



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 06:47 AM UTC

PDB ID : 3CMA / pdb_00003cma
Title : The structure of CCA and CCA-Phe-Cap-Bio bound to the large ribosomal subunit of *Haloarcula marismortui*
Authors : Simonovic, M.; Steitz, T.A.
Deposited on : 2008-03-21
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

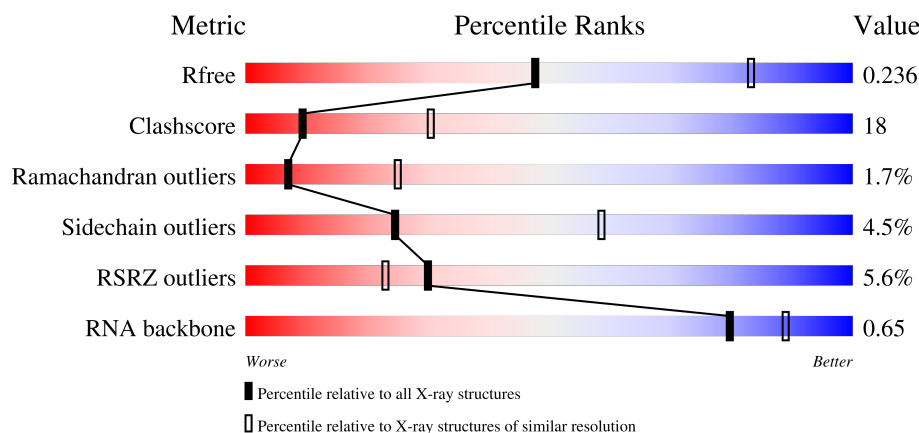
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	240	4% 51% 41% 6%
2	B	338	2% 40% 56%
3	C	246	57% 37% 6%
4	D	177	30% 28% 45% 6% 21%

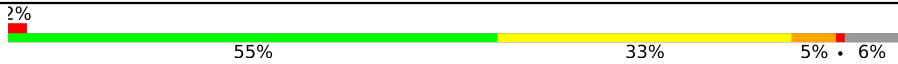
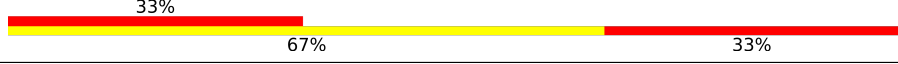
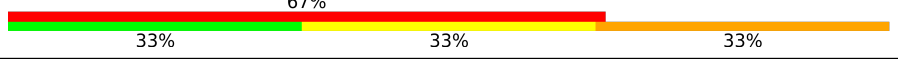
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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	240	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	
32	5	3	
33	6	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	MG	0	8049	-	-	-	X
34	MG	0	8063	-	-	-	X
34	MG	0	8071	-	-	-	X
34	MG	0	8081	-	-	-	X
34	MG	0	8090	-	-	-	X
36	SR	0	8920	-	-	-	X
36	SR	0	9006	-	-	-	X
37	NA	0	8509	-	-	-	X
37	NA	0	8522	-	-	-	X
37	NA	0	8546	-	-	-	X
37	NA	0	8553	-	-	-	X
37	NA	0	8571	-	-	-	X
37	NA	0	8573	-	-	-	X

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 99205 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1752	1072	351	324	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2624	1616	492	511	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1859	1130	344	384	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1093	685	194	210	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1356	840	223	289	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			889	551	140	197	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1281	798	239	238	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			518	323	80	114	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1119	696	198	222	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			993	609	188	192	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	S	0	0	0
			1117	670	221	226				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1557	943	332	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1444	895	261	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			864	529	160	175				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1135	683	228	224				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			734	450	140	144				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1148	713	208	223	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			640	389	110	138	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			949	568	179	202				

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1195	737	208	244	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			653	402	128	122	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			572	343	112	112	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			754	458	152	137	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59018	26346	10873	19054	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2596	1157	471	847	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	5	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			

- Molecule 33 is a RNA chain called RNA (5'-R(*CP*CP*(8AN))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	6	3	Total	C	N	O	P	0	0	0
			59	28	12	17	2			

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	2	Total	Mg	0	0
			2	2		
34	B	1	Total	Mg	0	0
			1	1		
34	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	K	1	Total 1	Mg 1	0	0
34	T	1	Total 1	Mg 1	0	0
34	Y	1	Total 1	Mg 1	0	0
34	2	1	Total 1	Mg 1	0	0
34	0	84	Total 84	Mg 84	0	0
34	9	1	Total 1	Mg 1	0	0

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	1	Total 1	Cl 1	0	0
35	B	1	Total 1	Cl 1	0	0
35	J	3	Total 3	Cl 3	0	0
35	K	1	Total 1	Cl 1	0	0
35	L	2	Total 2	Cl 2	0	0
35	M	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	Q	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	2	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	6	Total 6	Cl 6	0	0

- Molecule 36 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	3	Total 3	Sr 3	0	0
36	B	2	Total 2	Sr 2	0	0
36	F	1	Total 1	Sr 1	0	0
36	H	2	Total 2	Sr 2	0	0
36	R	1	Total 1	Sr 1	0	0
36	S	1	Total 1	Sr 1	0	0
36	T	2	Total 2	Sr 2	0	0
36	Y	1	Total 1	Sr 1	0	0
36	1	2	Total 2	Sr 2	0	0
36	3	3	Total 3	Sr 3	0	0
36	0	86	Total 86	Sr 86	0	0
36	9	3	Total 3	Sr 3	0	0

- Molecule 37 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	B	1	Total 1	Na 1	0	0
37	C	1	Total 1	Na 1	0	0
37	D	1	Total 1	Na 1	0	0
37	J	1	Total 1	Na 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	1	Total 1	Na 1	0	0
37	M	1	Total 1	Na 1	0	0
37	Q	1	Total 1	Na 1	0	0
37	R	2	Total 2	Na 2	0	0
37	S	1	Total 1	Na 1	0	0
37	0	64	Total 64	Na 64	0	0
37	9	1	Total 1	Na 1	0	0

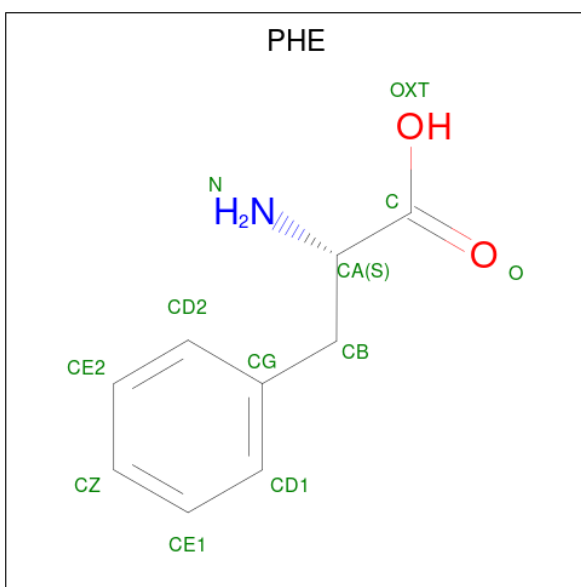
- Molecule 38 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 39 is POTASSIUM ION (CCD ID: K) (formula: K).

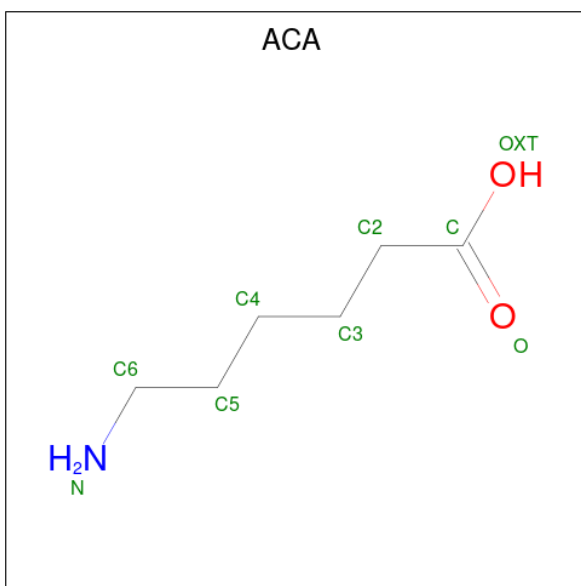
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	2	Total 2	K 2	0	0

- Molecule 40 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
40	6	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 41 is 6-AMINOHEXANOIC ACID (CCD ID: ACA) (formula: C₆H₁₃NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
41	6	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 42 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	A	128	Total O 128 128	0	0
42	B	165	Total O 165 165	0	0
42	C	170	Total O 170 170	0	0
42	D	49	Total O 49 49	0	0
42	E	48	Total O 48 48	0	0
42	F	31	Total O 31 31	0	0
42	G	19	Total O 19 19	0	0
42	H	77	Total O 77 77	0	0
42	I	11	Total O 11 11	0	0
42	J	63	Total O 63 63	0	0
42	K	54	Total O 54 54	0	0
42	L	92	Total O 92 92	0	0
42	M	136	Total O 136 136	0	0
42	N	64	Total O 64 64	0	0
42	O	43	Total O 43 43	0	0
42	P	69	Total O 69 69	0	0
42	Q	51	Total O 51 51	0	0
42	R	87	Total O 87 87	0	0
42	S	33	Total O 33 33	0	0
42	T	40	Total O 40 40	0	0
42	U	30	Total O 30 30	0	0
42	V	16	Total O 16 16	0	0

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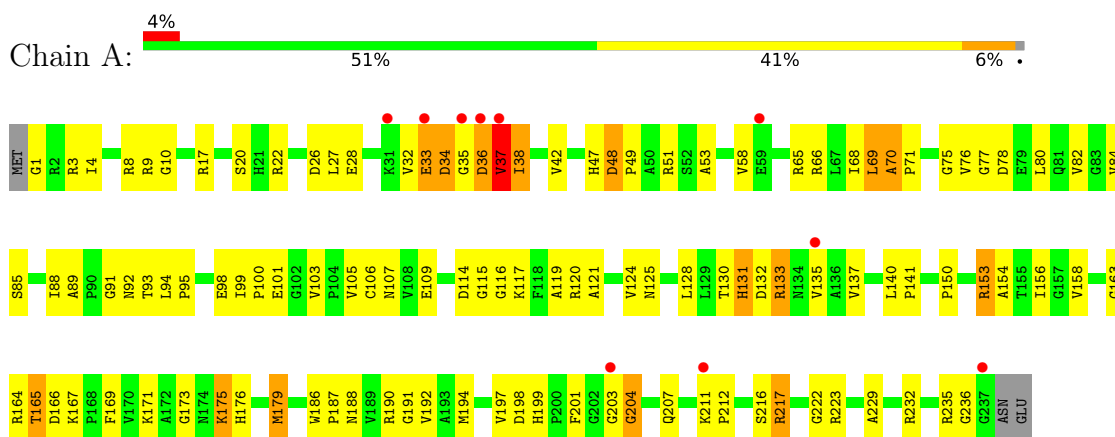
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	W	72	Total 72	O 72	0	0
42	X	25	Total 25	O 25	0	0
42	Y	108	Total 108	O 108	0	0
42	Z	30	Total 30	O 30	0	0
42	1	53	Total 53	O 53	0	0
42	2	42	Total 42	O 42	0	0
42	3	66	Total 66	O 66	0	0
42	0	5771	Total 5771	O 5771	0	0
42	9	148	Total 148	O 148	0	0
42	5	4	Total 4	O 4	0	0
42	6	3	Total 3	O 3	0	0

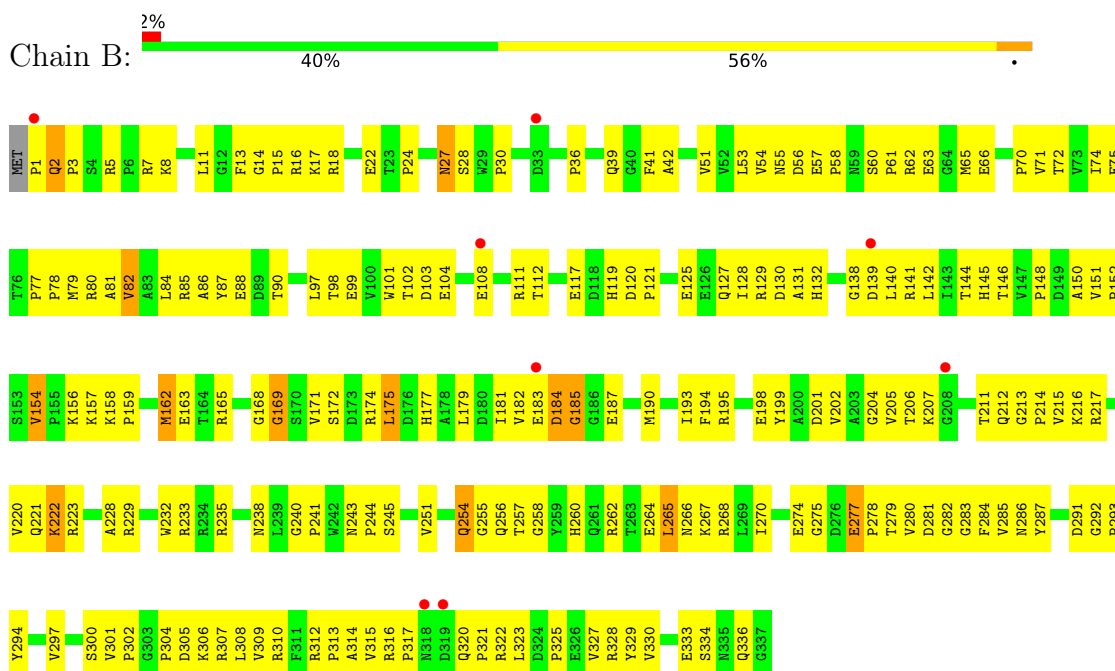
3 Residue-property plots [i](#)

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

- Molecule 1: 50S ribosomal protein L2P

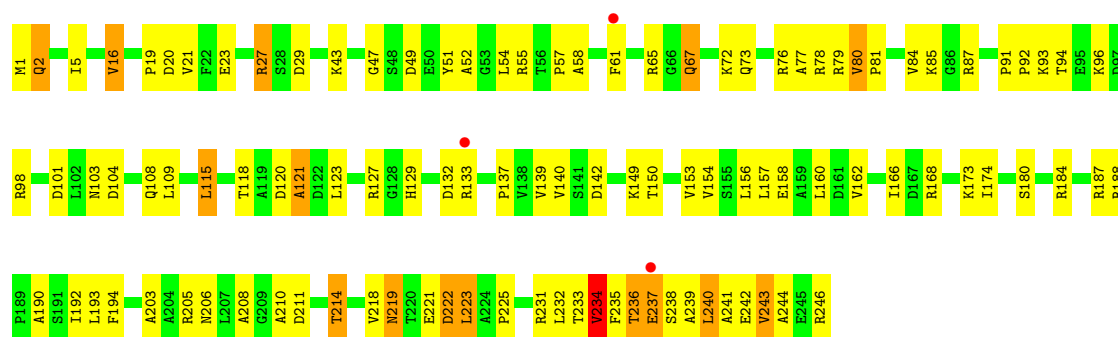


- Molecule 2: 50S ribosomal protein L3P

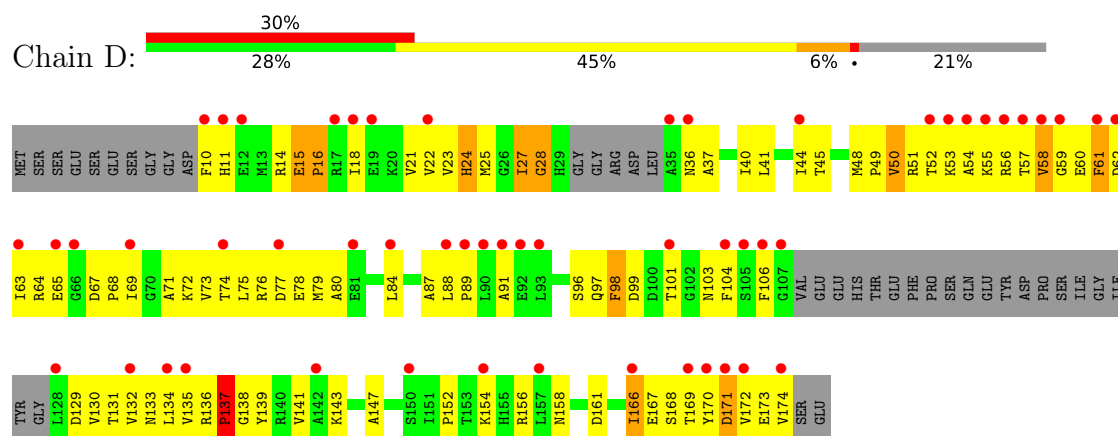


- Molecule 3: 50S ribosomal protein L4P

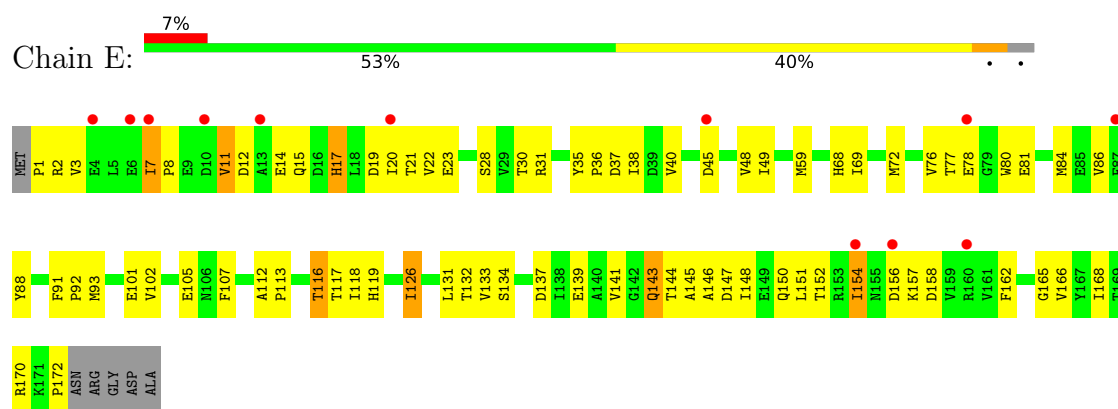




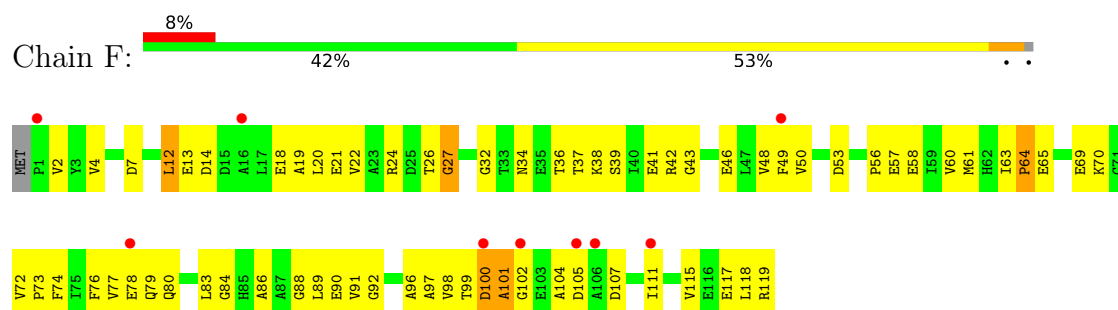
• Molecule 4: 50S ribosomal protein L5P



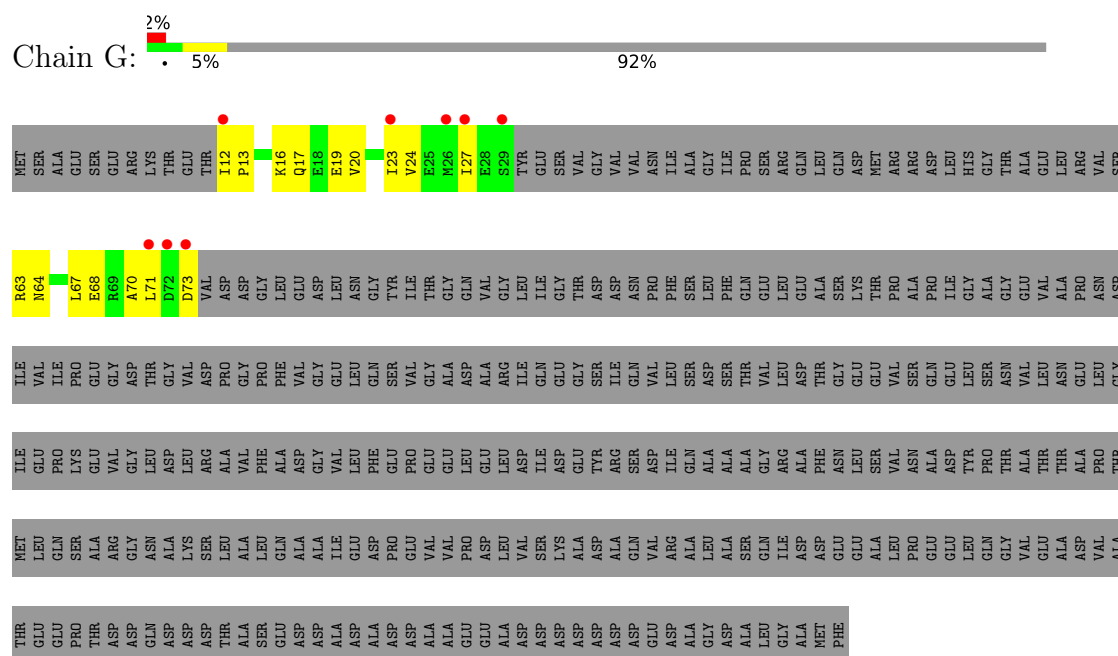
• Molecule 5: 50S ribosomal protein L6P



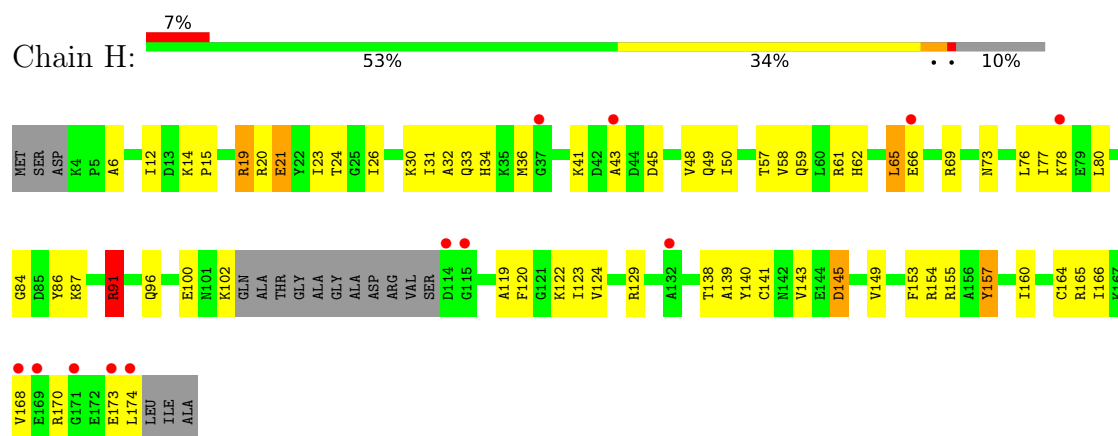
• Molecule 6: 50S ribosomal protein L7Ae



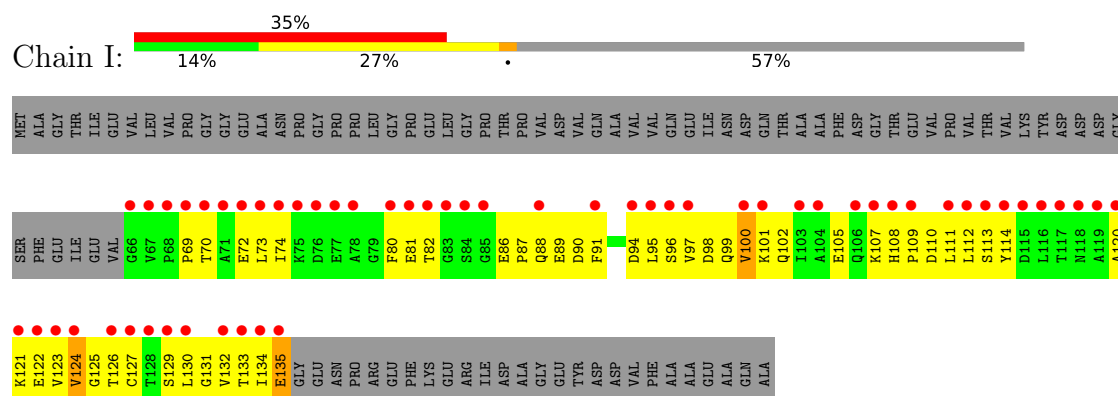
• Molecule 7: 50S ribosomal protein L10E



- Molecule 8: 50S ribosomal protein L10e

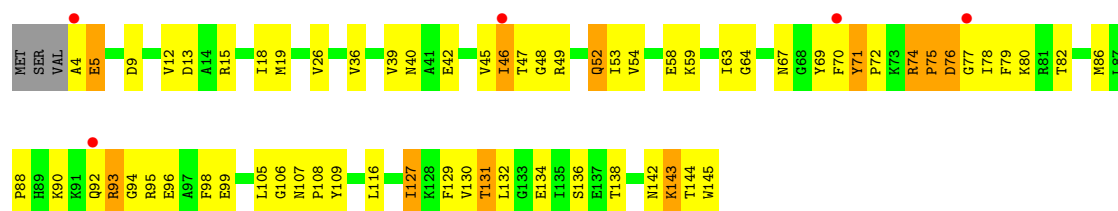


- Molecule 9: 50S ribosomal protein L11P



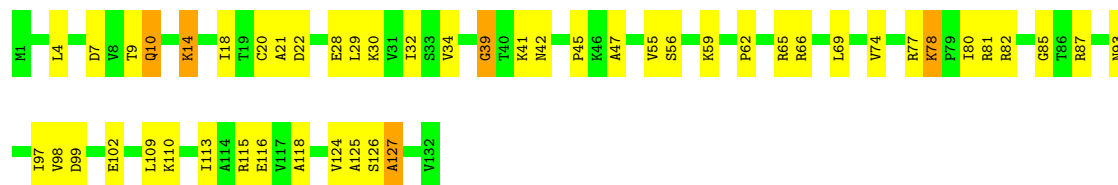
- Molecule 10: 50S ribosomal protein L13P





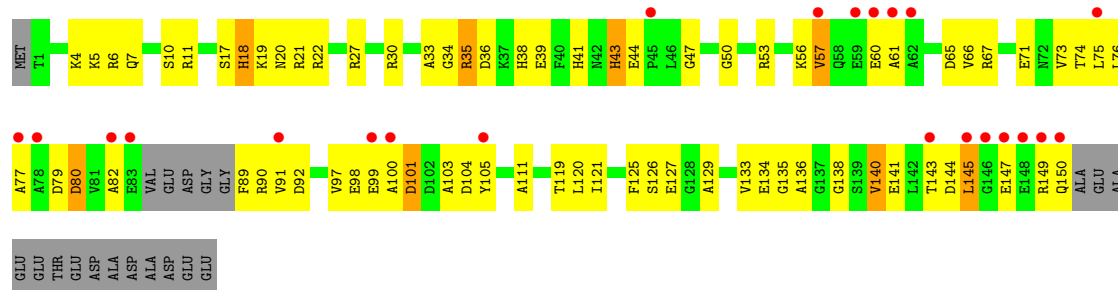
• Molecule 11: 50S ribosomal protein L14P

Chain K: 63% 33% .



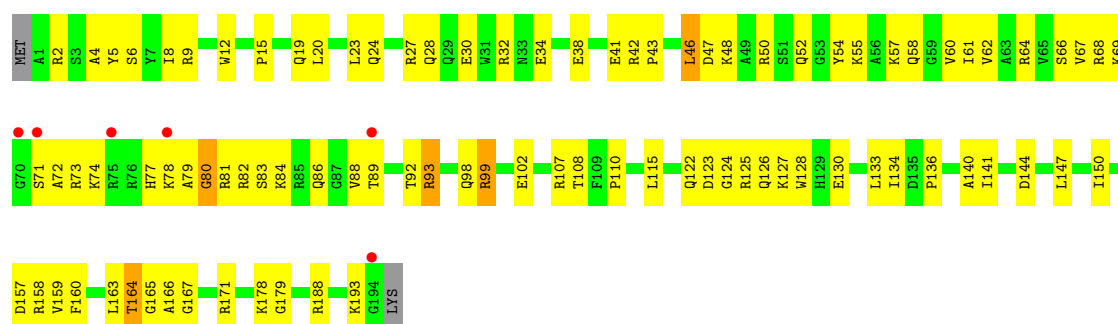
• Molecule 12: 50S ribosomal protein L15P

Chain L: 13% 42% 41% 5% 12%



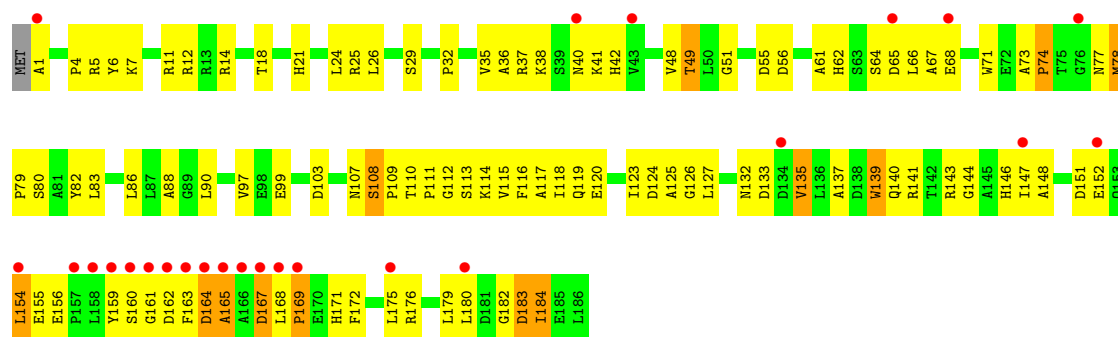
• Molecule 13: 50S ribosomal protein L15e

Chain M: 3% 52% 44% . .

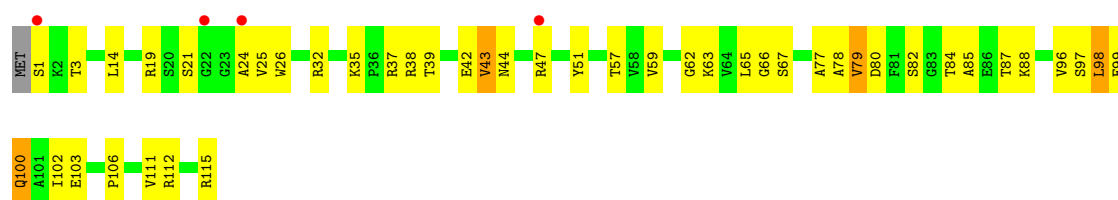


• Molecule 14: 50S ribosomal protein L18P

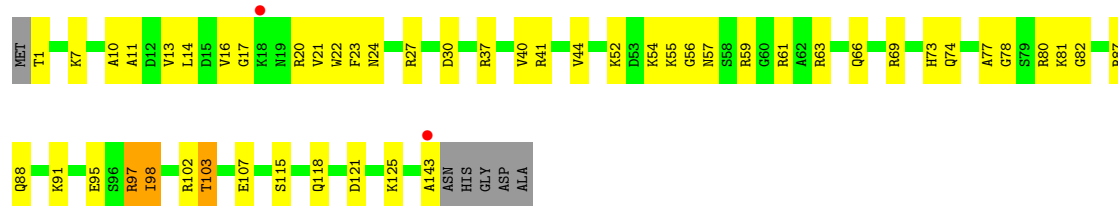
Chain N: 13% 44% 49% 7% .



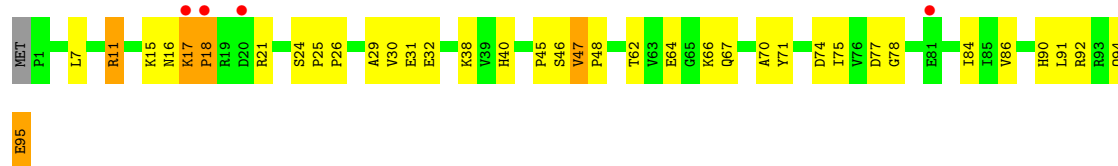
• Molecule 15: 50S ribosomal protein L18e



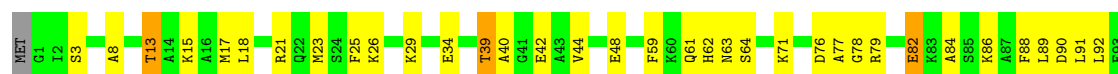
• Molecule 16: 50S ribosomal protein L19e

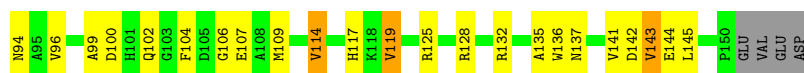


• Molecule 17: 50S ribosomal protein L21e

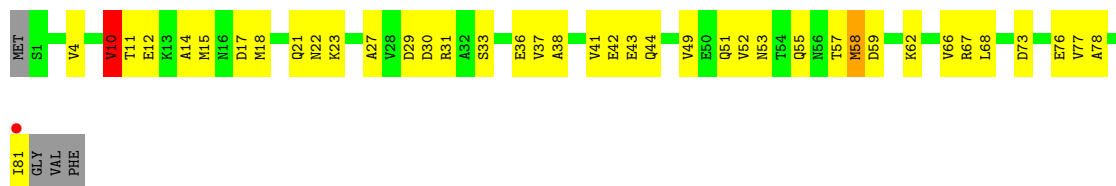


• Molecule 18: 50S ribosomal protein L22P

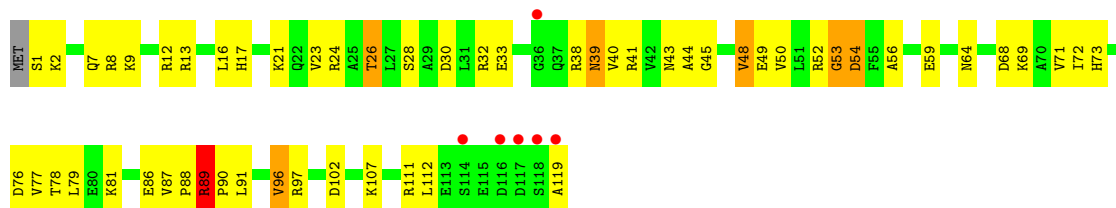




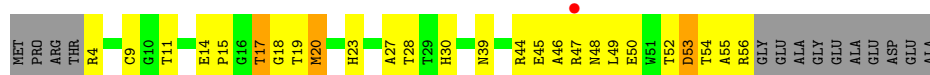
• Molecule 19: 50S ribosomal protein L23P



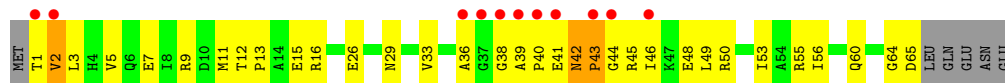
• Molecule 20: 50S ribosomal protein L24P



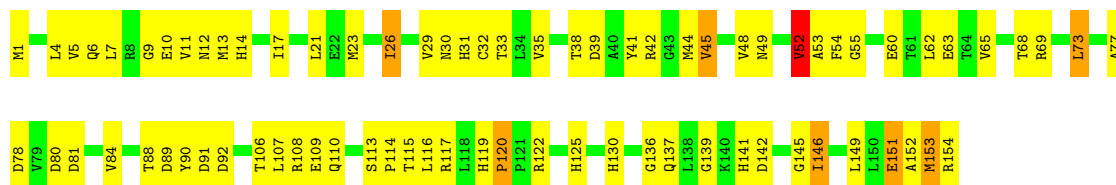
• Molecule 21: 50S ribosomal protein L24e



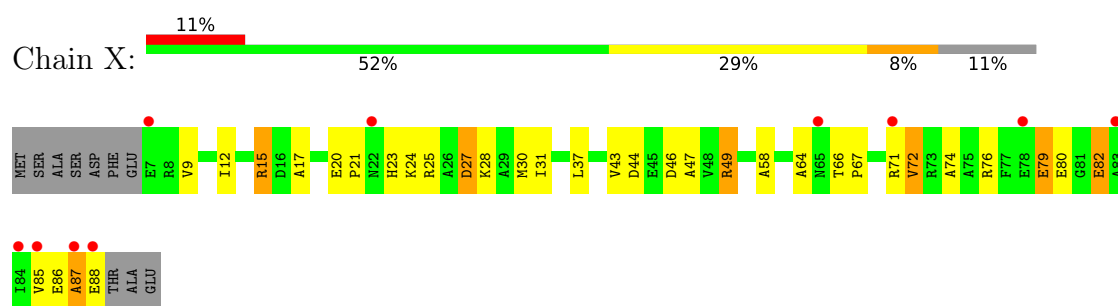
• Molecule 22: 50S ribosomal protein L29P



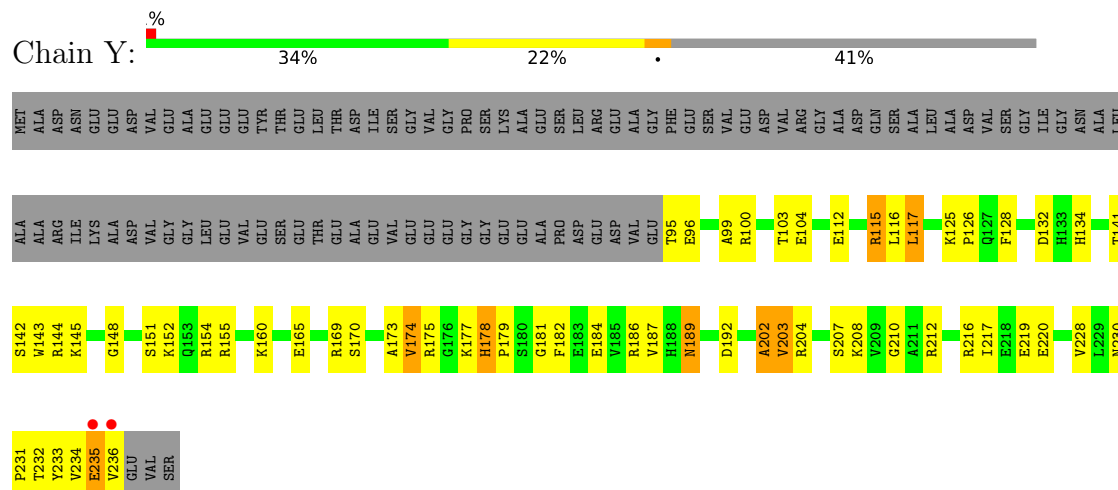
• Molecule 23: 50S ribosomal protein L30P



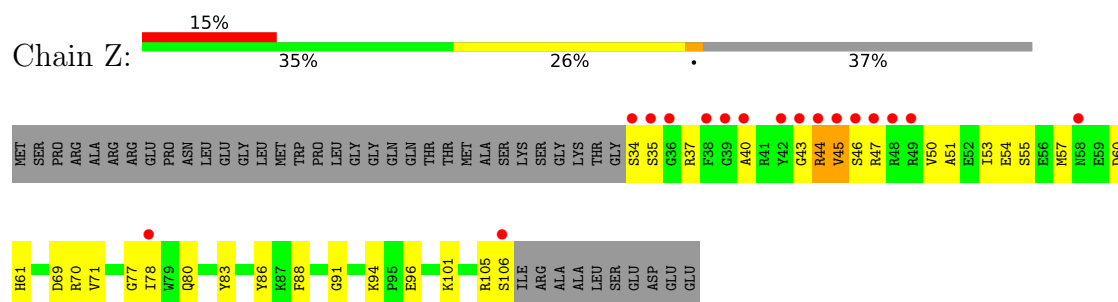
• Molecule 24: 50S ribosomal protein L31e



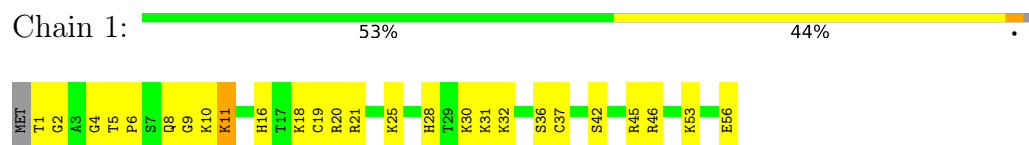
- Molecule 25: 50S ribosomal protein L32e



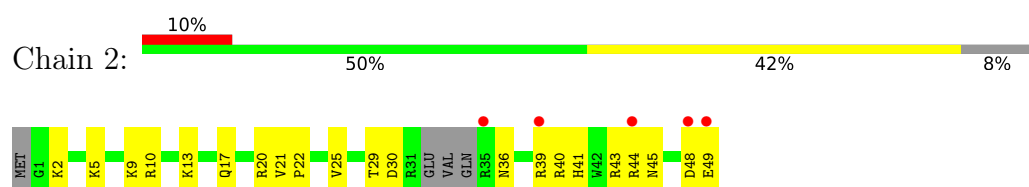
- Molecule 26: 50S ribosomal protein L37Ae



