



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 07:35 am BST

PDB ID : 3CMA
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

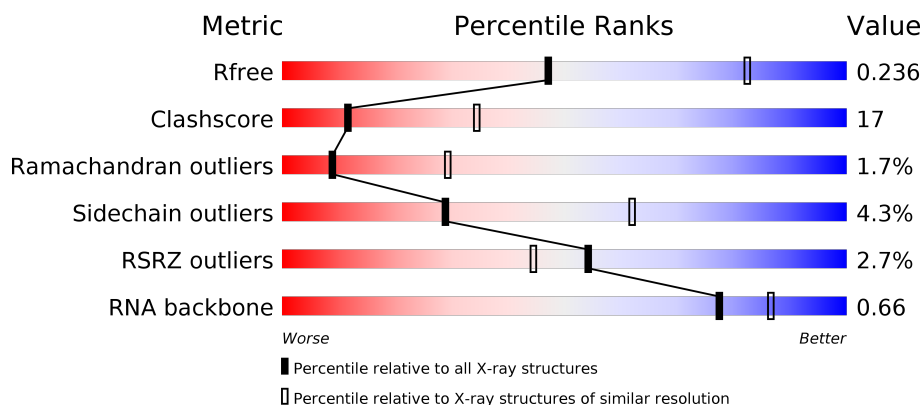
1 Overall quality at a glance

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.








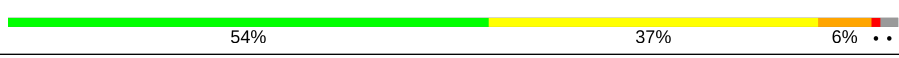



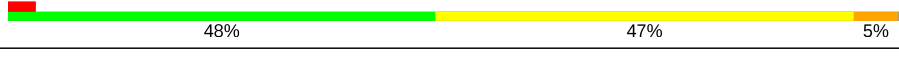

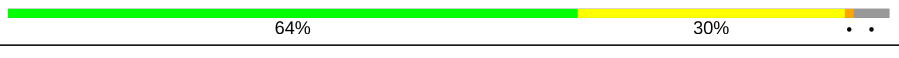





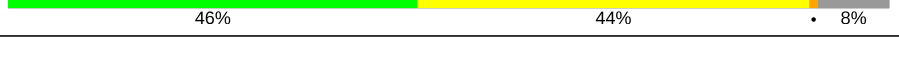


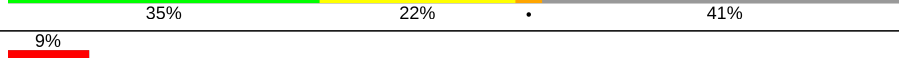
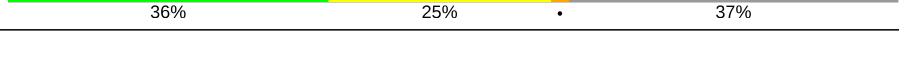

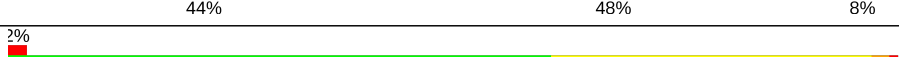

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div> <div>3%</div> <div>54%</div> <div>41%</div> <div>..</div> </div>
2	B	338	<div> <div>46%</div> <div>51%</div> <div>.</div> </div>
3	C	246	<div> <div>62%</div> <div>33%</div> <div>5%</div> </div>
4	D	177	<div> <div>13%</div> <div>28%</div> <div>46%</div> <div>..</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	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	8016	-	-	-	X
34	MG	0	8038	-	-	-	X
34	MG	0	8046	-	-	-	X
34	MG	0	8047	-	-	-	X
34	MG	0	8050	-	-	-	X
34	MG	0	8063	-	-	-	X
34	MG	0	8065	-	-	-	X
34	MG	0	8078	-	-	-	X
34	MG	0	8087	-	-	-	X
34	MG	0	8090	-	-	-	X
36	SR	0	8920	-	-	-	X
36	SR	0	8933	-	-	-	X
36	SR	0	9006	-	-	-	X
36	SR	0	9007	-	-	-	X
36	SR	B	8987	-	-	-	X
37	NA	0	8509	-	-	-	X
37	NA	0	8519	-	-	-	X
37	NA	0	8547	-	-	-	X
37	NA	0	8560	-	-	-	X
37	NA	0	8567	-	-	-	X
37	NA	0	8571	-	-	-	X
37	NA	0	8573	-	-	-	X
40	PHE	6	77	-	-	-	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		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 (three-letter code: MG) (formula: Mg).

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

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

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	6	Total 6	Cl 6	0	0
35	J	3	Total 3	Cl 3	0	0
35	Q	1	Total 1	Cl 1	0	0
35	K	1	Total 1	Cl 1	0	0
35	B	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	A	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	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	L	2	Total 2	Cl 2	0	0
35	2	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	M	1	Total Cl 1 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

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

- Molecule 37 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	64	Total Na 64 64	0	0
37	J	1	Total Na 1 1	0	0
37	Q	1	Total Na 1 1	0	0
37	D	1	Total Na 1 1	0	0

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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	R	2	Total 2	Na 2	0	0
37	9	1	Total 1	Na 1	0	0
37	L	1	Total 1	Na 1	0	0
37	S	1	Total 1	Na 1	0	0
37	M	1	Total 1	Na 1	0	0

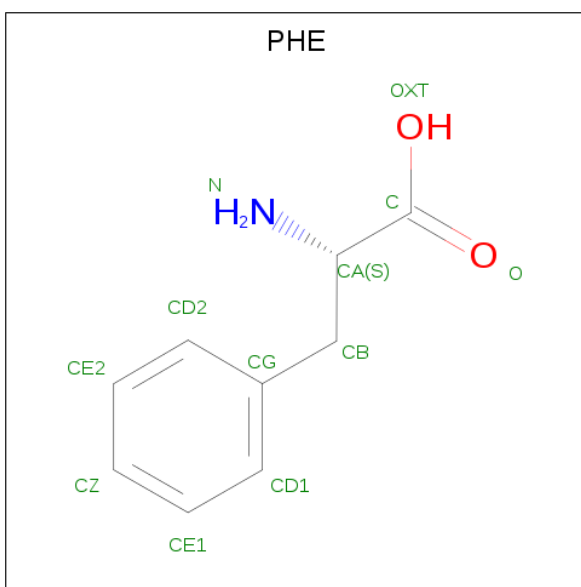
- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 39 is POTASSIUM ION (three-letter code: K) (formula: K).

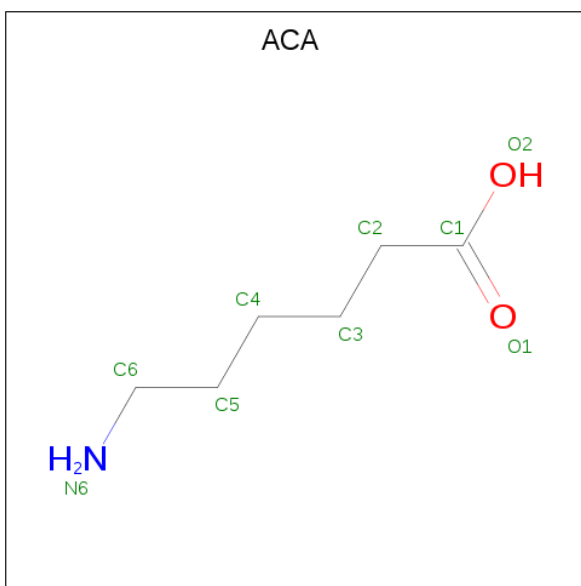
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	2	Total 2	K 2	0	0

- Molecule 40 is PHENYLALANINE (three-letter code: 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 (three-letter code: ACA) (formula: $C_6H_{13}NO_2$).



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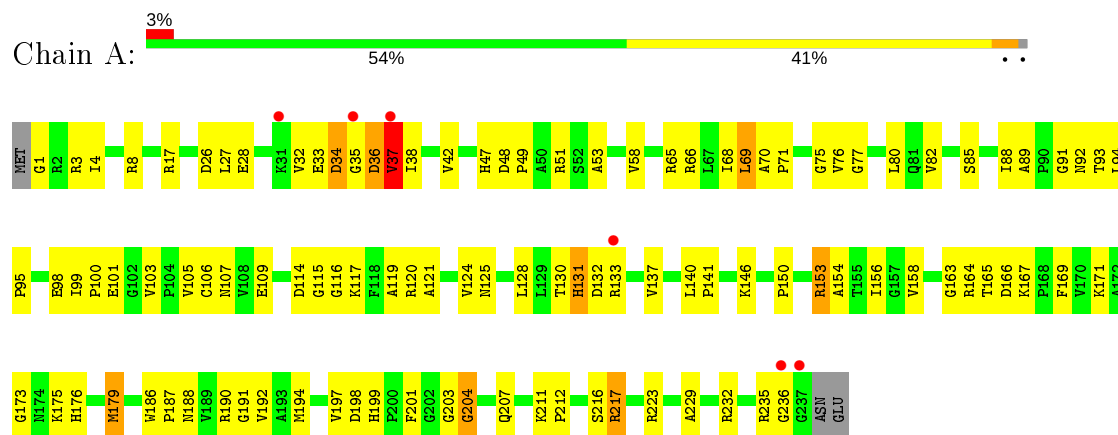
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	W	72	Total 72	O 72	0	0
42	X	25	Total 25	O 25	0	0
42	Y	108	Total 108	O 108	0	0
42	Z	30	Total 30	O 30	0	0
42	1	53	Total 53	O 53	0	0
42	2	42	Total 42	O 42	0	0
42	3	66	Total 66	O 66	0	0
42	0	5771	Total 5771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

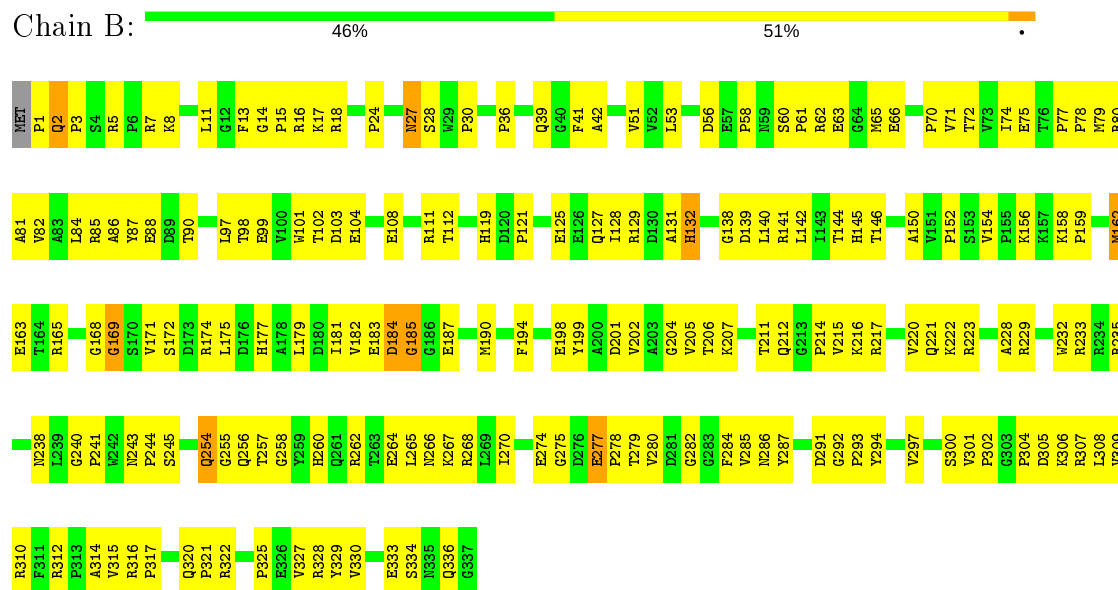
3 Residue-property plots [i](#)

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

• Molecule 1: 50S ribosomal protein L2P

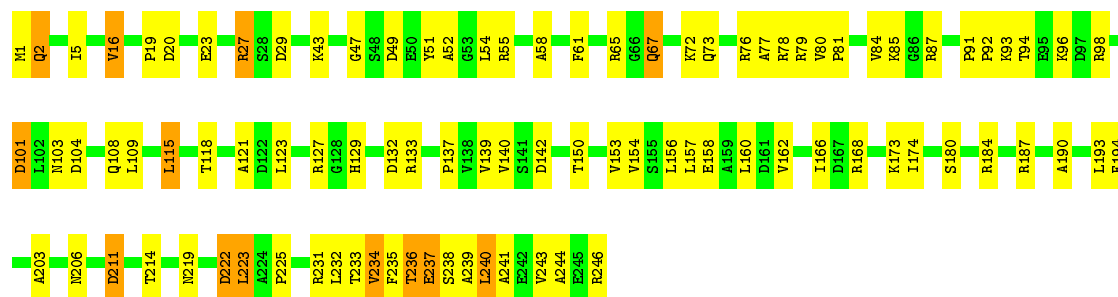


• Molecule 2: 50S ribosomal protein L3P

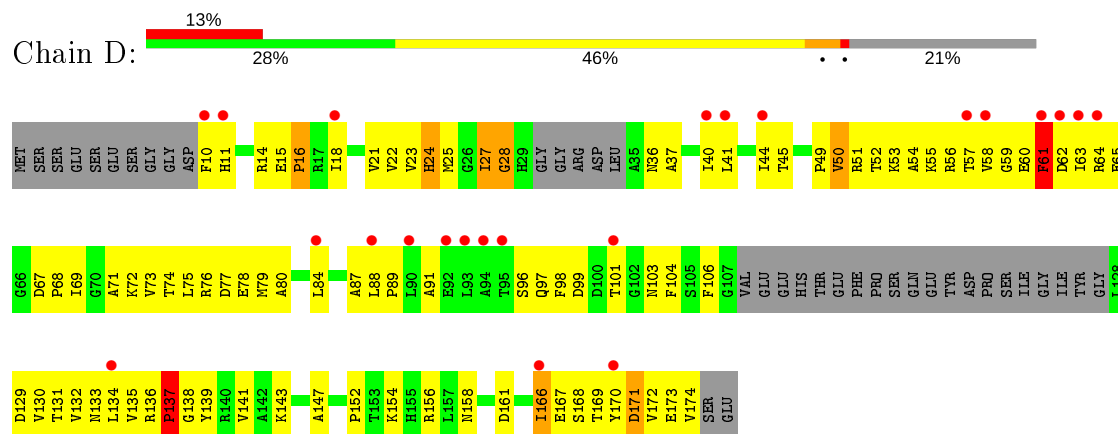


• Molecule 3: 50S ribosomal protein L4P

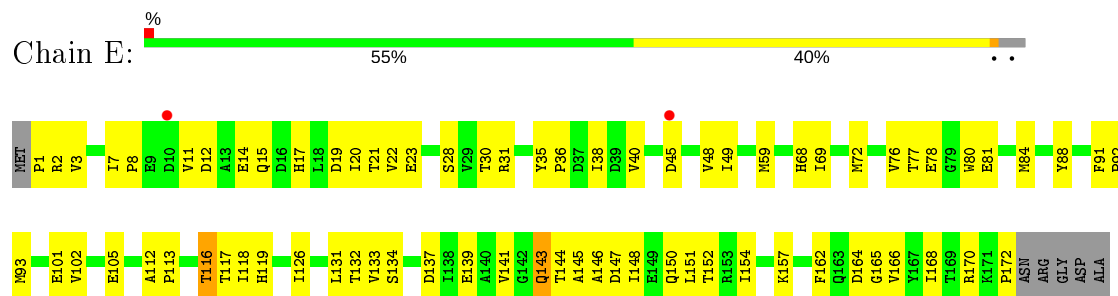




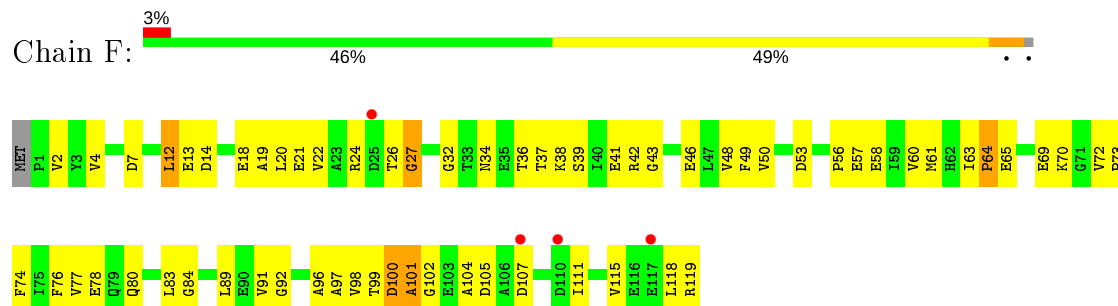
• Molecule 4: 50S ribosomal protein L5P



• Molecule 5: 50S ribosomal protein L6P

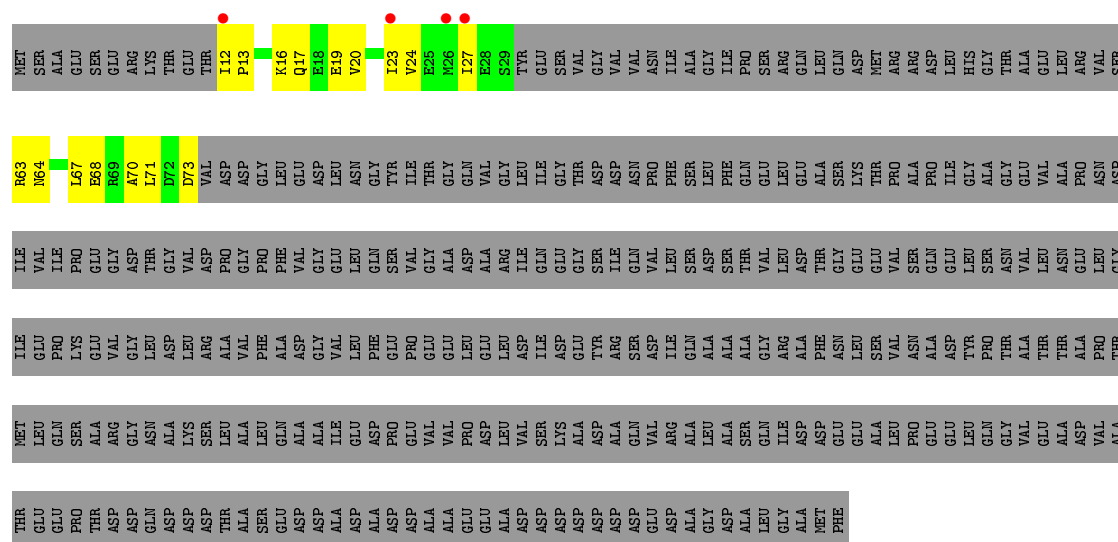


• Molecule 6: 50S ribosomal protein L7Ae

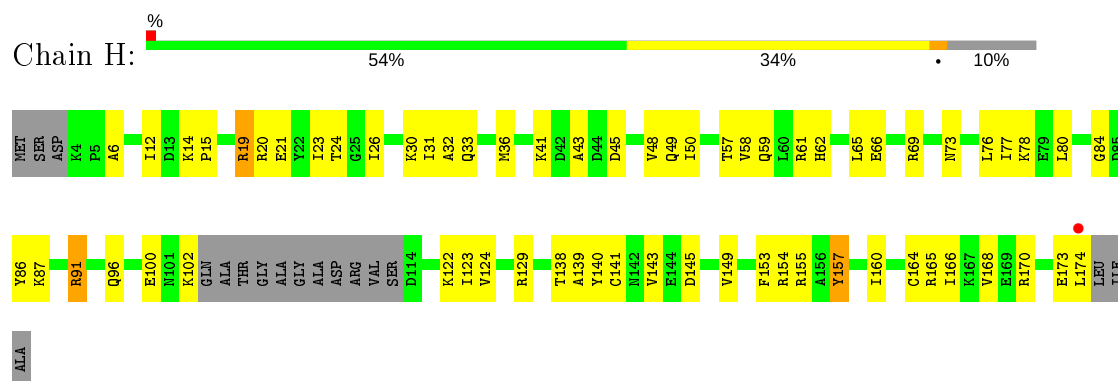


• Molecule 7: 50S ribosomal protein L10E

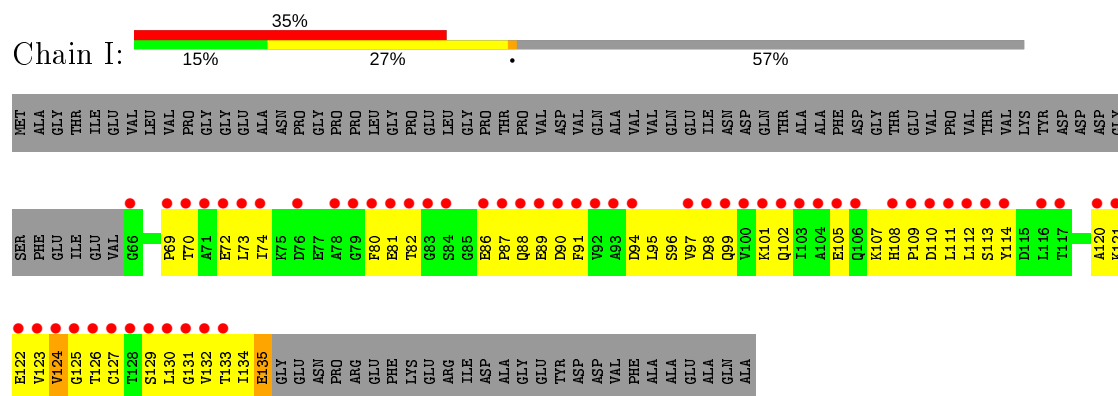




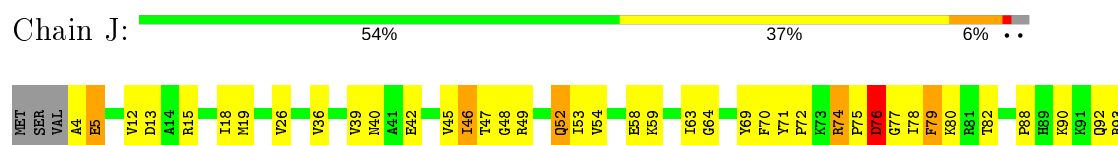
- Molecule 8: 50S ribosomal protein L10e

