



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:01 AM GMT

PDB ID : 3CCU  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2482C  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-26  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

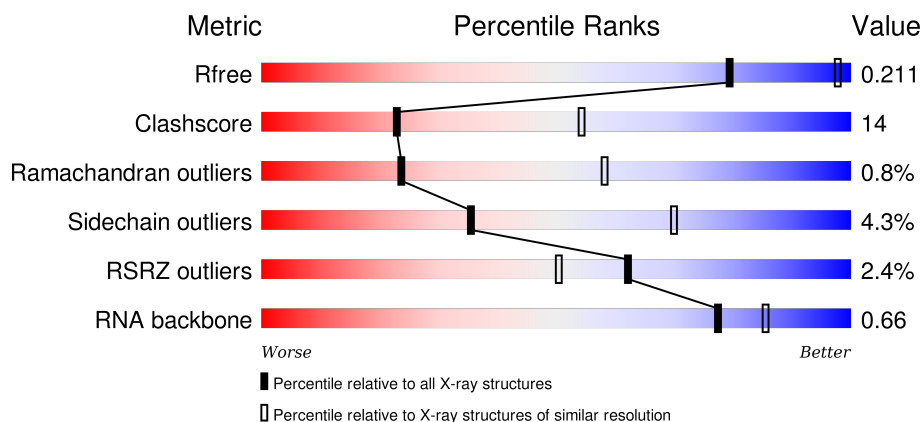
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



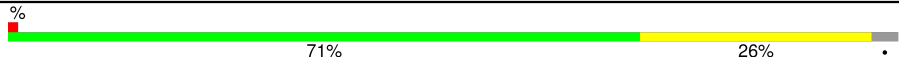

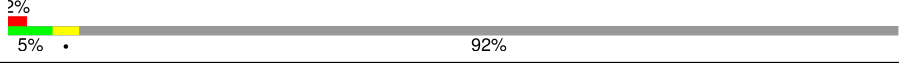

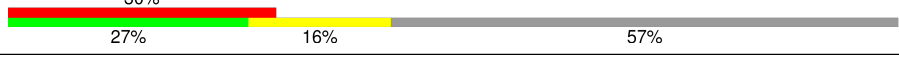
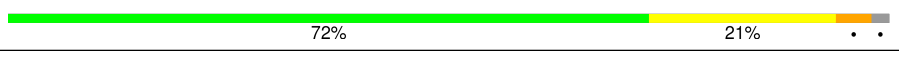
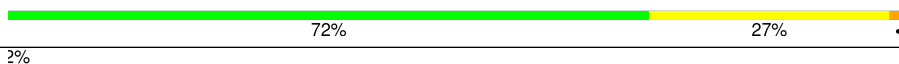

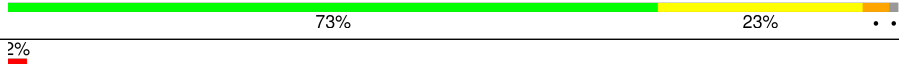


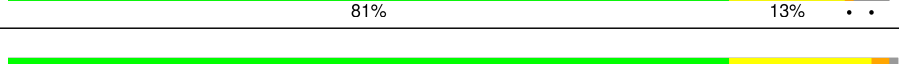
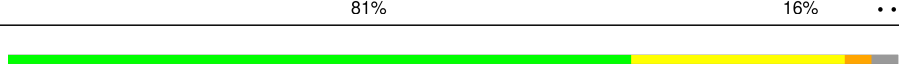
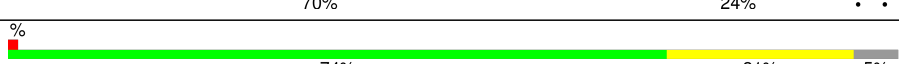


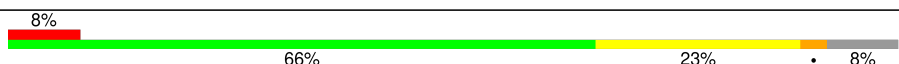
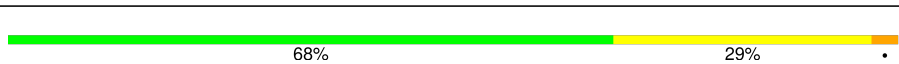
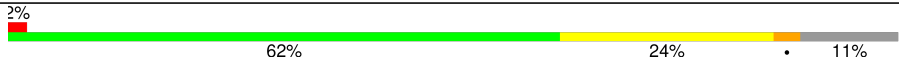
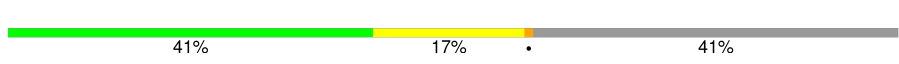
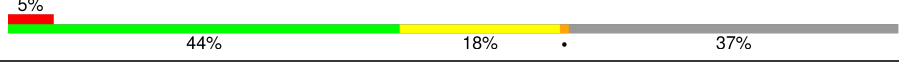
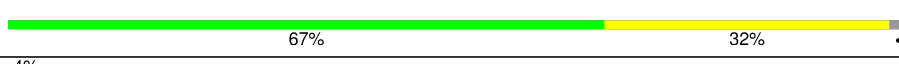
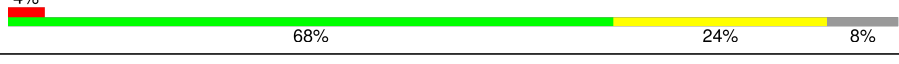