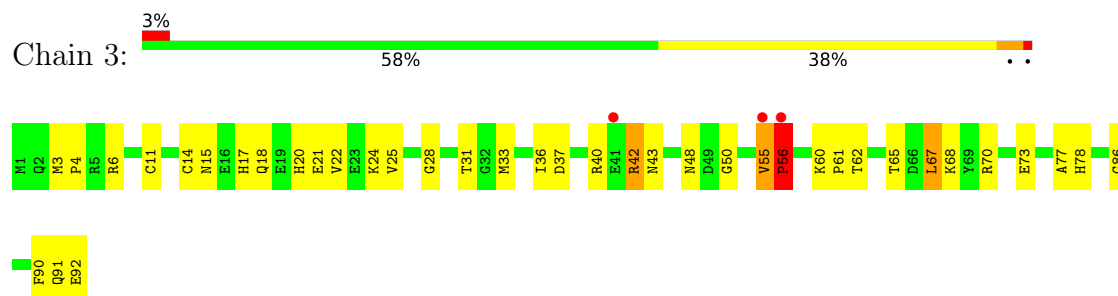
- Molecule 27: 50S ribosomal protein L37e



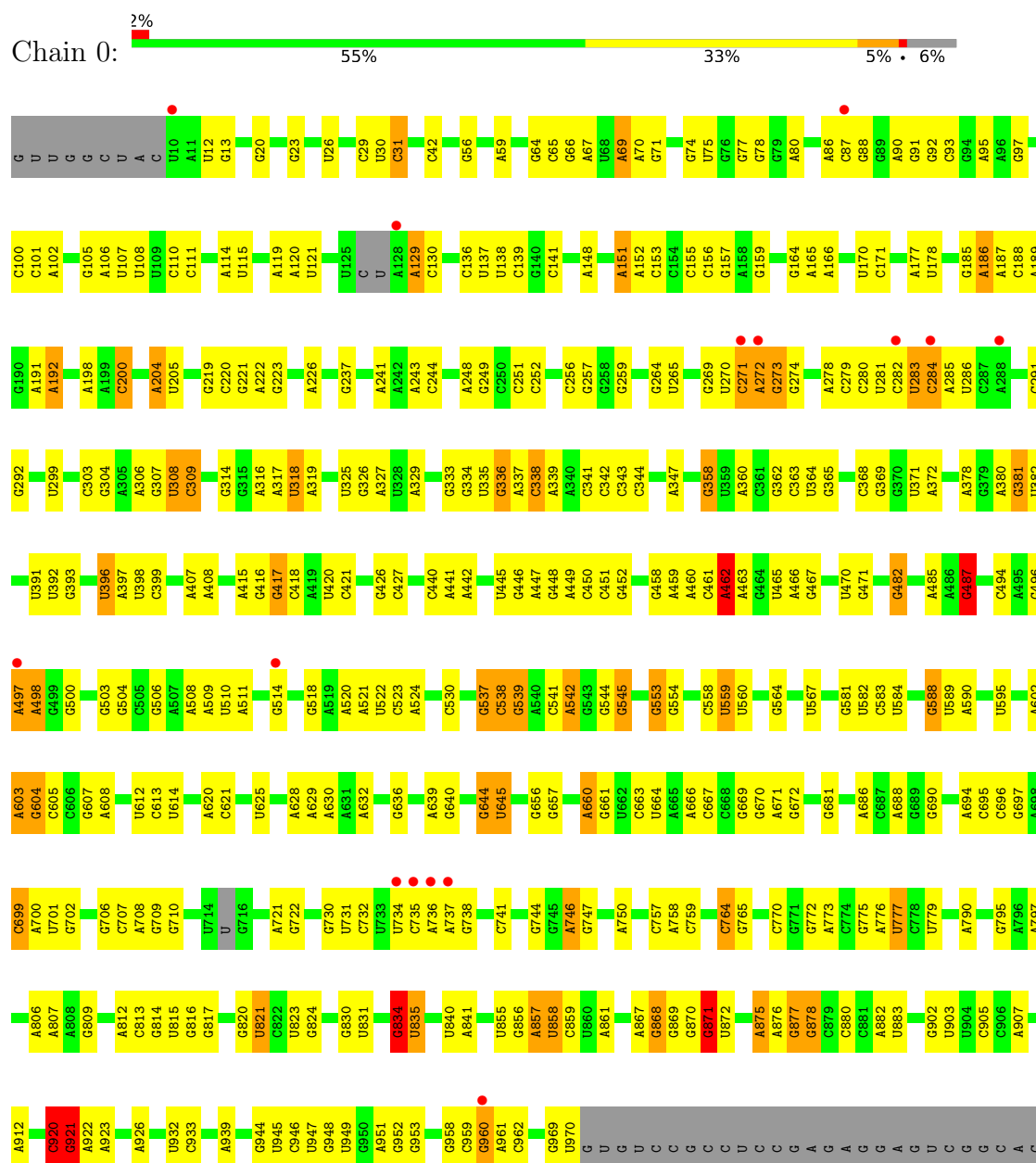
- Molecule 28: 50S ribosomal protein L39e



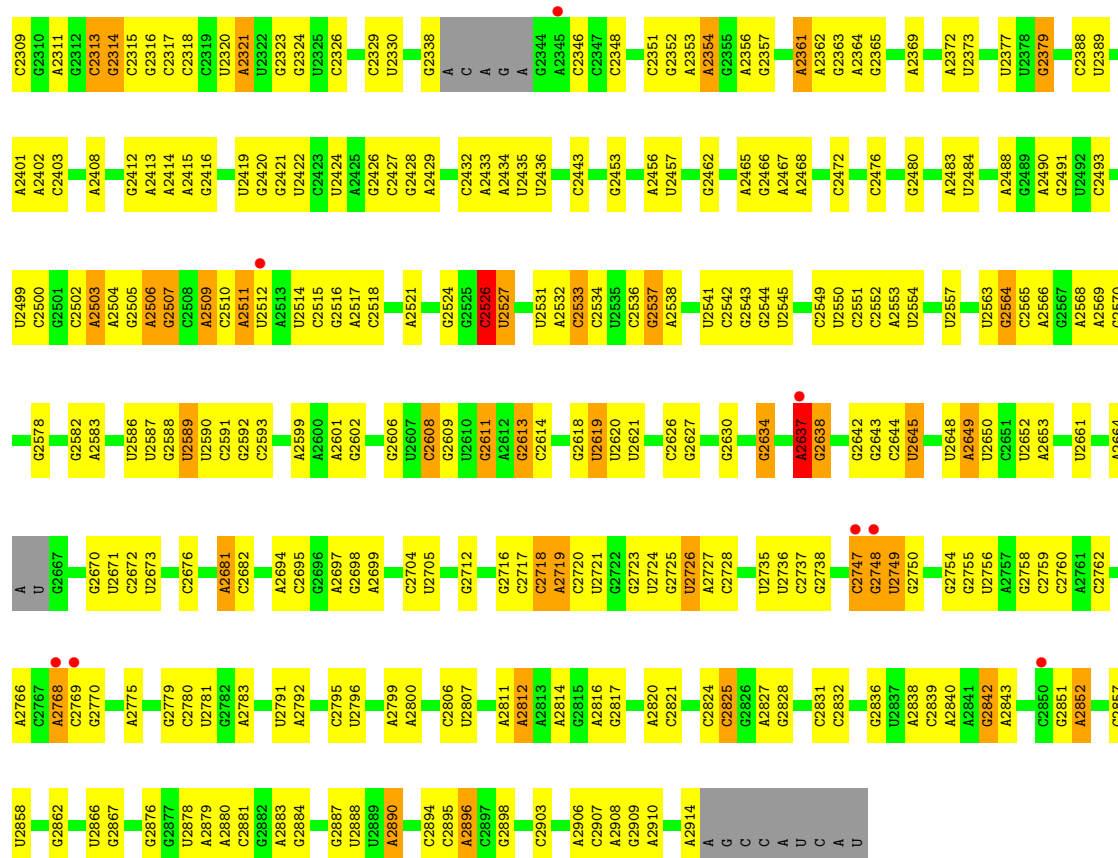
- Molecule 29: 50S ribosomal protein L44E



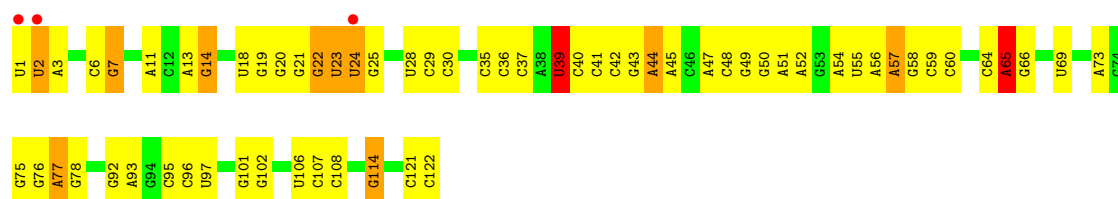
- Molecule 30: 23S RIBOSOMAL RNA



C	G2080	A1981	G1902	C1798	U1702	A1606	A1487	U1380	A1291	A1199	U1109	A
U	A2081	G2082	U1903	G1799	A1710	A1607	U1488	C1384	G1292	A1200	G1110	C999
A	A2083	U1985	A1909	G1799	A1710	A1615	G1497	C1385	U1293	C1201	C1101	C1006
C	U1992	U1910	A1909	C1803	C1714	A1616	G1497	G1386	A1294	A1202	U1116	A1007
C	C2087	C1993	C1911	A1804	C1715	C1617	U1500	G1387	U1298	G1203	U1117	C1008
G	A2088	A1994	G1806	G1806	A1716	U1625	A1501	C1387	U1299	U1205	G1118	
U	G2089	U1996	A1919	G1806	A1716	U1625	A1502	A1393	G1300	U1206	U1120	A1014
C	G2090	U1996	C1920	G1809	U1722	A1626	U1503	C1394	U1304	A1207	C1129	C1015
G	A1922	U2004	A1922	A1810	G1723	G1627	U1504	C1395	U1305	C1208	C1129	C1019
U	C2094	U2004	A1922	A1811	U1724	A1630	U1506	C1396	U1306	G1210	U1130	C1019
G	G2094	G2005	G1925	C1816	C1725	A1631	C1507	G1398	A1307	G1211	A1132	G1021
G	A2095	C2006	G1926	U1817	G1730	A1632	C1508	A1399	U1308	C1212		A1022
C	A2096	U2007	A1927	C1818	C1731	G1633	A1522	U1405	U1309	G1216	C1140	U1027
U	A2101	U2008	C1928	C1818	C1731	G1634	G1523	A1406	U1310	G1217	U1028	U1028
G	G2102	G2009	A1929	A1819	A1732	U1635	U1524	A1407	G1311	U1218		U1029
C	A2103	A2010	A1930	G1820	A1733	G1636	G1525	U1408	C1312	U1219	G1151	
A	C2104	A2011	A1931	A1829	A1736	A1637	G1526	G1409	U1313			
G	U2012	A2012	G1932	C1830	A1737	A1641	A1527	G1410	U1314	C1230	G1158	G1039
G	G2106	G2013	C1936	C1830	A1642	A1642	A1528	G1410	G1315	A1239	G1159	U1040
U	G2110	U2016	C1936	C1833	G1739	G1649	G1529	A1414	G1316	C1230	A1161	U1041
A	U2017	U2017	U1939	C1834	U1740	U1654	A1533	G1415	G1325	U1234	G1162	C1043
C	A2018	A2018	C1940	U1836	U1741	U1655	C1594	G1416	G1327	G1235	G1163	C1044
C	A2019	A2019	A1941	U1836	U1741	U1656	C1594	U1417	A1328	U1237	U1164	G1045
C	U2032	U2032	C1943	U1838	U1748	G1655	C1546	U1419	G1331	C1238	G1165	G1053
G	G2033	G2033	C1943	A1840	G1752	A1656	G1546	U1422	G1331	G1239	G1167	U1056
C	U2034	U2034	C1946	A1840	C1753	A1658	G1546	U1422	G1332	G1240	C1168	U1056
U	G1947	A1947	C1947	A1845	C1753	A1659	G1552	C1423	U1333	G1241	U1169	A1057
C	A2038	A2038	G1948	U1846	A1755	A1659	G1552	A1424	U1333	A1242	U1170	A1058
A	A2039	A2039	G1949	A1847	G1756	G1660	G1555	G1425	C1334	C1243	A1171	G1059
G	G2131	G1950	G1950	A1847	G1756	G1666	G1555	C1426	C1335	U1244	G1172	C1060
C	C2132	U2042	G1951	C1853	U1759	C1667	A1559	A1427	G1342	G1245	A1173	U1066
G	U2043	U2043	U	C1854	G1760	U1668	U	U1440	C1343	A1246	A1174	U1066
G	A2135	G2044	A	G1855	U1761	A1668	A1561	U1440	G1344	C1246	A1175	A1067
G	G2136	G2045	A	C1856	C1762	C1675	C1562	G1445	U1350	U1249	C1176	G1072
A	C	G2046	C	G1863	C1763	C1763	C1565	U1446	U1350	C1250	C1177	G1072
C	G	C2047	U	G1863	C1764	C1678	C1566	U1447	G1351	G1251	G1178	A1073
C	A	C2048	A	G1863	G1765	C1679	C1566	U1447	A1352	A1252	C1179	G1074
C	U	G2049	U	G1868	U1766	C1680	G1567	C1451	C1353	C1253	U1180	
C	G	G2050	G	G1877	U1766	G1681	G1564	C1451	G1354	C1253	A1181	A1078
C	G	A2051	A	C1873	U1771	A1682	A1573	A1458	A1355	G1260	A1182	A1078
C	A	G2053	C	U1874	C1772	G1683	C1574	A1458	A1356	C1260	C1183	C1080
G	U	A2054	C	C	G1773	A1684	C1574	A1458	A1357	U1266	C1184	A1081
A	G	A2055	C	G1877	G1774	A1685	G1588	U1461	A1357	G1267	U1185	
C	C		U1964	G1878	U1778	C1686	G1589	U1462	C1360	C1268	U1186	A1086
A	G	G2058	C1965	U1879	A1778	C1687	G1592	U1463	C1366	G1269	U1187	G1087
A	C	A	U1966	U1879	A1779	C1687	G1593	C1464	C1366	A1188	A1189	A1088
C	A	U2063	U1967	G1884	A1779	C1692	C1593	A1470	A1369	U1276	A1189	A1097
C	U	U2064	U1967	A1885	U1783	A1693	C1594	A1470	A1369	C1277	G1190	A1097
G	U	A1971	G1971	A1886	U1784	G1694	G1595	A1470	A1369	A1278	A1098	A1098
A	U	U1972	U1972	U1887	G1785	G1695	U1596	C1474	A1372	U1279	A1192	G1099
G	C	C2071	A1973	C1888	G1786	U1696	A1597	C1477	A1372	A1280	A1193	G1100
G	A	G2072	G1974	U1889	C1787	G1697	A1597	C1477	A1375	U1287	A1194	C1104
A	C	G2073	G2073	U1890	U1788	U1698	A1597	C1477	A1375	G1376	A1195	C1104
A	G	A2074	A1978	G1789	U1788	G1699	A1603	G1484	G1376	U1288	C1196	
C	A	A2074	G1979	U1789	C1790	G1700	A1604	A1485	G1378	C1289	G1197	A1107
U	A	C2079	U1980	C1894	U1791	A1700	G1695	A1486	A1379	C1290	U1199	A1107



• Molecule 31: 5S RIBOSOMAL RNA



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



• Molecule 33: RNA (5'-R(*CP*CP*(8AN))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.32Å 297.90Å 573.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 2.80 49.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.2 (49.79-2.80) 91.2 (49.79-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.245 0.186 , 0.236	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 73.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	99205	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SR, PSU, MG, NA, 1MA, OMG, ACA, CD, UR3, K, 8AN, CL, OMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.44	0/1784	0.99	6/2403 (0.2%)
2	B	0.45	0/2687	1.03	20/3644 (0.5%)
3	C	0.47	0/1883	0.98	7/2547 (0.3%)
4	D	0.38	0/1109	0.90	4/1493 (0.3%)
5	E	0.41	0/1380	0.92	4/1875 (0.2%)
6	F	0.39	0/899	0.85	2/1219 (0.2%)
7	G	0.38	0/241	0.78	0/324
8	H	0.40	0/1300	0.94	2/1738 (0.1%)
9	I	0.33	0/524	0.85	1/711 (0.1%)
10	J	0.44	0/1134	0.92	5/1525 (0.3%)
11	K	0.44	0/1002	1.02	5/1346 (0.4%)
12	L	0.40	0/1128	1.00	6/1504 (0.4%)
13	M	0.46	0/1580	0.88	3/2111 (0.1%)
14	N	0.38	0/1472	1.01	14/1994 (0.7%)
15	O	0.43	0/872	0.94	5/1176 (0.4%)
16	P	0.43	0/1145	0.87	2/1524 (0.1%)
17	Q	0.44	0/747	1.09	7/1001 (0.7%)
18	R	0.47	0/1170	0.94	4/1574 (0.3%)
19	S	0.41	0/646	0.86	3/870 (0.3%)
20	T	0.41	0/956	0.97	4/1284 (0.3%)
21	U	0.41	0/417	0.89	0/562
22	V	0.39	0/502	0.94	2/675 (0.3%)
23	W	0.54	1/1217 (0.1%)	1.17	6/1650 (0.4%)
24	X	0.45	0/662	0.94	2/890 (0.2%)
25	Y	0.45	0/1146	1.01	6/1536 (0.4%)
26	Z	0.35	0/582	0.94	1/776 (0.1%)
27	1	0.46	0/438	0.92	2/578 (0.3%)
28	2	0.45	0/401	0.82	0/529
29	3	0.43	0/769	0.90	5/1019 (0.5%)
30	0	0.38	0/65951	0.61	31/102855 (0.0%)
31	9	0.37	0/2897	0.62	2/4512 (0.0%)
32	5	0.47	0/65	1.38	1/99 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.49	0/40	0.80	0/60
All	All	0.40	1/98746 (0.0%)	0.73	162/147604 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
30	0	0	47
31	9	0	2
32	5	0	1
All	All	0	50

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	52	VAL	CB-CG2	-9.17	1.22	1.52

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	52	VAL	CG1-CB-CG2	22.05	159.32	110.80
23	W	52	VAL	CA-CB-CG2	-14.52	85.72	110.40
14	N	163	PHE	N-CA-C	-11.16	99.20	111.36
30	0	1979	G	C2'-C3'-O3'	10.42	125.13	109.50
20	T	54	ASP	N-CA-C	-9.70	101.44	113.28
12	L	57	VAL	N-CA-C	-9.19	104.38	113.20
1	A	222	GLY	N-CA-C	-7.85	105.14	114.48
2	B	222	LYS	N-CA-C	-7.70	98.49	110.42
2	B	323	LEU	N-CA-C	7.66	120.47	110.43
30	0	1942	A	C5'-C4'-C3'	7.52	127.28	116.00
18	R	141	VAL	N-CA-C	7.45	119.34	108.53
12	L	44	GLU	N-CA-C	-7.45	100.19	109.64
2	B	157	LYS	N-CA-C	-7.41	104.76	114.31
15	O	66	GLY	N-CA-C	7.31	124.37	115.31
22	V	42	ASN	CA-C-N	7.24	128.89	119.84
22	V	42	ASN	C-N-CA	7.24	128.89	119.84
2	B	154	VAL	CA-C-N	7.18	126.71	119.24
2	B	154	VAL	C-N-CA	7.18	126.71	119.24
3	C	188	ARG	N-CA-C	7.08	114.59	108.22
12	L	145	LEU	N-CA-C	-6.96	103.70	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	82	SER	N-CA-C	-6.94	101.38	110.53
31	9	39	U	N1-C1'-C2'	6.92	122.39	112.00
30	0	2726	U	N1-C1'-C2'	6.87	122.30	112.00
30	0	2637	A	C2'-C3'-O3'	6.72	119.58	109.50
17	Q	17	LYS	N-CA-C	-6.66	101.37	109.83
19	S	27	ALA	N-CA-C	-6.63	98.44	109.24
30	0	1592	G	N9-C1'-C2'	6.58	121.88	112.00
5	E	11	VAL	N-CA-C	6.58	118.89	108.89
24	X	12	ILE	N-CA-C	6.57	114.40	107.76
29	3	55	VAL	CA-C-N	6.54	128.01	119.84
29	3	55	VAL	C-N-CA	6.54	128.01	119.84
12	L	7	GLN	N-CA-C	6.53	119.22	111.71
30	0	1504	A	N9-C1'-C2'	6.51	121.76	112.00
14	N	135	VAL	N-CA-C	-6.50	106.66	112.90
2	B	265	LEU	N-CA-C	6.50	119.11	110.53
2	B	57	GLU	CA-C-N	6.48	126.06	119.19
2	B	57	GLU	C-N-CA	6.48	126.06	119.19
30	0	2291	A	N9-C1'-C2'	6.48	121.72	112.00
1	A	70	ALA	N-CA-C	6.47	117.80	109.72
30	0	2313	C	C5'-C4'-C3'	6.42	125.63	116.00
24	X	17	ALA	N-CA-C	-6.41	105.43	113.18
6	F	79	GLN	N-CA-C	6.38	119.14	109.95
25	Y	143	TRP	N-CA-C	6.38	119.61	110.10
3	C	205	ARG	N-CA-C	6.36	118.74	111.11
2	B	175	LEU	N-CA-C	-6.29	104.51	111.36
5	E	156	ASP	N-CA-C	6.21	118.57	111.11
30	0	834	G	C2'-C3'-O3'	-6.21	104.38	113.70
30	0	129	A	C2'-C3'-O3'	6.19	122.99	113.70
14	N	169	PRO	N-CA-C	-6.10	106.24	113.86
30	0	2301	A	N9-C1'-C2'	6.08	121.12	112.00
4	D	15	GLU	CA-C-N	6.06	127.42	119.84
4	D	15	GLU	C-N-CA	6.06	127.42	119.84
30	0	1819	G	C5'-C4'-C3'	6.06	125.09	116.00
30	0	871	G	C5'-C4'-O4'	-6.03	100.75	109.80
11	K	127	ALA	N-CA-C	-6.00	105.53	114.64
2	B	193	ILE	N-CA-C	5.99	116.75	111.90
12	L	47	GLY	N-CA-C	5.99	118.20	111.85
3	C	192	ILE	N-CA-C	5.96	117.27	109.58
30	0	1701	A	C5'-C4'-C3'	5.96	124.14	115.20
30	0	1352	A	C2'-C3'-O3'	5.95	118.42	109.50
17	Q	24	SER	CA-C-N	5.95	126.51	120.38
17	Q	24	SER	C-N-CA	5.95	126.51	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ASP	CA-C-N	5.95	126.10	119.32
1	A	48	ASP	C-N-CA	5.95	126.10	119.32
32	5	76	A	C5'-C4'-C3'	-5.95	107.08	116.00
5	E	17	HIS	CB-CA-C	-5.91	109.78	116.63
17	Q	47	VAL	N-CA-C	5.89	112.92	107.56
9	I	100	VAL	N-CA-C	-5.89	107.53	113.47
14	N	133	ASP	N-CA-C	5.88	118.44	111.33
12	L	76	LEU	N-CA-C	-5.86	106.76	112.97
30	O	2103	A	C2'-C3'-O3'	5.85	118.27	109.50
19	S	58	MET	N-CA-C	-5.84	106.39	112.93
10	J	71	TYR	CA-C-N	5.80	125.74	119.76
10	J	71	TYR	C-N-CA	5.80	125.74	119.76
23	W	113	SER	CA-C-N	5.78	126.17	119.47
23	W	113	SER	C-N-CA	5.78	126.17	119.47
20	T	89	ARG	CA-C-N	5.73	126.02	119.83
20	T	89	ARG	C-N-CA	5.73	126.02	119.83
13	M	8	ILE	N-CA-C	-5.73	105.15	110.53
30	O	462	A	N9-C1'-C2'	5.72	120.58	112.00
27	1	19	CYS	N-CA-C	5.71	118.04	108.96
30	O	883	U	N1-C1'-C2'	5.71	120.56	112.00
25	Y	230	ASN	CA-C-N	5.67	125.87	120.31
25	Y	230	ASN	C-N-CA	5.67	125.87	120.31
14	N	42	HIS	N-CA-C	5.67	118.48	109.81
14	N	116	PHE	N-CA-C	-5.65	105.50	112.90
18	R	137	ASN	N-CA-C	5.64	118.81	110.46
2	B	82	VAL	N-CA-C	5.62	118.12	111.09
1	A	135	VAL	N-CA-C	5.62	116.38	108.17
14	N	108	SER	CA-C-N	5.60	126.84	119.84
14	N	108	SER	C-N-CA	5.60	126.84	119.84
31	9	65	A	N9-C1'-C2'	5.59	120.39	112.00
16	P	103	THR	N-CA-C	-5.58	105.11	111.14
3	C	219	ASN	N-CA-C	5.58	118.70	109.94
10	J	67	ASN	N-CA-C	-5.58	105.20	111.28
14	N	117	ALA	N-CA-C	-5.58	105.10	111.07
30	O	2673	U	N1-C1'-C2'	5.58	120.37	112.00
25	Y	202	ALA	N-CA-C	-5.57	100.82	109.72
30	O	1700	C	C2'-C3'-O3'	-5.57	105.35	113.70
27	1	11	LYS	N-CA-C	5.55	117.76	107.99
5	E	37	ASP	N-CA-C	5.55	119.34	112.24
26	Z	94	LYS	N-CA-C	-5.54	102.47	110.40
18	R	3	SER	N-CA-C	-5.53	100.65	109.23
25	Y	178	HIS	N-CA-C	-5.53	102.16	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	34	HIS	N-CA-C	-5.50	107.22	114.04
30	0	920	C	C2'-C3'-O3'	-5.50	105.45	113.70
29	3	67	LEU	N-CA-C	5.50	117.77	109.41
19	S	10	VAL	N-CA-C	5.49	115.50	107.37
13	M	89	THR	N-CA-C	5.46	119.04	112.38
11	K	14	LYS	N-CA-C	-5.46	101.57	109.59
23	W	153	MET	N-CA-C	-5.44	106.52	112.72
29	3	43	ASN	N-CA-C	5.43	119.53	113.02
3	C	80	VAL	CA-C-N	5.42	125.76	119.47
3	C	80	VAL	C-N-CA	5.42	125.76	119.47
17	Q	29	ALA	N-CA-C	-5.38	106.89	113.50
11	K	78	LYS	CA-C-N	5.37	125.34	120.03
11	K	78	LYS	C-N-CA	5.37	125.34	120.03
1	A	133	ARG	N-CA-C	-5.36	106.41	113.17
3	C	221	GLU	N-CA-C	5.36	117.20	111.36
6	F	90	GLU	N-CA-C	-5.29	106.68	113.02
17	Q	47	VAL	CA-C-N	5.28	126.44	119.84
17	Q	47	VAL	C-N-CA	5.28	126.44	119.84
8	H	91	ARG	N-CA-C	5.27	119.34	113.01
10	J	9	ASP	N-CA-C	-5.27	105.59	112.23
20	T	16	LEU	N-CA-C	5.26	117.42	111.11
30	0	921	G	N9-C1'-C2'	5.23	119.85	112.00
30	0	2526	C	N1-C1'-C2'	5.22	119.83	112.00
2	B	130	ASP	N-CA-C	-5.20	105.51	111.07
23	W	35	VAL	N-CA-C	5.20	113.56	107.89
16	P	97	ARG	N-CA-C	5.19	116.62	111.07
15	O	43	VAL	N-CA-C	5.18	115.94	108.48
2	B	213	GLY	CA-C-N	5.18	125.22	119.32
2	B	213	GLY	C-N-CA	5.18	125.22	119.32
14	N	78	MET	CA-C-N	5.17	124.96	119.28
14	N	78	MET	C-N-CA	5.17	124.96	119.28
14	N	51	GLY	CA-C-N	5.16	124.77	119.56
14	N	51	GLY	C-N-CA	5.16	124.77	119.56
2	B	151	VAL	CA-C-N	5.14	124.64	119.19
2	B	151	VAL	C-N-CA	5.14	124.64	119.19
4	D	98	PHE	N-CA-C	5.14	117.87	109.59
2	B	22	GLU	N-CA-C	-5.13	106.28	112.54
30	0	1504	A	C4'-C3'-O3'	-5.13	105.30	113.00
30	0	1078	A	N9-C1'-C2'	5.13	119.70	112.00
30	0	2313	C	C5'-C4'-O4'	5.13	117.50	109.80
14	N	161	GLY	N-CA-C	-5.11	104.69	112.51
10	J	75	PRO	N-CA-C	-5.10	107.20	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	100	GLN	N-CA-C	-5.08	105.65	111.14
2	B	120	ASP	CA-C-N	5.08	124.52	119.24
2	B	120	ASP	C-N-CA	5.08	124.52	119.24
30	0	1819	G	C2'-C3'-O3'	-5.07	106.09	113.70
30	0	922	A	N9-C1'-C2'	5.07	119.60	112.00
2	B	117	GLU	N-CA-C	-5.07	107.76	114.04
4	D	48	MET	N-CA-C	5.07	116.07	109.64
15	O	79	VAL	N-CA-C	-5.06	104.76	111.09
11	K	124	VAL	N-CA-C	-5.05	105.57	110.42
25	Y	117	LEU	N-CA-C	-5.04	105.68	111.07
29	3	40	ARG	N-CA-C	-5.03	105.70	111.14
30	0	922	A	C4'-C3'-O3'	-5.02	105.47	113.00
18	R	34	GLU	N-CA-C	5.01	116.82	111.36
30	0	2726	U	C4'-C3'-O3'	-5.01	105.49	113.00
30	0	1737	A	C5'-C4'-C3'	-5.01	108.49	116.00
13	M	80	GLY	N-CA-C	5.00	117.21	111.36

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1039	G	Sidechain
30	0	1067	A	Sidechain
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain
30	0	1293	U	Sidechain
30	0	1309	U	Sidechain
30	0	1327	G	Sidechain
30	0	1342	C	Sidechain
30	0	1380	U	Sidechain
30	0	1458	A	Sidechain
30	0	148	A	Sidechain
30	0	1488	U	Sidechain
30	0	1681	G	Sidechain
30	0	1741	U	Sidechain
30	0	1819	G	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1993	C	Sidechain
30	0	2119	C	Sidechain

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Mol	Chain	Res	Type	Group
30	0	2316	G	Sidechain
30	0	2465	A	Sidechain
30	0	2466	G	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2524	G	Sidechain
30	0	2599	A	Sidechain
30	0	26	U	Sidechain
30	0	2630	G	Sidechain
30	0	2681	A	Sidechain
30	0	270	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	460	A	Sidechain
30	0	462	A	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	487	G	Sidechain
30	0	518	G	Sidechain
30	0	722	G	Sidechain
30	0	764	C	Sidechain
30	0	779	U	Sidechain
30	0	795	G	Sidechain
30	0	868	G	Sidechain
32	5	76	A	Sidechain
31	9	39	U	Sidechain
31	9	65	A	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1752	0	1764	137	0
2	B	2624	0	2530	193	0
3	C	1859	0	1811	104	0
4	D	1093	0	1083	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1356	0	1264	84	0
6	F	889	0	841	65	0
7	G	240	0	231	17	0
8	H	1281	0	1290	66	0
9	I	518	0	495	52	0
10	J	1119	0	1096	75	0
11	K	993	0	1025	59	0
12	L	1117	0	1071	75	0
13	M	1557	0	1571	90	0
14	N	1444	0	1399	104	0
15	O	864	0	868	54	0
16	P	1135	0	1120	47	0
17	Q	734	0	726	31	0
18	R	1148	0	1119	52	0
19	S	640	0	600	32	0
20	T	949	0	922	55	0
21	U	410	0	364	33	0
22	V	499	0	511	44	0
23	W	1195	0	1135	90	0
24	X	653	0	651	35	0
25	Y	1130	0	1133	65	0
26	Z	572	0	529	26	0
27	1	431	0	426	34	0
28	2	396	0	413	27	0
29	3	754	0	727	34	0
30	0	59018	0	29811	1011	0
31	9	2596	0	1324	76	0
32	5	59	0	35	10	0
33	6	59	0	35	1	0
34	0	84	0	0	0	0
34	2	1	0	0	0	0
34	9	1	0	0	0	0
34	A	2	0	0	0	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	6	0	0	0	0
35	2	1	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	B	1	0	0	0	0
35	J	3	0	0	2	0
35	K	1	0	0	1	0
35	L	2	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	86	0	0	0	0
36	1	2	0	0	0	0
36	3	3	0	0	0	0
36	9	3	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	H	2	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
36	T	2	0	0	0	0
36	Y	1	0	0	0	0
37	0	64	0	0	0	0
37	9	1	0	0	0	0
37	B	1	0	0	0	0
37	C	1	0	0	0	0
37	D	1	0	0	0	0
37	J	1	0	0	0	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	Q	1	0	0	0	0
37	R	2	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	2	0	0	0	0
40	6	11	0	8	0	0
41	6	8	0	6	0	0
42	0	5771	0	0	145	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	1	53	0	0	6	0
42	2	42	0	0	1	0
42	3	66	0	0	6	0
42	5	4	0	0	2	0
42	6	3	0	0	0	0
42	9	148	0	0	10	0
42	A	128	0	0	22	0
42	B	165	0	0	19	0
42	C	170	0	0	14	0
42	D	49	0	0	7	0
42	E	48	0	0	3	0
42	F	31	0	0	4	0
42	G	19	0	0	0	0
42	H	77	0	0	10	0
42	I	11	0	0	1	0
42	J	63	0	0	1	0
42	K	54	0	0	4	0
42	L	92	0	0	10	0
42	M	136	0	0	5	0
42	N	64	0	0	8	0
42	O	43	0	0	5	0
42	P	69	0	0	2	0
42	Q	51	0	0	0	0
42	R	87	0	0	3	0
42	S	33	0	0	4	0
42	T	40	0	0	3	0
42	U	30	0	0	2	0
42	V	16	0	0	4	0
42	W	72	0	0	8	0
42	X	25	0	0	4	0
42	Y	108	0	0	6	0
42	Z	30	0	0	4	0
All	All	99205	0	59934	2706	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 18.