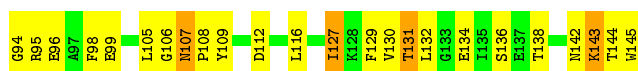


- Molecule 9: 50S ribosomal protein L11P

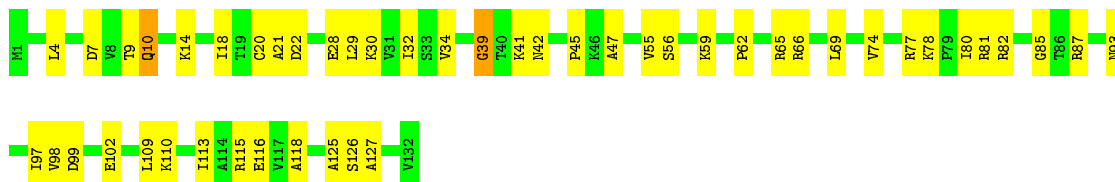


- Molecule 10: 50S ribosomal protein L13P

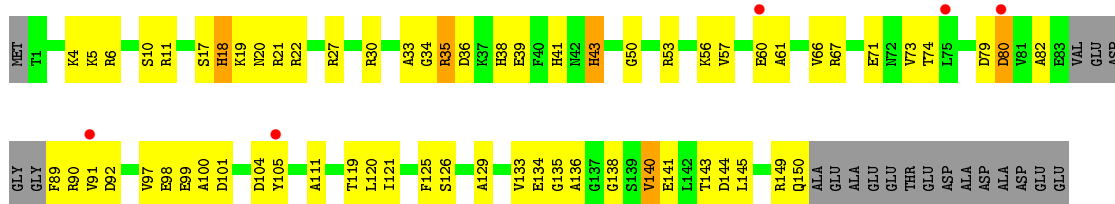




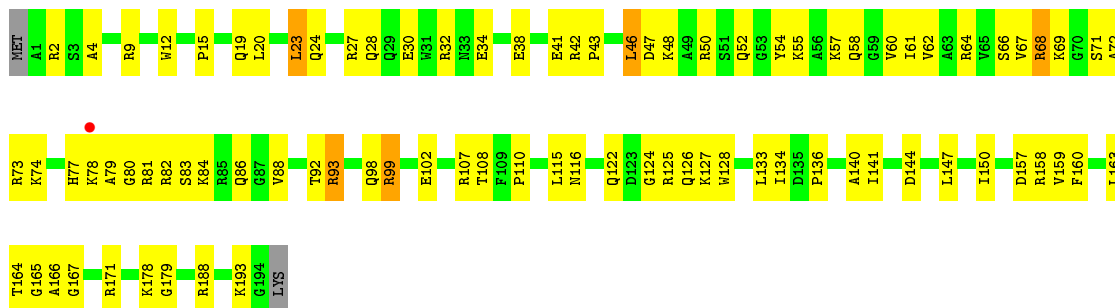
- Molecule 11: 50S ribosomal protein L14P



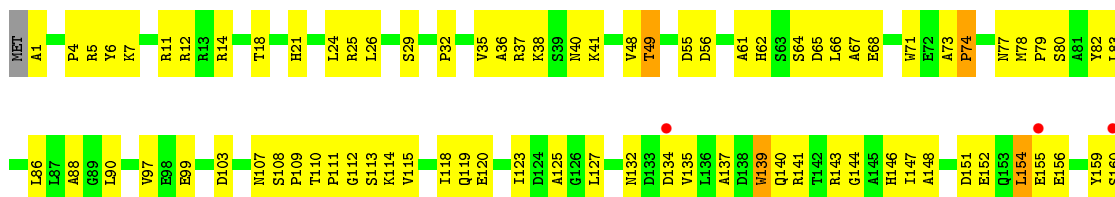
- Molecule 12: 50S ribosomal protein L15P



- Molecule 13: 50S ribosomal protein L15e

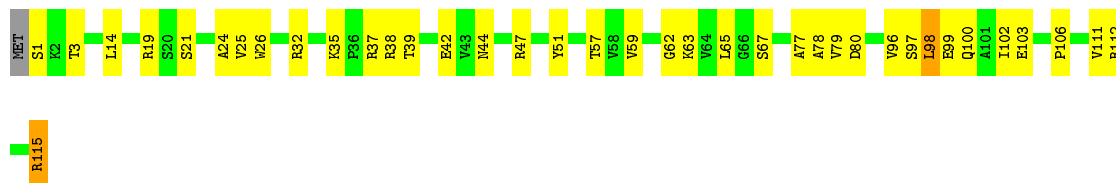


- Molecule 14: 50S ribosomal protein L18P

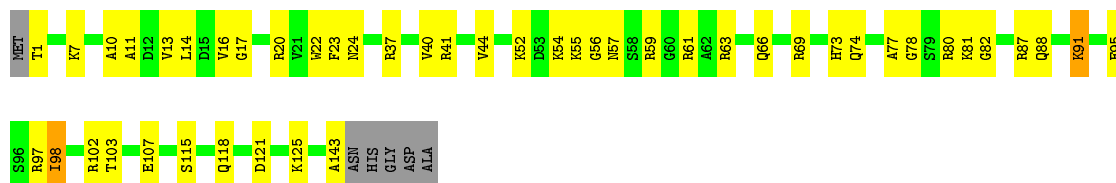




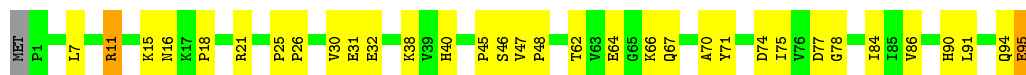
- Molecule 15: 50S ribosomal protein L18e



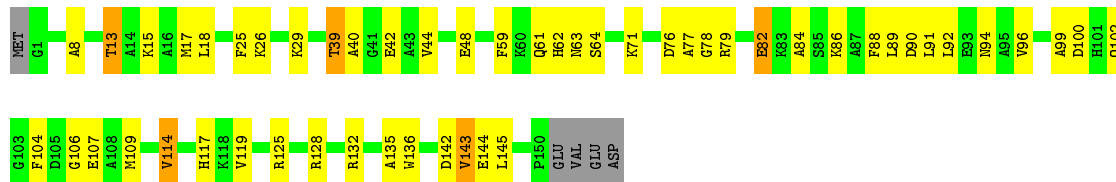
- Molecule 16: 50S ribosomal protein L19e



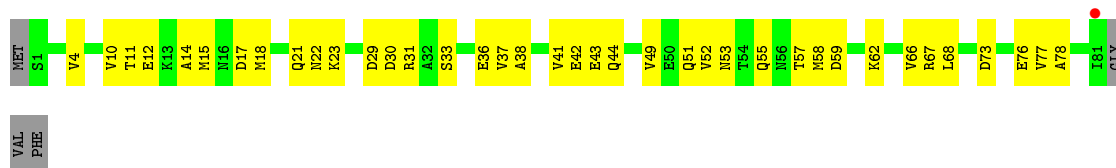
- Molecule 17: 50S ribosomal protein L21e



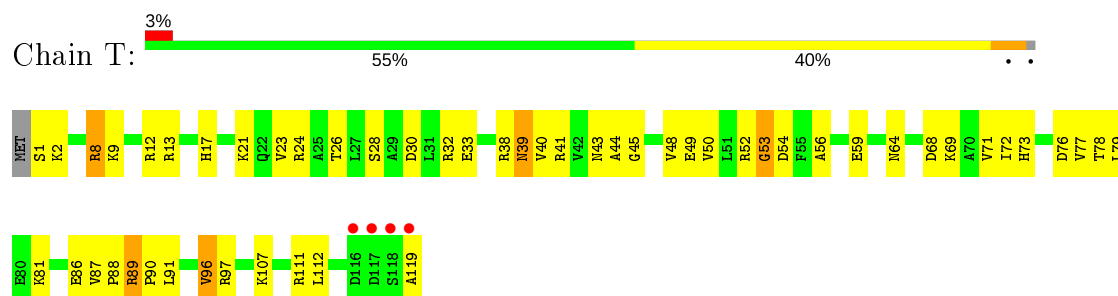
- Molecule 18: 50S ribosomal protein L22P



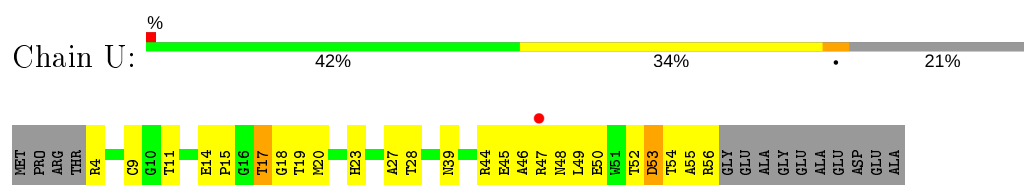
- Molecule 19: 50S ribosomal protein L23P



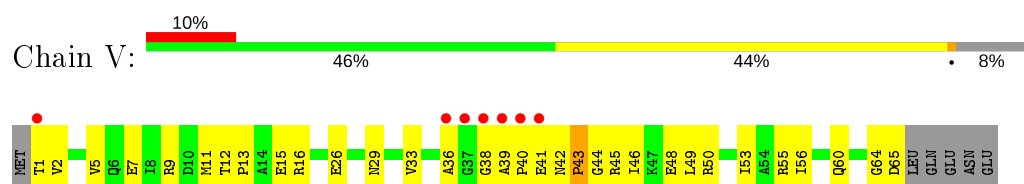
- Molecule 20: 50S ribosomal protein L24P



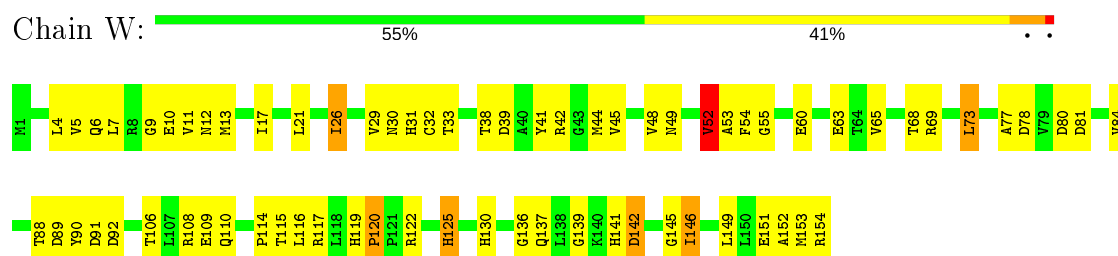
- Molecule 21: 50S ribosomal protein L24e



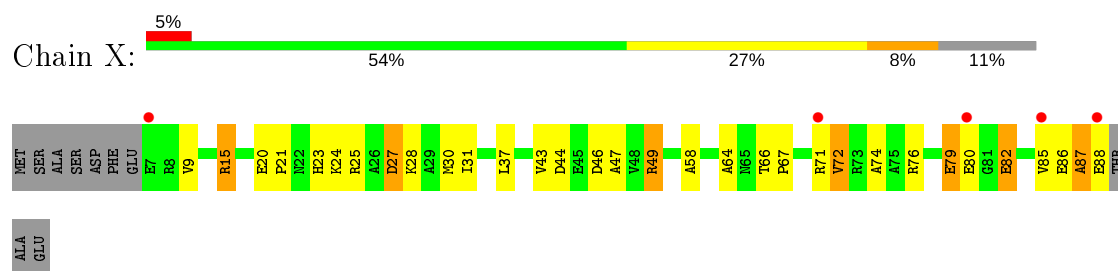
- Molecule 22: 50S ribosomal protein L29P



- Molecule 23: 50S ribosomal protein L30P

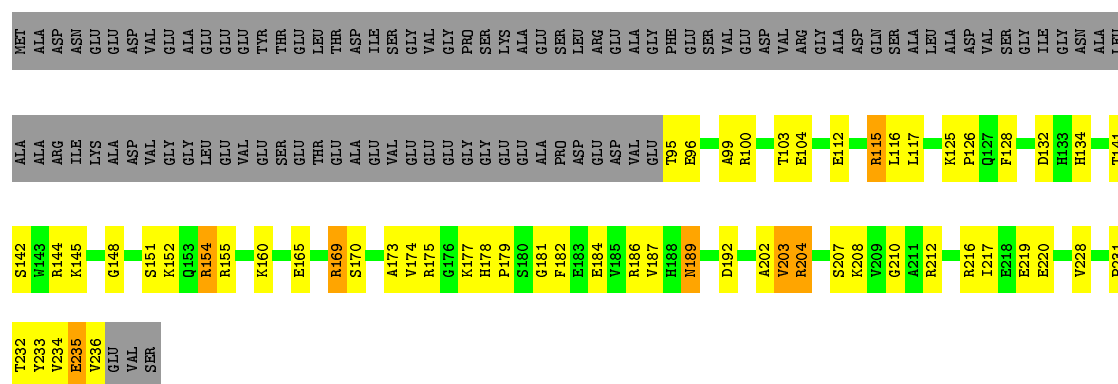


- Molecule 24: 50S ribosomal protein L31e

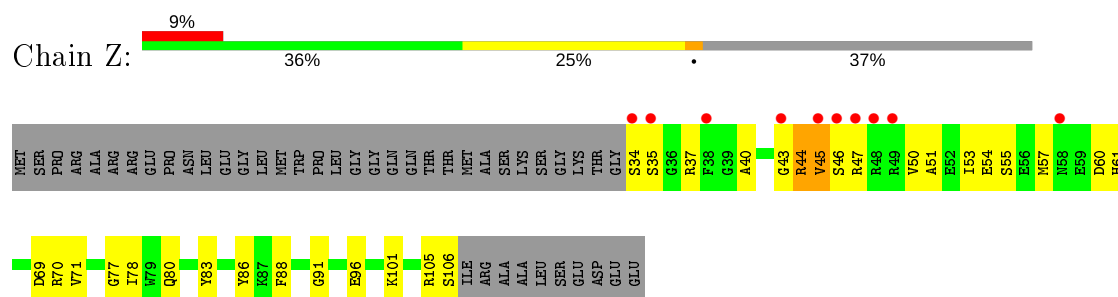


- Molecule 25: 50S ribosomal protein L32e

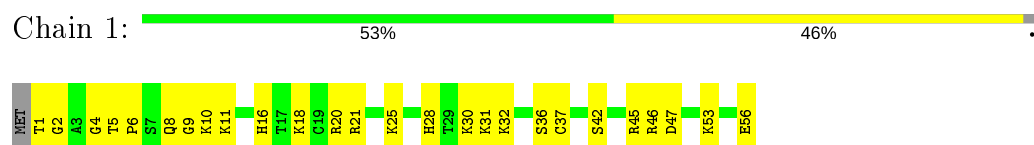




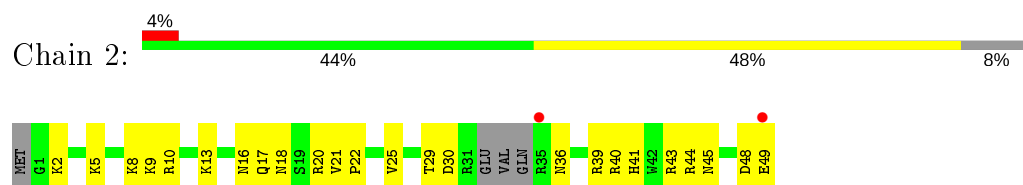
- Molecule 26: 50S ribosomal protein L37Ae



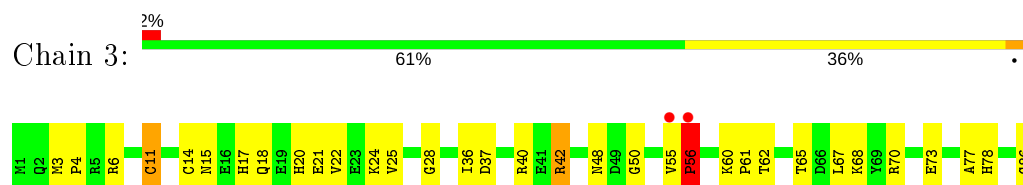
- Molecule 27: 50S ribosomal protein L37e



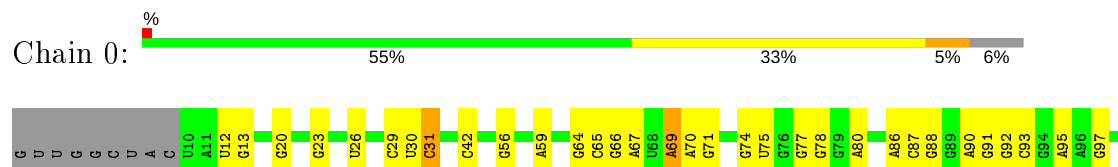
- Molecule 28: 50S ribosomal protein L39e



- Molecule 29: 50S ribosomal protein L44E



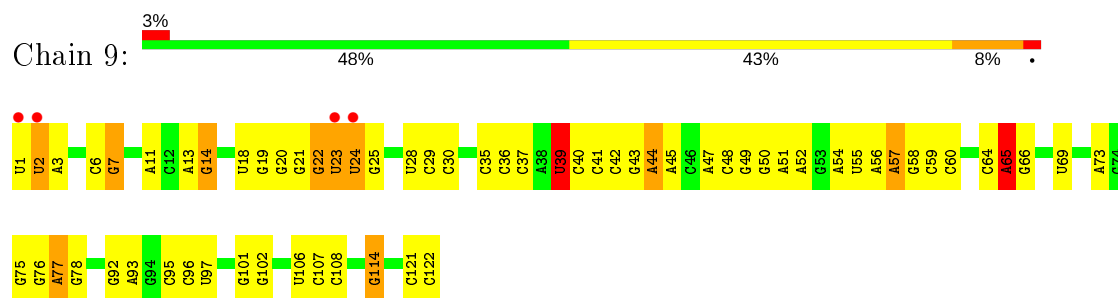
- Molecule 30: 23S RIBOSOMAL RNA



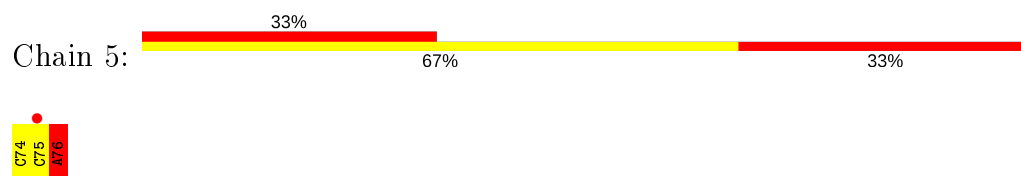
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G1523	A1406	G1310	G1213	C1140	C1019	A926	G814	G709	U612	G505	U398	A305	A198	G105
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A1526	G1409	U1314	U1219	G1151	A1022	C933	G816	U	A620	A508	A407	U308	U108	U108
A1527	G1410	G1315	C1229	G1158	A1022	G944	G817	G716	G621	A509	A408	C309	U109	U109
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G2897	U2803	U2803	U2803	U2590			C	C	C		U	U1928	G1820	U1731
U2898	U2804	U2804	U2804	U2591			C	C	C		U	U1929	G1821	U1732
A2899	U2805	U2805	U2805	U2592			C	C	C		U	U1930	G1822	U1733
C2900	U2806	U2806	U2806	U2593			C	C	C		U	U1931	G1823	U1734
G2901	U2807	U2807	U2807	U2594			C	C	C		U	U1932	G1824	U1735
A2902	U2808	U2808	U2808	U2595			C	C	C		U	U1933	G1825	U1736
C2903	U2809	U2809	U2809	U2596			C	C	C		U	U1934	G1826	U1737
G2904	U2810	U2810	U2810	U2597			C	C	C		U	U1935	G1827	U1738
A2905	U2811	U2811	U2811	U2598			C	C	C		U	U1936	G1828	U1739
C2906	U2812	U2812	U2812	U2599			C	C	C		U	U1937	G1829	U1740
G2907	U2813	U2813	U2813	U2600			C	C	C		U	U1938	G1830	U1741
A2908	U2814	U2814	U2814	U2601			C	C	C		U	U1939	G1831	U1742
C2909	U2815	U2815	U2815	U2602			C	C	C		U	U1940	G1832	U1743
G2910	U2816	U2816	U2816	U2603			C	C	C		U	U1941	G1833	U1744
A2911	U2817	U2817	U2817	U2604			C	C	C		U	U1942	G1834	U1745
C2912	U2818	U2818	U2818	U2605			C	C	C		U	U1943	G1835	U1746
G2913	U2819	U2819	U2819	U2606			C	C	C		U	U1944	G1836	U1747
A2914	U2820	U2820	U2820	U2607			C	C	C		U	U1945	G1837	U1748
C2915	U2821	U2821	U2821	U2608			C	C	C		U	U1946	G1838	U1749
G2916	U2822	U2822	U2822	U2609			C	C	C		U	U1947	G1839	U1750
A2917	U2823	U2823	U2823	U2610			C	C	C		U	U1948	G1840	U1751
C2918	U2824	U2824	U2824	U2611			C	C	C		U	U1949	G1841	U1752
G2919	U2825	U2825	U2825	U2612			C	C	C		U	U1950	G1842	U1753
A2920	U2826	U2826	U2826	U2613			C	C	C		U	U1951	G1843	U1754
C2921	U2827	U2827	U2827	U2614			C	C	C		U	U1952	G1844	U1755
G2922	U2828	U2828	U2828	U2615			C	C	C		U	U1953	G1845	U1756
A2923	U2829	U2829	U2829	U2616			C	C	C		U	U1954	G1846	U1757
C2924	U2830	U2830	U2830	U2617			C	C	C		U	U1955	G1847	U1758
G2925	U2831	U2831	U2831	U2618			C	C	C		U	U1956	G1848	U1759
A2926	U2832	U2832	U2832	U2619			C	C	C		U	U1957	G1849	U1760
C2927	U2833	U2833	U2833	U2620			C	C	C		U	U1958	G1850	U1761
G2928	U2834	U2834	U2834	U2621			C	C	C		U	U1959	G1851	U1762
A2929	U2835	U2835	U2835	U2622			C	C	C		U	U1960	G1852	U1763
C2930	U2836	U2836	U2836	U2623			C	C	C		U	U1961	G1853	U1764
G2931	U2837	U2837	U2837	U2624			C	C	C		U	U1962	G1854	U1765
A2932	U2838	U2838	U2838	U2625			C	C	C		U	U1963	G1855	U1766
C2933	U2839	U2839	U2839	U2626			C	C	C		U	U1964	G1856	U1767
G2934	U2840	U2840	U2840	U2627			C	C	C		U	U1965	G1857	U1768
A2935	U2841	U2841	U2841	U2628			C	C	C		U	U1966	G1858	U1769
C2936	U2842	U2842	U											