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>••</div> </div> </div>
2	B	338	<div> <div>65%</div> <div>31%</div> <div>•</div> </div>
3	C	246	<div> <div>74%</div> <div>23%</div> <div>•</div> </div>
4	D	177	<div> <div>15%</div> <div>44%</div> <div>35%</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	241	
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	

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
32	MG	0	8009	-	-	-	X
32	MG	0	8014	-	-	-	X
32	MG	0	8015	-	-	-	X
32	MG	0	8028	-	-	-	X
32	MG	0	8041	-	-	-	X
32	MG	0	8045	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	A	8051	-	-	-	X
33	K	0	8401	-	-	-	X
34	NA	0	8504	-	-	-	X
34	NA	0	8507	-	-	-	X
34	NA	0	8512	-	-	-	X
34	NA	0	8517	-	-	-	X
34	NA	0	8521	-	-	-	X
34	NA	0	8522	-	-	-	X
34	NA	0	8527	-	-	-	X
34	NA	0	8530	-	-	-	X
34	NA	0	8533	-	-	-	X
34	NA	0	8535	-	-	-	X
34	NA	0	8537	-	-	-	X
34	NA	0	8542	-	-	-	X
34	NA	0	8547	-	-	-	X
34	NA	0	8552	-	-	-	X
34	NA	0	8553	-	-	-	X
34	NA	0	8555	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8557	-	-	-	X
34	NA	0	8558	-	-	-	X
34	NA	0	8559	-	-	-	X
34	NA	0	8560	-	-	-	X
34	NA	0	8562	-	-	-	X
34	NA	0	8563	-	-	-	X
34	NA	0	8564	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	0	8565	-	-	-	X
34	NA	0	8567	-	-	-	X
34	NA	0	8569	-	-	-	X
34	NA	0	8575	-	-	-	X
34	NA	9	8572	-	-	-	X
35	CL	J	8801	-	-	X	-
36	SR	0	8903	-	-	-	X
36	SR	0	8904	-	-	-	X
36	SR	0	8926	-	-	-	X
36	SR	0	8947	-	-	-	X
36	SR	0	8969	-	-	-	X
36	SR	0	8992	-	-	-	X
36	SR	0	9001	-	-	-	X
36	SR	B	8987	-	-	-	X
36	SR	J	8986	-	-	-	X

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99119 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
			1753	1072	352	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
			2625	1616	493	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
			1860	1130	345	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
			1094	685	195	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
			1357	840	224	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
			890	551	141	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
			1282	798	240	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
			519	323	81	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
			1120	696	199	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
			994	609	189	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
			1118	670	222	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
			1558	943	333	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
			1445	895	262	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
			865	529	161	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
			1136	683	229	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
			735	450	141	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
			1149	713	209	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
			641	389	111	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
			950	568	180	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
			1196	737	209	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
			654	402	129	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	S	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
			573	343	113	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
			755	458	153	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
			59017	26348	10871	19053	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
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	84	Total	Mg	0	0
			84	84		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	2	Total	Mg	0	0
			2	2		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	9	2	Total	Mg	0	0
			2	2		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	H	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	9	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	9	Total Cl 9 9	0	0
35	J	3	Total Cl 3 3	0	0
35	K	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Y	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	92	Total 92	Sr 92	0	0
36	J	1	Total 1	Sr 1	0	0
36	1	2	Total 2	Sr 2	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	3	Total 3	Sr 3	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	3	Total 3	Sr 3	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	O	1	Total 1	Cd 1	0	0
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	3	1	Total 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5933	Total 5933	O 5933	0	0
38	9	144	Total 144	O 144	0	0
38	A	110	Total 110	O 110	0	0
38	B	144	Total 144	O 144	0	0
38	C	178	Total 178	O 178	0	0
38	D	45	Total 45	O 45	0	0
38	E	43	Total 43	O 43	0	0
38	F	27	Total 27	O 27	0	0
38	G	17	Total 17	O 17	0	0
38	H	69	Total 69	O 69	0	0
38	I	6	Total 6	O 6	0	0
38	J	53	Total 53	O 53	0	0
38	K	56	Total 56	O 56	0	0
38	L	92	Total 92	O 92	0	0
38	M	129	Total 129	O 129	0	0
38	N	63	Total 63	O 63	0	0
38	O	40	Total 40	O 40	0	0