All (2706) 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)
2:B:162:MET:HE3	2:B:310:ARG:HD2	1.22	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.25	1.15
3:C:236:THR:HG22	3:C:239:ALA:H	1.02	1.12
31:9:76:G:H3'	31:9:77:A:H5''	1.31	1.12
30:0:871:G:H5'	30:0:871:G:H8	1.20	1.06
4:D:25:MET:HE2	4:D:41:LEU:HG	1.36	1.05
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.41	1.03
14:N:37:ARG:NH1	31:9:6:C:H5''	1.72	1.03
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.24	1.02
30:0:541:C:H2'	30:0:542:A:H5''	1.40	1.02
10:J:82:THR:HG23	30:0:1242:A:H5'	1.41	1.02
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.43	1.01
30:0:871:G:H5'	30:0:871:G:C8	1.96	1.00
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.42	1.00
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.42	0.99
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.44	0.99
30:0:2542:C:H1'	42:0:7596:HOH:O	1.58	0.99
30:0:870:G:H2'	30:0:871:G:H5''	1.44	0.98
2:B:36:PRO:HG3	2:B:169:GLY:H	1.29	0.98
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.79	0.98
30:0:1160:G:H5'	30:0:1161:A:H5'	1.41	0.98
30:0:542:A:H5'	30:0:542:A:H8	1.28	0.98
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.26	0.97
28:2:41:HIS:H	28:2:45:ASN:HD22	1.09	0.97
20:T:9:LYS:HE3	20:T:13:ARG:NH1	1.80	0.97
14:N:144:GLY:O	14:N:147:ILE:HG22	1.64	0.97
30:0:541:C:C2'	30:0:542:A:H5''	1.94	0.97
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.45	0.96
1:A:153:ARG:HB2	1:A:153:ARG:HH11	1.28	0.96
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.46	0.96
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.82	0.95
22:V:1:THR:HG23	22:V:2:VAL:H	1.27	0.95
3:C:236:THR:HG22	3:C:239:ALA:N	1.81	0.95
16:P:115:SER:H	16:P:118:GLN:HE21	1.06	0.95
8:H:30:LYS:H	8:H:62:HIS:HD2	1.05	0.94
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.48	0.94
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.47	0.94
23:W:149:LEU:HG	23:W:153:MET:HE2	1.48	0.93
14:N:113:SER:HB2	42:N:8857:HOH:O	1.70	0.92
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.50	0.92
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.50	0.91
6:F:58:GLU:HA	6:F:61:MET:HE2	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.52	0.90
2:B:238:ASN:HD22	2:B:240:GLY:H	1.19	0.90
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.54	0.90
25:Y:235:GLU:CD	25:Y:235:GLU:H	1.80	0.89
4:D:57:THR:HG23	4:D:63:ILE:HA	1.55	0.89
2:B:162:MET:HE3	2:B:310:ARG:CD	2.02	0.89
11:K:10:GLN:HE21	11:K:10:GLN:H	1.15	0.88
29:3:65:THR:HG22	29:3:67:LEU:HG	1.56	0.88
2:B:179:LEU:O	2:B:183:GLU:HG2	1.72	0.88
23:W:13:MET:HE2	23:W:17:ILE:HG22	1.56	0.87
14:N:37:ARG:HH12	31:9:6:C:H5''	1.34	0.87
21:U:14:GLU:O	21:U:17:THR:HB	1.73	0.87
13:M:171:ARG:HD3	30:0:156:C:H5''	1.56	0.87
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.56	0.86
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.57	0.86
6:F:91:VAL:HG12	6:F:92:GLY:H	1.39	0.86
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.58	0.86
14:N:164:ASP:CG	14:N:167:ASP:HA	2.01	0.85
2:B:140:LEU:HA	42:B:9054:HOH:O	1.74	0.85
3:C:1:MET:HG2	3:C:2:GLN:H	1.41	0.85
3:C:236:THR:CG2	3:C:239:ALA:H	1.89	0.85
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.58	0.85
30:0:545:G:H5'	30:0:545:G:H8	1.40	0.85
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.58	0.85
16:P:115:SER:OG	16:P:118:GLN:HG3	1.76	0.84
2:B:275:GLY:O	2:B:291:ASP:HA	1.77	0.84
30:0:1377:C:H5'	30:0:1377:C:H6	1.40	0.84
30:0:1118:A:H62	30:0:1244:U:H3	1.22	0.84
29:3:48:ASN:HD21	30:0:2468:A:H61	1.24	0.84
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.58	0.84
30:0:2506:A:HO2'	30:0:2507:G:H8	0.85	0.84
2:B:162:MET:HG3	2:B:310:ARG:NH1	1.92	0.84
4:D:99:ASP:HB3	4:D:103:ASN:H	1.43	0.84
27:1:20:ARG:HG2	30:0:111:C:O2'	1.77	0.84
30:0:870:G:C2'	30:0:871:G:H5''	2.07	0.84
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.59	0.84
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.40	0.84
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.58	0.83
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.59	0.83
10:J:93:ARG:HB3	10:J:93:ARG:HH11	1.41	0.83
1:A:33:GLU:H	1:A:33:GLU:CD	1.86	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2073:G:H5''	42:0:4695:HOH:O	1.75	0.83
30:0:1116:U:HO2'	30:0:1118:A:H2	0.87	0.83
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.60	0.83
30:0:1451:C:H5'	30:0:1505:U:C5	2.14	0.83
30:0:2506:A:O2'	30:0:2507:G:H8	1.61	0.83
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.58	0.83
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.58	0.83
30:0:2586:U:H3	30:0:2592:G:H22	1.22	0.83
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.60	0.83
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.08	0.82
4:D:172:VAL:HG12	4:D:173:GLU:H	1.44	0.82
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.60	0.82
30:0:1474:C:H6	30:0:1474:C:H5'	1.44	0.82
30:0:282:C:H1'	30:0:368:C:N4	1.95	0.82
30:0:1160:G:C5'	30:0:1161:A:H5'	2.10	0.81
31:9:56:A:H2'	31:9:57:A:H5''	1.60	0.81
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.60	0.81
13:M:164:THR:HG22	13:M:166:ALA:H	1.44	0.81
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.61	0.81
30:0:1372:A:H3'	42:0:7983:HOH:O	1.79	0.81
13:M:107:ARG:HH11	13:M:107:ARG:HG3	1.45	0.81
9:I:82:THR:HG23	30:0:1168:C:H5''	1.63	0.81
30:0:2534:C:H1'	42:0:4378:HOH:O	1.80	0.81
3:C:233:THR:HG22	3:C:234:VAL:H	1.45	0.81
6:F:91:VAL:HG12	6:F:92:GLY:N	1.96	0.81
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.10	0.81
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.63	0.81
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.62	0.81
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.61	0.81
2:B:62:ARG:HA	2:B:65:MET:HE3	1.61	0.80
30:0:2005:G:H3'	30:0:2005:G:OP2	1.81	0.80
2:B:86:ALA:HA	42:B:9054:HOH:O	1.81	0.80
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.44	0.80
30:0:2717:C:C2'	30:0:2718:C:H5''	2.12	0.80
23:W:80:ASP:O	23:W:84:VAL:HG23	1.80	0.80
30:0:559:U:H6	30:0:559:U:H5'	1.45	0.80
4:D:154:LYS:H	4:D:154:LYS:HD2	1.45	0.80
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.62	0.80
30:0:1835:U:H5	30:0:1840:A:N7	1.79	0.80
6:F:58:GLU:CD	13:M:27:ARG:HH22	1.89	0.80
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.80	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:74:ARG:CB	10:J:74:ARG:HH11	1.95	0.79
30:0:1603:A:H5'	30:0:1605:G:O4'	1.80	0.79
30:0:2908:A:H2'	30:0:2909:G:O4'	1.82	0.79
30:0:541:C:H2'	30:0:542:A:C5'	2.13	0.79
30:0:1667:A:H8	30:0:1667:A:H5'	1.48	0.79
1:A:153:ARG:HH11	1:A:153:ARG:CB	1.94	0.79
8:H:30:LYS:H	8:H:62:HIS:CD2	1.97	0.79
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.64	0.79
30:0:877:G:H5'	30:0:878:G:OP1	1.82	0.79
20:T:112:LEU:HD23	20:T:119:ALA:HB3	1.63	0.78
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.65	0.78
30:0:506:G:H22	30:0:509:A:C5'	1.95	0.78
5:E:84:MET:HE1	5:E:148:ILE:HD12	1.65	0.78
30:0:1701:A:H4'	30:0:1702:U:H5''	1.65	0.78
14:N:132:ASN:O	14:N:135:VAL:HG12	1.84	0.78
18:R:39:THR:HG23	18:R:107:GLU:O	1.83	0.78
30:0:2717:C:H2'	30:0:2718:C:H5''	1.64	0.78
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.83	0.77
30:0:1300:G:H1'	42:0:5535:HOH:O	1.82	0.77
10:J:19:MET:HE2	10:J:79:PHE:HA	1.65	0.77
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.32	0.77
30:0:2812:A:H2	30:0:2814:A:H62	1.32	0.77
13:M:80:GLY:O	13:M:81:ARG:HD2	1.84	0.77
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.66	0.77
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.67	0.77
30:0:681:G:N3	30:0:681:G:H5'	1.99	0.77
30:0:969:G:H1	30:0:999:C:H42	1.32	0.77
9:I:73:LEU:HD12	9:I:107:LYS:NZ	1.98	0.77
27:1:16:HIS:HD2	30:0:470:U:O2'	1.67	0.77
30:0:506:G:H22	30:0:509:A:H5'	1.48	0.77
16:P:115:SER:H	16:P:118:GLN:NE2	1.82	0.77
4:D:36:ASN:HA	42:D:7500:HOH:O	1.83	0.77
30:0:1973:A:H5'	30:0:1973:A:H8	1.50	0.77
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.15	0.76
30:0:2637:A:H4'	30:0:2638:G:C5'	2.15	0.76
11:K:10:GLN:H	11:K:10:GLN:NE2	1.82	0.76
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.67	0.76
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.67	0.76
15:O:42:GLU:HB2	42:O:2176:HOH:O	1.85	0.76
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.66	0.76
30:0:1116:U:H3	30:0:1246:A:H62	1.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.16	0.76
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.68	0.76
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.66	0.76
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.68	0.76
30:0:1625:U:H4'	42:0:5518:HOH:O	1.86	0.76
2:B:211:THR:HG23	30:0:2840:A:OP1	1.85	0.76
10:J:77:GLY:HA2	10:J:80:LYS:H	1.50	0.76
30:0:855:U:H3'	42:0:4506:HOH:O	1.85	0.76
5:E:15:GLN:HG2	5:E:19:ASP:O	1.85	0.76
30:0:542:A:H5'	30:0:542:A:C8	2.18	0.75
30:0:1119:G:N2	30:0:1246:A:C2	2.54	0.75
30:0:1189:A:H3'	42:0:9461:HOH:O	1.84	0.75
1:A:199:HIS:CD2	1:A:201:PHE:H	2.04	0.75
3:C:236:THR:HG21	42:C:8573:HOH:O	1.85	0.75
10:J:46:ILE:HD11	10:J:53:ILE:HG21	1.67	0.75
8:H:49:GLN:HE21	8:H:140:TYR:HE2	1.35	0.75
30:0:1058:A:H2'	30:0:1060:C:H5''	1.68	0.75
30:0:1666:C:H2'	30:0:1667:A:H5'	1.69	0.75
2:B:267:LYS:HD3	42:0:3471:HOH:O	1.86	0.75
16:P:121:ASP:O	16:P:125:LYS:HG3	1.87	0.75
20:T:9:LYS:HE3	20:T:13:ARG:CZ	2.16	0.75
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.69	0.75
22:V:1:THR:HB	30:0:93:C:H5''	1.67	0.75
23:W:88:THR:HB	42:W:6679:HOH:O	1.85	0.75
24:X:25:ARG:HD3	24:X:64:ALA:O	1.87	0.75
11:K:39:GLY:HA2	42:K:4183:HOH:O	1.85	0.74
22:V:12:THR:HG22	22:V:15:GLU:CG	2.16	0.74
9:I:127:CYS:HB3	9:I:132:VAL:HB	1.69	0.74
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.27	0.74
8:H:23:ILE:HG23	8:H:123:ILE:HD11	1.69	0.74
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.67	0.74
31:9:59:C:H2'	31:9:60:C:C6	2.22	0.74
2:B:62:ARG:HA	2:B:65:MET:CE	2.17	0.74
8:H:30:LYS:N	8:H:62:HIS:HD2	1.83	0.74
27:1:1:THR:HA	42:0:3266:HOH:O	1.86	0.74
30:0:2291:A:C8	30:0:2309:C:H5'	2.23	0.74
30:0:1118:A:C8	30:0:1118:A:H3'	2.22	0.74
6:F:46:GLU:OE2	6:F:100:ASP:HA	1.87	0.74
30:0:1118:A:H3'	30:0:1118:A:H8	1.53	0.74
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.69	0.73
2:B:88:GLU:HB3	2:B:97:LEU:HD12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:MET:HG3	2:B:310:ARG:HH11	1.53	0.73
30:0:823:U:H3'	42:0:5309:HOH:O	1.88	0.73
14:N:110:THR:HB	14:N:113:SER:OG	1.88	0.73
21:U:52:THR:HG22	21:U:54:THR:H	1.52	0.73
30:0:1615:A:H5'	42:0:5048:HOH:O	1.87	0.73
22:V:56:ILE:HG22	22:V:60:GLN:HE21	1.53	0.73
30:0:1205:U:H2'	30:0:1206:U:H5''	1.70	0.73
30:0:1160:G:H5'	30:0:1161:A:C5'	2.17	0.73
5:E:84:MET:HE1	5:E:148:ILE:CD1	2.19	0.73
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.19	0.73
30:0:1838:U:O2'	30:0:2644:C:H5'	1.89	0.73
7:G:27:ILE:HD13	7:G:71:LEU:HD23	1.71	0.72
21:U:9:CYS:HA	21:U:52:THR:HG23	1.71	0.72
30:0:2420:G:O2'	30:0:2421:G:H5'	1.89	0.72
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.70	0.72
24:X:49:ARG:HG3	24:X:49:ARG:O	1.88	0.72
1:A:179:MET:HA	1:A:179:MET:HE3	1.70	0.72
3:C:5:ILE:HD11	3:C:16:VAL:HG22	1.71	0.72
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.19	0.72
30:0:1116:U:O2'	30:0:1118:A:H2	1.68	0.72
30:0:1887:U:H5	42:0:7407:HOH:O	1.72	0.72
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.72	0.72
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.72	0.71
4:D:25:MET:CE	4:D:37:ALA:HB1	2.21	0.71
26:Z:54:GLU:HA	26:Z:57:MET:HE2	1.71	0.71
13:M:58:GLN:HG3	42:M:8912:HOH:O	1.90	0.71
15:O:32:ARG:O	15:O:32:ARG:HD3	1.89	0.71
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.72	0.71
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.20	0.71
28:2:41:HIS:N	28:2:45:ASN:HD22	1.84	0.71
30:0:2637:A:H4'	30:0:2638:G:H5'	1.72	0.71
31:9:29:C:H2'	31:9:30:C:H5'	1.71	0.71
15:O:21:SER:OG	15:O:106:PRO:HB2	1.90	0.71
18:R:128:ARG:NH2	30:0:2054:A:N3	2.38	0.71
30:0:1166:A:H1'	30:0:1192:A:C2	2.26	0.71
31:9:75:G:H1	31:9:106:U:H3	1.39	0.71
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.72	0.71
30:0:1701:A:H2'	42:0:6861:HOH:O	1.91	0.71
30:0:2748:G:H2'	42:0:9326:HOH:O	1.90	0.71
12:L:6:ARG:HD3	30:0:1299:G:O6	1.91	0.71
1:A:199:HIS:HD2	1:A:201:PHE:H	1.37	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:32:ARG:NE	15:O:35:LYS:HD2	2.05	0.70
17:Q:38:LYS:HE2	17:Q:62:THR:OG1	1.92	0.70
30:0:1206:U:H5'	30:0:1206:U:H6	1.55	0.70
32:5:74:C:H2'	32:5:75:C:H5'	1.71	0.70
3:C:104:ASP:O	3:C:108:GLN:HG3	1.91	0.70
4:D:170:TYR:O	4:D:171:ASP:HB3	1.91	0.70
12:L:90:ARG:HA	12:L:119:THR:HB	1.73	0.70
14:N:80:SER:HB2	42:N:8836:HOH:O	1.91	0.70
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.27	0.70
12:L:80:ASP:HB2	12:L:90:ARG:O	1.92	0.70
22:V:39:ALA:N	22:V:40:PRO:HD2	2.06	0.70
4:D:25:MET:HE2	4:D:41:LEU:CG	2.17	0.70
12:L:18:HIS:HD2	30:0:902:G:N7	1.90	0.70
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.56	0.70
6:F:14:ASP:O	6:F:18:GLU:HG3	1.92	0.70
13:M:164:THR:HG22	13:M:166:ALA:N	2.05	0.70
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.74	0.69
30:0:2769:C:H2'	30:0:2770:G:O4'	1.92	0.69
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.05	0.69
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.08	0.69
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.72	0.69
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.90	0.69
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.07	0.69
30:0:271:C:H41	30:0:378:A:H2	1.38	0.69
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.74	0.69
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.73	0.69
42:M:8875:HOH:O	30:0:381:G:H5''	1.92	0.69
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.74	0.69
18:R:18:LEU:HD12	18:R:143:VAL:HG11	1.74	0.69
22:V:1:THR:HG23	22:V:2:VAL:N	2.04	0.69
3:C:2:GLN:HB3	42:C:8583:HOH:O	1.92	0.69
3:C:65:ARG:HG3	3:C:67:GLN:HB2	1.74	0.69
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.73	0.69
3:C:103:ASN:ND2	30:0:663:C:H5''	2.08	0.69
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.57	0.69
22:V:44:GLY:HA3	30:0:92:G:H4'	1.74	0.69
30:0:1206:U:H2'	30:0:1207:A:O4'	1.93	0.69
2:B:27:ASN:HD21	30:0:2807:U:P	2.16	0.69
30:0:1159:G:H21	30:0:1189:A:H8	1.40	0.69
2:B:36:PRO:HG3	2:B:169:GLY:N	2.06	0.69
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.41	0.68
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.58	0.68
23:W:122:ARG:HG3	23:W:122:ARG:HH11	1.57	0.68
30:0:2491:G:H1'	42:0:7670:HOH:O	1.93	0.68
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.41	0.68
5:E:93:MET:HE1	5:E:165:GLY:N	2.08	0.68
20:T:50:VAL:HG12	20:T:56:ALA:HA	1.75	0.68
30:0:1183:C:N4	30:0:1184:C:H41	1.90	0.68
30:0:1634:G:H3'	42:0:4762:HOH:O	1.92	0.68
4:D:172:VAL:HG12	4:D:173:GLU:N	2.08	0.68
11:K:28:GLU:HB3	11:K:59:LYS:HB2	1.75	0.68
30:0:871:G:H8	30:0:871:G:C5'	2.03	0.68
30:0:2533:C:H5'	30:0:2533:C:H6	1.58	0.68
1:A:33:GLU:O	1:A:34:ASP:HB2	1.94	0.68
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.76	0.68
26:Z:46:SER:O	26:Z:50:VAL:HG23	1.93	0.68
30:0:1730:G:H5'	30:0:1731:C:C5	2.28	0.68
2:B:56:ASP:OD1	2:B:322:ARG:HB3	1.94	0.68
11:K:87:ARG:HB2	21:U:19:THR:HG23	1.76	0.68
23:W:106:THR:OG1	23:W:109:GLU:HG3	1.93	0.68
28:2:20:ARG:HG2	42:2:5444:HOH:O	1.93	0.68
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.28	0.68
10:J:46:ILE:HD11	10:J:53:ILE:CG2	2.22	0.68
13:M:9:ARG:HD2	30:0:380:A:OP2	1.94	0.68
14:N:152:GLU:C	14:N:154:LEU:H	2.02	0.68
8:H:102:LYS:HD3	8:H:122:LYS:HD3	1.76	0.67
15:O:59:VAL:HG23	15:O:111:VAL:HG21	1.75	0.67
26:Z:44:ARG:HH21	30:0:1771:U:H5'	1.59	0.67
27:1:9:GLY:HA2	30:0:1687:C:O2	1.95	0.67
29:3:73:GLU:HB3	42:3:9053:HOH:O	1.94	0.67
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.24	0.67
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.76	0.67
30:0:545:G:H5'	30:0:545:G:C8	2.26	0.67
14:N:147:ILE:HD12	42:9:9090:HOH:O	1.93	0.67
30:0:2505:G:O2'	30:0:2506:A:H5'	1.95	0.67
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.75	0.67
11:K:81:ARG:HB2	11:K:87:ARG:HH11	1.59	0.67
30:0:1474:C:H5'	30:0:1474:C:C6	2.29	0.67
42:0:7596:HOH:O	32:5:76:A:C2	2.47	0.67
25:Y:212:ARG:HD2	42:Y:8911:HOH:O	1.95	0.67
3:C:77:ALA:C	3:C:78:ARG:CA	2.68	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.10	0.67
30:0:2502:C:H2'	30:0:2503:A:H5'	1.76	0.67
30:0:2851:G:O2'	30:0:2852:A:H5'	1.94	0.67
22:V:1:THR:HG23	22:V:2:VAL:HG23	1.76	0.67
4:D:57:THR:HA	42:D:5728:HOH:O	1.94	0.66
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.75	0.66
9:I:101:LYS:O	9:I:105:GLU:HG3	1.96	0.66
10:J:131:THR:HG22	10:J:134:GLU:H	1.60	0.66
19:S:51:GLN:HE21	19:S:53:ASN:HD21	1.43	0.66
23:W:149:LEU:CG	23:W:153:MET:HE2	2.24	0.66
30:0:2766:A:H5'	42:0:3471:HOH:O	1.94	0.66
3:C:78:ARG:HH11	3:C:78:ARG:HG3	1.60	0.66
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.76	0.66
20:T:49:GLU:OE2	20:T:97:ARG:HD2	1.95	0.66
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.78	0.66
21:U:11:THR:HG22	21:U:53:ASP:CG	2.21	0.66
5:E:93:MET:HE1	5:E:165:GLY:H	1.59	0.66
30:0:1878:G:HO2'	30:0:1879:U:H6	1.43	0.66
30:0:2320:U:H4'	30:0:2321:A:O4'	1.96	0.66
32:5:76:A:C5'	32:5:76:A:C8	2.79	0.66
14:N:37:ARG:NH1	31:9:6:C:OP1	2.28	0.66
18:R:39:THR:HB	18:R:42:GLU:HG3	1.76	0.66
25:Y:235:GLU:CD	25:Y:235:GLU:N	2.48	0.66
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.14	0.65
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.96	0.65
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.61	0.65
6:F:96:ALA:HA	42:F:3111:HOH:O	1.95	0.65
16:P:77:ALA:O	16:P:78:GLY:CA	2.44	0.65
31:9:78:G:N1	31:9:78:G:N7	2.43	0.65
22:V:12:THR:CG2	22:V:15:GLU:HG3	2.24	0.65
27:1:16:HIS:HE1	30:0:775:G:OP1	1.79	0.65
30:0:544:G:H2'	30:0:545:G:H5''	1.78	0.65
31:9:14:G:H5'	31:9:14:G:H8	1.61	0.65
15:O:3:THR:HB	30:0:656:G:H5'	1.76	0.65
30:0:1175:G:H1'	30:0:1193:A:H2'	1.78	0.65
18:R:114:VAL:HA	18:R:144:GLU:O	1.97	0.65
22:V:50:ARG:NH1	30:0:56:G:H5''	2.12	0.65
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.22	0.65
16:P:14:LEU:O	16:P:16:VAL:HG23	1.96	0.65
16:P:74:GLN:HG2	30:0:1786:C:OP1	1.97	0.65
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:39:VAL:HG13	10:J:106:GLY:O	1.97	0.65
18:R:99:ALA:CB	18:R:109:MET:HE1	2.16	0.65
31:9:76:G:C3'	31:9:77:A:H5''	2.20	0.65
1:A:153:ARG:HB2	1:A:153:ARG:NH1	2.06	0.65
14:N:77:ASN:C	14:N:80:SER:HB3	2.22	0.65
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.12	0.65
2:B:150:ALA:O	2:B:152:PRO:HD3	1.96	0.64
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.32	0.64
21:U:52:THR:HG22	21:U:54:THR:N	2.12	0.64
25:Y:116:LEU:HD12	25:Y:173:ALA:HB3	1.77	0.64
10:J:74:ARG:HH11	10:J:74:ARG:HB3	1.61	0.64
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.94	0.64
25:Y:154:ARG:NH1	25:Y:155:ARG:HG3	2.12	0.64
25:Y:154:ARG:HH12	25:Y:155:ARG:HG3	1.62	0.64
25:Y:174:VAL:HG13	25:Y:177:LYS:HD2	1.79	0.64
28:2:41:HIS:HD2	28:2:44:ARG:H	1.43	0.64
30:0:558:C:C2'	30:0:559:U:H5''	2.28	0.64
30:0:2578:G:H5'	30:0:2578:G:H8	1.63	0.64
31:9:73:A:H61	31:9:108:C:H42	1.45	0.64
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.78	0.64
1:A:163:GLY:HA2	1:A:166:ASP:OD2	1.96	0.64
2:B:185:GLY:HA2	42:B:9117:HOH:O	1.97	0.64
2:B:229:ARG:NH2	30:0:1753:C:O2	2.30	0.64
5:E:7:ILE:HG22	5:E:45:ASP:O	1.97	0.64
30:0:256:C:H2'	30:0:257:G:O4'	1.98	0.64
23:W:65:VAL:HA	23:W:68:THR:HG22	1.80	0.64
6:F:12:LEU:HD21	6:F:111:ILE:HG23	1.80	0.64
10:J:95:ARG:O	10:J:99:GLU:HG3	1.97	0.64
11:K:10:GLN:HE21	11:K:10:GLN:N	1.92	0.64
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.27	0.64
18:R:21:ARG:HB2	18:R:23:MET:HE2	1.80	0.64
28:2:36:ASN:HB3	28:2:39:ARG:HG3	1.79	0.64
3:C:184:ARG:NH2	30:0:450:C:OP1	2.30	0.64
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.80	0.64
23:W:110:GLN:HA	23:W:110:GLN:NE2	2.13	0.64
30:0:2851:G:C2'	30:0:2852:A:H5'	2.28	0.64
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.77	0.64
20:T:26:THR:HA	20:T:39:ASN:HB3	1.79	0.64
30:0:2073:G:OP2	30:0:2490:A:H5'	1.98	0.64
1:A:66:ARG:HH11	1:A:66:ARG:HB2	1.62	0.64
5:E:69:ILE:HA	5:E:72:MET:HE3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:88:GLN:HE22	30:0:1799:G:H21	1.45	0.64
9:I:129:SER:O	9:I:130:LEU:HD23	1.97	0.64
20:T:77:VAL:HG11	20:T:91:LEU:HD11	1.79	0.64
24:X:43:VAL:HG12	24:X:44:ASP:H	1.62	0.64
29:3:55:VAL:HG22	42:3:9004:HOH:O	1.97	0.64
30:0:1377:C:H5'	30:0:1377:C:C6	2.29	0.64
31:9:13:A:O2'	31:9:14:G:H5''	1.97	0.64
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.33	0.64
2:B:175:LEU:O	2:B:175:LEU:HD23	1.97	0.64
13:M:24:GLN:O	13:M:28:GLN:HG3	1.97	0.64
13:M:171:ARG:CD	30:0:156:C:H5''	2.26	0.64
31:9:50:G:H2'	31:9:51:A:C8	2.32	0.64
20:T:2:LYS:HG2	30:0:447:A:OP1	1.98	0.63
31:9:76:G:H3'	31:9:77:A:C5'	2.20	0.63
2:B:207:LYS:HG3	30:0:2717:C:OP1	1.98	0.63
14:N:36:ALA:HB1	14:N:118:ILE:HD12	1.81	0.63
20:T:54:ASP:OD2	30:0:316:A:H5'	1.97	0.63
20:T:71:VAL:HG11	20:T:90:PRO:CB	2.27	0.63
24:X:43:VAL:HG12	24:X:44:ASP:N	2.13	0.63
1:A:207:GLN:HA	42:A:9034:HOH:O	1.97	0.63
1:A:37:VAL:HG23	42:A:9070:HOH:O	1.98	0.63
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.81	0.63
23:W:21:LEU:HD22	23:W:26:ILE:HD13	1.81	0.63
27:1:25:LYS:O	27:1:25:LYS:HG2	1.99	0.63
30:0:1701:A:H4'	30:0:1702:U:C5'	2.29	0.63
30:0:2502:C:C2'	30:0:2503:A:H5'	2.29	0.63
32:5:76:A:H8	32:5:76:A:H5'	1.64	0.63
7:G:20:VAL:O	7:G:24:VAL:HG23	1.99	0.63
11:K:77:ARG:C	11:K:78:LYS:CA	2.72	0.63
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.34	0.63
31:9:24:U:H3'	31:9:25:G:H5'	1.80	0.63
5:E:23:GLU:HG2	5:E:28:SER:CB	2.28	0.63
12:L:35:ARG:C	12:L:35:ARG:HD3	2.24	0.63
23:W:39:ASP:OD1	23:W:42:ARG:NH2	2.32	0.63
31:9:56:A:C2'	31:9:57:A:H5''	2.28	0.63
5:E:84:MET:HE2	5:E:133:VAL:CG2	2.29	0.62
10:J:131:THR:HB	10:J:134:GLU:OE1	1.99	0.62
11:K:66:ARG:HH22	30:0:1994:A:P	2.22	0.62
32:5:76:A:C8	32:5:76:A:H5''	2.34	0.62
1:A:121:ALA:O	1:A:124:VAL:HG22	2.00	0.62
8:H:160:ILE:HD11	8:H:164:CYS:SG	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:57:THR:O	15:O:111:VAL:HG23	2.00	0.62
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.14	0.62
13:M:57:LYS:HE2	13:M:140:ALA:O	2.00	0.62
14:N:5:ARG:NH1	30:0:962:C:H1'	2.14	0.62
19:S:57:THR:HG22	19:S:58:MET:N	2.13	0.62
30:0:281:U:H2'	30:0:282:C:O4'	1.99	0.62
5:E:126:ILE:HB	5:E:131:LEU:HD23	1.80	0.62
14:N:164:ASP:OD1	14:N:167:ASP:HA	1.99	0.62
25:Y:165:GLU:HB3	42:0:7500:HOH:O	1.99	0.62
20:T:52:ARG:HD2	30:0:317:A:H5''	1.81	0.62
23:W:91:ASP:HB2	42:W:5425:HOH:O	1.99	0.62
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.14	0.62
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.82	0.62
22:V:1:THR:CG2	22:V:2:VAL:H	2.04	0.62
30:0:380:A:H2'	42:0:9029:HOH:O	1.98	0.62
1:A:88:ILE:O	1:A:88:ILE:HG22	1.98	0.62
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.99	0.62
14:N:169:PRO:O	14:N:172:PHE:HB3	2.00	0.62
30:0:2718:C:H6	30:0:2718:C:H5'	1.65	0.62
9:I:69:PRO:HA	30:0:1164:U:OP1	2.00	0.62
30:0:558:C:H2'	30:0:559:U:C5'	2.29	0.62
30:0:2896:A:H5''	42:0:6924:HOH:O	2.00	0.62
2:B:75:GLU:C	2:B:77:PRO:HD3	2.24	0.62
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.81	0.62
12:L:120:LEU:HD12	12:L:133:VAL:HG21	1.82	0.62
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.98	0.62
4:D:173:GLU:O	4:D:174:VAL:O	2.18	0.61
23:W:26:ILE:HB	42:W:5420:HOH:O	1.98	0.61
30:0:482:G:H4'	30:0:508:A:N1	2.15	0.61
1:A:107:ASN:OD1	1:A:120:ARG:HD2	2.00	0.61
8:H:168:VAL:HG13	42:H:9015:HOH:O	1.99	0.61
29:3:77:ALA:C	29:3:78:HIS:CA	2.73	0.61
30:0:2239:C:H2'	30:0:2240:U:H6	1.66	0.61
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.83	0.61
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.81	0.61
5:E:3:VAL:CG2	5:E:49:ILE:HB	2.31	0.61
30:0:2401:A:H2'	30:0:2402:A:C8	2.36	0.61
1:A:191:GLY:HA2	1:A:194:MET:CE	2.28	0.61
4:D:52:THR:HG21	30:0:2346:C:O2'	1.99	0.61
12:L:35:ARG:HB2	12:L:35:ARG:HH11	1.63	0.61
30:0:2472:C:O2'	30:0:2634:G:H4'	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:27:ARG:NH2	30:0:657:G:OP1	2.33	0.61
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.30	0.61
14:N:164:ASP:OD2	14:N:167:ASP:HA	2.01	0.61
17:Q:7:LEU:HD13	42:0:3528:HOH:O	2.01	0.61
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.81	0.61
24:X:80:GLU:HB3	42:X:5564:HOH:O	2.00	0.61
30:0:1666:C:O2'	30:0:1667:A:H5''	2.01	0.61
6:F:46:GLU:O	6:F:73:PRO:HD2	2.00	0.61
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.63	0.61
15:O:47:ARG:HH11	15:O:47:ARG:HG3	1.65	0.61
30:0:2795:C:O2'	30:0:2796:U:H5'	2.01	0.61
1:A:88:ILE:HD13	1:A:100:PRO:CD	2.29	0.61
1:A:211:LYS:O	30:0:1943:C:H4'	2.01	0.61
4:D:99:ASP:HB3	4:D:103:ASN:N	2.16	0.61
30:0:1184:C:H1'	42:0:9254:HOH:O	2.01	0.61
6:F:91:VAL:CG1	6:F:92:GLY:H	2.12	0.61
8:H:80:LEU:HD21	8:H:145:ASP:HB3	1.83	0.61
9:I:110:ASP:O	30:0:1163:G:H5'	2.01	0.61
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.48	0.61
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.83	0.61
20:T:41:ARG:HG2	20:T:41:ARG:HH11	1.64	0.61
30:0:272:A:H5'	30:0:273:G:OP2	2.00	0.61
30:0:1080:C:H4'	30:0:1081:A:OP1	1.99	0.61
30:0:2003:U:H4'	30:0:2004:U:H5	1.66	0.61
3:C:236:THR:H	3:C:239:ALA:HB3	1.65	0.60
5:E:7:ILE:HD11	5:E:11:VAL:HG12	1.83	0.60
30:0:1748:U:H4'	42:0:9307:HOH:O	2.00	0.60
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.83	0.60
8:H:49:GLN:NE2	8:H:140:TYR:HE2	1.97	0.60
17:Q:32:GLU:HA	17:Q:71:TYR:OH	2.01	0.60
30:0:1205:U:H2'	30:0:1206:U:C5'	2.31	0.60
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.84	0.60
10:J:107:ASN:ND2	10:J:109:TYR:H	1.99	0.60
13:M:77:HIS:C	13:M:78:LYS:CA	2.74	0.60
30:0:664:U:O4	30:0:681:G:H5''	2.01	0.60
3:C:81:PRO:HD3	42:0:4391:HOH:O	2.01	0.60
3:C:235:PHE:HE2	3:C:243:VAL:HG21	1.65	0.60
10:J:130:VAL:HG12	10:J:131:THR:H	1.65	0.60
16:P:91:LYS:O	16:P:95:GLU:HG3	2.01	0.60
16:P:115:SER:N	16:P:118:GLN:HE21	1.88	0.60
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2005:G:O2'	30:0:2008:U:OP2	2.18	0.60
4:D:135:VAL:HG21	4:D:139:TYR:CG	2.37	0.60
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.01	0.60
7:G:23:ILE:HD13	7:G:67:LEU:HD23	1.84	0.60
30:0:1165:G:H4'	30:0:1174:A:O2'	2.01	0.60
2:B:211:THR:HG21	42:0:9244:HOH:O	2.01	0.60
4:D:58:VAL:HG12	4:D:60:GLU:HG2	1.83	0.60
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.36	0.60
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.82	0.60
1:A:212:PRO:HB2	42:A:9038:HOH:O	2.02	0.60
19:S:52:VAL:HG22	19:S:66:VAL:HG22	1.84	0.60
28:2:41:HIS:CD2	28:2:44:ARG:H	2.19	0.60
30:0:2896:A:N3	30:0:2896:A:H2'	2.17	0.60
2:B:206:THR:HG21	30:0:2716:G:H5''	1.84	0.60
10:J:77:GLY:C	10:J:78:ILE:CA	2.75	0.60
21:U:49:LEU:HG	42:U:3805:HOH:O	2.02	0.60
1:A:36:ASP:OD2	1:A:85:SER:HB2	2.01	0.60
1:A:211:LYS:HB2	42:A:9094:HOH:O	2.01	0.60
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.83	0.60
13:M:41:GLU:O	13:M:42:ARG:HD3	2.02	0.60
14:N:40:ASN:ND2	31:9:28:U:H5''	2.17	0.60
30:0:65:C:O2'	30:0:66:G:H5'	2.01	0.60
30:0:1679:C:H5'	42:0:3233:HOH:O	2.02	0.60
30:0:2415:A:H2'	30:0:2416:G:H5'	1.84	0.60
1:A:48:ASP:HB3	42:A:9081:HOH:O	2.01	0.60
15:O:59:VAL:CG2	15:O:111:VAL:HG21	2.31	0.60
22:V:43:PRO:O	22:V:46:ILE:HG22	2.01	0.60
6:F:118:LEU:O	6:F:119:ARG:HB3	2.02	0.59
9:I:114:TYR:HE1	30:0:1186:C:H4'	1.67	0.59
30:0:544:G:C2'	30:0:545:G:H5''	2.31	0.59
30:0:1766:U:O2	30:0:1778:A:H5'	2.02	0.59
3:C:233:THR:HG22	3:C:234:VAL:N	2.16	0.59
19:S:37:VAL:O	19:S:41:VAL:HG23	2.03	0.59
30:0:1834:C:H2'	30:0:1840:A:N6	2.17	0.59
1:A:194:MET:HE3	1:A:199:HIS:HB2	1.85	0.59
28:2:41:HIS:HB3	28:2:44:ARG:HB2	1.83	0.59
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.21	0.59
25:Y:154:ARG:HH21	30:0:1293:U:H5'	1.67	0.59
25:Y:189:ASN:C	25:Y:189:ASN:HD22	2.09	0.59
30:0:2429:A:H5'	42:0:3404:HOH:O	2.02	0.59
31:9:39:U:HO2'	31:9:42:C:H5	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:GLN:O	30:0:2862:G:H4'	2.02	0.59
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.84	0.59
15:O:59:VAL:HG23	15:O:111:VAL:CG2	2.32	0.59
23:W:52:VAL:HG23	23:W:53:ALA:N	1.86	0.59
30:0:1180:U:H2'	30:0:1181:A:C8	2.37	0.59
2:B:177:HIS:O	2:B:181:ILE:HG13	2.03	0.59
5:E:145:ALA:HB1	5:E:168:ILE:CD1	2.32	0.59
9:I:107:LYS:HB3	9:I:110:ASP:HB2	1.83	0.59
12:L:4:LYS:HE2	30:0:645:U:OP2	2.02	0.59
16:P:55:LYS:HG2	16:P:56:GLY:N	2.17	0.59
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.33	0.59
30:0:2089:A:O2'	30:0:2090:G:H5'	2.02	0.59
12:L:143:THR:HG22	12:L:144:ASP:N	2.17	0.59
15:O:44:ASN:CG	15:O:67:SER:HB2	2.26	0.59
28:2:22:PRO:HG2	28:2:25:VAL:HG21	1.83	0.59
30:0:558:C:O2'	30:0:559:U:H5''	2.03	0.59
30:0:1632:A:H2'	30:0:1633:C:H5'	1.85	0.59
30:0:2827:A:H2'	30:0:2828:G:O4'	2.03	0.59
2:B:36:PRO:HB3	2:B:174:ARG:HB3	1.85	0.59
7:G:12:ILE:HG22	7:G:17:GLN:NE2	2.16	0.59
14:N:139:TRP:HA	14:N:139:TRP:HE3	1.68	0.59
18:R:117:HIS:HD2	30:0:20:G:H21	1.48	0.59
23:W:21:LEU:O	23:W:26:ILE:HG23	2.03	0.59
30:0:316:A:N3	30:0:336:G:O2'	2.34	0.59
30:0:459:A:H5''	42:0:2968:HOH:O	2.02	0.59
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.15	0.59
12:L:143:THR:HG22	12:L:145:LEU:H	1.68	0.59
28:2:10:ARG:NH2	30:0:121:U:OP2	2.35	0.59
30:0:1552:G:N2	30:0:1634:G:H1'	2.18	0.59
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.33	0.59
2:B:108:GLU:HB3	2:B:111:ARG:HD2	1.85	0.59
22:V:56:ILE:O	22:V:60:GLN:HG3	2.02	0.59
23:W:110:GLN:HA	23:W:110:GLN:HE21	1.67	0.59
2:B:144:THR:HB	42:B:9108:HOH:O	2.02	0.58
5:E:145:ALA:HB1	5:E:168:ILE:HD11	1.84	0.58
22:V:49:LEU:O	22:V:53:ILE:HG13	2.02	0.58
23:W:4:LEU:O	23:W:32:CYS:HA	2.03	0.58
30:0:1681:G:H5''	30:0:1682:A:H5'	1.84	0.58
30:0:2070:G:H5''	42:0:4653:HOH:O	2.03	0.58
1:A:201:PHE:HA	42:A:9062:HOH:O	2.03	0.58
6:F:37:THR:O	6:F:41:GLU:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:12:ILE:HG23	42:0:6294:HOH:O	2.02	0.58
14:N:86:LEU:O	14:N:90:LEU:HG	2.02	0.58
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.33	0.58
21:U:45:GLU:HB2	21:U:48:ASN:ND2	2.17	0.58
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	1.84	0.58
30:0:1116:U:O2'	30:0:1118:A:C2	2.49	0.58
30:0:1461:U:H2'	30:0:1462:C:C6	2.39	0.58
2:B:162:MET:CE	2:B:310:ARG:HD2	2.14	0.58
5:E:36:PRO:HD3	10:J:127:ILE:HD12	1.84	0.58
42:L:8846:HOH:O	30:0:2453:G:H5''	2.04	0.58
22:V:39:ALA:N	22:V:40:PRO:CD	2.66	0.58
2:B:297:VAL:HB	42:B:9083:HOH:O	2.03	0.58
5:E:31:ARG:NH1	5:E:68:HIS:CG	2.71	0.58
8:H:66:GLU:HA	42:H:9036:HOH:O	2.03	0.58
14:N:154:LEU:O	14:N:155:GLU:HB3	2.02	0.58
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.04	0.58
18:R:71:LYS:HE2	30:0:2831:C:O3'	2.03	0.58
19:S:29:ASP:OD1	19:S:31:ARG:HG3	2.04	0.58
20:T:53:GLY:HA3	42:0:7601:HOH:O	2.03	0.58
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.68	0.58
3:C:246:ARG:HB3	3:C:246:ARG:NH1	2.18	0.58
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.84	0.58
5:E:77:THR:C	5:E:78:GLU:CA	2.77	0.58
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.86	0.58
25:Y:184:GLU:OE1	25:Y:204:ARG:NH1	2.37	0.58
30:0:119:A:H2'	30:0:120:A:H5''	1.85	0.58
30:0:2419:U:H5''	30:0:2420:G:H5'	1.86	0.58
30:0:2626:C:H2'	30:0:2627:G:C8	2.39	0.58
2:B:53:LEU:HD21	2:B:270:ILE:HD12	1.85	0.58
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.39	0.58
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.37	0.58
17:Q:25:PRO:HB2	42:9:9081:HOH:O	2.03	0.58
23:W:130:HIS:O	23:W:136:GLY:HA3	2.03	0.58
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.38	0.58
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.18	0.58
30:0:1878:G:H1'	42:0:6945:HOH:O	2.03	0.58
30:0:2588:OMG:N2	42:0:7596:HOH:O	2.36	0.58
1:A:35:GLY:O	1:A:36:ASP:HB3	2.03	0.58
2:B:85:ARG:HB2	2:B:99:GLU:HG2	1.86	0.58
5:E:31:ARG:HH12	5:E:68:HIS:CG	2.21	0.58
12:L:73:VAL:HG23	12:L:74:THR:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:77:ALA:C	16:P:78:GLY:CA	2.76	0.58
19:S:10:VAL:HG11	22:V:36:ALA:HB2	1.84	0.58
19:S:22:ASN:ND2	19:S:68:LEU:HB2	2.18	0.58
25:Y:186:ARG:HG2	25:Y:186:ARG:HH11	1.68	0.58
30:0:951:A:C2'	30:0:952:G:H5'	2.34	0.58
3:C:174:ILE:CD1	30:0:338:C:H4'	2.34	0.58
4:D:152:PRO:HD2	31:9:57:A:O2'	2.04	0.58
9:I:121:LYS:HD3	30:0:1185:U:OP1	2.04	0.58
10:J:130:VAL:HG12	10:J:131:THR:N	2.18	0.58
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.03	0.58
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.86	0.58
30:0:1562:C:H42	30:0:2738:G:H1	1.52	0.58
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.84	0.58
23:W:88:THR:HG22	23:W:89:ASP:N	2.19	0.58
2:B:320:GLN:NE2	2:B:321:PRO:HD2	2.18	0.58
9:I:86:GLU:HB2	9:I:90:ASP:OD2	2.04	0.58
10:J:74:ARG:HH11	10:J:74:ARG:CG	2.16	0.58
29:3:70:ARG:HB3	42:3:9062:HOH:O	2.03	0.58
30:0:1333:U:H2'	30:0:1334:C:C6	2.39	0.58
30:0:1463:U:H2'	30:0:1464:C:C6	2.39	0.58
30:0:1973:A:H5'	30:0:1973:A:C8	2.37	0.58
30:0:2251:G:H2'	30:0:2252:A:C8	2.38	0.58
2:B:97:LEU:O	2:B:98:THR:HG23	2.04	0.57
2:B:139:ASP:OD2	2:B:165:ARG:HD2	2.04	0.57
4:D:25:MET:HE1	4:D:40:ILE:HD11	1.86	0.57
6:F:56:PRO:HB2	6:F:58:GLU:OE1	2.03	0.57
14:N:1:ALA:HB2	31:9:14:G:O2'	2.04	0.57
30:0:871:G:C8	30:0:871:G:C5'	2.80	0.57
2:B:238:ASN:HD22	2:B:240:GLY:N	1.96	0.57
2:B:254:GLN:HG2	2:B:255:GLY:N	2.17	0.57
6:F:26:THR:HG21	6:F:102:GLY:C	2.28	0.57
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.69	0.57
9:I:88:GLN:HA	9:I:91:PHE:HE2	1.69	0.57
26:Z:34:SER:OG	30:0:797:A:H4'	2.03	0.57
27:1:25:LYS:HD2	28:2:49:GLU:H	1.69	0.57
30:0:1700:C:H5''	30:0:1701:A:OP2	2.04	0.57
3:C:1:MET:HG2	3:C:2:GLN:N	2.15	0.57
3:C:236:THR:HA	42:C:8652:HOH:O	2.03	0.57
8:H:23:ILE:HG23	8:H:123:ILE:CD1	2.34	0.57
13:M:84:LYS:HG3	30:0:171:C:OP2	2.04	0.57
14:N:119:GLN:O	14:N:123:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:THR:HG21	42:O:5468:HOH:O	2.04	0.57
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.20	0.57
30:O:1182:C:H1'	30:O:1192:A:H8	1.67	0.57
30:O:2717:C:O2'	30:O:2718:C:H5''	2.04	0.57
10:J:4:ALA:O	10:J:5:GLU:HB2	2.02	0.57
10:J:54:VAL:O	10:J:58:GLU:HG3	2.05	0.57
14:N:37:ARG:NE	42:N:8833:HOH:O	2.37	0.57
18:R:77:ALA:O	18:R:78:GLY:CA	2.52	0.57
30:O:506:G:H22	30:O:509:A:H5''	1.69	0.57
21:U:50:GLU:HB3	30:O:2866:U:C4	2.40	0.57
30:O:282:C:O2'	30:O:283:U:H5'	2.04	0.57
4:D:167:GLU:C	4:D:169:THR:H	2.12	0.57
6:F:50:VAL:CG2	6:F:63:ILE:HG21	2.34	0.57
17:Q:77:ASP:C	17:Q:78:GLY:CA	2.77	0.57
18:R:39:THR:HB	18:R:42:GLU:CG	2.34	0.57
22:V:42:ASN:HB3	42:V:7247:HOH:O	2.05	0.57
30:O:946:C:H2'	30:O:947:U:C6	2.40	0.57
30:O:1189:A:H1'	30:O:1209:C:H1'	1.87	0.57
30:O:2064:U:H5'	30:O:2652:U:H4'	1.87	0.57
7:G:67:LEU:O	7:G:71:LEU:HG	2.05	0.57
10:J:52:GLN:HG3	10:J:53:ILE:N	2.17	0.57
14:N:86:LEU:HD21	14:N:180:LEU:CD1	2.35	0.57
30:O:292:G:H2'	30:O:358:G:N2	2.20	0.57
2:B:24:PRO:HG3	2:B:204:GLY:HA2	1.86	0.57
29:3:68:LYS:HE2	30:O:2436:U:H5'	1.86	0.57
30:O:78:G:N9	30:O:78:G:N3	2.52	0.57
30:O:241:A:C2	30:O:378:A:H4'	2.40	0.57
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.37	0.57
4:D:27:ILE:HD11	4:D:37:ALA:CB	2.35	0.57
4:D:131:THR:HG21	30:O:2348:C:H1'	1.87	0.57
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.19	0.57
14:N:32:PRO:HD2	14:N:99:GLU:O	2.05	0.57
15:O:77:ALA:C	15:O:78:ALA:CA	2.78	0.57
20:T:68:ASP:HB2	42:O:6493:HOH:O	2.04	0.57
21:U:14:GLU:OE1	21:U:15:PRO:HD2	2.04	0.57
23:W:151:GLU:O	23:W:154:ARG:HB2	2.05	0.57
26:Z:96:GLU:OE1	26:Z:101:LYS:HE2	2.03	0.57
30:O:699:C:H2'	30:O:744:G:O4'	2.05	0.57
30:O:820:G:H5'	30:O:821:U:H5'	1.86	0.57
30:O:1298:U:H2'	30:O:1299:G:C8	2.40	0.57
30:O:1299:G:H5'	42:O:4943:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1878:G:O2'	30:0:1879:U:H6	1.87	0.57
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.87	0.57
3:C:72:LYS:HG2	3:C:77:ALA:HA	1.85	0.57
18:R:39:THR:HB	18:R:42:GLU:CD	2.30	0.57
18:R:77:ALA:C	18:R:78:GLY:CA	2.78	0.57
25:Y:112:GLU:CD	25:Y:115:ARG:NH1	2.63	0.57
30:0:2361:A:H5'	30:0:2361:A:H8	1.70	0.57
13:M:188:ARG:HD3	30:0:155:C:OP2	2.05	0.56
19:S:33:SER:O	19:S:37:VAL:HG23	2.04	0.56
31:9:20:G:O2'	31:9:21:G:H5'	2.04	0.56
2:B:36:PRO:CG	2:B:169:GLY:H	2.09	0.56
2:B:141:ARG:HG2	2:B:165:ARG:HA	1.87	0.56
30:0:558:C:H2'	30:0:559:U:H5'	1.86	0.56
30:0:2090:G:H2'	30:0:2091:G:C8	2.40	0.56
2:B:175:LEU:HD23	2:B:175:LEU:C	2.29	0.56
4:D:64:ARG:NE	4:D:67:ASP:HB3	2.20	0.56
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.05	0.56
8:H:170:ARG:HD2	42:H:8991:HOH:O	2.04	0.56
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.06	0.56
22:V:12:THR:HG22	22:V:15:GLU:OE2	2.05	0.56
42:Z:8705:HOH:O	30:0:1886:A:H4'	2.06	0.56
31:9:92:G:H2'	31:9:93:A:C8	2.40	0.56
1:A:36:ASP:O	1:A:38:ILE:N	2.31	0.56
14:N:82:TYR:OH	14:N:176:ARG:NH1	2.39	0.56
20:T:76:ASP:C	20:T:78:THR:HG23	2.31	0.56
1:A:26:ASP:O	1:A:28:GLU:N	2.38	0.56
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.06	0.56
12:L:149:ARG:O	12:L:150:GLN:HB2	2.05	0.56
16:P:1:THR:O	30:0:1396:C:H1'	2.04	0.56
23:W:84:VAL:HG12	42:W:6679:HOH:O	2.03	0.56
30:0:960:G:H3'	30:0:960:G:N3	2.20	0.56
30:0:2004:U:H4'	42:0:6144:HOH:O	2.04	0.56
42:0:6025:HOH:O	32:5:76:A:H1'	2.05	0.56
1:A:192:VAL:HB	42:A:9067:HOH:O	2.05	0.56
12:L:133:VAL:HA	42:L:8879:HOH:O	2.05	0.56
30:0:1555:G:H4'	30:0:1630:A:H2	1.70	0.56
30:0:2356:A:H2'	30:0:2357:G:O4'	2.06	0.56
1:A:51:ARG:NH1	1:A:120:ARG:O	2.39	0.56
1:A:80:LEU:HD22	1:A:91:GLY:O	2.06	0.56
1:A:82:VAL:HG13	1:A:93:THR:HB	1.88	0.56
2:B:16:ARG:NH1	42:B:9097:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:99:GLU:N	15:O:99:GLU:OE1	2.39	0.56
24:X:66:THR:HG23	24:X:67:PRO:HD2	1.87	0.56
27:1:46:ARG:HA	42:0:3910:HOH:O	2.05	0.56
30:0:1829:A:H2'	30:0:1830:C:H5'	1.88	0.56
30:0:2426:G:H1'	42:0:6917:HOH:O	2.06	0.56
1:A:194:MET:HE3	1:A:199:HIS:CB	2.36	0.56
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.21	0.56
2:B:62:ARG:CA	2:B:65:MET:HE3	2.33	0.56
4:D:23:VAL:HG22	4:D:73:VAL:HB	1.86	0.56
8:H:48:VAL:HA	8:H:170:ARG:O	2.05	0.56
11:K:81:ARG:HD3	11:K:87:ARG:NH1	2.20	0.56
18:R:114:VAL:HB	18:R:145:LEU:HD12	1.88	0.56
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.71	0.56
30:0:447:A:O2'	30:0:448:G:H5'	2.06	0.56
30:0:603:A:H5''	30:0:604:G:OP1	2.06	0.56
4:D:18:ILE:HG12	4:D:134:LEU:CD2	2.36	0.56
16:P:11:ALA:HB1	16:P:16:VAL:O	2.06	0.56
30:0:2611:G:H3'	42:0:3252:HOH:O	2.04	0.56
4:D:77:ASP:C	4:D:78:GLU:CA	2.79	0.56
5:E:84:MET:HG2	5:E:168:ILE:HD13	1.88	0.56
5:E:137:ASP:OD1	5:E:139:GLU:HB2	2.05	0.56
6:F:111:ILE:O	6:F:115:VAL:HG23	2.06	0.56
23:W:38:THR:HG22	23:W:39:ASP:N	2.20	0.56
23:W:88:THR:HG22	23:W:89:ASP:H	1.71	0.56
23:W:154:ARG:NH1	30:0:588:G:O6	2.38	0.56
30:0:69:A:H5'	30:0:69:A:C8	2.40	0.56
4:D:99:ASP:HA	42:D:5675:HOH:O	2.06	0.55
6:F:65:GLU:O	6:F:69:GLU:HG2	2.07	0.55
20:T:2:LYS:HE2	42:T:2822:HOH:O	2.06	0.55
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.88	0.55
29:3:3:MET:HG3	29:3:4:PRO:HD2	1.88	0.55
30:0:101:C:H2'	30:0:102:A:C8	2.41	0.55
30:0:1201:C:H5''	42:0:7053:HOH:O	2.05	0.55
10:J:76:ASP:HA	42:J:5907:HOH:O	2.05	0.55
23:W:41:TYR:HA	23:W:44:MET:HE3	1.88	0.55
30:0:1189:A:O2'	30:0:1208:C:H2'	2.05	0.55
30:0:1209:C:H2'	30:0:1210:G:H8	1.71	0.55
30:0:1314:U:H5''	30:0:1316:G:O4'	2.06	0.55
30:0:2252:A:H2'	30:0:2253:G:O4'	2.06	0.55
4:D:58:VAL:HB	4:D:62:ASP:HB3	1.88	0.55
9:I:89:GLU:OE2	30:0:1181:A:H5'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:77:GLY:C	26:Z:78:ILE:CA	2.79	0.55
1:A:88:ILE:CD1	1:A:100:PRO:HD3	2.29	0.55
1:A:89:ALA:O	1:A:92:ASN:HB2	2.07	0.55
8:H:69:ARG:HD3	42:H:9036:HOH:O	2.05	0.55
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.36	0.55
30:0:304:G:H1'	30:0:347:A:N6	2.20	0.55
30:0:1835:U:C5	30:0:1840:A:N7	2.69	0.55
30:0:2072:G:C6	30:0:2533:C:H1'	2.41	0.55
3:C:27:ARG:HH11	3:C:27:ARG:CG	2.20	0.55
5:E:101:GLU:HB3	5:E:117:THR:HA	1.89	0.55
9:I:97:VAL:O	9:I:101:LYS:HG3	2.07	0.55
18:R:44:VAL:O	18:R:48:GLU:HG3	2.07	0.55
23:W:122:ARG:NH1	23:W:152:ALA:O	2.39	0.55
30:0:280:C:H2'	30:0:281:U:O4'	2.06	0.55
30:0:1909:A:N1	30:0:2128:G:H1'	2.22	0.55
31:9:23:U:O2'	31:9:24:U:H4'	2.07	0.55
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.87	0.55
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.21	0.55
9:I:108:HIS:N	9:I:109:PRO:HD2	2.22	0.55
13:M:71:SER:O	13:M:73:ARG:NH1	2.38	0.55
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.06	0.55
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.41	0.55
2:B:139:ASP:HB2	2:B:165:ARG:HE	1.70	0.55
3:C:154:VAL:O	3:C:158:GLU:HG3	2.07	0.55
4:D:49:PRO:HB3	42:D:5828:HOH:O	2.07	0.55
14:N:74:PRO:HG2	14:N:159:TYR:CE1	2.41	0.55
2:B:279:THR:HG22	2:B:280:VAL:N	2.22	0.55
8:H:141:CYS:HB2	42:H:8995:HOH:O	2.06	0.55
30:0:737:A:H2'	30:0:738:G:O4'	2.06	0.55
30:0:1350:U:H4'	42:0:5964:HOH:O	2.06	0.55
30:0:2362:A:H2'	30:0:2363:G:C8	2.42	0.55
2:B:16:ARG:HD3	42:B:9088:HOH:O	2.06	0.55
15:O:98:LEU:O	15:O:102:ILE:HG13	2.07	0.55
19:S:73:ASP:OD1	19:S:76:GLU:HG3	2.06	0.55
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.06	0.55
27:1:28:HIS:HE1	30:0:776:A:OP1	1.90	0.55
30:0:2103:A:O2'	30:0:2104:C:H5'	2.06	0.55
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.35	0.55
2:B:102:THR:HG21	2:B:182:VAL:O	2.06	0.55
3:C:168:ARG:NH2	3:C:190:ALA:O	2.40	0.55
30:0:1730:G:H5'	30:0:1731:C:H5	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2032:U:O2'	30:0:2033:G:H5''	2.06	0.55
1:A:36:ASP:C	1:A:38:ILE:H	2.13	0.54
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.89	0.54
30:0:1118:A:C8	30:0:1118:A:C3'	2.86	0.54
30:0:1309:U:O2'	30:0:1310:U:H5'	2.07	0.54
30:0:2531:U:O2'	30:0:2532:A:H5'	2.06	0.54
1:A:165:THR:HG22	42:A:9093:HOH:O	2.07	0.54
2:B:85:ARG:NH1	42:B:9118:HOH:O	2.39	0.54
2:B:232:TRP:CD1	2:B:235:ARG:HD2	2.43	0.54
5:E:152:THR:HG21	5:E:165:GLY:HA2	1.89	0.54
7:G:16:LYS:O	7:G:20:VAL:HG23	2.07	0.54
12:L:79:ASP:HB3	42:L:8862:HOH:O	2.06	0.54
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.88	0.54
19:S:43:GLU:HB3	42:S:7106:HOH:O	2.08	0.54
