52
10:D:159:PRO:O	10:D:163:VAL:HG23	2.09	0.52
27:U:39:ASN:ND2	27:U:44:ARG:HH11	2.07	0.52
1:0:2344:G:N3	1:0:2344:G:H2'	2.24	0.52
1:0:1242:A:H5'	16:J:82:THR:CG2	2.26	0.52
1:0:1189:A:O2'	1:0:1208:C:H2'	2.09	0.52
8:B:41:PHE:HB3	8:B:190:MET:CE	2.34	0.52
8:B:63:GLU:HG3	8:B:63:GLU:O	2.08	0.52
16:J:19:MET:HE2	16:J:79:PHE:HA	1.91	0.52
3:2:48:ASP:O	3:2:49:GLU:HB2	2.09	0.52
1:0:317:A:OP1	26:T:52:ARG:O	2.27	0.52
3:2:25:VAL:O	3:2:29:THR:HG23	2.09	0.52
1:0:1874:U:H2'	7:A:120:ARG:HG3	1.90	0.52
1:0:383:A:H2'	1:0:384:G:O4'	2.09	0.52
31:Y:203:VAL:HG12	31:Y:228:VAL:HG22	1.91	0.52
11:E:69:ILE:HA	11:E:72:MET:CE	2.39	0.52
9:C:22:PHE:HA	9:C:116:ALA:HA	1.91	0.52
15:I:97:VAL:CG1	15:I:101:LYS:HE3	2.40	0.52
7:A:76:VAL:CG2	32:Z:63:LYS:HB3	2.39	0.52
17:K:81:ARG:HB2	17:K:87:ARG:NH1	2.24	0.52
10:D:39:ASP:O	10:D:43:GLU:HG3	2.09	0.52
1:0:1342:C:O2'	1:0:1343:C:H5'	2.09	0.52
1:0:2002:C:H2'	1:0:2003:U:H5'	1.91	0.52
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.91	0.52
16:J:93:ARG:HH11	16:J:93:ARG:CB	2.16	0.52
7:A:153:ARG:NH1	7:A:153:ARG:HB2	2.19	0.52
7:A:179:MET:HA	7:A:179:MET:CE	2.40	0.52
1:0:2694:A:H4'	11:E:91:PHE:CE1	2.44	0.52
1:0:1086:A:C6	29:W:11:VAL:HG11	2.44	0.52
1:0:2821:C:H4'	8:B:116:PRO:HB3	1.90	0.52
6:9:64:C:H2'	6:9:65:A:H5'	1.91	0.52
1:0:1834:C:H2'	1:0:1840:A:H62	1.74	0.52
1:0:775:G:OP1	2:1:16:HIS:HE1	1.92	0.52
6:9:1:U:O3'	6:9:3:A:H5'	2.10	0.52
29:W:5:VAL:HG11	29:W:153:MET:CE	2.40	0.52
1:0:1266:U:H4'	31:Y:115:ARG:HH21	1.74	0.52
1:0:120:A:H2'	1:0:120:A:N3	2.25	0.52
7:A:74:VAL:O	32:Z:65:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:18:ALA:HA	21:O:23:GLY:O	2.10	0.52
1:O:1825:U:O2'	1:O:1826:C:H5'	2.09	0.52
22:P:115:SER:C	22:P:117:SER:H	2.12	0.52
9:C:127:ARG:HG2	9:C:127:ARG:NH1	2.24	0.52
9:C:1:MET:HG2	9:C:2:GLN:NE2	2.25	0.52
1:O:1666:C:C2'	1:O:1667:A:H5''	2.39	0.52
9:C:151:GLN:HA	9:C:151:GLN:NE2	2.25	0.52
11:E:105:GLU:HG2	11:E:113:PRO:HB3	1.91	0.52
8:B:62:ARG:HA	8:B:65:MET:CE	2.33	0.52
8:B:41:PHE:CD1	8:B:79:MET:HE2	2.43	0.52
17:K:20:CYS:HB2	17:K:29:LEU:HG	1.91	0.52
6:9:39:U:H3'	6:9:40:C:H5''	1.92	0.52
20:N:61:ALA:CB	20:N:88:ALA:HB2	2.40	0.52
6:9:49:G:O2'	6:9:50:G:H5'	2.10	0.52
1:O:1333:U:H2'	1:O:1334:C:C6	2.45	0.52
1:O:1268:C:H2'	1:O:1269:G:H8	1.75	0.52
1:O:371:U:H2'	1:O:372:A:H8	1.75	0.52
10:D:23:VAL:HG21	10:D:45:THR:CG2	2.39	0.52
15:I:69:PRO:HG2	15:I:72:GLU:HB2	1.92	0.52
20:N:164:ASP:OD2	20:N:168:LEU:HG	2.09	0.52
1:O:1926:G:H2'	1:O:1927:A:H8	1.75	0.52
6:9:28:U:H5''	20:N:40:ASN:HD21	1.72	0.52
6:9:2:U:P	6:9:3:A:H5'	2.49	0.52
7:A:94:LEU:HG	7:A:99:ILE:CD1	2.40	0.52
1:O:1010:C:H4'	20:N:4:PRO:HB2	1.91	0.52
17:K:7:ASP:OD2	17:K:81:ARG:NH2	2.43	0.52
7:A:134:ASN:O	7:A:150:PRO:HD3	2.10	0.52
18:L:104:ASP:O	18:L:105:TYR:HB3	2.10	0.52
1:O:2073:G:OP2	1:O:2490:A:H5'	2.10	0.52
31:Y:219:GLU:HG3	31:Y:220:GLU:N	2.25	0.52
9:C:39:GLN:O	9:C:43:LYS:HD3	2.09	0.52
10:D:135:VAL:HG22	10:D:136:ARG:N	2.24	0.51
1:O:797:A:H5'	32:Z:10:ARG:N	2.25	0.51
9:C:138:VAL:O	9:C:234:VAL:HA	2.10	0.51
20:N:73:ALA:HB1	20:N:74:PRO:HD2	1.91	0.51
19:M:31:TRP:HA	19:M:34:GLU:HG3	1.91	0.51
1:O:926:A:O2'	18:L:41:HIS:CD2	2.63	0.51
1:O:2135:A:O2'	1:O:2136:G:H5'	2.10	0.51
19:M:65:VAL:HG21	19:M:105:ALA:HB2	1.91	0.51
9:C:98:ARG:NH1	9:C:98:ARG:HG2	2.22	0.51
9:C:136:VAL:HG22	9:C:137:PRO:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:99:ILE:O	7:A:131:HIS:CE1	2.64	0.51
19:M:59:GLY:HA3	19:M:141:ILE:CD1	2.40	0.51
1:0:474:C:O3'	9:C:73:LEU:HD21	2.10	0.51
1:0:1008:C:H5''	14:H:19:ARG:HH12	1.75	0.51
1:0:2900:G:H2'	1:0:2901:C:O4'	2.10	0.51
1:0:2834:G:OP1	30:X:39:LYS:HE2	2.10	0.51
1:0:1422:U:H2'	1:0:1423:C:C6	2.45	0.51
32:Z:25:ARG:O	32:Z:29:ILE:HG13	2.10	0.51
1:0:1160:G:O2'	1:0:1190:G:H1'	2.10	0.51
13:G:64:ASN:H	13:G:64:ASN:ND2	2.08	0.51
1:0:2421:G:H3'	1:0:2422:U:H5''	1.91	0.51
1:0:2862:G:H4'	8:B:336:GLN:O	2.10	0.51
31:Y:189:ASN:ND2	31:Y:192:ASP:H	2.09	0.51
8:B:238:ASN:ND2	8:B:240:GLY:H	2.07	0.51
31:Y:184:GLU:OE1	31:Y:204:ARG:NH1	2.43	0.51
22:P:94:TRP:CZ2	22:P:98:ILE:HG13	2.45	0.51
15:I:111:LEU:HD22	15:I:122:GLU:OE1	2.10	0.51
17:K:41:LYS:O	17:K:42:ASN:HB2	2.10	0.51
10:D:88:LEU:HB2	10:D:89:PRO:HD3	1.92	0.51
26:T:43:ASN:HD22	26:T:108:ARG:NH2	2.08	0.51
19:M:99:ARG:CD	19:M:167:GLY:HA2	2.39	0.51
1:0:1205:U:H2'	1:0:1206:U:H5'	1.92	0.51
2:1:8:GLN:HE22	2:1:11:LYS:HZ2	1.59	0.51
6:9:73:A:H61	6:9:108:C:N4	2.07	0.51
20:N:15:GLU:HB3	20:N:17:ARG:HD2	1.93	0.51
1:0:2597:U:H2'	1:0:2598:U:H5'	1.91	0.51
1:0:2256:G:C2'	1:0:2257:G:H5'	2.41	0.51
1:0:474:C:O3'	9:C:73:LEU:CD2	2.59	0.51
1:0:947:U:H2'	1:0:948:G:C8	2.45	0.51
1:0:2435:U:OP1	4:3:28:GLY:HA3	2.11	0.51
1:0:24:G:N2	1:0:518:G:H1'	2.25	0.51
26:T:71:VAL:HG13	26:T:91:LEU:O	2.11	0.51
6:9:114:G:H2'	6:9:115:C:C6	2.46	0.51
7:A:217:ARG:CG	7:A:217:ARG:HH11	2.24	0.51
28:V:64:GLY:O	28:V:65:ASP:CB	2.58	0.51
9:C:16:VAL:HG12	9:C:17:ASP:H	1.76	0.51
9:C:47:GLY:HA2	9:C:92:PRO:HB2	1.92	0.51
11:E:101:GLU:HB3	11:E:117:THR:HA	1.92	0.51
20:N:179:LEU:HD23	20:N:184:ILE:CD1	2.41	0.51
8:B:195:ARG:HG2	8:B:323:LEU:HD22	1.93	0.51
26:T:9:LYS:CE	26:T:13:ARG:NH1	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2769:C:H2'	1:0:2770:G:C5'	2.40	0.51
32:Z:36:ASP:HB3	32:Z:45:ASP:HB3	1.92	0.51
8:B:217:ARG:HG3	8:B:257:THR:HG22	1.91	0.51
1:0:776:A:OP1	2:1:28:HIS:HE1	1.93	0.51
29:W:5:VAL:HG11	29:W:153:MET:HE3	1.91	0.51
29:W:107:LEU:O	29:W:112:LEU:HB2	2.11	0.51
12:F:39:SER:HB3	12:F:45:ALA:HB2	1.93	0.51
24:R:47:LEU:O	24:R:51:ILE:HG13	2.11	0.51
8:B:13:PHE:O	8:B:16:ARG:HD2	2.10	0.51
1:0:2105:C:H2'	1:0:2106:C:C6	2.45	0.51
1:0:2769:C:H2'	1:0:2770:G:H5'	1.93	0.51
7:A:66:ARG:HH11	7:A:66:ARG:CB	2.24	0.51
1:0:669:G:O2'	1:0:670:G:H5'	2.11	0.51
1:0:2104:C:O2	1:0:2485:A:N1	2.43	0.51
10:D:64:ARG:HB3	10:D:67:ASP:OD2	2.11	0.51
19:M:165:GLY:O	19:M:169:ARG:HG3	2.11	0.51
9:C:151:GLN:CA	9:C:151:GLN:HE21	2.24	0.51
31:Y:126:PRO:HG2	31:Y:128:PHE:CZ	2.46	0.51
4:3:3:MET:HG3	4:3:4:PRO:HD2	1.92	0.51
7:A:70:ALA:HB1	32:Z:65:THR:HG21	1.92	0.51
1:0:621:C:H5'	31:Y:132:ASP:OD2	2.11	0.51
1:0:2717:C:O2'	1:0:2718:C:H5"	2.10	0.51
30:X:47:ALA:O	30:X:82:GLU:HB2	2.10	0.51
6:9:73:A:N6	6:9:108:C:H42	2.07	0.51
1:0:2445:U:H2'	1:0:2446:G:C8	2.46	0.51
25:S:17:ASP:HB3	25:S:23:LYS:HB2	1.93	0.51
1:0:1165:G:H4'	1:0:1174:A:O2'	2.11	0.51
1:0:1644:C:H2'	1:0:1645:U:H6	1.75	0.51
1:0:559:U:H2'	1:0:560:U:O4'	2.11	0.50
7:A:179:MET:HG2	7:A:186:TRP:CB	2.41	0.50
24:R:53:GLY:HA2	24:R:80:TYR:CD2	2.47	0.50
1:0:1293:U:H5'	31:Y:154:ARG:HH21	1.76	0.50
1:0:820:G:O2'	1:0:856:G:H4'	2.11	0.50
6:9:64:C:C2'	6:9:65:A:H5'	2.41	0.50
7:A:125:ASN:HB3	7:A:158:VAL:HG12	1.93	0.50
1:0:157:G:H4'	19:M:95:LYS:HE2	1.93	0.50
1:0:960:G:H3'	1:0:960:G:N3	2.26	0.50
1:0:656:G:OP2	21:O:37:ARG:HD2	2.11	0.50
30:X:43:VAL:HG11	30:X:82:GLU:HA	1.93	0.50
21:O:47:ARG:HG3	21:O:47:ARG:NH1	2.26	0.50
10:D:55:LYS:HA	10:D:65:GLU:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:702:G:O2'	1:0:703:G:H5'	2.11	0.50
15:I:133:THR:HG22	15:I:134:ILE:N	2.27	0.50
1:0:2507:G:H2'	1:0:2510:C:H42	1.77	0.50
7:A:36:ASP:CB	7:A:83:GLY:HA3	2.41	0.50
1:0:1853:C:O2'	7:A:217:ARG:NH2	2.44	0.50
20:N:154:LEU:HD12	20:N:156:GLU:O	2.11	0.50
16:J:107:ASN:HD22	16:J:109:TYR:H	1.57	0.50
16:J:130:VAL:CG1	16:J:131:THR:N	2.74	0.50
12:F:56:PRO:CG	19:M:44:THR:HA	2.40	0.50
1:0:371:U:H2'	1:0:372:A:C8	2.46	0.50
10:D:86:THR:C	10:D:89:PRO:HD2	2.31	0.50
1:0:2533:C:H6	1:0:2533:C:C5'	2.18	0.50
1:0:1211:G:H5''	13:G:64:ASN:OD1	2.11	0.50
20:N:86:LEU:O	20:N:90:LEU:HG	2.12	0.50
12:F:46:GLU:OE1	12:F:100:ASP:HA	2.11	0.50
1:0:128:A:O2'	1:0:129:A:H5'	2.10	0.50
1:0:2613:G:O2'	1:0:2614:C:H5'	2.11	0.50
10:D:64:ARG:CD	10:D:67:ASP:HB3	2.41	0.50
25:S:37:VAL:O	25:S:41:VAL:HG23	2.12	0.50
1:0:1120:U:H5'	1:0:1121:G:OP2	2.11	0.50
9:C:165:ASP:O	9:C:168:ARG:HB3	2.11	0.50
28:V:42:ASN:N	28:V:43:PRO:HD3	2.27	0.50
21:O:21:SER:OG	21:O:106:PRO:HB2	2.11	0.50
10:D:172:VAL:HG12	10:D:173:GLU:N	2.26	0.50
1:0:138:U:OP2	1:0:139:C:H5	1.94	0.50
12:F:26:THR:HG21	12:F:102:GLY:C	2.32	0.50
10:D:13:MET:HA	10:D:137:PRO:HG2	1.93	0.50
17:K:66:ARG:HH11	17:K:66:ARG:HG2	1.77	0.50
29:W:76:ASP:O	29:W:77:ALA:C	2.49	0.50
20:N:15:GLU:HB3	20:N:17:ARG:HG3	1.92	0.50
1:0:1595:G:O2'	1:0:1596:U:H5'	2.11	0.50
1:0:65:C:O2'	1:0:66:G:H5'	2.11	0.50
22:P:83:LYS:O	22:P:86:ALA:HB3	2.12	0.50
1:0:449:A:N7	9:C:43:LYS:HG2	2.26	0.50
31:Y:99:ALA:HB2	31:Y:233:TYR:CZ	2.46	0.50
6:9:52:A:H2'	6:9:53:G:O4'	2.12	0.50
1:0:2443:C:H1'	18:L:56:LYS:HE3	1.94	0.50
7:A:55:VAL:HG23	7:A:68:ILE:O	2.11	0.50
8:B:315:VAL:HG23	8:B:316:ARG:HG2	1.94	0.50
1:0:1377:C:H5'	1:0:1377:C:C6	2.44	0.50
1:0:661:G:C5	1:0:686:A:C2	3.00	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1790:C:H2'	1:0:1791:U:H6	1.76	0.50
1:0:1636:G:O2'	1:0:1637:A:H5'	2.12	0.50
6:9:76:G:C3'	6:9:77:A:H5''	2.31	0.50
1:0:1942:A:O2'	1:0:1943:C:H5'	2.12	0.50
26:T:9:LYS:HE3	26:T:13:ARG:CZ	2.41	0.50
8:B:320:GLN:NE2	8:B:321:PRO:CD	2.73	0.50
1:0:1667:A:H2'	1:0:1668:U:C6	2.47	0.50
7:A:132:ASP:HB3	7:A:135:VAL:O	2.12	0.50
9:C:219:ASN:O	9:C:222:ASP:HB2	2.10	0.50
28:V:16:ARG:NH2	28:V:63:GLU:HG3	2.27	0.50
7:A:192:VAL:HG12	7:A:192:VAL:O	2.12	0.49
18:L:143:THR:CG2	18:L:144:ASP:N	2.75	0.49
10:D:18:ILE:HD13	10:D:84:LEU:CD1	2.41	0.49
1:0:1342:C:C2'	1:0:1343:C:H5'	2.42	0.49
1:0:671:A:O2'	1:0:672:G:H2'	2.12	0.49
29:W:130:HIS:O	29:W:136:GLY:HA3	2.12	0.49
14:H:86:TYR:CD1	14:H:86:TYR:C	2.85	0.49
26:T:69:LYS:O	26:T:71:VAL:HG23	2.12	0.49
7:A:192:VAL:HG12	7:A:207:GLN:HB3	1.93	0.49
8:B:51:VAL:CG2	8:B:327:VAL:HG13	2.42	0.49
1:0:2421:G:H3'	1:0:2422:U:C5'	2.43	0.49
20:N:151:ASP:OD1	20:N:154:LEU:HD13	2.12	0.49
1:0:1515:A:H2'	1:0:1516:U:C6	2.47	0.49
26:T:64:ASN:HB3	26:T:73:HIS:HB2	1.93	0.49
16:J:127:ILE:O	16:J:127:ILE:HG12	2.12	0.49
1:0:646:G:H5''	9:C:96:LYS:HD2	1.93	0.49
9:C:130:GLU:HA	9:C:130:GLU:OE1	2.11	0.49
1:0:1641:A:C2'	1:0:1642:A:H5'	2.42	0.49
13:G:20:VAL:O	13:G:24:VAL:HG23	2.12	0.49
25:S:52:VAL:C	25:S:53:ASN:HD22	2.16	0.49
26:T:38:ARG:HG3	26:T:38:ARG:NH1	2.26	0.49
11:E:24:GLY:HA3	11:E:76:VAL:HB	1.94	0.49
14:H:79:GLU:C	14:H:80:LEU:HD23	2.32	0.49
1:0:1116:U:O2'	1:0:1118:A:C2	2.54	0.49
6:9:91:C:H2'	6:9:92:G:O4'	2.12	0.49
8:B:7:ARG:NH1	8:B:11:LEU:HD21	2.27	0.49
1:0:894:A:C2	9:C:87:ARG:NH2	2.81	0.49
27:U:13:ILE:HG12	27:U:32:CYS:HB3	1.93	0.49
1:0:2899:A:H2'	1:0:2900:G:C8	2.48	0.49
20:N:67:ALA:HA	20:N:71:TRP:HB3	1.94	0.49
1:0:1352:A:N1	9:C:48:SER:HB3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:88:ILE:HD13	7:A:100:PRO:CD	2.36	0.49
8:B:190:MET:HE1	8:B:194:PHE:CD1	2.46	0.49
1:O:1450:C:O2'	1:O:1494:A:H5'	2.11	0.49
8:B:255:GLY:O	8:B:257:THR:HG23	2.12	0.49
7:A:186:TRP:CG	7:A:187:PRO:HA	2.47	0.49
1:O:1845:A:OP2	7:A:190:ARG:NH1	2.45	0.49
20:N:38:LYS:HE2	20:N:107:ASN:ND2	2.26	0.49
16:J:39:VAL:HG11	16:J:107:ASN:HB2	1.94	0.49
16:J:45:VAL:HG22	16:J:130:VAL:O	2.12	0.49
1:O:945:U:O2'	29:W:43:GLY:HA3	2.13	0.49
1:O:316:A:N3	1:O:336:G:O2'	2.45	0.49
1:O:1015:C:H2'	1:O:1016:U:C6	2.47	0.49
18:L:57:VAL:O	18:L:57:VAL:HG12	2.13	0.49
6:9:24:U:H3'	6:9:25:G:H5'	1.95	0.49
29:W:142:ASP:HB3	29:W:145:GLY:H	1.77	0.49
29:W:72:PRO:CG	29:W:77:ALA:HB3	2.30	0.49
10:D:63:ILE:O	10:D:64:ARG:C	2.50	0.49
6:9:56:A:O2'	10:D:14:ARG:HD3	2.12	0.49
20:N:152:GLU:HA	20:N:152:GLU:OE1	2.12	0.49
26:T:43:ASN:ND2	26:T:108:ARG:CZ	2.76	0.49
26:T:28:SER:O	26:T:32:ARG:HG3	2.12	0.49
1:O:88:G:H5'	1:O:88:G:H8	1.77	0.49
1:O:1167:G:H2'	1:O:1168:C:O4'	2.13	0.49
1:O:2511:A:H2'	1:O:2512:U:O4'	2.13	0.49
7:A:35:GLY:O	7:A:36:ASP:CB	2.50	0.49
8:B:304:PRO:HD2	8:B:307:ARG:CD	2.38	0.49
14:H:41:LYS:HD3	14:H:46:TYR:CZ	2.48	0.49
17:K:74:VAL:HG13	17:K:113:ILE:HG12	1.94	0.49
16:J:133:GLY:O	16:J:137:GLU:HG3	2.13	0.49
19:M:59:GLY:HA3	19:M:141:ILE:HD11	1.95	0.49
1:O:1717:A:H5''	22:P:54:LYS:HB2	1.93	0.49
10:D:101:THR:O	10:D:101:THR:HG22	2.12	0.49
30:X:76:ARG:O	30:X:77:PHE:HB3	2.12	0.49
1:O:318:U:O2'	1:O:338:C:H2'	2.13	0.49
31:Y:106:THR:CG2	31:Y:107:PRO:HD2	2.43	0.49
31:Y:112:GLU:CD	31:Y:115:ARG:NH1	2.66	0.49
20:N:83:LEU:HD13	20:N:175:LEU:HD23	1.95	0.49
1:O:1594:C:OP2	22:P:120:ARG:HD2	2.12	0.49
1:O:2353:A:H4'	1:O:2354:A:O5'	2.12	0.49
1:O:1450:C:C4'	1:O:1451:C:OP2	2.55	0.49
9:C:118:THR:CG2	9:C:137:PRO:HB3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J:6:PHE:O	16:J:8:ALA:N	2.45	0.49
1:0:1236:A:C8	16:J:63:ILE:HD11	2.48	0.49
9:C:5:ILE:HD11	9:C:16:VAL:CG2	2.43	0.49
1:0:451:C:O2'	1:0:452:G:H5'	2.13	0.49
9:C:7:ASP:OD1	9:C:11:ASN:HB2	2.12	0.49
8:B:195:ARG:N	8:B:198:GLU:OE1	2.46	0.49
11:E:5:LEU:HD21	11:E:66:GLN:HG3	1.94	0.49
1:0:920:C:H5'	1:0:921:G:C4	2.48	0.49
29:W:80:ASP:O	29:W:84:VAL:HG23	2.12	0.49
1:0:2314:G:C2'	1:0:2315:C:H5'	2.43	0.49
1:0:2509:A:H2'	1:0:2510:C:O4'	2.13	0.48
14:H:69:ARG:HH21	14:H:70:LEU:HD12	1.78	0.48
20:N:163:PHE:HZ	20:N:171:HIS:HD1	1.61	0.48
14:H:46:TYR:HE2	14:H:85:ASP:O	1.96	0.48
29:W:65:VAL:CA	29:W:68:THR:HG22	2.41	0.48
32:Z:11:SER:HB3	32:Z:23:ARG:HB2	1.95	0.48
1:0:1973:A:H2'	1:0:1974:G:O4'	2.13	0.48
16:J:131:THR:HB	16:J:134:GLU:HG3	1.94	0.48
24:R:80:TYR:O	24:R:82:GLU:N	2.45	0.48
1:0:969:G:H1	1:0:999:C:H42	1.60	0.48
1:0:2825:C:H4'	1:0:2826:G:O5'	2.13	0.48
26:T:43:ASN:HD22	26:T:108:ARG:CZ	2.26	0.48
10:D:94:ALA:HA	10:D:174:VAL:O	2.13	0.48
1:0:1594:C:O2'	1:0:1607:A:H4'	2.13	0.48
1:0:2904:U:H4'	30:X:8:ARG:NH1	2.27	0.48
1:0:166:A:N7	18:L:25:GLY:HA2	2.28	0.48
1:0:12:U:H2'	1:0:13:G:H5'	1.95	0.48
9:C:127:ARG:HH21	9:C:225:PRO:HG2	1.73	0.48
28:V:12:THR:CG2	28:V:15:GLU:H	2.26	0.48
1:0:2716:G:C5'	8:B:206:THR:HG21	2.41	0.48
11:E:23:GLU:HG2	11:E:28:SER:CB	2.43	0.48
1:0:1183:C:H42	1:0:1184:C:H41	1.59	0.48
30:X:10:VAL:HG11	30:X:36:HIS:CE1	2.47	0.48
1:0:968:G:O2'	1:0:969:G:H5'	2.13	0.48
28:V:27:LEU:HA	28:V:49:LEU:HD13	1.94	0.48
1:0:816:G:H5'	1:0:1598:A:H4'	1.95	0.48
1:0:926:A:O2'	18:L:41:HIS:HD2	1.96	0.48
31:Y:99:ALA:HB2	31:Y:233:TYR:CE2	2.48	0.48
6:9:61:C:H2'	6:9:62:A:H8	1.77	0.48
1:0:2758:G:H2'	1:0:2759:C:C6	2.49	0.48
10:D:35:ALA:C	10:D:37:ALA:H	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D:28:GLY:CA	10:D:69:ILE:HG23	2.38	0.48
16:J:75:PRO:HB3	16:J:132:LEU:HB3	1.95	0.48
1:0:319:A:H4'	1:0:338:C:C4	2.49	0.48
9:C:27:ARG:HG3	9:C:27:ARG:HH11	1.78	0.48
20:N:183:ASP:O	20:N:184:ILE:O	2.31	0.48
1:0:960:G:N3	1:0:960:G:C2'	2.76	0.48
24:R:114:VAL:HG13	24:R:114:VAL:O	2.13	0.48
9:C:173:LYS:HB3	9:C:187:ARG:HG3	1.94	0.48
10:D:37:ALA:O	10:D:40:ILE:HG12	2.13	0.48
1:0:2055:A:H4'	24:R:132:ARG:NH2	2.29	0.48
22:P:10:ALA:HA	22:P:13:VAL:HG12	1.94	0.48
8:B:36:PRO:HA	8:B:168:GLY:HA3	1.95	0.48
17:K:28:GLU:HG2	17:K:58:THR:HB	1.96	0.48
16:J:54:VAL:HG11	16:J:138:THR:HG21	1.94	0.48
1:0:1654:U:H2'	7:A:47:HIS:HD2	1.77	0.48
26:T:71:VAL:HG12	26:T:72:ILE:N	2.28	0.48
6:9:56:A:C3'	6:9:57:A:H5''	2.44	0.48
8:B:279:THR:HG22	8:B:280:VAL:N	2.28	0.48
22:P:38:GLU:HA	22:P:41:ARG:NH1	2.29	0.48
20:N:12:ARG:HD3	20:N:18:THR:OG1	2.13	0.48
1:0:426:G:H2'	1:0:427:C:O4'	2.14	0.48
1:0:2361:A:H8	1:0:2361:A:H5'	1.79	0.48
10:D:27:ILE:HB	10:D:69:ILE:O	2.13	0.48
1:0:2502:C:H2'	1:0:2503:A:C5'	2.42	0.48
9:C:118:THR:HG22	9:C:137:PRO:HB3	1.94	0.48
1:0:1185:U:H2'	1:0:1186:C:C6	2.48	0.48
16:J:15:ARG:NH1	16:J:43:ARG:NH1	2.62	0.48
22:P:10:ALA:HA	22:P:13:VAL:CG1	2.44	0.48
1:0:1333:U:H2'	1:0:1334:C:H6	1.79	0.48
29:W:108:ARG:HG3	29:W:114:PRO:HG3	1.94	0.48
1:0:23:G:H1'	1:0:520:A:N6	2.29	0.48
1:0:812:A:H2'	1:0:813:C:O4'	2.13	0.48
7:A:109:GLU:HG2	7:A:116:GLY:H	1.78	0.48
23:Q:64:GLU:OE1	23:Q:64:GLU:HA	2.13	0.48
10:D:140:ARG:HG3	10:D:140:ARG:HH11	1.78	0.48
14:H:12:ILE:HG12	14:H:59:GLN:HG2	1.96	0.48
15:I:94:ASP:HA	15:I:133:THR:O	2.13	0.48
1:0:2506:A:O2'	1:0:2507:G:O5'	2.31	0.48
12:F:58:GLU:HA	12:F:61:MET:CE	2.42	0.48
26:T:19:ARG:NH1	26:T:68:ASP:O	2.46	0.48
7:A:179:MET:HG2	7:A:186:TRP:CG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1845:A:O3'	7:A:187:PRO:HB2	2.14	0.48
7:A:43:VAL:CG2	7:A:59:GLU:HG3	2.44	0.48
1:0:2064:U:H4'	1:0:2653:A:OP1	2.14	0.48
15:I:73:LEU:HD12	15:I:107:LYS:NZ	2.28	0.48
18:L:72:ASN:O	18:L:76:LEU:HG	2.14	0.48
1:0:952:G:OP1	23:Q:42:LYS:HE2	2.14	0.48
7:A:97:ALA:HB2	7:A:150:PRO:HB2	1.94	0.48
10:D:95:THR:OG1	10:D:174:VAL:HG13	2.13	0.48
1:0:2329:C:O2'	1:0:2330:U:H5'	2.13	0.48
1:0:1321:A:H2'	1:0:1322:G:C8	2.49	0.48
25:S:8:PRO:HD2	28:V:32:ALA:HA	1.95	0.48
1:0:1904:A:H2'	1:0:1905:U:O4'	2.13	0.48
30:X:74:ALA:CB	30:X:85:VAL:HG22	2.44	0.48
14:H:122:LYS:O	14:H:124:VAL:HG13	2.13	0.48
8:B:207:LYS:HG2	8:B:304:PRO:HB3	1.94	0.48
16:J:19:MET:HE1	16:J:132:LEU:CD2	2.41	0.48
29:W:64:THR:O	29:W:68:THR:HG22	2.13	0.48
10:D:136:ARG:HD2	10:D:155:HIS:O	2.14	0.48
11:E:84:MET:HB2	11:E:131:LEU:HB2	1.96	0.48
1:0:539:G:H2'	1:0:540:A:C8	2.48	0.48
22:P:9:LEU:O	22:P:13:VAL:HG12	2.14	0.48
20:N:42:HIS:HB3	20:N:62:HIS:CE1	2.49	0.48
1:0:204:A:H2'	1:0:205:U:H5'	1.95	0.48
1:0:1471:A:H2'	1:0:1472:C:C6	2.48	0.48
6:9:51:A:H5'	20:N:160:SER:HB3	1.95	0.48
1:0:1151:G:OP1	13:G:63:ARG:NH1	2.46	0.48
1:0:558:C:H2'	1:0:559:U:H5''	1.95	0.48
1:0:1753:C:O2	8:B:229:ARG:NH2	2.46	0.48
1:0:1839:A:H5'	1:0:2643:G:H4'	1.96	0.48
1:0:1878:G:O2'	1:0:1879:U:P	2.71	0.48
1:0:2897:C:H2'	1:0:2898:G:H8	1.76	0.48
1:0:625:U:H5''	1:0:1044:C:N4	2.29	0.48
1:0:1289:C:O2'	1:0:1290:G:H5'	2.14	0.48
10:D:25:MET:HE1	10:D:41:LEU:HG	1.96	0.48
19:M:102:GLU:CD	19:M:164:THR:HG21	2.34	0.48
24:R:119:VAL:HG12	24:R:119:VAL:O	2.14	0.48
1:0:1495:C:H1'	1:0:1573:A:H1'	1.96	0.48
1:0:2044:G:OP1	30:X:23:HIS:HE1	1.97	0.48
19:M:157:ASP:HB3	19:M:160:PHE:HD1	1.78	0.48
1:0:1163:G:H5'	15:I:110:ASP:O	2.14	0.48
1:0:37:A:H2'	1:0:38:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:139:TRP:HA	20:N:139:TRP:CE3	2.49	0.48
16:J:77:GLY:O	16:J:78:ILE:C	2.52	0.47
15:I:94:ASP:OD1	15:I:133:THR:HB	2.15	0.47
7:A:36:ASP:HA	7:A:83:GLY:HA3	1.95	0.47
1:0:285:A:C2	1:0:368:C:H4'	2.49	0.47
24:R:9:ASP:O	24:R:13:THR:HB	2.14	0.47
1:0:2781:U:H1'	11:E:139:GLU:OE2	2.13	0.47
32:Z:19:GLY:O	32:Z:23:ARG:HG2	2.14	0.47
20:N:114:LYS:O	20:N:117:ALA:HB3	2.14	0.47
29:W:1:MET:N	29:W:103:GLU:OE2	2.47	0.47
29:W:26:ILE:O	29:W:26:ILE:CG1	2.61	0.47
8:B:162:MET:HG3	8:B:310:ARG:CZ	2.44	0.47
1:0:1184:C:O2'	1:0:1185:U:OP2	2.29	0.47
31:Y:154:ARG:NH1	31:Y:155:ARG:HG3	2.29	0.47
32:Z:72:GLU:HB2	32:Z:77:LYS:HE3	1.95	0.47
21:O:105:ASN:HD21	21:O:109:SER:N	2.13	0.47
21:O:80:ASP:OD1	21:O:81:PHE:N	2.46	0.47
1:0:17:G:H2'	1:0:18:C:C6	2.49	0.47
26:T:37:GLN:OE1	26:T:118:SER:HA	2.15	0.47
1:0:2072:G:C6	1:0:2533:C:H1'	2.50	0.47
19:M:99:ARG:HE	19:M:170:ASN:HD22	1.61	0.47
1:0:558:C:C2'	1:0:559:U:C5'	2.92	0.47
16:J:108:PRO:HG2	16:J:109:TYR:CD1	2.50	0.47
10:D:104:PHE:CE2	10:D:166:ILE:HD13	2.49	0.47
24:R:119:VAL:CG2	24:R:142:ASP:HB2	2.44	0.47
28:V:20:LEU:HD11	28:V:53:ILE:HG23	1.96	0.47
1:0:926:A:H5'	18:L:39:GLU:OE2	2.14	0.47
1:0:1790:C:H2'	1:0:1791:U:C6	2.48	0.47
29:W:7:LEU:HD12	29:W:53:ALA:HB2	1.96	0.47
19:M:54:TYR:CG	19:M:55:LYS:N	2.82	0.47
1:0:1925:G:H5'	4:3:29:ARG:NH1	2.26	0.47
14:H:29:SER:HA	14:H:62:HIS:HD2	1.78	0.47
15:I:108:HIS:N	15:I:109:PRO:CD	2.77	0.47
1:0:820:G:C6	7:A:171:LYS:HB2	2.49	0.47
1:0:308:U:H5'	1:0:309:C:OP1	2.14	0.47
1:0:958:G:H2'	1:0:959:C:C6	2.49	0.47
1:0:1055:G:OP2	14:H:99:ARG:NH1	2.48	0.47
8:B:41:PHE:CZ	8:B:79:MET:HG3	2.49	0.47
24:R:39:THR:O	24:R:40:ALA:C	2.51	0.47
17:K:28:GLU:OE2	17:K:58:THR:HG21	2.15	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L:82:ALA:O	18:L:83:GLU:C	2.53	0.47
9:C:107:ARG:CZ	9:C:107:ARG:HB3	2.45	0.47
31:Y:186:ARG:HG2	31:Y:186:ARG:HH11	1.78	0.47
30:X:70:ILE:HG23	30:X:70:ILE:O	2.15	0.47
1:O:1166:A:H1'	1:O:1192:A:C2	2.50	0.47
24:R:18:LEU:HG	24:R:91:LEU:HD13	1.97	0.47
17:K:113:ILE:HG22	17:K:114:ALA:O	2.15	0.47
1:O:2781:U:H2'	1:O:2782:G:H5'	1.96	0.47
8:B:171:VAL:O	8:B:175:LEU:HB2	2.14	0.47
1:O:657:G:H2'	1:O:658:C:C6	2.50	0.47
7:A:65:ARG:C	7:A:66:ARG:HG3	2.35	0.47
4:3:69:TYR:HB2	4:3:78:HIS:CE1	2.49	0.47
4:3:69:TYR:CZ	4:3:80:ARG:HD2	2.50	0.47
20:N:49:THR:CG2	20:N:50:LEU:N	2.77	0.47
12:F:56:PRO:HG2	19:M:44:THR:HA	1.95	0.47
23:Q:32:GLU:HA	23:Q:71:TYR:OH	2.15	0.47
17:K:34:VAL:HG22	17:K:47:ALA:HB2	1.95	0.47
14:H:157:TYR:C	14:H:157:TYR:CD1	2.87	0.47
25:S:51:GLN:HB3	25:S:67:ARG:NH1	2.29	0.47
20:N:58:LEU:HD12	20:N:58:LEU:N	2.30	0.47
21:O:53:GLN:HG2	21:O:56:GLU:OE1	2.14	0.47
19:M:164:THR:HG22	19:M:166:ALA:H	1.79	0.47
1:O:1205:U:C2'	1:O:1206:U:H5''	2.41	0.47
9:C:115:LEU:HD13	9:C:223:LEU:CD2	2.42	0.47
1:O:2780:C:C1'	11:E:143:GLN:HE21	2.27	0.47
32:Z:10:ARG:HB2	32:Z:27:ALA:CB	2.45	0.47
32:Z:10:ARG:HG3	32:Z:11:SER:N	2.29	0.47
14:H:88:MET:HA	14:H:139:ALA:HA	1.97	0.47
12:F:15:ASP:O	12:F:18:GLU:HB2	2.14	0.47
1:O:1279:U:O2	1:O:1279:U:H2'	2.13	0.47
1:O:969:G:H1	1:O:999:C:N4	2.12	0.47
9:C:233:THR:HG22	9:C:234:VAL:N	2.28	0.47
20:N:43:VAL:O	20:N:84:THR:HG21	2.13	0.47
1:O:475:G:OP1	9:C:73:LEU:HD22	2.15	0.47
12:F:26:THR:HG21	12:F:103:GLU:HB2	1.97	0.47
29:W:1:MET:N	29:W:37:GLU:HG3	2.30	0.47
19:M:49:ALA:HB1	19:M:54:TYR:HB2	1.97	0.47
9:C:104:ASP:O	9:C:108:GLN:HG3	2.15	0.47
1:O:2472:C:O2'	1:O:2634:G:H4'	2.13	0.47
29:W:21:LEU:HD21	29:W:48:VAL:HG13	1.97	0.47
20:N:72:GLU:HG2	20:N:72:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:U:31:PHE:CG	27:U:37:GLU:HG2	2.50	0.47
18:L:65:ASP:CG	18:L:111:ALA:HB3	2.35	0.47
1:0:809:G:H2'	1:0:810:G:H8	1.79	0.47
8:B:80:ARG:HA	8:B:186:GLY:O	2.15	0.47
9:C:20:ASP:O	9:C:23:GLU:HB2	2.15	0.47