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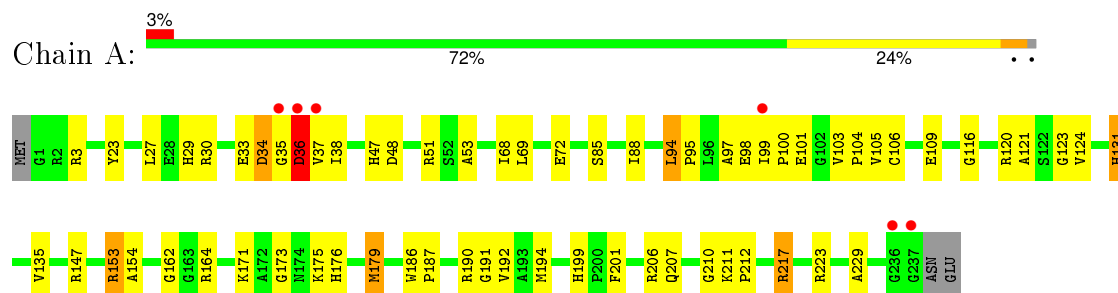
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	P	66	Total 66	O 66	0	0
38	Q	46	Total 46	O 46	0	0
38	R	76	Total 76	O 76	0	0
38	S	39	Total 39	O 39	0	0
38	T	35	Total 35	O 35	0	0
38	U	28	Total 28	O 28	0	0
38	V	13	Total 13	O 13	0	0
38	W	69	Total 69	O 69	0	0
38	X	27	Total 27	O 27	0	0
38	Y	91	Total 91	O 91	0	0
38	Z	25	Total 25	O 25	0	0
38	1	56	Total 56	O 56	0	0
38	2	38	Total 38	O 38	0	0
38	3	65	Total 65	O 65	0	0