2:B:14:GLY:HA2	2:B:15:PRO:C	2.32	0.54
5:E:119:HIS:HE1	5:E:147:ASP:OD2	1.90	0.54
5:E:131:LEU:HD12	5:E:166:VAL:HG11	1.90	0.54
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.08	0.54
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.73	0.54
15:O:25:VAL:HG12	30:0:709:G:O2'	2.07	0.54
20:T:1:SER:HB2	30:0:447:A:P	2.47	0.54
20:T:32:ARG:NH1	20:T:38:ARG:HH12	2.04	0.54
20:T:38:ARG:NH1	42:T:6217:HOH:O	2.41	0.54
24:X:47:ALA:HB1	24:X:82:GLU:CB	2.37	0.54
30:0:1205:U:C2'	30:0:1206:U:H5''	2.36	0.54
31:9:1:U:H5'	31:9:121:C:O2	2.07	0.54
31:9:14:G:H5'	31:9:14:G:C8	2.42	0.54
31:9:39:U:H3'	31:9:40:C:H5''	1.88	0.54
2:B:2:GLN:NE2	30:0:2545:U:OP2	2.40	0.54
3:C:43:LYS:HG2	30:0:449:A:N7	2.22	0.54
12:L:39:GLU:OE2	30:0:926:A:H5'	2.08	0.54
26:Z:51:ALA:HA	42:Z:8712:HOH:O	2.08	0.54
30:0:1189:A:H1'	30:0:1209:C:C1'	2.37	0.54
2:B:145:HIS:HD2	2:B:159:PRO:HB3	1.72	0.54
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.73	0.54
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.08	0.54
13:M:178:LYS:HB2	42:0:7676:HOH:O	2.07	0.54
20:T:23:VAL:HG23	20:T:41:ARG:HG3	1.90	0.54
25:Y:148:GLY:O	25:Y:154:ARG:HD3	2.06	0.54
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	1.90	0.54
26:Z:54:GLU:HB2	42:Z:8712:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:136:C:H2'	30:0:137:U:O4'	2.08	0.54
30:0:151:A:H2'	30:0:152:A:O4'	2.08	0.54
30:0:602:A:O2'	30:0:605:C:H4'	2.06	0.54
30:0:1218:U:H2'	30:0:1219:U:C6	2.42	0.54
30:0:2324:G:N2	30:0:2377:U:H1'	2.22	0.54
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.89	0.54
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.42	0.54
13:M:164:THR:CG2	13:M:165:GLY:N	2.70	0.54
13:M:171:ARG:NH2	30:0:189:A:OP1	2.39	0.54
22:V:7:GLU:O	22:V:11:MET:HG3	2.08	0.54
30:0:138:U:H5''	30:0:139:C:OP2	2.07	0.54
30:0:1592:G:H2'	30:0:1593:C:C6	2.42	0.54
30:0:1730:G:C5'	30:0:1731:C:C6	2.90	0.54
30:0:2894:C:O2'	30:0:2895:C:H5'	2.07	0.54
1:A:8:ARG:HG2	42:A:9029:HOH:O	2.07	0.54
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.90	0.54
2:B:162:MET:HE3	2:B:310:ARG:HH11	1.72	0.54
8:H:20:ARG:HD3	8:H:26:ILE:HD12	1.90	0.54
11:K:87:ARG:NH2	30:0:2720:C:O2	2.41	0.54
12:L:50:GLY:C	30:0:2453:G:H4'	2.32	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.07	0.54
23:W:48:VAL:O	23:W:48:VAL:HG12	2.07	0.54
23:W:78:ASP:HB2	42:W:6694:HOH:O	2.07	0.54
30:0:137:U:H2'	30:0:139:C:C5	2.41	0.54
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.08	0.54
4:D:135:VAL:HG22	4:D:136:ARG:N	2.23	0.54
7:G:64:ASN:O	7:G:68:GLU:HG3	2.07	0.54
10:J:107:ASN:C	10:J:107:ASN:HD22	2.16	0.54
15:O:39:THR:O	15:O:115:ARG:NH2	2.41	0.54
15:O:96:VAL:CG1	15:O:100:GLN:HB2	2.38	0.54
27:1:25:LYS:HE2	42:1:7213:HOH:O	2.07	0.54
1:A:65:ARG:C	1:A:66:ARG:HG3	2.32	0.54
2:B:243:ASN:HA	2:B:244:PRO:C	2.32	0.54
9:I:111:LEU:HD22	9:I:122:GLU:OE1	2.07	0.54
20:T:43:ASN:C	20:T:45:GLY:H	2.16	0.54
27:1:9:GLY:HA3	30:0:1695:G:H1'	1.90	0.54
30:0:185:G:H4'	30:0:186:A:H4'	1.89	0.54
30:0:1342:C:C2'	30:0:1343:C:H5'	2.37	0.54
30:0:2265:U:H2'	30:0:2266:A:C8	2.42	0.54
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.44	0.54
8:H:31:ILE:HA	8:H:66:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:145:LEU:HD23	12:L:145:LEU:O	2.08	0.54
14:N:115:VAL:HG22	42:N:8857:HOH:O	2.08	0.54
15:O:25:VAL:HG23	15:O:26:TRP:N	2.22	0.54
21:U:52:THR:CG2	21:U:54:THR:HB	2.38	0.54
23:W:23:MET:HE1	30:O:944:G:C8	2.44	0.54
25:Y:117:LEU:HD13	25:Y:174:VAL:HG11	1.90	0.54
30:O:1406:A:H4'	30:O:1407:A:H5''	1.89	0.54
30:O:1559:A:H1'	42:O:6694:HOH:O	2.07	0.54
3:C:157:LEU:HD13	3:C:166:ILE:HD11	1.90	0.53
8:H:61:ARG:HG3	8:H:61:ARG:NH1	2.22	0.53
30:O:612:U:H2'	30:O:613:C:C6	2.44	0.53
30:O:1132:A:N6	30:O:1229:C:H2'	2.23	0.53
31:9:2:U:OP2	31:9:3:A:H5'	2.08	0.53
1:A:94:LEU:HD21	1:A:156:ILE:HD11	1.90	0.53
12:L:91:VAL:CG1	12:L:120:LEU:HD23	2.38	0.53
13:M:30:GLU:O	13:M:34:GLU:HG3	2.08	0.53
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.08	0.53
13:M:179:GLY:O	30:O:399:C:H5'	2.08	0.53
14:N:62:HIS:HB3	14:N:65:ASP:OD1	2.08	0.53
22:V:5:VAL:HG12	22:V:9:ARG:NH1	2.23	0.53
30:O:2372:A:H2'	30:O:2373:U:C6	2.43	0.53
3:C:20:ASP:O	3:C:23:GLU:HB2	2.08	0.53
30:O:834:G:H3'	30:O:835:U:H4'	1.90	0.53
30:O:920:C:H4'	30:O:921:G:C2	2.44	0.53
31:9:57:A:H2'	31:9:58:G:H5'	1.89	0.53
3:C:140:VAL:HB	42:C:8652:HOH:O	2.08	0.53
4:D:18:ILE:HG12	4:D:134:LEU:HD23	1.91	0.53
4:D:50:VAL:O	4:D:71:ALA:HA	2.07	0.53
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.89	0.53
5:E:81:GLU:O	5:E:172:PRO:HD3	2.09	0.53
14:N:37:ARG:NH1	31:9:6:C:C5'	2.59	0.53
23:W:41:TYR:O	23:W:45:VAL:HG22	2.08	0.53
29:3:73:GLU:HB2	42:3:9021:HOH:O	2.09	0.53
30:O:1278:A:H4'	30:O:1279:U:C4	2.43	0.53
30:O:2047:C:H5'	42:O:3721:HOH:O	2.07	0.53
30:O:2748:G:C5'	42:O:9326:HOH:O	2.57	0.53
30:O:2878:U:H2'	30:O:2879:A:O4'	2.09	0.53
1:A:4:ILE:HG22	1:A:198:ASP:O	2.09	0.53
4:D:60:GLU:O	4:D:61:PHE:C	2.51	0.53
8:H:77:ILE:C	8:H:78:LYS:CA	2.81	0.53
29:3:3:MET:O	29:3:90:PHE:HA	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:204:A:C2'	30:0:205:U:H5'	2.37	0.53
30:0:1527:A:H1'	30:0:1528:A:C8	2.43	0.53
30:0:1878:G:O2'	30:0:1879:U:P	2.67	0.53
4:D:27:ILE:HD11	4:D:37:ALA:HB3	1.90	0.53
5:E:144:THR:O	5:E:148:ILE:HG13	2.08	0.53
19:S:55:GLN:HE22	30:0:1446:U:H2'	1.72	0.53
19:S:77:VAL:C	19:S:78:ALA:CA	2.81	0.53
30:0:1528:A:H2'	30:0:1529:G:O4'	2.08	0.53
30:0:2239:C:H2'	30:0:2240:U:C6	2.44	0.53
9:I:124:VAL:O	9:I:124:VAL:HG12	2.09	0.53
30:0:1042:U:O2'	30:0:1043:C:H5'	2.08	0.53
30:0:2351:C:H2'	30:0:2352:G:O4'	2.08	0.53
30:0:2453:G:H5'	42:0:5543:HOH:O	2.08	0.53
30:0:2728:C:H4'	30:0:2894:C:HO2'	1.74	0.53
30:0:2824:C:O3'	30:0:2825:C:H6	1.91	0.53
9:I:94:ASP:OD1	9:I:133:THR:HB	2.08	0.53
28:2:20:ARG:HG3	28:2:21:VAL:N	2.24	0.53
30:0:95:A:H5''	30:0:97:G:O4'	2.09	0.53
30:0:790:A:H1'	30:0:1710:A:H2'	1.91	0.53
30:0:1666:C:H2'	30:0:1667:A:C5'	2.38	0.53
30:0:1714:C:O2'	30:0:1715:C:H5'	2.09	0.53
30:0:1730:G:H5''	30:0:1731:C:H6	1.74	0.53
30:0:2266:A:H2'	30:0:2267:G:C8	2.44	0.53
30:0:2583:A:H3'	42:0:5454:HOH:O	2.08	0.53
30:0:2755:G:H1'	42:0:5534:HOH:O	2.09	0.53
1:A:186:TRP:CG	1:A:187:PRO:HA	2.43	0.53
6:F:4:VAL:HG13	6:F:76:PHE:CE1	2.44	0.53
10:J:71:TYR:CD1	10:J:72:PRO:HD2	2.44	0.53
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.43	0.53
30:0:192:A:H5'	42:0:9428:HOH:O	2.08	0.53
30:0:2551:C:O2'	30:0:2552:C:H5'	2.08	0.53
2:B:212:GLN:HA	30:0:1733:A:H4'	1.90	0.53
4:D:143:LYS:O	31:9:45:A:H4'	2.09	0.53
12:L:90:ARG:NH2	12:L:121:ILE:HD11	2.24	0.53
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.28	0.53
30:0:969:G:H1	30:0:999:C:N4	2.03	0.53
30:0:1878:G:O2'	30:0:1879:U:C6	2.57	0.53
2:B:277:GLU:N	2:B:278:PRO:HD2	2.23	0.52
3:C:236:THR:HG22	3:C:239:ALA:CB	2.40	0.52
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.73	0.52
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:74:ARG:NH1	10:J:76:ASP:OD2	2.41	0.52
11:K:30:LYS:O	11:K:55:VAL:HG13	2.09	0.52
19:S:67:ARG:HD3	42:S:3430:HOH:O	2.08	0.52
30:0:2314:G:C2'	30:0:2315:C:H5'	2.39	0.52
2:B:51:VAL:HG22	2:B:327:VAL:HG13	1.92	0.52
42:C:8658:HOH:O	30:0:656:G:H1'	2.10	0.52
4:D:53:LYS:O	4:D:54:ALA:HB2	2.08	0.52
12:L:71:GLU:HG2	30:0:700:A:C2	2.45	0.52
14:N:162:ASP:HA	42:N:8830:HOH:O	2.08	0.52
21:U:45:GLU:HB2	21:U:48:ASN:HD22	1.73	0.52
25:Y:154:ARG:HH12	25:Y:155:ARG:CG	2.22	0.52
25:Y:203:VAL:CG1	25:Y:228:VAL:HG22	2.39	0.52
30:0:1067:A:H5'	42:0:5209:HOH:O	2.10	0.52
30:0:1972:U:H2'	30:0:1973:A:H5'	1.91	0.52
30:0:2769:C:C2'	30:0:2770:G:H5'	2.38	0.52
9:I:98:ASP:HA	9:I:101:LYS:HD2	1.92	0.52
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.92	0.52
13:M:9:ARG:NH2	30:0:378:A:OP1	2.42	0.52
13:M:107:ARG:HG3	13:M:107:ARG:NH1	2.17	0.52
14:N:151:ASP:OD1	14:N:154:LEU:HD13	2.10	0.52
14:N:160:SER:HB3	31:9:51:A:H5'	1.91	0.52
20:T:69:LYS:O	20:T:71:VAL:HG23	2.09	0.52
22:V:50:ARG:HH12	30:0:56:G:H5''	1.72	0.52
30:0:325:U:H2'	30:0:326:G:H8	1.74	0.52
30:0:558:C:H2'	30:0:559:U:H5''	1.90	0.52
30:0:564:G:H1'	42:0:7127:HOH:O	2.10	0.52
30:0:1595:G:O2'	30:0:1596:U:H5'	2.08	0.52
2:B:58:PRO:HA	2:B:63:GLU:CD	2.34	0.52
22:V:55:ARG:NE	42:V:4428:HOH:O	2.37	0.52
30:0:164:G:H3'	42:0:4517:HOH:O	2.10	0.52
30:0:204:A:H2'	30:0:205:U:H5'	1.90	0.52
30:0:1130:U:H2'	30:0:1131:G:O4'	2.08	0.52
30:0:1279:U:O2	30:0:1279:U:H2'	2.10	0.52
30:0:1778:A:H2'	30:0:1779:A:H5'	1.91	0.52
31:9:3:A:H2	31:9:21:G:N3	2.08	0.52
31:9:59:C:H2'	31:9:60:C:H6	1.71	0.52
2:B:222:LYS:HE2	42:0:4152:HOH:O	2.09	0.52
2:B:223:ARG:O	2:B:228:ALA:HB2	2.09	0.52
3:C:49:ASP:HB3	3:C:52:ALA:HB2	1.89	0.52
5:E:126:ILE:HB	5:E:131:LEU:CD2	2.39	0.52
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:125:ALA:C	11:K:127:ALA:H	2.17	0.52
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.44	0.52
30:0:364:U:H2'	30:0:365:G:O4'	2.09	0.52
30:0:1426:C:H3'	42:0:9544:HOH:O	2.09	0.52
30:0:1477:C:H5'	30:0:1868:G:C5'	2.39	0.52
30:0:2507:G:H2'	30:0:2510:C:H42	1.75	0.52
30:0:2717:C:H2'	30:0:2718:C:C5'	2.36	0.52
30:0:2748:G:H4'	30:0:2749:U:H5'	1.91	0.52
14:N:179:LEU:HA	14:N:184:ILE:HD12	1.92	0.52
20:T:71:VAL:HG12	20:T:72:ILE:N	2.24	0.52
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.30	0.52
23:W:122:ARG:HG3	23:W:122:ARG:NH1	2.23	0.52
27:1:4:GLY:O	27:1:8:GLN:HG2	2.10	0.52
30:0:2353:A:H4'	30:0:2354:A:O5'	2.10	0.52
31:9:3:A:H2'	42:9:9045:HOH:O	2.08	0.52
2:B:214:PRO:HD2	42:0:2992:HOH:O	2.08	0.52
4:D:10:PHE:CE1	4:D:11:HIS:HB3	2.45	0.52
8:H:174:LEU:HA	42:H:9026:HOH:O	2.10	0.52
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.92	0.52
30:0:299:U:H5'	42:0:9133:HOH:O	2.09	0.52
30:0:2003:U:H4'	30:0:2004:U:C5	2.45	0.52
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.45	0.52
23:W:4:LEU:HB2	23:W:33:THR:CG2	2.40	0.52
23:W:90:TYR:N	23:W:90:TYR:CD1	2.78	0.52
1:A:175:LYS:HG3	30:0:1847:A:OP1	2.10	0.52
2:B:280:VAL:HG12	2:B:334:SER:HA	1.91	0.52
10:J:19:MET:HE1	10:J:78:ILE:HG22	1.91	0.52
14:N:78:MET:HB2	14:N:146:HIS:CE1	2.45	0.52
27:1:36:SER:O	27:1:46:ARG:HD3	2.09	0.52
30:0:834:G:H4'	30:0:835:U:OP2	2.09	0.52
30:0:1352:A:O2'	30:0:1353:C:OP1	2.23	0.52
30:0:1700:C:P	42:0:6861:HOH:O	2.66	0.52
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.25	0.52
4:D:172:VAL:CG1	4:D:173:GLU:H	2.19	0.52
13:M:60:VAL:C	13:M:61:ILE:HD12	2.35	0.52
27:1:42:SER:HB2	42:1:354:HOH:O	2.09	0.52
28:2:48:ASP:O	28:2:49:GLU:HB2	2.10	0.52
29:3:15:ASN:O	30:0:2408:A:H4'	2.10	0.52
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.74	0.51
1:A:173:GLY:O	1:A:176:HIS:HB3	2.10	0.51
6:F:48:VAL:HG12	6:F:97:ALA:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:120:ALA:O	9:I:124:VAL:HG23	2.10	0.51
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.44	0.51
14:N:152:GLU:C	14:N:154:LEU:N	2.66	0.51
15:O:35:LYS:HD3	42:0:5468:HOH:O	2.10	0.51
18:R:64:SER:OG	30:0:1369:A:H4'	2.11	0.51
30:0:462:A:H2'	42:0:5731:HOH:O	2.10	0.51
30:0:1380:U:O4	30:0:2748:G:O2'	2.23	0.51
30:0:2488:A:H61	30:0:2534:C:H42	1.58	0.51
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.23	0.51
8:H:32:ALA:O	8:H:33:GLN:HG3	2.10	0.51
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.59	0.51
14:N:21:HIS:HD2	42:0:5578:HOH:O	1.91	0.51
20:T:28:SER:O	20:T:32:ARG:HG3	2.11	0.51
21:U:50:GLU:O	21:U:56:ARG:HG3	2.10	0.51
23:W:4:LEU:HB2	23:W:33:THR:HG22	1.92	0.51
30:0:137:U:OP1	30:0:259:G:O2'	2.29	0.51
30:0:2338:G:H1	30:0:2346:C:H42	1.58	0.51
30:0:2563:U:H2'	30:0:2565:C:O5'	2.10	0.51
1:A:33:GLU:CD	1:A:33:GLU:N	2.60	0.51
2:B:17:LYS:O	2:B:260:HIS:CD2	2.64	0.51
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.40	0.51
8:H:139:ALA:HB3	8:H:149:VAL:HG21	1.93	0.51
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.24	0.51
12:L:97:VAL:HG12	12:L:98:GLU:O	2.11	0.51
14:N:11:ARG:HD3	31:9:114:G:O6	2.09	0.51
19:S:21:GLN:NE2	30:0:1508:C:H5'	2.25	0.51
30:0:407:A:O2'	30:0:408:A:H5'	2.11	0.51
30:0:1667:A:H2'	30:0:1668:U:C6	2.45	0.51
30:0:1790:C:H2'	30:0:1791:U:H6	1.75	0.51
2:B:81:ALA:HB1	2:B:142:LEU:HD13	1.92	0.51
2:B:190:MET:CE	2:B:194:PHE:CD1	2.94	0.51
2:B:305:ASP:O	2:B:306:LYS:HB2	2.11	0.51
3:C:241:ALA:O	3:C:244:ALA:HB3	2.11	0.51
8:H:59:GLN:HE22	8:H:96:GLN:HG2	1.75	0.51
10:J:90:LYS:HB2	35:J:8802:CL:CL	2.47	0.51
10:J:93:ARG:HH11	10:J:93:ARG:CB	2.17	0.51
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.90	0.51
16:P:73:HIS:HE1	30:0:1789:G:O6	1.94	0.51
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.91	0.51
25:Y:95:THR:N	25:Y:236:VAL:O	2.43	0.51
27:1:20:ARG:HH21	30:0:120:A:H5'	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2103:A:N7	30:0:2538:A:N6	2.58	0.51
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.92	0.51
15:O:97:SER:OG	15:O:100:GLN:HG3	2.09	0.51
21:U:23:HIS:HB2	21:U:27:ALA:HB3	1.93	0.51
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.10	0.51
30:0:1183:C:H5	30:0:1192:A:OP1	1.94	0.51
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.46	0.51
5:E:133:VAL:HG12	5:E:141:VAL:HG13	1.93	0.51
6:F:27:GLY:HA3	6:F:101:ALA:O	2.10	0.51
6:F:57:GLU:O	6:F:61:MET:HG3	2.10	0.51
9:I:91:PHE:HA	9:I:131:GLY:HA3	1.91	0.51
10:J:80:LYS:HE2	10:J:98:PHE:CZ	2.46	0.51
21:U:17:THR:CG2	21:U:18:GLY:N	2.74	0.51
29:3:60:LYS:NZ	30:0:2428:G:N7	2.54	0.51
30:0:625:U:H5''	30:0:1044:C:N4	2.25	0.51
30:0:2241:C:O2'	30:0:2242:U:H5'	2.10	0.51
30:0:2456:A:H2'	30:0:2457:U:C6	2.46	0.51
1:A:130:THR:HB	1:A:137:VAL:HB	1.91	0.51
2:B:18:ARG:HE	2:B:256:GLN:NE2	2.08	0.51
6:F:21:GLU:O	6:F:24:ARG:HG3	2.10	0.51
11:K:109:LEU:CD1	11:K:113:ILE:HD11	2.37	0.51
14:N:41:LYS:HD3	42:9:9064:HOH:O	2.10	0.51
16:P:55:LYS:CG	16:P:56:GLY:N	2.74	0.51
42:X:4132:HOH:O	30:0:2895:C:H4'	2.10	0.51
4:D:57:THR:HG23	4:D:63:ILE:CA	2.35	0.51
10:J:75:PRO:HD3	10:J:136:SER:OG	2.09	0.51
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.93	0.51
13:M:47:ASP:CG	13:M:48:LYS:N	2.69	0.51
21:U:47:ARG:HG2	21:U:54:THR:HG22	1.93	0.51
24:X:72:VAL:HG22	24:X:85:VAL:HG12	1.91	0.51
25:Y:112:GLU:CD	25:Y:115:ARG:HH12	2.18	0.51
28:2:40:ARG:HG3	28:2:45:ASN:HB2	1.91	0.51
30:0:304:G:H1'	30:0:347:A:H61	1.75	0.51
30:0:441:A:H1'	30:0:442:A:N7	2.25	0.51
3:C:206:ASN:HB2	30:0:329:A:OP2	2.11	0.51
5:E:84:MET:HE2	5:E:133:VAL:HG23	1.92	0.51
10:J:63:ILE:HD11	30:0:1236:A:C8	2.46	0.51
13:M:9:ARG:HB2	13:M:47:ASP:OD2	2.11	0.51
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.10	0.51
28:2:5:LYS:O	28:2:9:LYS:HG3	2.11	0.51
30:0:398:U:H2'	30:0:399:C:C6	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1829:A:C2'	30:0:1830:C:H5'	2.40	0.51
30:0:1833:U:O2'	30:0:1834:C:H5'	2.11	0.51
31:9:64:C:C2'	31:9:65:A:H5'	2.41	0.51
3:C:27:ARG:NH1	3:C:29:ASP:OD2	2.44	0.51
3:C:101:ASP:HB2	30:0:750:A:O3'	2.11	0.51
7:G:64:ASN:HD22	7:G:64:ASN:N	2.09	0.51
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.41	0.51
23:W:65:VAL:HG12	23:W:116:LEU:HD13	1.93	0.51
23:W:88:THR:HG22	23:W:90:TYR:CD1	2.43	0.51
24:X:74:ALA:CB	24:X:85:VAL:HG22	2.41	0.51
30:0:876:A:H2'	30:0:876:A:N3	2.25	0.51
30:0:1183:C:H2'	42:0:7062:HOH:O	2.11	0.51
30:0:1566:C:H2'	30:0:1567:G:H8	1.76	0.51
30:0:1755:A:H2'	30:0:1756:G:O4'	2.11	0.51
30:0:2414:A:H2'	30:0:2415:A:C8	2.46	0.51
5:E:93:MET:HE2	5:E:107:PHE:HD1	1.76	0.50
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.41	0.50
18:R:114:VAL:HG13	18:R:114:VAL:O	2.12	0.50
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.39	0.50
23:W:137:GLN:HG3	23:W:137:GLN:O	2.11	0.50
29:3:61:PRO:HG2	42:0:9341:HOH:O	2.10	0.50
30:0:248:A:H5'	30:0:249:G:OP2	2.11	0.50
30:0:1159:G:H1	30:0:1208:C:H42	1.59	0.50
30:0:1171:A:H2'	30:0:1172:G:H5'	1.93	0.50
1:A:179:MET:HG2	1:A:186:TRP:HB2	1.92	0.50
2:B:294:TYR:HE2	42:B:9134:HOH:O	1.93	0.50
6:F:69:GLU:O	6:F:70:LYS:HG2	2.11	0.50
13:M:102:GLU:CD	13:M:164:THR:HG21	2.36	0.50
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.11	0.50
20:T:112:LEU:CD2	20:T:119:ALA:HB3	2.38	0.50
21:U:56:ARG:O	21:U:56:ARG:CD	2.60	0.50
5:E:11:VAL:HG12	5:E:12:ASP:N	2.27	0.50
24:X:85:VAL:HG12	24:X:86:GLU:N	2.26	0.50
30:0:558:C:C2'	30:0:559:U:C5'	2.89	0.50
30:0:1529:G:H5'	42:0:9181:HOH:O	2.09	0.50
1:A:103:VAL:O	1:A:105:VAL:HG23	2.11	0.50
1:A:179:MET:HG2	1:A:186:TRP:CB	2.41	0.50
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.39	0.50
3:C:153:VAL:O	3:C:157:LEU:HG	2.11	0.50
6:F:41:GLU:OE2	13:M:2:ARG:HB2	2.11	0.50
25:Y:234:VAL:HG12	25:Y:235:GLU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:29:C:O2'	30:0:30:U:H5'	2.11	0.50
30:0:530:C:H4'	30:0:612:U:H4'	1.92	0.50
30:0:559:U:H2'	30:0:560:U:O4'	2.11	0.50
30:0:1909:A:H2'	30:0:1910:A:C8	2.47	0.50
2:B:1:PRO:HG3	30:0:2591:C:OP1	2.11	0.50
4:D:170:TYR:O	4:D:171:ASP:CB	2.59	0.50
15:O:99:GLU:HG3	42:O:6044:HOH:O	2.10	0.50
19:S:58:MET:HE2	30:0:1418:U:C4	2.46	0.50
20:T:32:ARG:NH1	20:T:38:ARG:NH1	2.59	0.50
22:V:5:VAL:HG23	42:V:2271:HOH:O	2.11	0.50
25:Y:96:GLU:O	25:Y:235:GLU:HA	2.11	0.50
30:0:110:C:H2'	30:0:111:C:H6	1.75	0.50
30:0:1414:A:H2'	30:0:1415:G:O4'	2.11	0.50
30:0:1819:G:H2'	30:0:1820:G:C5'	2.42	0.50
4:D:63:ILE:HG13	4:D:64:ARG:N	2.25	0.50
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.76	0.50
8:H:96:GLN:NE2	8:H:129:ARG:NH2	2.59	0.50
18:R:39:THR:HG22	18:R:42:GLU:H	1.75	0.50
18:R:136:TRP:CE2	30:0:2053:G:H4'	2.47	0.50
23:W:29:VAL:O	23:W:30:ASN:HB2	2.10	0.50
2:B:42:ALA:HB1	2:B:308:LEU:HD11	1.93	0.50
10:J:47:THR:HG21	30:0:1244:U:H2'	1.94	0.50
30:0:1941:A:H4'	42:0:5079:HOH:O	2.11	0.50
30:0:2115:U:H2'	30:0:2116:U:C6	2.46	0.50
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.10	0.50
2:B:217:ARG:CG	2:B:257:THR:HG22	2.35	0.50
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.77	0.50
14:N:141:ARG:HH12	31:9:35:C:H2'	1.77	0.50
16:P:40:VAL:O	16:P:44:VAL:HG23	2.12	0.50
30:0:1667:A:H5'	30:0:1667:A:C8	2.36	0.50
30:0:2114:C:O2'	30:0:2115:U:H5'	2.10	0.50
2:B:215:VAL:HA	2:B:220:VAL:HG22	1.93	0.50
2:B:314:ALA:CB	2:B:317:PRO:HG3	2.41	0.50
3:C:72:LYS:CG	3:C:77:ALA:HA	2.42	0.50
3:C:79:ARG:O	3:C:87:ARG:HG2	2.12	0.50
5:E:80:TRP:O	5:E:134:SER:HA	2.12	0.50
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.40	0.50
17:Q:11:ARG:NH1	30:0:2363:G:O3'	2.45	0.50
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.93	0.50
25:Y:112:GLU:OE2	25:Y:115:ARG:NH1	2.43	0.50
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:37:ARG:HD3	42:0:5547:HOH:O	2.12	0.50
30:0:945:U:H2'	30:0:946:C:C6	2.47	0.50
30:0:1183:C:H41	30:0:1192:A:P	2.35	0.50
30:0:2326:C:H4'	30:0:2412:G:H4'	1.94	0.50
31:9:39:U:H1'	31:9:44:A:H61	1.77	0.50
3:C:132:ASP:O	3:C:133:ARG:HB2	2.11	0.49
3:C:173:LYS:HE3	30:0:1311:G:O6	2.11	0.49
4:D:60:GLU:O	4:D:60:GLU:HG3	2.12	0.49
6:F:77:VAL:C	6:F:78:GLU:CA	2.85	0.49
17:Q:67:GLN:NE2	30:0:2403:C:O2	2.45	0.49
22:V:29:ASN:O	22:V:33:VAL:HG23	2.12	0.49
30:0:285:A:H2'	30:0:286:U:O4'	2.11	0.49
30:0:396:U:O2'	30:0:418:C:H4'	2.11	0.49
30:0:589:U:H2'	30:0:590:A:H8	1.76	0.49
30:0:1783:A:O2'	30:0:1784:U:H5'	2.12	0.49
30:0:1925:G:O2'	30:0:1926:G:H5'	2.12	0.49
1:A:105:VAL:HG12	1:A:106:CYS:N	2.28	0.49
3:C:1:MET:HG2	3:C:2:GLN:NE2	2.27	0.49
4:D:76:ARG:NE	31:9:44:A:O4'	2.45	0.49
4:D:138:GLY:HA2	31:9:29:C:O3'	2.12	0.49
9:I:102:GLN:HA	9:I:105:GLU:OE2	2.12	0.49
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.48	0.49
30:0:110:C:H2'	30:0:111:C:C6	2.47	0.49
30:0:336:G:H5''	42:0:4598:HOH:O	2.11	0.49
30:0:812:A:H2'	30:0:813:C:C6	2.47	0.49
30:0:1187:U:O2'	30:0:1189:A:H2	1.95	0.49
30:0:1200:A:H3'	42:0:6584:HOH:O	2.10	0.49
30:0:1741:U:O2'	30:0:2723:G:H4'	2.12	0.49
30:0:2505:G:C2'	30:0:2506:A:H5'	2.42	0.49
1:A:109:GLU:HG2	1:A:116:GLY:H	1.76	0.49
1:A:140:LEU:HB3	1:A:141:PRO:HD2	1.94	0.49
2:B:265:LEU:HD21	2:B:316:ARG:HD3	1.93	0.49
9:I:72:GLU:C	9:I:74:ILE:H	2.20	0.49
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.27	0.49
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.93	0.49
12:L:66:VAL:HG23	12:L:67:ARG:N	2.27	0.49
14:N:29:SER:HB3	30:0:2415:A:O2'	2.12	0.49
19:S:4:VAL:HG11	19:S:37:VAL:HA	1.94	0.49
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.27	0.49
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.77	0.49
30:0:333:G:O2'	30:0:334:G:H5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2326:C:H4'	30:0:2412:G:C4'	2.42	0.49
3:C:43:LYS:HG2	30:0:449:A:C8	2.48	0.49
5:E:1:PRO:HG2	5:E:59:MET:SD	2.52	0.49
6:F:101:ALA:HA	42:F:5413:HOH:O	2.11	0.49
6:F:107:ASP:O	6:F:111:ILE:HG13	2.12	0.49
7:G:63:ARG:O	7:G:67:LEU:HG	2.13	0.49
8:H:57:THR:O	8:H:58:VAL:HG13	2.13	0.49
8:H:61:ARG:HG3	42:H:9007:HOH:O	2.13	0.49
10:J:42:GLU:O	10:J:131:THR:HG23	2.12	0.49
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.47	0.49
12:L:136:ALA:HB3	42:L:8879:HOH:O	2.12	0.49
13:M:164:THR:CG2	13:M:166:ALA:H	2.19	0.49
16:P:103:THR:O	16:P:107:GLU:HG3	2.13	0.49
19:S:57:THR:HG22	19:S:59:ASP:N	2.26	0.49
42:S:2012:HOH:O	30:0:1507:C:H4'	2.12	0.49
30:0:1545:C:H2'	30:0:1546:G:O4'	2.12	0.49
30:0:1736:A:H1'	42:0:9369:HOH:O	2.10	0.49
3:C:77:ALA:O	3:C:78:ARG:CA	2.60	0.49
3:C:156:LEU:O	3:C:160:LEU:HG	2.10	0.49
8:H:32:ALA:C	8:H:33:GLN:HG3	2.38	0.49
10:J:45:VAL:HG23	10:J:130:VAL:O	2.13	0.49
13:M:84:LYS:NZ	30:0:391:U:OP2	2.46	0.49
15:O:14:LEU:HG	15:O:102:ILE:HD11	1.95	0.49
17:Q:64:GLU:HG3	17:Q:74:ASP:OD2	2.13	0.49
20:T:64:ASN:HB3	20:T:73:HIS:HB2	1.95	0.49
30:0:407:A:H5'	42:0:6851:HOH:O	2.12	0.49
30:0:2758:G:H2'	30:0:2759:C:C6	2.48	0.49
30:0:2832:C:H5	42:0:9015:HOH:O	1.96	0.49
1:A:66:ARG:CB	1:A:66:ARG:NH1	2.76	0.49
3:C:194:PHE:HA	3:C:234:VAL:HG13	1.94	0.49
9:I:96:SER:OG	9:I:99:GLN:HG3	2.12	0.49
9:I:134:ILE:HG22	9:I:135:GLU:N	2.27	0.49
12:L:92:ASP:HA	12:L:121:ILE:HB	1.95	0.49
14:N:11:ARG:HG3	14:N:14:ARG:HH12	1.77	0.49
16:P:16:VAL:HG12	16:P:17:GLY:N	2.28	0.49
22:V:56:ILE:HG22	22:V:60:GLN:NE2	2.24	0.49
23:W:119:HIS:HD2	23:W:120:PRO:O	1.96	0.49
30:0:932:U:H2'	30:0:933:C:C6	2.48	0.49
31:9:73:A:N6	31:9:108:C:H42	2.09	0.49
1:A:51:ARG:HB2	42:A:9081:HOH:O	2.11	0.49
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.43	0.49
5:E:36:PRO:HD3	10:J:127:ILE:CD1	2.42	0.49
14:N:11:ARG:HA	14:N:14:ARG:CZ	2.43	0.49
14:N:82:TYR:HE1	14:N:120:GLU:HG2	1.78	0.49
14:N:183:ASP:O	14:N:184:ILE:O	2.30	0.49
15:O:32:ARG:HH21	15:O:35:LYS:HZ3	1.61	0.49
30:0:697:G:H4'	30:0:730:G:O3'	2.13	0.49
31:9:96:C:H2'	31:9:97:U:C6	2.48	0.49
1:A:232:ARG:NH2	1:A:236:GLY:O	2.45	0.49
2:B:77:PRO:C	2:B:78:PRO:HG3	2.38	0.49
4:D:156:ARG:HG3	4:D:156:ARG:HH11	1.78	0.49
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.43	0.49
9:I:70:THR:OG1	9:I:107:LYS:HE2	2.13	0.49
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.94	0.49
30:0:221:G:H2'	30:0:222:A:C8	2.48	0.49
30:0:1166:A:H1'	30:0:1192:A:H2	1.78	0.49
30:0:1304:U:H2'	30:0:1305:C:C6	2.48	0.49
30:0:1461:U:H2'	30:0:1462:C:H6	1.78	0.49
2:B:183:GLU:O	2:B:184:ASP:C	2.56	0.49
4:D:54:ALA:HB2	4:D:69:ILE:CD1	2.40	0.49
6:F:99:THR:HG23	6:F:99:THR:O	2.13	0.49
9:I:123:VAL:C	9:I:125:GLY:H	2.21	0.49
10:J:92:GLN:HG2	10:J:96:GLU:OE2	2.13	0.49
23:W:11:VAL:O	23:W:12:ASN:HB2	2.13	0.49
24:X:30:MET:HG2	30:0:1384:C:H5'	1.95	0.49
25:Y:208:LYS:HB3	30:0:1312:G:O2'	2.13	0.49
30:0:951:A:H2'	30:0:952:G:H5'	1.94	0.49
30:0:1506:U:H6	30:0:1506:U:H5'	1.78	0.49
30:0:1803:C:H2'	30:0:1804:A:C8	2.48	0.49
30:0:2866:U:H4'	30:0:2867:G:H5'	1.94	0.49
5:E:101:GLU:HB2	5:E:116:THR:O	2.12	0.49
10:J:86:MET:HE2	30:0:1241:G:N3	2.27	0.49
14:N:77:ASN:C	14:N:78:MET:CA	2.86	0.49
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.28	0.49
18:R:92:LEU:HD23	18:R:145:LEU:HD21	1.94	0.49
26:Z:34:SER:HB2	42:Z:8712:HOH:O	2.13	0.49
30:0:284:C:H4'	30:0:285:A:H8	1.78	0.49
30:0:1406:A:H4'	30:0:1407:A:C5'	2.43	0.49
30:0:1730:G:C5'	30:0:1731:C:H6	2.25	0.49
30:0:1759:A:N3	30:0:1818:C:H2'	2.28	0.49
2:B:258:GLY:H	2:B:260:HIS:CE1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:ILE:HG13	4:D:41:LEU:N	2.27	0.48
4:D:76:ARG:NH1	31:9:42:C:O2	2.45	0.48
8:H:86:TYR:CD1	8:H:86:TYR:C	2.91	0.48
13:M:58:GLN:NE2	30:0:259:G:H21	2.11	0.48
16:P:82:GLY:O	30:0:1761:U:H4'	2.13	0.48
25:Y:178:HIS:CG	25:Y:179:PRO:HD2	2.48	0.48
30:0:1666:C:C2'	30:0:1667:A:C5'	2.90	0.48
1:A:82:VAL:HG22	1:A:93:THR:HB	1.95	0.48
1:A:109:GLU:HG2	1:A:116:GLY:N	2.28	0.48
3:C:142:ASP:CG	3:C:238:SER:HG	2.21	0.48
9:I:82:THR:CG2	30:0:1168:C:H5''	2.38	0.48
15:O:44:ASN:OD1	15:O:67:SER:HB2	2.12	0.48
16:P:81:LYS:HG2	42:0:3445:HOH:O	2.12	0.48
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.13	0.48
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.49	0.48
30:0:952:G:N3	30:0:2302:A:H2'	2.28	0.48
31:9:28:U:H2'	31:9:29:C:C6	2.48	0.48
2:B:321:PRO:HA	42:B:9143:HOH:O	2.12	0.48
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.43	0.48
14:N:165:ALA:C	14:N:167:ASP:H	2.21	0.48
20:T:71:VAL:HG12	20:T:72:ILE:H	1.78	0.48
21:U:52:THR:HG22	21:U:54:THR:HB	1.95	0.48
22:V:64:GLY:O	22:V:65:ASP:CB	2.60	0.48
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.78	0.48
30:0:553:G:H2'	30:0:554:G:H5'	1.95	0.48
30:0:2063:U:O4	30:0:2083:A:H2	1.95	0.48
5:E:2:ARG:HH21	5:E:48:VAL:HG21	1.77	0.48
12:L:80:ASP:HB3	12:L:90:ARG:HB3	1.96	0.48
14:N:78:MET:HB2	14:N:146:HIS:HE1	1.79	0.48
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.78	0.48
15:O:96:VAL:HG13	15:O:100:GLN:CD	2.38	0.48
17:Q:95:GLU:HA	30:0:949:U:H4'	1.95	0.48
18:R:125:ARG:HG2	42:R:8947:HOH:O	2.14	0.48
19:S:57:THR:HG22	19:S:59:ASP:H	1.78	0.48
30:0:1185:U:H2'	30:0:1186:C:C6	2.49	0.48
30:0:1819:G:H2'	30:0:1820:G:H4'	1.93	0.48
30:0:2443:C:H3'	42:0:4356:HOH:O	2.13	0.48
30:0:2619:UR3:H2'	30:0:2620:U:C6	2.49	0.48
1:A:95:PRO:HA	1:A:153:ARG:HA	1.96	0.48
1:A:128:LEU:HG	42:A:9050:HOH:O	2.13	0.48
8:H:14:LYS:HE2	42:0:4714:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:THR:O	8:H:123:ILE:HD12	2.14	0.48
11:K:41:LYS:HE3	42:0:6399:HOH:O	2.13	0.48
13:M:71:SER:HB2	13:M:92:THR:HG22	1.96	0.48
13:M:125:ARG:HD3	42:0:5827:HOH:O	2.12	0.48
16:P:143:ALA:HA	42:P:194:HOH:O	2.12	0.48
17:Q:45:PRO:O	30:0:2365:G:H4'	2.14	0.48
19:S:57:THR:CG2	19:S:58:MET:N	2.76	0.48
24:X:28:LYS:HD2	24:X:31:ILE:HD12	1.94	0.48
29:3:42:ARG:HH11	29:3:42:ARG:HG3	1.79	0.48
30:0:625:U:H5'	42:0:4074:HOH:O	2.12	0.48
30:0:1098:A:H2'	30:0:1099:G:O4'	2.13	0.48
30:0:1632:A:C2'	30:0:1633:C:H5'	2.43	0.48
30:0:2372:A:H2'	30:0:2373:U:H6	1.78	0.48
1:A:66:ARG:HB2	1:A:66:ARG:NH1	2.27	0.48
1:A:75:GLY:HA2	26:Z:88:PHE:HA	1.95	0.48
2:B:125:GLU:O	2:B:129:ARG:HG3	2.13	0.48
2:B:280:VAL:HG13	2:B:333:GLU:O	2.13	0.48
3:C:77:ALA:O	3:C:78:ARG:HG3	2.13	0.48
42:C:8558:HOH:O	15:O:3:THR:HG21	2.12	0.48
4:D:167:GLU:OE2	4:D:173:GLU:HB3	2.12	0.48
13:M:61:ILE:HD12	13:M:61:ILE:N	2.29	0.48
14:N:4:PRO:HG3	31:9:69:U:OP1	2.14	0.48
15:O:62:GLY:O	15:O:79:VAL:HG23	2.14	0.48
26:Z:77:GLY:O	26:Z:78:ILE:CA	2.62	0.48
27:1:45:ARG:NH2	42:1:2086:HOH:O	2.41	0.48
30:0:1451:C:H5'	30:0:1505:U:H5	1.73	0.48
30:0:1946:C:H2'	30:0:1971:G:C8	2.49	0.48
30:0:2613:G:O2'	30:0:2614:C:H5'	2.13	0.48
8:H:12:ILE:HD12	8:H:57:THR:CG2	2.44	0.48
23:W:26:ILE:O	23:W:26:ILE:HG12	2.13	0.48
30:0:1175:G:H1'	30:0:1193:A:C2'	2.42	0.48
30:0:1198:U:H2'	30:0:1200:A:OP2	2.13	0.48
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.49	0.48
3:C:150:THR:HA	3:C:203:ALA:O	2.14	0.48
5:E:143:GLN:NE2	30:0:2779:G:H21	2.12	0.48
11:K:55:VAL:HG12	11:K:56:SER:N	2.28	0.48
12:L:30:ARG:HD3	30:0:164:G:H4'	1.94	0.48
18:R:104:PHE:HB3	18:R:109:MET:HE2	1.95	0.48
25:Y:112:GLU:O	25:Y:116:LEU:HG	2.14	0.48
28:2:40:ARG:HA	28:2:45:ASN:ND2	2.29	0.48
30:0:1058:A:H2'	30:0:1060:C:C5'	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:PHE:HB2	2:B:16:ARG:NH1	2.28	0.48
2:B:72:THR:HB	42:B:9083:HOH:O	2.12	0.48
2:B:77:PRO:HA	2:B:293:PRO:HB2	1.95	0.48
6:F:19:ALA:O	6:F:22:VAL:HG22	2.13	0.48
7:G:12:ILE:HA	42:0:6294:HOH:O	2.13	0.48
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.95	0.48
10:J:39:VAL:CG1	10:J:40:ASN:N	2.76	0.48
12:L:143:THR:CG2	12:L:144:ASP:N	2.76	0.48
13:M:159:VAL:HG12	35:M:8818:CL:CL	2.51	0.48
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.96	0.48
17:Q:16:ASN:HD21	17:Q:45:PRO:HD2	1.79	0.48
23:W:139:GLY:O	23:W:141:HIS:HD2	1.96	0.48
30:0:2032:U:H2'	30:0:2033:G:C5'	2.43	0.48
30:0:2748:G:H4'	30:0:2749:U:C5'	2.43	0.48
3:C:58:ALA:HA	3:C:73:GLN:NE2	2.28	0.48
4:D:96:SER:C	4:D:98:PHE:H	2.22	0.48
6:F:32:GLY:N	42:F:3111:HOH:O	2.47	0.48
9:I:87:PRO:HD3	42:0:4123:HOH:O	2.14	0.48
12:L:17:SER:C	12:L:19:LYS:H	2.21	0.48
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.96	0.48
20:T:40:VAL:HG23	20:T:119:ALA:C	2.39	0.48
22:V:26:GLU:OE2	22:V:45:ARG:HD3	2.13	0.48
24:X:20:GLU:CD	24:X:21:PRO:HD2	2.39	0.48
30:0:200:C:H2'	42:0:4329:HOH:O	2.14	0.48
30:0:603:A:H4'	30:0:604:G:O5'	2.13	0.48
30:0:2748:G:H5'	42:0:9326:HOH:O	2.13	0.48
1:A:186:TRP:CD1	1:A:187:PRO:HA	2.49	0.47
1:A:204:GLY:N	30:0:2634:G:OP2	2.47	0.47
2:B:42:ALA:HB2	2:B:162:MET:CE	2.43	0.47
2:B:104:GLU:HB2	42:B:9117:HOH:O	2.14	0.47
16:P:7:LYS:HD3	16:P:23:PHE:CZ	2.49	0.47
16:P:69:ARG:HA	16:P:73:HIS:O	2.14	0.47
22:V:39:ALA:O	22:V:41:GLU:N	2.42	0.47
27:1:56:GLU:HG2	27:1:56:GLU:OXT	2.14	0.47
30:0:343:C:H2'	30:0:344:C:H6	1.79	0.47
30:0:757:C:H2'	30:0:758:A:C8	2.48	0.47
30:0:1171:A:N6	30:0:1172:G:C2	2.82	0.47
30:0:1181:A:H2'	30:0:1182:C:H5'	1.96	0.47
30:0:2499:U:H2'	30:0:2500:C:H6	1.78	0.47
2:B:17:LYS:O	2:B:260:HIS:HD2	1.96	0.47
3:C:51:TYR:CE2	27:1:53:LYS:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:138:GLY:N	42:D:7597:HOH:O	2.46	0.47
5:E:69:ILE:HA	5:E:72:MET:CE	2.44	0.47
10:J:47:THR:HG22	10:J:48:GLY:N	2.28	0.47
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.94	0.47
18:R:39:THR:O	18:R:40:ALA:C	2.56	0.47
25:Y:189:ASN:C	25:Y:189:ASN:ND2	2.72	0.47
29:3:56:PRO:HA	42:0:6865:HOH:O	2.12	0.47
30:0:690:G:H4'	30:0:741:C:O2	2.14	0.47
30:0:1060:C:H6	30:0:1060:C:H5'	1.79	0.47
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.42	0.47
4:D:141:VAL:HG21	31:9:57:A:C8	2.48	0.47
9:I:127:CYS:C	9:I:129:SER:H	2.22	0.47
10:J:39:VAL:HG11	10:J:107:ASN:HB2	1.96	0.47
23:W:77:ALA:C	23:W:78:ASP:CA	2.87	0.47
24:X:79:GLU:CD	24:X:80:GLU:H	2.22	0.47
25:Y:103:THR:HG22	25:Y:104:GLU:OE2	2.14	0.47
28:2:40:ARG:HG3	28:2:45:ASN:CB	2.44	0.47
30:0:451:C:O2'	30:0:452:G:H5'	2.14	0.47
30:0:1422:U:H2'	30:0:1423:C:C6	2.49	0.47
30:0:1940:C:H4'	42:0:9143:HOH:O	2.13	0.47
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.95	0.47
2:B:132:HIS:NE2	2:B:171:VAL:HG23	2.29	0.47
8:H:91:ARG:NH1	8:H:138:THR:OG1	2.47	0.47
12:L:99:GLU:C	12:L:101:ASP:H	2.21	0.47
14:N:61:ALA:CB	14:N:88:ALA:HB2	2.44	0.47
14:N:73:ALA:HB1	14:N:74:PRO:CD	2.44	0.47
30:0:947:U:O2'	30:0:948:G:H5'	2.15	0.47
32:5:74:C:C2'	32:5:75:C:H5'	2.41	0.47
2:B:282:GLY:O	30:0:2898:G:H1'	2.15	0.47
3:C:27:ARG:NH1	3:C:27:ARG:HG2	2.29	0.47
10:J:39:VAL:HG11	10:J:107:ASN:CG	2.40	0.47
21:U:4:ARG:NH1	21:U:4:ARG:HG2	2.30	0.47
24:X:87:ALA:O	24:X:88:GLU:CB	2.63	0.47
30:0:292:G:H1'	30:0:360:A:H61	1.80	0.47
30:0:1066:U:H2'	30:0:1067:A:C8	2.49	0.47
30:0:1416:G:C2'	30:0:1417:G:H5'	2.45	0.47
30:0:2323:G:H5''	42:0:5629:HOH:O	2.14	0.47
30:0:2670:G:O2'	30:0:2671:U:H5'	2.13	0.47
30:0:2836:G:O2'	30:0:2838:A:N7	2.43	0.47
1:A:76:VAL:HG12	1:A:77:GLY:N	2.29	0.47
2:B:51:VAL:HG13	2:B:53:LEU:CD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:139:VAL:HG13	42:C:8649:HOH:O	2.14	0.47
12:L:35:ARG:HB2	12:L:35:ARG:NH1	2.30	0.47
12:L:150:GLN:HB3	42:L:8876:HOH:O	2.15	0.47
23:W:31:HIS:HB3	23:W:115:THR:HG21	1.95	0.47
23:W:60:GLU:O	23:W:63:GLU:HB2	2.14	0.47
23:W:122:ARG:NH2	42:O:6126:HOH:O	2.47	0.47
30:O:90:A:H2'	30:O:91:G:O4'	2.13	0.47
30:O:666:A:H2'	30:O:667:C:O4'	2.15	0.47
30:O:1203:G:O2'	30:O:1204:C:H5'	2.15	0.47
30:O:1447:U:H3'	30:O:1506:U:O2	2.15	0.47
30:O:1641:A:H2'	30:O:1642:A:H5'	1.95	0.47
30:O:1902:G:H2'	30:O:1903:U:O4'	2.15	0.47
30:O:2554:U:H1'	42:O:6960:HOH:O	2.14	0.47
31:9:24:U:H3'	31:9:25:G:C5'	2.43	0.47
1:A:32:VAL:HG12	1:A:34:ASP:H	1.80	0.47
1:A:117:LYS:HA	42:A:9014:HOH:O	2.14	0.47
2:B:36:PRO:HA	2:B:168:GLY:CA	2.30	0.47
2:B:36:PRO:HB3	2:B:174:ARG:CB	2.44	0.47
3:C:115:LEU:O	3:C:118:THR:HB	2.14	0.47
4:D:21:VAL:HA	4:D:131:THR:O	2.15	0.47
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.97	0.47
5:E:116:THR:CG2	5:E:151:LEU:HD22	2.39	0.47
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.50	0.47
12:L:98:GLU:O	12:L:99:GLU:HB2	2.15	0.47
17:Q:75:ILE:CD1	17:Q:84:ILE:HD11	2.45	0.47
19:S:42:GLU:HG2	19:S:49:VAL:HG23	1.96	0.47
20:T:8:ARG:NH1	30:O:31:C:OP2	2.47	0.47
22:V:11:MET:HB3	22:V:15:GLU:HB2	1.96	0.47
23:W:4:LEU:HD22	23:W:52:VAL:HB	1.95	0.47
23:W:21:LEU:CD2	23:W:48:VAL:HG11	2.33	0.47
23:W:130:HIS:C	23:W:136:GLY:HA3	2.39	0.47
24:X:27:ASP:OD2	24:X:27:ASP:N	2.48	0.47
30:O:120:A:H2'	30:O:120:A:N3	2.30	0.47
30:O:343:C:O2'	30:O:344:C:H5'	2.15	0.47
30:O:629:A:H2'	30:O:630:A:O4'	2.15	0.47
30:O:867:A:H2	30:O:880:C:O2	1.97	0.47
30:O:946:C:H2'	30:O:947:U:H6	1.78	0.47
30:O:1006:A:N1	30:O:2311:A:H1'	2.30	0.47
30:O:1174:A:C5	30:O:1201:C:H4'	2.50	0.47
30:O:1416:G:H2'	30:O:1417:G:H5'	1.97	0.47
30:O:2506:A:O2'	30:O:2507:G:O5'	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2828:G:O5'	30:0:2828:G:H8	1.98	0.47
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.97	0.47
5:E:7:ILE:CG1	5:E:11:VAL:HB	2.45	0.47
9:I:70:THR:O	9:I:74:ILE:HG13	2.15	0.47
19:S:15:MET:O	19:S:18:MET:HB3	2.14	0.47
20:T:9:LYS:HD2	42:0:4630:HOH:O	2.15	0.47
25:Y:144:ARG:CZ	42:Y:8923:HOH:O	2.63	0.47
30:0:958:G:O2'	30:0:959:C:H5'	2.15	0.47
30:0:1118:A:H8	30:0:1119:G:H5''	1.78	0.47
30:0:2281:C:C2'	30:0:2282:U:H5'	2.44	0.47
32:5:76:A:C5'	32:5:76:A:H8	2.20	0.47
2:B:212:GLN:OE1	2:B:216:LYS:HD3	2.15	0.47
4:D:99:ASP:CB	4:D:103:ASN:HB2	2.45	0.47
4:D:166:ILE:O	4:D:169:THR:N	2.48	0.47
9:I:126:THR:HG22	9:I:126:THR:O	2.15	0.47
14:N:110:THR:HB	14:N:113:SER:HG	1.80	0.47
14:N:155:GLU:O	14:N:156:GLU:HG3	2.14	0.47
20:T:73:HIS:HD2	20:T:88:PRO:HG3	1.79	0.47
30:0:251:C:O2'	30:0:252:C:H5'	2.14	0.47
30:0:861:A:H4'	30:0:1697:G:H4'	1.97	0.47
30:0:1249:U:H2'	30:0:1250:C:C6	2.49	0.47
30:0:2289:G:H21	30:0:2291:A:H2	1.61	0.47
30:0:2756:U:N3	30:0:2896:A:C2	2.77	0.47
6:F:49:PHE:HE1	6:F:98:VAL:HG23	1.79	0.47
9:I:127:CYS:C	9:I:129:SER:N	2.73	0.47
14:N:164:ASP:OD1	14:N:167:ASP:OD1	2.33	0.47
18:R:100:ASP:C	18:R:102:GLN:H	2.23	0.47
20:T:21:LYS:HA	20:T:24:ARG:HG3	1.97	0.47
22:V:38:GLY:C	22:V:40:PRO:HD2	2.39	0.47
30:0:1167:G:H2'	30:0:1168:C:O4'	2.14	0.47
30:0:1419:U:H2'	30:0:1685:A:C2	2.49	0.47
30:0:1684:A:H5'	30:0:1692:C:OP1	2.15	0.47
30:0:1930:A:H2'	30:0:1931:A:C8	2.50	0.47
30:0:1947:G:H2'	30:0:1948:G:H8	1.79	0.47
30:0:2016:U:O5'	30:0:2016:U:H6	1.97	0.47
30:0:2072:G:N2	42:0:7670:HOH:O	2.48	0.47
30:0:2102:G:H2'	42:0:9547:HOH:O	2.14	0.47
2:B:24:PRO:HB2	2:B:310:ARG:HG3	1.96	0.46
2:B:321:PRO:HG3	42:B:9077:HOH:O	2.14	0.46
5:E:14:GLU:O	5:E:15:GLN:HB2	2.14	0.46
10:J:63:ILE:HG22	10:J:64:GLY:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:69:LYS:HG3	13:M:126:GLN:CA	2.45	0.46
20:T:86:GLU:HB2	42:T:6653:HOH:O	2.15	0.46
30:0:420:U:H2'	30:0:421:C:C6	2.50	0.46
30:0:708:A:H2'	30:0:709:G:O4'	2.15	0.46
30:0:1278:A:H2'	30:0:1280:A:C8	2.50	0.46
30:0:1522:A:H2'	30:0:1523:G:H5'	1.97	0.46
30:0:2880:A:H2'	30:0:2881:C:H5'	1.97	0.46
2:B:3:PRO:HG2	42:0:9679:HOH:O	2.15	0.46
2:B:233:ARG:HG2	2:B:233:ARG:NH1	2.29	0.46
13:M:12:TRP:O	13:M:15:PRO:HD3	2.15	0.46
13:M:24:GLN:NE2	13:M:27:ARG:NH1	2.62	0.46
15:O:37:ARG:HD2	30:0:656:G:OP2	2.15	0.46
17:Q:94:GLN:O	17:Q:95:GLU:HB2	2.15	0.46
20:T:30:ASP:O	20:T:33:GLU:HB3	2.15	0.46
23:W:31:HIS:CE1	23:W:117:ARG:HG2	2.50	0.46
42:Y:8884:HOH:O	30:0:1355:A:H5''	2.14	0.46
29:3:36:ILE:HG23	29:3:37:ASP:N	2.30	0.46
29:3:77:ALA:HB3	30:0:2436:U:O3'	2.15	0.46
30:0:59:A:H5'	42:0:5192:HOH:O	2.14	0.46
30:0:806:A:H2'	30:0:807:A:O4'	2.15	0.46
30:0:1592:G:O2'	30:0:1593:C:O4'	2.32	0.46
30:0:1787:C:H4'	30:0:2883:A:O4'	2.16	0.46
30:0:2426:G:H5''	30:0:2427:C:O4'	2.15	0.46
30:0:2618:G:N2	42:0:6025:HOH:O	2.36	0.46
30:0:2769:C:O2'	30:0:2770:G:H5'	2.15	0.46
2:B:82:VAL:CG1	2:B:101:TRP:CZ3	2.97	0.46
2:B:98:THR:HG22	30:0:2820:A:OP1	2.14	0.46
2:B:258:GLY:HA2	42:0:4877:HOH:O	2.15	0.46
3:C:55:ARG:NH2	27:1:56:GLU:OE2	2.40	0.46
4:D:24:HIS:HB2	4:D:72:LYS:HB3	1.96	0.46
4:D:169:THR:C	4:D:170:TYR:HD1	2.23	0.46
7:G:64:ASN:N	7:G:64:ASN:ND2	2.63	0.46
9:I:130:LEU:HA	42:I:7210:HOH:O	2.15	0.46
10:J:93:ARG:HB3	10:J:93:ARG:NH1	2.21	0.46
11:K:81:ARG:HD3	11:K:87:ARG:CZ	2.46	0.46
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.50	0.46
18:R:82:GLU:O	18:R:86:LYS:HG3	2.15	0.46
23:W:1:MET:HE1	23:W:62:LEU:HD22	1.97	0.46
30:0:12:U:H2'	30:0:13:G:H5'	1.95	0.46
2:B:171:VAL:HG23	2:B:172:SER:N	2.30	0.46
8:H:14:LYS:HB3	42:H:9006:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:79:PRO:HG3	14:N:143:ARG:C	2.39	0.46
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.83	0.46
22:V:16:ARG:NH1	22:V:65:ASP:O	2.49	0.46
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.31	0.46
24:X:23:HIS:NE2	24:X:24:LYS:HD2	2.31	0.46
27:1:5:THR:N	27:1:6:PRO:HD2	2.30	0.46
29:3:24:LYS:HE3	29:3:90:PHE:HE1	1.81	0.46
30:0:334:G:H2'	30:0:335:U:O4'	2.16	0.46
30:0:1158:G:O2'	30:0:1159:G:H5'	2.15	0.46
30:0:1592:G:H2'	30:0:1593:C:H6	1.80	0.46
30:0:1931:A:H2'	30:0:1932:G:H5'	1.97	0.46
30:0:2274:A:O2'	30:0:2275:G:H5'	2.15	0.46
1:A:167:LYS:HB2	26:Z:53:ILE:HD13	1.97	0.46
2:B:5:ARG:HD2	2:B:8:LYS:NZ	2.31	0.46
2:B:294:TYR:CD1	2:B:294:TYR:C	2.93	0.46
4:D:135:VAL:HG22	4:D:136:ARG:H	1.80	0.46
8:H:149:VAL:HG22	42:H:9033:HOH:O	2.15	0.46
8:H:165:ARG:HD2	42:H:9038:HOH:O	2.14	0.46
13:M:158:ARG:HB2	13:M:163:LEU:HB2	1.96	0.46
16:P:91:LYS:HA	42:0:3945:HOH:O	2.15	0.46
17:Q:16:ASN:HB2	42:0:7759:HOH:O	2.15	0.46
28:2:29:THR:O	28:2:30:ASP:C	2.59	0.46
29:3:70:ARG:NH1	29:3:70:ARG:HG2	2.30	0.46
30:0:407:A:H3'	42:0:5323:HOH:O	2.15	0.46
30:0:757:C:H4'	42:0:5053:HOH:O	2.15	0.46
2:B:98:THR:HG21	2:B:127:GLN:OE1	2.16	0.46
5:E:31:ARG:NH1	42:E:5919:HOH:O	2.48	0.46
6:F:38:LYS:HE3	30:0:244:C:OP2	2.15	0.46
14:N:103:ASP:C	14:N:103:ASP:OD1	2.58	0.46
21:U:9:CYS:O	21:U:53:ASP:HB2	2.15	0.46
29:3:17:HIS:O	29:3:18:GLN:HG3	2.16	0.46
30:0:291:C:H2'	30:0:292:G:O4'	2.16	0.46
30:0:407:A:H2'	30:0:408:A:C8	2.51	0.46
30:0:1131:G:C6	30:0:1230:A:C4	3.02	0.46
30:0:1603:A:H5''	30:0:1605:G:H5'	1.97	0.46
30:0:1679:C:O2'	30:0:1685:A:N1	2.46	0.46
30:0:2265:U:H2'	30:0:2266:A:H8	1.80	0.46
30:0:2531:U:C2'	30:0:2532:A:H5'	2.46	0.46
30:0:2649:A:H5'	30:0:2649:A:H8	1.81	0.46
1:A:36:ASP:O	1:A:36:ASP:CG	2.59	0.46
3:C:193:LEU:HD22	3:C:222:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:61:GLN:CD	42:R:8945:HOH:O	2.59	0.46
20:T:12:ARG:NH2	30:0:31:C:OP1	2.49	0.46
30:0:1119:G:N2	30:0:1246:A:N1	2.63	0.46
30:0:1172:G:H1'	42:0:5820:HOH:O	2.14	0.46
30:0:2105:C:H2'	30:0:2106:C:C6	2.51	0.46
31:9:78:G:N3	31:9:78:G:C8	2.84	0.46
1:A:131:HIS:O	1:A:132:ASP:HB2	2.16	0.46
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.79	0.46
2:B:84:LEU:O	2:B:99:GLU:HA	2.16	0.46
4:D:22:VAL:CG2	4:D:74:THR:HG22	2.42	0.46
5:E:7:ILE:HD11	5:E:11:VAL:C	2.40	0.46
6:F:38:LYS:HA	6:F:41:GLU:OE1	2.15	0.46
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.15	0.46
10:J:19:MET:CE	10:J:132:LEU:HD11	2.33	0.46
12:L:20:ASN:HA	42:L:8872:HOH:O	2.16	0.46
12:L:80:ASP:CB	12:L:90:ARG:HB3	2.46	0.46
17:Q:7:LEU:HD12	30:0:2424:U:H1'	1.97	0.46
30:0:1021:G:O2'	30:0:1022:A:H5'	2.15	0.46
30:0:1201:C:H2'	30:0:1202:A:H5'	1.97	0.46
30:0:1393:A:H2'	30:0:1394:C:C6	2.50	0.46
30:0:1398:G:H2'	30:0:1399:A:C8	2.51	0.46
30:0:1985:U:C2	30:0:1996:U:O4'	2.69	0.46
30:0:2039:A:H4'	30:0:2760:C:O2'	2.16	0.46
30:0:2047:C:H2'	30:0:2048:C:H6	1.81	0.46
30:0:2820:A:H2'	30:0:2821:C:C6	2.50	0.46
1:A:101:GLU:O	1:A:103:VAL:HG23	2.16	0.46
2:B:128:ILE:O	2:B:131:ALA:HB3	2.16	0.46
5:E:15:GLN:NE2	5:E:17:HIS:O	2.48	0.46
6:F:20:LEU:HD13	6:F:98:VAL:HG22	1.97	0.46
6:F:86:ALA:C	6:F:88:GLY:H	2.24	0.46
12:L:89:PHE:N	42:L:8877:HOH:O	2.48	0.46
14:N:115:VAL:HG13	42:9:9109:HOH:O	2.16	0.46
15:O:26:TRP:N	42:O:3062:HOH:O	2.49	0.46
15:O:32:ARG:HH21	15:O:35:LYS:NZ	2.12	0.46
18:R:79:ARG:HB3	30:0:2050:G:OP1	2.15	0.46
25:Y:177:LYS:HD3	25:Y:181:GLY:O	2.16	0.46
30:0:694:A:H2'	30:0:695:C:H5'	1.97	0.46
30:0:1180:U:H1'	42:0:4123:HOH:O	2.16	0.46
30:0:2019:A:H5'	42:0:5396:HOH:O	2.15	0.46
30:0:2588:OMG:N2	42:5:3737:HOH:O	2.49	0.46
1:A:42:VAL:HG12	1:A:76:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:MET:SD	30:0:875:A:C2	3.09	0.46
2:B:305:ASP:O	2:B:306:LYS:CB	2.63	0.46
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.49	0.46
8:H:43:ALA:HB1	8:H:140:TYR:CE2	2.51	0.46
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.31	0.46
12:L:10:SER:O	12:L:11:ARG:HB3	2.16	0.46
13:M:54:TYR:CG	13:M:55:LYS:N	2.84	0.46
19:S:33:SER:OG	19:S:36:GLU:HG3	2.15	0.46
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.98	0.46
30:0:445:U:O2'	30:0:446:G:H5'	2.16	0.46
30:0:920:C:H5''	30:0:921:G:O5'	2.16	0.46
30:0:1014:A:H5''	31:9:101:G:O2'	2.16	0.46
30:0:1183:C:H42	30:0:1184:C:H41	1.59	0.46
30:0:1761:U:H2'	30:0:1762:C:C6	2.51	0.46
30:0:1971:G:N2	30:0:2009:G:H2'	2.31	0.46
30:0:2775:A:C6	30:0:2799:A:C8	3.04	0.46
31:9:49:G:H5''	42:9:9090:HOH:O	2.16	0.46
31:9:95:C:O2'	31:9:96:C:H5'	2.16	0.46
2:B:77:PRO:C	2:B:78:PRO:CA	2.89	0.45
2:B:245:SER:OG	30:0:2094:G:H4'	2.17	0.45
3:C:115:LEU:CD2	3:C:243:VAL:HG13	2.41	0.45
4:D:84:LEU:HA	4:D:87:ALA:HB3	1.98	0.45
4:D:104:PHE:CZ	4:D:132:VAL:HG21	2.51	0.45
10:J:88:PRO:O	10:J:94:GLY:HA3	2.16	0.45
13:M:57:LYS:HZ2	13:M:144:ASP:HB2	1.81	0.45
15:O:25:VAL:CG1	30:0:710:G:H5'	2.46	0.45
15:O:32:ARG:HD3	15:O:32:ARG:C	2.42	0.45
19:S:11:THR:H	19:S:14:ALA:HB3	1.81	0.45
23:W:119:HIS:CG	42:0:6126:HOH:O	2.69	0.45
30:0:226:A:H1'	30:0:393:G:C5	2.51	0.45
30:0:282:C:H1'	30:0:368:C:H42	1.76	0.45
30:0:530:C:C4'	30:0:612:U:H4'	2.46	0.45
30:0:816:G:C6	30:0:817:G:N1	2.84	0.45
30:0:820:G:O2'	30:0:856:G:H4'	2.16	0.45
30:0:1159:G:H1	30:0:1208:C:N4	2.14	0.45