- 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 85.22 – 2.39	Depositor EDS
% Data completeness (in resolution range)	91.2 (49.79-2.80) 90.7 (85.22-2.39)	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 0.184 , 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)	0.31 , 71.5	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: ACA, OMG, 8AN, CL, SR, NA, K, MG, CD, OMU, UR3, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.33	0/1784	0.64	0/2403
2	B	0.35	0/2687	0.66	0/3644
3	C	0.37	0/1883	0.62	0/2547
4	D	0.31	0/1109	0.56	0/1493
5	E	0.33	0/1380	0.61	0/1875
6	F	0.32	0/899	0.56	0/1219
7	G	0.29	0/241	0.47	0/324
8	H	0.34	0/1300	0.64	0/1738
9	I	0.27	0/524	0.50	0/711
10	J	0.36	0/1134	0.60	0/1525
11	K	0.36	0/1002	0.68	0/1346
12	L	0.33	0/1128	0.63	0/1504
13	M	0.36	0/1580	0.60	0/2111
14	N	0.29	0/1472	0.61	0/1994
15	O	0.33	0/872	0.60	0/1176
16	P	0.35	0/1145	0.54	0/1524
17	Q	0.35	0/747	0.67	0/1001
18	R	0.37	0/1170	0.63	0/1574
19	S	0.33	0/646	0.56	0/870
20	T	0.33	0/956	0.62	0/1284
21	U	0.34	0/417	0.60	0/562
22	V	0.28	0/502	0.53	0/675
23	W	0.54	1/1217 (0.1%)	1.06	2/1650 (0.1%)
24	X	0.33	0/662	0.59	0/890
25	Y	0.36	0/1146	0.65	0/1536
26	Z	0.34	0/582	0.59	0/776
27	1	0.40	0/438	0.63	0/578
28	2	0.34	0/401	0.55	0/529
29	3	0.38	0/769	0.58	0/1019
30	0	0.39	0/65951	0.69	20/102855 (0.0%)
31	9	0.35	0/2897	0.71	1/4512 (0.0%)
32	5	0.64	0/65	1.28	2/99 (2.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.38	0/40	0.60	0/60
All	All	0.38	1/98746 (0.0%)	0.68	25/147604 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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	-14.55	1.22	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	52	VAL	CG1-CB-CG2	30.26	159.32	110.90
23	W	52	VAL	CA-CB-CG2	-16.79	85.72	110.90
30	0	1979	G	C2'-C3'-O3'	7.10	125.13	109.50
30	0	1942	A	C5'-C4'-C3'	7.05	127.28	116.00
30	0	2313	C	C5'-C4'-O4'	7.00	117.50	109.10
30	0	871	G	C5'-C4'-O4'	-6.96	100.75	109.10
30	0	1942	A	C5'-C4'-O4'	6.65	117.08	109.10
31	9	39	U	N1-C1'-C2'	6.45	122.39	114.00
30	0	2726	U	N1-C1'-C2'	6.38	122.30	114.00
30	0	1592	G	N9-C1'-C2'	6.06	121.88	114.00
30	0	2313	C	C5'-C4'-C3'	6.02	125.63	116.00
30	0	1504	A	N9-C1'-C2'	5.97	121.76	114.00
30	0	2291	A	N9-C1'-C2'	5.94	121.72	114.00
30	0	129	A	C2'-C3'-O3'	5.80	122.99	113.70
30	0	1819	G	C5'-C4'-C3'	5.68	125.09	116.00
30	0	2467	A	C1'-O4'-C4'	-5.63	105.39	109.90
32	5	76	A	C5'-C4'-C3'	-5.57	107.08	116.00
30	0	2301	A	N9-C1'-C2'	5.48	121.12	114.00
30	0	1504	A	C1'-O4'-C4'	-5.29	105.66	109.90
30	0	1942	A	C1'-O4'-C4'	-5.28	105.68	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2313	C	C1'-O4'-C4'	-5.14	105.78	109.90
30	0	1701	A	C5'-C4'-C3'	5.08	124.14	116.00
30	0	462	A	N9-C1'-C2'	5.07	120.58	114.00
32	5	76	A	C5'-C4'-O4'	-5.06	103.03	109.10
30	0	883	U	N1-C1'-C2'	5.05	120.56	114.00

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
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

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Mol	Chain	Res	Type	Group
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	129	0
2	B	2624	0	2530	190	0
3	C	1859	0	1811	97	0
4	D	1093	0	1083	96	0
5	E	1356	0	1264	77	0
6	F	889	0	841	63	0
7	G	240	0	231	17	0
8	H	1281	0	1290	63	0
9	I	518	0	495	49	0
10	J	1119	0	1096	74	0
11	K	993	0	1025	57	0
12	L	1117	0	1071	69	0
13	M	1557	0	1571	86	0
14	N	1444	0	1399	101	0
15	O	864	0	868	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	1135	0	1120	46	0
17	Q	734	0	726	29	0
18	R	1148	0	1119	51	0
19	S	640	0	600	30	0
20	T	949	0	922	54	0
21	U	410	0	364	32	0
22	V	499	0	511	41	0
23	W	1195	0	1135	89	0
24	X	653	0	651	34	0
25	Y	1130	0	1133	63	0
26	Z	572	0	529	25	0
27	1	431	0	426	35	0
28	2	396	0	413	27	0
29	3	754	0	727	33	0
30	0	59018	0	29811	1006	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	12	0	0
42	0	5771	0	0	145	0
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	21	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	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	59940	2631	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 17.