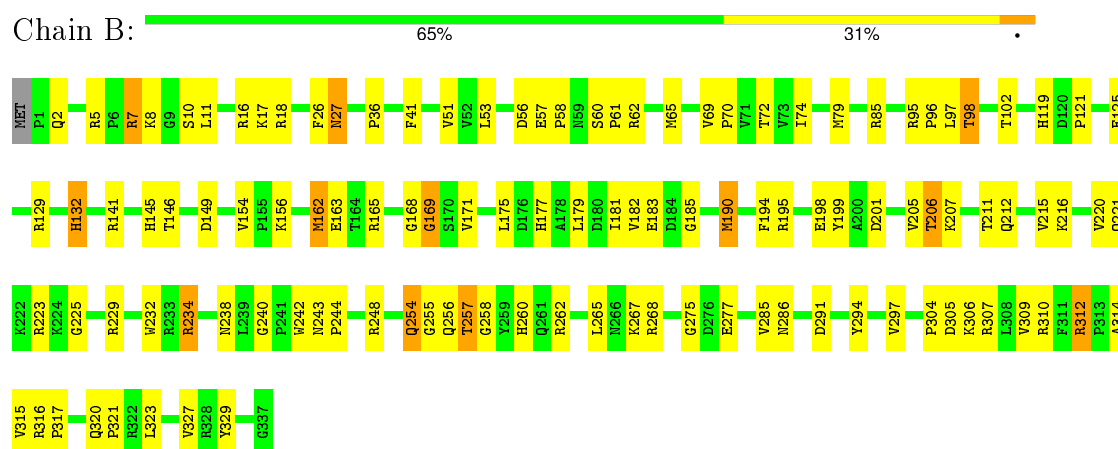
### 3 Residue-property plots

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

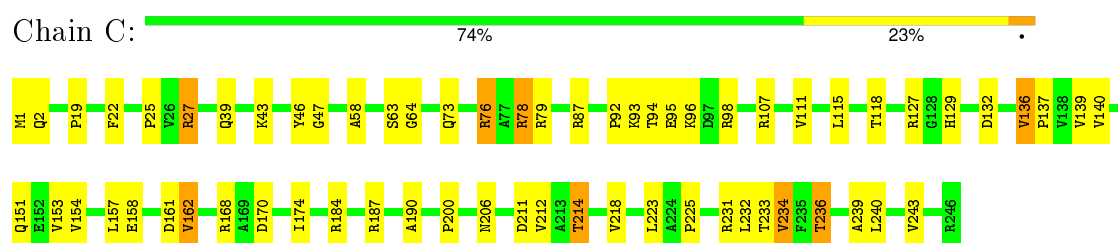
- Molecule 1: 50S ribosomal protein L2P



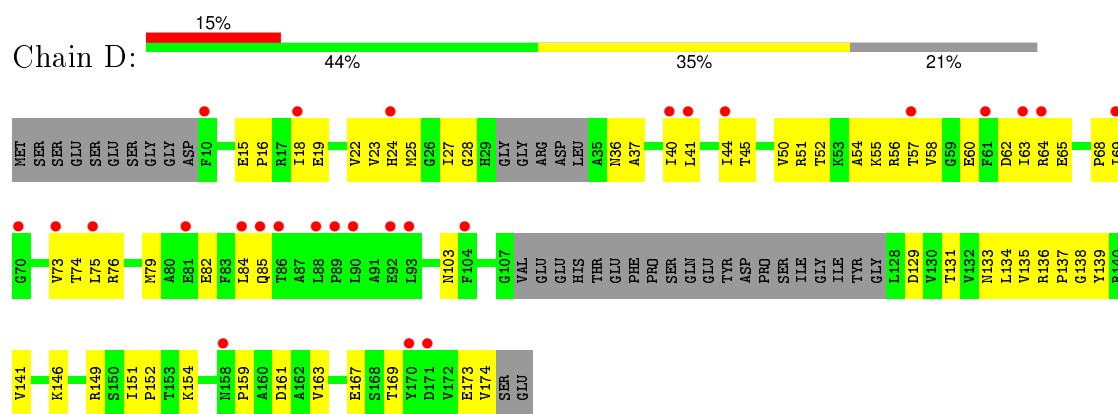
- Molecule 2: 50S ribosomal protein L3P



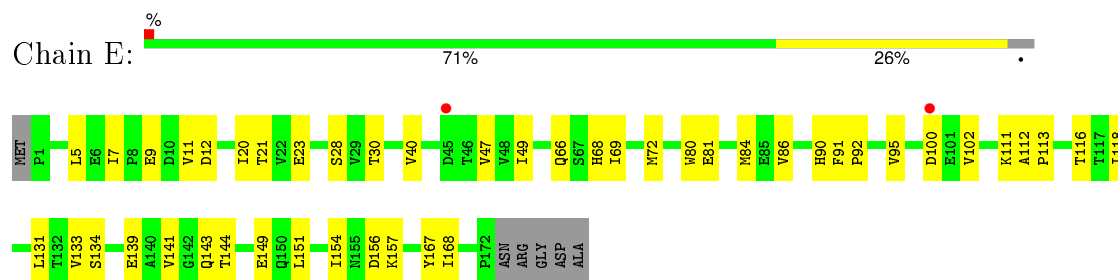
- Molecule 3: 50S ribosomal protein L4P



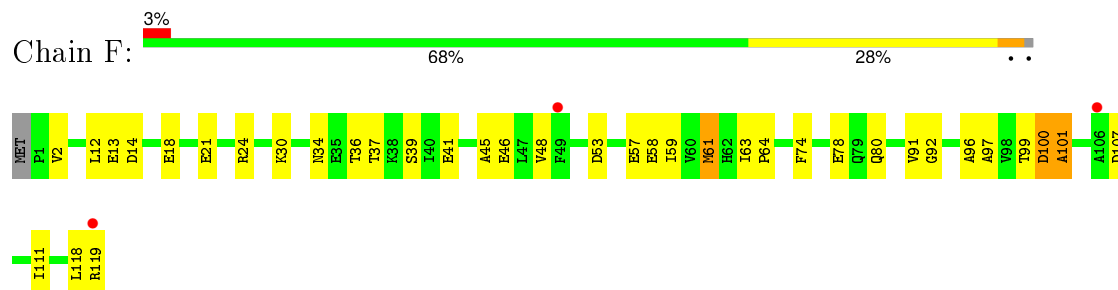
- Molecule 4: 50S ribosomal protein L5P



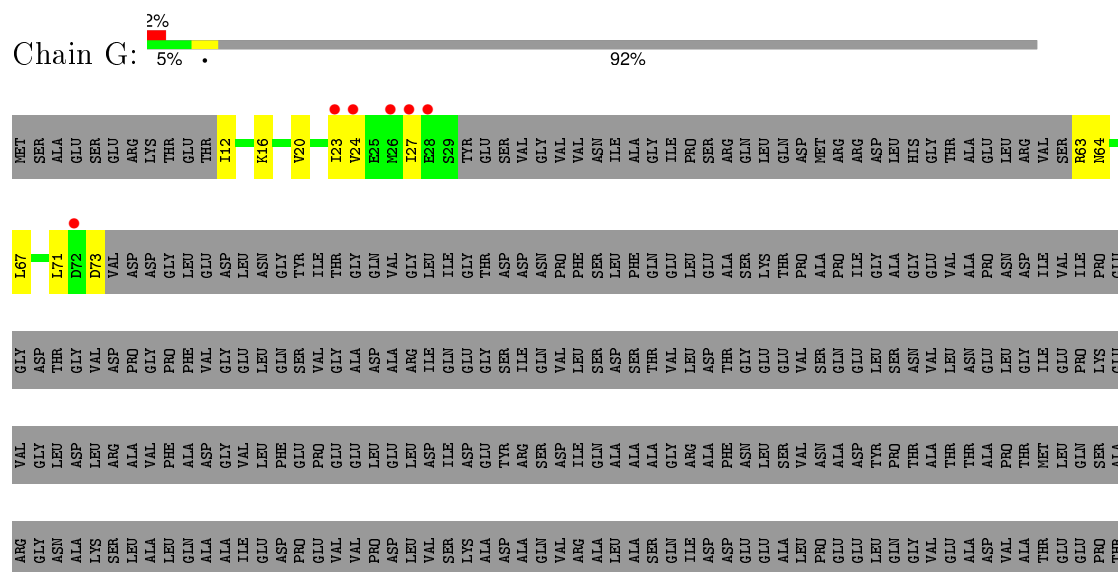
- Molecule 5: 50S ribosomal protein L6P