1:0:2785:C:H4'	1:0:2786:G:OP2	2.15	0.47
1:0:1206:U:H2'	1:0:1207:A:O4'	2.15	0.47
1:0:2256:G:H2'	1:0:2257:G:C5'	2.45	0.47
10:D:10:PHE:CD1	10:D:11:HIS:N	2.83	0.47
1:0:308:U:C4	1:0:342:C:H1'	2.50	0.47
1:0:960:G:H2'	1:0:960:G:N3	2.30	0.47
1:0:2724:U:H2'	1:0:2725:G:O4'	2.15	0.47
9:C:49:ASP:HB3	9:C:52:ALA:HB2	1.96	0.47
4:3:91:GLN:O	4:3:92:GLU:HB2	2.14	0.47
1:0:1506:U:H6	1:0:1506:U:H5'	1.79	0.47
15:I:87:PRO:HB3	15:I:129:SER:O	2.15	0.47
29:W:139:GLY:O	29:W:141:HIS:HD2	1.97	0.47
10:D:146:LYS:HZ1	20:N:107:ASN:ND2	2.12	0.47
1:0:1328:A:OP1	31:Y:169:ARG:CD	2.63	0.47
1:0:1973:A:H5'	1:0:1973:A:C8	2.47	0.47
8:B:5:ARG:NH1	8:B:8:LYS:HE2	2.30	0.47
29:W:122:ARG:HG3	29:W:152:ALA:O	2.15	0.47
1:0:1787:C:OP1	22:P:68:LYS:HE2	2.15	0.47
6:9:49:G:H2'	6:9:50:G:O4'	2.15	0.47
18:L:53:ARG:NH2	18:L:57:VAL:HG12	2.30	0.47
21:O:105:ASN:HD21	21:O:109:SER:H	1.63	0.47
1:0:1576:G:H2'	1:0:1577:U:O4'	2.15	0.47
31:Y:205:ILE:HB	31:Y:230:ASN:HD21	1.79	0.47
8:B:75:GLU:C	8:B:77:PRO:HD3	2.35	0.47
22:P:141:ILE:O	22:P:143:ALA:N	2.38	0.47
1:0:2846:C:H4'	8:B:156:LYS:HB3	1.95	0.47
29:W:4:LEU:O	29:W:32:CYS:HA	2.15	0.46
10:D:54:ALA:CB	10:D:69:ILE:HD12	2.45	0.46
9:C:46:TYR:CE2	9:C:98:ARG:NH1	2.82	0.46
1:0:506:G:N2	1:0:508:A:H3'	2.30	0.46
1:0:1845:A:P	7:A:190:ARG:HH11	2.38	0.46
7:A:59:GLU:HG2	7:A:65:ARG:HD3	1.97	0.46
1:0:1298:U:H2'	1:0:1299:G:C8	2.50	0.46
1:0:745:G:H5''	1:0:746:A:OP1	2.15	0.46
30:X:66:THR:HG23	30:X:67:PRO:HD2	1.97	0.46
1:0:441:A:H1'	1:0:442:A:N7	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:34:GLY:O	8:B:35:GLN:O	2.33	0.46
1:0:2717:C:H5'	8:B:302:PRO:HA	1.96	0.46
8:B:41:PHE:CB	8:B:190:MET:HE3	2.38	0.46
30:X:43:VAL:HG12	30:X:47:ALA:HB3	1.95	0.46
10:D:27:ILE:HG22	10:D:28:GLY:N	2.30	0.46
16:J:42:GLU:HG2	16:J:43:ARG:N	2.29	0.46
15:I:70:THR:HA	15:I:107:LYS:HZ3	1.81	0.46
19:M:80:GLY:O	19:M:81:ARG:HD2	2.16	0.46
1:0:2793:A:H2'	1:0:2794:G:H5'	1.97	0.46
1:0:1314:U:H5''	1:0:1316:G:O4'	2.14	0.46
1:0:503:G:H2'	1:0:504:G:H8	1.80	0.46
1:0:711:G:C2	1:0:718:C:C2	3.03	0.46
1:0:2670:G:O2'	1:0:2671:U:H5'	2.14	0.46
1:0:2768:A:O2'	1:0:2769:C:H5'	2.15	0.46
1:0:398:U:H2'	1:0:399:C:C6	2.50	0.46
1:0:820:G:C5	7:A:171:LYS:HB2	2.50	0.46
26:T:40:VAL:HG22	26:T:41:ARG:N	2.30	0.46
1:0:1375:A:C2'	1:0:1376:G:H5'	2.45	0.46
14:H:49:GLN:NE2	14:H:140:TYR:HE2	2.10	0.46
27:U:17:THR:CG2	27:U:18:GLY:N	2.79	0.46
1:0:2839:C:H2'	1:0:2840:A:H5''	1.96	0.46
7:A:55:VAL:HG21	7:A:67:LEU:HB3	1.98	0.46
30:X:7:GLU:HG2	30:X:8:ARG:N	2.31	0.46
1:0:440:C:H2'	1:0:441:A:C8	2.50	0.46
1:0:1398:G:H2'	1:0:1399:A:C8	2.51	0.46
1:0:222:A:H2'	1:0:223:G:O4'	2.15	0.46
1:0:2894:C:O2'	1:0:2895:C:H5'	2.15	0.46
1:0:1041:U:H4'	1:0:1295:G:H5'	1.98	0.46
32:Z:50:GLN:HB2	32:Z:54:ILE:HG22	1.96	0.46
1:0:1181:A:O4'	15:I:87:PRO:HG2	2.16	0.46
29:W:139:GLY:O	29:W:141:HIS:CD2	2.68	0.46
1:0:285:A:H2'	1:0:286:U:O4'	2.15	0.46
26:T:52:ARG:O	26:T:53:GLY:O	2.34	0.46
1:0:1185:U:OP1	15:I:121:LYS:HD3	2.15	0.46
13:G:71:LEU:C	13:G:73:ASP:H	2.19	0.46
1:0:2582:G:O3'	17:K:41:LYS:HA	2.16	0.46
1:0:35:U:H5'	9:C:47:GLY:O	2.16	0.46
1:0:106:A:H2'	1:0:107:U:O4'	2.16	0.46
16:J:97:ALA:O	16:J:101:VAL:HG23	2.16	0.46
1:0:542:A:H2'	1:0:543:G:O4'	2.16	0.46
14:H:100:GLU:HB3	14:H:124:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:44:VAL:O	24:R:48:GLU:HG3	2.16	0.46
14:H:60:LEU:O	14:H:65:LEU:HD21	2.16	0.46
12:F:100:ASP:O	12:F:101:ALA:O	2.33	0.46
12:F:16:ALA:HA	12:F:111:ILE:HD13	1.96	0.46
7:A:125:ASN:CB	7:A:158:VAL:HG12	2.46	0.46
26:T:18:GLU:O	26:T:21:LYS:HG2	2.16	0.46
1:0:524:A:H5'	24:R:29:LYS:HE2	1.97	0.46
1:0:263:U:O4'	12:F:59:ILE:HD13	2.15	0.46
19:M:122:GLN:OE1	19:M:127:LYS:HE2	2.16	0.46
1:0:1029:U:O2'	1:0:1273:C:OP1	2.31	0.46
18:L:90:ARG:HH11	18:L:90:ARG:HG3	1.81	0.46
30:X:37:LEU:CD1	30:X:85:VAL:HG21	2.35	0.46
17:K:29:LEU:HB3	17:K:55:VAL:CG1	2.39	0.46
20:N:47:LEU:HD12	20:N:92:ALA:HB1	1.96	0.46
27:U:52:THR:HG21	27:U:54:THR:HB	1.98	0.46
19:M:9:ARG:HB2	19:M:47:ASP:OD2	2.16	0.46
10:D:18:ILE:HA	10:D:134:LEU:HD23	1.96	0.46
1:0:2676:C:H4'	16:J:70:PHE:CD1	2.51	0.46
1:0:945:U:H2'	1:0:946:C:H6	1.79	0.46
1:0:1268:C:H2'	1:0:1269:G:C8	2.50	0.46
1:0:569:A:H5''	1:0:587:A:N1	2.31	0.46
1:0:603:A:H4'	1:0:604:G:O5'	2.16	0.46
10:D:78:GLU:O	10:D:82:GLU:HG3	2.16	0.46
27:U:52:THR:HG22	27:U:54:THR:HB	1.96	0.46
1:0:553:G:O4'	1:0:1325:G:H5'	2.15	0.46
1:0:2850:C:C6	1:0:2850:C:H5'	2.48	0.46
28:V:42:ASN:O	28:V:44:GLY:N	2.49	0.46
7:A:109:GLU:HG2	7:A:116:GLY:N	2.31	0.46
1:0:107:U:H2'	1:0:108:U:H5'	1.98	0.46
29:W:19:ASP:O	29:W:23:MET:HG3	2.15	0.46
1:0:1579:C:H4'	1:0:1580:A:OP1	2.15	0.46
1:0:2708:G:H2'	1:0:2709:G:O4'	2.16	0.46
1:0:1805:G:H2'	1:0:1806:G:H8	1.80	0.46
1:0:1384:C:H5'	30:X:30:MET:HG2	1.96	0.46
1:0:553:G:P	31:Y:204:ARG:NH2	2.87	0.46
7:A:105:VAL:HG12	7:A:106:CYS:N	2.30	0.46
1:0:907:A:H4'	1:0:1328:A:C2	2.51	0.46
14:H:123:ILE:HD12	14:H:123:ILE:N	2.31	0.46
16:J:131:THR:HG22	16:J:133:GLY:H	1.80	0.46
29:W:73:LEU:HA	29:W:73:LEU:HD12	1.78	0.46
26:T:24:ARG:HH21	26:T:39:ASN:HD22	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:42:VAL:HG21	7:A:74:VAL:CG1	2.46	0.46
16:J:46:ILE:O	16:J:46:ILE:HG12	2.15	0.46
1:0:1182:C:H1'	1:0:1192:A:H8	1.80	0.46
1:0:542:A:H5'	1:0:542:A:C8	2.40	0.46
9:C:235:PHE:CE2	9:C:243:VAL:HG21	2.45	0.46
17:K:115:ARG:HG3	17:K:116:GLU:N	2.31	0.46
1:0:2521:A:P	14:H:6:ALA:HB3	2.56	0.46
9:C:54:LEU:HD23	9:C:79:ARG:HG3	1.97	0.46
11:E:68:HIS:O	11:E:72:MET:HG3	2.16	0.46
1:0:2443:C:H5'	18:L:57:VAL:HG21	1.98	0.46
1:0:266:G:OP2	19:M:55:LYS:HE2	2.16	0.46
9:C:133:ARG:NE	9:C:135:GLU:O	2.49	0.46
9:C:170:ASP:O	9:C:171:GLU:HG3	2.16	0.46
21:O:39:THR:O	21:O:115:ARG:NH2	2.49	0.46
11:E:16:ASP:O	11:E:17:HIS:HB2	2.16	0.46
28:V:26:GLU:OE2	28:V:45:ARG:NH1	2.49	0.46
29:W:13:MET:HE2	29:W:18:GLN:CA	2.36	0.45
17:K:125:ALA:C	17:K:127:ALA:H	2.19	0.45
13:G:71:LEU:C	13:G:73:ASP:N	2.69	0.45
25:S:32:ALA:HA	25:S:36:GLU:OE1	2.16	0.45
1:0:2815:G:N7	16:J:80:LYS:NZ	2.64	0.45
1:0:821:U:H2'	1:0:822:C:H6	1.81	0.45
1:0:920:C:H5''	1:0:921:G:O5'	2.16	0.45
1:0:1850:U:H2'	1:0:1851:G:H8	1.81	0.45
1:0:860:U:H2'	1:0:861:A:C8	2.51	0.45
1:0:2356:A:H2'	1:0:2357:G:O4'	2.16	0.45
1:0:2028:U:H2'	1:0:2029:C:C6	2.50	0.45
1:0:911:G:H5'	1:0:932:U:OP1	2.16	0.45
30:X:27:ASP:OD2	30:X:27:ASP:N	2.46	0.45
9:C:98:ARG:HH11	9:C:98:ARG:CG	2.23	0.45
8:B:238:ASN:HD22	8:B:240:GLY:N	2.08	0.45
6:9:8:G:O6	20:N:11:ARG:NH1	2.49	0.45
1:0:2781:U:C2'	1:0:2782:G:H5'	2.46	0.45
14:H:30:LYS:N	14:H:62:HIS:HD2	2.13	0.45
1:0:137:U:OP1	1:0:259:G:O2'	2.34	0.45
1:0:2379:G:N7	1:0:2408:A:N1	2.64	0.45
8:B:81:ALA:O	8:B:186:GLY:HA3	2.17	0.45
30:X:34:ARG:NH1	30:X:48:VAL:O	2.46	0.45
8:B:14:GLY:HA2	8:B:15:PRO:C	2.36	0.45
1:0:366:U:H2'	1:0:367:G:O4'	2.16	0.45
4:3:42:ARG:HH11	4:3:42:ARG:HG3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:88:ILE:CD1	7:A:100:PRO:HD3	2.39	0.45
12:F:57:GLU:O	12:F:61:MET:HG3	2.16	0.45
7:A:105:VAL:HG11	7:A:154:ALA:CB	2.46	0.45
13:G:71:LEU:O	13:G:73:ASP:N	2.49	0.45
32:Z:72:GLU:CB	32:Z:77:LYS:HE3	2.46	0.45
1:O:815:U:O2'	1:O:1598:A:H4'	2.16	0.45
7:A:55:VAL:CG2	7:A:67:LEU:HB3	2.47	0.45
26:T:73:HIS:CD2	26:T:88:PRO:HG3	2.51	0.45
16:J:127:ILE:HG22	36:J:8801:CL:CL	2.53	0.45
1:O:204:A:C2'	1:O:205:U:H5'	2.45	0.45
1:O:2504:A:H4'	14:H:74:ARG:HH11	1.81	0.45
22:P:55:LYS:CG	22:P:56:GLY:N	2.79	0.45
1:O:682:A:H2'	1:O:683:G:O4'	2.16	0.45
10:D:91:ALA:HB2	10:D:106:PHE:CE2	2.51	0.45
1:O:1419:U:H2'	1:O:1685:A:C2	2.51	0.45
1:O:2090:G:H2'	1:O:2091:G:C8	2.51	0.45
30:X:73:ARG:NH2	30:X:88:GLU:OE2	2.50	0.45
6:9:95:C:O2'	6:9:96:C:H5'	2.16	0.45
1:O:2506:A:N6	1:O:2511:A:O2'	2.49	0.45
29:W:3:ALA:O	29:W:54:PHE:HA	2.16	0.45
1:O:1058:A:H2'	1:O:1060:C:C5'	2.44	0.45
18:L:54:PRO:HG2	18:L:57:VAL:CG2	2.46	0.45
1:O:1878:G:O2'	1:O:1879:U:C6	2.67	0.45
1:O:2880:A:H2'	1:O:2881:C:H5'	1.99	0.45
1:O:1783:A:O2'	1:O:1784:U:H5'	2.16	0.45
1:O:363:C:O2'	1:O:364:U:H5'	2.17	0.45
24:R:124:GLY:HA3	24:R:136:TRP:O	2.16	0.45
1:O:1829:A:H2'	1:O:1830:C:H5'	1.99	0.45
1:O:1557:G:O2'	1:O:1558:C:H5'	2.16	0.45
10:D:169:THR:O	10:D:169:THR:HG22	2.17	0.45
15:I:87:PRO:HB2	15:I:129:SER:HA	1.99	0.45
1:O:1209:C:H2'	1:O:1210:G:H8	1.81	0.45
29:W:48:VAL:HG12	29:W:48:VAL:O	2.17	0.45
19:M:166:ALA:HA	19:M:169:ARG:NH1	2.32	0.45
14:H:41:LYS:HE2	14:H:45:ASP:CB	2.40	0.45
17:K:113:ILE:CG2	17:K:114:ALA:N	2.79	0.45
20:N:79:PRO:HB3	20:N:172:PHE:CD1	2.52	0.45
28:V:39:ALA:O	28:V:41:GLU:N	2.50	0.45
1:O:2564:G:OP2	1:O:2565:C:H5''	2.15	0.45
8:B:280:VAL:HG12	8:B:334:SER:HA	1.97	0.45
28:V:44:GLY:O	28:V:48:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:154:ARG:HA	14:H:157:TYR:CE2	2.51	0.45
6:9:22:G:H5'	6:9:23:U:OP1	2.16	0.45
30:X:20:GLU:OE1	30:X:21:PRO:HD2	2.17	0.45
14:H:53:ILE:HA	14:H:134:GLU:O	2.17	0.45
8:B:215:VAL:HA	8:B:220:VAL:HG22	1.97	0.45
1:0:2276:U:H2'	1:0:2277:U:C6	2.51	0.45
1:0:2667:G:H1'	1:0:2914:A:N3	2.31	0.45
20:N:178:THR:O	20:N:181:ASP:HB3	2.17	0.45
1:0:188:C:H5''	19:M:163:LEU:HD21	1.99	0.45
24:R:17:MET:CE	24:R:19:ARG:CZ	2.94	0.45
3:2:36:ASN:HB3	3:2:39:ARG:CG	2.46	0.45
18:L:145:LEU:C	18:L:145:LEU:HD23	2.37	0.45
21:O:25:VAL:O	21:O:29:VAL:HG23	2.16	0.45
1:0:2265:U:H2'	1:0:2266:A:H8	1.78	0.45
1:0:638:C:H2'	1:0:639:A:H8	1.80	0.45
1:0:105:G:O2'	1:0:106:A:H5'	2.16	0.45
1:0:2089:A:O2'	1:0:2090:G:H5'	2.17	0.45
8:B:109:LEU:HD11	8:B:113:LEU:HD12	1.99	0.45
1:0:113:A:OP2	1:0:114:A:H2'	2.16	0.45
1:0:152:A:O2'	1:0:153:C:H5'	2.15	0.45
16:J:36:VAL:HG12	16:J:37:ALA:N	2.32	0.45
25:S:57:THR:CG2	25:S:58:MET:N	2.80	0.45
29:W:90:TYR:CE2	29:W:99:ALA:HB2	2.52	0.45
14:H:87:LYS:HZ2	14:H:87:LYS:HB2	1.82	0.45
26:T:96:VAL:HG13	26:T:97:ARG:N	2.30	0.45
27:U:6:CYS:C	27:U:8:TYR:H	2.19	0.45
10:D:55:LYS:O	10:D:56:ARG:HB2	2.17	0.45
1:0:1483:C:O2'	1:0:1484:G:H5'	2.17	0.45
9:C:85:LYS:HA	9:C:85:LYS:HD2	1.86	0.45
4:3:65:THR:CG2	4:3:67:LEU:HG	2.46	0.45
1:0:2387:U:H2'	1:0:2388:C:C6	2.51	0.45
12:F:117:GLU:C	12:F:119:ARG:H	2.18	0.45
1:0:2005:G:H3'	1:0:2005:G:OP2	2.17	0.45
28:V:12:THR:HG23	28:V:15:GLU:H	1.82	0.45
8:B:264:GLU:HG2	8:B:267:LYS:CE	2.42	0.45
24:R:39:THR:HB	24:R:42:GLU:CD	2.36	0.45
1:0:1071:G:H4'	31:Y:154:ARG:HH22	1.80	0.45
22:P:94:TRP:CH2	22:P:98:ILE:HG13	2.52	0.45
11:E:72:MET:O	11:E:76:VAL:HG22	2.16	0.45
1:0:764:C:H2'	1:0:765:G:O4'	2.16	0.45
8:B:82:VAL:HG12	8:B:101:TRP:CE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:K:24:THR:HG21	17:K:105:ARG:HB3	1.98	0.45
8:B:150:ALA:O	8:B:152:PRO:HD3	2.17	0.45
16:J:14:ALA:O	16:J:17:CYS:HB2	2.17	0.45
29:W:26:ILE:O	29:W:26:ILE:HG13	2.16	0.45
19:M:164:THR:HG23	19:M:165:GLY:N	2.32	0.45
14:H:102:LYS:HD3	14:H:122:LYS:CD	2.40	0.45
1:O:2768:A:C2'	1:O:2769:C:O4'	2.61	0.45
1:O:1925:G:O2'	1:O:1926:G:H5'	2.17	0.45
9:C:7:ASP:C	9:C:9:ASP:H	2.20	0.45
26:T:49:GLU:OE2	26:T:97:ARG:HD2	2.17	0.45
1:O:816:G:C6	1:O:817:G:N1	2.85	0.45
1:O:2003:U:H4'	1:O:2004:U:H5	1.81	0.45
1:O:2594:C:O2'	1:O:2595:U:H5'	2.17	0.45
12:F:13:GLU:OE2	12:F:78:GLU:HG2	2.17	0.45
1:O:1097:A:H5''	29:W:125:HIS:NE2	2.32	0.45
22:P:114:LEU:HA	22:P:118:GLN:NE2	2.32	0.45
20:N:47:LEU:HD23	20:N:47:LEU:HA	1.78	0.45
1:O:380:A:OP2	19:M:9:ARG:HD2	2.17	0.45
13:G:24:VAL:HA	13:G:27:ILE:HD12	1.99	0.45
18:L:145:LEU:O	18:L:147:GLU:N	2.50	0.45
1:O:2001:G:O2'	1:O:2002:C:H5'	2.16	0.45
1:O:2314:G:H2'	1:O:2315:C:H5'	1.99	0.45
1:O:2708:G:N2	17:K:1:MET:O	2.47	0.45
14:H:72:ALA:HB2	14:H:156:ALA:HB2	1.99	0.45
1:O:2453:G:H4'	18:L:50:GLY:C	2.37	0.45
1:O:1119:G:N2	1:O:1246:A:H2	2.10	0.44
6:9:39:U:HO2'	6:9:42:C:H5	1.64	0.44
14:H:50:ILE:HD12	14:H:149:VAL:CG1	2.47	0.44
28:V:23:LEU:HD22	28:V:49:LEU:HD23	1.98	0.44
1:O:2719:A:C2	8:B:70:PRO:HG3	2.52	0.44
1:O:2301:A:H5''	1:O:2302:A:H5'	1.99	0.44
1:O:11:A:H5'	1:O:12:U:OP2	2.17	0.44
1:O:941:G:C5	1:O:942:U:C4	3.05	0.44
14:H:91:ARG:NH1	14:H:138:THR:OG1	2.43	0.44
9:C:140:VAL:HG12	9:C:141:SER:N	2.32	0.44
1:O:1909:A:H2'	1:O:1910:A:C8	2.52	0.44
1:O:195:C:H2'	1:O:196:G:H5'	2.00	0.44
14:H:12:ILE:HD12	14:H:57:THR:HG22	2.00	0.44
8:B:162:MET:CG	8:B:310:ARG:HD3	2.44	0.44
17:K:109:LEU:CD1	17:K:113:ILE:HD11	2.47	0.44
29:W:90:TYR:N	29:W:90:TYR:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:97:VAL:O	15:I:101:LYS:HG3	2.18	0.44
18:L:67:ARG:HB2	18:L:112:GLY:HA3	1.99	0.44
10:D:76:ARG:O	10:D:77:ASP:HB2	2.17	0.44
1:O:1641:A:H2'	1:O:1642:A:C5'	2.45	0.44
8:B:56:ASP:HB3	8:B:322:ARG:HE	1.82	0.44
20:N:86:LEU:HD21	20:N:180:LEU:HD11	1.99	0.44
16:J:45:VAL:HG11	16:J:121:LEU:HD22	1.99	0.44
1:O:2598:U:O2	1:O:2600:A:H8	2.00	0.44
11:E:69:ILE:HA	11:E:72:MET:HE2	1.99	0.44
20:N:139:TRP:HA	20:N:139:TRP:HE3	1.82	0.44
1:O:1762:C:H2'	1:O:1763:C:H6	1.82	0.44
1:O:497:A:H2'	1:O:498:A:C5'	2.46	0.44
1:O:2729:C:H4'	1:O:2893:C:O2	2.17	0.44
1:O:2099:G:H21	5:8:5:MEA:CE1	2.31	0.44
1:O:2498:C:O2'	1:O:2499:U:H5'	2.17	0.44
7:A:30:ARG:HB3	7:A:30:ARG:HE	1.62	0.44
9:C:236:THR:O	9:C:237:GLU:C	2.54	0.44
32:Z:60:CYS:O	32:Z:61:ASP:HB2	2.17	0.44
15:I:95:LEU:O	15:I:134:ILE:HG23	2.17	0.44
10:D:60:GLU:O	10:D:60:GLU:HG3	2.17	0.44
11:E:84:MET:HE1	11:E:148:ILE:HD12	1.99	0.44
8:B:180:ASP:O	8:B:181:ILE:C	2.56	0.44
22:P:142:ASP:O	22:P:143:ALA:O	2.36	0.44
1:O:1398:G:O2'	1:O:1399:A:H5'	2.17	0.44
30:X:21:PRO:HG2	30:X:24:LYS:HD3	1.99	0.44
8:B:83:ALA:HB2	8:B:101:TRP:CD2	2.53	0.44
11:E:77:THR:OG1	11:E:78:GLU:N	2.51	0.44
1:O:21:G:H5''	24:R:1:GLY:O	2.18	0.44
6:9:57:A:H8	10:D:141:VAL:HG21	1.82	0.44
1:O:1168:C:H5'	15:I:83:GLY:CA	2.46	0.44
1:O:1205:U:C2'	1:O:1206:U:C5'	2.93	0.44
8:B:140:LEU:HD13	8:B:175:LEU:HA	1.99	0.44
32:Z:10:ARG:CG	32:Z:11:SER:H	2.27	0.44
13:G:23:ILE:HD13	13:G:67:LEU:HD23	1.99	0.44
4:3:69:TYR:O	4:3:77:ALA:HA	2.17	0.44
1:O:920:C:H4'	1:O:921:G:C2	2.52	0.44
14:H:167:LYS:HE2	14:H:169:GLU:OE1	2.16	0.44
29:W:35:VAL:HG22	29:W:36:PRO:O	2.18	0.44
1:O:1307:A:H2'	1:O:1308:A:C8	2.52	0.44
1:O:1947:G:N2	1:O:1966:U:C2	2.85	0.44
1:O:1262:C:H1'	29:W:120:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2869:G:H2'	1:0:2870:C:C6	2.52	0.44
7:A:27:LEU:HD12	7:A:69:LEU:HD22	1.99	0.44
10:D:25:MET:CE	10:D:41:LEU:HG	2.48	0.44
32:Z:57:CYS:O	32:Z:61:ASP:HA	2.17	0.44
8:B:62:ARG:NH2	8:B:66:GLU:O	2.50	0.44
1:0:1587:U:H2'	1:0:1588:G:O4'	2.18	0.44
1:0:236:A:H8	1:0:236:A:OP1	2.00	0.44
7:A:192:VAL:CG1	7:A:207:GLN:HB3	2.48	0.44
8:B:243:ASN:HA	8:B:244:PRO:C	2.37	0.44
14:H:139:ALA:HB3	14:H:149:VAL:HG21	2.00	0.44
1:0:308:U:H5'	26:T:97:ARG:NH2	2.33	0.44
29:W:149:LEU:HG	29:W:153:MET:CE	2.48	0.44
1:0:947:U:H2'	1:0:948:G:H8	1.81	0.44
1:0:64:G:H2'	1:0:65:C:O4'	2.17	0.44
24:R:114:VAL:HA	24:R:144:GLU:O	2.18	0.44
1:0:512:G:O3'	1:0:513:A:H8	2.01	0.44
7:A:214:SER:HA	7:A:227:ASP:O	2.17	0.44
1:0:705:C:H2'	1:0:706:G:O4'	2.17	0.44
1:0:241:A:C2	1:0:378:A:H4'	2.52	0.44
1:0:1175:G:H1'	1:0:1193:A:H2'	2.00	0.44
6:9:3:A:H2	6:9:21:G:N3	2.15	0.44
1:0:553:G:H2'	1:0:554:G:H5'	1.99	0.44
16:J:39:VAL:CG1	16:J:107:ASN:HB2	2.47	0.44
1:0:47:G:N3	1:0:114:A:C2	2.86	0.44
1:0:853:C:H2'	1:0:854:G:O4'	2.17	0.44
1:0:1872:C:H5	7:A:20:SER:HB3	1.82	0.44
1:0:1652:C:OP2	32:Z:49:ARG:NH2	2.50	0.44
12:F:48:VAL:CG2	12:F:74:PHE:HB3	2.47	0.44
1:0:2717:C:H2'	1:0:2718:C:C5'	2.34	0.44
15:I:95:LEU:HD23	15:I:99:GLN:OE1	2.17	0.44
1:0:283:U:C5	1:0:284:C:N3	2.85	0.44
17:K:113:ILE:HG22	17:K:114:ALA:N	2.31	0.44
3:2:40:ARG:HG3	3:2:45:ASN:CB	2.48	0.44
1:0:67:A:H5''	1:0:69:A:C8	2.53	0.44
20:N:154:LEU:HG	20:N:155:GLU:N	2.33	0.44
1:0:944:G:H21	29:W:44:MET:HE1	1.83	0.44
11:E:125:GLU:HB2	11:E:132:THR:CG2	2.47	0.44
1:0:2064:U:H5'	1:0:2652:U:O3'	2.18	0.44
15:I:70:THR:HA	15:I:107:LYS:NZ	2.32	0.44
1:0:474:C:O2'	9:C:73:LEU:HD21	2.18	0.44
1:0:2002:C:C2'	1:0:2003:U:H5'	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2897:C:O2'	1:0:2898:G:H5'	2.18	0.44
9:C:133:ARG:HG2	9:C:134:ASP:N	2.33	0.44
26:T:89:ARG:O	26:T:89:ARG:HG3	2.17	0.44
1:0:2032:U:H2'	1:0:2033:G:C5'	2.48	0.44
15:I:80:PHE:CD2	15:I:92:VAL:HG12	2.53	0.44
29:W:63:GLU:HG2	29:W:93:ILE:HG22	1.99	0.44
1:0:1287:A:O4'	29:W:117:ARG:HD3	2.17	0.44
26:T:71:VAL:CG1	26:T:72:ILE:N	2.80	0.44
26:T:35:TYR:CD2	26:T:112:LEU:HD22	2.53	0.44
28:V:12:THR:OG1	28:V:13:PRO:HD2	2.18	0.44
1:0:877:G:C5'	1:0:878:G:OP1	2.63	0.44
1:0:2780:C:H2'	1:0:2781:U:C6	2.53	0.44
21:O:25:VAL:HG23	21:O:26:TRP:N	2.33	0.44
3:2:29:THR:C	3:2:31:ARG:N	2.70	0.44
1:0:2600:A:H2'	1:0:2601:A:O4'	2.18	0.44
21:O:32:ARG:HE	21:O:35:LYS:HD2	1.83	0.44
8:B:195:ARG:HD2	8:B:324:ASP:OD1	2.17	0.44
29:W:142:ASP:CB	29:W:145:GLY:H	2.30	0.44
14:H:53:ILE:HD11	14:H:167:LYS:HD3	2.00	0.44
1:0:2619:UR3:H2'	1:0:2620:U:C6	2.53	0.44
20:N:144:GLY:O	20:N:147:ILE:CG2	2.65	0.44
1:0:432:G:O2'	1:0:433:C:H5'	2.18	0.44
1:0:2478:U:O2'	1:0:2479:A:H5'	2.17	0.44
1:0:1168:C:H5''	15:I:83:GLY:H	1.82	0.44
19:M:164:THR:CG2	19:M:166:ALA:H	2.31	0.44
17:K:55:VAL:CG1	17:K:56:SER:N	2.81	0.44
17:K:13:GLU:OE2	17:K:44:LEU:HB2	2.17	0.44
1:0:1316:G:H1'	1:0:1340:G:N2	2.33	0.44
1:0:2599:A:C2	1:0:2684:A:H4'	2.52	0.44
1:0:1855:G:H4'	1:0:1856:C:O5'	2.17	0.44
2:1:26:SER:HB3	2:1:35:SER:OG	2.18	0.44
1:0:2424:U:H1'	23:Q:7:LEU:HD12	2.00	0.44
11:E:119:HIS:HE1	11:E:147:ASP:OD2	2.01	0.44
1:0:2866:U:C4	27:U:50:GLU:HB3	2.52	0.44
12:F:110:ASP:O	12:F:114:LYS:HG3	2.17	0.44
9:C:14:GLY:O	9:C:15:GLU:HB3	2.18	0.44
1:0:1930:A:H2'	1:0:1931:A:C8	2.53	0.44
1:0:1593:C:OP1	22:P:117:SER:HB3	2.16	0.43
7:A:36:ASP:HB2	7:A:83:GLY:C	2.38	0.43
8:B:55:ASN:HB3	8:B:63:GLU:CA	2.41	0.43
24:R:145:LEU:HD12	24:R:146:ILE:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2676:C:H4'	16:J:70:PHE:HE1	1.81	0.43
1:0:668:C:H2'	1:0:669:G:H8	1.83	0.43
29:W:119:HIS:HD2	29:W:120:PRO:O	2.00	0.43
1:0:1849:G:H1'	1:0:2011:A:N1	2.33	0.43
1:0:1385:G:O3'	30:X:49:ARG:NH1	2.51	0.43
18:L:35:ARG:O	18:L:40:PHE:HA	2.18	0.43
6:9:11:A:P	23:Q:19:ARG:HH21	2.41	0.43
1:0:613:C:H2'	1:0:614:U:H6	1.82	0.43
1:0:2761:A:C4	1:0:2763:G:C8	3.06	0.43
17:K:131:ILE:HG22	17:K:131:ILE:O	2.17	0.43
28:V:12:THR:HG23	28:V:14:ALA:H	1.83	0.43
10:D:136:ARG:H	10:D:136:ARG:HG2	1.59	0.43
11:E:11:VAL:HG13	11:E:23:GLU:O	2.19	0.43
7:A:192:VAL:CG1	7:A:192:VAL:O	2.65	0.43
7:A:94:LEU:N	7:A:94:LEU:CD2	2.81	0.43
1:0:485:A:O2'	1:0:487:G:H5'	2.18	0.43
8:B:36:PRO:HB3	8:B:174:ARG:HA	1.99	0.43
1:0:2256:G:H2'	1:0:2257:G:H5'	1.99	0.43
22:P:55:LYS:HG2	22:P:56:GLY:N	2.33	0.43
1:0:2619:UR3:O2	1:0:2619:UR3:O4'	2.35	0.43
1:0:1855:G:O6	7:A:142:SER:HB3	2.18	0.43
1:0:303:C:H2'	1:0:304:G:O4'	2.19	0.43
11:E:20:ILE:CD1	11:E:40:VAL:HG11	2.48	0.43
8:B:44:TYR:OH	8:B:148:PRO:HG3	2.18	0.43
24:R:46:TYR:O	24:R:50:VAL:HG23	2.18	0.43
1:0:2455:A:H2'	1:0:2456:A:O4'	2.18	0.43
17:K:72:VAL:HG11	17:K:121:PHE:CD1	2.53	0.43
1:0:2401:A:H2'	1:0:2402:A:C8	2.54	0.43
10:D:128:LEU:C	10:D:128:LEU:HD23	2.38	0.43
16:J:52:GLN:HG3	16:J:53:ILE:H	1.83	0.43
1:0:559:U:C5'	1:0:559:U:H6	2.23	0.43
8:B:17:LYS:O	8:B:260:HIS:CD2	2.72	0.43
7:A:86:ALA:HB1	7:A:92:ASN:HD22	1.83	0.43
1:0:1925:G:H5''	4:3:29:ARG:HH22	1.82	0.43
6:9:28:U:H2'	6:9:29:C:C6	2.54	0.43
26:T:40:VAL:HG23	26:T:119:ALA:C	2.37	0.43
1:0:2326:C:H4'	1:0:2412:G:C4'	2.48	0.43
1:0:419:A:H1'	1:0:1921:A:C2	2.52	0.43
1:0:2740:G:H2'	1:0:2741:A:O4'	2.17	0.43
1:0:790:A:H1'	1:0:1710:A:H2'	2.00	0.43
11:E:86:VAL:CG1	11:E:129:GLU:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1882:C:O2'	1:0:2012:U:OP2	2.33	0.43
1:0:2769:C:C2'	1:0:2770:G:C5'	2.96	0.43
16:J:19:MET:HE1	16:J:132:LEU:HD11	2.01	0.43
8:B:217:ARG:CD	8:B:257:THR:HG22	2.49	0.43
11:E:81:GLU:HA	11:E:133:VAL:O	2.18	0.43
9:C:7:ASP:O	9:C:9:ASP:N	2.51	0.43
17:K:81:ARG:HD3	17:K:87:ARG:NH2	2.32	0.43
2:1:28:HIS:CD2	2:1:30:LYS:HB2	2.53	0.43
1:0:932:U:H2'	1:0:933:C:C6	2.53	0.43
10:D:21:VAL:HA	10:D:131:THR:O	2.18	0.43
1:0:1407:A:O2'	1:0:1408:U:H3'	2.18	0.43
1:0:1345:A:H2'	1:0:1346:U:C6	2.53	0.43
1:0:2115:U:H2'	1:0:2116:U:C6	2.53	0.43
28:V:29:ASN:O	28:V:33:VAL:HG23	2.18	0.43
6:9:34:A:H8	6:9:34:A:O5'	2.02	0.43
1:0:876:A:H2'	1:0:876:A:N3	2.33	0.43
6:9:13:A:N3	20:N:14:ARG:NH2	2.66	0.43
19:M:47:ASP:CG	19:M:48:LYS:N	2.72	0.43
29:W:38:THR:CG2	29:W:39:ASP:N	2.81	0.43
24:R:80:TYR:CD1	24:R:80:TYR:N	2.86	0.43
28:V:42:ASN:N	28:V:43:PRO:CD	2.81	0.43
31:Y:112:GLU:OE2	31:Y:115:ARG:NH1	2.51	0.43
9:C:57:PRO:HG2	9:C:73:LEU:HD13	2.00	0.43
11:E:69:ILE:HA	11:E:72:MET:HE3	2.00	0.43
1:0:1003:U:H4'	14:H:91:ARG:O	2.19	0.43
1:0:1940:C:H5''	7:A:234:GLY:HA3	2.00	0.43
29:W:42:ARG:HA	29:W:45:VAL:CG2	2.49	0.43
32:Z:56:GLN:HA	32:Z:62:TYR:O	2.17	0.43
7:A:211:LYS:CB	7:A:212:PRO:HD2	2.33	0.43
1:0:777:U:O2'	2:1:11:LYS:HG2	2.18	0.43
6:9:107:C:O2'	6:9:108:C:H5'	2.19	0.43
11:E:84:MET:HE1	11:E:133:VAL:CG2	2.49	0.43
16:J:107:ASN:C	16:J:107:ASN:ND2	2.71	0.43
8:B:280:VAL:CG1	8:B:334:SER:HA	2.49	0.43
1:0:1375:A:O2'	1:0:1376:G:H5'	2.18	0.43
1:0:2728:C:H4'	1:0:2894:C:O2'	2.19	0.43
2:1:2:GLY:O	2:1:6:PRO:HG2	2.18	0.43
25:S:19:ASP:O	25:S:20:PHE:HD2	2.01	0.43
18:L:98:GLU:C	18:L:99:GLU:HG3	2.38	0.43
1:0:1617:C:C4	1:0:1643:C:H4'	2.53	0.43
9:C:132:ASP:O	9:C:161:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:243:A:H61	1:0:269:G:H1'	1.83	0.43
9:C:78:ARG:CG	9:C:78:ARG:NH1	2.73	0.43
8:B:55:ASN:HB3	8:B:64:GLY:H	1.83	0.43
8:B:57:GLU:O	8:B:63:GLU:HB3	2.19	0.43
9:C:98:ARG:NH1	9:C:98:ARG:CG	2.81	0.43
24:R:39:THR:HG22	24:R:42:GLU:H	1.84	0.43
1:0:100:C:H4'	26:T:16:LEU:HB2	2.01	0.43
1:0:2420:G:H2'	1:0:2421:G:C8	2.54	0.43
10:D:99:ASP:N	10:D:103:ASN:O	2.39	0.43
29:W:122:ARG:NH1	29:W:122:ARG:HG3	2.33	0.43
1:0:1015:C:H2'	1:0:1016:U:H6	1.81	0.43