30:0:2016:U:H2'	30:0:2017:U:O4'	2.16	0.45
30:0:2032:U:H2'	30:0:2033:G:H5'	1.97	0.45
30:0:2649:A:H5'	30:0:2649:A:C8	2.51	0.45
16:P:59:ARG:O	16:P:63:ARG:HG3	2.16	0.45
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.98	0.45
17:Q:86:VAL:HG11	17:Q:91:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:100:ASP:C	18:R:102:GLN:N	2.73	0.45
30:0:1636:G:O2'	30:0:1637:A:H5'	2.17	0.45
30:0:1730:G:H5'	30:0:1731:C:C6	2.51	0.45
30:0:2314:G:H2'	30:0:2315:C:H5'	1.98	0.45
31:9:49:G:O2'	31:9:50:G:H5'	2.16	0.45
31:9:73:A:H61	31:9:108:C:N4	2.10	0.45
1:A:69:LEU:HD21	1:A:120:ARG:HB3	1.99	0.45
1:A:164:ARG:NE	42:A:9064:HOH:O	2.49	0.45
3:C:54:LEU:HD23	3:C:79:ARG:HG3	1.99	0.45
3:C:162:VAL:CG2	3:C:232:LEU:HD21	2.47	0.45
3:C:214:THR:HG23	42:C:8637:HOH:O	2.16	0.45
11:K:80:ILE:HG23	42:K:7064:HOH:O	2.16	0.45
12:L:22:ARG:HG2	42:0:3882:HOH:O	2.16	0.45
12:L:30:ARG:HD2	42:0:2938:HOH:O	2.15	0.45
14:N:109:PRO:HB3	30:0:2413:A:N7	2.31	0.45
14:N:167:ASP:C	14:N:168:LEU:HG	2.42	0.45
30:0:2649:A:H2'	42:0:6956:HOH:O	2.15	0.45
31:9:39:U:H3'	31:9:40:C:C5'	2.47	0.45
1:A:26:ASP:O	1:A:26:ASP:CG	2.58	0.45
13:M:79:ALA:HB1	30:0:770:C:OP1	2.16	0.45
20:T:77:VAL:C	20:T:78:THR:CA	2.90	0.45
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.16	0.45
24:X:87:ALA:O	24:X:88:GLU:HB3	2.16	0.45
30:0:303:C:H2'	30:0:304:G:O4'	2.16	0.45
30:0:612:U:H2'	30:0:613:C:H6	1.82	0.45
30:0:824:G:N2	42:0:6927:HOH:O	2.48	0.45
31:9:64:C:O2'	31:9:65:A:H5'	2.15	0.45
2:B:62:ARG:HG2	2:B:62:ARG:HH11	1.82	0.45
3:C:27:ARG:CG	3:C:27:ARG:NH1	2.77	0.45
10:J:39:VAL:HG12	10:J:40:ASN:CG	2.42	0.45
11:K:62:PRO:HG3	11:K:65:ARG:NH2	2.31	0.45
16:P:41:ARG:O	16:P:44:VAL:HB	2.17	0.45
18:R:119:VAL:O	18:R:119:VAL:HG13	2.16	0.45
23:W:38:THR:CG2	23:W:39:ASP:N	2.78	0.45
23:W:42:ARG:HA	23:W:45:VAL:CG2	2.47	0.45
30:0:1230:A:H8	30:0:1230:A:OP1	2.00	0.45
30:0:2533:C:H5'	30:0:2533:C:C6	2.43	0.45
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.49	0.45
3:C:236:THR:O	3:C:237:GLU:C	2.59	0.45
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.48	0.45
12:L:41:HIS:HD2	30:0:926:A:O2'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:64:SER:C	14:N:66:LEU:H	2.24	0.45
14:N:154:LEU:C	14:N:156:GLU:H	2.25	0.45
23:W:55:GLY:CA	23:W:146:ILE:HG13	2.46	0.45
25:Y:142:SER:OG	30:0:1331:G:OP2	2.28	0.45
30:0:42:C:H3'	42:0:5033:HOH:O	2.16	0.45
30:0:106:A:O2'	30:0:107:U:H5'	2.17	0.45
30:0:583:C:H2'	30:0:584:U:H6	1.82	0.45
30:0:669:G:O2'	30:0:670:G:H5'	2.16	0.45
30:0:1044:C:H5	42:0:7405:HOH:O	2.00	0.45
30:0:1377:C:O2'	30:0:1378:G:H5''	2.17	0.45
30:0:1566:C:H2'	30:0:1567:G:C8	2.52	0.45
30:0:2038:A:O2'	30:0:2039:A:H5'	2.16	0.45
2:B:80:ARG:HB2	2:B:145:HIS:CE1	2.51	0.45
2:B:254:GLN:HG3	42:B:9001:HOH:O	2.16	0.45
4:D:91:ALA:HB2	4:D:106:PHE:CD2	2.52	0.45
21:U:39:ASN:ND2	21:U:44:ARG:HH11	2.15	0.45
26:Z:51:ALA:O	26:Z:55:SER:HB2	2.15	0.45
30:0:2768:A:O2'	30:0:2769:C:H5'	2.17	0.45
31:9:18:U:H2'	31:9:19:G:H8	1.82	0.45
2:B:232:TRP:HD1	2:B:235:ARG:HD2	1.82	0.45
2:B:268:ARG:NH2	2:B:325:PRO:HG3	2.32	0.45
4:D:21:VAL:HG23	4:D:80:ALA:HB1	1.99	0.45
4:D:52:THR:O	4:D:68:PRO:HA	2.16	0.45
5:E:2:ARG:NH2	5:E:48:VAL:HG21	2.32	0.45
5:E:22:VAL:HG12	5:E:76:VAL:HG11	1.99	0.45
6:F:70:LYS:C	6:F:72:VAL:H	2.24	0.45
8:H:157:TYR:CD1	8:H:157:TYR:C	2.93	0.45
14:N:7:LYS:HB3	30:0:2353:A:O2'	2.17	0.45
22:V:16:ARG:HH12	22:V:65:ASP:C	2.25	0.45
24:X:30:MET:CE	24:X:58:ALA:HB3	2.46	0.45
25:Y:112:GLU:HA	25:Y:112:GLU:OE1	2.17	0.45
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.99	0.45
30:0:939:A:N1	30:0:1027:G:O2'	2.45	0.45
30:0:1202:A:H2'	30:0:1203:G:O4'	2.17	0.45
30:0:2831:C:H2'	30:0:2832:C:H5'	1.99	0.45
1:A:125:ASN:CB	1:A:158:VAL:HG12	2.47	0.45
1:A:130:THR:HG22	1:A:131:HIS:N	2.30	0.45
2:B:233:ARG:HG2	2:B:233:ARG:HH11	1.81	0.45
8:H:143:VAL:HG21	8:H:173:GLU:HG2	1.98	0.45
12:L:27:ARG:HD2	30:0:757:C:OP1	2.17	0.45
15:O:63:LYS:HG3	15:O:80:ASP:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:103:GLU:O	15:O:106:PRO:HD3	2.16	0.45
26:Z:54:GLU:HG2	26:Z:57:MET:CE	2.47	0.45
28:2:2:LYS:HG3	30:0:1486:A:C5	2.52	0.45
30:0:1739:G:O2'	30:0:1740:U:H5'	2.17	0.45
30:0:2047:C:H2'	30:0:2048:C:C6	2.52	0.45
9:I:108:HIS:N	9:I:109:PRO:CD	2.80	0.45
12:L:75:LEU:C	12:L:77:ALA:H	2.25	0.45
13:M:64:ARG:HD2	42:M:8887:HOH:O	2.17	0.45
19:S:30:ASP:HA	19:S:62:LYS:HE3	1.98	0.45
20:T:48:VAL:O	20:T:59:GLU:HA	2.17	0.45
20:T:79:LEU:HG	20:T:89:ARG:HB2	1.99	0.45
22:V:5:VAL:CG1	22:V:9:ARG:NH1	2.80	0.45
4:D:59:GLY:O	4:D:61:PHE:N	2.50	0.44
5:E:22:VAL:O	5:E:28:SER:HA	2.17	0.44
5:E:170:ARG:NH2	42:E:4761:HOH:O	2.50	0.44
6:F:39:SER:O	6:F:43:GLY:N	2.50	0.44
8:H:36:MET:HB3	8:H:73:ASN:ND2	2.32	0.44
8:H:49:GLN:NE2	8:H:140:TYR:CE2	2.73	0.44
13:M:102:GLU:OE2	13:M:164:THR:HG21	2.16	0.44
20:T:41:ARG:HG2	20:T:41:ARG:NH1	2.31	0.44
24:X:71:ARG:HD3	42:X:7542:HOH:O	2.16	0.44
29:3:62:THR:HB	42:3:9041:HOH:O	2.17	0.44
30:0:1165:G:O2'	30:0:1174:A:H4'	2.17	0.44
30:0:2432:C:O2'	30:0:2433:A:H5'	2.17	0.44
30:0:2754:G:H2'	30:0:2755:G:O4'	2.17	0.44
31:9:78:G:N2	31:9:102:G:H2'	2.33	0.44
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.18	0.44
1:A:58:VAL:HG21	1:A:80:LEU:HD12	1.98	0.44
2:B:42:ALA:CB	2:B:162:MET:HE1	2.47	0.44
42:B:9118:HOH:O	30:0:2672:C:H1'	2.17	0.44
3:C:233:THR:CG2	3:C:234:VAL:H	2.24	0.44
6:F:50:VAL:HG21	6:F:63:ILE:HG21	1.99	0.44
9:I:129:SER:HB3	30:0:1192:A:N6	2.32	0.44
42:K:4183:HOH:O	30:0:2712:G:H5'	2.17	0.44
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.52	0.44
13:M:82:ARG:O	13:M:84:LYS:N	2.50	0.44
42:N:8814:HOH:O	31:9:36:C:H4'	2.17	0.44
21:U:44:ARG:HB3	42:U:3805:HOH:O	2.17	0.44
30:0:416:G:OP1	30:0:417:G:H5'	2.18	0.44
30:0:559:U:H5'	30:0:559:U:C6	2.37	0.44
30:0:661:G:C5	30:0:686:A:C2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1342:C:H2'	30:0:1343:C:H5'	1.99	0.44
30:0:1839:A:H5'	30:0:2643:G:H4'	1.99	0.44
30:0:2379:G:N7	30:0:2408:A:N1	2.64	0.44
30:0:2589:U:H2'	30:0:2590:U:C6	2.52	0.44
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.99	0.44
3:C:84:VAL:O	3:C:85:LYS:HB2	2.17	0.44
5:E:88:TYR:CE1	5:E:92:PRO:HA	2.52	0.44
6:F:83:LEU:HD11	6:F:96:ALA:HB3	1.98	0.44
11:K:22:ASP:C	11:K:22:ASP:OD1	2.60	0.44
13:M:167:GLY:O	13:M:171:ARG:HG3	2.18	0.44
18:R:40:ALA:HB3	18:R:107:GLU:HA	1.99	0.44
20:T:17:HIS:HB3	30:0:100:C:O2	2.17	0.44
21:U:56:ARG:O	21:U:56:ARG:HD2	2.17	0.44
25:Y:189:ASN:CA	25:Y:217:ILE:HD11	2.38	0.44
30:0:77:G:C2'	30:0:78:G:H5'	2.47	0.44
30:0:1204:C:H2'	30:0:1205:U:O4'	2.16	0.44
30:0:2816:A:H5''	30:0:2817:G:H5'	1.98	0.44
5:E:93:MET:HE2	5:E:107:PHE:CD1	2.53	0.44
5:E:158:ASP:C	5:E:158:ASP:OD1	2.60	0.44
6:F:7:ASP:O	6:F:118:LEU:HD21	2.18	0.44
12:L:101:ASP:C	12:L:103:ALA:H	2.25	0.44
13:M:133:LEU:O	13:M:134:ILE:HD13	2.17	0.44
14:N:40:ASN:HD21	31:9:28:U:H5''	1.81	0.44
14:N:141:ARG:HH21	31:9:48:C:H4'	1.82	0.44
15:O:14:LEU:CG	15:O:102:ILE:HD11	2.48	0.44
18:R:94:ASN:ND2	30:0:500:G:O2'	2.49	0.44
21:U:4:ARG:HG2	21:U:4:ARG:HH11	1.82	0.44
23:W:65:VAL:HA	23:W:68:THR:CG2	2.47	0.44
25:Y:144:ARG:NE	42:Y:8923:HOH:O	2.51	0.44
30:0:308:U:H5'	30:0:309:C:OP1	2.16	0.44
30:0:1774:G:H1'	42:0:5396:HOH:O	2.16	0.44
30:0:2857:C:H2'	30:0:2858:U:C6	2.52	0.44
1:A:36:ASP:C	1:A:38:ILE:N	2.76	0.44
2:B:145:HIS:CD2	2:B:159:PRO:HB3	2.51	0.44
3:C:174:ILE:HD11	30:0:338:C:H4'	1.98	0.44
3:C:180:SER:HB3	42:C:8647:HOH:O	2.18	0.44
10:J:39:VAL:HG11	10:J:107:ASN:CB	2.48	0.44
11:K:14:LYS:CB	11:K:45:PRO:HG2	2.42	0.44
13:M:57:LYS:NZ	13:M:144:ASP:HB2	2.32	0.44
13:M:60:VAL:HG22	13:M:134:ILE:HD12	1.99	0.44
14:N:37:ARG:HA	14:N:37:ARG:HD3	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:51:TYR:CD1	30:0:721:A:H4'	2.52	0.44
23:W:108:ARG:NH2	23:W:114:PRO:HG2	2.32	0.44
30:0:380:A:O4'	30:0:382:U:H1'	2.18	0.44
30:0:629:A:C2	30:0:2074:A:C2	3.06	0.44
30:0:1427:A:H61	30:0:1440:U:C1'	2.30	0.44
30:0:1805:G:O2'	30:0:1806:G:H5'	2.18	0.44
2:B:264:GLU:OE2	2:B:302:PRO:HD3	2.18	0.44
2:B:284:PHE:HB2	2:B:287:TYR:HB3	1.99	0.44
3:C:85:LYS:HD3	42:0:3695:HOH:O	2.17	0.44
3:C:225:PRO:O	30:0:1308:A:H4'	2.17	0.44
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.17	0.44
4:D:158:ASN:HB2	4:D:161:ASP:OD2	2.17	0.44
5:E:162:PHE:N	5:E:162:PHE:CD1	2.85	0.44
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.33	0.44
9:I:72:GLU:C	9:I:74:ILE:N	2.76	0.44
11:K:41:LYS:HA	30:0:2582:G:O3'	2.17	0.44
12:L:104:ASP:O	12:L:105:TYR:HB3	2.17	0.44
12:L:121:ILE:HG12	12:L:141:GLU:HB2	2.00	0.44
13:M:82:ARG:C	13:M:84:LYS:N	2.76	0.44
13:M:134:ILE:HG23	13:M:141:ILE:CD1	2.38	0.44
18:R:84:ALA:O	18:R:88:PHE:HD1	2.01	0.44
23:W:44:MET:CE	30:0:944:G:H21	2.30	0.44
24:X:15:ARG:HB3	24:X:15:ARG:HH11	1.83	0.44
30:0:157:G:H3'	42:0:4825:HOH:O	2.16	0.44
30:0:318:U:H5'	30:0:339:A:C2	2.53	0.44
30:0:463:A:H5'	30:0:465:U:O4'	2.17	0.44
30:0:2906:A:H5'	30:0:2907:C:O4'	2.18	0.44
31:9:29:C:C2'	31:9:30:C:H5'	2.43	0.44
1:A:217:ARG:CG	1:A:217:ARG:NH1	2.80	0.44
2:B:238:ASN:ND2	2:B:240:GLY:H	2.01	0.44
2:B:266:ASN:OD1	2:B:317:PRO:HA	2.17	0.44
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.86	0.44
11:K:21:ALA:HB1	11:K:110:LYS:O	2.18	0.44
15:O:97:SER:H	15:O:100:GLN:NE2	2.16	0.44
18:R:135:ALA:O	30:0:2054:A:H4'	2.18	0.44
19:S:81:ILE:C	19:S:81:ILE:HD12	2.43	0.44
23:W:115:THR:HG23	42:W:5420:HOH:O	2.18	0.44
26:Z:40:ALA:HA	30:0:1773:G:C8	2.51	0.44
27:1:45:ARG:HB3	42:1:988:HOH:O	2.18	0.44
30:0:336:G:H2'	42:0:4598:HOH:O	2.16	0.44
30:0:764:C:H2'	30:0:765:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:814:G:H2'	30:0:815:U:C6	2.52	0.44
30:0:1333:U:H2'	30:0:1334:C:H6	1.81	0.44
30:0:1603:A:H5''	30:0:1604:G:H3'	2.00	0.44
30:0:1682:A:H5''	42:0:3364:HOH:O	2.18	0.44
30:0:2253:G:O2'	30:0:2254:G:H5'	2.18	0.44
30:0:2543:G:H2'	30:0:2544:G:O4'	2.18	0.44
31:9:7:G:H5'	42:9:9099:HOH:O	2.18	0.44
1:A:212:PRO:HA	30:0:1943:C:O4'	2.17	0.44
2:B:132:HIS:CE1	2:B:171:VAL:HG21	2.53	0.44
2:B:281:ASP:C	2:B:283:GLY:H	2.24	0.44
2:B:300:SER:HB3	42:0:5521:HOH:O	2.18	0.44
3:C:242:GLU:C	3:C:244:ALA:N	2.75	0.44
4:D:156:ARG:HG3	4:D:156:ARG:NH1	2.32	0.44
10:J:64:GLY:HA3	35:J:8821:CL:CL	2.55	0.44
13:M:124:GLY:HA3	30:0:2132:C:H1'	1.99	0.44
14:N:6:TYR:HB3	31:9:11:A:N6	2.32	0.44
14:N:112:GLY:HA2	14:N:137:ALA:H	1.82	0.44
14:N:182:GLY:O	14:N:184:ILE:HG22	2.18	0.44
18:R:39:THR:CB	18:R:42:GLU:HG3	2.47	0.44
19:S:10:VAL:HG11	22:V:36:ALA:CB	2.48	0.44
25:Y:145:LYS:HE2	42:Y:8917:HOH:O	2.17	0.44
30:0:177:A:H2'	30:0:178:U:O4'	2.17	0.44
30:0:522:U:O2'	30:0:1366:C:H5'	2.17	0.44
30:0:613:C:H2'	30:0:614:U:H6	1.83	0.44
30:0:746:A:H4'	30:0:747:G:H5'	1.99	0.44
30:0:1207:A:H5'	30:0:1208:C:OP2	2.18	0.44
30:0:2032:U:C2'	30:0:2033:G:H5''	2.48	0.44
30:0:2608:C:H2'	42:0:4450:HOH:O	2.18	0.44
30:0:2718:C:H5'	30:0:2718:C:C6	2.50	0.44
30:0:2879:A:H2'	30:0:2880:A:O4'	2.17	0.44
31:9:13:A:H3'	31:9:14:G:H5'	2.00	0.44
2:B:274:GLU:HA	2:B:292:GLY:O	2.17	0.44
4:D:103:ASN:ND2	4:D:134:LEU:H	2.16	0.44
6:F:48:VAL:HG23	6:F:74:PHE:CB	2.47	0.44
6:F:101:ALA:HB3	6:F:105:ASP:OD1	2.18	0.44
7:G:13:PRO:HD2	7:G:16:LYS:HD2	1.99	0.44
10:J:12:VAL:HG21	10:J:116:LEU:HD11	1.99	0.44
10:J:142:ASN:O	10:J:144:THR:N	2.51	0.44
12:L:134:GLU:HA	12:L:138:GLY:O	2.18	0.44
13:M:159:VAL:HG13	13:M:160:PHE:N	2.32	0.44
14:N:140:GLN:O	14:N:143:ARG:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:84:THR:O	15:O:85:ALA:C	2.60	0.44
23:W:9:GLY:H	30:0:1086:A:P	2.41	0.44
24:X:49:ARG:NH1	30:0:1385:G:O3'	2.51	0.44
25:Y:182:PHE:CG	25:Y:202:ALA:HB2	2.53	0.44
27:1:28:HIS:O	27:1:32:LYS:N	2.45	0.44
30:0:660:A:H4'	30:0:661:G:O5'	2.18	0.44
30:0:1160:G:H5'	30:0:1161:A:C4'	2.48	0.44
30:0:1252:A:H2'	30:0:1253:C:O4'	2.18	0.44
30:0:1697:G:H1'	42:0:9075:HOH:O	2.17	0.44
30:0:2323:G:H5'	42:0:7820:HOH:O	2.17	0.44
42:C:8558:HOH:O	30:0:656:G:H4'	2.18	0.43
6:F:48:VAL:HG12	6:F:97:ALA:HB2	2.00	0.43
8:H:19:ARG:HH21	8:H:21:GLU:CD	2.25	0.43
8:H:59:GLN:HG2	8:H:129:ARG:HG2	1.99	0.43
12:L:73:VAL:HG23	12:L:74:THR:N	2.31	0.43
15:O:38:ARG:NH1	42:O:7674:HOH:O	2.50	0.43
23:W:10:GLU:HG3	23:W:11:VAL:N	2.32	0.43
24:X:23:HIS:C	24:X:24:LYS:HG3	2.42	0.43
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.53	0.43
30:0:152:A:O2'	30:0:153:C:H5'	2.17	0.43
30:0:187:A:H3'	30:0:188:C:H6	1.83	0.43
30:0:243:A:H61	30:0:269:G:H1'	1.83	0.43
30:0:314:G:N2	30:0:316:A:H3'	2.33	0.43
30:0:538:C:H5''	30:0:539:G:C8	2.51	0.43
30:0:671:A:O2'	30:0:672:G:H2'	2.18	0.43
30:0:855:U:H5'	42:0:9252:HOH:O	2.18	0.43
30:0:1790:C:H2'	30:0:1791:U:C6	2.53	0.43
30:0:1855:G:H4'	30:0:1856:C:O5'	2.17	0.43
30:0:2346:C:H6	30:0:2346:C:O5'	2.01	0.43
30:0:2511:A:H4'	42:0:6305:HOH:O	2.18	0.43
3:C:57:PRO:O	3:C:58:ALA:C	2.60	0.43
4:D:10:PHE:O	4:D:14:ARG:HG3	2.18	0.43
9:I:96:SER:HB3	9:I:99:GLN:NE2	2.34	0.43
11:K:14:LYS:HD2	35:K:8812:CL:CL	2.55	0.43
11:K:28:GLU:CB	11:K:59:LYS:HB2	2.44	0.43
12:L:27:ARG:NH2	12:L:30:ARG:HG2	2.33	0.43
15:O:24:ALA:HB3	30:0:710:G:OP1	2.17	0.43
17:Q:77:ASP:O	17:Q:78:GLY:CA	2.66	0.43
18:R:59:PHE:O	18:R:63:ASN:HB3	2.18	0.43
27:1:18:LYS:HA	27:1:25:LYS:HA	2.00	0.43
30:0:319:A:H4'	30:0:338:C:C5	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1309:U:C2'	30:0:1310:U:H5'	2.49	0.43
30:0:1659:A:H2'	30:0:1660:G:O4'	2.17	0.43
30:0:1730:G:H5''	30:0:1731:C:C6	2.53	0.43
30:0:1979:G:O2'	30:0:1980:U:OP1	2.34	0.43
30:0:2510:C:H42	30:0:2564:G:H22	1.66	0.43
30:0:2537:G:O5'	30:0:2538:A:H5''	2.18	0.43
1:A:235:ARG:HB2	42:A:9026:HOH:O	2.17	0.43
16:P:37:ARG:NH2	30:0:1502:A:OP1	2.50	0.43
19:S:49:VAL:HG13	19:S:66:VAL:HG13	2.00	0.43
19:S:73:ASP:HB3	19:S:76:GLU:OE1	2.17	0.43
23:W:142:ASP:HB3	23:W:145:GLY:H	1.84	0.43
29:3:65:THR:CG2	29:3:67:LEU:HG	2.39	0.43
30:0:841:A:H5''	42:0:7715:HOH:O	2.17	0.43
30:0:951:A:O2'	30:0:952:G:H5'	2.18	0.43
30:0:1477:C:H5'	30:0:1868:G:H5'	2.00	0.43
30:0:2645:U:OP2	30:0:2645:U:H6	2.02	0.43
2:B:154:VAL:HG12	2:B:156:LYS:HG2	2.00	0.43
3:C:115:LEU:HD12	3:C:115:LEU:HA	1.80	0.43
5:E:84:MET:SD	5:E:168:ILE:HD13	2.58	0.43
6:F:117:GLU:C	6:F:119:ARG:H	2.25	0.43
9:I:81:GLU:OE1	9:I:81:GLU:N	2.51	0.43
11:K:82:ARG:O	11:K:85:GLY:N	2.50	0.43
15:O:65:LEU:HD13	30:0:746:A:C6	2.53	0.43
16:P:41:ARG:HH22	30:0:1500:U:P	2.41	0.43
19:S:38:ALA:O	19:S:42:GLU:HG3	2.19	0.43
23:W:65:VAL:CA	23:W:68:THR:HG22	2.48	0.43
30:0:1056:U:H2'	30:0:1057:A:O4'	2.19	0.43
30:0:1803:C:H2'	30:0:1804:A:H8	1.82	0.43
30:0:2507:G:H2'	30:0:2510:C:N4	2.32	0.43
3:C:234:VAL:HG13	3:C:234:VAL:O	2.18	0.43
14:N:21:HIS:HB2	42:N:8831:HOH:O	2.19	0.43
14:N:111:PRO:HD2	31:9:37:C:H4'	2.00	0.43
18:R:106:GLY:HA2	18:R:109:MET:CE	2.47	0.43
20:T:43:ASN:O	20:T:45:GLY:N	2.50	0.43
28:2:10:ARG:NH1	28:2:49:GLU:CD	2.77	0.43
30:0:95:A:O5'	30:0:97:G:H5'	2.19	0.43
30:0:2557:U:H3'	42:0:7487:HOH:O	2.18	0.43
30:0:2748:G:H8	42:0:9326:HOH:O	2.01	0.43
30:0:2768:A:H2'	30:0:2769:C:O4'	2.19	0.43
31:9:54:A:O2'	31:9:55:U:H5'	2.18	0.43
1:A:132:ASP:OD1	1:A:133:ARG:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.51	0.43
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.84	0.43
4:D:88:LEU:HB2	4:D:89:PRO:HD3	2.00	0.43
10:J:59:LYS:O	10:J:63:ILE:HG13	2.19	0.43
11:K:62:PRO:HG3	11:K:65:ARG:HH22	1.82	0.43
11:K:69:LEU:HD12	11:K:97:ILE:HD13	2.01	0.43
13:M:5:TYR:O	13:M:6:SER:C	2.62	0.43
14:N:97:VAL:HG12	14:N:127:LEU:HD11	1.99	0.43
14:N:182:GLY:O	14:N:183:ASP:C	2.61	0.43
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.13	0.43
22:V:1:THR:CB	30:0:93:C:H5''	2.44	0.43
22:V:45:ARG:HA	22:V:48:GLU:HB2	2.00	0.43
30:0:23:G:H1'	30:0:520:A:N6	2.34	0.43
30:0:706:G:N2	30:0:707:C:H41	2.16	0.43
30:0:1926:G:H2'	30:0:1927:A:C8	2.53	0.43
30:0:2769:C:H2'	30:0:2770:G:C5'	2.49	0.43
1:A:34:ASP:C	1:A:36:ASP:H	2.26	0.43
1:A:114:ASP:OD1	1:A:115:GLY:N	2.52	0.43
1:A:176:HIS:CD2	30:0:857:A:H4'	2.54	0.43
1:A:223:ARG:NH2	42:A:9054:HOH:O	2.51	0.43
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.48	0.43
5:E:15:GLN:HG3	5:E:20:ILE:HG12	2.01	0.43
5:E:118:ILE:HG23	5:E:144:THR:HG21	2.00	0.43
17:Q:31:GLU:OE1	17:Q:31:GLU:HA	2.19	0.43
28:2:13:LYS:O	28:2:17:GLN:HG3	2.18	0.43
42:3:9017:HOH:O	30:0:2468:A:H4'	2.18	0.43
30:0:77:G:H2'	30:0:78:G:H5'	2.00	0.43
30:0:264:G:H1'	30:0:265:U:H5	1.84	0.43
30:0:521:A:H2'	30:0:522:U:H5'	2.00	0.43
30:0:878:G:H4'	30:0:1835:U:H4'	2.01	0.43
30:0:1524:U:H6	30:0:1524:U:H5''	1.83	0.43
30:0:2506:A:O2'	30:0:2507:G:P	2.77	0.43
33:6:75:C:H5''	33:6:76:8AN:O1P	2.18	0.43
1:A:1:GLY:HA2	1:A:197:VAL:HG23	2.00	0.43
1:A:42:VAL:O	1:A:76:VAL:HG13	2.19	0.43
2:B:201:ASP:HB2	2:B:312:ARG:HD2	2.01	0.43
2:B:285:VAL:O	2:B:286:ASN:HB2	2.18	0.43
3:C:193:LEU:HA	3:C:211:ASP:O	2.19	0.43
5:E:146:ALA:O	5:E:150:GLN:HG2	2.19	0.43
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.99	0.43
8:H:153:PHE:HD1	8:H:166:ILE:HG23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:87:PRO:HB2	9:I:129:SER:HA	2.01	0.43
11:K:115:ARG:HG3	11:K:116:GLU:N	2.33	0.43
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.48	0.43
17:Q:86:VAL:HG13	17:Q:91:LEU:HD11	1.99	0.43
22:V:12:THR:HG22	22:V:15:GLU:CD	2.43	0.43
30:0:317:A:H5'	42:0:4644:HOH:O	2.18	0.43
30:0:497:A:H2'	30:0:498:A:C5'	2.49	0.43
30:0:607:G:H2'	30:0:608:A:O4'	2.19	0.43
30:0:1120:U:H5''	30:0:1120:U:C6	2.54	0.43
30:0:1180:U:H2'	30:0:1181:A:H8	1.81	0.43
30:0:1603:A:H5'	30:0:1605:G:C4'	2.48	0.43
30:0:1921:A:C6	30:0:1922:A:C2	3.07	0.43
30:0:2550:U:O2'	30:0:2551:C:H5'	2.19	0.43
1:A:71:PRO:HA	1:A:158:VAL:O	2.19	0.43
1:A:105:VAL:HG11	1:A:154:ALA:HB1	2.00	0.43
1:A:217:ARG:HG2	1:A:229:ALA:HB2	2.01	0.43
2:B:279:THR:CG2	2:B:280:VAL:N	2.81	0.43
5:E:132:THR:HB	42:E:2227:HOH:O	2.19	0.43
9:I:91:PHE:HA	9:I:131:GLY:CA	2.49	0.43
14:N:73:ALA:HB1	14:N:74:PRO:HD2	2.00	0.43
16:P:80:ARG:HG2	16:P:87:ARG:NH2	2.34	0.43
22:V:50:ARG:HD3	42:V:2826:HOH:O	2.18	0.43
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.82	0.43
25:Y:152:LYS:HB3	25:Y:160:LYS:HG3	2.01	0.43
25:Y:155:ARG:NH1	42:Y:8864:HOH:O	2.52	0.43
25:Y:184:GLU:CD	25:Y:204:ARG:NH1	2.77	0.43
27:1:10:LYS:HG3	42:1:2979:HOH:O	2.18	0.43
30:0:559:U:H6	30:0:559:U:C5'	2.25	0.43
30:0:1117:A:C2	30:0:1244:U:C2	3.07	0.43
30:0:1268:C:H2'	30:0:1269:G:H8	1.84	0.43
30:0:1698:U:O5'	30:0:1698:U:H6	2.02	0.43
1:A:9:ARG:O	1:A:10:GLY:C	2.61	0.43
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.85	0.43
3:C:19:PRO:CD	3:C:240:LEU:HD22	2.49	0.43
4:D:25:MET:CE	4:D:40:ILE:HD11	2.49	0.43
4:D:136:ARG:HB3	4:D:137:PRO:HD2	2.01	0.43
6:F:4:VAL:HG13	6:F:76:PHE:CD1	2.54	0.43
9:I:130:LEU:HB2	9:I:132:VAL:HG23	2.00	0.43
11:K:9:THR:HA	42:0:4173:HOH:O	2.19	0.43
17:Q:46:SER:O	17:Q:48:PRO:HD3	2.18	0.43
23:W:125:HIS:NE2	30:0:1097:A:H5''	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:485:A:N3	30:0:487:G:H5'	2.34	0.43
30:0:523:C:H2'	30:0:524:A:H8	1.84	0.43
30:0:1657:A:H2'	30:0:1658:A:C8	2.54	0.43
30:0:2456:A:H2'	30:0:2457:U:H6	1.83	0.43
30:0:2618:G:N3	32:5:76:A:C2	2.87	0.43
30:0:2697:A:H2'	30:0:2698:G:O4'	2.19	0.43
1:A:211:LYS:NZ	42:A:9049:HOH:O	2.47	0.42
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.84	0.42
2:B:152:PRO:HA	42:B:9043:HOH:O	2.19	0.42
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.83	0.42
2:B:312:ARG:O	2:B:313:PRO:C	2.62	0.42
6:F:80:GLN:HB3	42:F:2563:HOH:O	2.19	0.42
8:H:76:LEU:HD21	8:H:149:VAL:HA	2.01	0.42
8:H:157:TYR:C	8:H:157:TYR:HD1	2.26	0.42
12:L:35:ARG:NH1	12:L:43:HIS:CD2	2.87	0.42
13:M:98:GLN:O	13:M:102:GLU:HG3	2.19	0.42
13:M:157:ASP:HB3	13:M:160:PHE:HD1	1.84	0.42
14:N:114:LYS:O	14:N:118:ILE:HG13	2.19	0.42
14:N:147:ILE:HG23	14:N:148:ALA:N	2.34	0.42
15:O:97:SER:H	15:O:100:GLN:HE21	1.67	0.42
20:T:81:LYS:HG3	20:T:87:VAL:HG13	2.00	0.42
30:0:876:A:N3	30:0:876:A:C2'	2.82	0.42
30:0:1947:G:H2'	30:0:1948:G:C8	2.54	0.42
30:0:2106:C:H1'	30:0:2484:U:O2	2.19	0.42
30:0:2611:G:H5'	30:0:2613:G:C8	2.53	0.42
3:C:118:THR:HG23	42:C:8504:HOH:O	2.19	0.42
3:C:120:ASP:O	3:C:121:ALA:C	2.62	0.42
3:C:157:LEU:CD1	3:C:166:ILE:HD11	2.49	0.42
5:E:68:HIS:O	5:E:72:MET:HG3	2.18	0.42
12:L:41:HIS:CD2	30:0:926:A:O2'	2.73	0.42
12:L:50:GLY:HA2	30:0:2453:G:O3'	2.19	0.42
13:M:123:ASP:C	13:M:123:ASP:OD1	2.61	0.42
15:O:19:ARG:NH1	30:0:1276:U:H3'	2.34	0.42
16:P:16:VAL:HG13	16:P:20:ARG:CZ	2.49	0.42
17:Q:17:LYS:O	17:Q:18:PRO:C	2.61	0.42
29:3:48:ASN:ND2	29:3:50:GLY:H	2.17	0.42
30:0:426:G:O2'	30:0:427:C:H5'	2.19	0.42
30:0:772:G:H2'	30:0:773:A:O4'	2.19	0.42
30:0:1210:G:O2'	30:0:1211:G:H5'	2.19	0.42
30:0:1574:C:O5'	30:0:1574:C:H6	2.03	0.42
30:0:2064:U:H5'	30:0:2652:U:O3'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2087:C:O2'	30:0:2088:C:H5'	2.20	0.42
30:0:2756:U:O2	30:0:2896:A:H2	2.02	0.42
31:9:49:G:C2'	31:9:50:G:H5'	2.50	0.42
32:5:74:C:N4	42:5:3737:HOH:O	2.39	0.42
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.86	0.42
2:B:87:TYR:O	2:B:138:GLY:N	2.42	0.42
2:B:119:HIS:O	2:B:121:PRO:HD3	2.19	0.42
5:E:101:GLU:HA	5:E:118:ILE:HG13	2.02	0.42
6:F:86:ALA:C	6:F:88:GLY:N	2.77	0.42
7:G:12:ILE:HG22	7:G:17:GLN:HE21	1.82	0.42
8:H:62:HIS:HA	8:H:65:LEU:HD23	2.02	0.42
13:M:71:SER:CB	13:M:92:THR:HG22	2.49	0.42
13:M:188:ARG:HB2	30:0:156:C:OP2	2.18	0.42
14:N:143:ARG:HE	14:N:143:ARG:HB3	1.61	0.42
21:U:52:THR:HG21	21:U:54:THR:HB	2.01	0.42
23:W:154:ARG:NH2	42:W:321:HOH:O	2.51	0.42
30:0:2129:U:H2'	30:0:2130:C:C6	2.54	0.42
2:B:87:TYR:OH	2:B:163:GLU:OE2	2.27	0.42
3:C:149:LYS:NZ	30:0:327:A:OP1	2.42	0.42
4:D:88:LEU:N	4:D:89:PRO:CD	2.82	0.42
14:N:82:TYR:CD2	14:N:82:TYR:C	2.97	0.42
25:Y:184:GLU:CD	25:Y:204:ARG:HH11	2.27	0.42
30:0:523:C:H2'	30:0:524:A:C8	2.54	0.42
30:0:960:G:N3	30:0:960:G:C2'	2.83	0.42
30:0:1378:G:O4'	30:0:2747:C:N4	2.48	0.42
30:0:2569:A:H2'	30:0:2570:G:O5'	2.20	0.42
1:A:211:LYS:CB	42:A:9094:HOH:O	2.65	0.42
2:B:75:GLU:O	2:B:77:PRO:HD3	2.19	0.42
4:D:55:LYS:HA	4:D:65:GLU:HG3	2.01	0.42
4:D:99:ASP:OD2	4:D:101:THR:HB	2.18	0.42
5:E:137:ASP:OD1	5:E:139:GLU:N	2.52	0.42
13:M:46:LEU:HD22	13:M:50:ARG:CD	2.50	0.42
14:N:108:SER:HA	14:N:109:PRO:HD3	1.75	0.42
15:O:32:ARG:O	15:O:35:LYS:HB2	2.20	0.42
16:P:97:ARG:HD2	42:P:163:HOH:O	2.19	0.42
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.45	0.42
20:T:102:ASP:C	20:T:102:ASP:OD1	2.63	0.42
27:1:28:HIS:HD2	27:1:31:LYS:H	1.66	0.42
29:3:70:ARG:HG2	29:3:70:ARG:HH11	1.84	0.42
30:0:371:U:H2'	30:0:372:A:H8	1.84	0.42
30:0:858:U:H2'	30:0:859:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1307:A:H2'	30:0:1308:A:C8	2.55	0.42
30:0:1819:G:H2'	30:0:1820:G:C4'	2.50	0.42
31:9:107:C:H5	42:9:9060:HOH:O	2.02	0.42
1:A:20:SER:C	1:A:22:ARG:N	2.77	0.42
3:C:51:TYR:O	3:C:54:LEU:HB2	2.20	0.42
11:K:66:ARG:HD2	30:0:1992:U:OP2	2.19	0.42
12:L:18:HIS:HB2	30:0:903:U:O4	2.20	0.42
15:O:1:SER:HA	42:O:7521:HOH:O	2.18	0.42
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.84	0.42
30:0:595:U:O5'	30:0:595:U:H6	2.03	0.42
30:0:696:C:O2'	30:0:697:G:H5'	2.20	0.42
30:0:1139:U:H2'	30:0:1140:C:C6	2.54	0.42
30:0:1589:G:C2	30:0:1605:G:N3	2.87	0.42
30:0:2435:U:H1'	42:0:6264:HOH:O	2.19	0.42
1:A:188:ASN:HA	42:A:9046:HOH:O	2.19	0.42
1:A:194:MET:CE	1:A:199:HIS:HB2	2.49	0.42
2:B:51:VAL:CG2	2:B:330:VAL:HG22	2.47	0.42
2:B:56:ASP:HB3	2:B:322:ARG:HH21	1.83	0.42
2:B:244:PRO:HB3	30:0:1234:U:N3	2.34	0.42
3:C:237:GLU:HB2	42:C:8632:HOH:O	2.19	0.42
5:E:7:ILE:HD11	5:E:11:VAL:CG1	2.48	0.42
5:E:84:MET:HB2	5:E:131:LEU:HB2	2.00	0.42
11:K:87:ARG:CZ	42:K:4854:HOH:O	2.67	0.42
12:L:89:PHE:N	12:L:89:PHE:CD1	2.87	0.42
12:L:140:VAL:HB	42:L:8861:HOH:O	2.18	0.42
22:V:1:THR:C	22:V:3:LEU:N	2.77	0.42
24:X:66:THR:CG2	24:X:67:PRO:HD2	2.50	0.42
30:0:440:C:H2'	30:0:441:A:C8	2.54	0.42
30:0:553:G:O4'	30:0:1325:G:H5'	2.19	0.42
30:0:1386:G:O2'	30:0:1387:G:H5'	2.20	0.42
30:0:2042:U:H2'	30:0:2043:U:C6	2.53	0.42
30:0:2064:U:H4'	30:0:2653:A:OP1	2.18	0.42
30:0:2842:G:H2'	30:0:2843:A:H5'	2.01	0.42
31:9:56:A:C3'	31:9:57:A:H5''	2.50	0.42
1:A:179:MET:HA	1:A:179:MET:CE	2.46	0.42
2:B:84:LEU:HB2	2:B:182:VAL:HG21	2.01	0.42
4:D:106:PHE:CZ	4:D:130:VAL:HG11	2.54	0.42
5:E:31:ARG:HH12	5:E:68:HIS:CE1	2.37	0.42
8:H:41:LYS:HE2	8:H:45:ASP:HB3	2.02	0.42
11:K:99:ASP:OD1	11:K:99:ASP:C	2.63	0.42
12:L:17:SER:C	12:L:19:LYS:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:41:HIS:HE1	42:0:3673:HOH:O	2.03	0.42
13:M:193:LYS:HB3	30:0:392:U:C5'	2.50	0.42
15:O:87:THR:O	15:O:88:LYS:C	2.63	0.42
16:P:13:VAL:HG21	16:P:41:ARG:HG2	2.00	0.42
27:1:11:LYS:HG2	30:0:777:U:O2'	2.20	0.42
30:0:506:G:N1	30:0:509:A:OP2	2.51	0.42
30:0:816:G:H5'	30:0:1598:A:H4'	2.02	0.42
30:0:1182:C:H1'	30:0:1192:A:C8	2.52	0.42
30:0:1298:U:H2'	30:0:1299:G:H8	1.81	0.42
30:0:1405:U:H4'	30:0:1406:A:H5''	2.02	0.42
30:0:2592:G:H2'	30:0:2593:C:C6	2.55	0.42
31:9:47:A:C2	31:9:48:C:C2	3.08	0.42
1:A:77:GLY:C	1:A:78:ASP:CA	2.93	0.42
1:A:150:PRO:HB3	42:A:9069:HOH:O	2.20	0.42
2:B:60:SER:HA	2:B:61:PRO:HD3	1.94	0.42
5:E:84:MET:CG	5:E:168:ILE:HD13	2.50	0.42
10:J:12:VAL:HG22	10:J:116:LEU:HD21	2.02	0.42
13:M:32:ARG:NH2	42:M:8901:HOH:O	2.53	0.42
14:N:25:ARG:HB3	30:0:2415:A:C2	2.55	0.42
17:Q:91:LEU:C	17:Q:92:ARG:HG2	2.44	0.42
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.35	0.42
21:U:17:THR:HG23	21:U:18:GLY:N	2.35	0.42
23:W:39:ASP:HB2	42:W:3580:HOH:O	2.20	0.42
25:Y:125:LYS:HB2	25:Y:126:PRO:HD2	2.02	0.42
30:0:292:G:H1'	30:0:360:A:N6	2.34	0.42
30:0:503:G:H2'	30:0:504:G:H8	1.84	0.42
30:0:537:G:H4'	30:0:538:C:O5'	2.20	0.42
30:0:644:G:H5'	30:0:644:G:N3	2.35	0.42
30:0:695:C:H2'	30:0:696:C:C6	2.55	0.42
31:9:59:C:O5'	31:9:59:C:H6	2.03	0.42
1:A:17:ARG:HD2	42:A:9018:HOH:O	2.19	0.42
1:A:190:ARG:HD2	30:0:1884:G:O6	2.19	0.42
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.84	0.42
5:E:35:TYR:HB3	5:E:38:ILE:HD12	2.02	0.42
10:J:63:ILE:CG2	10:J:64:GLY:N	2.82	0.42
13:M:67:VAL:HA	42:M:8841:HOH:O	2.20	0.42
14:N:48:VAL:HG11	14:N:55:ASP:HB3	2.00	0.42
18:R:26:LYS:HD3	18:R:62:HIS:CG	2.55	0.42
20:T:1:SER:H2	20:T:7:GLN:NE2	2.17	0.42
30:0:734:U:O2'	30:0:736:A:N7	2.49	0.42
30:0:1165:G:H4'	30:0:1174:A:HO2'	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1741:U:H5''	42:0:3670:HOH:O	2.20	0.42
30:0:2388:C:O2'	30:0:2389:U:H5'	2.19	0.42
30:0:2506:A:H1'	42:0:4621:HOH:O	2.20	0.42
30:0:2568:A:H2'	30:0:2569:A:O4'	2.20	0.42
30:0:2644:C:O2'	30:0:2645:U:H5'	2.19	0.42
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.85	0.41
2:B:241:PRO:HG3	30:0:2606:G:N2	2.34	0.41
3:C:120:ASP:C	3:C:120:ASP:OD1	2.63	0.41
5:E:81:GLU:HA	5:E:133:VAL:O	2.20	0.41
5:E:84:MET:HG2	5:E:168:ILE:HA	2.02	0.41
6:F:38:LYS:O	6:F:42:ARG:HG3	2.19	0.41
8:H:23:ILE:CG2	8:H:123:ILE:CD1	2.97	0.41
8:H:50:ILE:HD12	8:H:149:VAL:CG1	2.49	0.41
12:L:133:VAL:HB	42:L:8861:HOH:O	2.20	0.41
20:T:43:ASN:OD1	30:0:80:A:H3'	2.19	0.41
30:0:170:U:H2'	30:0:171:C:H5'	2.01	0.41
30:0:553:G:C2'	30:0:554:G:H5'	2.50	0.41
30:0:1074:G:H4'	30:0:1260:G:C6	2.55	0.41
30:0:1183:C:C5	30:0:1192:A:OP1	2.71	0.41
30:0:1209:C:O2'	30:0:1210:G:H5'	2.20	0.41
30:0:1236:A:H2'	30:0:1237:U:O4'	2.20	0.41
30:0:1342:C:O2'	30:0:1343:C:H5'	2.19	0.41
30:0:2499:U:O2'	30:0:2500:C:H5'	2.19	0.41
30:0:2512:U:H4'	30:0:2514:U:O4	2.20	0.41
30:0:2642:G:H2'	30:0:2643:G:O4'	2.19	0.41
7:G:19:GLU:O	7:G:23:ILE:HG13	2.20	0.41
12:L:33:ALA:HB2	30:0:165:A:H5''	2.01	0.41
16:P:98:ILE:HD12	16:P:102:ARG:CZ	2.50	0.41
23:W:88:THR:HG23	23:W:110:GLN:CB	2.43	0.41
24:X:49:ARG:O	24:X:49:ARG:CG	2.65	0.41
30:0:583:C:H2'	30:0:584:U:C6	2.55	0.41
30:0:814:G:H2'	30:0:815:U:H6	1.85	0.41
30:0:912:A:C4	30:0:1294:A:C2	3.08	0.41
30:0:1100:G:O2'	30:0:1107:A:N1	2.50	0.41
30:0:2257:G:H4'	30:0:2259:C:C2	2.55	0.41
30:0:2329:C:H2'	30:0:2330:U:C6	2.56	0.41
1:A:105:VAL:HG11	1:A:154:ALA:CB	2.50	0.41
2:B:139:ASP:CB	2:B:165:ARG:HE	2.32	0.41
2:B:316:ARG:HB2	30:0:2768:A:C8	2.55	0.41
3:C:67:GLN:HG2	42:C:8627:HOH:O	2.19	0.41
8:H:59:GLN:NE2	8:H:96:GLN:HG2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:143:LYS:HG3	10:J:145:TRP:CE2	2.55	0.41
12:L:126:SER:O	12:L:129:ALA:HB3	2.20	0.41
12:L:145:LEU:C	12:L:147:GLU:N	2.77	0.41
14:N:48:VAL:HG13	14:N:55:ASP:HB3	1.99	0.41
15:O:112:ARG:HD2	42:0:3574:HOH:O	2.21	0.41
17:Q:94:GLN:NE2	30:0:1019:C:O2	2.53	0.41
24:X:9:VAL:HG12	42:X:6893:HOH:O	2.21	0.41
25:Y:117:LEU:HD13	25:Y:174:VAL:CG1	2.48	0.41
25:Y:216:ARG:O	25:Y:219:GLU:HG2	2.20	0.41
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.18	0.41
29:3:22:VAL:HG11	29:3:67:LEU:HD13	2.02	0.41
30:0:307:G:H3'	30:0:342:C:OP2	2.20	0.41
30:0:494:C:H2'	30:0:496:G:OP2	2.20	0.41
30:0:636:G:H1'	30:0:2058:G:C4	2.55	0.41
30:0:1207:A:H8	30:0:1207:A:OP2	2.03	0.41
30:0:1366:C:H1'	42:0:3161:HOH:O	2.20	0.41
30:0:1910:A:H2'	30:0:1911:C:C6	2.56	0.41
30:0:2281:C:H2'	30:0:2282:U:H5'	2.02	0.41
2:B:28:SER:HB3	30:0:2807:U:OP1	2.21	0.41
2:B:70:PRO:HG3	30:0:2719:A:C2	2.55	0.41
2:B:255:GLY:O	2:B:257:THR:HG23	2.19	0.41
2:B:333:GLU:HB2	21:U:14:GLU:OE2	2.20	0.41
3:C:78:ARG:O	3:C:80:VAL:N	2.51	0.41
3:C:109:LEU:HD12	3:C:109:LEU:O	2.19	0.41
3:C:123:LEU:HD23	3:C:123:LEU:HA	1.87	0.41
4:D:44:ILE:HG12	4:D:44:ILE:O	2.21	0.41
12:L:98:GLU:O	12:L:99:GLU:CB	2.68	0.41
12:L:129:ALA:O	12:L:133:VAL:HG23	2.20	0.41
14:N:35:VAL:HG11	31:9:6:C:H4'	2.03	0.41
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.55	0.41
30:0:187:A:H3'	30:0:188:C:C6	2.56	0.41
30:0:541:C:O2'	30:0:542:A:H5''	2.20	0.41
30:0:970:U:O5'	30:0:970:U:H6	2.04	0.41
30:0:1039:G:H2'	30:0:1040:A:O4'	2.20	0.41
30:0:1211:G:H2'	30:0:1212:C:C6	2.55	0.41
30:0:1565:C:O4'	30:0:2738:G:H1'	2.21	0.41
30:0:1649:G:H1'	42:0:6370:HOH:O	2.20	0.41
30:0:1972:U:H2'	30:0:1973:A:C5'	2.50	0.41
30:0:1973:A:H2'	30:0:1974:G:O4'	2.21	0.41
30:0:2072:G:H3'	30:0:2073:G:H5''	2.03	0.41
30:0:2271:G:H8	42:0:4562:HOH:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2637:A:H4'	30:0:2638:G:O5'	2.20	0.41
1:A:169:PHE:O	1:A:171:LYS:N	2.47	0.41
2:B:66:GLU:OE1	2:B:328:ARG:HD2	2.20	0.41
2:B:198:GLU:HA	42:B:9143:HOH:O	2.20	0.41
2:B:235:ARG:HD3	30:0:2091:G:O3'	2.21	0.41
3:C:21:VAL:C	3:C:23:GLU:H	2.27	0.41
3:C:61:PHE:CD2	3:C:65:ARG:CZ	3.04	0.41
6:F:77:VAL:C	6:F:78:GLU:C	2.89	0.41
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.32	0.41
9:I:98:ASP:C	9:I:100:VAL:H	2.28	0.41
10:J:75:PRO:O	10:J:76:ASP:C	2.63	0.41
10:J:107:ASN:HD22	10:J:108:PRO:N	2.19	0.41
12:L:36:ASP:HB2	42:L:8839:HOH:O	2.20	0.41
12:L:67:ARG:HB2	12:L:111:ALA:O	2.21	0.41
13:M:46:LEU:HD22	13:M:50:ARG:HD2	2.02	0.41
25:Y:100:ARG:HD2	25:Y:232:THR:HB	2.02	0.41
25:Y:186:ARG:HG2	25:Y:186:ARG:NH1	2.33	0.41
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	2.02	0.41
30:0:222:A:H2'	30:0:223:G:O4'	2.20	0.41
30:0:415:A:O2'	30:0:416:G:H5'	2.20	0.41
30:0:1291:A:H2	42:0:6129:HOH:O	2.03	0.41
30:0:1741:U:H3'	42:0:3670:HOH:O	2.20	0.41
30:0:2081:A:H2'	30:0:2082:G:O4'	2.21	0.41
1:A:69:LEU:C	1:A:69:LEU:HD12	2.45	0.41
2:B:277:GLU:N	2:B:278:PRO:CD	2.84	0.41
4:D:25:MET:CE	4:D:41:LEU:HG	2.27	0.41
6:F:84:GLY:O	6:F:89:LEU:HB2	2.21	0.41
8:H:100:GLU:HB3	8:H:124:VAL:HG11	2.03	0.41
12:L:34:GLY:HA2	42:0:6243:HOH:O	2.19	0.41
12:L:57:VAL:HG12	12:L:57:VAL:O	2.20	0.41
12:L:125:PHE:CZ	12:L:140:VAL:HG22	2.56	0.41
14:N:124:ASP:C	14:N:126:GLY:H	2.28	0.41
21:U:20:MET:CG	21:U:28:THR:HG23	2.50	0.41
28:2:2:LYS:HG3	30:0:1486:A:C4	2.55	0.41
29:3:6:ARG:NH1	29:3:21:GLU:HG3	2.35	0.41
30:0:2296:C:H2'	30:0:2297:U:H6	1.85	0.41
30:0:2704:C:H2'	30:0:2705:U:O4'	2.20	0.41
30:0:2831:C:C2'	30:0:2832:C:H5'	2.51	0.41
3:C:219:ASN:O	3:C:222:ASP:OD1	2.38	0.41
4:D:27:ILE:HD11	4:D:37:ALA:HB2	2.01	0.41
4:D:167:GLU:C	4:D:169:THR:N	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:7:ILE:HG13	5:E:11:VAL:HB	2.03	0.41
5:E:21:THR:HG23	5:E:30:THR:OG1	2.20	0.41
9:I:80:PHE:N	9:I:80:PHE:CD1	2.89	0.41
10:J:13:ASP:OD1	10:J:15:ARG:HB3	2.20	0.41
13:M:68:ARG:O	13:M:68:ARG:HD3	2.20	0.41
23:W:13:MET:O	23:W:14:HIS:C	2.64	0.41
24:X:43:VAL:HG12	24:X:47:ALA:HB3	2.02	0.41
25:Y:207:SER:HB3	30:0:1335:C:OP2	2.20	0.41
26:Z:54:GLU:HA	26:Z:57:MET:HB3	2.02	0.41
27:1:2:GLY:O	27:1:6:PRO:HG2	2.20	0.41
30:0:278:A:H2'	30:0:279:C:O4'	2.20	0.41
30:0:1375:A:H1'	30:0:2045:G:O5'	2.21	0.41
30:0:1497:G:H4'	30:0:1627:G:O2'	2.21	0.41
30:0:2072:G:H3'	30:0:2073:G:C5'	2.51	0.41
30:0:2135:A:O2'	30:0:2136:G:H5'	2.21	0.41
31:9:39:U:H1'	31:9:44:A:N6	2.35	0.41
2:B:54:VAL:O	2:B:55:ASN:C	2.64	0.41
2:B:112:THR:OG1	2:B:158:LYS:HG3	2.20	0.41
6:F:60:VAL:O	6:F:60:VAL:CG1	2.69	0.41
20:T:40:VAL:HG23	20:T:119:ALA:OXT	2.21	0.41
28:2:48:ASP:O	28:2:49:GLU:CB	2.68	0.41
29:3:28:GLY:HA3	30:0:2434:A:O3'	2.20	0.41
29:3:91:GLN:O	29:3:92:GLU:HB2	2.20	0.41
30:0:220:C:H1'	42:0:6586:HOH:O	2.21	0.41
30:0:875:A:H5'	30:0:876:A:N7	2.35	0.41
30:0:1445:G:N2	30:0:1678:A:H1'	2.36	0.41
30:0:1533:A:H4'	30:0:1534:C:O4'	2.20	0.41
30:0:1809:G:N2	30:0:1811:A:H3'	2.35	0.41
30:0:1816:C:H2'	30:0:1817:U:O4'	2.21	0.41
30:0:2724:U:H2'	30:0:2725:G:O4'	2.20	0.41
31:9:35:C:H5''	42:9:9078:HOH:O	2.21	0.41
1:A:20:SER:C	1:A:22:ARG:H	2.29	0.41
1:A:51:ARG:HD2	30:0:1874:U:OP1	2.20	0.41
1:A:53:ALA:HB3	42:A:9081:HOH:O	2.19	0.41
1:A:82:VAL:HA	1:A:93:THR:O	2.21	0.41
2:B:79:MET:O	2:B:187:GLU:HA	2.21	0.41
2:B:82:VAL:HG11	2:B:101:TRP:CZ3	2.55	0.41
2:B:202:VAL:HG11	2:B:301:VAL:HG13	2.02	0.41
3:C:93:LYS:O	3:C:98:ARG:NH2	2.53	0.41
3:C:168:ARG:NH1	30:0:1310:U:OP2	2.54	0.41
4:D:52:THR:CG2	30:0:2346:C:O3'	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:154:LYS:H	4:D:154:LYS:CD	2.19	0.41
5:E:105:GLU:HG2	5:E:113:PRO:HB3	2.02	0.41
6:F:20:LEU:HB2	6:F:49:PHE:CZ	2.56	0.41
6:F:26:THR:CG2	6:F:102:GLY:HA3	2.50	0.41
8:H:119:ALA:O	8:H:120:PHE:C	2.64	0.41
8:H:154:ARG:NH2	30:0:2503:A:OP1	2.53	0.41
9:I:87:PRO:HB3	9:I:129:SER:C	2.46	0.41
9:I:95:LEU:HG	9:I:132:VAL:CG1	2.51	0.41
9:I:96:SER:H	9:I:99:GLN:CD	2.28	0.41
11:K:9:THR:O	11:K:10:GLN:C	2.64	0.41
13:M:77:HIS:CE1	13:M:86:GLN:HG2	2.55	0.41
14:N:171:HIS:CE1	42:N:8862:HOH:O	2.74	0.41
16:P:22:TRP:CH2	16:P:24:ASN:HA	2.56	0.41
16:P:37:ARG:HH21	30:0:1502:A:P	2.44	0.41
18:R:8:ALA:HB3	18:R:15:LYS:HE2	2.02	0.41
18:R:21:ARG:CB	18:R:23:MET:HE2	2.49	0.41
18:R:44:VAL:HG13	18:R:89:LEU:HD22	2.03	0.41
19:S:23:LYS:HE2	42:S:3430:HOH:O	2.19	0.41
20:T:40:VAL:HG22	20:T:41:ARG:N	2.35	0.41
20:T:77:VAL:N	20:T:78:THR:HG23	2.35	0.41
21:U:50:GLU:O	21:U:56:ARG:CG	2.69	0.41
22:V:42:ASN:O	22:V:44:GLY:N	2.53	0.41
23:W:7:LEU:HD23	23:W:7:LEU:HA	1.92	0.41
23:W:106:THR:O	23:W:107:LEU:C	2.64	0.41
26:Z:80:GLN:HA	26:Z:86:TYR:O	2.21	0.41
27:1:1:THR:HB	42:0:7939:HOH:O	2.21	0.41
28:2:25:VAL:O	28:2:29:THR:HG23	2.21	0.41
29:3:6:ARG:HA	29:3:20:HIS:O	2.21	0.41
30:0:74:G:H2'	30:0:75:U:C6	2.56	0.41
30:0:362:G:O2'	30:0:363:C:H5'	2.21	0.41
30:0:731:U:H2'	30:0:732:C:C6	2.56	0.41
30:0:813:C:H2'	30:0:814:G:O4'	2.21	0.41
30:0:907:A:H4'	30:0:1328:A:C2	2.56	0.41
30:0:945:U:H2'	30:0:946:C:H6	1.86	0.41
30:0:1165:G:H1'	30:0:1174:A:H1'	2.02	0.41
30:0:1343:C:H2'	30:0:1344:G:O5'	2.21	0.41
30:0:1409:G:C2	30:0:1410:G:C8	3.09	0.41
30:0:1603:A:C5'	30:0:1605:G:H5'	2.50	0.41
30:0:1902:G:N2	30:0:1936:C:C2	2.88	0.41
30:0:1980:U:O2'	30:0:1981:A:H5'	2.20	0.41
30:0:2290:U:H2'	42:0:7931:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2515:C:H2'	30:0:2516:G:O4'	2.20	0.41
30:0:2517:A:C2'	30:0:2518:C:H5'	2.50	0.41
30:0:2526:C:O2'	30:0:2527:U:H5'	2.21	0.41
30:0:2806:C:H2'	30:0:2807:U:C6	2.56	0.41
31:9:22:G:H5'	31:9:23:U:OP1	2.20	0.41
4:D:24:HIS:HB2	4:D:72:LYS:CB	2.51	0.41
12:L:5:LYS:NZ	30:0:1353:C:N3	2.69	0.41
12:L:65:ASP:CG	12:L:111:ALA:HB3	2.46	0.41
15:O:26:TRP:HA	15:O:26:TRP:CE3	2.56	0.41
16:P:27:ARG:HH21	16:P:30:ASP:CG	2.29	0.41
20:T:9:LYS:CE	20:T:13:ARG:NH1	2.67	0.41
20:T:87:VAL:HB	20:T:88:PRO:HD2	2.03	0.41
22:V:13:PRO:HA	22:V:16:ARG:NH1	2.35	0.41
27:1:11:LYS:HA	42:1:5026:HOH:O	2.22	0.41
30:0:101:C:H2'	30:0:102:A:H8	1.84	0.41
30:0:542:A:C5'	30:0:542:A:C8	2.98	0.41
30:0:1588:G:H1'	30:0:1607:A:N6	2.36	0.41
30:0:2089:A:C2'	30:0:2090:G:H5'	2.50	0.41
30:0:2509:A:H2'	30:0:2510:C:O4'	2.20	0.41
2:B:146:THR:C	2:B:148:PRO:HD3	2.46	0.40
2:B:265:LEU:CD2	2:B:316:ARG:HD3	2.52	0.40
3:C:80:VAL:HA	3:C:81:PRO:HD3	1.87	0.40
5:E:170:ARG:HE	5:E:170:ARG:HB2	1.63	0.40
8:H:61:ARG:O	8:H:65:LEU:HD22	2.21	0.40
10:J:75:PRO:HD3	10:J:136:SER:CB	2.51	0.40
11:K:18:ILE:HG22	11:K:93:ASN:HB2	2.03	0.40
13:M:48:LYS:HE3	13:M:52:GLN:NE2	2.36	0.40
13:M:93:ARG:HD2	30:0:1470:A:OP1	2.22	0.40
13:M:134:ILE:O	13:M:136:PRO:HD3	2.21	0.40
20:T:96:VAL:HG13	20:T:97:ARG:N	2.36	0.40
22:V:39:ALA:C	22:V:41:GLU:H	2.27	0.40
23:W:110:GLN:HE21	23:W:110:GLN:CA	2.30	0.40
25:Y:141:THR:HG23	42:0:7305:HOH:O	2.21	0.40
29:3:86:GLY:HA3	30:0:2318:C:OP1	2.21	0.40
30:0:243:A:H2	30:0:274:G:N3	2.19	0.40
30:0:466:A:H2'	30:0:467:G:O4'	2.20	0.40
30:0:541:C:C3'	30:0:542:A:H5''	2.49	0.40
30:0:567:U:H6	30:0:567:U:O5'	2.04	0.40
30:0:639:A:H2'	30:0:640:G:C8	2.55	0.40
30:0:1166:A:H61	30:0:1180:U:H3	1.69	0.40
30:0:2361:A:H2'	30:0:2362:A:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2698:G:H2'	30:0:2699:A:C8	2.56	0.40
2:B:101:TRP:HB2	2:B:119:HIS:CD2	2.57	0.40
2:B:205:VAL:O	2:B:307:ARG:NE	2.49	0.40
2:B:254:GLN:NE2	42:B:9065:HOH:O	2.53	0.40
3:C:208:ALA:C	3:C:210:ALA:H	2.29	0.40
3:C:214:THR:HB	42:C:8522:HOH:O	2.22	0.40
4:D:10:PHE:CD1	4:D:10:PHE:C	2.99	0.40
12:L:126:SER:O	12:L:127:GLU:C	2.64	0.40
24:X:23:HIS:HE1	30:0:2044:G:OP1	2.04	0.40
26:Z:45:VAL:CG2	30:0:1887:U:OP1	2.69	0.40
30:0:1014:A:H2'	30:0:1015:C:H5'	2.02	0.40
30:0:1117:A:H2'	42:0:5743:HOH:O	2.20	0.40
30:0:1889:C:H2'	30:0:1890:U:O4'	2.21	0.40
30:0:2079:G:H2'	30:0:2080:G:O4'	2.21	0.40
30:0:2250:G:H2'	30:0:2251:G:O4'	2.21	0.40
30:0:2504:A:H2'	30:0:2505:G:O4'	2.21	0.40
30:0:2566:A:H2	30:0:2695:C:O2	2.04	0.40
30:0:2887:G:H2'	30:0:2888:U:O4'	2.20	0.40
1:A:203:GLY:HA2	42:A:9022:HOH:O	2.21	0.40
2:B:145:HIS:HD2	2:B:146:THR:O	2.04	0.40
4:D:169:THR:HG22	4:D:170:TYR:HD1	1.86	0.40
10:J:49:ARG:NH1	30:0:1119:G:OP1	2.55	0.40
11:K:98:VAL:HG13	11:K:102:GLU:CA	2.51	0.40
11:K:125:ALA:O	11:K:127:ALA:N	2.47	0.40
12:L:61:ALA:HB2	12:L:105:TYR:CZ	2.55	0.40
13:M:74:LYS:HE2	30:0:159:G:OP1	2.21	0.40
13:M:107:ARG:O	13:M:110:PRO:HD3	2.21	0.40
14:N:41:LYS:HE3	42:9:9021:HOH:O	2.20	0.40
15:O:32:ARG:HG2	15:O:32:ARG:HH11	1.86	0.40
17:Q:47:VAL:HB	17:Q:90:HIS:CE1	2.57	0.40
19:S:29:ASP:OD1	19:S:31:ARG:NH1	2.55	0.40
21:U:20:MET:HE2	21:U:30:HIS:NE2	2.36	0.40
23:W:55:GLY:HA3	23:W:146:ILE:HG13	2.03	0.40
30:0:64:G:H2'	30:0:65:C:O4'	2.22	0.40
30:0:107:U:H2'	30:0:108:U:H5'	2.02	0.40
30:0:1190:G:H2'	42:0:4926:HOH:O	2.20	0.40
30:0:1573:A:H2'	30:0:1574:C:O4'	2.21	0.40
30:0:2549:C:H2'	30:0:2550:U:O4'	2.21	0.40
30:0:2661:U:H3	30:0:2812:A:H62	1.70	0.40
2:B:102:THR:HB	42:B:9117:HOH:O	2.21	0.40
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:36:ASN:HB3	42:D:7502:HOH:O	2.21	0.40
7:G:27:ILE:HD12	7:G:70:ALA:HB1	2.03	0.40
10:J:107:ASN:HD22	10:J:109:TYR:H	1.70	0.40
11:K:66:ARG:NH2	30:0:1994:A:OP1	2.54	0.40
13:M:108:THR:O	13:M:110:PRO:HD2	2.20	0.40
13:M:147:LEU:O	13:M:150:ILE:HG22	2.22	0.40
16:P:37:ARG:O	16:P:41:ARG:HG3	2.21	0.40
16:P:57:ASN:HB3	42:0:7671:HOH:O	2.21	0.40
18:R:76:ASP:HA	42:R:8919:HOH:O	2.20	0.40
20:T:107:LYS:O	20:T:111:ARG:HB2	2.21	0.40
23:W:21:LEU:HA	23:W:21:LEU:HD23	1.78	0.40
25:Y:210:GLY:N	30:0:1313:A:H5''	2.36	0.40
25:Y:210:GLY:H	30:0:1313:A:H5''	1.86	0.40
28:2:5:LYS:HD2	30:0:1675:C:H5''	2.03	0.40
30:0:368:C:H2'	30:0:369:G:H5'	2.02	0.40
30:0:581:G:O2'	30:0:582:U:H5'	2.21	0.40
30:0:1423:C:O2'	30:0:1424:A:H5'	2.21	0.40
30:0:1484:G:H2'	42:0:3018:HOH:O	2.21	0.40
30:0:2415:A:C2'	30:0:2416:G:H5'	2.49	0.40
30:0:2883:A:H2'	30:0:2884:G:O4'	2.20	0.40
30:0:2909:G:O2'	30:0:2910:A:H5'	2.21	0.40
1:A:125:ASN:HB3	1:A:158:VAL:HG12	2.03	0.40
4:D:27:ILE:HG21	42:D:5858:HOH:O	2.21	0.40
6:F:13:GLU:OE1	6:F:77:VAL:HG13	2.22	0.40
11:K:98:VAL:CG1	11:K:99:ASP:N	2.84	0.40
12:L:53:ARG:NH2	12:L:57:VAL:CG1	2.81	0.40
29:3:31:THR:HB	29:3:33:MET:HE3	2.04	0.40
30:0:69:A:H5'	30:0:69:A:H8	1.84	0.40
30:0:105:G:O2'	30:0:106:A:H5'	2.21	0.40
30:0:185:G:C4'	30:0:186:A:H4'	2.52	0.40
30:0:306:A:H2'	30:0:341:C:O2'	2.22	0.40
30:0:790:A:H1'	30:0:1710:A:C2'	2.51	0.40
30:0:830:G:O2'	30:0:831:U:H5'	2.21	0.40
30:0:1522:A:H2'	30:0:1523:G:C5'	2.51	0.40
30:0:1764:C:H2'	30:0:1765:G:O4'	2.22	0.40
30:0:1773:G:N2	30:0:1774:G:C8	2.89	0.40
30:0:1894:C:N4	30:0:1939:U:H2'	2.36	0.40
30:0:1948:G:H2'	30:0:1949:G:O4'	2.21	0.40
30:0:2735:U:H2'	30:0:2736:U:C6	2.56	0.40
30:0:2839:C:H2'	30:0:2840:A:H5''	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/240 (97%)	197 (84%)	31 (13%)	5 (2%)	5	20
2	B	333/338 (98%)	300 (90%)	29 (9%)	4 (1%)	10	34
3	C	242/246 (98%)	215 (89%)	25 (10%)	2 (1%)	16	44
4	D	132/177 (75%)	98 (74%)	23 (17%)	11 (8%)	0	1
5	E	168/178 (94%)	159 (95%)	9 (5%)	0	100	100
6	F	115/120 (96%)	97 (84%)	13 (11%)	5 (4%)	2	7
7	G	25/348 (7%)	22 (88%)	3 (12%)	0	100	100
8	H	154/177 (87%)	131 (85%)	21 (14%)	2 (1%)	9	31
9	I	66/162 (41%)	45 (68%)	19 (29%)	2 (3%)	3	12
10	J	138/145 (95%)	126 (91%)	9 (6%)	3 (2%)	5	19
11	K	128/132 (97%)	117 (91%)	9 (7%)	2 (2%)	7	27
12	L	139/165 (84%)	115 (83%)	19 (14%)	5 (4%)	2	10
13	M	190/196 (97%)	171 (90%)	17 (9%)	2 (1%)	11	36
14	N	182/187 (97%)	156 (86%)	18 (10%)	8 (4%)	2	7
15	O	111/116 (96%)	103 (93%)	8 (7%)	0	100	100
16	P	139/149 (93%)	133 (96%)	6 (4%)	0	100	100
17	Q	91/96 (95%)	82 (90%)	8 (9%)	1 (1%)	11	36
18	R	146/155 (94%)	132 (90%)	13 (9%)	1 (1%)	18	47
19	S	77/85 (91%)	73 (95%)	4 (5%)	0	100	100
20	T	115/120 (96%)	109 (95%)	4 (4%)	2 (2%)	7	25
21	U	51/67 (76%)	46 (90%)	4 (8%)	1 (2%)	6	21
22	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	7	27
23	W	150/154 (97%)	140 (93%)	9 (6%)	1 (1%)	18	47
24	X	78/92 (85%)	70 (90%)	7 (9%)	1 (1%)	9	31
25	Y	140/240 (58%)	135 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	69/116 (60%)	60 (87%)	6 (9%)	3 (4%)	2	7
27	1	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
28	2	42/50 (84%)	36 (86%)	6 (14%)	0	100	100
29	3	88/92 (96%)	83 (94%)	4 (4%)	1 (1%)	11	36
All	All	3659/4471 (82%)	3256 (89%)	340 (9%)	63 (2%)	7	25