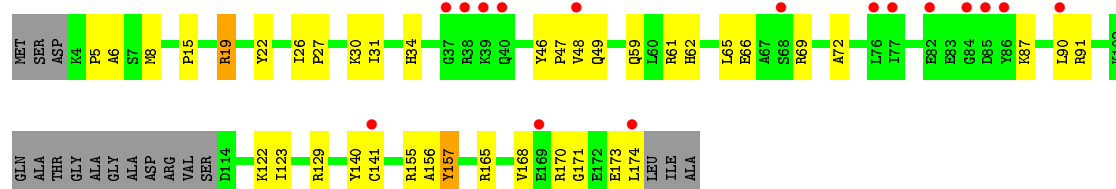
- Molecule 6: 50S ribosomal protein L7Ae



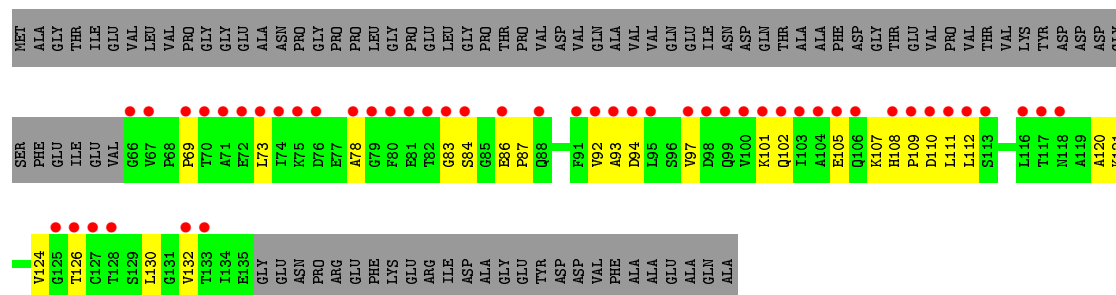
- Molecule 7: 50S ribosomal protein L10E



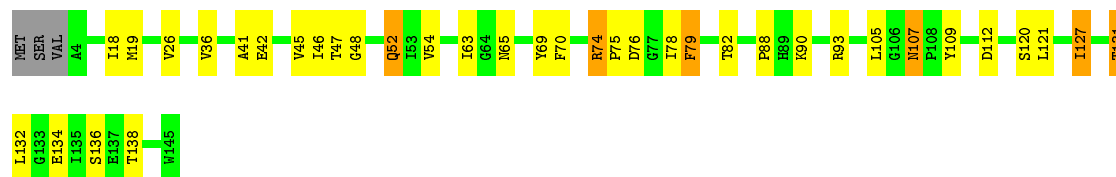
- Molecule 8: 50S ribosomal protein L10e



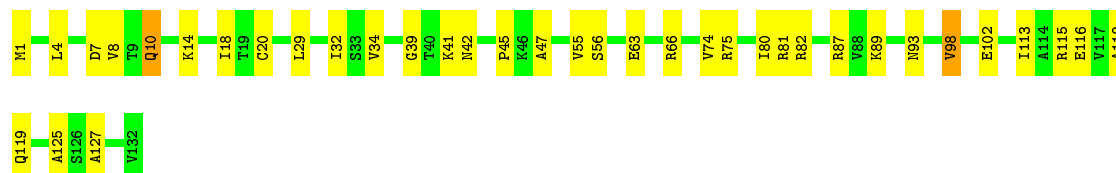
- Molecule 9: 50S ribosomal protein L11P



- Molecule 10: 50S ribosomal protein L13P

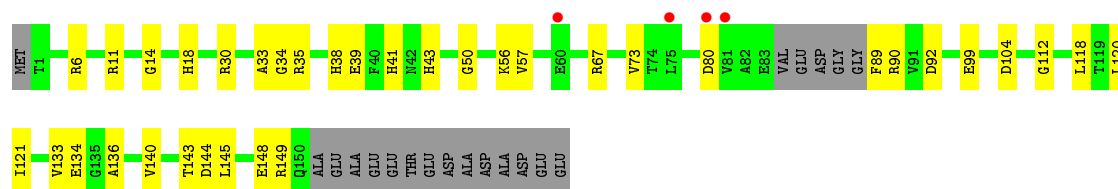


- Molecule 11: 50S ribosomal protein L14P



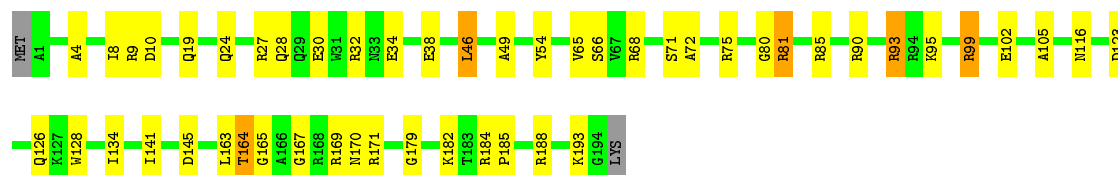
- Molecule 12: 50S ribosomal protein L15P