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.19	0.43
1:0:1165:G:C4'	1:0:1174:A:O2'	2.66	0.43
4:3:34:LYS:HD2	4:3:34:LYS:N	2.33	0.43
9:C:127:ARG:HD2	9:C:229:PRO:O	2.17	0.43
29:W:4:LEU:HD23	29:W:4:LEU:HA	1.77	0.43
24:R:91:LEU:CD2	24:R:143:VAL:HG22	2.48	0.43
1:0:482:G:H4'	1:0:508:A:N1	2.34	0.43
29:W:88:THR:HG23	29:W:110:GLN:CB	2.47	0.43
20:N:143:ARG:HG2	20:N:172:PHE:CD2	2.53	0.43
1:0:110:C:H2'	1:0:111:C:C6	2.54	0.43
9:C:200:PRO:HB3	9:C:212:VAL:CG2	2.49	0.43
1:0:694:A:C2'	1:0:695:C:H5'	2.48	0.43
8:B:195:ARG:CZ	8:B:323:LEU:HD13	2.49	0.43
23:Q:93:ARG:NH1	23:Q:93:ARG:HG3	2.33	0.43
1:0:1025:C:H5'	29:W:23:MET:O	2.19	0.43
1:0:249:G:O2'	1:0:250:C:H5'	2.19	0.43
31:Y:187:VAL:CG2	31:Y:192:ASP:HB2	2.30	0.43
7:A:32:VAL:O	7:A:33:GLU:C	2.57	0.43
7:A:100:PRO:O	7:A:103:VAL:HG23	2.19	0.43
11:E:84:MET:HG2	11:E:168:ILE:HA	2.01	0.43
32:Z:10:ARG:HB2	32:Z:27:ALA:HB1	2.01	0.43
1:0:1819:G:H2'	1:0:1820:G:C4'	2.45	0.43
11:E:6:GLU:HG2	11:E:46:THR:HG22	2.01	0.43
1:0:2270:G:C4'	7:A:223:ARG:HH12	2.31	0.43
31:Y:234:VAL:HG12	31:Y:235:GLU:N	2.34	0.43
1:0:2831:C:C2'	1:0:2832:C:H5'	2.49	0.43
20:N:170:GLU:HA	20:N:173:ASP:OD2	2.19	0.43
1:0:758:A:H2'	1:0:759:C:O4'	2.19	0.43
12:F:106:ALA:O	12:F:109:GLU:HB3	2.18	0.43
1:0:1544:U:H2'	1:0:1545:C:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:I:72:GLU:C	15:I:74:ILE:N	2.71	0.43
8:B:307:ARG:CB	8:B:307:ARG:HH11	2.31	0.43
6:9:14:G:O2'	20:N:1:ALA:HB2	2.19	0.43
9:C:136:VAL:HA	9:C:137:PRO:C	2.39	0.43
7:A:57:ALA:HA	7:A:67:LEU:HD23	2.00	0.43
29:W:125:HIS:CD2	29:W:127:GLY:H	2.37	0.43
9:C:140:VAL:CG1	9:C:141:SER:N	2.82	0.43
1:0:2866:U:H4'	1:0:2867:G:H5'	2.01	0.43
29:W:42:ARG:HA	29:W:45:VAL:HG22	2.00	0.43
1:0:1681:G:H5''	1:0:1682:A:H5'	2.00	0.43
1:0:1597:A:O4'	22:P:95:GLU:HG2	2.19	0.43
1:0:2281:C:H2'	1:0:2282:U:H5'	2.01	0.43
1:0:2133:U:H4'	1:0:2134:G:C5'	2.49	0.43
1:0:466:A:H2'	1:0:467:G:O4'	2.18	0.43
10:D:156:ARG:HG3	10:D:156:ARG:HH11	1.84	0.43
1:0:1168:C:C5'	15:I:83:GLY:H	2.32	0.42
30:X:43:VAL:HG22	30:X:76:ARG:NH1	2.34	0.42
1:0:2715:G:N2	8:B:264:GLU:OE1	2.41	0.42
7:A:217:ARG:NH1	7:A:217:ARG:CG	2.80	0.42
29:W:10:GLU:HG3	29:W:11:VAL:N	2.33	0.42
14:H:80:LEU:HD11	14:H:145:ASP:HB3	2.01	0.42
24:R:25:PHE:CE2	24:R:29:LYS:HE2	2.54	0.42
9:C:4:THR:HB	9:C:135:GLU:OE2	2.19	0.42
8:B:82:VAL:O	8:B:82:VAL:HG12	2.19	0.42
1:0:581:G:O2'	1:0:582:U:H5'	2.19	0.42
1:0:121:U:OP2	3:2:10:ARG:NH2	2.41	0.42
27:U:20:MET:CG	27:U:28:THR:HG23	2.49	0.42
3:2:28:LYS:O	3:2:28:LYS:HG2	2.19	0.42
29:W:48:VAL:CG1	29:W:52:VAL:HB	2.46	0.42
1:0:2781:U:H2'	1:0:2782:G:C5'	2.49	0.42
8:B:313:PRO:O	8:B:314:ALA:C	2.57	0.42
10:D:103:ASN:ND2	10:D:134:LEU:H	2.17	0.42
1:0:2269:C:C2'	1:0:2270:G:H5'	2.48	0.42
1:0:1787:C:O2'	1:0:1788:U:H5'	2.19	0.42
19:M:42:ARG:HA	19:M:43:PRO:HD3	1.87	0.42
1:0:1852:A:H4'	7:A:230:SER:HB2	2.01	0.42
26:T:41:ARG:NH1	26:T:42:VAL:O	2.51	0.42
12:F:118:LEU:O	12:F:119:ARG:OXT	2.37	0.42
31:Y:145:LYS:O	31:Y:147:ARG:HG2	2.18	0.42
1:0:940:G:C5	1:0:1027:G:C2	3.07	0.42
1:0:2515:C:H2'	1:0:2516:G:O4'	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1249:U:H2'	1:0:1250:C:C6	2.54	0.42
1:0:1250:C:O2'	1:0:1251:C:H5'	2.20	0.42
9:C:19:PRO:HD2	9:C:240:LEU:CD2	2.50	0.42
1:0:2112:A:H2'	1:0:2113:G:C8	2.54	0.42
18:L:81:VAL:HG12	18:L:81:VAL:O	2.19	0.42
1:0:1943:C:O4'	7:A:212:PRO:HA	2.18	0.42
1:0:1180:U:H2'	1:0:1181:A:O4'	2.19	0.42
17:K:75:ARG:O	17:K:93:ASN:HA	2.19	0.42
1:0:2345:A:H3'	1:0:2346:C:C6	2.54	0.42
9:C:27:ARG:CG	9:C:27:ARG:HH11	2.32	0.42
11:E:91:PHE:CD2	11:E:109:GLY:HA2	2.54	0.42
20:N:50:LEU:HA	20:N:50:LEU:HD12	1.93	0.42
26:T:73:HIS:CD2	26:T:88:PRO:CB	3.02	0.42
17:K:34:VAL:CG2	17:K:47:ALA:HB2	2.49	0.42
8:B:109:LEU:HD11	8:B:113:LEU:CD1	2.50	0.42
9:C:84:VAL:O	9:C:85:LYS:HB2	2.19	0.42
1:0:704:C:H2'	1:0:705:C:H6	1.84	0.42
26:T:79:LEU:O	26:T:87:VAL:HG22	2.19	0.42
1:0:2906:A:H5'	1:0:2907:C:O4'	2.19	0.42
17:K:64:MET:HA	17:K:67:GLN:NE2	2.35	0.42
1:0:2644:C:O2'	1:0:2645:U:H5'	2.18	0.42
1:0:629:A:H2'	1:0:630:A:O4'	2.20	0.42
20:N:82:TYR:CD2	20:N:82:TYR:C	2.93	0.42
1:0:1524:U:OP1	1:0:1524:U:H4'	2.19	0.42
1:0:875:A:C2	7:A:194:MET:SD	3.12	0.42
11:E:102:VAL:HG11	11:E:148:ILE:HG12	2.01	0.42
29:W:73:LEU:O	29:W:74:GLU:HG3	2.19	0.42
1:0:2379:G:H5'	1:0:2381:C:O4'	2.20	0.42
16:J:84:ARG:HB2	16:J:98:PHE:CE1	2.55	0.42
1:0:2720:C:O2	17:K:87:ARG:NH2	2.52	0.42
1:0:1500:U:P	22:P:41:ARG:HH22	2.42	0.42
8:B:181:ILE:HG22	8:B:186:GLY:HA2	2.01	0.42
1:0:1391:G:H2'	1:0:1392:A:H5'	2.01	0.42
10:D:20:LYS:HA	10:D:75:LEU:O	2.20	0.42
7:A:41:THR:HG23	7:A:77:GLY:O	2.19	0.42
15:I:87:PRO:HB3	15:I:129:SER:C	2.40	0.42
1:0:1592:G:O2'	1:0:1593:C:O5'	2.38	0.42
6:9:47:A:C2	6:9:48:C:C2	3.07	0.42
1:0:484:A:N1	1:0:506:G:H4'	2.34	0.42
11:E:11:VAL:HG12	11:E:12:ASP:H	1.81	0.42
11:E:7:ILE:HA	11:E:8:PRO:HD3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:39:ALA:C	28:V:41:GLU:N	2.73	0.42
1:0:2547:C:OP2	8:B:5:ARG:NH1	2.53	0.42
18:L:73:VAL:HG21	18:L:116:HIS:CE1	2.55	0.42
1:0:2269:C:H2'	1:0:2270:G:H5'	2.00	0.42
19:M:59:GLY:C	19:M:141:ILE:HD11	2.40	0.42
29:W:149:LEU:HG	29:W:153:MET:HE2	2.02	0.42
1:0:2634:G:OP2	7:A:204:GLY:N	2.50	0.42
8:B:34:GLY:O	8:B:35:GLN:C	2.58	0.42
11:E:18:LEU:HD13	11:E:34:TRP:CG	2.55	0.42
12:F:28:ALA:CB	12:F:99:THR:HG23	2.50	0.42
1:0:1503:U:H2'	1:0:1504:A:O4'	2.19	0.42
21:O:77:ALA:HA	21:O:96:VAL:O	2.19	0.42
1:0:1842:A:C4	1:0:1979:G:C6	3.08	0.42
1:0:1104:C:H4'	16:J:88:PRO:HD3	2.01	0.42
1:0:2656:G:C2'	1:0:2657:G:H5'	2.50	0.42
20:N:32:PRO:HD2	20:N:99:GLU:O	2.19	0.42
1:0:1811:A:H2'	1:0:1812:G:H5'	2.01	0.42
26:T:3:GLN:HA	26:T:4:PRO:HD3	1.94	0.42
30:X:43:VAL:CG1	30:X:44:ASP:N	2.81	0.42
1:0:533:U:H2'	1:0:2814:A:C6	2.54	0.42
17:K:74:VAL:HG21	17:K:96:VAL:HG23	2.01	0.42
30:X:22:ASN:HA	30:X:25:ARG:HG3	2.00	0.42
12:F:43:GLY:C	12:F:45:ALA:H	2.22	0.42
1:0:1878:G:O2'	1:0:1879:U:OP2	2.37	0.42
1:0:2684:A:H2'	1:0:2685:C:C6	2.55	0.42
1:0:1754:A:H2'	1:0:1755:A:O4'	2.20	0.42
8:B:119:HIS:O	8:B:121:PRO:HD3	2.20	0.42
1:0:292:G:H2'	1:0:358:G:N2	2.33	0.42
30:X:26:ALA:HB2	30:X:63:ARG:HA	2.01	0.42
1:0:799:C:O2'	1:0:800:G:H5'	2.18	0.42
25:S:12:GLU:OE1	25:S:12:GLU:N	2.50	0.42
1:0:1160:G:H5'	1:0:1161:A:O4'	2.20	0.42
9:C:1:MET:HG2	9:C:2:GLN:HE21	1.83	0.42
25:S:57:THR:HG22	25:S:58:MET:N	2.34	0.42
23:Q:21:ARG:HG2	23:Q:22:GLY:H	1.85	0.42
20:N:11:ARG:HA	20:N:14:ARG:CZ	2.49	0.42
1:0:2419:U:H5''	1:0:2420:G:C5'	2.48	0.42
2:1:37:CYS:SG	2:1:39:PHE:HB2	2.60	0.42
16:J:131:THR:CG2	16:J:133:GLY:H	2.32	0.42
1:0:2270:G:H4'	7:A:223:ARG:NH1	2.32	0.42
12:F:21:GLU:HA	12:F:24:ARG:HE	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:16:VAL:HG12	22:P:17:GLY:N	2.35	0.42
1:0:2727:A:H2'	1:0:2728:C:H5'	2.02	0.42
7:A:45:ILE:HG22	32:Z:54:ILE:HG12	2.02	0.42
18:L:90:ARG:HG3	18:L:90:ARG:NH1	2.34	0.42
1:0:2326:C:H4'	1:0:2412:G:H4'	2.02	0.42
1:0:2338:G:O3'	10:D:107:GLY:O	2.36	0.42
1:0:134:U:C2	1:0:145:A:C2	3.08	0.42
1:0:51:G:O2'	1:0:52:A:H5'	2.20	0.42
6:9:80:A:H2'	6:9:81:C:O4'	2.19	0.42
8:B:153:SER:HB2	8:B:287:TYR:CZ	2.54	0.42
10:D:170:TYR:CD1	10:D:170:TYR:N	2.88	0.42
15:I:114:TYR:CD1	15:I:114:TYR:N	2.88	0.42
10:D:60:GLU:O	10:D:61:PHE:C	2.57	0.42
6:9:29:C:C2'	6:9:30:C:H5'	2.46	0.42
11:E:145:ALA:HB1	11:E:168:ILE:HD11	2.01	0.42
15:I:117:THR:O	15:I:121:LYS:HG3	2.19	0.42
14:H:50:ILE:HD12	14:H:149:VAL:HG11	2.01	0.42
11:E:116:THR:CG2	11:E:151:LEU:HD22	2.49	0.42
8:B:7:ARG:CG	8:B:7:ARG:HH11	2.32	0.42
1:0:2039:A:OP2	8:B:234:ARG:NH2	2.53	0.42
1:0:2831:C:H2'	1:0:2832:C:C5'	2.49	0.42
23:Q:32:GLU:O	23:Q:93:ARG:NH2	2.53	0.42
1:0:809:G:H2'	1:0:810:G:C8	2.54	0.42
19:M:67:VAL:HB	19:M:97:ILE:HG23	2.02	0.42
1:0:2325:U:O2'	1:0:2411:C:H1'	2.20	0.42
1:0:2241:C:H2'	1:0:2242:U:C6	2.55	0.42
1:0:216:A:O2'	1:0:217:C:H5'	2.19	0.42
3:2:9:LYS:O	3:2:12:ALA:HB3	2.19	0.42
1:0:626:U:C4	1:0:627:G:C6	3.07	0.42
1:0:1098:A:H2'	1:0:1099:G:O4'	2.19	0.42
1:0:827:A:H2'	1:0:828:G:O4'	2.18	0.42
10:D:44:ILE:HG23	10:D:45:THR:HG23	2.02	0.42
1:0:1181:A:N1	1:0:1192:A:O2'	2.52	0.42
20:N:166:ALA:O	20:N:167:ASP:HB2	2.20	0.42
10:D:60:GLU:O	10:D:62:ASP:N	2.53	0.42
20:N:151:ASP:O	20:N:154:LEU:HB2	2.20	0.42
1:0:1477:C:H5'	1:0:1868:G:H5'	2.01	0.42
1:0:947:U:O2'	1:0:948:G:H5'	2.19	0.42
1:0:80:A:H5''	26:T:41:ARG:CZ	2.50	0.42
29:W:67:ALA:HB2	29:W:93:ILE:HD13	2.02	0.42
1:0:1675:C:H5''	3:2:5:LYS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:685:C:O2	1:0:748:C:H4'	2.20	0.42
6:9:31:C:H2'	6:9:32:G:O4'	2.20	0.42
9:C:129:HIS:CE1	9:C:231:ARG:HA	2.55	0.42
20:N:116:PHE:HB3	20:N:136:LEU:HD23	2.01	0.42
1:0:2050:G:OP1	24:R:79:ARG:HB3	2.20	0.42
3:2:20:ARG:HG2	3:2:21:VAL:N	2.35	0.42
1:0:1600:G:H8	1:0:1600:G:OP2	2.03	0.42
1:0:870:G:C3'	1:0:871:G:H5''	2.50	0.42
1:0:2505:G:C2'	1:0:2506:A:H5'	2.49	0.42
17:K:55:VAL:O	17:K:68:VAL:HA	2.20	0.42
11:E:126:ILE:HB	11:E:131:LEU:HD21	2.01	0.42
8:B:51:VAL:HG23	8:B:330:VAL:HG22	2.01	0.42
8:B:266:ASN:OD1	8:B:317:PRO:HA	2.20	0.42
8:B:165:ARG:CG	8:B:166:VAL:N	2.83	0.42
1:0:255:A:H2'	1:0:256:C:O4'	2.19	0.42
8:B:69:VAL:HA	8:B:70:PRO:HD3	1.88	0.42
22:P:14:LEU:O	22:P:16:VAL:HG23	2.19	0.42
23:Q:93:ARG:HG3	23:Q:93:ARG:HH11	1.85	0.42
1:0:1909:A:N1	1:0:2128:G:H1'	2.34	0.42
29:W:41:TYR:O	29:W:45:VAL:HG22	2.20	0.42
1:0:1544:U:H2'	1:0:1545:C:C6	2.55	0.42
1:0:2281:C:C2'	1:0:2282:U:H5'	2.50	0.42
4:3:6:ARG:NH1	4:3:21:GLU:HG3	2.35	0.42
18:L:89:PHE:N	18:L:117:GLU:O	2.53	0.42
31:Y:189:ASN:ND2	31:Y:189:ASN:C	2.73	0.41
15:I:87:PRO:C	15:I:89:GLU:H	2.23	0.41
1:0:559:U:H5'	1:0:559:U:C6	2.36	0.41
30:X:76:ARG:NH1	30:X:76:ARG:CG	2.81	0.41
29:W:88:THR:CG2	29:W:110:GLN:NE2	2.82	0.41
1:0:1853:C:OP1	7:A:231:LYS:HG3	2.19	0.41
13:G:15:TRP:CE2	13:G:16:LYS:HG3	2.55	0.41
1:0:949:U:H4'	23:Q:95:GLU:HA	2.02	0.41
4:3:24:LYS:HE3	4:3:90:PHE:HE1	1.84	0.41
29:W:11:VAL:O	29:W:12:ASN:HB2	2.20	0.41
1:0:2614:C:O2'	1:0:2615:U:H5'	2.20	0.41
1:0:1903:U:O2'	1:0:1904:A:C8	2.72	0.41
1:0:37:A:H2'	1:0:38:G:H8	1.85	0.41
1:0:1308:A:O4'	9:C:226:GLY:HA3	2.20	0.41
1:0:886:A:OP2	1:0:2113:G:H5'	2.20	0.41
1:0:74:G:H2'	1:0:75:U:C6	2.54	0.41
8:B:233:ARG:HH11	8:B:233:ARG:HG2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:9:57:A:C8	10:D:141:VAL:HG21	2.56	0.41
15:I:130:LEU:HB2	15:I:132:VAL:HG23	2.02	0.41
28:V:64:GLY:O	28:V:65:ASP:OD1	2.38	0.41
11:E:24:GLY:CA	11:E:76:VAL:HB	2.51	0.41
10:D:173:GLU:OE1	10:D:174:VAL:HG23	2.20	0.41
6:9:52:A:O2'	6:9:53:G:H5'	2.20	0.41
1:0:182:G:O3'	19:M:157:ASP:OD2	2.38	0.41
1:0:958:G:O2'	1:0:959:C:H5'	2.20	0.41
1:0:107:U:C2'	1:0:108:U:H5'	2.50	0.41
1:0:1855:G:H8	7:A:144:GLU:OE2	2.04	0.41
1:0:1304:U:H2'	1:0:1305:C:C6	2.55	0.41
14:H:92:LYS:HG3	14:H:130:VAL:HG22	2.01	0.41
1:0:602:A:O2'	1:0:605:C:H4'	2.19	0.41
1:0:1890:U:H4'	1:0:2010:A:C6	2.56	0.41
11:E:15:GLN:HB3	11:E:42:VAL:CG2	2.50	0.41
15:I:67:VAL:HG13	15:I:68:PRO:HD2	2.02	0.41
7:A:34:ASP:OD1	7:A:35:GLY:N	2.47	0.41
29:W:54:PHE:CZ	29:W:140:LYS:HB2	2.55	0.41
20:N:11:ARG:HG3	20:N:14:ARG:CZ	2.50	0.41
20:N:86:LEU:HD21	20:N:180:LEU:CD1	2.50	0.41
1:0:1299:G:N7	18:L:6:ARG:NH1	2.67	0.41
16:J:95:ARG:O	16:J:99:GLU:HB2	2.21	0.41
22:P:13:VAL:HG11	22:P:40:VAL:HG11	2.03	0.41
28:V:8:ILE:HG21	28:V:59:ILE:HG13	2.02	0.41
20:N:42:HIS:CB	20:N:62:HIS:HE1	2.34	0.41
1:0:2821:C:H4'	8:B:116:PRO:CB	2.50	0.41
1:0:221:G:H2'	1:0:222:A:C8	2.55	0.41
18:L:24:ALA:HB2	18:L:30:ARG:HD2	2.02	0.41
9:C:191:SER:OG	9:C:192:ILE:N	2.53	0.41
1:0:1883:U:O2'	1:0:1884:G:H5'	2.19	0.41
1:0:1461:U:H2'	1:0:1462:C:C6	2.55	0.41
1:0:2507:G:H2'	1:0:2510:C:N4	2.35	0.41
14:H:69:ARG:NH2	14:H:70:LEU:HD12	2.36	0.41
28:V:12:THR:HG23	28:V:14:ALA:N	2.35	0.41
32:Z:37:HIS:O	32:Z:45:ASP:HA	2.21	0.41
1:0:2714:U:H4'	8:B:10:SER:HB2	2.02	0.41
10:D:139:TYR:CE2	10:D:143:LYS:HE2	2.56	0.41
31:Y:184:GLU:OE2	31:Y:204:ARG:HD2	2.21	0.41
9:C:27:ARG:HG3	9:C:29:ASP:OD1	2.19	0.41
1:0:1820:G:C6	1:0:2030:A:C2	3.08	0.41
16:J:80:LYS:HE2	16:J:98:PHE:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:926:A:H1'	18:L:38:HIS:O	2.20	0.41
29:W:7:LEU:CD1	29:W:53:ALA:HB2	2.50	0.41
8:B:232:TRP:CD1	8:B:235:ARG:HD2	2.55	0.41
26:T:79:LEU:HG	26:T:89:ARG:HB2	2.01	0.41
26:T:81:LYS:HD2	26:T:87:VAL:HG11	2.02	0.41
1:0:2088:C:H1'	1:0:2841:A:N1	2.35	0.41
19:M:68:ARG:HD3	19:M:68:ARG:O	2.20	0.41
1:0:545:G:H2'	1:0:546:C:O4'	2.19	0.41
22:P:115:SER:C	22:P:117:SER:N	2.74	0.41
7:A:88:ILE:HG21	7:A:100:PRO:HG3	2.01	0.41
8:B:190:MET:CE	8:B:194:PHE:CD1	3.04	0.41
30:X:47:ALA:HB1	30:X:82:GLU:CB	2.47	0.41
1:0:111:C:H2'	1:0:112:G:O4'	2.21	0.41
8:B:53:LEU:HD21	8:B:270:ILE:HD12	2.02	0.41
29:W:38:THR:HG22	29:W:39:ASP:H	1.82	0.41
18:L:73:VAL:CG1	18:L:118:LEU:HD21	2.50	0.41
1:0:2719:A:H2'	1:0:2720:C:H5'	2.01	0.41
2:1:28:HIS:O	2:1:32:LYS:N	2.47	0.41
1:0:517:U:H2'	1:0:518:G:H5'	2.02	0.41
19:M:50:ARG:N	19:M:54:TYR:HB3	2.36	0.41
1:0:790:A:H2'	1:0:791:A:O4'	2.21	0.41
1:0:2520:G:H5'	14:H:64:SER:OG	2.20	0.41
17:K:78:LYS:HA	17:K:79:PRO:HD3	1.91	0.41
8:B:102:THR:HG22	8:B:182:VAL:HG12	2.03	0.41
7:A:75:GLY:HA2	32:Z:64:PHE:HA	2.02	0.41
32:Z:53:GLY:HA2	32:Z:67:GLY:O	2.20	0.41
19:M:133:LEU:N	19:M:133:LEU:HD12	2.34	0.41
20:N:72:GLU:HB3	20:N:171:HIS:HE1	1.86	0.41
1:0:560:U:H2'	1:0:561:G:H8	1.85	0.41
14:H:46:TYR:HA	14:H:47:PRO:HD3	1.80	0.41
31:Y:154:ARG:NH1	31:Y:155:ARG:CG	2.84	0.41
1:0:949:U:O2'	23:Q:40:HIS:HE1	2.03	0.41
1:0:1421:C:O2'	1:0:1422:U:H5'	2.20	0.41
1:0:445:U:H2'	1:0:446:G:H8	1.84	0.41
1:0:2842:G:H5'	24:R:68:HIS:O	2.20	0.41
1:0:2672:C:H2'	1:0:2673:U:H6	1.85	0.41
14:H:5:PRO:HB2	14:H:7:SER:OG	2.20	0.41
1:0:1160:G:H5''	1:0:1161:A:H5'	1.98	0.41
25:S:57:THR:C	25:S:59:ASP:H	2.24	0.41
14:H:41:LYS:HD3	14:H:46:TYR:CE1	2.55	0.41
1:0:538:C:H5''	1:0:539:G:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:106:PRO:HG2	21:O:107:GLU:OE1	2.20	0.41
1:O:1514:C:O2'	1:O:1515:A:H5'	2.21	0.41
14:H:79:GLU:O	14:H:80:LEU:HD23	2.20	0.41
1:O:249:G:H2'	1:O:250:C:C6	2.56	0.41
9:C:40:ALA:HB3	9:C:100:LEU:HD12	2.03	0.41
1:O:2864:U:C5	1:O:2865:G:C6	3.09	0.41
1:O:1821:A:O2'	1:O:1822:A:H5'	2.21	0.41
3:2:8:LYS:HE3	25:S:58:MET:SD	2.61	0.41
8:B:307:ARG:CG	8:B:307:ARG:HH11	2.33	0.41
6:9:13:A:OP1	6:9:113:C:H5'	2.20	0.41
29:W:88:THR:HG22	29:W:90:TYR:HD1	1.84	0.41
24:R:44:VAL:HG13	24:R:89:LEU:HD22	2.03	0.41
8:B:51:VAL:HG23	8:B:329:TYR:O	2.21	0.41
1:O:2270:G:O3'	7:A:223:ARG:NH1	2.54	0.41
17:K:4:LEU:HD23	17:K:4:LEU:HA	1.94	0.41
1:O:1771:U:O2'	1:O:1773:G:N7	2.53	0.41
14:H:61:ARG:HG3	14:H:61:ARG:NH1	2.36	0.41
19:M:184:ARG:CZ	19:M:184:ARG:HB2	2.50	0.41
1:O:1086:A:P	29:W:9:GLY:H	2.44	0.41
18:L:34:GLY:HA3	18:L:38:HIS:CE1	2.55	0.41
1:O:2445:U:H2'	1:O:2446:G:H8	1.85	0.41
1:O:1165:G:C4'	1:O:1174:A:HO2'	2.33	0.41
1:O:958:G:H2'	1:O:959:C:H6	1.84	0.41
1:O:1762:C:H2'	1:O:1763:C:C6	2.56	0.41
18:L:89:PHE:CD1	18:L:89:PHE:N	2.89	0.41
25:S:6:LYS:HB2	25:S:27:ALA:O	2.19	0.41
1:O:10:U:O4	1:O:532:A:OP2	2.38	0.41
24:R:59:PHE:HZ	24:R:81:PRO:HG3	1.85	0.41
1:O:1242:A:OP2	16:J:60:ARG:NH2	2.50	0.41
17:K:98:VAL:HG13	17:K:102:GLU:HA	1.98	0.41
8:B:265:LEU:HD21	8:B:316:ARG:HD3	2.03	0.41
12:F:63:ILE:HB	12:F:64:PRO:CD	2.45	0.41
2:1:8:GLN:NE2	2:1:11:LYS:NZ	2.62	0.41
1:O:2714:U:H2'	1:O:2715:G:C8	2.56	0.41
1:O:111:C:O2'	1:O:112:G:H5'	2.21	0.41
1:O:553:G:C2'	1:O:554:G:H5'	2.51	0.41
7:A:105:VAL:CG1	7:A:106:CYS:N	2.83	0.41
1:O:1972:U:C2'	1:O:1973:A:C5'	2.99	0.41
7:A:66:ARG:CB	7:A:66:ARG:NH1	2.83	0.41
20:N:24:LEU:HD13	23:Q:26:PRO:HB3	2.02	0.41
1:O:2271:G:N3	1:O:2271:G:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:61:GLU:C	7:A:63:GLY:H	2.24	0.41
1:0:1778:A:H2'	1:0:1779:A:H5'	2.03	0.41
22:P:38:GLU:HA	22:P:41:ARG:HH11	1.86	0.41
1:0:820:G:H5'	1:0:821:U:C5'	2.51	0.41
10:D:159:PRO:O	10:D:162:ALA:HB3	2.20	0.41
20:N:71:TRP:CE3	20:N:175:LEU:HD23	2.56	0.41
1:0:746:A:C6	21:O:65:LEU:HD13	2.56	0.41
21:O:96:VAL:HG12	21:O:97:SER:N	2.36	0.41
1:0:1755:A:H2'	1:0:1756:G:O4'	2.20	0.41
1:0:164:G:O3'	18:L:30:ARG:HB2	2.21	0.41
23:Q:24:SER:HB3	23:Q:28:ARG:HH21	1.86	0.41
8:B:87:TYR:HA	8:B:95:ARG:O	2.21	0.41
26:T:23:VAL:C	26:T:93:THR:HG21	2.42	0.41
11:E:31:ARG:HB3	11:E:31:ARG:HE	1.76	0.41
9:C:13:ASP:OD1	9:C:13:ASP:O	2.39	0.41
2:1:53:LYS:HB3	9:C:51:TYR:CE2	2.56	0.41
1:0:1139:U:H2'	1:0:1140:C:C6	2.56	0.41
1:0:424:C:H2'	1:0:425:U:C6	2.56	0.41
1:0:1335:C:OP2	31:Y:207:SER:HB3	2.20	0.41
1:0:1706:G:H1'	1:0:1712:A:H61	1.86	0.41
22:P:89:ASN:HB3	22:P:92:GLU:OE1	2.21	0.41
8:B:24:PRO:HG2	8:B:204:GLY:HA2	2.03	0.41
1:0:1933:G:O2'	1:0:1934:A:H5'	2.21	0.41
10:D:35:ALA:C	10:D:37:ALA:N	2.74	0.41
29:W:29:VAL:O	29:W:30:ASN:HB2	2.21	0.41
9:C:46:TYR:HE2	9:C:98:ARG:HH12	1.68	0.41
12:F:58:GLU:HG3	12:F:61:MET:HE1	2.03	0.41
1:0:1588:G:C6	1:0:1589:G:N1	2.89	0.41
9:C:115:LEU:HA	9:C:115:LEU:HD12	1.89	0.41
18:L:145:LEU:C	18:L:147:GLU:N	2.75	0.41
29:W:131:PRO:HD2	29:W:134:GLU:OE1	2.21	0.41
8:B:285:VAL:O	8:B:286:ASN:HB2	2.20	0.41
15:I:95:LEU:HD12	15:I:132:VAL:CG1	2.51	0.40
17:K:101:ASN:O	17:K:102:GLU:HB2	2.21	0.40
1:0:2630:G:O6	7:A:206:ARG:NH2	2.54	0.40
1:0:1477:C:C5'	1:0:1868:G:H5''	2.50	0.40
11:E:24:GLY:N	11:E:76:VAL:HB	2.36	0.40
8:B:24:PRO:O	8:B:25:ARG:HD3	2.22	0.40
1:0:2438:G:H2'	1:0:2439:C:O4'	2.21	0.40
1:0:1707:G:N2	1:0:1709:G:H3'	2.36	0.40
29:W:83:TRP:CE2	29:W:87:HIS:CD2	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:R:17:MET:CE	24:R:19:ARG:NH2	2.79	0.40
1:0:69:A:H2'	1:0:70:A:OP2	2.21	0.40
1:0:968:G:C1'	14:H:35:LYS:HD2	2.51	0.40
21:O:96:VAL:CG1	21:O:100:GLN:HB2	2.51	0.40
1:0:291:C:H2'	1:0:292:G:O4'	2.22	0.40
8:B:233:ARG:NH1	8:B:233:ARG:HG2	2.37	0.40
1:0:858:U:H2'	1:0:859:C:C6	2.56	0.40
1:0:653:U:H2'	1:0:654:A:C8	2.56	0.40
10:D:24:HIS:HB2	10:D:72:LYS:HB3	2.03	0.40
12:F:7:ASP:O	12:F:9:PRO:HD3	2.21	0.40
1:0:724:G:O2'	1:0:725:C:H5'	2.21	0.40
14:H:4:LYS:HE2	14:H:100:GLU:OE2	2.22	0.40
14:H:123:ILE:CD1	14:H:123:ILE:N	2.84	0.40
1:0:1747:A:C8	17:K:44:LEU:HD13	2.57	0.40
1:0:1311:G:O6	9:C:173:LYS:HE3	2.21	0.40
1:0:2091:G:O3'	8:B:235:ARG:HD3	2.22	0.40
18:L:97:VAL:HG12	18:L:98:GLU:O	2.21	0.40
1:0:1051:C:H2'	1:0:1052:G:O4'	2.21	0.40
31:Y:130:ARG:HB2	31:Y:142:SER:O	2.21	0.40
9:C:153:VAL:O	9:C:157:LEU:HG	2.21	0.40
11:E:83:GLY:HA3	11:E:170:ARG:HE	1.87	0.40
1:0:1815:A:H4'	1:0:2751:C:O4'	2.21	0.40
1:0:1463:U:H2'	1:0:1464:C:C6	2.56	0.40
14:H:41:LYS:HD3	14:H:46:TYR:OH	2.21	0.40
1:0:2346:C:O3'	10:D:52:THR:CG2	2.69	0.40
3:2:30:ASP:O	3:2:31:ARG:HB2	2.22	0.40
9:C:151:GLN:O	9:C:154:VAL:HB	2.21	0.40
22:P:13:VAL:HG11	22:P:40:VAL:CG1	2.52	0.40
22:P:16:VAL:HG12	22:P:20:ARG:HB2	2.04	0.40
4:3:22:VAL:HG11	4:3:67:LEU:HD13	2.02	0.40
1:0:1947:G:N2	1:0:1965:C:O2	2.55	0.40
1:0:271:C:H41	1:0:378:A:H2	1.65	0.40
11:E:20:ILE:HD11	11:E:40:VAL:HG11	2.03	0.40
1:0:581:G:H4'	1:0:1254:C:O2'	2.20	0.40
1:0:401:C:O2'	19:M:92:THR:HB	2.21	0.40
1:0:461:C:N3	1:0:479:G:H5'	2.37	0.40
11:E:103:VAL:HG21	11:E:115:ARG:NH2	2.37	0.40
32:Z:42:CYS:SG	32:Z:44:GLU:CB	3.09	0.40
10:D:23:VAL:HG12	10:D:130:VAL:HG22	2.04	0.40
1:0:1167:G:H2'	1:0:1168:C:C6	2.57	0.40
7:A:32:VAL:HG12	7:A:34:ASP:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:57:GLU:HB2	19:M:23:LEU:HD11	2.03	0.40
7:A:81:GLN:HB2	7:A:92:ASN:HD22	1.83	0.40
24:R:17:MET:HE3	24:R:19:ARG:CZ	2.52	0.40
1:0:907:A:H5''	31:Y:164:VAL:HG12	2.02	0.40
1:0:1080:C:H6	1:0:1080:C:O5'	2.05	0.40
22:P:131:PHE:CD1	22:P:137:LEU:HD13	2.56	0.40
26:T:24:ARG:HH21	26:T:39:ASN:ND2	2.19	0.40
28:V:1:THR:HG23	28:V:3:LEU:H	1.86	0.40
1:0:2598:U:O2	1:0:2600:A:C8	2.74	0.40
25:S:11:THR:H	25:S:14:ALA:HB3	1.85	0.40
1:0:792:G:O2'	1:0:793:A:H5'	2.21	0.40
1:0:2642:G:H2'	1:0:2643:G:O4'	2.21	0.40
1:0:2543:G:H2'	1:0:2544:G:O4'	2.22	0.40
14:H:31:ILE:HA	14:H:66:GLU:OE1	2.21	0.40
1:0:2385:G:H2'	1:0:2386:U:C6	2.57	0.40
20:N:102:LEU:HG	20:N:104:ILE:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
3	2	42/50 (84%)	39 (93%)	3 (7%)	0	100	100
4	3	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	17	50
5	8	2/7 (29%)	2 (100%)	0	0	100	100
7	A	235/240 (98%)	202 (86%)	28 (12%)	5 (2%)	9	29
8	B	335/338 (99%)	294 (88%)	35 (10%)	6 (2%)	11	34
9	C	244/246 (99%)	216 (88%)	27 (11%)	1 (0%)	39	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	D	134/177 (76%)	97 (72%)	28 (21%)	9 (7%)	1	4
11	E	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
12	F	117/120 (98%)	101 (86%)	11 (9%)	5 (4%)	3	10
13	G	25/348 (7%)	22 (88%)	3 (12%)	0	100	100
14	H	156/177 (88%)	142 (91%)	12 (8%)	2 (1%)	15	44
15	I	68/162 (42%)	43 (63%)	22 (32%)	3 (4%)	3	10
16	J	140/145 (97%)	127 (91%)	7 (5%)	6 (4%)	3	10
17	K	130/132 (98%)	119 (92%)	11 (8%)	0	100	100
18	L	141/165 (86%)	115 (82%)	23 (16%)	3 (2%)	9	29
19	M	192/195 (98%)	176 (92%)	15 (8%)	1 (0%)	34	69
20	N	184/187 (98%)	161 (88%)	17 (9%)	6 (3%)	5	16
21	O	113/116 (97%)	107 (95%)	5 (4%)	1 (1%)	21	55
22	P	141/149 (95%)	131 (93%)	6 (4%)	4 (3%)	6	21
23	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
24	R	148/155 (96%)	134 (90%)	13 (9%)	1 (1%)	26	62
25	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
26	T	117/120 (98%)	103 (88%)	12 (10%)	2 (2%)	11	36
27	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
28	V	63/71 (89%)	55 (87%)	6 (10%)	2 (3%)	5	17
29	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	15	44
30	X	80/92 (87%)	71 (89%)	7 (9%)	2 (2%)	7	24
31	Y	140/241 (58%)	131 (94%)	8 (6%)	1 (1%)	26	62
32	Z	71/83 (86%)	59 (83%)	9 (13%)	3 (4%)	3	11
All	All	3707/4444 (83%)	3293 (89%)	348 (9%)	66 (2%)	11	34