All (2631) 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)
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:H8	30:0:871:G:H5'	1.20	1.06
14:N:37:ARG:NH1	31:9:6:C:H5''	1.72	1.03
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.41	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:C8	30:0:871:G:H5'	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:541:C:C2'	30:0:542:A:H5''	1.94	0.97
14:N:144:GLY:O	14:N:147:ILE:HG22	1.64	0.97
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.28	0.96
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.46	0.96
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.48	0.95
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
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
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
2:B:162:MET:HE3	2:B:310:ARG:HD2	1.51	0.90
4:D:57:THR:HG23	4:D:63:ILE:HA	1.55	0.89
11:K:10:GLN:H	11:K:10:GLN:HE21	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
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
4:D:25:MET:HE2	4:D:41:LEU:HG	1.54	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
2:B:140:LEU:HA	42:B:9054:HOH:O	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:545:G:H8	30:0:545:G:H5'	1.40	0.85
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.58	0.85
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.58	0.85
25:Y:235:GLU:H	25:Y:235:GLU:CD	1.80	0.85
16:P:115:SER:OG	16:P:118:GLN:HG3	1.76	0.84
30:0:1377:C:H6	30:0:1377:C:H5'	1.40	0.84
2:B:275:GLY:O	2:B:291:ASP:HA	1.77	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
30:0:2506:A:HO2'	30:0:2507:G:H8	0.85	0.84
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.58	0.84
30:0:870:G:C2'	30:0:871:G:H5''	2.07	0.84
27:1:20:ARG:HG2	30:0:111:C:O2'	1.77	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
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:HH11	10:J:93:ARG:HB3	1.41	0.83
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
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
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.60	0.83
30:0:2586:U:H3	30:0:2592:G:H22	1.22	0.83
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.58	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
30:0:1474:C:H6	30:0:1474:C:H5'	1.44	0.82
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.60	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
30:0:1372:A:H3'	42:0:7983:HOH:O	1.79	0.81
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.61	0.81
13:M:107:ARG:HH11	13:M:107:ARG:HG3	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2534:C:H1'	42:0:4378:HOH:O	1.80	0.81
9:I:82:THR:HG23	30:0:1168:C:H5''	1.63	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
14:N:164:ASP:CG	14:N:167:ASP:HA	2.01	0.81
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.61	0.81
30:0:2005:G:H3'	30:0:2005:G:OP2	1.81	0.80
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.44	0.80
2:B:86:ALA:HA	42:B:9054:HOH:O	1.81	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:H5'	30:0:559:U:H6	1.45	0.80
30:0:1835:U:H5	30:0:1840:A:N7	1.79	0.80
4:D:154:LYS:HD2	4:D:154:LYS:H	1.45	0.80
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.62	0.80
30:0:1603:A:H5'	30:0:1605:G:O4'	1.80	0.79
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.80	0.79
10:J:74:ARG:CB	10:J:74:ARG:HH11	1.95	0.79
30:0:2908:A:H2'	30:0:2909:G:O4'	1.82	0.79
30:0:1667:A:H8	30:0:1667:A:H5'	1.48	0.79
30:0:541:C:H2'	30:0:542:A:C5'	2.13	0.79
30:0:877:G:H5'	30:0:878:G:OP1	1.82	0.79
1:A:153:ARG:CB	1:A:153:ARG:HH11	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
1:A:33:GLU:CD	1:A:33:GLU:H	1.86	0.79
20:T:112:LEU:HD23	20:T:119:ALA:HB3	1.63	0.78
30:0:506:G:H22	30:0:509:A:C5'	1.95	0.78
4:D:54:ALA:HB2	4:D:69: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
30:0:2717:C:H2'	30:0:2718:C:H5''	1.64	0.78
18:R:39:THR:HG23	18:R:107:GLU:O	1.83	0.78
30:0:1300:G:H1'	42:0:5535:HOH:O	1.82	0.77
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.83	0.77
30:0:2812:A:H2	30:0:2814:A:H62	1.32	0.77
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.32	0.77
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:MET:CE	2:B:310:ARG:HD2	2.14	0.77
13:M:80:GLY:O	13:M:81:ARG:HD2	1.84	0.77
30:0:681:G:H5'	30:0:681:G:N3	1.99	0.77
30:0:969:G:H1	30:0:999:C:H42	1.32	0.77
2:B:162:MET:HE3	2:B:310:ARG:HH11	1.47	0.77
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.67	0.77
9:I:73:LEU:HD12	9:I:107:LYS:NZ	1.98	0.77
30:0:506:G:H22	30:0:509:A:H5'	1.48	0.77
27:1:16:HIS:HD2	30:0:470:U:O2'	1.67	0.77
16:P:115:SER:H	16:P:118:GLN:NE2	1.82	0.77
30:0:1973:A:H5'	30:0:1973:A:H8	1.50	0.77
4:D:36:ASN:HA	42:D:7500:HOH:O	1.83	0.77
30:0:2637:A:H4'	30:0:2638:G:C5'	2.15	0.76
16:P:80:ARG:HG2	16:P:87:ARG:CZ	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
30:0:1116:U:H3	30:0:1246:A:H62	1.34	0.76
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.66	0.76
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.16	0.76
30:0:1625:U:H4'	42:0:5518:HOH:O	1.86	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
2:B:211:THR:HG23	30:0:2840:A:OP1	1.85	0.76
30:0:855:U:H3'	42:0:4506:HOH:O	1.85	0.76
10:J:77:GLY:HA2	10:J:80:LYS:H	1.50	0.76
5:E:15:GLN:HG2	5:E:19:ASP:O	1.85	0.76
30:0:1189:A:H3'	42:0:9461:HOH:O	1.84	0.75
30:0:1119:G:N2	30:0:1246:A:C2	2.54	0.75
30:0:542:A:H5'	30:0:542:A:C8	2.18	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
30:0:1058:A:H2'	30:0:1060:C:H5''	1.68	0.75
8:H:49:GLN:HE21	8:H:140:TYR:HE2	1.35	0.75
30:0:1666:C:H2'	30:0:1667:A:H5'	1.69	0.75
4:D:25:MET:HE1	4:D:37:ALA:HB1	1.68	0.75
2:B:267:LYS:HD3	42:0:3471:HOH:O	1.86	0.75
10:J:19:MET:HE2	10:J:79:PHE:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:1:THR:HB	30:0:93:C:H5''	1.67	0.75
16:P:121:ASP:O	16:P:125:LYS:HG3	1.87	0.75
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.69	0.75
20:T:9:LYS:HE3	20:T:13:ARG:CZ	2.16	0.75
6:F:58:GLU:CD	13:M:27:ARG:HH22	1.89	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
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.27	0.74
9:I:127:CYS:HB3	9:I:132:VAL:HB	1.69	0.74
31:9:59:C:H2'	31:9:60:C:C6	2.22	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
2:B:62:ARG:HA	2:B:65:MET:CE	2.17	0.74
30:0:2291:A:C8	30:0:2309:C:H5'	2.23	0.74
27:1:1:THR:HA	42:0:3266:HOH:O	1.86	0.74
8:H:30:LYS:N	8:H:62:HIS:HD2	1.83	0.74
30:0:1118:A:H3'	30:0:1118:A:C8	2.22	0.74
30:0:1118:A:H3'	30:0:1118:A:H8	1.53	0.74
6:F:46:GLU:OE2	6:F:100:ASP:HA	1.87	0.74
30:0:823:U:H3'	42:0:5309:HOH:O	1.88	0.73
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.69	0.73
2:B:162:MET:HG3	2:B:310:ARG:HH11	1.53	0.73
2:B:88:GLU:HB3	2:B:97:LEU:HD12	1.70	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
30:0:1205:U:H2'	30:0:1206:U:H5''	1.70	0.73
22:V:56:ILE:HG22	22:V:60:GLN:HE21	1.53	0.73
30:0:1160:G:H5'	30:0:1161:A:C5'	2.17	0.73
30:0:1838:U:O2'	30:0:2644:C:H5'	1.89	0.73
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.19	0.73
30:0:2420:G:O2'	30:0:2421:G:H5'	1.89	0.72
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
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
3:C:5:ILE:HD11	3:C:16:VAL:HG22	1.71	0.72
30:0:1116:U:O2'	30:0:1118:A:H2	1.68	0.72
5:E:84:MET:HE1	5:E:148:ILE:HD12	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.19	0.72
23:W:149:LEU:HG	23:W:153:MET:HE2	1.71	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
13:M:58:GLN:HG3	42:M:8912:HOH:O	1.90	0.71
15:O:32:ARG:HD3	15:O:32:ARG:O	1.89	0.71
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.72	0.71
30:0:2637:A:H4'	30:0:2638:G:H5'	1.72	0.71
28:2:41:HIS:N	28:2:45:ASN:HD22	1.84	0.71
31:9:29:C:H2'	31:9:30:C:H5'	1.71	0.71
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.20	0.71
15:O:21:SER:OG	15:O:106:PRO:HB2	1.90	0.71
18:R:99:ALA:HB1	18:R:109:MET:CE	2.20	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
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
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.72	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
30:0:1206:U:H6	30:0:1206:U:H5'	1.55	0.70
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
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
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
2:B:62:ARG:HA	2:B:65:MET:HE3	1.73	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
30:0:2769:C:H2'	30:0:2770:G:O4'	1.92	0.69
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.05	0.69
30:0:271:C:H41	30:0:378:A:H2	1.38	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
42:M:8875:HOH:O	30:0:381:G:H5''	1.92	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
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
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
3:C:103:ASN:ND2	30:0:663:C:H5''	2.08	0.69
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.57	0.69
30:0:1159:G:H21	30:0:1189:A:H8	1.40	0.69
2:B:27:ASN:HD21	30:0:2807:U:P	2.16	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
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
30:0:2491:G:H1'	42:0:7670:HOH:O	1.93	0.68
23:W:122:ARG:HH11	23:W:122:ARG:HG3	1.57	0.68
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.41	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
20:T:50:VAL:HG12	20:T:56:ALA:HA	1.75	0.68
30:0:2533:C:H5'	30:0:2533:C:H6	1.58	0.68
30:0:871:G:H8	30:0:871:G:C5'	2.03	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
30:0:1730:G:H5'	30:0:1731:C:C5	2.28	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
28:2:20:ARG:HG2	42:2:5444:HOH:O	1.93	0.68
2:B:56:ASP:OD1	2:B:322:ARG:HB3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
26:Z:44:ARG:HH21	30:0:1771:U:H5'	1.59	0.67
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.24	0.67
30:0:545:G:C8	30:0:545:G:H5'	2.26	0.67
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.76	0.67
30:0:2505:G:O2'	30:0:2506:A:H5'	1.95	0.67
14:N:147:ILE:HD12	42:9:9090:HOH:O	1.93	0.67
30:0:1474:C:C6	30:0:1474:C:H5'	2.29	0.67
42:0:7596:HOH:O	32:5:76:A:C2	2.47	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
25:Y:212:ARG:HD2	42:Y:8911:HOH:O	1.95	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
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.10	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
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
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.76	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
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:169:ARG:HD2	30:0:1328:A:OP1	1.96	0.65
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:78:G:N1	31:9:78:G:N7	2.43	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
30:0:544:G:H2'	30:0:545:G:H5''	1.78	0.65
27:1:16:HIS:HE1	30:0:775:G:OP1	1.79	0.65
31:9:14:G:H5'	31:9:14:G:H8	1.61	0.65
22:V:12:THR:CG2	22:V:15:GLU:HG3	2.24	0.65
30:0:1175:G:H1'	30:0:1193:A:H2'	1.78	0.65
15:O:3:THR:HB	30:0:656:G:H5'	1.76	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
16:P:74:GLN:HG2	30:0:1786:C:OP1	1.97	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
23:W:52:VAL:HG23	23:W:53:ALA:N	1.86	0.65
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.27	0.65
31:9:76:G:C3'	31:9:77:A:H5''	2.20	0.65
6:F:58:GLU:HA	6:F:61:MET:HE2	1.78	0.65
10:J:39:VAL:HG13	10:J:106:GLY:O	1.97	0.65
1:A:153:ARG:NH1	1:A:153:ARG:HB2	2.06	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
30:0:2578:G:H5'	30:0:2578:G:H8	1.63	0.64
30:0:558:C:C2'	30:0:559:U:H5''	2.28	0.64
28:2:41:HIS:HD2	28:2:44:ARG:H	1.43	0.64
31:9:73:A:H61	31:9:108:C:H42	1.45	0.64
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.32	0.64
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.61	0.64
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.94	0.64
25:Y:154:ARG:HH12	25:Y:155:ARG:HG3	1.62	0.64
25:Y:154:ARG:NH1	25:Y:155:ARG:HG3	2.12	0.64
25:Y:174:VAL:HG13	25:Y:177:LYS:HD2	1.79	0.64
2:B:229:ARG:NH2	30:0:1753:C:O2	2.30	0.64
30:0:256:C:H2'	30:0:257:G:O4'	1.98	0.64
1:A:163:GLY:HA2	1:A:166:ASP:OD2	1.96	0.64
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.78	0.64
2:B:185:GLY:HA2	42:B:9117:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:7:ILE:HG22	5:E:45:ASP:O	1.97	0.64
23:W:65:VAL:HA	23:W:68:THR:HG22	1.80	0.64
28:2:36:ASN:HB3	28:2:39:ARG:HG3	1.79	0.64
1:A:191:GLY:HA2	1:A:194:MET:CE	2.28	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:N	11:K:10:GLN:HE21	1.92	0.64
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.27	0.64
30:0:2851:G:C2'	30:0:2852:A:H5'	2.28	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:NE2	23:W:110:GLN:HA	2.13	0.64
25:Y:235:GLU:CD	25:Y:235:GLU:N	2.48	0.64
30:0:2073:G:OP2	30:0:2490:A:H5'	1.98	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
16:P:88:GLN:HE22	30:0:1799:G:H21	1.45	0.64
1:A:66:ARG:HH11	1:A:66:ARG:HB2	1.62	0.64
30:0:1377:C:H5'	30:0:1377:C:C6	2.29	0.64
29:3:55:VAL:HG22	42:3:9004:HOH:O	1.97	0.64
31:9:13:A:O2'	31:9:14:G:H5''	1.97	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
31:9:50:G:H2'	31:9:51:A:C8	2.32	0.64
2:B:175:LEU:O	2:B:175:LEU:HD23	1.97	0.64
13:M:171:ARG:CD	30:0:156:C:H5''	2.26	0.64
13:M:24:GLN:O	13:M:28:GLN:HG3	1.97	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
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
27:1:25:LYS:O	27:1:25:LYS:HG2	1.99	0.63
32:5:76:A:H8	32:5:76:A:H5'	1.64	0.63
1:A:37:VAL:HG23	42:A:9070:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
27:1:28: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
7:G:20:VAL:O	7:G:24:VAL:HG23	1.99	0.63
14:N:152:GLU:C	14:N:154:LEU:H	2.02	0.63
31:9:56:A:C2'	31:9:57:A:H5''	2.28	0.63
5:E:23:GLU:HG2	5:E:28:SER:CB	2.28	0.63
23:W:39:ASP:OD1	23:W:42:ARG:NH2	2.32	0.63
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
10:J:131:THR:HB	10:J:134:GLU:OE1	1.99	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
15:O:57:THR:O	15:O:111:VAL:HG23	2.00	0.62
30:0:281:U:H2'	30:0:282:C:O4'	1.99	0.62
14:N:5:ARG:NH1	30:0:962:C:H1'	2.14	0.62
13:M:57:LYS:HE2	13:M:140:ALA:O	2.00	0.62
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.14	0.62
19:S:57:THR:HG22	19:S:58:MET:N	2.13	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
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.62	0.62
23:W:91:ASP:HB2	42:W:5425:HOH:O	1.99	0.62
30:0:380:A:H2'	42:0:9029:HOH:O	1.98	0.62
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.82	0.62
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.14	0.62
22:V:1:THR:CG2	22:V:2:VAL:H	2.04	0.62
30:0:2718:C:H6	30:0:2718:C:H5'	1.65	0.62
1:A:88:ILE:HG22	1:A:88:ILE:O	1.98	0.62
3:C:77:ALA:C	3:C:78:ARG:CA	2.68	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
9:I:69:PRO:HA	30:0:1164:U:OP1	2.00	0.62
30:0:2896:A:H5''	42:0:6924:HOH:O	2.00	0.62
30:0:558:C:H2'	30:0:559:U:C5'	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:482:G:H4'	30:0:508:A:N1	2.15	0.61
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
30:0:2239:C:H2'	30:0:2240:U:H6	1.66	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
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.83	0.61
30:0:2401:A:H2'	30:0:2402:A:C8	2.36	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
4:D:52:THR:HG21	30:0:2346:C:O2'	1.99	0.61
30:0:2472:C:O2'	30:0:2634:G:H4'	1.99	0.61
12:L:35:ARG:HB2	12:L:35:ARG:HH11	1.63	0.61
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
30:0:1666:C:O2'	30:0:1667:A:H5''	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
30:0:2795:C:O2'	30:0:2796:U:H5'	2.01	0.61
4:D:25:MET:CE	4:D:41:LEU:HG	2.27	0.61
6:F:46:GLU:O	6:F:73:PRO:HD2	2.00	0.61
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.65	0.61
30:0:1184:C:H1'	42:0:9254:HOH:O	2.01	0.61
1:A:211:LYS:O	30:0:1943:C:H4'	2.01	0.61
1:A:88:ILE:HD13	1:A:100:PRO:CD	2.29	0.61
4:D:99:ASP:HB3	4:D:103:ASN:N	2.16	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
30:0:272:A:H5'	30:0:273:G:OP2	2.00	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
20:T:41:ARG:HG2	20:T:41:ARG:HH11	1.64	0.61
30:0:1748:U:H4'	42:0:9307:HOH:O	2.00	0.60
30:0:2005:G:O2'	30:0:2008:U:OP2	2.18	0.60
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
30:0:1205:U:H2'	30:0:1206:U:C5'	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
21:U:11:THR:HG22	21:U:53:ASP:CG	2.21	0.60
30:0:664:U:O4	30:0:681:G:H5''	2.01	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
3:C:235:PHE:HE2	3:C:243:VAL:HG21	1.65	0.60
3:C:81:PRO:HD3	42:0:4391:HOH:O	2.01	0.60
10:J:130:VAL:HG12	10:J:131:THR:H	1.65	0.60
16:P:115:SER:N	16:P:118:GLN:HE21	1.88	0.60
16:P:91:LYS:O	16:P:95:GLU:HG3	2.01	0.60
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.01	0.60
30:0:1165:G:H4'	30:0:1174:A:O2'	2.01	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
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:154:ILE:HD11	5:E:157:LYS:HB2	1.82	0.60
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.36	0.60
30:0:2896:A:N3	30:0:2896:A:H2'	2.17	0.60
28:2:41:HIS:CD2	28:2:44:ARG:H	2.19	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
2:B:206:THR:HG21	30:0:2716:G:H5''	1.84	0.60
21:U:49:LEU:HG	42:U:3805:HOH:O	2.02	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
30:0:65:C:O2'	30:0:66:G:H5'	2.01	0.60
1:A:211:LYS:HB2	42:A:9094:HOH:O	2.01	0.60
1:A:36:ASP:OD2	1:A:85:SER:HB2	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
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
9:I:114:TYR:HE1	30:0:1186:C:H4'	1.67	0.59
30:0:1766:U:O2	30:0:1778:A:H5'	2.02	0.59
30:0:544:G:C2'	30:0:545:G:H5''	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:118:LEU:O	6:F:119:ARG:HB3	2.02	0.59
30:0:1834:C:H2'	30:0:1840:A:N6	2.17	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
28:2:41:HIS:HB3	28:2:44:ARG:HB2	1.83	0.59
10:J:19:MET:CE	10:J:132:LEU:HD11	2.33	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
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
30:0:1180:U:H2'	30:0:1181:A:C8	2.37	0.59
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
30:0:2089:A:O2'	30:0:2090:G:H5'	2.02	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
30:0:1632: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
30:0:558:C:O2'	30:0:559:U:H5''	2.03	0.59
28:2:22:PRO:HG2	28:2:25:VAL:HG21	1.83	0.59
12:L:143:THR:HG22	12:L:144:ASP:N	2.17	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: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
14:N:77:ASN:C	14:N:80:SER:HB3	2.22	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
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
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.15	0.59
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.84	0.59
12:L:143:THR:HG22	12:L:145:LEU:H	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:GLN:HG3	10:J:53:ILE:N	2.17	0.59
22:V:56:ILE:O	22:V:60:GLN:HG3	2.02	0.59
23:W:110:GLN:HE21	23:W:110:GLN:HA	1.67	0.59
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
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
30:0:1116: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
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
7:G:12:ILE:HG23	42:0:6294:HOH:O	2.02	0.58
10:J:19:MET:HE1	10:J:132:LEU:HD21	1.85	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
42:L:8846:HOH:O	30:0:2453:G:H5''	2.04	0.58
5:E:36:PRO:HD3	10:J:127:ILE:HD12	1.84	0.58
22:V:39:ALA:N	22:V:40:PRO:CD	2.66	0.58
18:R:71:LYS:HE2	30:0:2831:C:O3'	2.03	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
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
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
3:C:246:ARG:NH1	3:C:246:ARG:HB3	2.18	0.58
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.68	0.58
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.84	0.58
11:K:77:ARG:C	11:K:78:LYS:CA	2.72	0.58
12:L:35:ARG:HD3	12:L:35:ARG:C	2.24	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
30:0:1878:G:H1'	42:0:6945:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2588:OMG:N2	42:0:7596:HOH:O	2.36	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
30:0:951:A:C2'	30:0:952:G:H5'	2.34	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
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
30:0:1562:C:H42	30:0:2738:G:H1	1.52	0.58
4:D:152:PRO:HD2	31:9:57:A:O2'	2.04	0.58
3:C:174:ILE:CD1	30:0:338:C:H4'	2.34	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
23:W:5:VAL:HG11	23:W:153:MET:HE3	1.85	0.58
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.86	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
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
29:3:70:ARG:HB3	42:3:9062:HOH:O	2.03	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:CG	10:J:74:ARG:HH11	2.16	0.58
30:0:871:G:C8	30:0:871:G:C5'	2.80	0.57
2:B:139:ASP:OD2	2:B:165:ARG:HD2	2.04	0.57
2:B:97:LEU:O	2:B:98:THR:HG23	2.04	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
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.69	0.57
30:0:1700:C:H5''	30:0:1701:A:OP2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:25:LYS:HD2	28:2:49:GLU:H	1.69	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
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
30:0:1182:C:H1'	30:0:1192:A:H8	1.67	0.57
30:0:2717:C:O2'	30:0:2718:C:H5''	2.04	0.57
3:C:236:THR:HA	42:C:8652:HOH:O	2.03	0.57
3:C:1:MET:HG2	3:C:2:GLN:N	2.15	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
15:O:39:THR:HG21	42:0:5468:HOH:O	2.04	0.57
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.20	0.57
30:0:506:G:H22	30:0:509:A:H5''	1.69	0.57
10:J:54:VAL:O	10:J:58:GLU:HG3	2.05	0.57
10:J:4:ALA:O	10:J:5:GLU:HB2	2.02	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
30:0:282:C:O2'	30:0:283:U:H5'	2.04	0.57
21:U:50:GLU:HB3	30:0:2866:U:C4	2.40	0.57
30:0:1189:A:H1'	30:0:1209:C:H1'	1.87	0.57
30:0:2064:U:H5'	30:0:2652:U:H4'	1.87	0.57
30:0:946:C:H2'	30:0:947:U:C6	2.40	0.57
6:F:50:VAL:CG2	6:F:63:ILE:HG21	2.34	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
30:0:292:G:H2'	30:0:358:G:N2	2.20	0.57
7:G:67:LEU:O	7:G:71:LEU:HG	2.05	0.57
14:N:86:LEU:HD21	14:N:180:LEU:CD1	2.35	0.57
30:0:241:A:C2	30:0:378:A:H4'	2.40	0.57
30:0:78:G:N3	30:0:78:G:N9	2.52	0.57
29:3:68:LYS:HE2	30:0:2436:U:H5'	1.86	0.57
2:B:24:PRO:HG3	2:B:204:GLY:HA2	1.86	0.57
30:0:1298:U:H2'	30:0:1299:G:C8	2.40	0.57
30:0:1299:G:H5'	42:0:4943:HOH:O	2.04	0.57
30:0:1878:G:O2'	30:0:1879:U:H6	1.87	0.57
30:0:699:C:H2'	30:0:744:G:O4'	2.05	0.57
30:0:820:G:H5'	30:0:821:U:H5'	1.86	0.57
29:3:77:ALA:C	29:3:78:HIS:CA	2.73	0.57
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:GLU:C	2:B:77:PRO:HD3	2.24	0.57
4:D:131:THR:HG21	30:0:2348:C:H1'	1.87	0.57
4:D:27:ILE:HD11	4:D:37:ALA:CB	2.35	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
20:T:68:ASP:HB2	42:0:6493: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
30:0:2361:A:H8	30:0:2361:A:H5'	1.70	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
31:9:20:G:O2'	31:9:21:G:H5'	2.04	0.56
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
30:0:2090:G:H2'	30:0:2091:G:C8	2.40	0.56
30:0:558:C:H2'	30:0:559:U:H5'	1.86	0.56
2:B:141:ARG:HG2	2:B:165:ARG:HA	1.87	0.56
2:B:36:PRO:CG	2:B:169:GLY:H	2.09	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
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
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.05	0.56
4:D:64:ARG:NE	4:D:67:ASP:HB3	2.20	0.56
22:V:12:THR:HG22	22:V:15:GLU:OE2	2.05	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
30:0:2004:U:H4'	42:0:6144:HOH:O	2.04	0.56
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.06	0.56
30:0:960:G:H3'	30:0:960:G:N3	2.20	0.56
42:0:6025:HOH:O	32:5:76:A:H1'	2.05	0.56
1:A:26:ASP:O	1:A:28:GLU:N	2.38	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
30:0:1555: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: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
30:0:1829:A:H2'	30:0:1830:C:H5'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2426:G:H1'	42:0:6917:HOH:O	2.06	0.56
27:1:46:ARG:HA	42:0:3910:HOH:O	2.05	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
15:O:99:GLU:OE1	15:O:99:GLU:N	2.39	0.56
24:X:66:THR:HG23	24:X:67:PRO:HD2	1.87	0.56
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.21	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: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
23:W:38:THR:HG22	23:W:39:ASP:N	2.20	0.56
24:X:76:ARG:HG3	24:X:76:ARG:HH11	1.71	0.56
30:0:2611:G:H3'	42:0:3252:HOH:O	2.04	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
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
5:E:137:ASP:OD1	5:E:139:GLU:HB2	2.05	0.56
5:E:84:MET:HG2	5:E:168:ILE:HD13	1.88	0.56
6:F:111:ILE:O	6:F:115:VAL:HG23	2.06	0.56
13:M:77:HIS:C	13:M:78:LYS:CA	2.74	0.56
23:W:88:THR:HG22	23:W:89:ASP:H	1.71	0.56
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
29:3:3:MET:HG3	29:3:4:PRO:HD2	1.88	0.55
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
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
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
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)
29:3:60:LYS:NZ	30:0:2428:G:N7	2.54	0.55
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.88	0.55
4:D:58:VAL:HB	4:D:62:ASP:HB3	1.88	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
30:0:304:G:H1'	30:0:347:A:N6	2.20	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
10:J:77:GLY:C	10:J:78:ILE:CA	2.75	0.55
30:0:1909:A:N1	30:0:2128:G:H1'	2.22	0.55
30:0:280:C:H2'	30:0:281:U:O4'	2.06	0.55
31:9:23:U:O2'	31:9:24:U:H4'	2.07	0.55
3:C:27:ARG:CG	3:C:27:ARG:HH11	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
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.41	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
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
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
30:0:737:A:H2'	30:0:738:G:O4'	2.06	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
30:0:2103:A:O2'	30:0:2104:C:H5'	2.06	0.55
27:1:28:HIS:HE1	30:0:776:A:OP1	1.90	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
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: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
25:Y:189:ASN:HD22	25:Y:189:ASN:C	2.09	0.55
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
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.89	0.54
1:A:165:THR:HG22	42:A:9093:HOH:O	2.07	0.54
2:B:232:TRP:CD1	2:B:235:ARG:HD2	2.43	0.54
2:B:85:ARG:NH1	42:B:9118:HOH:O	2.39	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
30:0:1205:U:C2'	30:0:1206:U:H5''	2.36	0.54
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.08	0.54
15:O:25:VAL:HG12	30:0:709:G:O2'	2.07	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
5:E:131:LEU:HD12	5:E:166:VAL:HG11	1.90	0.54
5:E:119:HIS:HE1	5:E:147:ASP:OD2	1.90	0.54
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.73	0.54
15:O:44:ASN:CG	15:O:67:SER:HB2	2.26	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
30:0:1189:A:H1'	30:0:1209:C:C1'	2.37	0.54
3:C:43:LYS:HG2	30:0:449:A:N7	2.22	0.54
2:B:2:GLN:NE2	30:0:2545:U:OP2	2.40	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
30:0:1218:U:H2'	30:0:1219:U:C6	2.42	0.54
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
30:0:2324:G:N2	30:0:2377:U:H1'	2.22	0.54
30:0:602:A:O2'	30:0:605:C:H4'	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:R:29:LYS:NZ	42:R:8945:HOH:O	2.40	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
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
13:M:171:ARG:NH2	30:0:189:A:OP1	2.39	0.54
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.42	0.54
30:0:2894:C:O2'	30:0:2895:C:H5'	2.07	0.54
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.89	0.54
13:M:164:THR:CG2	13:M:165:GLY:N	2.70	0.54
22:V:7:GLU:O	22:V:11:MET:HG3	2.08	0.54
30:0:137:U:H2'	30:0:139:C:C5	2.41	0.54
11:K:87:ARG:NH2	30:0:2720:C:O2	2.41	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
8:H:20:ARG:HD3	8:H:26:ILE:HD12	1.90	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.07	0.54
23:W:48:VAL:HG12	23:W:48:VAL:O	2.07	0.54
23:W:78:ASP:HB2	42:W:6694:HOH:O	2.07	0.54
27:1:25:LYS:HE2	42:1:7213:HOH:O	2.07	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
15:O:96:VAL:CG1	15:O:100:GLN:HB2	2.38	0.54
15:O:39:THR:O	15:O:115:ARG:NH2	2.41	0.54
30:0:1342:C:C2'	30:0:1343:C:H5'	2.37	0.54
30:0:185:G:H4'	30:0:186:A:H4'	1.89	0.54
30:0:2265:U:H2'	30:0:2266:A:C8	2.42	0.54
27:1:9:GLY:HA3	30:0:1695:G:H1'	1.90	0.54
6:F:26:THR:HG21	6:F:102:GLY:C	2.28	0.54
9:I:111:LEU:HD22	9:I:122:GLU:OE1	2.07	0.54
30:0:1406:A:H4'	30:0:1407:A:H5''	1.89	0.54
30:0:1559:A:H1'	42:0:6694:HOH:O	2.07	0.54
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.44	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:31:ILE:HA	8:H:66:GLU:OE1	2.08	0.54
12:L:145:LEU:O	12:L:145:LEU:HD23	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
25:Y:117:LEU:HD13	25:Y:174:VAL:HG11	1.90	0.54
30:0:1132:A:N6	30:0:1229:C:H2'	2.23	0.53
30:0:612:U:H2'	30:0:613:C:C6	2.44	0.53
31:9:2:U:OP2	31:9:3:A:H5'	2.08	0.53
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
30:0:2372:A:H2'	30:0:2373:U:C6	2.43	0.53
13:M:179:GLY:O	30:0:399:C:H5'	2.08	0.53
1:A:94:LEU:HD21	1:A:156:ILE:HD11	1.90	0.53
4:D:167:GLU:C	4:D:169:THR:H	2.12	0.53
5:E:77:THR:C	5:E:78:GLU:CA	2.77	0.53
12:L:91:VAL:CG1	12:L:120:LEU:HD23	2.38	0.53
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.08	0.53
13:M:30:GLU:O	13:M:34:GLU:HG3	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
30:0:834:G:H3'	30:0:835:U:H4'	1.90	0.53
30:0:920:C:H4'	30:0:921:G:C2	2.44	0.53
31:9:57:A:H2'	31:9:58:G:H5'	1.89	0.53
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.90	0.53
3:C:20:ASP:O	3:C:23:GLU:HB2	2.08	0.53
30:0:1278:A:H4'	30:0:1279:U:C4	2.43	0.53
30:0:2047:C:H5'	42:0:3721:HOH:O	2.07	0.53
30:0:2748:G:C5'	42:0:9326:HOH:O	2.57	0.53
30:0:2878:U:H2'	30:0:2879:A:O4'	2.09	0.53
29:3:73:GLU:HB2	42:3:9021:HOH:O	2.09	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:81:GLU:O	5:E:172:PRO:HD3	2.09	0.53
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.89	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
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
30:0:204:A:C2'	30:0:205:U:H5'	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:3:MET:O	29:3:90:PHE:HA	2.07	0.53
1:A:4:ILE:HG22	1:A:198:ASP:O	2.09	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
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
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
30:0:2824:C:O3'	30:0:2825:C:H6	1.91	0.53
9:I:124:VAL:O	9:I:124:VAL:HG12	2.09	0.53
16:P:77:ALA:C	16:P:78:GLY:CA	2.76	0.53
30:0:1666:C:H2'	30:0:1667:A:C5'	2.38	0.53
30:0:790:A:H1'	30:0:1710:A:H2'	1.91	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
30:0:95:A:H5''	30:0:97:G:O4'	2.09	0.53
28:2:20:ARG:HG3	28:2:21:VAL:N	2.24	0.53
9:I:94:ASP:OD1	9:I:133:THR:HB	2.08	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
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.43	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
23:W:5:VAL:HG11	23:W:153:MET:CE	2.39	0.53
2:B:212:GLN:HA	30:0:1733:A:H4'	1.90	0.53
30:0:1878:G:O2'	30:0:1879:U:C6	2.57	0.53
30:0:969:G:H1	30:0:999:C:N4	2.03	0.53
4:D:143:LYS:O	31:9:45:A:H4'	2.09	0.53
2:B:175:LEU:C	2:B:175:LEU:HD23	2.29	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
30:0:2314:G:C2'	30:0:2315:C:H5'	2.39	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.91	0.52
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
30:0:1067: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
42:C:8658:HOH:O	30:0:656:G:H1'	2.10	0.52
12:L:71:GLU:HG2	30:0:700:A:C2	2.45	0.52
2:B:51:VAL:HG22	2:B:327:VAL:HG13	1.92	0.52
4:D:53:LYS:O	4:D:54:ALA:HB2	2.08	0.52
14:N:162:ASP:HA	42:N:8830:HOH:O	2.08	0.52
17:Q:77:ASP:C	17:Q:78:GLY:CA	2.77	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
30:0:1595:G:O2'	30:0:1596:U:H5'	2.08	0.52
30:0:325:U:H2'	30:0:326:G:H8	1.74	0.52
13:M:9:ARG:NH2	30:0:378:A:OP1	2.42	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
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:107:ARG:NH1	13:M:107:ARG:HG3	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
30:0:1130: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
30:0:164:G:H3'	42:0:4517:HOH:O	2.10	0.52
30:0:1778:A:H2'	30:0:1779:A:H5'	1.91	0.52
30:0:204:A:H2'	30:0:205:U:H5'	1.90	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
22:V:55:ARG:NE	42:V:4428:HOH:O	2.37	0.52
8:H:15:PRO:HG3	30:0:1053:G:OP1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2748:G:H4'	30:0:2749:U:H5'	1.91	0.52
30:0:364:U:H2'	30:0:365:G:O4'	2.09	0.52
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.44	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
15:O:77:ALA:C	15:O:78:ALA:CA	2.78	0.52
30:0:2353:A:H4'	30:0:2354:A:O5'	2.10	0.52
27:1:4:GLY:O	27:1:8:GLN:HG2	2.10	0.52
31:9:3:A:H2'	42:9:9045:HOH:O	2.08	0.52
14:N:179:LEU:HA	14:N:184:ILE:HD12	1.92	0.52
18:R:39:THR:HB	18:R:42:GLU:CD	2.30	0.52
18:R:77:ALA:C	18:R:78:GLY:CA	2.78	0.52
20:T:71:VAL:HG12	20:T:72:ILE:N	2.24	0.52
23:W:122:ARG:NH1	23:W:122:ARG:HG3	2.23	0.52
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.30	0.52
30:0:2003:U:H4'	30:0:2004:U:C5	2.45	0.52
30:0:299:U:H5'	42:0:9133:HOH:O	2.09	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
25:Y:112:GLU:CD	25:Y:115:ARG:NH1	2.63	0.52
2:B:62:ARG:HA	2:B:65:MET:HE2	1.91	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
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
1:A:175:LYS:HG3	30:0:1847:A:OP1	2.10	0.52
30:0:834:G:H4'	30:0:835:U:OP2	2.09	0.52
27:1:36:SER:O	27:1:46:ARG:HD3	2.09	0.52
2:B:280:VAL:HG12	2:B:334:SER:HA	1.91	0.52
14:N:78:MET:HB2	14:N:146:HIS:CE1	2.45	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
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
18:R:64:SER:OG	30:0:1369:A:H4'	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2488:A:H61	30:0:2534:C:H42	1.58	0.51
30:0:462:A:H2'	42:0:5731:HOH:O	2.10	0.51
1:A:173:GLY:O	1:A:176:HIS:HB3	2.10	0.51
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.74	0.51
6:F:48:VAL:HG12	6:F:97:ALA:CB	2.40	0.51
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
15:O:35:LYS:HD3	42:0:5468:HOH:O	2.10	0.51
20:T:76:ASP:C	20:T:78:THR:HG23	2.31	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
30:0:137:U:OP1	30:0:259:G:O2'	2.29	0.51
1:A:217:ARG:CG	1:A:217:ARG:HH11	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
30:0:1667: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
30:0:407:A:O2'	30:0:408:A:H5'	2.11	0.51
14:N:11:ARG:HD3	31:9:114:G:O6	2.09	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
6:F:58:GLU:HG3	6:F:61:MET:HE1	1.92	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
19:S:21:GLN:NE2	30:0:1508:C:H5'	2.25	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
30:0:2103:A:N7	30:0:2538:A:N6	2.58	0.51
27:1:20:ARG:HH21	30:0:120:A:H5'	1.75	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
2:B:81:ALA:HB1	2:B:142:LEU:HD13	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:95:THR:N	25:Y:236:VAL:O	2.43	0.51
30:0:1183:C:H5	30:0:1192:A:OP1	1.94	0.51
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.10	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
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
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
42:X:4132:HOH:O	30:0:2895:C:H4'	2.10	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
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
28:2:40:ARG:HG3	28:2:45:ASN:HB2	1.91	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
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
10:J:63:ILE:HD11	30:0:1236:A:C8	2.46	0.51
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
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.10	0.51
3:C:206:ASN:HB2	30:0:329:A:OP2	2.11	0.51
30:0:398:U:H2'	30:0:399:C:C6	2.46	0.51
28:2:5:LYS:O	28:2:9:LYS:HG3	2.11	0.51
31:9:64:C:C2'	31:9:65:A:H5'	2.41	0.51
13:M:9:ARG:HB2	13:M:47:ASP:OD2	2.11	0.51
30:0:1183:C:H2'	42:0:7062:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:101:ASP:HB2	30:0:750:A:O3'	2.11	0.51
30:0:876:A:N3	30:0:876:A:H2'	2.25	0.51
3:C:27:ARG:NH1	3:C:29:ASP:OD2	2.44	0.51
4:D:77:ASP:C	4:D:78:GLU:CA	2.79	0.51
7:G:64:ASN:N	7:G:64:ASN:HD22	2.09	0.51
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.41	0.51
23:W:13:MET:CE	23:W:17:ILE:HG22	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
26:Z:77:GLY:C	26:Z:78:ILE:CA	2.79	0.51
30:0:1171:A:H2'	30:0:1172:G:H5'	1.93	0.50
30:0:1159:G:H1	30:0:1208:C:H42	1.59	0.50
30:0:248:A:H5'	30:0:249:G:OP2	2.11	0.50
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.41	0.50
29:3:61:PRO:HG2	42:0:9341:HOH:O	2.10	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
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
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
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.93	0.50
30:0:1529:G:H5'	42:0:9181:HOH:O	2.09	0.50
30:0:558:C:C2'	30:0:559:U:C5'	2.89	0.50
5:E:11:VAL:HG12	5:E:12:ASP:N	2.27	0.50
23:W:149:LEU:HG	23:W:153:MET:CE	2.40	0.50
24:X:85:VAL:HG12	24:X:86:GLU:N	2.26	0.50
30:0:1909:A:H2'	30:0:1910:A:C8	2.47	0.50
30:0:29:C:O2'	30:0:30:U:H5'	2.11	0.50
30:0:559:U:H2'	30:0:560:U:O4'	2.11	0.50
30:0:530:C:H4'	30:0:612:U:H4'	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.76	0.50
4:D:63:ILE:HG13	4:D:64:ARG:N	2.25	0.50
8:H:96:GLN:NE2	8:H:129:ARG:NH2	2.59	0.50
18:R:136:TRP:CE2	30:0:2053:G:H4'	2.47	0.50
18:R:39:THR:HG22	18:R:42:GLU:H	1.75	0.50
23:W:29:VAL:O	23:W:30:ASN:HB2	2.10	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
2:B:42:ALA:HB1	2:B:308:LEU:HD11	1.93	0.50
30:0:1667:A:C8	30:0:1667:A:H5'	2.36	0.50
30:0:2114:C:O2'	30:0:2115:U:H5'	2.10	0.50
14:N:141:ARG:HH12	31:9:35:C:H2'	1.77	0.50
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.10	0.50
1:A:36:ASP:C	1:A:38:ILE:H	2.13	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
16:P:40:VAL:O	16:P:44:VAL:HG23	2.12	0.50
30:0:1183:C:H41	30:0:1192:A:P	2.35	0.50
17:Q:11:ARG:NH1	30:0:2363:G:O3'	2.45	0.50
30:0:2326:C:H4'	30:0:2412:G:H4'	1.94	0.50
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.94	0.50
30:0:945:U:H2'	30:0:946:C:C6	2.47	0.50
31:9:39:U:H1'	31:9:44:A:H61	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.40	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
26:Z:37:ARG:HD3	42:0:5547:HOH:O	2.12	0.50
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
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
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
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
30:0:110:C:H2'	30:0:111: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
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
4:D:138:GLY:HA2	31:9:29:C:O3'	2.12	0.49
4:D:76:ARG:NE	31:9:44:A:O4'	2.45	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
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
30:0:2326:C:H4'	30:0:2412:G:C4'	2.42	0.49
14:N:29:SER:HB3	30:0:2415:A:O2'	2.12	0.49
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.93	0.49
30:0:333:G:O2'	30:0:334:G:H5'	2.12	0.49
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.77	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
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.27	0.49
12:L:50:GLY:C	30:0:2453:G:H4'	2.32	0.49
12:L:66:VAL:HG23	12:L:67:ARG:N	2.27	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
42:S:2012:HOH:O	30:0:1507:C:H4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:43:LYS:HG2	30:0:449:A:C8	2.48	0.49
1:A:65:ARG:C	1:A:66:ARG:HG3	2.32	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
6:F:58:GLU:HA	6:F:61:MET:CE	2.42	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
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
13:M:84:LYS:NZ	30:0:391:U:OP2	2.46	0.49
30:0:407:A:H5'	42:0:6851:HOH:O	2.12	0.49
2:B:14:GLY:HA2	2:B:15:PRO:C	2.32	0.49
3:C:156:LEU:O	3:C:160:LEU:HG	2.10	0.49
3:C:77:ALA:O	3:C:78:ARG:CA	2.60	0.49
10:J:45:VAL:HG23	10:J:130:VAL:O	2.13	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:43:ASN:C	20:T:45:GLY:H	2.16	0.49
20:T:64:ASN:HB3	20:T:73:HIS:HB2	1.95	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:66:ARG:NH1	1:A:66:ARG:CB	2.76	0.49
2:B:243:ASN:HA	2:B:244:PRO:C	2.32	0.49
3:C:194:PHE:HA	3:C:234:VAL:HG13	1.94	0.49
9:I:134:ILE:HG22	9:I:135:GLU:N	2.27	0.49
9:I:96:SER:OG	9:I:99:GLN:HG3	2.12	0.49
10:J:107:ASN:HD22	10:J:107:ASN:C	2.16	0.49
10:J:47:THR:HG22	10:J:48:GLY:N	2.28	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
15:O:44:ASN:OD1	15:O:67:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:396:U:HO2'	30:0:418:C:H4'	1.78	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: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
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:82:TYR:HE1	14:N:120:GLU:HG2	1.78	0.49
14:N:11:ARG:HA	14:N:14:ARG:CZ	2.43	0.49
14:N:183:ASP:O	14:N:184:ILE:O	2.30	0.49
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.94	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
30:0:221:G:H2'	30:0:222:A:C8	2.48	0.49
1:A:232:ARG:NH2	1:A:236:GLY:O	2.45	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:19:MET:HE1	10:J:132:LEU:CD2	2.43	0.49
19:S:77:VAL:C	19:S:78:ALA:CA	2.81	0.49
24:X:30:MET:HG2	30:0:1384:C:H5'	1.95	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
30:0:951:A:H2'	30:0:952:G:H5'	1.94	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
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
25:Y:208:LYS:HB3	30:0:1312:G:O2'	2.13	0.49
30:0:1406:A:H4'	30:0:1407:A:C5'	2.43	0.49
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.46	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
30:0:284:C:H4'	30:0:285:A:H8	1.78	0.49
5:E:101:GLU:HB2	5:E:116:THR:O	2.12	0.49
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:1666:C:C2'	30:0:1667:A:C5'	2.90	0.48
13:M:58:GLN:NE2	30:0:259:G:H21	2.11	0.48
4:D:76:ARG:NH1	31:9:42:C:O2	2.45	0.48
2:B:258:GLY:H	2:B:260:HIS:CE1	2.31	0.48
4:D:40:ILE:HG13	4:D:41:LEU:N	2.27	0.48
4:D:60:GLU:O	4:D:61:PHE:C	2.51	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
9:I:82:THR:CG2	30:0:1168:C:H5''	2.38	0.48
30:0:952:G:N3	30:0:2302:A:H2'	2.28	0.48
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.49	0.48
31:9:28:U:H2'	31:9:29:C:C6	2.48	0.48
1:A:109:GLU:HG2	1:A:116:GLY:N	2.28	0.48
1:A:82:VAL:HG22	1:A:93:THR:HB	1.95	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
30:0:2063:U:O4	30:0:2083:A:H2	1.95	0.48
30:0:553:G:H2'	30:0:554:G:H5'	1.95	0.48
2:B:321:PRO:HA	42:B:9143:HOH:O	2.12	0.48
8:H:77:ILE:C	8:H:78:LYS:CA	2.81	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
30:0:1185: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
17:Q:95:GLU:HA	30:0:949:U:H4'	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:143:ARG:HH21	14:N:169:PRO:HB2	1.78	0.48
14:N:78:MET:HB2	14:N:146:HIS:HE1	1.79	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
30:0:1098: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
30:0:625:U:H5'	42:0:4074:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:42:ARG:HH11	29:3:42:ARG:HG3	1.79	0.48
1:A:128:LEU:HG	42:A:9050:HOH:O	2.13	0.48
1:A:95:PRO:HA	1:A:153:ARG:HA	1.96	0.48
8:H:24:THR:O	8:H:123:ILE:HD12	2.14	0.48
8:H:14:LYS:HE2	42:0:4714:HOH:O	2.14	0.48
11:K:41:LYS:HE3	42:0:6399:HOH:O	2.13	0.48
13:M:125:ARG:HD3	42:0:5827:HOH:O	2.12	0.48
13:M:71:SER:HB2	13:M:92:THR:HG22	1.96	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
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
27:1:45:ARG:NH2	42:1:2086:HOH:O	2.41	0.48
14:N:4:PRO:HG3	31:9:69:U:OP1	2.14	0.48
1:A:66:ARG:NH1	1:A:66:ARG:HB2	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
4:D:167:GLU:OE2	4:D:173:GLU:HB3	2.12	0.48
13:M:61:ILE:N	13:M:61:ILE:HD12	2.29	0.48
42:C:8558:HOH:O	15:O:3:THR:HG21	2.12	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
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
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
30:0:1058:A:H2'	30:0:1060:C:C5'	2.41	0.48
5:E:143:GLN:NE2	30:0:2779:G:H21	2.12	0.48
28:2:40:ARG:HA	28:2:45:ASN:ND2	2.29	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
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
25:Y:112:GLU:O	25:Y:116:LEU:HG	2.14	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