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	34	ASP
1	A	37	VAL
4	D	27	ILE
4	D	171	ASP
6	F	101	ALA
12	L	80	ASP
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
18	R	114	VAL
21	U	55	ALA
26	Z	44	ARG
26	Z	105	ARG
29	3	56	PRO
1	A	204	GLY
4	D	16	PRO
4	D	97	GLN
4	D	147	ALA
6	F	27	GLY
9	I	113	SER
12	L	82	ALA
14	N	165	ALA
14	N	167	ASP
20	T	44	ALA
20	T	53	GLY
22	V	43	PRO
24	X	87	ALA
1	A	119	ALA
2	B	184	ASP
3	C	121	ALA
4	D	61	PHE

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Mol	Chain	Res	Type
4	D	137	PRO
6	F	104	ALA
8	H	19	ARG
10	J	143	LYS
11	K	126	SER
12	L	21	ARG
23	W	49	ASN
26	Z	45	VAL
2	B	185	GLY
4	D	28	GLY
4	D	56	ARG
4	D	168	SER
13	M	83	SER
2	B	2	GLN
4	D	166	ILE
6	F	100	ASP
8	H	84	GLY
10	J	5	GLU
10	J	76	ASP
14	N	68	GLU
14	N	164	ASP
12	L	100	ALA
13	M	88	VAL
14	N	74	PRO
2	B	169	GLY
3	C	234	VAL
9	I	124	VAL
6	F	64	PRO
11	K	39	GLY
12	L	135	GLY
17	Q	18	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/182 (98%)	163 (92%)	15 (8%)	10	32
2	B	281/283 (99%)	270 (96%)	11 (4%)	28	64
3	C	192/193 (100%)	174 (91%)	18 (9%)	8	27
4	D	116/148 (78%)	111 (96%)	5 (4%)	26	60
5	E	151/156 (97%)	144 (95%)	7 (5%)	24	58
6	F	92/94 (98%)	91 (99%)	1 (1%)	65	87
7	G	27/282 (10%)	26 (96%)	1 (4%)	30	65
8	H	133/145 (92%)	127 (96%)	6 (4%)	24	58
9	I	58/130 (45%)	57 (98%)	1 (2%)	53	83
10	J	117/121 (97%)	111 (95%)	6 (5%)	21	54
11	K	105/106 (99%)	103 (98%)	2 (2%)	50	81
12	L	113/127 (89%)	107 (95%)	6 (5%)	20	52
13	M	157/160 (98%)	151 (96%)	6 (4%)	29	64
14	N	148/150 (99%)	145 (98%)	3 (2%)	48	80
15	O	93/94 (99%)	91 (98%)	2 (2%)	45	78
16	P	113/117 (97%)	110 (97%)	3 (3%)	39	74
17	Q	79/80 (99%)	77 (98%)	2 (2%)	42	76
18	R	117/122 (96%)	110 (94%)	7 (6%)	17	47
19	S	71/74 (96%)	67 (94%)	4 (6%)	19	50
20	T	104/106 (98%)	99 (95%)	5 (5%)	23	56
21	U	44/53 (83%)	41 (93%)	3 (7%)	14	42
22	V	51/57 (90%)	50 (98%)	1 (2%)	48	80
23	W	129/130 (99%)	122 (95%)	7 (5%)	20	51
24	X	65/74 (88%)	58 (89%)	7 (11%)	6	21
25	Y	120/195 (62%)	113 (94%)	7 (6%)	18	49
26	Z	59/94 (63%)	58 (98%)	1 (2%)	53	83
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	42 (100%)	0	100	100
29	3	78/79 (99%)	75 (96%)	3 (4%)	29	64
All	All	3079/3645 (84%)	2939 (96%)	140 (4%)	24	58