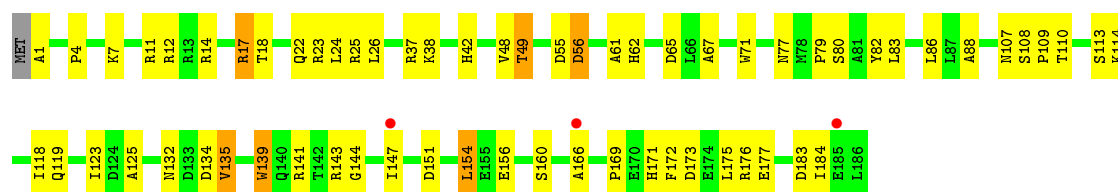
- Molecule 13: 50S ribosomal protein L15e

Chain M: 73% 23% ..



- Molecule 14: 50S ribosomal protein L18P

Chain N: 2% 65% 31% ..



- Molecule 15: 50S ribosomal protein L18e

Chain O: 84% 16% .



- Molecule 16: 50S ribosomal protein L19e

Chain P: 81% 13% ..



- Molecule 17: 50S ribosomal protein L21e

Chain Q: 81% 16% ..

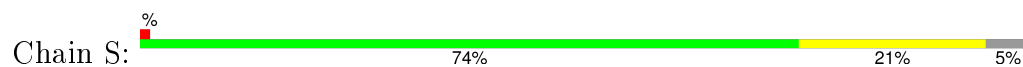


- Molecule 18: 50S ribosomal protein L22P

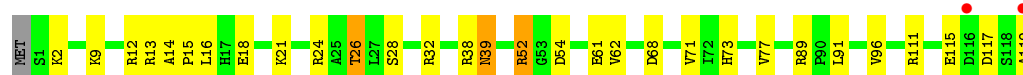
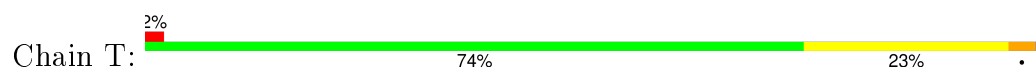
Chain R: 70% 24% ..



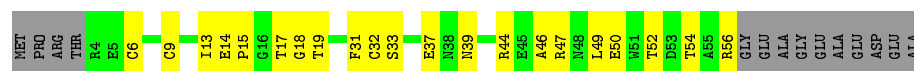
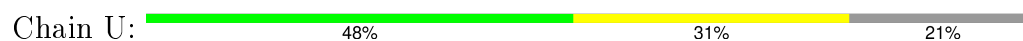
- Molecule 19: 50S ribosomal protein L23P



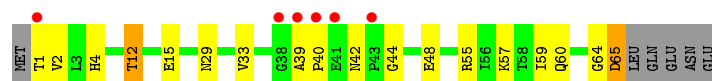
- Molecule 20: 50S ribosomal protein L24P



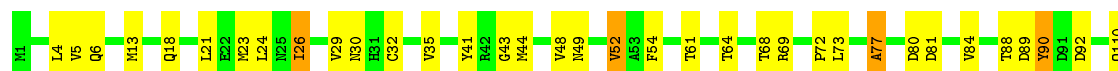
- Molecule 21: 50S ribosomal protein L24e