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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:77:PRO:HA	2:B:293:PRO:HB2	1.95	0.48
2:B:72:THR:HB	42:B:9083:HOH:O	2.12	0.48
5:E:14:GLU:O	5:E:15:GLN:HB2	2.14	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
30:0:200:C:H2'	42:0:4329:HOH:O	2.14	0.48
30:0:2748:G:H5'	42:0:9326:HOH:O	2.13	0.48
30:0:603:A:H4'	30:0:604:G:O5'	2.13	0.48
3:C:58:ALA:HA	3:C:73:GLN:NE2	2.28	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
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.96	0.48
22:V:26:GLU:OE2	22:V:45:ARG:HD3	2.13	0.48
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
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
27:1:56:GLU:OXT	27:1:56:GLU:HG2	2.14	0.47
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:104:GLU:HB2	42:B:9117:HOH:O	2.14	0.47
2:B:42:ALA:HB2	2:B:162:MET:CE	2.43	0.47
16:P:69:ARG:HA	16:P:73:HIS:O	2.14	0.47
16:P:7:LYS:HD3	16:P:23:PHE:CZ	2.49	0.47
22:V:39:ALA:O	22:V:41:GLU:N	2.42	0.47
30:0:1060:C:H6	30:0:1060:C:H5'	1.79	0.47
30:0:690:G:H4'	30:0:741:C:O2	2.14	0.47
29:3:56:PRO:HA	42:0:6865:HOH:O	2.12	0.47
2:B:17:LYS:O	2:B:260:HIS:HD2	1.96	0.47
2:B:58:PRO:HA	2:B:63:GLU:CD	2.34	0.47
3:C:51:TYR:CE2	27:1:53:LYS:HB3	2.49	0.47
4:D:138:GLY:N	42:D:7597:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:69:ILE:HA	5:E:72:MET:CE	2.44	0.47
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.94	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
30:0:451:C:O2'	30:0:452:G:H5'	2.14	0.47
28:2:40:ARG:HG3	28:2:45:ASN:CB	2.44	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
10:J:39:VAL:HG11	10:J:107:ASN:HB2	1.96	0.47
11:K:125:ALA:C	11:K:127:ALA:H	2.17	0.47
25:Y:103:THR:HG22	25:Y:104:GLU:OE2	2.14	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: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
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
30:0:1066: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
2:B:282:GLY:O	30:0:2898:G:H1'	2.15	0.47
30:0:292:G:H1'	30:0:360:A:H61	1.80	0.47
3:C:27:ARG:NH1	3:C:27:ARG:HG2	2.29	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
30:0:1203:G:O2'	30:0:1204:C:H5'	2.15	0.47
30:0:1447:U:H3'	30:0:1506:U:O2	2.15	0.47
30:0:1641:A:H2'	30:0:1642:A:H5'	1.95	0.47
30:0:1902:G:H2'	30:0:1903:U:O4'	2.15	0.47
30:0:2554:U:H1'	42:0:6960:HOH:O	2.14	0.47
30:0:666:A:H2'	30:0:667:C:O4'	2.15	0.47
30:0:90:A:H2'	30:0:91:G:O4'	2.13	0.47
31:9:24:U:H3'	31:9:25:G:C5'	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
3:C:139:VAL:HG13	42:C:8649:HOH:O	2.14	0.47
12:L:150:GLN:HB3	42:L:8876:HOH:O	2.15	0.47
12:L:35:ARG:HB2	12:L:35:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:122:ARG:NH2	42:O:6126:HOH:O	2.47	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
30:O:1174:A:C5	30:O:1201:C:H4'	2.50	0.47
30:O:120:A:H2'	30:O:120:A:N3	2.30	0.47
30:O:1006:A:N1	30:O:2311:A:H1'	2.30	0.47
30:O:2506:A:O2'	30:O:2507:G:O5'	2.33	0.47
30:O:2828:G:H8	30:O:2828:G:O5'	1.98	0.47
30:O:629:A:H2'	30:O:630:A:O4'	2.15	0.47
1:A:117:LYS:HA	42:A:9014:HOH:O	2.14	0.47
2:B:36:PRO:HB3	2:B:174:ARG:CB	2.44	0.47
2:B:36:PRO:HA	2:B:168:GLY:CA	2.30	0.47
3:C:115:LEU:O	3:C:118:THR:HB	2.14	0.47
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.50	0.47
23:W:21:LEU:CD2	23:W:48:VAL:HG11	2.33	0.47
23:W:4:LEU:HD22	23:W:52:VAL:HB	1.95	0.47
24:X:27:ASP:OD2	24:X:27:ASP:N	2.48	0.47
30:O:1416:G:H2'	30:O:1417:G:H5'	1.97	0.47
30:O:343:C:O2'	30:O:344:C:H5'	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
1:A:32:VAL:HG12	1:A:34:ASP:H	1.80	0.47
2:B:42:ALA:HB2	2:B:162:MET:HE2	1.95	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
12:L:98:GLU:O	12:L:99:GLU:HB2	2.15	0.47
13:M:60:VAL:C	13:M:61:ILE:HD12	2.35	0.47
14:N:152:GLU:C	14:N:154:LEU:N	2.66	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
30:O:1118:A:H8	30:O:1119:G:H5''	1.78	0.47
30:O:2281:C:C2'	30:O:2282:U:H5'	2.44	0.47
30:O:958:G:O2'	30:O:959:C:H5'	2.15	0.47
32:5:76:A:H8	32:5:76:A:C5'	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:1249:U:H2'	30:0:1250:C:C6	2.49	0.47
30:0:861:A:H4'	30:0:1697:G:H4'	1.97	0.47
30:0:2289:G:H21	30:0:2291:A:H2	1.61	0.47
30:0:251:C:O2'	30:0:252:C:H5'	2.14	0.47
30:0:2756:U:N3	30:0:2896:A:C2	2.77	0.47
2:B:212:GLN:OE1	2:B:216:LYS:HD3	2.15	0.47
2:B:42:ALA:CB	2:B:162:MET:HE2	2.45	0.47
4:D:166:ILE:O	4:D:169:THR:N	2.48	0.47
4:D:99:ASP:CB	4:D:103:ASN:HB2	2.45	0.47
9:I:126:THR:O	9:I:126:THR:HG22	2.15	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
30:0:1167:G:H2'	30:0:1168:C:O4'	2.14	0.47
30:0:1684:A:H5'	30:0:1692:C:OP1	2.15	0.47
30:0:1419:U:H2'	30:0:1685:A:C2	2.49	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:H6	30:0:2016:U:O5'	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
6:F:49:PHE:HE1	6:F:98:VAL:HG23	1.79	0.47
14:N:164:ASP:OD1	14:N:167:ASP:OD1	2.33	0.47
20:T:21:LYS:HA	20:T:24:ARG:HG3	1.97	0.47
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
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
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
10:J:63:ILE:HG22	10:J:64:GLY:N	2.30	0.46
13:M:69:LYS:HG3	13:M:126:GLN:CA	2.45	0.46
18:R:17:MET:HE2	42:R:8953:HOH:O	2.15	0.46
20:T:86:GLU:HB2	42:T:6653:HOH:O	2.15	0.46
42:Y:8884:HOH:O	30:0:1355:A:H5''	2.14	0.46
30:0:1592:G:O2'	30:0:1593:C:O4'	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1787:C:H4'	30:0:2883:A:O4'	2.16	0.46
30:0:59:A:H5'	42:0:5192:HOH:O	2.14	0.46
15:O:37:ARG:HD2	30:0:656:G:OP2	2.15	0.46
30:0:806:A:H2'	30:0:807:A:O4'	2.15	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
2:B:233:ARG:NH1	2:B:233:ARG:HG2	2.29	0.46
2:B:3:PRO:HG2	42:0:9679:HOH:O	2.15	0.46
2:B:62:ARG:CA	2:B:65:MET:HE3	2.43	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:32:ARG:HH21	15:O:35:LYS:NZ	2.12	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
30:0:12:U:H2'	30:0:13:G:H5'	1.95	0.46
3:C:55:ARG:NH2	27:1:56:GLU:OE2	2.40	0.46
2:B:258:GLY:HA2	42:0:4877:HOH:O	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
4:D:24:HIS:HB2	4:D:72:LYS:HB3	1.96	0.46
5:E:93:MET:HE1	5:E:165:GLY:N	2.31	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:NH1	10:J:93:ARG:HB3	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
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
30:0:334:G:H2'	30:0:335:U:O4'	2.16	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
29:3:70:ARG:NH1	29:3:70:ARG:HG2	2.30	0.46
2:B:5:ARG:HD2	2:B:8:LYS:NZ	2.31	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
13:M:47:ASP:CG	13:M:48:LYS:N	2.69	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
25:Y:112:GLU:CD	25:Y:115:ARG:HH12	2.18	0.46
1:A:167:LYS:HB2	26:Z:53:ILE:HD13	1.97	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
30:0:2265: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
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
29:3:17:HIS:O	29:3:18:GLN:HG3	2.16	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
21:U:9:CYS:O	21:U:53:ASP:HB2	2.15	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
3:C:193:LEU:HD22	3:C:222:ASP:O	2.15	0.46
14:N:110:THR:HB	14:N:113:SER:HG	1.81	0.46
20:T:12:ARG:NH2	30:0:31:C:OP1	2.49	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
30:0:2047:C:H2'	30:0:2048:C:H6	1.81	0.46
17:Q:7:LEU:HD12	30:0:2424:U:H1'	1.97	0.46
30:0:2039:A:H4'	30:0:2760:C:O2'	2.16	0.46
30:0:2820:A:H2'	30:0:2821:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:69:ILE:HA	5:E:72:MET:HE3	1.96	0.46
6:F:38:LYS:HA	6:F:41:GLU:OE1	2.15	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
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.15	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
18:R:79:ARG:HB3	30:0:2050:G:OP1	2.15	0.46
30:0:2588:OMG:N2	42:5:3737:HOH:O	2.49	0.46
30:0:694:A:H2'	30:0:695:C:H5'	1.97	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
12:L:89:PHE:N	42:L:8877:HOH:O	2.48	0.46
13:M:102:GLU:CD	13:M:164:THR:HG21	2.36	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
25:Y:177:LYS:HD3	25:Y:181:GLY:O	2.16	0.46
30:0:1014:A:H5''	31:9:101:G:O2'	2.16	0.46
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.49	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
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
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.98	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
1:A:179:MET:HA	1:A:179:MET:CE	2.46	0.46
1:A:194:MET:SD	30:0:875:A:C2	3.09	0.46
1:A:42:VAL:HG12	1:A:76:VAL:HA	1.97	0.46
2:B:305:ASP:O	2:B:306:LYS:CB	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:245:SER:OG	30:0:2094:G:H4'	2.17	0.45
30:0:2649:A:H5'	30:0:2649:A:C8	2.51	0.45
30:0:282:C:H1'	30:0:368:C:H42	1.76	0.45
30:0:226:A:H1'	30:0:393:G:C5	2.51	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
3:C:115:LEU:CD2	3:C:243:VAL:HG13	2.41	0.45
4:D:104:PHE:CZ	4:D:132:VAL:HG21	2.51	0.45
4:D:84:LEU:HA	4:D:87:ALA:HB3	1.98	0.45
10:J:88:PRO:O	10:J:94:GLY:HA3	2.16	0.45
15:O:25:VAL:CG1	30:0:710:G:H5'	2.46	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
30:0:1636: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
17:Q:40:HIS:HE1	30:0:949:U:O2'	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
16:P:59:ARG:O	16:P:63:ARG:HG3	2.16	0.45
17:Q:86:VAL:HG11	17:Q:91:LEU:HD21	1.97	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: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:214:THR:HG23	42:C:8637:HOH:O	2.16	0.45
3:C:162:VAL:CG2	3:C:232:LEU:HD21	2.47	0.45
3:C:142:ASP:CG	3:C:238:SER:HG	2.20	0.45
3:C:54:LEU:HD23	3:C:79:ARG:HG3	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:41:PHE:CD1	2:B:79:MET:HE2	2.51	0.45
13:M:79:ALA:HB1	30:0:770:C:OP1	2.16	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
30:0:1230:A:OP1	30:0:1230:A:H8	2.00	0.45
30:0:2533:C:C6	30:0:2533:C:H5'	2.43	0.45
2:B:62:ARG:HG2	2:B:62:ARG:HH11	1.82	0.45
3:C:27:ARG:NH1	3:C:27:ARG:CG	2.77	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:HG13	18:R:119:VAL:O	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
30:0:1044:C:H5	42:0:7405:HOH:O	2.00	0.45
30:0:106:A:O2'	30:0:107:U:H5'	2.17	0.45
25:Y:142:SER:OG	30:0:1331:G:OP2	2.28	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
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.49	0.45
30:0:2038:A:O2'	30:0:2039:A:H5'	2.16	0.45
30:0:42:C:H3'	42:0:5033:HOH:O	2.16	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
12:L:41:HIS:HD2	30:0:926:A:O2'	1.99	0.45
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.48	0.45
23:W:55:GLY:CA	23:W:146:ILE:HG13	2.46	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: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
6:F:77:VAL:C	6:F:78:GLU:CA	2.85	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
30:0:1202: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:52:THR:O	4:D:68:PRO:HA	2.16	0.45
5:E:22:VAL:HG12	5:E:76:VAL:HG11	1.99	0.45
5:E:2:ARG:NH2	5:E:48:VAL:HG21	2.32	0.45
14:N:7:LYS:HB3	30:0:2353:A:O2'	2.17	0.45
24:X:30:MET:CE	24:X:58:ALA:HB3	2.46	0.45
25:Y:112:GLU:OE1	25:Y:112:GLU:HA	2.17	0.45
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.99	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
12:L:27:ARG:HD2	30:0:757:C:OP1	2.17	0.45
28:2:2:LYS:HG3	30:0:1486:A:C5	2.52	0.45
1:A:130:THR:HG22	1:A:131:HIS:N	2.30	0.45
1:A:125:ASN:CB	1:A:158:VAL:HG12	2.47	0.45
2:B:233:ARG:HH11	2:B:233:ARG:HG2	1.81	0.45
8:H:143:VAL:HG21	8:H:173:GLU:HG2	1.98	0.45
15:O:103:GLU:O	15:O:106:PRO:HD3	2.16	0.45
15:O:63:LYS:HG3	15:O:80:ASP:O	2.16	0.45
26:Z:54:GLU:HG2	26:Z:57:MET:CE	2.47	0.45
9:I:108:HIS:N	9:I:109:PRO:CD	2.80	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
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
29:3:62:THR:HB	42:3:9041:HOH:O	2.17	0.44
31:9:78:G:N2	31:9:102:G:H2'	2.33	0.44
4:D:59:GLY:O	4:D:61:PHE:N	2.50	0.44
5:E:170:ARG:NH2	42:E:4761:HOH:O	2.50	0.44
5:E:22:VAL:O	5:E:28:SER:HA	2.17	0.44
6:F:39:SER:O	6:F:43:GLY:N	2.50	0.44
8:H:49:GLN:NE2	8:H:140:TYR:CE2	2.73	0.44
8:H:32:ALA:C	8:H:33:GLN:HG3	2.38	0.44
8:H:36:MET:HB3	8:H:73:ASN:ND2	2.32	0.44
13:M:102:GLU:OE2	13:M:164:THR:HG21	2.16	0.44
20:T:41:ARG:NH1	20:T:41:ARG:HG2	2.31	0.44
24:X:71:ARG:HD3	42:X:7542:HOH:O	2.16	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.18	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
42:B:9118:HOH:O	30:0:2672:C:H1'	2.17	0.44
42:K:4183:HOH:O	30:0:2712:G:H5'	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
42:N:8814:HOH:O	31:9:36:C:H4'	2.17	0.44
1:A:58:VAL:HG21	1:A:80:LEU:HD12	1.98	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
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
21:U:44:ARG:HB3	42:U:3805:HOH:O	2.17	0.44
20:T:17:HIS:HB3	30:0:100:C:O2	2.17	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
30:0:77:G:C2'	30:0:78:G:H5'	2.47	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
9:I:72:GLU:C	9:I:74:ILE:H	2.20	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
21:U:56:ARG:HD2	21:U:56:ARG:O	2.17	0.44
25:Y:189:ASN:CA	25:Y:217:ILE:HD11	2.38	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
30:0:308:U:H5'	30:0:309:C:OP1	2.16	0.44
18:R:94:ASN:ND2	30:0:500:G:O2'	2.49	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
2:B:77:PRO:C	2:B:78:PRO:HG3	2.38	0.44
6:F:7:ASP:O	6:F:118:LEU:HD21	2.18	0.44
9:I:123:VAL:C	9:I:125:GLY:H	2.21	0.44
13:M:133:LEU:O	13:M:134:ILE:HD13	2.17	0.44
15:O:14:LEU:CG	15:O:102:ILE:HD11	2.48	0.44
21:U:4:ARG:HH11	21:U:4:ARG:HG2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:1427: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
3:C:174:ILE:HD11	30:0:338:C:H4'	1.98	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
2:B:145:HIS:CD2	2:B:159:PRO:HB3	2.51	0.44
2:B:183:GLU:O	2:B:184:ASP:C	2.56	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
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
3:C:225:PRO:O	30:0:1308:A:H4'	2.17	0.44
30:0:157:G:H3'	42:0:4825:HOH:O	2.16	0.44
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.17	0.44
30:0:2906:A:H5'	30:0:2907:C:O4'	2.18	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
30:0:485:A:HO2'	30:0:487:G:H8	1.65	0.44
31:9:29:C:C2'	31:9:30:C:H5'	2.43	0.44
1:A:33:GLU:CD	1:A:33:GLU:N	2.60	0.44
2:B:284:PHE:HB2	2:B:287:TYR:HB3	1.99	0.44
2:B:264:GLU:OE2	2:B:302:PRO:HD3	2.18	0.44
3:C:85:LYS:HD3	42:0:3695:HOH:O	2.17	0.44
4:D:158:ASN:HB2	4:D:161:ASP:OD2	2.17	0.44
5:E:162:PHE:CD1	5:E:162:PHE:N	2.85	0.44
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.33	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:134:ILE:HG23	13:M:141:ILE:CD1	2.38	0.44
14:N:77:ASN:C	14:N:78:MET:CA	2.86	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
30:0:1333:U:H2'	30:0:1334:C:H6	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
30:0:814:G:H2'	30:0:815:U:C6	2.52	0.44
27:1:45:ARG:HB3	42:1:988:HOH:O	2.18	0.44
31:9:7:G:H5'	42:9:9099:HOH:O	2.18	0.44
1:A:217:ARG:NH1	1:A:217:ARG:CG	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
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
30:0:1207:A:H5'	30:0:1208:C:OP2	2.18	0.44
30:0:177:A:H2'	30:0:178:U:O4'	2.17	0.44
1:A:212:PRO:HA	30:0:1943:C:O4'	2.17	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
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
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.66	0.44
31:9:13:A:H3'	31:9:14:G:H5'	2.00	0.44
2:B:132:HIS:CE1	2:B:171:VAL:HG21	2.53	0.44
2:B:300:SER:HB3	42:0:5521:HOH:O	2.18	0.44
4:D:156:ARG:HG3	4:D:156:ARG:NH1	2.32	0.44
8:H:86:TYR:C	8:H:86:TYR:CD1	2.91	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: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
14:N:6:TYR:HB3	31:9:11:A:N6	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:145:LYS:HE2	42:Y:8917:HOH:O	2.17	0.44
23:W:9:GLY:H	30:0:1086:A:P	2.41	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
30:0:660:A:H4'	30:0:661:G:O5'	2.18	0.44
27:1:28:HIS:O	27:1:32:LYS:N	2.45	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:101:ALA:HB3	6:F:105:ASP:OD1	2.18	0.44
6:F:48:VAL:HG23	6:F:74:PHE:CB	2.47	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
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
30:0:152:A:O2'	30:0:153:C:H5'	2.17	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
30:0:187:A:H3'	30:0:188:C:H6	1.83	0.43
30:0:2346:C:O5'	30:0:2346:C:H6	2.01	0.43
30:0:243:A:H61	30:0:269:G:H1'	1.83	0.43
30:0:2511:A:H4'	42:0:6305:HOH:O	2.18	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
42:C:8558:HOH:O	30:0:656:G:H4'	2.18	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
6:F:48:VAL:HG12	6:F:97:ALA:HB2	2.00	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
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.53	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1979:G:O2'	30:0:1980:U:OP1	2.34	0.43
30:0:2537:G:O5'	30:0:2538:A:H5''	2.18	0.43
30:0:2510:C:H42	30:0:2564:G:H22	1.66	0.43
30:0:319:A:H4'	30:0:338:C:C5	2.53	0.43
27:1:18:LYS:HA	27:1:25:LYS:HA	2.00	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:17:SER:C	12:L:19:LYS:H	2.21	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:39:THR:O	18:R:40:ALA:C	2.56	0.43
18:R:59:PHE:O	18:R:63:ASN:HB3	2.18	0.43
30:0:1477:C:H5'	30:0:1868:G:H5'	2.00	0.43
30:0:2645:U:H6	30:0:2645:U:OP2	2.02	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
29:3:65:THR:CG2	29:3:67:LEU:HG	2.39	0.43
1:A:235:ARG:HB2	42:A:9026:HOH:O	2.17	0.43
9:I:127:CYS:C	9:I:129:SER:H	2.22	0.43
14:N:165:ALA:C	14:N:167:ASP:H	2.21	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
30:0:1056:U:H2'	30:0:1057:A:O4'	2.19	0.43
16:P:41:ARG:HH22	30:0:1500:U:P	2.41	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
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
9:I:81:GLU:N	9:I:81:GLU:OE1	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
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
30:0:2557: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2768:A:H2'	30:0:2769:C:O4'	2.19	0.43
30:0:95:A:O5'	30:0:97:G:H5'	2.19	0.43
31:9:54:A:O2'	31:9:55:U:H5'	2.18	0.43
3:C:234:VAL:HG13	3:C:234:VAL:O	2.18	0.43
14:N:111:PRO:HD2	31:9:37:C:H4'	2.00	0.43
14:N:21:HIS:HB2	42:N:8831:HOH:O	2.19	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
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.51	0.43
30:0:1926:G:H2'	30:0:1927:A:C8	2.53	0.43
30:0:23:G:H1'	30:0:520:A:N6	2.34	0.43
30:0:2769:C:H2'	30:0:2770:G:C5'	2.49	0.43
30:0:706:G:N2	30:0:707:C:H41	2.16	0.43
22:V:1:THR:CB	30:0:93:C:H5''	2.44	0.43
1:A:132:ASP:OD1	1:A:133:ARG:N	2.49	0.43
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.84	0.43
4:D:25:MET:CE	4:D:40:ILE:HD11	2.49	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
14:N:97:VAL:HG12	14:N:127:LEU:HD11	1.99	0.43
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.13	0.43
22:V:45:ARG:HA	22:V:48:GLU:HB2	2.00	0.43
23:W:13:MET:HE3	23:W:17:ILE:HG22	2.00	0.43
30:0:1524:U:H6	30:0:1524:U:H5''	1.83	0.43
42:3:9017:HOH:O	30:0:2468:A:H4'	2.18	0.43
30:0:2506:A:O2'	30:0:2507:G:P	2.77	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
30:0:77:G:H2'	30:0:78:G:H5'	2.00	0.43
1:A:176:HIS:CD2	30:0:857:A:H4'	2.54	0.43
30:0:878:G:H4'	30:0:1835:U:H4'	2.01	0.43
28:2:13:LYS:O	28:2:17:GLN:HG3	2.18	0.43
33:6:75:C:H5''	33:6:76:8AN:O1P	2.18	0.43
1:A:114:ASP:OD1	1:A:115:GLY:N	2.52	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
4:D:96:SER:C	4:D:98:PHE:H	2.22	0.43
5:E:118:ILE:HG23	5:E:144:THR:HG21	2.00	0.43
5:E:15:GLN:HG3	5:E:20:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:96:VAL:HG13	15:O:100:GLN:CD	2.38	0.43
17:Q:31:GLU:OE1	17:Q:31:GLU:HA	2.19	0.43
20:T:40:VAL:HG23	20:T:119:ALA:C	2.39	0.43
24:X:20:GLU:CD	24:X:21:PRO:HD2	2.39	0.43
30:0:1120:U:C6	30:0:1120:U:H5'	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
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
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:285:VAL:O	2:B:286:ASN:HB2	2.18	0.43
2:B:201:ASP:HB2	2:B:312:ARG:HD2	2.01	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
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
25:Y:189:ASN:ND2	25:Y:189:ASN:C	2.72	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:H6	30:0:1698:U:O5'	2.02	0.43
30:0:559:U:C5'	30:0:559:U:H6	2.25	0.43
27:1:10:LYS:HG3	42:1:2979:HOH:O	2.18	0.43
1:A:105:VAL:HG11	1:A:154:ALA:HB1	2.00	0.43
1:A:71:PRO:HA	1:A:158:VAL:O	2.19	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
12:L:99:GLU:C	12:L:101:ASP:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:79:GLU:CD	24:X:80:GLU:H	2.22	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
23:W:125:HIS:NE2	30:0:1097:A:H5''	2.34	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
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
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: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:77:ALA:C	23:W:78:ASP:CA	2.87	0.43
30:0:1947:G:H2'	30:0:1948:G:C8	2.54	0.42
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.84	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
30:0:876:A:N3	30:0:876:A:C2'	2.82	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
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
10:J:39:VAL:HG11	10:J:107:ASN:CG	2.40	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
30:0:1210: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
30:0:2087:C:O2'	30:0:2088:C:H5'	2.20	0.42
30:0:2064:U:H5'	30:0:2652:U:O3'	2.19	0.42
30:0:2756:U:O2	30:0:2896:A:H2	2.02	0.42
30:0:426:G:O2'	30:0:427:C:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:772:G:H2'	30:0:773:A:O4'	2.19	0.42
29:3:48:ASN:ND2	29:3:50:GLY:H	2.17	0.42
32:5:74:C:N4	42:5:3737:HOH:O	2.39	0.42
31:9:49:G:C2'	31:9:50:G:H5'	2.50	0.42
1:A:194:MET:CE	1:A:199:HIS:HB2	2.49	0.42
3:C:118:THR:HG23	42:C:8504:HOH:O	2.19	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
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
30:0:2129:U:H2'	30:0:2130:C:C6	2.54	0.42
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.86	0.42
2:B:119:HIS:O	2:B:121:PRO:HD3	2.19	0.42
2:B:87:TYR:O	2:B:138:GLY:N	2.42	0.42
5:E:101:GLU:HA	5:E:118:ILE:HG13	2.02	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:188:ARG:HB2	30:0:156:C:OP2	2.18	0.42
13:M:71:SER:CB	13:M:92:THR:HG22	2.49	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
30:0:1378: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
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
2:B:87:TYR:OH	2:B:163:GLU:OE2	2.27	0.42
4:D:88:LEU:N	4:D:89:PRO:CD	2.82	0.42
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
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
27:1:28:HIS:HD2	27:1:31:LYS:H	1.66	0.42
29:3:70:ARG:HH11	29:3:70:ARG:HG2	1.84	0.42
31:9:107:C:H5	42:9:9060:HOH:O	2.02	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:99:ASP:OD2	4:D:101:THR:HB	2.18	0.42
4:D:55:LYS:HA	4:D:65:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
2:B:244:PRO:HB3	30:0:1234:U:N3	2.34	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
30:0:440:C:H2'	30:0:441:A:C8	2.54	0.42
31:9:56:A:C3'	31:9:57:A:H5''	2.50	0.42
1:A:188:ASN:HA	42:A:9046:HOH:O	2.19	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
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:140:VAL:HB	42:L:8861:HOH:O	2.18	0.42
12:L:89:PHE:CD1	12:L:89:PHE:N	2.87	0.42
24:X:66:THR:CG2	24:X:67:PRO:HD2	2.50	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
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
27:1:11:LYS:HG2	30:0:777:U:O2'	2.20	0.42
31:9:47:A:C2	31:9:48:C:C2	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:I:127:CYS:C	9:I:129:SER:N	2.73	0.42
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
16:P:13:VAL:HG21	16:P:41:ARG:HG2	2.00	0.42
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.35	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:N3	30:0:644:G:H5'	2.35	0.42
30:0:695:C:H2'	30:0:696:C:C6	2.55	0.42
30:0:766:A:HO2'	30:0:767:A:H8	1.67	0.42
31:9:59:C:H6	31:9:59:C:O5'	2.03	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
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
30:0:1741: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: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
2:B:294:TYR:CD1	2:B:294:TYR:C	2.93	0.42
2:B:77:PRO:C	2:B:78:PRO:CA	2.89	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:100:ASP:C	18:R:102:GLN:H	2.23	0.42
18:R:26:LYS:HD3	18:R:62:HIS:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
30:0:1074:G:H4'	30:0:1260:G:C6	2.55	0.41
30:0:1342:C:O2'	30:0:1343:C:H5'	2.19	0.41
30:0:170:U:H2'	30:0:171:C:H5'	2.01	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
30:0:553:G:C2'	30:0:554:G:H5'	2.50	0.41
20:T:43:ASN:OD1	30:0:80:A:H3'	2.19	0.41
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
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
14:N:79:PRO:HG3	14:N:143:ARG:C	2.39	0.41
22:V:38:GLY:C	22:V:40:PRO:HD2	2.39	0.41
30:0:912:A:C4	30:0:1294:A:C2	3.08	0.41
12:L:33:ALA:HB2	30:0:165:A:H5''	2.01	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
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
4:D:169:THR:C	4:D:170:TYR:HD1	2.23	0.41
7:G:19:GLU:O	7:G:23:ILE:HG13	2.20	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:CG	24:X:49:ARG:O	2.65	0.41
17:Q:94:GLN:NE2	30:0:1019:C:O2	2.53	0.41
30:0:1207:A:OP2	30:0:1207:A:H8	2.03	0.41
30:0:1366:C:H1'	42:0:3161:HOH:O	2.20	0.41
30:0:1806:G:HO2'	30:0:2883:A:H2	1.65	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.18	0.41
28:2:29:THR:O	28:2:30:ASP:C	2.59	0.41
29:3:22:VAL:HG11	29:3:67:LEU:HD13	2.02	0.41
1:A:105:VAL:HG11	1:A:154:ALA:CB	2.50	0.41
1:A:194:MET:HE1	1:A:199:HIS:HB2	2.01	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
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
14:N:103:ASP:OD1	14:N:103:ASP:C	2.58	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
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
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
30:0:187:A:H3'	30:0:188:C:C6	2.56	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
30:0:2637:A:H4'	30:0:2638:G:O5'	2.20	0.41
2:B:70:PRO:HG3	30:0:2719:A:C2	2.55	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
2:B:255:GLY:O	2:B:257:THR:HG23	2.19	0.41
2:B:28:SER:HB3	30:0:2807:U:OP1	2.21	0.41
3:C:109:LEU:O	3:C:109:LEU:HD12	2.19	0.41
3:C:123:LEU:HA	3:C:123:LEU:HD23	1.87	0.41
3:C:78:ARG:O	3:C:80:VAL:N	2.51	0.41
4:D:44:ILE:HG12	4:D:44:ILE:O	2.21	0.41
12:L:129:ALA:O	12:L:133:VAL:HG23	2.20	0.41
12:L:98:GLU:O	12:L:99:GLU:CB	2.68	0.41
14:N:35:VAL:HG11	31:9:6:C:H4'	2.03	0.41
2:B:333:GLU:HB2	21:U:14:GLU:OE2	2.20	0.41
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:169:PHE:O	1:A:171:LYS:N	2.47	0.41
1:A:36:ASP:CG	1:A:36:ASP:O	2.59	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
2:B:66:GLU:OE1	2:B:328:ARG:HD2	2.20	0.41
3:C:61:PHE:CD2	3:C:65:ARG:CZ	3.04	0.41
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.32	0.41
10:J:107:ASN:HD22	10:J:108:PRO:N	2.19	0.41
12:L:67:ARG:HB2	12:L:111:ALA:O	2.21	0.41
12:L:36:ASP:HB2	42:L:8839:HOH:O	2.20	0.41
13:M:46:LEU:HD22	13:M:50:ARG:HD2	2.02	0.41
25:Y:186:ARG:HG2	25:Y:186:ARG:NH1	2.33	0.41
25:Y:100:ARG:HD2	25:Y:232:THR:HB	2.02	0.41
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	2.02	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
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
2:B:277:GLU:N	2:B:278:PRO:CD	2.84	0.41
5:E:7:ILE:HD11	5:E:11:VAL:C	2.40	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:125:PHE:CZ	12:L:140:VAL:HG22	2.56	0.41
12:L:34:GLY:HA2	42:0:6243:HOH:O	2.19	0.41
12:L:57:VAL:O	12:L:57:VAL:HG12	2.20	0.41
18:R:61:GLN:CD	42:R:8945:HOH:O	2.59	0.41
21:U:20:MET:CG	21:U:28:THR:HG23	2.50	0.41
23:W:130:HIS:C	23:W:136:GLY:HA3	2.39	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
30:0:278:A:H2'	30:0:279:C:O4'	2.20	0.41
27:1:2:GLY:O	27:1:6:PRO:HG2	2.20	0.41
31:9:39:U:H1'	31:9:44:A:N6	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD3	13:M:68:ARG:O	2.20	0.41
20:T:96:VAL:CG1	20:T:97:ARG:N	2.84	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
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
30:0:220:C:H1'	42:0:6586:HOH:O	2.21	0.41
30:0:2724:U:H2'	30:0:2725:G:O4'	2.20	0.41
30:0:875:A:H5'	30:0:876:A:N7	2.35	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
31:9:35:C:H5''	42:9:9078:HOH:O	2.21	0.41
2:B:112:THR:OG1	2:B:158:LYS:HG3	2.20	0.41
6:F:60:VAL:CG1	6:F:60:VAL:O	2.69	0.41
20:T:40:VAL:HG23	20:T:119:ALA:OXT	2.21	0.41
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.43	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
8:H:154:ARG:NH2	30:0:2503:A:OP1	2.53	0.41
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
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
31:9:22:G:H5'	31:9:23:U:OP1	2.20	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
2:B:79:MET:O	2:B:187:GLU:HA	2.21	0.41
3:C:168:ARG:NH1	30:0:1310:U:OP2	2.54	0.41
3:C:93:LYS:O	3:C:98:ARG:NH2	2.53	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
4:D:52:THR:CG2	30:0:2346:C:O3'	2.69	0.41
5:E:105:GLU:HG2	5:E:113:PRO:HB3	2.02	0.41
6:F:26:THR:CG2	6:F:102:GLY:HA3	2.50	0.41
8:H:157:TYR:CD1	8:H:157:TYR:C	2.93	0.41
13:M:77:HIS:CE1	13:M:86:GLN:HG2	2.55	0.41
15:O:32:ARG:HD3	15:O:32:ARG:C	2.42	0.41
18:R:8:ALA:HB3	18:R:15:LYS:HE2	2.02	0.41
18:R:44:VAL:HG13	18:R:89:LEU:HD22	2.03	0.41
30:0:1165:G:H1'	30:0:1174:A:H1'	2.02	0.41
30:0:907:A:H4'	30:0:1328:A:C2	2.56	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
30:0:2290:U:H2'	42:0:7931:HOH:O	2.19	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
30:0:74:G:H2'	30:0:75:U:C6	2.56	0.41
30:0:813:C:H2'	30:0:814:G:O4'	2.21	0.41
30:0:945:U:H2'	30:0:946:C:H6	1.86	0.41
29:3:6:ARG:HA	29:3:20:HIS:O	2.21	0.41
1:A:82:VAL:HA	1:A:93:THR:O	2.21	0.41
2:B:202:VAL:HG11	2:B:301:VAL:HG13	2.02	0.41
2:B:82:VAL:HG11	2:B:101:TRP:CZ3	2.55	0.41
6:F:20:LEU:HB2	6:F:49:PHE:CZ	2.56	0.41
9:I:95:LEU:HG	9:I:132:VAL:CG1	2.51	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
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
26:Z:80:GLN:HA	26:Z:86:TYR:O	2.21	0.41
30:0:101:C:H2'	30:0:102:A:H8	1.84	0.41
12:L:5:LYS:NZ	30:0:1353:C:N3	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:542:A:C5'	30:0:542:A:C8	2.98	0.41
27:1:11:LYS:HA	42:1:5026:HOH:O	2.22	0.41
1:A:26:ASP:CG	1:A:26:ASP:O	2.58	0.41
4:D:24:HIS:HB2	4:D:72:LYS:CB	2.51	0.41
14:N:167:ASP:C	14:N:168:LEU:HG	2.42	0.41
15:O:26:TRP:HA	15:O:26:TRP:CE3	2.56	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
23:W:13:MET:HE2	23:W:17:ILE:HG22	2.02	0.41
30:0:1166:A:H61	30:0:1180:U:H3	1.69	0.40
13:M:93:ARG:HD2	30:0:1470:A:OP1	2.22	0.40
1:A:146:LYS:NZ	30:0:1855:G:O3'	2.53	0.40
30:0:2361:A:H2'	30:0:2362:A:O4'	2.21	0.40
30:0:243:A:H2	30:0:274:G:N3	2.19	0.40
30:0:2698:G:H2'	30:0:2699:A:C8	2.56	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:O5'	30:0:567:U:H6	2.04	0.40
30:0:639:A:H2'	30:0:640:G:C8	2.55	0.40
29:3:86:GLY:HA3	30:0:2318:C:OP1	2.21	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:134:ILE:O	13:M:136:PRO:HD3	2.21	0.40
13:M:48:LYS:HE3	13:M:52:GLN:NE2	2.36	0.40
20:T:77:VAL:C	20:T:78:THR:CA	2.90	0.40
20:T:96:VAL:HG13	20:T:97:ARG:N	2.36	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
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
26:Z:45:VAL:CG2	30:0:1887:U:OP1	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2887:G:H2'	30:0:2888:U:O4'	2.20	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:214:THR:HB	42:C:8522:HOH:O	2.22	0.40
10:J:39:VAL:HG12	10:J:40:ASN:CG	2.42	0.40
11:K:22:ASP:OD1	11:K:22:ASP:C	2.60	0.40
24:X:23:HIS:HE1	30:0:2044:G:OP1	2.04	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
30:0:64:G:H2'	30:0:65:C:O4'	2.22	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
3:C:236:THR:O	3:C:237:GLU:C	2.59	0.40
4:D:169:THR:HG22	4:D:170:TYR:HD1	1.86	0.40
6:F:70:LYS:C	6:F:72:VAL:H	2.24	0.40
9:I:133:THR:HG22	9:I:134:ILE:N	2.37	0.40
10:J:49:ARG:NH1	30:0:1119:G:OP1	2.55	0.40
11:K:125:ALA:O	11:K:127:ALA:N	2.47	0.40
11:K:98:VAL:HG13	11:K:102:GLU:CA	2.51	0.40
12:L:61:ALA:HB2	12:L:105:TYR:CZ	2.55	0.40
13:M:107:ARG:O	13:M:110:PRO:HD3	2.21	0.40
13:M:74:LYS:HE2	30:0:159:G:OP1	2.21	0.40
14:N:154:LEU:C	14:N:156:GLU:H	2.25	0.40
14:N:41:LYS:HE3	42:9:9021:HOH:O	2.20	0.40
14:N:64:SER:C	14:N:66:LEU:H	2.24	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
18:R:100:ASP:C	18:R:102:GLN:N	2.73	0.40
19:S:29:ASP:OD1	19:S:31:ARG:NH1	2.55	0.40
23:W:55:GLY:HA3	23:W:146:ILE:HG13	2.03	0.40
25:Y:210:GLY:N	30:0:1313:A:H5''	2.36	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
28:2:5:LYS:HD2	30:0:1675:C:H5''	2.03	0.40
11:K:66:ARG:NH2	30:0:1994:A:OP1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2909:G:O2'	30:0:2910:A:H5'	2.21	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
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
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
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:104:PHE:HB2	18:R:109:MET:HE1	2.03	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:HD23	23:W:21:LEU:HA	1.78	0.40
25:Y:210:GLY:H	30:0:1313:A:H5''	1.86	0.40
30:0:105:G:O2'	30:0:106:A: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
30:0:185:G:C4'	30:0:186:A:H4'	2.52	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
30:0:306:A:H2'	30:0:341:C:O2'	2.22	0.40
30:0:69:A:H5'	30:0:69:A:H8	1.84	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
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
22:V:16:ARG:HH12	22:V:65:ASP:C	2.25	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%)	7	23
2	B	333/338 (98%)	300 (90%)	29 (9%)	4 (1%)	13	39
3	C	242/246 (98%)	215 (89%)	25 (10%)	2 (1%)	19	49
4	D	132/177 (75%)	98 (74%)	23 (17%)	11 (8%)	1	2
5	E	168/178 (94%)	159 (95%)	9 (5%)	0	100	100
6	F	115/120 (96%)	97 (84%)	13 (11%)	5 (4%)	2	8
7	G	25/348 (7%)	22 (88%)	3 (12%)	0	100	100
8	H	154/177 (87%)	131 (85%)	21 (14%)	2 (1%)	12	36
9	I	66/162 (41%)	45 (68%)	19 (29%)	2 (3%)	4	15
10	J	138/145 (95%)	126 (91%)	9 (6%)	3 (2%)	6	22
11	K	128/132 (97%)	117 (91%)	9 (7%)	2 (2%)	9	31
12	L	139/165 (84%)	115 (83%)	19 (14%)	5 (4%)	3	11
13	M	190/196 (97%)	171 (90%)	17 (9%)	2 (1%)	14	41
14	N	182/187 (97%)	156 (86%)	18 (10%)	8 (4%)	2	8
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%)	14	41
18	R	146/155 (94%)	132 (90%)	13 (9%)	1 (1%)	22	53
19	S	77/85 (91%)	73 (95%)	4 (5%)	0	100	100
20	T	115/120 (96%)	109 (95%)	4 (4%)	2 (2%)	9	29
21	U	51/67 (76%)	46 (90%)	4 (8%)	1 (2%)	7	24
22	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	9	31
23	W	150/154 (97%)	140 (93%)	9 (6%)	1 (1%)	22	53
24	X	78/92 (85%)	70 (90%)	7 (9%)	1 (1%)	12	36
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	8
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%)	14	41
All	All	3659/4471 (82%)	3256 (89%)	340 (9%)	63 (2%)	9	29