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	34	ASP
10	D	63	ILE
10	D	137	PRO
12	F	101	ALA
16	J	5	GLU
18	L	80	ASP

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Mol	Chain	Res	Type
20	N	154	LEU
20	N	164	ASP
20	N	183	ASP
20	N	184	ILE
28	V	43	PRO
30	X	87	ALA
32	Z	20	ARG
32	Z	81	ARG
8	B	206	THR
9	C	8	LEU
10	D	61	PHE
10	D	138	GLY
12	F	44	SER
14	H	19	ARG
14	H	143	VAL
16	J	7	ASP
21	O	20	SER
22	P	116	SER
26	T	53	GLY
7	A	36	ASP
8	B	35	GLN
8	B	184	ASP
10	D	27	ILE
10	D	64	ARG
16	J	143	LYS
20	N	139	TRP
22	P	132	ASP
29	W	77	ALA
30	X	70	ILE
8	B	2	GLN
8	B	185	GLY
10	D	173	GLU
12	F	100	ASP
15	I	95	LEU
16	J	76	ASP
18	L	105	TYR
22	P	97	ARG
22	P	142	ASP
24	R	81	PRO
26	T	46	ASP
29	W	49	ASN
32	Z	21	VAL

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Mol	Chain	Res	Type
7	A	119	ALA
12	F	61	MET
4	3	58	GLY
7	A	37	VAL
8	B	138	GLY
10	D	16	PRO
10	D	97	GLN
12	F	70	LYS
15	I	133	THR
16	J	65	ASN
16	J	89	HIS
31	Y	198	GLY
20	N	161	GLY
28	V	40	PRO
18	L	146	GLY
7	A	211	LYS
15	I	109	PRO
19	M	88	VAL