- Molecule 22: 50S ribosomal protein L29P



- Molecule 23: 50S ribosomal protein L30P

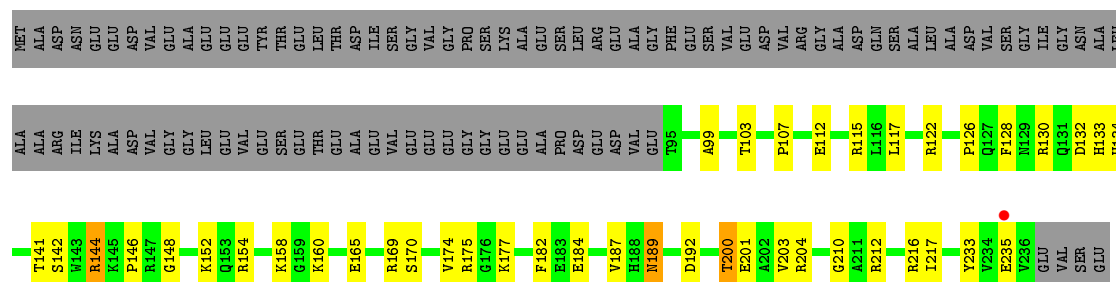


- Molecule 24: 50S ribosomal protein L31e

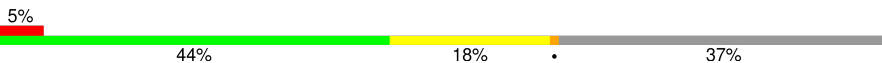


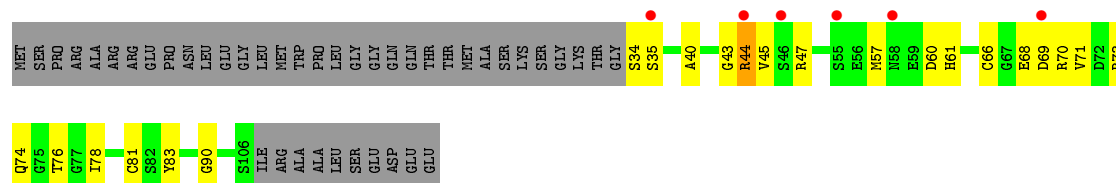
- Molecule 25: 50S ribosomal protein L32e

Chain Y: 



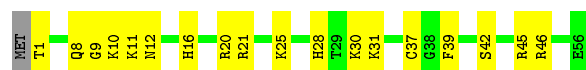
- Molecule 26: 50S ribosomal protein L37Ae

Chain Z: 



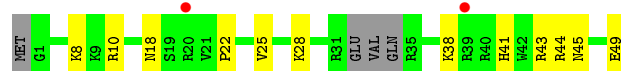
- Molecule 27: 50S ribosomal protein L37e

Chain 1: 



- Molecule 28: 50S ribosomal protein L39e

Chain 2: 



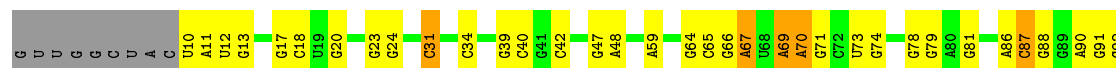
- Molecule 29: 50S ribosomal protein L44E

Chain 3: 



- Molecule 30: 23S RIBOSOMAL RNA

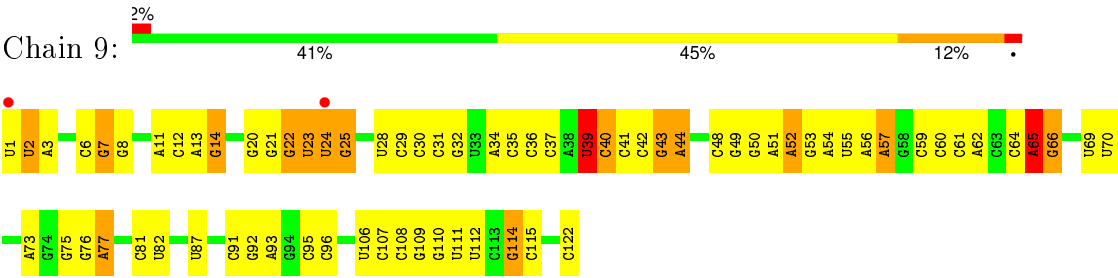
Chain 0: 