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%)	168 (94%)	10 (6%)	21	51
2	B	281/283 (99%)	271 (96%)	10 (4%)	35	69
3	C	192/193 (100%)	176 (92%)	16 (8%)	11	32
4	D	116/148 (78%)	111 (96%)	5 (4%)	29	62
5	E	151/156 (97%)	147 (97%)	4 (3%)	46	79
6	F	92/94 (98%)	91 (99%)	1 (1%)	73	92
7	G	27/282 (10%)	26 (96%)	1 (4%)	34	68
8	H	133/145 (92%)	129 (97%)	4 (3%)	41	75
9	I	58/130 (45%)	57 (98%)	1 (2%)	60	87
10	J	117/121 (97%)	108 (92%)	9 (8%)	13	35
11	K	105/106 (99%)	103 (98%)	2 (2%)	57	85
12	L	113/127 (89%)	108 (96%)	5 (4%)	28	61
13	M	157/160 (98%)	150 (96%)	7 (4%)	27	60
14	N	148/150 (99%)	144 (97%)	4 (3%)	44	78
15	O	93/94 (99%)	91 (98%)	2 (2%)	52	83
16	P	113/117 (97%)	110 (97%)	3 (3%)	44	78
17	Q	79/80 (99%)	77 (98%)	2 (2%)	47	80
18	R	117/122 (96%)	111 (95%)	6 (5%)	24	55
19	S	71/74 (96%)	68 (96%)	3 (4%)	30	63
20	T	104/106 (98%)	100 (96%)	4 (4%)	33	67
21	U	44/53 (83%)	42 (96%)	2 (4%)	27	60
22	V	51/57 (90%)	51 (100%)	0	100	100
23	W	129/130 (99%)	122 (95%)	7 (5%)	22	53
24	X	65/74 (88%)	58 (89%)	7 (11%)	6	19
25	Y	120/195 (62%)	111 (92%)	9 (8%)	13	37
26	Z	59/94 (63%)	58 (98%)	1 (2%)	60	87
27	1	46/47 (98%)	45 (98%)	1 (2%)	52	83
28	2	42/46 (91%)	40 (95%)	2 (5%)	25	58
29	3	78/79 (99%)	73 (94%)	5 (6%)	17	45
All	All	3079/3645 (84%)	2946 (96%)	133 (4%)	29	62