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	
2	1	46/47 (98%)	46 (100%)	0	100	100
3	2	42/46 (91%)	40 (95%)	2 (5%)	31	66
4	3	79/79 (100%)	78 (99%)	1 (1%)	76	94
5	8	2/2 (100%)	2 (100%)	0	100	100
7	A	179/182 (98%)	169 (94%)	10 (6%)	26	59
8	B	282/283 (100%)	263 (93%)	19 (7%)	20	50
9	C	193/193 (100%)	176 (91%)	17 (9%)	12	35
10	D	117/148 (79%)	110 (94%)	7 (6%)	24	56
11	E	152/156 (97%)	147 (97%)	5 (3%)	45	79
12	F	93/94 (99%)	92 (99%)	1 (1%)	80	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	G	27/283 (10%)	26 (96%)	1 (4%)	41	76
14	H	134/145 (92%)	131 (98%)	3 (2%)	60	89
15	I	58/130 (45%)	57 (98%)	1 (2%)	68	92
16	J	118/121 (98%)	110 (93%)	8 (7%)	20	49
17	K	106/106 (100%)	103 (97%)	3 (3%)	51	84
18	L	113/127 (89%)	107 (95%)	6 (5%)	28	61
19	M	158/159 (99%)	152 (96%)	6 (4%)	40	74
20	N	149/150 (99%)	145 (97%)	4 (3%)	52	85
21	O	93/94 (99%)	90 (97%)	3 (3%)	46	80
22	P	113/117 (97%)	108 (96%)	5 (4%)	35	69
23	Q	79/80 (99%)	77 (98%)	2 (2%)	55	86
24	R	117/122 (96%)	112 (96%)	5 (4%)	35	70
25	S	71/74 (96%)	69 (97%)	2 (3%)	51	84
26	T	105/106 (99%)	99 (94%)	6 (6%)	25	58
27	U	44/52 (85%)	43 (98%)	1 (2%)	58	88
28	V	51/57 (90%)	49 (96%)	2 (4%)	39	74
29	W	130/130 (100%)	123 (95%)	7 (5%)	27	60
30	X	66/74 (89%)	59 (89%)	7 (11%)	8	24
31	Y	120/196 (61%)	116 (97%)	4 (3%)	45	79
32	Z	60/68 (88%)	60 (100%)	0	100	100
All	All	3097/3621 (86%)	2959 (96%)	138 (4%)	34	68