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	33	GLU
1	A	36	ASP
1	A	37	VAL
1	A	38	ILE
1	A	68	ILE
1	A	69	LEU
1	A	84	VAL
1	A	131	HIS
1	A	153	ARG
1	A	165	THR
1	A	175	LYS
1	A	179	MET
1	A	216	SER
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN
2	B	71	VAL
2	B	90	THR
2	B	103	ASP
2	B	162	MET
2	B	195	ARG
2	B	251	VAL
2	B	254	GLN
2	B	277	GLU
3	C	2	GLN
3	C	16	VAL
3	C	27	ARG
3	C	67	GLN
3	C	76	ARG
3	C	91	PRO
3	C	94	THR
3	C	115	LEU
3	C	187	ARG
3	C	214	THR
3	C	218	VAL
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	237	GLU

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Mol	Chain	Res	Type
3	C	240	LEU
3	C	243	VAL
4	D	24	HIS
4	D	50	VAL
4	D	58	VAL
4	D	133	ASN
4	D	137	PRO
5	E	7	ILE
5	E	86	VAL
5	E	102	VAL
5	E	116	THR
5	E	126	ILE
5	E	143	GLN
5	E	154	ILE
6	F	12	LEU
7	G	73	ASP
8	H	21	GLU
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	145	ASP
8	H	157	TYR
9	I	135	GLU
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	93	ARG
10	J	127	ILE
10	J	131	THR
11	K	7	ASP
11	K	10	GLN
12	L	18	HIS
12	L	35	ARG
12	L	43	HIS
12	L	60	GLU
12	L	101	ASP
12	L	140	VAL
13	M	46	LEU
13	M	93	ARG
13	M	99	ARG
13	M	115	LEU
13	M	130	GLU

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Mol	Chain	Res	Type
13	M	164	THR
14	N	26	LEU
14	N	49	THR
14	N	139	TRP
15	O	43	VAL
15	O	98	LEU
16	P	21	VAL
16	P	52	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	95	GLU
18	R	13	THR
18	R	17	MET
18	R	39	THR
18	R	82	GLU
18	R	90	ASP
18	R	119	VAL
18	R	143	VAL
19	S	10	VAL
19	S	12	GLU
19	S	17	ASP
19	S	44	GLN
20	T	26	THR
20	T	39	ASN
20	T	48	VAL
20	T	89	ARG
20	T	96	VAL
21	U	17	THR
21	U	20	MET
21	U	53	ASP
22	V	2	VAL
23	W	26	ILE
23	W	45	VAL
23	W	52	VAL
23	W	73	LEU
23	W	120	PRO
23	W	146	ILE
23	W	151	GLU
24	X	15	ARG
24	X	27	ASP
24	X	46	ASP
24	X	49	ARG

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Mol	Chain	Res	Type
24	X	72	VAL
24	X	79	GLU
24	X	82	GLU
25	Y	115	ARG
25	Y	174	VAL
25	Y	189	ASN
25	Y	203	VAL
25	Y	220	GLU
25	Y	231	PRO
25	Y	235	GLU
26	Z	106	SER
29	3	14	CYS
29	3	42	ARG
29	3	56	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (112) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	188	ASN
1	A	199	HIS
1	A	218	ASN
2	B	27	ASN
2	B	55	ASN
2	B	145	HIS
2	B	221	GLN
2	B	230	GLN
2	B	238	ASN
2	B	254	GLN
2	B	256	GLN
2	B	260	HIS
2	B	286	ASN
2	B	318	ASN
2	B	320	GLN
2	B	332	ASN
3	C	2	GLN
3	C	11	ASN
3	C	39	GLN
3	C	73	GLN
3	C	108	GLN
3	C	129	HIS
4	D	103	ASN

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Mol	Chain	Res	Type
4	D	133	ASN
5	E	106	ASN
5	E	119	HIS
5	E	143	GLN
5	E	150	GLN
6	F	80	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	142	ASN
8	H	158	ASN
9	I	88	GLN
9	I	99	GLN
9	I	106	GLN
10	J	25	GLN
10	J	29	GLN
10	J	107	ASN
11	K	10	GLN
12	L	18	HIS
12	L	41	HIS
12	L	42	ASN
12	L	43	HIS
13	M	24	GLN
13	M	26	GLN
13	M	58	GLN
13	M	122	GLN
13	M	170	ASN
14	N	21	HIS
14	N	22	GLN
14	N	107	ASN
14	N	119	GLN
14	N	140	GLN
15	O	100	GLN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS

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Mol	Chain	Res	Type
18	R	22	GLN
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
18	R	122	GLN
19	S	25	GLN
19	S	44	GLN
19	S	53	ASN
19	S	55	GLN
20	T	7	GLN
20	T	11	GLN
20	T	37	GLN
20	T	39	ASN
20	T	64	ASN
20	T	73	HIS
21	U	39	ASN
21	U	48	ASN
22	V	29	ASN
22	V	60	GLN
23	W	28	HIS
23	W	59	GLN
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
25	Y	119	GLN
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	153	GLN
25	Y	189	ASN
26	Z	58	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	2	GLN

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Mol	Chain	Res	Type
29	3	13	HIS
29	3	15	ASN
29	3	30	GLN
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	257 (9%)	30 (1%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
32	5	2/3 (66%)	1 (50%)	0
33	6	1/3 (33%)	0	0
All	All	2869/3051 (94%)	274 (9%)	31 (1%)

All (274) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	200	C
30	0	204	A
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A

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Mol	Chain	Res	Type
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	497	A
30	0	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	645	U
30	0	660	A
30	0	688	A
30	0	701	U
30	0	702	G
30	0	735	C
30	0	746	A
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U

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Mol	Chain	Res	Type
30	0	835	U
30	0	840	U
30	0	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	882	A
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1129	C
30	0	1130	U
30	0	1151	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A

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Mol	Chain	Res	Type
30	0	1193	A
30	0	1205	U
30	0	1206	U
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1287	A
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1357	A
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1559	A
30	0	1592	G
30	0	1617	C
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1686	C
30	0	1692	C
30	0	1693	A
30	0	1701	A
30	0	1722	U
30	0	1723	G

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Mol	Chain	Res	Type
30	0	1725	C
30	0	1731	C
30	0	1738	C
30	0	1752	G
30	0	1778	A
30	0	1779	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1873	G
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1943	C
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2004	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2101	A
30	0	2102	G
30	0	2103	A
30	0	2104	C
30	0	2110	G
30	0	2238	A
30	0	2243	C
30	0	2258	A

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Mol	Chain	Res	Type
30	0	2271	G
30	0	2272	G
30	0	2313	C
30	0	2314	G
30	0	2317	C
30	0	2321	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2467	A
30	0	2476	C
30	0	2480	G
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2526	C
30	0	2527	U
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2609	G
30	0	2611	G
30	0	2613	G
30	0	2634	G
30	0	2637	A
30	0	2638	G
30	0	2645	U
30	0	2648	U
30	0	2649	A
30	0	2650	U
30	0	2664	A
30	0	2681	A

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Mol	Chain	Res	Type
30	0	2682	C
30	0	2718	C
30	0	2719	A
30	0	2726	U
30	0	2727	A
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2783	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	39	U
31	9	41	C
31	9	43	G
31	9	44	A
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C
32	5	76	A

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	129	A
30	0	338	C
30	0	603	A
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1237	U
30	0	1352	A
30	0	1506	U
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1730	G
30	0	1942	A
30	0	1979	G
30	0	2103	A
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2637	A
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2791	U
30	0	2852	A
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	1MA	0	628	30	21,25,26	0.73	1 (4%)	30,37,40	0.94	2 (6%)
30	PSU	0	2621	30	18,21,22	1.65	2 (11%)	21,30,33	1.36	3 (14%)
30	OMG	0	2588	30,32	23,26,27	0.29	0	32,38,41	0.40	0
33	8AN	6	76	33	21,24,25	1.02	1 (4%)	26,35,38	1.22	3 (11%)
30	UR3	0	2619	30	19,22,23	0.56	0	26,32,35	0.78	1 (3%)
30	OMU	0	2587	30	19,22,23	0.36	0	25,31,34	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	1MA	0	628	30	-	1/7/25/26	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMG	0	2588	30,32	-	0/9/27/28	0/3/3/3
33	8AN	6	76	33	-	3/7/25/26	0/3/3/3
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	5.77	1.44	1.36
30	0	2621	PSU	C6-C5	2.78	1.38	1.35
33	6	76	8AN	C3'-N3'	-2.64	1.43	1.47
30	0	628	1MA	C6-N6	2.32	1.33	1.28