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	37	VAL
1	A	68	ILE
1	A	69	LEU
1	A	131	HIS
1	A	153	ARG
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	132	HIS
2	B	162	MET
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	101	ASP
3	C	115	LEU
3	C	187	ARG
3	C	211	ASP
3	C	222	ASP
3	C	223	LEU
3	C	236	THR
3	C	237	GLU
3	C	240	LEU
4	D	24	HIS
4	D	50	VAL
4	D	61	PHE
4	D	133	ASN
4	D	137	PRO
5	E	102	VAL

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Mol	Chain	Res	Type
5	E	116	THR
5	E	143	GLN
5	E	164	ASP
6	F	12	LEU
7	G	73	ASP
8	H	21	GLU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
9	I	135	GLU
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	76	ASP
10	J	79	PHE
10	J	107	ASN
10	J	112	ASP
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	140	VAL
13	M	23	LEU
13	M	46	LEU
13	M	68	ARG
13	M	93	ARG
13	M	99	ARG
13	M	115	LEU
13	M	116	ASN
14	N	26	LEU
14	N	49	THR
14	N	134	ASP
14	N	139	TRP
15	O	98	LEU
15	O	115	ARG
16	P	52	LYS
16	P	91	LYS
16	P	98	ILE

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Mol	Chain	Res	Type
17	Q	11	ARG
17	Q	95	GLU
18	R	13	THR
18	R	39	THR
18	R	82	GLU
18	R	90	ASP
18	R	142	ASP
18	R	143	VAL
19	S	12	GLU
19	S	17	ASP
19	S	44	GLN
20	T	8	ARG
20	T	39	ASN
20	T	89	ARG
20	T	96	VAL
21	U	17	THR
21	U	53	ASP
23	W	26	ILE
23	W	52	VAL
23	W	73	LEU
23	W	120	PRO
23	W	125	HIS
23	W	142	ASP
23	W	146	ILE
24	X	15	ARG
24	X	27	ASP
24	X	46	ASP
24	X	49	ARG
24	X	72	VAL
24	X	79	GLU
24	X	82	GLU
25	Y	115	ARG
25	Y	154	ARG
25	Y	169	ARG
25	Y	189	ASN
25	Y	203	VAL
25	Y	204	ARG
25	Y	220	GLU
25	Y	231	PRO
25	Y	235	GLU
26	Z	106	SER
27	1	47	ASP

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Mol	Chain	Res	Type
28	2	16	ASN
28	2	18	ASN
29	3	11	CYS
29	3	14	CYS
29	3	40	ARG
29	3	42	ARG
29	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	254	GLN
2	B	256	GLN
2	B	260	HIS
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	129	HIS
3	C	163	HIS
4	D	47	GLN
4	D	103	ASN
4	D	133	ASN
5	E	15	GLN
5	E	106	ASN
5	E	119	HIS
5	E	143	GLN
5	E	150	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
9	I	88	GLN

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Mol	Chain	Res	Type
10	J	25	GLN
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
12	L	42	ASN
12	L	43	HIS
12	L	116	HIS
13	M	24	GLN
13	M	26	GLN
13	M	58	GLN
13	M	122	GLN
13	M	129	HIS
13	M	137	ASN
13	M	170	ASN
14	N	21	HIS
14	N	40	ASN
14	N	107	ASN
14	N	119	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
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
19	S	44	GLN
19	S	51	GLN
19	S	55	GLN
20	T	7	GLN
20	T	37	GLN
20	T	39	ASN
20	T	64	ASN

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Mol	Chain	Res	Type
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	133	HIS
25	Y	134	HIS
25	Y	149	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	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%)	248 (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%)	265 (9%)	31 (1%)

All (265) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
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	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

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Mol	Chain	Res	Type
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
30	0	2271	G
30	0	2272	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	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

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Mol	Chain	Res	Type
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
30	0	2682	C
30	0	2719	A
30	0	2726	U
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

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Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
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 [i](#)

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	OMU	0	2587	30	14,22,23	0.96	1 (7%)	14,31,34	1.18	1 (7%)
30	UR3	0	2619	30	14,22,23	0.89	1 (7%)	15,32,35	0.76	0
30	PSU	0	2621	30	17,21,22	1.67	3 (17%)	20,30,33	5.43	4 (20%)
33	8AN	6	76	33	19,24,25	1.15	1 (5%)	13,35,38	1.79	3 (23%)
30	1MA	0	628	30	15,25,26	0.78	0	15,37,40	1.44	1 (6%)
30	OMG	0	2588	32,30	18,26,27	1.03	2 (11%)	20,38,41	2.59	5 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/7/27/28	0/2/2/2
30	UR3	0	2619	30	-	0/5/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
33	8AN	6	76	33	-	3/3/25/26	0/3/3/3
30	1MA	0	628	30	-	0/3/25/26	0/3/3/3
30	OMG	0	2588	32,30	-	0/5/27/28	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.92	1.48	1.52
30	0	2588	OMG	C6-N1	3.29	1.38	1.33
30	0	2621	PSU	C4-N3	3.06	1.38	1.33
30	0	2621	PSU	C2-N1	3.04	1.44	1.38
33	6	76	8AN	C3'-N3'	-2.63	1.43	1.47
30	0	2587	OMU	C4-N3	2.41	1.37	1.33
30	0	2588	OMG	C8-N7	-2.02	1.31	1.34
30	0	2619	UR3	C6-C5	-2.01	1.33	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.58	114.45	128.43
30	0	2621	PSU	C4-N3-C2	13.94	126.92	115.14
30	0	2588	OMG	C5-C6-N1	-8.75	111.46	123.43
30	0	2621	PSU	C5-C4-N3	-7.90	115.18	125.36
30	0	2588	OMG	C6-N1-C2	5.77	125.10	115.93
30	0	628	1MA	C2-N3-C4	-4.74	110.66	116.58
30	0	2587	OMU	C5-C4-N3	-3.97	114.57	123.31
33	6	76	8AN	O2'-C2'-C3'	3.74	121.22	111.47
33	6	76	8AN	O4'-C4'-C3'	3.51	109.19	104.15
30	0	2588	OMG	C2-N3-C4	-3.03	111.89	115.36
30	0	2621	PSU	C6-N1-C2	2.90	120.15	115.36
30	0	2588	OMG	C6-C5-C4	-2.26	118.64	120.80
30	0	2588	OMG	N3-C2-N1	-2.25	124.22	127.22
33	6	76	8AN	C5-C6-N6	2.02	123.42	120.35

There are no chirality outliers.

All (3) 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'

There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2588	OMG	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z > 2$
41	ACA	6	78	-	7,7,8	1.80	2 (28%)	6,6,8	0.78	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
41	ACA	6	78	-	-	1/4/5/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	6	78	ACA	C3-C2	-3.83	1.37	1.52
41	6	78	ACA	O1-C1	2.00	1.31	1.19

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	6	78	ACA	C2-C3-C4-C5

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%)	-0.52	6 (2%) 57 47	22, 45, 81, 106	0
2	B	337/338 (99%)	-0.75	0 100 100	20, 45, 72, 88	0
3	C	246/246 (100%)	-0.63	0 100 100	17, 41, 65, 82	0
4	D	140/177 (79%)	0.81	23 (16%) 1 1	54, 93, 129, 137	0
5	E	172/178 (96%)	-0.47	2 (1%) 79 73	38, 60, 81, 91	0
6	F	119/120 (99%)	0.28	4 (3%) 45 35	41, 70, 106, 115	0
7	G	29/348 (8%)	0.78	4 (13%) 2 1	66, 93, 107, 109	0
8	H	160/177 (90%)	-0.28	1 (0%) 89 86	34, 56, 93, 104	0
9	I	70/162 (43%)	3.97	57 (81%) 0 0	143, 158, 174, 175	0
10	J	142/145 (97%)	-0.71	0 100 100	28, 44, 63, 81	0
11	K	132/132 (100%)	-0.83	0 100 100	25, 39, 60, 72	0
12	L	145/165 (87%)	0.02	5 (3%) 45 35	20, 61, 109, 127	0
13	M	194/196 (98%)	-0.69	1 (0%) 91 88	24, 40, 63, 74	0
14	N	186/187 (99%)	-0.23	6 (3%) 47 37	37, 60, 119, 126	0
15	O	115/116 (99%)	-0.51	0 100 100	33, 53, 68, 74	0
16	P	143/149 (95%)	-0.75	0 100 100	30, 45, 58, 67	0
17	Q	95/96 (98%)	-0.64	0 100 100	30, 42, 60, 74	0
18	R	150/155 (96%)	-0.72	0 100 100	23, 37, 59, 70	0
19	S	81/85 (95%)	-0.28	1 (1%) 79 73	37, 53, 74, 95	0
20	T	119/120 (99%)	-0.33	4 (3%) 45 35	36, 51, 80, 121	0
21	U	53/67 (79%)	-0.45	1 (1%) 66 59	32, 47, 71, 81	0
22	V	65/71 (91%)	0.99	7 (10%) 5 3	44, 74, 117, 125	0
23	W	154/154 (100%)	-0.70	0 100 100	30, 45, 66, 80	0
24	X	82/92 (89%)	-0.32	5 (6%) 21 13	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%)	-0.73	0 100 100	18, 39, 62, 85	0
26	Z	73/116 (62%)	0.55	10 (13%) 3 1	44, 82, 99, 108	0
27	1	56/57 (98%)	-0.81	0 100 100	21, 28, 36, 43	0
28	2	46/50 (92%)	-0.45	2 (4%) 35 25	30, 52, 68, 86	0
29	3	92/92 (100%)	-0.42	2 (2%) 62 52	34, 53, 71, 80	0
30	0	2749/2923 (94%)	-0.70	31 (1%) 80 75	17, 40, 89, 186	0
31	9	122/122 (100%)	-0.74	4 (3%) 46 36	33, 61, 86, 151	0
32	5	3/3 (100%)	1.88	1 (33%) 0 0	81, 81, 83, 86	0
33	6	2/3 (66%)	0.85	0 100 100	96, 96, 96, 104	0
All	All	6651/7522 (88%)	-0.49	177 (2%) 54 44	17, 46, 98, 186	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	40	PRO	13.2
9	I	66	GLY	11.4
9	I	74	ILE	9.9
22	V	1	THR	8.5
4	D	57	THR	8.4
9	I	100	VAL	8.3
9	I	70	THR	8.1
22	V	39	ALA	8.0
14	N	166	ALA	7.8
9	I	103	ILE	7.8
9	I	111	LEU	7.7
9	I	72	GLU	7.5
9	I	80	PHE	7.0
9	I	128	THR	7.0
20	T	119	ALA	7.0
4	D	63	ILE	6.9
22	V	38	GLY	6.8
9	I	104	ALA	6.8
9	I	71	ALA	6.8
26	Z	34	SER	6.7
26	Z	46	SER	6.4
9	I	99	GLN	6.2
9	I	97	VAL	6.1
9	I	91	PHE	5.8
9	I	98	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
9	I	132	VAL	5.7
9	I	78	ALA	5.6
30	0	1172	G	5.3
26	Z	35	SER	5.3
9	I	76	ASP	5.2
20	T	116	ASP	5.2
9	I	131	GLY	5.1
9	I	133	THR	5.1
30	0	1199	A	5.0
9	I	82	THR	5.0
4	D	90	LEU	4.9
9	I	86	GLU	4.8
9	I	69	PRO	4.8
9	I	108	HIS	4.5
30	0	1198	U	4.5
9	I	93	ALA	4.4
22	V	36	ALA	4.4
9	I	123	VAL	4.3
4	D	95	THR	4.3
9	I	81	GLU	4.2
9	I	109	PRO	4.2
19	S	81	ILE	4.2
9	I	113	SER	4.1
9	I	94	ASP	4.1
30	0	1169	U	4.1
31	9	1	U	4.0
26	Z	49	ARG	4.0
26	Z	45	VAL	3.9
7	G	23	ILE	3.9
9	I	88	GLN	3.9
14	N	155	GLU	3.9
4	D	166	ILE	3.9
30	0	1177	A	3.8
4	D	170	TYR	3.8
28	2	49	GLU	3.8
30	0	1200	A	3.8
9	I	102	GLN	3.8
14	N	160	SER	3.7
9	I	127	CYS	3.7
9	I	92	VAL	3.6
30	0	735	C	3.6
30	0	1163	G	3.5