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	2	16	ASN
3	2	18	ASN
4	3	15	ASN
7	A	3	ARG
7	A	33	GLU
7	A	36	ASP
7	A	69	LEU
7	A	78	ASP
7	A	94	LEU
7	A	131	HIS

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Mol	Chain	Res	Type
7	A	153	ARG
7	A	179	MET
7	A	217	ARG
8	B	7	ARG
8	B	11	LEU
8	B	27	ASN
8	B	49	THR
8	B	56	ASP
8	B	97	LEU
8	B	132	HIS
8	B	162	MET
8	B	190	MET
8	B	195	ARG
8	B	234	ARG
8	B	251	VAL
8	B	254	GLN
8	B	256	GLN
8	B	264	GLU
8	B	277	GLU
8	B	304	PRO
8	B	307	ARG
8	B	312	ARG
9	C	2	GLN
9	C	16	VAL
9	C	27	ARG
9	C	42	ARG
9	C	76	ARG
9	C	98	ARG
9	C	101	ASP
9	C	115	LEU
9	C	162	VAL
9	C	187	ARG
9	C	199	GLU
9	C	214	THR
9	C	223	LEU
9	C	234	VAL
9	C	236	THR
9	C	237	GLU
9	C	240	LEU
10	D	24	HIS
10	D	100	ASP
10	D	133	ASN

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Mol	Chain	Res	Type
10	D	136	ARG
10	D	137	PRO
10	D	149	ARG
10	D	153	THR
11	E	7	ILE
11	E	15	GLN
11	E	16	ASP
11	E	156	ASP
11	E	164	ASP
12	F	99	THR
13	G	64	ASN
14	H	33	GLN
14	H	87	LYS
14	H	157	TYR
15	I	114	TYR
16	J	7	ASP
16	J	45	VAL
16	J	46	ILE
16	J	52	GLN
16	J	74	ARG
16	J	79	PHE
16	J	107	ASN
16	J	112	ASP
17	K	10	GLN
17	K	107	THR
17	K	129	THR
18	L	30	ARG
18	L	35	ARG
18	L	80	ASP
18	L	90	ARG
18	L	99	GLU
18	L	101	ASP
19	M	46	LEU
19	M	68	ARG
19	M	93	ARG
19	M	99	ARG
19	M	116	ASN
19	M	164	THR
20	N	17	ARG
20	N	26	LEU
20	N	53	ASN
20	N	56	ASP

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Mol	Chain	Res	Type
21	O	3	THR
21	O	28	ASP
21	O	38	ARG
22	P	21	VAL
22	P	61	ARG
22	P	73	HIS
22	P	91	LYS
22	P	98	ILE
23	Q	57	ASP
23	Q	95	GLU
24	R	13	THR
24	R	39	THR
24	R	82	GLU
24	R	132	ARG
24	R	143	VAL
25	S	12	GLU
25	S	53	ASN
26	T	19	ARG
26	T	23	VAL
26	T	26	THR
26	T	39	ASN
26	T	89	ARG
26	T	112	LEU
27	U	47	ARG
28	V	43	PRO
28	V	65	ASP
29	W	4	LEU
29	W	26	ILE
29	W	52	VAL
29	W	73	LEU
29	W	142	ASP
29	W	146	ILE
29	W	151	GLU
30	X	15	ARG
30	X	27	ASP
30	X	44	ASP
30	X	49	ARG
30	X	72	VAL
30	X	82	GLU
30	X	88	GLU
31	Y	163	THR
31	Y	186	ARG

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Mol	Chain	Res	Type
31	Y	189	ASN
31	Y	203	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	8	GLN
2	1	16	HIS
2	1	28	HIS
3	2	16	ASN
3	2	18	ASN
3	2	41	HIS
3	2	45	ASN
4	3	30	GLN
4	3	48	ASN
7	A	47	HIS
7	A	92	ASN
7	A	125	ASN
7	A	176	HIS
7	A	199	HIS
8	B	27	ASN
8	B	145	HIS
8	B	238	ASN
8	B	260	HIS
8	B	320	GLN
8	B	332	ASN
9	C	2	GLN
9	C	39	GLN
9	C	129	HIS
9	C	151	GLN
10	D	97	GLN
10	D	103	ASN
10	D	133	ASN
11	E	106	ASN
11	E	119	HIS
11	E	143	GLN
13	G	64	ASN
14	H	34	HIS
14	H	59	GLN
14	H	62	HIS
14	H	73	ASN
14	H	148	HIS

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Mol	Chain	Res	Type
15	I	88	GLN
15	I	108	HIS
16	J	52	GLN
16	J	107	ASN
17	K	10	GLN
17	K	42	ASN
18	L	18	HIS
18	L	41	HIS
18	L	42	ASN
18	L	58	GLN
18	L	116	HIS
19	M	24	GLN
19	M	58	GLN
19	M	137	ASN
19	M	170	ASN
19	M	190	ASN
20	N	40	ASN
20	N	107	ASN
20	N	153	GLN
22	P	50	GLN
22	P	66	GLN
22	P	89	ASN
22	P	118	GLN
23	Q	16	ASN
23	Q	40	HIS
24	R	61	GLN
24	R	94	ASN
24	R	98	ASN
24	R	113	HIS
24	R	117	HIS
25	S	25	GLN
25	S	53	ASN
26	T	39	ASN
26	T	43	ASN
26	T	64	ASN
26	T	73	HIS
27	U	39	ASN
28	V	4	HIS
28	V	29	ASN
28	V	60	GLN
29	W	2	HIS
29	W	12	ASN