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	6	76	8AN	O2'-C2'-C3'	3.64	121.22	111.61
30	0	2621	PSU	C6-C5-C4	3.42	120.48	118.17
33	6	76	8AN	O4'-C4'-C3'	3.41	109.19	104.22
30	0	2621	PSU	O2-C2-N1	2.99	125.87	122.79
30	0	628	1MA	CM1-N1-C6	2.95	124.72	120.15
30	0	2621	PSU	C6-N1-C2	-2.74	120.15	122.69
30	0	628	1MA	N1-C2-N3	2.65	129.14	126.00
30	0	2619	UR3	C4-N3-C2	2.57	126.64	124.58
33	6	76	8AN	C2'-C1'-N9	2.48	119.47	113.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	6	76	8AN	O4'-C4'-C5'-O5'
33	6	76	8AN	C4'-C5'-O5'-P
33	6	76	8AN	C3'-C4'-C5'-O5'
30	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2588	OMG	2	0
33	6	76	8AN	1	0
30	0	2619	UR3	1	0
30	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 304 are monoatomic - leaving 2 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	$\# Z > 2$
40	PHE	6	77	-	10,11,12	2.16	4 (40%)	8,13,15	0.52	0
41	ACA	6	78	-	6,7,8	1.88	1 (16%)	5,6,8	0.63	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	PHE	6	77	-	-	5/5/6/8	0/1/1/1
41	ACA	6	78	-	-	2/5/5/6	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	6	77	PHE	CE2-CD2	4.03	1.45	1.38
41	6	78	ACA	C3-C2	-3.62	1.37	1.52
40	6	77	PHE	CE1-CD1	2.92	1.43	1.38
40	6	77	PHE	CB-CG	2.14	1.56	1.51
40	6	77	PHE	CD1-CG	2.05	1.43	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	6	77	PHE	O-C-CA-CB
40	6	77	PHE	C-CA-CB-CG
41	6	78	ACA	O-C-C2-C3
41	6	78	ACA	C2-C3-C4-C5
40	6	77	PHE	N-CA-CB-CG
40	6	77	PHE	CA-CB-CG-CD1
40	6	77	PHE	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	0.20	10 (4%) 40 32	22, 45, 81, 106	0
2	B	337/338 (99%)	0.09	8 (2%) 59 49	20, 45, 72, 88	0
3	C	246/246 (100%)	0.05	3 (1%) 76 68	17, 41, 65, 82	0
4	D	140/177 (79%)	1.99	53 (37%) 1 0	54, 93, 129, 137	0
5	E	172/178 (96%)	0.61	12 (6%) 22 16	38, 60, 81, 91	0
6	F	119/120 (99%)	0.82	9 (7%) 20 14	41, 70, 106, 115	0
7	G	29/348 (8%)	1.52	8 (27%) 1 1	66, 93, 107, 109	0
8	H	160/177 (90%)	0.58	12 (7%) 20 15	34, 56, 93, 104	0
9	I	70/162 (43%)	3.16	56 (80%) 0 0	143, 158, 174, 175	0
10	J	142/145 (97%)	0.12	5 (3%) 47 38	28, 44, 63, 81	0
11	K	132/132 (100%)	-0.17	0 100 100	25, 39, 60, 72	0
12	L	145/165 (87%)	0.74	22 (15%) 5 4	20, 61, 109, 127	0
13	M	194/196 (98%)	0.09	6 (3%) 51 41	24, 40, 63, 74	0
14	N	186/187 (99%)	0.89	25 (13%) 7 5	37, 60, 119, 126	0
15	O	115/116 (99%)	0.36	4 (3%) 47 38	33, 53, 68, 74	0
16	P	143/149 (95%)	0.07	2 (1%) 73 64	30, 45, 58, 67	0
17	Q	95/96 (98%)	0.20	4 (4%) 40 32	30, 42, 60, 74	0
18	R	150/155 (96%)	-0.21	0 100 100	23, 37, 59, 70	0
19	S	81/85 (95%)	0.18	1 (1%) 76 68	37, 53, 74, 95	0
20	T	119/120 (99%)	0.38	6 (5%) 34 26	36, 51, 80, 121	0
21	U	53/67 (79%)	0.09	1 (1%) 66 57	32, 46, 71, 81	0
22	V	65/71 (91%)	1.28	11 (16%) 4 3	44, 74, 117, 125	0
23	W	154/154 (100%)	0.08	0 100 100	30, 45, 66, 80	0
24	X	82/92 (89%)	0.55	10 (12%) 8 6	37, 52, 83, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/240 (59%)	-0.14	2 (1%) 73 64	18, 39, 62, 85	0
26	Z	73/116 (62%)	1.44	17 (23%) 2 1	44, 82, 99, 108	0
27	1	56/57 (98%)	-0.47	0 100 100	21, 28, 36, 43	0
28	2	46/50 (92%)	0.60	5 (10%) 10 8	30, 52, 68, 86	0
29	3	92/92 (100%)	0.42	3 (3%) 49 39	34, 53, 71, 80	0
30	0	2749/2923 (94%)	-0.39	69 (2%) 58 48	17, 40, 89, 186	0
31	9	122/122 (100%)	0.16	3 (2%) 58 48	33, 61, 86, 151	0
32	5	3/3 (100%)	1.80	1 (33%) 1 1	81, 81, 83, 86	0
33	6	2/3 (66%)	2.64	2 (100%) 0 0	96, 96, 96, 104	0
All	All	6651/7522 (88%)	0.08	370 (5%) 30 23	17, 46, 98, 186	0

All (370) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	7.7
9	I	100	VAL	7.3
4	D	10	PHE	6.9
9	I	71	ALA	6.7
9	I	128	THR	6.7
28	2	49	GLU	6.6
26	Z	46	SER	6.4
4	D	63	ILE	6.4
26	Z	35	SER	6.4
22	V	39	ALA	6.0
9	I	132	VAL	6.0
4	D	57	THR	5.8
24	X	88	GLU	5.8
12	L	78	ALA	5.8
22	V	2	VAL	5.6
9	I	73	LEU	5.6
8	H	174	LEU	5.5
9	I	74	ILE	5.5
4	D	55	LYS	5.3
9	I	120	ALA	5.3
26	Z	106	SER	5.3
30	0	1199	A	5.2
14	N	166	ALA	5.2
4	D	90	LEU	5.2
14	N	168	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
5	E	45	ASP	4.9
9	I	70	THR	4.9
30	0	2748	G	4.8
22	V	38	GLY	4.8
9	I	67	VAL	4.8
22	V	40	PRO	4.8
26	Z	34	SER	4.7
22	V	36	ALA	4.6
9	I	116	LEU	4.6
31	9	1	U	4.6
5	E	6	GLU	4.5
9	I	83	GLY	4.5
4	D	107	GLY	4.5
9	I	103	ILE	4.5
9	I	72	GLU	4.5
12	L	60	GLU	4.4
4	D	174	VAL	4.4
4	D	171	ASP	4.4
4	D	18	ILE	4.4
9	I	104	ALA	4.3
29	3	41	GLU	4.3
29	3	56	PRO	4.3
14	N	154	LEU	4.2
9	I	127	CYS	4.2
14	N	163	PHE	4.2
9	I	119	ALA	4.1
7	G	26	MET	4.1
31	9	2	U	4.1
4	D	62	ASP	4.1
1	A	237	GLY	4.1
14	N	134	ASP	4.0
13	M	78	LYS	4.0
4	D	134	LEU	4.0
9	I	133	THR	4.0
9	I	124	VAL	4.0
8	H	169	GLU	3.9
26	Z	36	GLY	3.9
24	X	85	VAL	3.9
9	I	97	VAL	3.9
30	0	2769	C	3.9
30	0	1172	G	3.9
4	D	53	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
8	H	171	GLY	3.8
14	N	160	SER	3.8
1	A	37	VAL	3.8
9	I	134	ILE	3.8
12	L	82	ALA	3.8
30	0	271	C	3.8
4	D	93	LEU	3.8
10	J	4	ALA	3.8
9	I	112	LEU	3.8
4	D	135	VAL	3.7
29	3	55	VAL	3.7
4	D	61	PHE	3.7
9	I	109	PRO	3.7
4	D	11	HIS	3.6
12	L	75	LEU	3.6
30	0	1175	G	3.6
30	0	2237	G	3.6
4	D	106	PHE	3.6
4	D	44	ILE	3.6
9	I	123	VAL	3.6
4	D	17	ARG	3.6
30	0	1173	A	3.6
30	0	1177	A	3.6
30	0	2637	A	3.6
12	L	150	GLN	3.5
30	0	1197	G	3.5
26	Z	45	VAL	3.5
9	I	106	GLN	3.5
9	I	113	SER	3.5
14	N	169	PRO	3.5
26	Z	42	TYR	3.5
22	V	41	GLU	3.5
9	I	129	SER	3.5
14	N	1	ALA	3.5
4	D	104	PHE	3.5
30	0	1161	A	3.5
9	I	111	LEU	3.5
26	Z	38	PHE	3.4
17	Q	20	ASP	3.4
20	T	116	ASP	3.4
13	M	75	ARG	3.4
30	0	737	A	3.4

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Mol	Chain	Res	Type	RSRZ
8	H	114	ASP	3.4
7	G	12	ILE	3.4
30	0	1165	G	3.4
9	I	66	GLY	3.4
6	F	78	GLU	3.4
9	I	77	GLU	3.4
14	N	167	ASP	3.4
24	X	65	ASN	3.3
12	L	99	GLU	3.3
12	L	148	GLU	3.3
26	Z	47	ARG	3.3
24	X	83	ALA	3.3
30	0	1160	G	3.3
4	D	88	LEU	3.3
12	L	62	ALA	3.3
12	L	100	ALA	3.3
26	Z	40	ALA	3.3
14	N	158	LEU	3.3
28	2	35	ARG	3.3
22	V	37	GLY	3.3
9	I	108	HIS	3.2
12	L	83	GLU	3.2
1	A	36	ASP	3.2
5	E	10	ASP	3.2
4	D	54	ALA	3.2
9	I	88	GLN	3.2
30	0	514	G	3.2
4	D	172	VAL	3.2
9	I	69	PRO	3.2
20	T	119	ALA	3.2
22	V	43	PRO	3.2
20	T	118	SER	3.1
26	Z	58	ASN	3.1
30	0	10	U	3.1
30	0	1170	U	3.1
5	E	154	ILE	3.1
6	F	105	ASP	3.1
30	0	2345	A	3.1
2	B	1	PRO	3.1
14	N	159	TYR	3.1
4	D	89	PRO	3.1
30	0	1168	C	3.1

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Mol	Chain	Res	Type	RSRZ
30	0	1169	U	3.0
30	0	1200	A	3.0
30	0	1951	G	3.0
30	0	1182	C	3.0
3	C	61	PHE	3.0
26	Z	49	ARG	3.0
20	T	117	ASP	3.0
30	0	1196	C	3.0
4	D	154	LYS	2.9
9	I	101	LYS	2.9
21	U	47	ARG	2.9
30	0	1192	A	2.9
7	G	71	LEU	2.9
9	I	118	ASN	2.9
14	N	162	ASP	2.9
4	D	52	THR	2.9
30	0	1176	C	2.9
4	D	59	GLY	2.9
13	M	70	GLY	2.9
30	0	272	A	2.9
9	I	75	LYS	2.9
16	P	18	LYS	2.9
9	I	82	THR	2.9
12	L	146	GLY	2.9
30	0	1184	C	2.9
30	0	960	G	2.9
9	I	107	LYS	2.9
30	0	734	U	2.8
30	0	735	C	2.8
17	Q	17	LYS	2.8
4	D	36	ASN	2.8
17	Q	18	PRO	2.8
4	D	128	LEU	2.8
30	0	1162	G	2.8
30	0	1195	G	2.8
24	X	87	ALA	2.8
9	I	117	THR	2.8
26	Z	43	GLY	2.8
4	D	92	GLU	2.8
12	L	149	ARG	2.8
4	D	35	ALA	2.8
30	0	1164	U	2.8

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Mol	Chain	Res	Type	RSRZ
26	Z	39	GLY	2.8
4	D	56	ARG	2.7
5	E	4	GLU	2.7
30	0	497	A	2.7
9	I	130	LEU	2.7
4	D	19	GLU	2.7
33	6	74	C	2.7
30	0	736	A	2.7
4	D	74	THR	2.7
7	G	73	ASP	2.7
12	L	77	ALA	2.7
30	0	284	C	2.7
9	I	114	TYR	2.7
8	H	168	VAL	2.7
9	I	91	PHE	2.7
30	0	1171	A	2.7
30	0	1198	U	2.7
30	0	1964	U	2.7
9	I	80	PHE	2.6
4	D	169	THR	2.6
1	A	31	LYS	2.6
12	L	57	VAL	2.6
5	E	7	ILE	2.6
4	D	170	TYR	2.6
14	N	161	GLY	2.6
4	D	58	VAL	2.6
7	G	23	ILE	2.6
4	D	142	ALA	2.6
10	J	70	PHE	2.6
15	O	24	ALA	2.6
1	A	203	GLY	2.6
14	N	76	GLY	2.6
14	N	152	GLU	2.6
6	F	106	ALA	2.6
33	6	75	C	2.5
30	0	1174	A	2.5
30	0	2768	A	2.5
17	Q	81	GLU	2.5
9	I	78	ALA	2.5
4	D	77	ASP	2.5
9	I	121	LYS	2.5
9	I	85	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
30	0	1191	A	2.5
5	E	13	ALA	2.5
26	Z	44	ARG	2.5
4	D	105	SER	2.5
4	D	150	SER	2.5
6	F	16	ALA	2.5
8	H	43	ALA	2.5
5	E	156	ASP	2.5
9	I	76	ASP	2.5
7	G	27	ILE	2.5
8	H	37	GLY	2.5
5	E	87	PHE	2.5
16	P	143	ALA	2.5
28	2	44	ARG	2.5
1	A	211	LYS	2.5
30	0	2747	C	2.5
30	0	1178	G	2.5
6	F	102	GLY	2.4
8	H	115	GLY	2.4
13	M	194	GLY	2.4
31	9	24	U	2.4
4	D	157	LEU	2.4
7	G	29	SER	2.4
20	T	114	SER	2.4
4	D	91	ALA	2.4
14	N	165	ALA	2.4
4	D	166	ILE	2.4
30	0	1201	C	2.4
30	0	1202	A	2.4
9	I	122	GLU	2.4
9	I	135	GLU	2.4
30	0	1167	G	2.4
30	0	1929	G	2.4
12	L	143	THR	2.4
12	L	145	LEU	2.4
12	L	91	VAL	2.4
14	N	65	ASP	2.4
30	0	999	C	2.4
12	L	147	GLU	2.4
30	0	1207	A	2.4
10	J	92	GLN	2.4
12	L	105	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
13	M	89	THR	2.4
30	0	1966	U	2.4
4	D	69	ILE	2.4
22	V	46	ILE	2.4
2	B	318	ASN	2.3
24	X	22	ASN	2.3
28	2	39	ARG	2.3
6	F	49	PHE	2.3
6	F	1	PRO	2.3
24	X	71	ARG	2.3
9	I	115	ASP	2.3
9	I	95	LEU	2.3
30	0	288	A	2.3
28	2	48	ASP	2.3
9	I	126	THR	2.3
30	0	87	C	2.3
30	0	128	A	2.3
4	D	65	GLU	2.3
2	B	33	ASP	2.3
3	C	133	ARG	2.3
15	O	1	SER	2.3
10	J	77	GLY	2.3
4	D	12	GLU	2.2
5	E	78	GLU	2.2
8	H	173	GLU	2.2
25	Y	235	GLU	2.2
14	N	180	LEU	2.2
9	I	94	ASP	2.2
4	D	101	THR	2.2
14	N	157	PRO	2.2
2	B	208	GLY	2.2
4	D	66	GLY	2.2
30	0	1967	U	2.2
4	D	81	GLU	2.2
30	0	1166	A	2.2
32	5	74	C	2.2
7	G	72	ASP	2.2
14	N	164	ASP	2.2
2	B	108	GLU	2.2
24	X	7	GLU	2.2
30	0	1203	G	2.2
30	0	1206	U	2.2

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Mol	Chain	Res	Type	RSRZ
26	Z	48	ARG	2.2
30	0	1181	A	2.2
1	A	59	GLU	2.2
3	C	237	GLU	2.2
12	L	61	ALA	2.2
24	X	78	GLU	2.2
5	E	20	ILE	2.2
14	N	40	ASN	2.2
30	0	1524	U	2.2
2	B	139	ASP	2.2
14	N	43	VAL	2.2
30	0	1193	A	2.2
30	0	1183	C	2.2
13	M	71	SER	2.2
8	H	66	GLU	2.2
12	L	59	GLU	2.2
6	F	111	ILE	2.1
9	I	68	PRO	2.1
14	N	147	ILE	2.1
26	Z	78	ILE	2.1
1	A	135	VAL	2.1
2	B	319	ASP	2.1
6	F	100	ASP	2.1
15	O	22	GLY	2.1
14	N	175	LEU	2.1
1	A	33	GLU	2.1
9	I	96	SER	2.1
19	S	81	ILE	2.1
30	0	1204	C	2.1
4	D	132	VAL	2.1
25	Y	236	VAL	2.1
1	A	35	GLY	2.1
4	D	84	LEU	2.1
22	V	44	GLY	2.1
24	X	84	ILE	2.1
30	0	2850	C	2.1
12	L	45	PRO	2.1
20	T	36	GLY	2.1
2	B	183	GLU	2.1
9	I	84	SER	2.0
30	0	282	C	2.0
15	O	47	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
8	H	132	ALA	2.0
5	E	160	ARG	2.0
10	J	46	ILE	2.0
8	H	78	LYS	2.0
9	I	81	GLU	2.0
14	N	68	GLU	2.0
30	0	2512	U	2.0
30	0	1525	G	2.0
4	D	22	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	8AN	6	76	22/23	0.88	0.20	84,92,94,95	0
30	UR3	0	2619	21/22	0.95	0.10	33,35,40,41	0
30	1MA	0	628	23/24	0.97	0.07	25,28,29,30	0
30	PSU	0	2621	20/21	0.97	0.08	29,31,38,39	0
30	OMG	0	2588	24/25	0.97	0.09	24,29,31,33	0
30	OMU	0	2587	21/22	0.98	0.07	24,28,32,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	NA	0	8571	1/1	0.11	0.51	131,131,131,131	0
37	NA	0	8573	1/1	0.50	0.48	107,107,107,107	0
34	MG	0	8016	1/1	0.56	0.27	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	MG	0	8049	1/1	0.57	0.43	141,141,141,141	0
34	MG	0	8063	1/1	0.58	0.48	87,87,87,87	0
34	MG	0	8065	1/1	0.58	0.26	84,84,84,84	0
34	MG	B	8042	1/1	0.59	0.32	92,92,92,92	0
34	MG	0	8090	1/1	0.60	0.76	126,126,126,126	0
34	MG	0	8038	1/1	0.64	0.21	112,112,112,112	0
36	SR	0	9001	1/1	0.70	0.16	155,155,155,155	0
36	SR	0	8983	1/1	0.71	0.24	195,195,195,195	0
37	NA	0	8509	1/1	0.74	0.41	83,83,83,83	0
37	NA	0	8522	1/1	0.74	0.43	64,64,64,64	0
36	SR	0	8942	1/1	0.74	0.35	186,186,186,186	0
36	SR	0	9006	1/1	0.74	0.43	199,199,199,199	0
34	MG	0	8081	1/1	0.75	0.64	103,103,103,103	0
37	NA	0	8555	1/1	0.75	0.28	64,64,64,64	0
40	PHE	6	77	11/12	0.75	0.39	72,73,77,80	0
34	MG	0	8078	1/1	0.76	0.37	104,104,104,104	0
37	NA	0	8548	1/1	0.76	0.18	27,27,27,27	0
34	MG	0	8037	1/1	0.77	0.35	70,70,70,70	0
34	MG	0	8071	1/1	0.78	0.41	98,98,98,98	0
37	NA	0	8553	1/1	0.78	0.42	100,100,100,100	0
37	NA	0	8546	1/1	0.79	0.45	79,79,79,79	0
34	MG	0	8062	1/1	0.79	0.24	76,76,76,76	0
37	NA	0	8559	1/1	0.79	0.36	75,75,75,75	0
37	NA	0	8561	1/1	0.80	0.54	89,89,89,89	0
37	NA	0	8564	1/1	0.80	0.27	68,68,68,68	0
36	SR	0	8920	1/1	0.80	0.43	200,200,200,200	0
37	NA	0	8506	1/1	0.80	0.21	65,65,65,65	0
34	MG	0	8010	1/1	0.80	0.37	103,103,103,103	0
36	SR	0	8959	1/1	0.81	0.10	131,131,131,131	0
37	NA	0	8547	1/1	0.81	0.27	66,66,66,66	0
34	MG	0	8045	1/1	0.81	0.56	147,147,147,147	0
37	NA	0	8502	1/1	0.81	0.26	55,55,55,55	0
37	NA	0	8535	1/1	0.81	0.32	64,64,64,64	0
39	K	0	8402	1/1	0.81	0.18	81,81,81,81	0
37	NA	0	8556	1/1	0.81	0.16	39,39,39,39	0
36	SR	B	8987	1/1	0.82	0.41	200,200,200,200	0
37	NA	0	8560	1/1	0.82	0.39	107,107,107,107	0
39	K	0	8401	1/1	0.82	0.20	66,66,66,66	0
36	SR	0	8994	1/1	0.82	0.51	200,200,200,200	0
34	MG	0	8085	1/1	0.82	0.25	91,91,91,91	0
41	ACA	6	78	8/9	0.82	0.35	74,74,81,82	0
37	NA	0	8567	1/1	0.83	0.38	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	NA	0	8520	1/1	0.83	0.22	43,43,43,43	0
36	SR	0	8998	1/1	0.83	0.25	159,159,159,159	0
37	NA	9	8572	1/1	0.83	0.39	85,85,85,85	0
37	NA	0	8551	1/1	0.83	0.23	53,53,53,53	0
36	SR	S	8961	1/1	0.83	0.19	189,189,189,189	0
37	NA	0	8518	1/1	0.83	0.24	68,68,68,68	0
37	NA	0	8565	1/1	0.83	0.17	59,59,59,59	0
37	NA	0	8501	1/1	0.84	0.42	100,100,100,100	0
37	NA	0	8519	1/1	0.84	0.22	53,53,53,53	0
36	SR	0	8969	1/1	0.84	0.30	154,154,154,154	0
34	MG	0	8017	1/1	0.84	0.25	80,80,80,80	0
34	MG	0	8069	1/1	0.84	0.39	88,88,88,88	0
34	MG	0	8029	1/1	0.85	0.46	87,87,87,87	0
37	NA	0	8514	1/1	0.85	0.24	53,53,53,53	0
37	NA	0	8562	1/1	0.85	0.43	61,61,61,61	0
35	CL	3	8804	1/1	0.85	0.18	88,88,88,88	0
34	MG	A	8051	1/1	0.85	0.13	58,58,58,58	0
34	MG	0	8046	1/1	0.85	0.49	99,99,99,99	0
37	NA	0	8569	1/1	0.85	0.14	44,44,44,44	0
34	MG	0	8079	1/1	0.86	0.24	64,64,64,64	0
34	MG	0	8056	1/1	0.86	0.23	69,69,69,69	0
36	SR	0	8933	1/1	0.86	0.31	168,168,168,168	0
36	SR	9	8980	1/1	0.86	0.14	155,155,155,155	0
36	SR	9	9003	1/1	0.86	0.14	127,127,127,127	0
37	NA	B	8552	1/1	0.86	0.21	69,69,69,69	0
37	NA	D	8543	1/1	0.86	0.23	60,60,60,60	0
37	NA	Q	8540	1/1	0.86	0.13	48,48,48,48	0
34	MG	0	8064	1/1	0.86	0.12	51,51,51,51	0
36	SR	0	8996	1/1	0.86	0.17	148,148,148,148	0
34	MG	0	8091	1/1	0.87	0.19	59,59,59,59	0
36	SR	0	8986	1/1	0.87	0.14	114,114,114,114	0
37	NA	0	8541	1/1	0.87	0.32	80,80,80,80	0
34	MG	0	8040	1/1	0.87	0.23	75,75,75,75	0
34	MG	0	8033	1/1	0.87	0.12	59,59,59,59	0
37	NA	S	8510	1/1	0.88	0.11	58,58,58,58	0
36	SR	0	9000	1/1	0.88	0.13	137,137,137,137	0
34	MG	0	8035	1/1	0.88	0.31	94,94,94,94	0
34	MG	T	8057	1/1	0.88	0.19	65,65,65,65	0
37	NA	0	8531	1/1	0.88	0.19	37,37,37,37	0
37	NA	0	8507	1/1	0.88	0.35	88,88,88,88	0
37	NA	0	8536	1/1	0.88	0.28	69,69,69,69	0
37	NA	J	8538	1/1	0.88	0.14	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	MG	0	8047	1/1	0.88	0.33	89,89,89,89	0
37	NA	0	8516	1/1	0.88	0.15	42,42,42,42	0
37	NA	0	8558	1/1	0.89	0.30	56,56,56,56	0
36	SR	0	8976	1/1	0.89	0.14	124,124,124,124	0
37	NA	0	8524	1/1	0.89	0.10	37,37,37,37	0
37	NA	0	8575	1/1	0.89	0.28	59,59,59,59	0
37	NA	0	8525	1/1	0.89	0.32	63,63,63,63	0
34	MG	0	8002	1/1	0.89	0.23	62,62,62,62	0
34	MG	9	8074	1/1	0.89	0.28	53,53,53,53	0
37	NA	0	8508	1/1	0.89	0.09	31,31,31,31	0
36	SR	0	9007	1/1	0.89	0.46	200,200,200,200	0
36	SR	0	8951	1/1	0.90	0.10	107,107,107,107	0
34	MG	0	8024	1/1	0.90	0.19	80,80,80,80	0
37	NA	0	8557	1/1	0.90	0.30	57,57,57,57	0
34	MG	0	8053	1/1	0.90	0.20	54,54,54,54	0
36	SR	0	8971	1/1	0.90	0.14	157,157,157,157	0
37	NA	0	8521	1/1	0.90	0.23	61,61,61,61	0
34	MG	0	8092	1/1	0.90	0.09	48,48,48,48	0
34	MG	2	8060	1/1	0.90	0.13	42,42,42,42	0
34	MG	0	8076	1/1	0.90	0.21	81,81,81,81	0
37	NA	0	8529	1/1	0.90	0.08	20,20,20,20	0
36	SR	0	8944	1/1	0.91	0.12	113,113,113,113	0
37	NA	0	8554	1/1	0.91	0.21	53,53,53,53	0
37	NA	0	8534	1/1	0.91	0.31	78,78,78,78	0
37	NA	0	8570	1/1	0.91	0.28	53,53,53,53	0
34	MG	0	8077	1/1	0.91	0.08	37,37,37,37	0
34	MG	0	8089	1/1	0.91	0.07	35,35,35,35	0
37	NA	0	8574	1/1	0.91	0.32	48,48,48,48	0
37	NA	0	8512	1/1	0.91	0.21	43,43,43,43	0
34	MG	0	8048	1/1	0.91	0.10	43,43,43,43	0
37	NA	0	8505	1/1	0.91	0.23	29,29,29,29	0
37	NA	0	8528	1/1	0.91	0.09	42,42,42,42	0
37	NA	0	8549	1/1	0.91	0.12	61,61,61,61	0
37	NA	M	8539	1/1	0.91	0.10	33,33,33,33	0
34	MG	0	8030	1/1	0.92	0.31	188,188,188,188	0
34	MG	0	8044	1/1	0.92	0.10	47,47,47,47	0
37	NA	0	8550	1/1	0.92	0.17	43,43,43,43	0
34	MG	0	8082	1/1	0.92	0.19	64,64,64,64	0
35	CL	A	8809	1/1	0.92	0.18	57,57,57,57	0
37	NA	0	8523	1/1	0.92	0.18	49,49,49,49	0
37	NA	R	8533	1/1	0.92	0.23	42,42,42,42	0
37	NA	0	8566	1/1	0.92	0.15	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	NA	0	8517	1/1	0.92	0.18	40,40,40,40	0
37	NA	R	8532	1/1	0.92	0.14	29,29,29,29	0
36	SR	0	9004	1/1	0.93	0.10	107,107,107,107	0
34	MG	0	8087	1/1	0.93	0.30	106,106,106,106	0
37	NA	0	8511	1/1	0.93	0.21	48,48,48,48	0
36	SR	0	8955	1/1	0.93	0.10	115,115,115,115	0
36	SR	0	8991	1/1	0.93	0.16	147,147,147,147	0
37	NA	0	8526	1/1	0.93	0.07	47,47,47,47	0
35	CL	B	8819	1/1	0.93	0.23	56,56,56,56	0
34	MG	0	8080	1/1	0.93	0.12	62,62,62,62	0
36	SR	B	8950	1/1	0.93	0.08	89,89,89,89	0
36	SR	0	8975	1/1	0.93	0.10	115,115,115,115	0
34	MG	0	8032	1/1	0.93	0.08	44,44,44,44	0
34	MG	0	8027	1/1	0.94	0.12	44,44,44,44	0
36	SR	0	8956	1/1	0.94	0.10	105,105,105,105	0
36	SR	0	8958	1/1	0.94	0.07	68,68,68,68	0
37	NA	0	8542	1/1	0.94	0.10	38,38,38,38	0
37	NA	0	8544	1/1	0.94	0.45	67,67,67,67	0
34	MG	0	8015	1/1	0.94	0.14	45,45,45,45	0
36	SR	0	8962	1/1	0.94	0.07	96,96,96,96	0
36	SR	0	8965	1/1	0.94	0.11	88,88,88,88	0
34	MG	0	8068	1/1	0.94	0.21	74,74,74,74	0
36	SR	0	8928	1/1	0.94	0.07	87,87,87,87	0
36	SR	0	8974	1/1	0.94	0.11	110,110,110,110	0
36	SR	9	8968	1/1	0.94	0.08	105,105,105,105	0
34	MG	0	8005	1/1	0.94	0.15	30,30,30,30	0
35	CL	J	8802	1/1	0.94	0.08	66,66,66,66	0
34	MG	0	8050	1/1	0.94	0.31	162,162,162,162	0
37	NA	0	8530	1/1	0.94	0.12	38,38,38,38	0
34	MG	0	8073	1/1	0.94	0.14	62,62,62,62	0
36	SR	0	8988	1/1	0.94	0.07	110,110,110,110	0
34	MG	0	8039	1/1	0.95	0.10	32,32,32,32	0
36	SR	A	8929	1/1	0.95	0.10	105,105,105,105	0
36	SR	0	8997	1/1	0.95	0.07	116,116,116,116	0
34	MG	0	8055	1/1	0.95	0.14	30,30,30,30	0
34	MG	0	8023	1/1	0.95	0.07	21,21,21,21	0
34	MG	0	8067	1/1	0.95	0.11	48,48,48,48	0
36	SR	0	8915	1/1	0.95	0.06	73,73,73,73	0
37	NA	0	8563	1/1	0.95	0.15	55,55,55,55	0
36	SR	0	8916	1/1	0.95	0.08	65,65,65,65	0
34	MG	0	8008	1/1	0.95	0.06	13,13,13,13	0
35	CL	K	8812	1/1	0.95	0.07	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	NA	0	8513	1/1	0.95	0.07	29,29,29,29	0
36	SR	0	8931	1/1	0.95	0.08	74,74,74,74	0
37	NA	0	8545	1/1	0.95	0.06	40,40,40,40	0
35	CL	M	8818	1/1	0.95	0.06	33,33,33,33	0
36	SR	0	8941	1/1	0.95	0.07	71,71,71,71	0
37	NA	C	8503	1/1	0.95	0.11	22,22,22,22	0
36	SR	0	8982	1/1	0.95	0.10	105,105,105,105	0
35	CL	Q	8811	1/1	0.95	0.09	68,68,68,68	0
36	SR	0	8984	1/1	0.95	0.09	89,89,89,89	0
35	CL	Y	8820	1/1	0.95	0.07	35,35,35,35	0
36	SR	0	8945	1/1	0.95	0.08	89,89,89,89	0
36	SR	0	8946	1/1	0.95	0.09	86,86,86,86	0
36	SR	0	8966	1/1	0.96	0.11	86,86,86,86	0
37	NA	L	8568	1/1	0.96	0.12	30,30,30,30	0
36	SR	3	8999	1/1	0.96	0.07	70,70,70,70	0
36	SR	0	8970	1/1	0.96	0.06	88,88,88,88	0
36	SR	0	8914	1/1	0.96	0.12	75,75,75,75	0
36	SR	0	8973	1/1	0.96	0.06	91,91,91,91	0
34	MG	0	8059	1/1	0.96	0.10	58,58,58,58	0
35	CL	N	8807	1/1	0.96	0.08	62,62,62,62	0
36	SR	0	8919	1/1	0.96	0.06	82,82,82,82	0
37	NA	0	8504	1/1	0.96	0.07	20,20,20,20	0
36	SR	0	8981	1/1	0.96	0.13	107,107,107,107	0
35	CL	O	8808	1/1	0.96	0.12	63,63,63,63	0
36	SR	0	8923	1/1	0.96	0.09	66,66,66,66	0
36	SR	0	8926	1/1	0.96	0.12	81,81,81,81	0
36	SR	0	8985	1/1	0.96	0.12	116,116,116,116	0
34	MG	0	8052	1/1	0.96	0.06	37,37,37,37	0
34	MG	0	8007	1/1	0.96	0.06	37,37,37,37	0
34	MG	0	8031	1/1	0.96	0.09	48,48,48,48	0
36	SR	0	8992	1/1	0.96	0.14	102,102,102,102	0
37	NA	0	8515	1/1	0.96	0.09	20,20,20,20	0
36	SR	0	8993	1/1	0.96	0.09	126,126,126,126	0
36	SR	0	8935	1/1	0.96	0.07	64,64,64,64	0
36	SR	0	8995	1/1	0.96	0.09	86,86,86,86	0
36	SR	0	8938	1/1	0.96	0.08	101,101,101,101	0
35	CL	0	8813	1/1	0.96	0.07	53,53,53,53	0
35	CL	0	8815	1/1	0.96	0.09	61,61,61,61	0
35	CL	0	8816	1/1	0.96	0.16	60,60,60,60	0
35	CL	0	8817	1/1	0.96	0.09	42,42,42,42	0
34	MG	0	8034	1/1	0.96	0.06	31,31,31,31	0
36	SR	A	8977	1/1	0.96	0.09	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	CL	J	8821	1/1	0.96	0.09	61,61,61,61	0
34	MG	0	8075	1/1	0.96	0.04	35,35,35,35	0
36	SR	0	8957	1/1	0.96	0.13	122,122,122,122	0
36	SR	F	9005	1/1	0.96	0.10	85,85,85,85	0
36	SR	H	8972	1/1	0.96	0.15	119,119,119,119	0
35	CL	L	8810	1/1	0.96	0.14	52,52,52,52	0
36	SR	Y	9002	1/1	0.96	0.10	118,118,118,118	0
34	MG	0	8041	1/1	0.97	0.10	31,31,31,31	0
36	SR	0	8967	1/1	0.97	0.06	92,92,92,92	0
37	NA	0	8527	1/1	0.97	0.08	40,40,40,40	0
36	SR	1	8952	1/1	0.97	0.07	60,60,60,60	0
36	SR	0	8936	1/1	0.97	0.07	59,59,59,59	0
34	MG	0	8084	1/1	0.97	0.12	31,31,31,31	0
36	SR	0	8901	1/1	0.97	0.06	44,44,44,44	0
36	SR	0	8908	1/1	0.97	0.06	66,66,66,66	0
35	CL	0	8822	1/1	0.97	0.28	53,53,53,53	0
36	SR	0	9008	1/1	0.97	0.08	80,80,80,80	0
34	MG	0	8043	1/1	0.97	0.12	37,37,37,37	0
34	MG	Y	8086	1/1	0.97	0.19	46,46,46,46	0
36	SR	0	8947	1/1	0.97	0.07	84,84,84,84	0
36	SR	0	8917	1/1	0.97	0.07	61,61,61,61	0
34	MG	0	8088	1/1	0.97	0.11	37,37,37,37	0
34	MG	0	8013	1/1	0.97	0.06	28,28,28,28	0
35	CL	0	8805	1/1	0.97	0.06	46,46,46,46	0
34	MG	0	8001	1/1	0.97	0.12	22,22,22,22	0
36	SR	0	8927	1/1	0.97	0.11	67,67,67,67	0
38	CD	O	8705	1/1	0.97	0.07	103,103,103,103	0
36	SR	0	8960	1/1	0.97	0.07	98,98,98,98	0
34	MG	0	8036	1/1	0.97	0.15	47,47,47,47	0
36	SR	0	8963	1/1	0.97	0.09	70,70,70,70	0
36	SR	T	8911	1/1	0.97	0.05	52,52,52,52	0
36	SR	0	8943	1/1	0.98	0.06	65,65,65,65	0
36	SR	3	8953	1/1	0.98	0.06	103,103,103,103	0
36	SR	0	8989	1/1	0.98	0.06	71,71,71,71	0
36	SR	0	8990	1/1	0.98	0.08	39,39,39,39	0
35	CL	2	8803	1/1	0.98	0.08	51,51,51,51	0
34	MG	K	8054	1/1	0.98	0.08	18,18,18,18	0
36	SR	0	8905	1/1	0.98	0.11	49,49,49,49	0
34	MG	0	8093	1/1	0.98	0.10	25,25,25,25	0
36	SR	0	8954	1/1	0.98	0.06	67,67,67,67	0
34	MG	0	8066	1/1	0.98	0.17	32,32,32,32	0
34	MG	0	8014	1/1	0.98	0.10	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	MG	0	8009	1/1	0.98	0.18	1,1,1,1	0
35	CL	J	8801	1/1	0.98	0.14	58,58,58,58	0
36	SR	0	8918	1/1	0.98	0.06	41,41,41,41	0
34	MG	A	8025	1/1	0.98	0.06	40,40,40,40	0
34	MG	0	8083	1/1	0.98	0.06	36,36,36,36	0
36	SR	0	8921	1/1	0.98	0.06	51,51,51,51	0
36	SR	0	8964	1/1	0.98	0.04	92,92,92,92	0
36	SR	0	8922	1/1	0.98	0.04	62,62,62,62	0
36	SR	A	8930	1/1	0.98	0.11	72,72,72,72	0
36	SR	0	8924	1/1	0.98	0.11	65,65,65,65	0
36	SR	0	8925	1/1	0.98	0.11	66,66,66,66	0
34	MG	0	8070	1/1	0.98	0.11	62,62,62,62	0
35	CL	L	8814	1/1	0.98	0.15	49,49,49,49	0
34	MG	0	8011	1/1	0.98	0.07	17,17,17,17	0
34	MG	0	8072	1/1	0.98	0.06	25,25,25,25	0
34	MG	0	8061	1/1	0.98	0.08	17,17,17,17	0
34	MG	0	8018	1/1	0.98	0.15	9,9,9,9	0
34	MG	0	8019	1/1	0.98	0.07	9,9,9,9	0
36	SR	0	8937	1/1	0.98	0.04	59,59,59,59	0
38	CD	Z	8703	1/1	0.98	0.03	62,62,62,62	0
37	NA	0	8537	1/1	0.98	0.03	22,22,22,22	0
36	SR	T	8939	1/1	0.98	0.05	70,70,70,70	0
35	CL	R	8806	1/1	0.98	0.06	36,36,36,36	0
34	MG	0	8021	1/1	0.98	0.09	24,24,24,24	0
36	SR	0	8948	1/1	0.99	0.07	57,57,57,57	0
36	SR	0	8949	1/1	0.99	0.04	49,49,49,49	0
36	SR	0	8978	1/1	0.99	0.06	60,60,60,60	0
36	SR	0	8904	1/1	0.99	0.07	39,39,39,39	0
36	SR	R	8912	1/1	0.99	0.08	64,64,64,64	0
36	SR	0	8906	1/1	0.99	0.07	49,49,49,49	0
34	MG	C	8012	1/1	0.99	0.08	13,13,13,13	0
36	SR	0	8909	1/1	0.99	0.10	59,59,59,59	0
36	SR	0	8910	1/1	0.99	0.03	40,40,40,40	0
36	SR	0	8934	1/1	0.99	0.08	67,67,67,67	0
34	MG	0	8026	1/1	0.99	0.10	35,35,35,35	0
34	MG	0	8006	1/1	0.99	0.06	6,6,6,6	0
34	MG	0	8028	1/1	0.99	0.11	1,1,1,1	0
36	SR	1	8913	1/1	0.99	0.05	42,42,42,42	0
36	SR	0	8940	1/1	0.99	0.05	53,53,53,53	0
34	MG	0	8020	1/1	0.99	0.18	24,24,24,24	0
34	MG	0	8003	1/1	0.99	0.07	18,18,18,18	0
36	SR	3	8932	1/1	0.99	0.07	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
38	CD	1	8702	1/1	0.99	0.04	50,50,50,50	0
36	SR	H	8907	1/1	0.99	0.05	41,41,41,41	0
34	MG	0	8004	1/1	0.99	0.06	13,13,13,13	0
36	SR	0	8902	1/1	0.99	0.07	32,32,32,32	0
36	SR	0	8903	1/1	0.99	0.09	44,44,44,44	0
38	CD	U	8701	1/1	1.00	0.03	50,50,50,50	0
34	MG	0	8022	1/1	1.00	0.10	12,12,12,12	0
34	MG	0	8058	1/1	1.00	0.13	1,1,1,1	0
38	CD	3	8704	1/1	1.00	0.01	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.