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Mol	Chain	Res	Type	RSRZ
9	I	84	SER	3.5
4	D	92	GLU	3.4
9	I	120	ALA	3.4
9	I	101	LYS	3.4
9	I	106	GLN	3.4
30	0	1164	U	3.4
4	D	93	LEU	3.4
26	Z	48	ARG	3.4
22	V	37	GLY	3.4
30	0	1196	C	3.4
31	9	2	U	3.3
4	D	101	THR	3.3
30	0	1170	U	3.3
4	D	134	LEU	3.3
1	A	237	GLY	3.3
26	Z	58	ASN	3.2
9	I	116	LEU	3.2
9	I	129	SER	3.1
9	I	90	ASP	3.1
9	I	73	LEU	3.1
9	I	79	GLY	3.0
30	0	1951	G	3.0
1	A	236	GLY	3.0
9	I	105	GLU	3.0
1	A	37	VAL	3.0
9	I	83	GLY	2.9
26	Z	43	GLY	2.9
30	0	1965	C	2.9
21	U	47	ARG	2.9
4	D	88	LEU	2.9
30	0	970	U	2.8
4	D	84	LEU	2.8
5	E	45	ASP	2.8
7	G	26	MET	2.8
9	I	130	LEU	2.8
30	0	1202	A	2.8
32	5	75	C	2.8
4	D	10	PHE	2.7
9	I	126	THR	2.7
4	D	18	ILE	2.7
6	F	110	ASP	2.7
4	D	11	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
9	I	121	LYS	2.7
6	F	25	ASP	2.6
14	N	134	ASP	2.6
9	I	122	GLU	2.6
24	X	88	GLU	2.6
12	L	75	LEU	2.5
30	0	1181	A	2.5
20	T	118	SER	2.5
12	L	60	GLU	2.5
26	Z	47	ARG	2.5
29	3	56	PRO	2.5
30	0	1967	U	2.5
20	T	117	ASP	2.5
30	0	1173	A	2.5
30	0	1966	U	2.4
30	0	514	G	2.4
30	0	2637	A	2.4
12	L	91	VAL	2.4
4	D	62	ASP	2.4
31	9	23	U	2.4
9	I	87	PRO	2.4
24	X	71	ARG	2.4
14	N	163	PHE	2.3
1	A	31	LYS	2.3
1	A	35	GLY	2.3
30	0	1165	G	2.3
12	L	105	TYR	2.3
9	I	112	LEU	2.3
4	D	61	PHE	2.3
30	0	1171	A	2.3
30	0	1175	G	2.3
29	3	55	VAL	2.2
9	I	110	ASP	2.2
8	H	174	LEU	2.2
7	G	27	ILE	2.2
4	D	64	ARG	2.2
9	I	114	TYR	2.2
5	E	10	ASP	2.2
6	F	117	GLU	2.2
14	N	165	ALA	2.2
30	0	1197	G	2.2
24	X	80	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
6	F	107	ASP	2.2
1	A	133	ARG	2.2
4	D	40	ILE	2.2
22	V	41	GLU	2.2
28	2	35	ARG	2.2
4	D	41	LEU	2.1
30	0	1180	U	2.1
4	D	44	ILE	2.1
4	D	94	ALA	2.1
30	0	1195	G	2.1
26	Z	38	PHE	2.1
9	I	124	VAL	2.1
9	I	89	GLU	2.1
31	9	24	U	2.1
9	I	125	GLY	2.1
24	X	85	VAL	2.1
30	0	1168	C	2.1
30	0	1206	U	2.1
30	0	1176	C	2.1
9	I	117	THR	2.1
12	L	80	ASP	2.0
24	X	7	GLU	2.0
7	G	12	ILE	2.0
30	0	282	C	2.0
4	D	58	VAL	2.0
13	M	78	LYS	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
33	8AN	6	76	22/23	0.87	0.28	84,92,94,95	0
30	PSU	0	2621	20/21	0.97	0.14	29,31,38,39	0
30	UR3	0	2619	21/22	0.97	0.14	33,35,40,41	0
30	1MA	0	628	23/24	0.97	0.15	25,28,29,30	0
30	OMG	0	2588	24/25	0.97	0.11	24,29,31,33	0
30	OMU	0	2587	21/22	0.98	0.09	24,28,32,33	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
36	SR	0	8942	1/1	-0.19	0.23	186,186,186,186	0
34	MG	0	8063	1/1	-0.06	0.42	87,87,87,87	0
36	SR	0	8933	1/1	0.01	0.41	168,168,168,168	0
34	MG	0	8038	1/1	0.08	2.39	112,112,112,112	0
34	MG	0	8090	1/1	0.17	1.00	126,126,126,126	0
37	NA	0	8573	1/1	0.27	0.99	107,107,107,107	0
34	MG	0	8087	1/1	0.28	1.17	106,106,106,106	0
37	NA	0	8560	1/1	0.34	0.62	107,107,107,107	0
36	SR	0	8996	1/1	0.47	0.11	148,148,148,148	0
34	MG	0	8016	1/1	0.48	0.87	98,98,98,98	0
37	NA	0	8547	1/1	0.48	0.40	66,66,66,66	0
37	NA	0	8571	1/1	0.49	0.69	131,131,131,131	0
34	MG	0	8079	1/1	0.50	0.34	64,64,64,64	0
36	SR	0	9007	1/1	0.51	0.72	200,200,200,200	0
36	SR	0	8920	1/1	0.52	0.70	200,200,200,200	0
37	NA	0	8567	1/1	0.52	0.44	75,75,75,75	0
39	K	0	8402	1/1	0.52	0.22	81,81,81,81	0
36	SR	0	9006	1/1	0.55	0.57	199,199,199,199	0
36	SR	0	8959	1/1	0.60	0.06	131,131,131,131	0
40	PHE	6	77	11/12	0.62	0.45	72,73,77,80	0
36	SR	0	8969	1/1	0.63	0.20	154,154,154,154	0
36	SR	B	8987	1/1	0.65	0.42	200,200,200,200	0
37	NA	0	8525	1/1	0.65	0.32	63,63,63,63	0
34	MG	0	8065	1/1	0.66	0.41	84,84,84,84	0
37	NA	Q	8540	1/1	0.66	0.10	48,48,48,48	0
37	NA	0	8559	1/1	0.66	0.36	75,75,75,75	0
37	NA	0	8506	1/1	0.67	0.20	65,65,65,65	0
35	CL	3	8804	1/1	0.67	0.09	88,88,88,88	0
34	MG	0	8030	1/1	0.69	0.15	188,188,188,188	0
34	MG	T	8057	1/1	0.69	0.13	65,65,65,65	0
37	NA	0	8522	1/1	0.70	0.15	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8078	1/1	0.71	0.88	104,104,104,104	0
36	SR	0	8976	1/1	0.72	0.22	124,124,124,124	0
34	MG	0	8046	1/1	0.72	0.82	99,99,99,99	0
36	SR	0	8998	1/1	0.73	0.20	159,159,159,159	0
34	MG	0	8085	1/1	0.73	0.34	91,91,91,91	0
37	NA	0	8546	1/1	0.74	0.25	79,79,79,79	0
37	NA	0	8541	1/1	0.74	0.39	80,80,80,80	0
37	NA	9	8572	1/1	0.75	0.09	85,85,85,85	0
41	ACA	6	78	8/9	0.75	0.37	74,74,81,82	0
34	MG	0	8050	1/1	0.76	0.58	162,162,162,162	0
34	MG	0	8005	1/1	0.76	0.33	30,30,30,30	0
36	SR	0	9001	1/1	0.77	0.09	155,155,155,155	0
34	MG	0	8047	1/1	0.77	0.88	89,89,89,89	0
37	NA	0	8507	1/1	0.77	0.37	88,88,88,88	0
37	NA	0	8509	1/1	0.79	0.41	83,83,83,83	0
37	NA	0	8511	1/1	0.79	0.19	48,48,48,48	0
34	MG	0	8092	1/1	0.80	0.12	48,48,48,48	0
37	NA	0	8519	1/1	0.80	0.54	53,53,53,53	0
34	MG	0	8037	1/1	0.80	0.14	70,70,70,70	0
37	NA	0	8564	1/1	0.80	0.08	68,68,68,68	0
34	MG	0	8053	1/1	0.80	0.11	54,54,54,54	0
36	SR	S	8961	1/1	0.80	0.08	189,189,189,189	0
36	SR	A	8929	1/1	0.81	0.06	105,105,105,105	0
37	NA	0	8516	1/1	0.81	0.19	42,42,42,42	0
36	SR	0	8974	1/1	0.81	0.19	110,110,110,110	0
39	K	0	8401	1/1	0.81	0.24	66,66,66,66	0
34	MG	0	8059	1/1	0.81	0.13	58,58,58,58	0
37	NA	0	8536	1/1	0.82	0.15	69,69,69,69	0
37	NA	0	8569	1/1	0.82	0.21	44,44,44,44	0
37	NA	0	8565	1/1	0.82	0.32	59,59,59,59	0
34	MG	0	8048	1/1	0.82	0.16	43,43,43,43	0
37	NA	0	8557	1/1	0.83	0.10	57,57,57,57	0
37	NA	0	8542	1/1	0.83	0.22	38,38,38,38	0
37	NA	0	8535	1/1	0.83	0.39	64,64,64,64	0
34	MG	0	8056	1/1	0.83	0.17	69,69,69,69	0
34	MG	0	8081	1/1	0.83	0.52	103,103,103,103	0
37	NA	M	8539	1/1	0.83	0.11	33,33,33,33	0
34	MG	0	8069	1/1	0.83	0.25	88,88,88,88	0
37	NA	0	8555	1/1	0.83	0.72	64,64,64,64	0
34	MG	0	8040	1/1	0.84	0.20	75,75,75,75	0
37	NA	0	8556	1/1	0.84	0.17	39,39,39,39	0
37	NA	0	8566	1/1	0.84	0.24	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	NA	D	8543	1/1	0.84	0.07	60,60,60,60	0
37	NA	0	8549	1/1	0.84	0.34	61,61,61,61	0
34	MG	0	8089	1/1	0.84	0.15	35,35,35,35	0
37	NA	J	8538	1/1	0.84	0.21	31,31,31,31	0
34	MG	0	8082	1/1	0.85	0.31	64,64,64,64	0
34	MG	0	8076	1/1	0.85	0.52	81,81,81,81	0
34	MG	B	8042	1/1	0.85	0.11	92,92,92,92	0
37	NA	0	8508	1/1	0.85	0.12	31,31,31,31	0
37	NA	B	8552	1/1	0.85	0.45	69,69,69,69	0
34	MG	0	8024	1/1	0.85	0.25	80,80,80,80	0
37	NA	0	8504	1/1	0.85	0.20	20,20,20,20	0
34	MG	0	8064	1/1	0.85	0.18	51,51,51,51	0
34	MG	0	8091	1/1	0.85	0.10	59,59,59,59	0
34	MG	0	8062	1/1	0.86	0.60	76,76,76,76	0
34	MG	A	8051	1/1	0.86	0.39	58,58,58,58	0
34	MG	0	8033	1/1	0.86	0.09	59,59,59,59	0
36	SR	0	8951	1/1	0.86	0.09	107,107,107,107	0
36	SR	0	8955	1/1	0.86	0.09	115,115,115,115	0
36	SR	0	8994	1/1	0.86	0.53	200,200,200,200	0
37	NA	0	8528	1/1	0.86	0.10	42,42,42,42	0
37	NA	0	8518	1/1	0.86	0.21	68,68,68,68	0
34	MG	0	8010	1/1	0.87	0.34	103,103,103,103	0
36	SR	0	8944	1/1	0.87	0.13	113,113,113,113	0
36	SR	0	9000	1/1	0.88	0.18	137,137,137,137	0
37	NA	0	8531	1/1	0.88	0.21	37,37,37,37	0
34	MG	0	8023	1/1	0.88	0.14	21,21,21,21	0
37	NA	0	8521	1/1	0.88	0.39	61,61,61,61	0
37	NA	0	8558	1/1	0.88	0.65	56,56,56,56	0
34	MG	0	8049	1/1	0.88	0.55	141,141,141,141	0
36	SR	9	8980	1/1	0.89	0.05	155,155,155,155	0
34	MG	0	8001	1/1	0.89	0.24	22,22,22,22	0
37	NA	0	8551	1/1	0.89	0.28	53,53,53,53	0
36	SR	9	8968	1/1	0.89	0.09	105,105,105,105	0
35	CL	0	8813	1/1	0.90	0.08	53,53,53,53	0
37	NA	S	8510	1/1	0.90	0.15	58,58,58,58	0
37	NA	0	8517	1/1	0.90	0.41	40,40,40,40	0
37	NA	0	8530	1/1	0.90	0.23	38,38,38,38	0
34	MG	0	8075	1/1	0.90	0.08	35,35,35,35	0
34	MG	0	8039	1/1	0.91	0.22	32,32,32,32	0
36	SR	9	9003	1/1	0.91	0.06	127,127,127,127	0
34	MG	0	8077	1/1	0.91	0.09	37,37,37,37	0
37	NA	0	8505	1/1	0.91	0.40	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	NA	0	8570	1/1	0.91	0.15	53,53,53,53	0
34	MG	0	8002	1/1	0.91	0.42	62,62,62,62	0
37	NA	0	8523	1/1	0.91	0.19	49,49,49,49	0
36	SR	0	8971	1/1	0.91	0.07	157,157,157,157	0
34	MG	0	8027	1/1	0.91	0.13	44,44,44,44	0
36	SR	0	8988	1/1	0.91	0.06	110,110,110,110	0
37	NA	0	8515	1/1	0.91	0.15	20,20,20,20	0
36	SR	0	8993	1/1	0.91	0.05	126,126,126,126	0
37	NA	0	8520	1/1	0.92	0.17	43,43,43,43	0
34	MG	0	8032	1/1	0.92	0.07	44,44,44,44	0
36	SR	0	8919	1/1	0.92	0.12	82,82,82,82	0
34	MG	0	8029	1/1	0.92	0.27	87,87,87,87	0
37	NA	0	8545	1/1	0.92	0.15	40,40,40,40	0
37	NA	0	8501	1/1	0.92	0.32	100,100,100,100	0
34	MG	0	8021	1/1	0.92	0.07	24,24,24,24	0
36	SR	H	8972	1/1	0.92	0.11	119,119,119,119	0
37	NA	0	8514	1/1	0.92	0.40	53,53,53,53	0
36	SR	0	8995	1/1	0.92	0.15	86,86,86,86	0
36	SR	0	8983	1/1	0.92	0.23	195,195,195,195	0
36	SR	Y	9002	1/1	0.93	0.11	118,118,118,118	0
37	NA	0	8575	1/1	0.93	0.15	59,59,59,59	0
34	MG	0	8067	1/1	0.93	0.29	48,48,48,48	0
36	SR	0	8982	1/1	0.93	0.12	105,105,105,105	0
36	SR	0	8986	1/1	0.93	0.12	114,114,114,114	0
36	SR	0	8956	1/1	0.93	0.12	105,105,105,105	0
34	MG	0	8080	1/1	0.93	0.16	62,62,62,62	0
36	SR	0	9004	1/1	0.93	0.16	107,107,107,107	0
35	CL	J	8821	1/1	0.93	0.17	61,61,61,61	0
34	MG	0	8073	1/1	0.93	0.09	62,62,62,62	0
36	SR	0	8957	1/1	0.93	0.12	122,122,122,122	0
34	MG	0	8017	1/1	0.93	0.66	80,80,80,80	0
37	NA	0	8527	1/1	0.94	0.20	40,40,40,40	0
34	MG	0	8008	1/1	0.94	0.12	13,13,13,13	0
36	SR	0	8916	1/1	0.94	0.13	65,65,65,65	0
36	SR	0	8975	1/1	0.94	0.04	115,115,115,115	0
37	NA	0	8554	1/1	0.94	0.46	53,53,53,53	0
34	MG	0	8004	1/1	0.94	0.21	13,13,13,13	0
37	NA	R	8533	1/1	0.94	0.14	42,42,42,42	0
37	NA	0	8512	1/1	0.94	0.43	43,43,43,43	0
34	MG	0	8013	1/1	0.94	0.04	28,28,28,28	0
34	MG	0	8044	1/1	0.94	0.08	47,47,47,47	0
37	NA	0	8550	1/1	0.94	0.20	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8036	1/1	0.94	0.15	47,47,47,47	0
34	MG	0	8068	1/1	0.94	0.24	74,74,74,74	0
36	SR	F	9005	1/1	0.94	0.12	85,85,85,85	0
34	MG	Y	8086	1/1	0.94	0.19	46,46,46,46	0
37	NA	0	8562	1/1	0.94	0.46	61,61,61,61	0
34	MG	0	8035	1/1	0.94	0.18	94,94,94,94	0
35	CL	O	8808	1/1	0.94	0.10	63,63,63,63	0
36	SR	0	8966	1/1	0.94	0.13	86,86,86,86	0
37	NA	0	8544	1/1	0.94	0.34	67,67,67,67	0
36	SR	0	8967	1/1	0.95	0.11	92,92,92,92	0
35	CL	Q	8811	1/1	0.95	0.06	68,68,68,68	0
35	CL	0	8822	1/1	0.95	0.15	53,53,53,53	0
35	CL	A	8809	1/1	0.95	0.07	57,57,57,57	0
36	SR	0	8941	1/1	0.95	0.14	71,71,71,71	0
36	SR	0	8928	1/1	0.95	0.08	87,87,87,87	0
34	MG	0	8014	1/1	0.95	0.21	9,9,9,9	0
34	MG	0	8043	1/1	0.95	0.15	37,37,37,37	0
36	SR	0	8936	1/1	0.95	0.16	59,59,59,59	0
36	SR	0	8985	1/1	0.95	0.07	116,116,116,116	0
35	CL	N	8807	1/1	0.95	0.06	62,62,62,62	0
36	SR	0	8962	1/1	0.95	0.09	96,96,96,96	0
35	CL	J	8801	1/1	0.95	0.10	58,58,58,58	0
34	MG	0	8055	1/1	0.95	0.29	30,30,30,30	0
36	SR	B	8950	1/1	0.95	0.17	89,89,89,89	0
37	NA	0	8524	1/1	0.95	0.09	37,37,37,37	0
37	NA	0	8502	1/1	0.95	0.21	55,55,55,55	0
37	NA	0	8553	1/1	0.95	0.51	100,100,100,100	0
35	CL	0	8805	1/1	0.96	0.07	46,46,46,46	0
36	SR	0	9008	1/1	0.96	0.14	80,80,80,80	0
37	NA	0	8563	1/1	0.96	0.24	55,55,55,55	0
35	CL	J	8802	1/1	0.96	0.06	66,66,66,66	0
34	MG	0	8066	1/1	0.96	0.24	32,32,32,32	0
37	NA	L	8568	1/1	0.96	0.18	30,30,30,30	0
34	MG	0	8041	1/1	0.96	0.26	31,31,31,31	0
35	CL	L	8814	1/1	0.96	0.07	49,49,49,49	0
37	NA	0	8537	1/1	0.96	0.04	22,22,22,22	0
36	SR	0	8938	1/1	0.96	0.07	101,101,101,101	0
37	NA	0	8529	1/1	0.96	0.04	20,20,20,20	0
36	SR	0	8923	1/1	0.96	0.17	66,66,66,66	0
35	CL	Y	8820	1/1	0.96	0.05	35,35,35,35	0
36	SR	A	8977	1/1	0.96	0.10	95,95,95,95	0
34	MG	0	8007	1/1	0.96	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8083	1/1	0.96	0.09	36,36,36,36	0
34	MG	0	8071	1/1	0.96	0.49	98,98,98,98	0
36	SR	0	8917	1/1	0.96	0.17	61,61,61,61	0
36	SR	0	8960	1/1	0.96	0.08	98,98,98,98	0
36	SR	0	8984	1/1	0.96	0.10	89,89,89,89	0
34	MG	0	8031	1/1	0.96	0.12	48,48,48,48	0
36	SR	0	8997	1/1	0.96	0.05	116,116,116,116	0
34	MG	0	8052	1/1	0.96	0.07	37,37,37,37	0
34	MG	0	8093	1/1	0.97	0.12	25,25,25,25	0
38	CD	O	8705	1/1	0.97	0.03	103,103,103,103	0
36	SR	0	8922	1/1	0.97	0.14	62,62,62,62	0
34	MG	C	8012	1/1	0.97	0.22	13,13,13,13	0
37	NA	0	8574	1/1	0.97	0.44	48,48,48,48	0
35	CL	M	8818	1/1	0.97	0.08	33,33,33,33	0
37	NA	0	8513	1/1	0.97	0.15	29,29,29,29	0
37	NA	R	8532	1/1	0.97	0.09	29,29,29,29	0
34	MG	0	8028	1/1	0.97	0.26	1,1,1,1	0
36	SR	0	8965	1/1	0.97	0.11	88,88,88,88	0
36	SR	0	8958	1/1	0.97	0.11	68,68,68,68	0
35	CL	0	8817	1/1	0.97	0.06	42,42,42,42	0
35	CL	2	8803	1/1	0.97	0.07	51,51,51,51	0
36	SR	0	8954	1/1	0.97	0.12	67,67,67,67	0
36	SR	0	8945	1/1	0.97	0.13	89,89,89,89	0
36	SR	0	8943	1/1	0.97	0.13	65,65,65,65	0
37	NA	0	8526	1/1	0.97	0.12	47,47,47,47	0
36	SR	0	8964	1/1	0.97	0.07	92,92,92,92	0
37	NA	0	8534	1/1	0.97	0.69	78,78,78,78	0
36	SR	0	8991	1/1	0.97	0.10	147,147,147,147	0
34	MG	9	8074	1/1	0.97	0.24	53,53,53,53	0
36	SR	0	8906	1/1	0.97	0.17	49,49,49,49	0
36	SR	0	8947	1/1	0.97	0.17	84,84,84,84	0
35	CL	0	8816	1/1	0.98	0.11	60,60,60,60	0
34	MG	0	8011	1/1	0.98	0.20	17,17,17,17	0
37	NA	0	8548	1/1	0.98	0.20	27,27,27,27	0
36	SR	0	8973	1/1	0.98	0.10	91,91,91,91	0
34	MG	0	8018	1/1	0.98	0.26	9,9,9,9	0
36	SR	A	8930	1/1	0.98	0.13	72,72,72,72	0
34	MG	0	8003	1/1	0.98	0.17	18,18,18,18	0
37	NA	C	8503	1/1	0.98	0.23	22,22,22,22	0
36	SR	0	8978	1/1	0.98	0.16	60,60,60,60	0
35	CL	L	8810	1/1	0.98	0.05	52,52,52,52	0
36	SR	1	8952	1/1	0.98	0.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8019	1/1	0.98	0.19	9,9,9,9	0
36	SR	0	8934	1/1	0.98	0.18	67,67,67,67	0
34	MG	0	8084	1/1	0.98	0.11	31,31,31,31	0
36	SR	3	8999	1/1	0.98	0.12	70,70,70,70	0
34	MG	0	8088	1/1	0.98	0.18	37,37,37,37	0
34	MG	0	8015	1/1	0.98	0.18	45,45,45,45	0
34	MG	0	8020	1/1	0.98	0.20	24,24,24,24	0
34	MG	0	8045	1/1	0.98	0.56	147,147,147,147	0
36	SR	0	8946	1/1	0.98	0.17	86,86,86,86	0
36	SR	0	8963	1/1	0.98	0.16	70,70,70,70	0
34	MG	0	8034	1/1	0.98	0.12	31,31,31,31	0
34	MG	0	8006	1/1	0.98	0.15	6,6,6,6	0
37	NA	0	8561	1/1	0.98	0.33	89,89,89,89	0
36	SR	0	8914	1/1	0.98	0.22	75,75,75,75	0
36	SR	0	8935	1/1	0.98	0.11	64,64,64,64	0
36	SR	0	8992	1/1	0.98	0.07	102,102,102,102	0
34	MG	2	8060	1/1	0.98	0.12	42,42,42,42	0
36	SR	0	8903	1/1	0.98	0.16	44,44,44,44	0
34	MG	A	8025	1/1	0.98	0.06	40,40,40,40	0
36	SR	0	8931	1/1	0.98	0.13	74,74,74,74	0
34	MG	0	8070	1/1	0.98	0.22	62,62,62,62	0
36	SR	0	8908	1/1	0.99	0.13	66,66,66,66	0
36	SR	0	8905	1/1	0.99	0.22	49,49,49,49	0
36	SR	0	8937	1/1	0.99	0.19	59,59,59,59	0
36	SR	0	8904	1/1	0.99	0.16	39,39,39,39	0
35	CL	B	8819	1/1	0.99	0.34	56,56,56,56	0
35	CL	K	8812	1/1	0.99	0.06	43,43,43,43	0
36	SR	0	8901	1/1	0.99	0.13	44,44,44,44	0
36	SR	0	8949	1/1	0.99	0.13	49,49,49,49	0
36	SR	0	8924	1/1	0.99	0.18	65,65,65,65	0
36	SR	0	8918	1/1	0.99	0.14	41,41,41,41	0
38	CD	Z	8703	1/1	0.99	0.08	62,62,62,62	0
36	SR	0	8940	1/1	0.99	0.12	53,53,53,53	0
34	MG	0	8061	1/1	0.99	0.20	17,17,17,17	0
36	SR	0	8921	1/1	0.99	0.13	51,51,51,51	0
34	MG	0	8009	1/1	0.99	0.30	1,1,1,1	0
34	MG	K	8054	1/1	0.99	0.17	18,18,18,18	0
36	SR	3	8953	1/1	0.99	0.12	103,103,103,103	0
36	SR	3	8932	1/1	0.99	0.15	68,68,68,68	0
36	SR	0	8902	1/1	0.99	0.17	32,32,32,32	0
36	SR	0	8925	1/1	0.99	0.15	66,66,66,66	0
36	SR	0	8915	1/1	0.99	0.10	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	SR	R	8912	1/1	0.99	0.18	64,64,64,64	0
36	SR	0	8989	1/1	0.99	0.11	71,71,71,71	0
36	SR	0	8948	1/1	0.99	0.16	57,57,57,57	0
34	MG	0	8058	1/1	0.99	0.20	1,1,1,1	0
34	MG	0	8072	1/1	0.99	0.14	25,25,25,25	0
35	CL	R	8806	1/1	0.99	0.08	36,36,36,36	0
36	SR	1	8913	1/1	0.99	0.15	42,42,42,42	0
36	SR	T	8939	1/1	0.99	0.09	70,70,70,70	0
36	SR	0	8970	1/1	0.99	0.05	88,88,88,88	0
36	SR	0	8927	1/1	0.99	0.17	67,67,67,67	0
38	CD	1	8702	1/1	0.99	0.09	50,50,50,50	0
34	MG	0	8026	1/1	0.99	0.14	35,35,35,35	0
36	SR	0	8990	1/1	0.99	0.17	39,39,39,39	0
36	SR	0	8981	1/1	0.99	0.15	107,107,107,107	0
34	MG	0	8022	1/1	0.99	0.19	12,12,12,12	0
36	SR	0	8926	1/1	1.00	0.16	81,81,81,81	0
36	SR	H	8907	1/1	1.00	0.15	41,41,41,41	0
35	CL	0	8815	1/1	1.00	0.06	61,61,61,61	0
36	SR	0	8909	1/1	1.00	0.17	59,59,59,59	0
36	SR	T	8911	1/1	1.00	0.10	52,52,52,52	0
38	CD	3	8704	1/1	1.00	0.09	54,54,54,54	0
38	CD	U	8701	1/1	1.00	0.11	50,50,50,50	0
36	SR	0	8910	1/1	1.00	0.12	40,40,40,40	0

6.5 Other polymers

There are no such residues in this entry.