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Mol	Chain	Res	Type
29	W	27	HIS
29	W	28	HIS
29	W	59	GLN
29	W	87	HIS
29	W	110	GLN
29	W	119	HIS
29	W	125	HIS
29	W	141	HIS
30	X	23	HIS
30	X	36	HIS
31	Y	134	HIS
31	Y	149	GLN
31	Y	189	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	239 (8%)	27 (0%)
6	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	255 (8%)	28 (0%)

All (255) 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	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	185	G
1	0	186	A
1	0	187	A

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Mol	Chain	Res	Type
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	285	A
1	0	308	U
1	0	309	C
1	0	319	A
1	0	331	A
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	461	C
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	516	A
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

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Mol	Chain	Res	Type
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	821	U
1	0	835	U
1	0	840	U
1	0	846	A
1	0	857	A
1	0	858	U
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
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	1137	G

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Mol	Chain	Res	Type
1	0	1164	U
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1193	A
1	0	1205	U
1	0	1206	U
1	0	1208	C
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	1380	U
1	0	1407	A
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1488	U
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1564	C
1	0	1580	A
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

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Mol	Chain	Res	Type
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
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	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A

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Mol	Chain	Res	Type
1	0	2271	G
1	0	2272	G
1	0	2291	A
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	2465	A
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
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	2634	G
1	0	2645	U
1	0	2649	A
1	0	2664	A
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

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Mol	Chain	Res	Type
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2850	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2914	A
6	9	2	U
6	9	7	G
6	9	14	G
6	9	22	G
6	9	23	U
6	9	24	U
6	9	25	G
6	9	40	C
6	9	41	C
6	9	43	G
6	9	52	A
6	9	57	A
6	9	66	G
6	9	77	A
6	9	114	G
6	9	122	C

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	318	U
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	1237	U

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Mol	Chain	Res	Type
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1506	U
1	0	1685	A
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2644	C
1	0	2649	A
1	0	2718	C
1	0	2761	A
1	0	2791	U
6	9	65	A

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

10 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	12,22,23	1.07	1 (8%)	19,31,34	3.15	2 (10%)
1	OMG	0	2588	1	17,26,27	0.99	1 (5%)	21,38,41	2.56	3 (14%)
1	UR3	0	2619	1	12,22,23	0.89	0	16,32,35	0.87	0
1	PSU	0	2621	1	13,21,22	1.49	2 (15%)	18,30,33	6.11	4 (22%)
1	1MA	0	628	1	14,25,26	1.02	1 (7%)	15,37,40	1.14	1 (6%)
5	MHW	8	1	33,5	9,9,10	1.78	3 (33%)	8,11,13	0.78	0
5	DBB	8	3	5	4,5,6	0.64	0	3,5,7	1.49	1 (33%)
5	MEA	8	5	5	10,12,13	1.65	4 (40%)	10,14,16	1.26	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MHV	8	6	5	7,9,10	1.14	1 (14%)	8,11,13	1.29	0
5	004	8	7	5	9,10,11	2.04	2 (22%)	10,12,14	2.28	3 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
5	MHW	8	1	33,5	-	0/2/2/4	0/1/1/1
5	DBB	8	3	5	-	0/2/4/6	0/0/0/0
5	MEA	8	5	5	-	0/4/8/10	0/1/1/1
5	MHV	8	6	5	-	0/1/12/14	0/1/1/1
5	004	8	7	5	-	0/4/6/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.45	1.48	1.52
5	8	5	MEA	CE2-CZ	2.08	1.43	1.38
5	8	5	MEA	CA-N	2.14	1.51	1.47
5	8	7	004	CD2-CG2	2.21	1.43	1.38
1	0	2621	PSU	C4-N3	2.39	1.37	1.33
5	8	5	MEA	CD1-CG	2.40	1.43	1.38
5	8	6	MHV	CB-CG	2.44	1.54	1.50
5	8	1	MHW	CA-N	2.47	1.39	1.35
5	8	1	MHW	CA-C	2.63	1.52	1.48
5	8	5	MEA	CE2-CD2	2.64	1.44	1.38
1	0	2587	OMU	C4-N3	2.67	1.38	1.33
1	0	628	1MA	C6-N6	2.85	1.34	1.29
5	8	1	MHW	CB-CA	2.86	1.44	1.40
1	0	2588	OMG	C6-N1	3.05	1.38	1.33
5	8	7	004	CB-CA	5.51	1.57	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.44	114.66	128.33
1	0	2588	OMG	C5-C6-N1	-8.78	111.58	123.59
1	0	628	1MA	C2-N3-C4	-3.59	110.83	116.40
1	0	2587	OMU	C5-C4-N3	-3.27	114.73	123.12
5	8	5	MEA	O-C-CA	-3.24	116.88	125.44
5	8	3	DBB	O-C-CA	-2.57	118.79	125.49
5	8	7	004	CB-CA-N	-2.44	106.80	112.54
1	0	2588	OMG	N3-C2-N1	-2.26	124.00	127.44
1	0	2621	PSU	C5-C1'-C2'	-2.12	111.76	115.52
5	8	7	004	CG2-CB-CA	2.68	125.32	120.70
1	0	2621	PSU	C6-N1-C2	2.85	120.05	115.47
5	8	7	004	C-CA-N	5.55	121.16	109.12
1	0	2588	OMG	C6-N1-C2	6.77	125.34	115.94
1	0	2587	OMU	C4-N3-C2	13.12	127.13	114.14
1	0	2621	PSU	C4-N3-C2	13.78	127.16	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2619	UR3	2	0
5	8	5	MEA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 231 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
37	VIR	0	9000	-	34,40,40	2.45	17 (50%)	37,55,55	1.91	8 (21%)

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
37	VIR	0	9000	-	-	0/42/58/58	0/1/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9000	VIR	C28-C29	-5.64	1.17	1.32
37	0	9000	VIR	C16-C17	-3.38	1.48	1.54
37	0	9000	VIR	C13-C14	-2.92	1.46	1.51
37	0	9000	VIR	C1-C37	-2.60	1.38	1.47
37	0	9000	VIR	C17-C19	-2.55	1.47	1.50
37	0	9000	VIR	C4-C3	-2.19	1.49	1.53
37	0	9000	VIR	O38-C37	2.02	1.25	1.21
37	0	9000	VIR	O36-C32	2.07	1.48	1.44
37	0	9000	VIR	C1-N5	2.12	1.42	1.39
37	0	9000	VIR	C6-N5	2.22	1.44	1.39
37	0	9000	VIR	O15-C14	2.66	1.26	1.21
37	0	9000	VIR	C21-C20	2.69	1.56	1.50
37	0	9000	VIR	C34-C33	3.04	1.63	1.52
37	0	9000	VIR	C28-C26	3.58	1.55	1.48
37	0	9000	VIR	C30-C32	4.21	1.63	1.54
37	0	9000	VIR	C26-N25	4.31	1.40	1.34
37	0	9000	VIR	C4-N5	4.81	1.55	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9000	VIR	C28-C26-N25	-4.85	103.70	114.87
37	0	9000	VIR	C8-C6-N5	-2.98	111.19	118.55
37	0	9000	VIR	C12-C8-C6	-2.10	122.48	129.47
37	0	9000	VIR	O7-C6-C8	2.04	123.28	118.75
37	0	9000	VIR	C31-C30-C32	2.29	115.45	111.08
37	0	9000	VIR	O36-C37-C1	2.29	114.00	110.77
37	0	9000	VIR	O7-C6-N5	3.30	125.51	119.98
37	0	9000	VIR	O27-C26-C28	6.40	135.33	123.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	0.05	41 (1%) 76 68	20, 45, 89, 150	0
2	1	56/57 (98%)	-0.18	0 100 100	25, 32, 36, 40	0
3	2	46/50 (92%)	0.82	8 (17%) 2 1	28, 59, 93, 108	0
4	3	92/92 (100%)	0.98	11 (11%) 6 3	42, 60, 72, 82	0
5	8	2/7 (28%)	0.06	0 100 100	40, 40, 40, 41	0
6	9	122/122 (100%)	0.17	2 (1%) 74 66	35, 62, 88, 150	0
7	A	237/240 (98%)	0.29	12 (5%) 32 21	26, 53, 88, 108	0
8	B	337/338 (99%)	0.06	4 (1%) 81 73	25, 51, 77, 89	0
9	C	246/246 (100%)	0.03	0 100 100	21, 43, 68, 77	0
10	D	140/177 (79%)	2.38	74 (52%) 0 0	55, 98, 121, 131	0
11	E	172/178 (96%)	0.75	13 (7%) 17 9	42, 64, 86, 95	0
12	F	119/120 (99%)	0.54	9 (7%) 17 9	46, 69, 92, 107	0
13	G	29/348 (8%)	1.79	12 (41%) 0 0	70, 87, 93, 97	0
14	H	160/177 (90%)	0.46	7 (4%) 38 26	37, 56, 91, 103	0
15	I	70/162 (43%)	3.45	50 (71%) 0 0	105, 121, 139, 140	0
16	J	142/145 (97%)	0.09	1 (0%) 89 84	34, 48, 66, 85	0
17	K	132/132 (100%)	0.04	3 (2%) 64 52	28, 48, 68, 79	0
18	L	145/165 (87%)	0.79	20 (13%) 4 2	24, 64, 104, 118	0
19	M	194/195 (99%)	-0.15	0 100 100	28, 41, 57, 63	0
20	N	186/187 (99%)	0.69	24 (12%) 5 2	37, 63, 108, 116	0
21	O	115/116 (99%)	0.09	1 (0%) 85 79	35, 51, 70, 73	0
22	P	143/149 (95%)	0.18	2 (1%) 78 69	33, 53, 70, 75	0
23	Q	95/96 (98%)	0.04	1 (1%) 82 74	35, 42, 58, 75	0
24	R	150/155 (96%)	-0.06	0 100 100	30, 42, 61, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	S	81/85 (95%)	0.02	2 (2%) 61 48	40, 59, 77, 84	0
26	T	119/120 (99%)	0.46	7 (5%) 26 16	36, 54, 82, 98	0
27	U	53/66 (80%)	0.51	6 (11%) 7 3	40, 53, 70, 80	0
28	V	65/71 (91%)	1.79	23 (35%) 0 0	51, 72, 112, 117	0
29	W	154/154 (100%)	-0.21	0 100 100	32, 45, 62, 74	0
30	X	82/92 (89%)	0.37	5 (6%) 25 15	39, 54, 76, 93	0
31	Y	142/241 (58%)	-0.01	2 (1%) 78 69	24, 42, 64, 87	0
32	Z	73/83 (87%)	1.47	24 (32%) 0 0	64, 78, 91, 99	0
All	All	6648/7488 (88%)	0.28	364 (5%) 29 18	20, 50, 97, 150	0

All (364) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	V	1	THR	11.6
15	I	128	THR	9.0
28	V	40	PRO	8.6
10	D	18	ILE	7.7
10	D	63	ILE	7.7
15	I	112	LEU	7.5
15	I	132	VAL	7.5
15	I	74	ILE	7.2
15	I	83	GLY	6.6
10	D	69	ILE	6.5
15	I	70	THR	6.1
15	I	113	SER	5.9
10	D	27	ILE	5.8
15	I	88	GLN	5.8
28	V	43	PRO	5.8
15	I	80	PHE	5.7
28	V	39	ALA	5.7
32	Z	11	SER	5.6
15	I	71	ALA	5.5
32	Z	22	SER	5.5
10	D	26	GLY	5.5
10	D	134	LEU	5.4
10	D	25	MET	5.4
18	L	60	GLU	5.3
1	0	2237	G	5.3
15	I	104	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
28	V	38	GLY	5.3
15	I	111	LEU	5.3
10	D	57	THR	5.3
10	D	85	GLN	5.3
10	D	24	HIS	5.2
14	H	174	LEU	5.2
15	I	72	GLU	5.2
15	I	90	ASP	5.2
10	D	88	LEU	5.1
10	D	44	ILE	5.1
15	I	109	PRO	5.1
15	I	92	VAL	5.0
10	D	64	ARG	5.0
15	I	91	PHE	4.9
10	D	62	ASP	4.9
15	I	97	VAL	4.9
10	D	75	LEU	4.9
15	I	105	GLU	4.8
10	D	10	PHE	4.8
7	A	237	GLY	4.7
3	2	49	GLU	4.7
28	V	41	GLU	4.7
3	2	35	ARG	4.6
15	I	100	VAL	4.6
15	I	98	ASP	4.5
10	D	165	PHE	4.5
15	I	82	THR	4.5
6	9	1	U	4.4
32	Z	45	ASP	4.4
10	D	56	ARG	4.4
13	G	71	LEU	4.4
1	0	1173	A	4.4
3	2	39	ARG	4.3
15	I	108	HIS	4.3
10	D	61	PHE	4.3
10	D	17	ARG	4.3
20	N	164	ASP	4.3
15	I	129	SER	4.3
10	D	106	PHE	4.2
15	I	79	GLY	4.2
10	D	87	ALA	4.2
10	D	130	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
10	D	128	LEU	4.1
15	I	86	GLU	4.1
15	I	133	THR	4.1
10	D	23	VAL	4.1
11	E	45	ASP	4.1
4	3	1	MET	4.0
18	L	106	VAL	4.0
7	A	38	ILE	4.0
32	Z	34	ASN	4.0
32	Z	25	ARG	4.0
4	3	83	TRP	3.9
15	I	73	LEU	3.9
28	V	8	ILE	3.9
15	I	93	ALA	3.9
10	D	84	LEU	3.9
10	D	104	PHE	3.9
15	I	130	LEU	3.9
15	I	84	SER	3.9
15	I	78	ALA	3.9
10	D	58	VAL	3.9
12	F	119	ARG	3.8
20	N	166	ALA	3.8
12	F	106	ALA	3.8
32	Z	18	TYR	3.8
32	Z	26	VAL	3.8
10	D	68	PRO	3.8
4	3	22	VAL	3.7
8	B	1	PRO	3.7
10	D	16	PRO	3.7
18	L	105	TYR	3.7
1	0	1172	G	3.6
26	T	119	ALA	3.7
10	D	74	THR	3.6
15	I	123	VAL	3.6
10	D	171	ASP	3.6
10	D	170	TYR	3.6
7	A	37	VAL	3.6
20	N	147	ILE	3.6
13	G	23	ILE	3.6
28	V	7	GLU	3.6
10	D	41	LEU	3.6
10	D	86	THR	3.6

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Mol	Chain	Res	Type	RSRZ
10	D	93	LEU	3.6
10	D	166	ILE	3.6
15	I	76	ASP	3.5
10	D	90	LEU	3.5
10	D	45	THR	3.5
18	L	97	VAL	3.5
10	D	65	GLU	3.5
20	N	151	ASP	3.5
10	D	83	PHE	3.5
10	D	67	ASP	3.5
15	I	106	GLN	3.5
20	N	159	TYR	3.5
10	D	172	VAL	3.5
10	D	66	GLY	3.5
15	I	102	GLN	3.4
1	0	1199	A	3.4
27	U	47	ARG	3.4
1	0	2238	A	3.4
32	Z	44	GLU	3.4
10	D	102	GLY	3.3
10	D	72	LYS	3.3
20	N	145	ALA	3.3
28	V	37	GLY	3.3
18	L	104	ASP	3.3
10	D	28	GLY	3.2
4	3	8	ASN	3.2
10	D	98	PHE	3.2
18	L	99	GLU	3.2
28	V	3	LEU	3.2
15	I	81	GLU	3.2
10	D	135	VAL	3.1
27	U	52	THR	3.1
15	I	99	GLN	3.1
10	D	11	HIS	3.1
10	D	29	HIS	3.1
10	D	133	ASN	3.1
1	0	1171	A	3.1
10	D	47	GLN	3.0
32	Z	14	PHE	3.0
7	A	36	ASP	3.0
32	Z	20	ARG	3.0
1	0	735	C	3.0

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Mol	Chain	Res	Type	RSRZ
20	N	172	PHE	3.0
28	V	59	ILE	3.0
18	L	102	ASP	3.0
31	Y	235	GLU	3.0
4	3	15	ASN	3.0
1	0	2637	A	3.0
18	L	80	ASP	3.0
1	0	2346	C	3.0
28	V	49	LEU	3.0
10	D	70	GLY	2.9
1	0	960	G	2.9
13	G	27	ILE	2.9
27	U	54	THR	2.9
10	D	50	VAL	2.9
10	D	51	ARG	2.9
20	N	140	GLN	2.9
14	H	68	SER	2.9
1	0	1181	A	2.9
20	N	150	TYR	2.9
11	E	154	ILE	2.8
32	Z	19	GLY	2.8
20	N	158	LEU	2.8
7	A	64	ASP	2.8
23	Q	95	GLU	2.8
10	D	73	VAL	2.8
18	L	108	VAL	2.8
18	L	140	VAL	2.8
1	0	2344	G	2.8
1	0	10	U	2.8
10	D	19	GLU	2.7
17	K	101	ASN	2.7
10	D	169	THR	2.7
32	Z	16	ALA	2.7
28	V	44	GLY	2.7
10	D	71	ALA	2.7
32	Z	59	TYR	2.7
20	N	160	SER	2.7
13	G	24	VAL	2.7
13	G	63	ARG	2.7
32	Z	41	ASN	2.6
13	G	68	GLU	2.6
20	N	162	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
18	L	110	GLY	2.6
30	X	88	GLU	2.6
1	0	282	C	2.6
6	9	24	U	2.6
20	N	157	PRO	2.6
14	H	40	GLN	2.6
13	G	65	THR	2.6
31	Y	95	THR	2.6
18	L	91	VAL	2.6
27	U	48	ASN	2.6
1	0	2345	A	2.6
15	I	87	PRO	2.6
25	S	76	GLU	2.6
3	2	44	ARG	2.6
15	I	131	GLY	2.6
15	I	126	THR	2.6
8	B	57	GLU	2.6
10	D	15	GLU	2.6
10	D	80	ALA	2.6
20	N	165	ALA	2.6
26	T	116	ASP	2.6
1	0	1202	A	2.6
11	E	107	PHE	2.5
10	D	81	GLU	2.5
20	N	68	GLU	2.5
11	E	10	ASP	2.5
13	G	15	TRP	2.5
32	Z	23	ARG	2.5
1	0	1525	G	2.5
1	0	1948	G	2.5
4	3	2	GLN	2.5
15	I	127	CYS	2.5
15	I	101	LYS	2.5
12	F	117	GLU	2.5
28	V	9	ARG	2.5
12	F	28	ALA	2.5
20	N	148	ALA	2.5
4	3	88	LEU	2.5
10	D	162	ALA	2.5
1	0	1929	G	2.5
1	0	1951	G	2.5
28	V	2	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
25	S	81	ILE	2.5
18	L	141	GLU	2.5
30	X	80	GLU	2.5
1	0	1175	G	2.5
12	F	44	SER	2.5
3	2	41	HIS	2.5
18	L	59	GLU	2.5
28	V	56	ILE	2.5
11	E	95	VAL	2.5
18	L	96	VAL	2.5
8	B	109	LEU	2.4
10	D	43	GLU	2.4
18	L	100	ALA	2.4
1	0	1192	A	2.4
1	0	1168	C	2.4
28	V	31	ARG	2.4
20	N	67	ALA	2.4
1	0	1169	U	2.4
10	D	129	ASP	2.4
14	H	53	ILE	2.4
7	A	82	VAL	2.4
16	J	92	GLN	2.4
1	0	370	G	2.4
1	0	1947	G	2.4
11	E	87	PHE	2.4
4	3	91	GLN	2.4
7	A	31	LYS	2.4
12	F	45	ALA	2.3
32	Z	27	ALA	2.3
32	Z	15	GLY	2.3
10	D	53	LYS	2.3
4	3	3	MET	2.3
28	V	33	VAL	2.3
27	U	55	ALA	2.3
30	X	41	PHE	2.3
20	N	149	GLU	2.3
8	B	318	ASN	2.3
27	U	51	TRP	2.3
1	0	1170	U	2.3
13	G	64	ASN	2.3
4	3	62	THR	2.3
1	0	1163	G	2.3

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Mol	Chain	Res	Type	RSRZ
15	I	94	ASP	2.3
20	N	138	ASP	2.3
1	0	1000	C	2.3
32	Z	29	ILE	2.3
4	3	41	GLU	2.3
7	A	34	ASP	2.3
13	G	66	LEU	2.3
15	I	125	GLY	2.3
11	E	6	GLU	2.3
32	Z	10	ARG	2.3
13	G	70	ALA	2.2
14	H	149	VAL	2.2
3	2	48	ASP	2.2
1	0	1198	U	2.2
11	E	42	VAL	2.2
10	D	52	THR	2.2
10	D	89	PRO	2.2
14	H	89	THR	2.2
20	N	139	TRP	2.2
1	0	1928	C	2.2
32	Z	43	GLY	2.2
32	Z	58	SER	2.2
10	D	101	THR	2.2
12	F	98	VAL	2.2
32	Z	21	VAL	2.2
1	0	497	A	2.2
28	V	36	ALA	2.2
1	0	369	G	2.2
20	N	152	GLU	2.2
10	D	22	VAL	2.2
17	K	119	GLN	2.2
30	X	85	VAL	2.2
11	E	108	LEU	2.2
20	N	154	LEU	2.2
14	H	72	ALA	2.2
15	I	110	ASP	2.2
1	0	1190	G	2.2
15	I	116	LEU	2.2
26	T	101	LEU	2.2
1	0	280	C	2.2
11	E	156	ASP	2.2
18	L	101	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
11	E	48	VAL	2.2
26	T	115	GLU	2.1
30	X	7	GLU	2.1
17	K	132	VAL	2.1
1	0	1913	C	2.1
12	F	100	ASP	2.1
1	0	285	A	2.1
7	A	85	SER	2.1
18	L	89	PHE	2.1
20	N	64	SER	2.1
20	N	183	ASP	2.1
1	0	1177	A	2.1
26	T	40	VAL	2.1
26	T	112	LEU	2.1
12	F	19	ALA	2.1
7	A	236	GLY	2.1
26	T	117	ASP	2.1
1	0	1965	C	2.1
28	V	6	GLN	2.1
13	G	25	GLU	2.1
10	D	132	VAL	2.1
15	I	135	GLU	2.1
10	D	157	LEU	2.1
1	0	2769	C	2.1
11	E	11	VAL	2.1
32	Z	36	ASP	2.1
1	0	970	U	2.1
28	V	45	ARG	2.1
15	I	121	LYS	2.0
28	V	42	ASN	2.0
11	E	131	LEU	2.0
7	A	35	GLY	2.0
3	2	38	LYS	2.0
32	Z	30	GLU	2.0
22	P	71	TYR	2.0
3	2	36	ASN	2.0
10	D	103	ASN	2.0
18	L	93	VAL	2.0
18	L	124	ASP	2.0
7	A	80	LEU	2.0
21	O	98	LEU	2.0
28	V	62	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
15	I	134	ILE	2.0
22	P	67	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	OMG	0	2588	24/25	0.98	0.15	-	28,30,34,36	0
1	OMU	0	2587	21/22	0.98	0.17	-	31,34,37,40	0
1	1MA	0	628	23/24	0.98	0.16	-	26,28,29,30	0
1	UR3	0	2619	21/22	0.98	0.17	-	26,32,37,38	0
5	MHV	8	6	9/10	0.96	0.17	-	42,43,45,48	0
5	MHW	8	1	9/10	0.92	0.21	-	37,40,43,44	0
5	MEA	8	5	12/13	0.95	0.21	-	39,40,43,43	0
1	PSU	0	2621	20/21	0.98	0.14	-	25,29,33,34	0
5	004	8	7	10/11	0.97	0.22	-	41,45,48,49	0
5	DBB	8	3	6/7	0.95	0.17	-	36,40,40,41	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	8573	1/1	0.94	0.84	59.27	68,68,68,68	0
35	NA	0	8561	1/1	0.86	0.61	52.62	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8071	1/1	0.55	0.67	46.04	68,68,68,68	0
35	NA	0	8535	1/1	0.46	0.59	41.56	44,44,44,44	0
33	MG	0	8038	1/1	0.90	0.54	41.23	26,26,26,26	0
33	MG	0	8060	1/1	0.67	0.51	39.62	51,51,51,51	0
35	NA	0	8572	1/1	0.85	0.60	36.84	58,58,58,58	0
35	NA	0	8563	1/1	0.72	0.34	32.27	44,44,44,44	0
33	MG	0	8072	1/1	0.86	0.50	31.99	63,63,63,63	0
33	MG	0	8091	1/1	0.66	0.39	31.76	55,55,55,55	0
33	MG	0	8084	1/1	0.49	0.48	30.80	43,43,43,43	0
33	MG	0	8111	1/1	0.60	0.48	30.55	42,42,42,42	0
35	NA	0	8571	1/1	0.71	0.55	28.71	62,62,62,62	0
33	MG	0	8096	1/1	0.53	0.35	28.64	46,46,46,46	0
33	MG	0	8018	1/1	0.78	0.41	28.30	43,43,43,43	0
33	MG	K	8069	1/1	0.89	0.45	27.42	45,45,45,45	0
35	NA	0	8526	1/1	0.93	0.68	25.76	51,51,51,51	0
33	MG	0	8012	1/1	0.60	0.57	22.67	36,36,36,36	0
35	NA	0	8502	1/1	0.80	0.30	22.67	44,44,44,44	0
33	MG	Y	8108	1/1	0.88	0.35	22.24	36,36,36,36	0
35	NA	0	8576	1/1	0.69	0.40	21.85	69,69,69,69	0
35	NA	9	8582	1/1	0.87	0.51	20.62	78,78,78,78	0
35	NA	0	8556	1/1	0.95	0.48	20.60	40,40,40,40	0
35	NA	0	8521	1/1	0.84	0.56	20.33	61,61,61,61	0
33	MG	0	8054	1/1	0.74	0.32	19.99	32,32,32,32	0
33	MG	0	8032	1/1	0.56	0.35	17.76	26,26,26,26	0
33	MG	0	8080	1/1	0.85	0.23	15.84	36,36,36,36	0
33	MG	0	8058	1/1	0.52	0.47	15.48	39,39,39,39	0
35	NA	0	8550	1/1	0.61	0.26	14.37	34,34,34,34	0
35	NA	0	8577	1/1	0.78	0.56	14.00	44,44,44,44	0
35	NA	0	8570	1/1	0.65	0.26	13.63	58,58,58,58	0
33	MG	0	8117	1/1	0.96	0.39	13.46	47,47,47,47	0
35	NA	0	8560	1/1	0.80	0.36	12.83	56,56,56,56	0
33	MG	0	8035	1/1	0.91	0.33	12.47	42,42,42,42	0
33	MG	0	8013	1/1	0.75	0.34	12.26	32,32,32,32	0
35	NA	0	8527	1/1	0.62	0.39	11.98	51,51,51,51	0
33	MG	0	8015	1/1	0.84	0.33	11.28	30,30,30,30	0
33	MG	0	8047	1/1	0.88	0.28	11.01	70,70,70,70	0
33	MG	0	8077	1/1	0.97	0.35	10.99	29,29,29,29	0
33	MG	0	8019	1/1	0.75	0.38	10.97	27,27,27,27	0
35	NA	L	8579	1/1	0.84	0.48	10.92	67,67,67,67	0
35	NA	0	8566	1/1	0.74	0.30	10.65	46,46,46,46	0
33	MG	0	8052	1/1	0.72	0.30	10.52	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8532	1/1	0.75	0.28	10.31	42,42,42,42	0
35	NA	0	8525	1/1	0.85	0.28	10.19	51,51,51,51	0
33	MG	0	8049	1/1	0.72	0.60	10.18	73,73,73,73	0
33	MG	A	8065	1/1	0.66	0.46	10.14	43,43,43,43	0
33	MG	0	8017	1/1	0.90	0.37	10.05	27,27,27,27	0
36	CL	0	8815	1/1	0.89	0.22	9.92	84,84,84,84	0
35	NA	0	8575	1/1	0.88	0.32	8.83	45,45,45,45	0
35	NA	0	8523	1/1	0.87	0.26	8.40	35,35,35,35	0
33	MG	0	8003	1/1	0.69	0.27	8.29	31,31,31,31	0
33	MG	0	8020	1/1	0.91	0.27	7.31	20,20,20,20	0
35	NA	0	8503	1/1	0.92	0.27	7.10	45,45,45,45	0
35	NA	0	8531	1/1	0.86	0.25	7.05	46,46,46,46	0
35	NA	0	8505	1/1	0.66	0.24	6.65	32,32,32,32	0
35	NA	0	8565	1/1	0.42	0.31	6.27	53,53,53,53	0
35	NA	A	8545	1/1	0.72	0.39	6.17	49,49,49,49	0
33	MG	B	8055	1/1	0.69	0.30	5.94	38,38,38,38	0
33	MG	0	8053	1/1	0.79	0.26	5.52	40,40,40,40	0
35	NA	0	8510	1/1	0.92	0.24	5.38	40,40,40,40	0
33	MG	B	8056	1/1	0.91	0.41	5.12	50,50,50,50	0
35	NA	M	8547	1/1	0.85	0.25	5.04	31,31,31,31	0
33	MG	0	8004	1/1	0.67	0.24	4.92	39,39,39,39	0
33	MG	0	8044	1/1	0.88	0.23	3.99	43,43,43,43	0
35	NA	R	8585	1/1	0.77	0.36	3.91	82,82,82,82	0
37	VIR	0	9000	38/38	0.96	0.22	3.84	24,36,40,44	0
33	MG	0	8109	1/1	0.67	0.21	3.64	20,20,20,20	0
35	NA	0	8564	1/1	0.92	0.39	3.51	45,45,45,45	0
35	NA	0	8553	1/1	0.87	0.30	3.35	30,30,30,30	0
33	MG	0	8006	1/1	0.87	0.22	2.86	32,32,32,32	0
33	MG	0	8002	1/1	0.90	0.20	2.72	28,28,28,28	0
34	K	0	8402	1/1	0.88	0.22	2.67	66,66,66,66	0
33	MG	0	8008	1/1	0.81	0.19	2.53	35,35,35,35	0
33	MG	0	8010	1/1	0.80	0.20	2.18	34,34,34,34	0
35	NA	0	8567	1/1	0.88	0.17	1.99	64,64,64,64	0
33	MG	0	8074	1/1	0.65	0.24	1.90	34,34,34,34	0
33	MG	0	8106	1/1	0.70	0.21	1.82	38,38,38,38	0
36	CL	0	8816	1/1	0.96	0.20	1.61	57,57,57,57	0
36	CL	B	8819	1/1	0.97	0.23	1.45	46,46,46,46	0
35	NA	R	8537	1/1	0.60	0.21	1.35	44,44,44,44	0
35	NA	C	8504	1/1	0.77	0.28	1.25	40,40,40,40	0
33	MG	0	8001	1/1	0.63	0.18	1.17	33,33,33,33	0
33	MG	0	8102	1/1	0.77	0.21	0.48	80,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	Q	8548	1/1	0.85	0.21	0.33	32,32,32,32	0
33	MG	0	8086	1/1	0.78	0.24	0.11	47,47,47,47	0
35	NA	0	8520	1/1	0.83	0.17	0.02	28,28,28,28	0
36	CL	3	8804	1/1	0.93	0.28	-0.18	68,68,68,68	0
36	CL	O	8808	1/1	0.91	0.22	-0.38	84,84,84,84	0
33	MG	0	8007	1/1	0.87	0.15	-0.42	18,18,18,18	0
35	NA	0	8543	1/1	0.91	0.17	-0.46	46,46,46,46	0
33	MG	0	8033	1/1	0.81	0.15	-0.65	32,32,32,32	0
33	MG	3	8078	1/1	0.83	0.17	-1.00	45,45,45,45	0
35	NA	J	8546	1/1	0.86	0.16	-1.12	48,48,48,48	0
35	NA	0	8524	1/1	0.95	0.10	-1.31	43,43,43,43	0
35	NA	0	8538	1/1	0.93	0.12	-1.31	42,42,42,42	0
33	MG	0	8064	1/1	0.95	0.12	-1.48	30,30,30,30	0
36	CL	0	8805	1/1	0.90	0.14	-1.56	58,58,58,58	0
35	NA	0	8533	1/1	0.87	0.14	-1.56	43,43,43,43	0
35	NA	0	8517	1/1	0.84	0.12	-1.57	46,46,46,46	0
33	MG	0	8057	1/1	0.91	0.15	-1.64	38,38,38,38	0
36	CL	0	8812	1/1	0.94	0.12	-1.66	43,43,43,43	0
35	NA	0	8509	1/1	0.94	0.10	-1.79	38,38,38,38	0
38	CD	U	8701	1/1	1.00	0.09	-1.93	58,58,58,58	0
36	CL	M	8818	1/1	0.98	0.13	-1.98	40,40,40,40	0
36	CL	J	8821	1/1	0.98	0.10	-2.03	48,48,48,48	0
38	CD	1	8702	1/1	0.99	0.05	-2.25	58,58,58,58	0
35	NA	0	8544	1/1	0.86	0.10	-2.31	24,24,24,24	0
38	CD	Z	8703	1/1	0.99	0.06	-2.53	84,84,84,84	0
38	CD	3	8704	1/1	0.97	0.07	-2.58	69,69,69,69	0
35	NA	0	8539	1/1	0.92	0.12	-2.73	35,35,35,35	0
36	CL	0	8813	1/1	0.99	0.11	-2.99	50,50,50,50	0
33	MG	T	8073	1/1	0.90	0.07	-3.43	66,66,66,66	0
33	MG	0	8067	1/1	0.98	0.10	-7.30	44,44,44,44	0
33	MG	0	8040	1/1	0.62	0.52	-	56,56,56,56	0
36	CL	N	8807	1/1	0.87	0.22	-	62,62,62,62	0
35	NA	0	8514	1/1	0.73	0.17	-	33,33,33,33	0
33	MG	0	8085	1/1	0.73	0.32	-	53,53,53,53	0
33	MG	0	8062	1/1	0.56	0.37	-	61,61,61,61	0
35	NA	H	8522	1/1	0.87	0.16	-	55,55,55,55	0
33	MG	0	8014	1/1	0.60	0.32	-	22,22,22,22	0
33	MG	0	8094	1/1	0.78	0.28	-	72,72,72,72	0
36	CL	0	8803	1/1	0.98	0.13	-	54,54,54,54	0
33	MG	0	8115	1/1	0.52	0.33	-	49,49,49,49	0
35	NA	0	8549	1/1	0.81	0.28	-	46,46,46,46	0
33	MG	0	8113	1/1	0.67	0.24	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8501	1/1	0.91	0.33	-	23,23,23,23	0
36	CL	Y	8820	1/1	0.96	0.10	-	43,43,43,43	0
35	NA	0	8529	1/1	0.49	0.24	-	66,66,66,66	0
33	MG	0	8098	1/1	0.86	0.21	-	25,25,25,25	0
33	MG	2	8076	1/1	0.57	0.39	-	57,57,57,57	0
36	CL	0	8817	1/1	0.94	0.13	-	49,49,49,49	0
33	MG	0	8009	1/1	0.57	0.35	-	28,28,28,28	0
35	NA	0	8578	1/1	0.67	0.43	-	58,58,58,58	0
33	MG	0	8110	1/1	0.80	0.25	-	52,52,52,52	0
33	MG	0	8100	1/1	0.79	0.40	-	63,63,63,63	0
36	CL	A	8809	1/1	0.93	0.28	-	68,68,68,68	0
33	MG	0	8024	1/1	0.93	0.22	-	22,22,22,22	0
35	NA	0	8558	1/1	0.88	0.89	-	61,61,61,61	0
35	NA	0	8568	1/1	0.52	0.75	-	58,58,58,58	0
33	MG	0	8063	1/1	0.81	0.67	-	62,62,62,62	0
35	NA	0	8506	1/1	0.78	1.28	-	41,41,41,41	0
33	MG	0	8022	1/1	0.51	0.25	-	59,59,59,59	0
35	NA	0	8554	1/1	0.92	0.20	-	38,38,38,38	0
33	MG	0	8005	1/1	0.87	0.28	-	31,31,31,31	0
36	CL	L	8810	1/1	0.97	0.18	-	53,53,53,53	0
33	MG	0	8103	1/1	0.82	0.26	-	47,47,47,47	0
35	NA	0	8542	1/1	0.90	0.38	-	41,41,41,41	0
33	MG	0	8105	1/1	0.84	0.19	-	50,50,50,50	0
33	MG	0	8039	1/1	0.64	0.32	-	42,42,42,42	0
33	MG	0	8021	1/1	0.85	0.39	-	36,36,36,36	0
33	MG	0	8043	1/1	0.66	0.23	-	45,45,45,45	0
35	NA	0	8507	1/1	0.81	0.23	-	59,59,59,59	0
35	NA	0	8581	1/1	0.70	0.37	-	89,89,89,89	0
33	MG	0	8075	1/1	0.44	0.36	-	51,51,51,51	0
33	MG	0	8050	1/1	0.76	0.16	-	77,77,77,77	0
33	MG	0	8045	1/1	0.88	0.22	-	54,54,54,54	0
33	MG	0	8092	1/1	0.57	0.51	-	66,66,66,66	0
35	NA	0	8583	1/1	0.24	0.59	-	56,56,56,56	0
36	CL	0	8822	1/1	0.82	0.41	-	81,81,81,81	0
33	MG	0	8027	1/1	0.75	0.28	-	44,44,44,44	0
33	MG	0	8029	1/1	0.68	0.45	-	37,37,37,37	0
35	NA	0	8574	1/1	0.88	0.88	-	44,44,44,44	0
35	NA	0	8528	1/1	0.90	0.32	-	38,38,38,38	0
35	NA	0	8534	1/1	0.85	0.12	-	40,40,40,40	0
36	CL	0	8814	1/1	0.99	0.13	-	49,49,49,49	0
33	MG	0	8107	1/1	0.32	0.27	-	49,49,49,49	0
35	NA	0	8511	1/1	0.75	0.27	-	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8104	1/1	0.79	0.21	-	51,51,51,51	0
35	NA	0	8555	1/1	0.82	0.59	-	72,72,72,72	0
33	MG	0	8025	1/1	0.85	0.25	-	31,31,31,31	0
33	MG	0	8068	1/1	0.78	0.30	-	77,77,77,77	0
33	MG	0	8016	1/1	0.52	0.24	-	32,32,32,32	0
35	NA	0	8584	1/1	0.55	0.42	-	51,51,51,51	0
33	MG	0	8061	1/1	0.75	0.24	-	31,31,31,31	0
33	MG	0	8048	1/1	0.89	0.27	-	49,49,49,49	0
38	CD	O	8705	1/1	0.94	0.09	-	88,88,88,88	0
35	NA	0	8559	1/1	0.66	0.63	-	52,52,52,52	0
33	MG	0	8112	1/1	0.86	0.38	-	42,42,42,42	0
33	MG	0	8101	1/1	0.79	0.23	-	50,50,50,50	0
33	MG	0	8116	1/1	0.93	0.15	-	20,20,20,20	0
35	NA	0	8519	1/1	0.76	0.21	-	25,25,25,25	0
33	MG	0	8046	1/1	0.84	0.11	-	48,48,48,48	0
33	MG	0	8083	1/1	0.74	0.33	-	39,39,39,39	0
36	CL	J	8801	1/1	0.91	0.19	-	63,63,63,63	0
33	MG	0	8026	1/1	0.92	0.19	-	22,22,22,22	0
33	MG	9	8095	1/1	0.91	0.09	-	55,55,55,55	0
33	MG	0	8041	1/1	0.71	0.26	-	42,42,42,42	0
35	NA	0	8562	1/1	0.80	0.29	-	43,43,43,43	0
35	NA	0	8569	1/1	0.73	0.64	-	73,73,73,73	0
33	MG	0	8070	1/1	0.75	0.13	-	45,45,45,45	0
33	MG	0	8037	1/1	0.76	0.23	-	32,32,32,32	0
35	NA	0	8518	1/1	0.87	0.42	-	30,30,30,30	0
35	NA	0	8513	1/1	0.78	0.40	-	56,56,56,56	0
36	CL	0	8811	1/1	0.94	0.14	-	53,53,53,53	0
33	MG	0	8097	1/1	0.59	0.19	-	29,29,29,29	0
35	NA	0	8541	1/1	0.79	0.27	-	39,39,39,39	0
33	MG	0	8023	1/1	0.63	0.31	-	41,41,41,41	0
33	MG	0	8118	1/1	0.82	0.28	-	34,34,34,34	0
35	NA	0	8516	1/1	0.70	0.37	-	42,42,42,42	0
33	MG	0	8036	1/1	0.83	0.48	-	36,36,36,36	0
36	CL	J	8802	1/1	0.93	0.19	-	63,63,63,63	0
33	MG	0	8059	1/1	0.91	0.34	-	38,38,38,38	0
33	MG	0	8079	1/1	0.76	0.27	-	36,36,36,36	0
33	MG	0	8093	1/1	0.83	0.26	-	49,49,49,49	0
33	MG	0	8090	1/1	0.55	0.63	-	53,53,53,53	0
35	NA	0	8552	1/1	0.73	0.33	-	59,59,59,59	0
36	CL	R	8806	1/1	0.89	0.13	-	41,41,41,41	0
35	NA	0	8515	1/1	0.90	0.48	-	47,47,47,47	0
35	NA	S	8512	1/1	0.77	0.14	-	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8580	1/1	0.81	0.33	-	49,49,49,49	0
33	MG	0	8034	1/1	0.90	0.23	-	24,24,24,24	0
35	NA	0	8530	1/1	0.77	0.26	-	40,40,40,40	0
33	MG	0	8088	1/1	0.78	0.17	-	21,21,21,21	0
35	NA	0	8536	1/1	0.88	0.25	-	47,47,47,47	0
33	MG	0	8011	1/1	0.62	0.39	-	11,11,11,11	0
33	MG	0	8042	1/1	0.91	0.15	-	31,31,31,31	0
33	MG	0	8114	1/1	0.89	0.40	-	47,47,47,47	0
33	MG	0	8051	1/1	0.63	0.40	-	60,60,60,60	0
33	MG	0	8089	1/1	0.51	0.66	-	77,77,77,77	0
33	MG	0	8087	1/1	0.71	0.14	-	51,51,51,51	0
33	MG	0	8082	1/1	0.68	0.43	-	63,63,63,63	0
35	NA	0	8540	1/1	0.90	0.27	-	34,34,34,34	0
33	MG	0	8030	1/1	0.67	0.19	-	21,21,21,21	0
33	MG	0	8099	1/1	0.89	0.19	-	49,49,49,49	0
33	MG	0	8031	1/1	0.83	0.23	-	27,27,27,27	0
33	MG	0	8028	1/1	0.74	0.28	-	35,35,35,35	0
33	MG	0	8066	1/1	0.62	0.27	-	62,62,62,62	0
35	NA	0	8508	1/1	0.42	0.27	-	56,56,56,56	0
35	NA	0	8557	1/1	0.91	0.09	-	50,50,50,50	0
33	MG	0	8081	1/1	0.84	0.16	-	44,44,44,44	0
35	NA	9	8551	1/1	0.72	0.24	-	49,49,49,49	0

6.5 Other polymers

There are no such residues in this entry.