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C1483	C1394	G1214	G1151	U1041	G960	G869	C765	G661	U170	U170	G350	G264	U170	A95
G1484	C1395	G1215	A1152	U1042	A961	G870	C766	G662	G564	A466	G358	U265	C171	A96
C1492	C1396	G1216	G1153	U1043	C962	G871	C767	G663	U567	G467	G358	C271	A177	G97
A1493	C1397	U1218	G1154	C1044	G963	U872	C768	A671	C570	U470	U364	A272	U178	A98
A1494	C1398	U1219	G1155	G1045	G964	U873	C769	G672	C571	U471	G365	G273	C179	A99
C1495	C1399	G1221	G1156	U1046	G965	U874	C770	A673	G574	G482	G366	U277	G182	C100
G1496	C1400	G1222	G1157	U1047	G966	U875	C771	C677	A575	U482	U366	U278	U179	A102
G1497	G1401	G1223	G1158	U1048	G967	U876	C772	C678	G576	G483	G367	A279	G183	A106
C1498	G1402	G1224	G1159	U1049	G968	U877	C773	C679	A577	U483	U368	C280	A186	U107
A1499	A1403	G1225	G1160	U1050	G969	U878	C774	C680	A578	U484	G368	C281	A187	C111
G1500	A1404	G1226	G1161	U1051	G970	U879	C775	C681	A579	U485	G369	C282	A188	G112
C1501	A1405	G1227	G1162	U1052	G971	U880	C776	C682	A580	U486	G370	C283	A189	A113
A1502	A1406	G1228	G1163	U1053	G972	U881	C777	C683	A581	U487	G371	C284	A190	A114
C1503	A1407	G1229	G1164	U1054	G973	U882	C778	C684	A582	U488	G372	A285	A191	U115
A1504	A1408	G1230	G1165	U1055	G974	U883	C779	C685	A583	U489	G373	U286	A192	C119
U1505	A1409	G1231	G1166	U1056	G975	U884	C780	C686	A584	U490	G374	C287	A193	A116
U1506	A1410	G1232	G1167	U1057	G976	U885	C781	C687	A585	U491	G375	C288	A194	A117
C1507	A1411	G1233	G1168	U1058	G977	U886	C782	C688	A586	U492	G376	C289	A195	A118
U1511	A1412	G1234	G1169	U1059	G978	U887	C783	C689	A587	U493	G377	C290	A196	U121
G1512	A1413	G1235	U1170	U1060	G979	U888	C784	C690	A588	U494	G378	C291	A197	U122
C1513	A1414	G1236	U1171	U1061	G980	U889	C785	C691	A589	U495	G379	C292	A198	U123
G1514	A1415	G1237	U1172	U1062	G981	U890	C786	C692	A590	U496	G380	C293	A199	U124
A1515	A1416	G1238	U1173	U1063	G982	U891	C787	C693	A591	U497	G381	C294	A200	C120
C1516	A1417	G1239	U1174	U1064	G983	U892	C788	C694	A592	U498	G382	C295	A201	G124
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G1520	A1419	G1241	U1176	U1066	G985	U894	C790	C696	A594	U500	G384	C297	A203	C
C1521	A1420	G1242	U1177	U1067	G986	U895	C791	C697	A595	U501	G385	C298	A204	U
A1522	A1421	G1243	U1178	U1068	G987	U896	C792	C698	A596	U502	G386	C299	A205	A128
G1523	A1422	G1244	U1179	U1069	G988	U897	C793	C699	A597	U503	G387	C300	A206	A129
C1524	A1423	G1245	U1180	U1070	G989	U898	C794	C700	A598	U504	G388	C301	A207	C130
A1525	A1424	G1246	U1181	U1071	G990	U899	C795	C701	A599	U505	G389	C302	A208	
C1526	A1425	G1247	U1182	U1072	G991	U900	C796	C702	A600	U506	G390	C303	A209	
A1527	A1426	G1248	U1183	U1073	G992	U901	C797	C703	A601	U507	G391	C304	A210	
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	A1448	G1270	U1205	U1095	G1014	U923	C819	C725	A623	U529	G413	C326	A232	
	A1449	G1271	U1206	U1096	G1015	U924	C820	C726	A624	U530	G414	C327	A233	
	A1450	G1272	U1207	U1097	G1016	U925	C821	C727	A625	U531	G415	C328	A234	
	A1451	G1273	U1208	U1098	G1017	U926	C822	C728	A626	U532	G416	C329	A235	
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	A1477	G1299	U1234	U1124	G1043	U952	C848	C754	A652	U558	G442	C355	A261	
	A1478	G1300	U1235	U1125	G1044	U953	C849	C755	A653	U559	G443	C356	A262	

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A2783	G2592	U2499	U2499	U2411	G2324	U	A	A2100	U1977	U1897	G1805	C1714	C1623
A2784	C2593	C2502	C2502	G2412	U2325	C	C	A2101	A1978	G1902	G1815	C1715	C1624
C2787	U2594	A2503	A2503	A2413	C2326	G	A	A2103	A1994	U1903	A1815	A1716	U1625
A2880	G2595	A2504	A2504	A2414	G2328	A	A	C2104	A1995	A1904	C1818	A1717	A1626
C2881	A2697	U2597	A2506	A2415	C2329	G	G	C2105	U1996	U1905	G1819	U1722	G1627
G2882	G2698	U2598	G2507	G2416	U2330	U	U	C2106	U2004	A1909	G1820	G1723	A1632
A2890	C2698	A2599	G2507	G2416	C2331	C	C	G2110	G2005	A1919	G1823	U1724	C1633
C2893	U2710	A2600	C2508	U2419	G2336	A	A	G2111	C2006	C1920	G1824	G1730	U1635
C2894	U2711	A2601	A2509	G2420	C2337	G	C	C2112	A2011	A1922	A1829	A1732	A1641
A2896	G2712	G2602	C2510	G2421	G2338	A	U	C2122	U2012	G1923	C1830	A1733	A1642
C2897	G2713	U2607	A2511	U2422	C2344	C	C	G2128	G1925	G1926	C1834	C1735	G1649
A2898	U2714	C2608	A2512	G2426	A	C	G	U2116	U2008	A1921	U1835	A1739	C1650
A2899	G2715	C2608	A2513	G2426	C	C	C	G2121	G2009	A1922	U1835	U1740	C1653
G2900	G2716	U2514	U2514	C2432	A	A	C	C2122	A2011	A1924	C1839	U1741	C1652
A2902	C2717	C2515	G2516	A2433	G	U	U	U2115	U2012	G1925	U1840	A1742	U1654
C2903	G2718	U2615	G2516	A2434	A2345	C	C	U2116	G2013	G1926	C1841	A1746	G1655
U2904	C2720	G2616	A2521	U2435	C2346	G	C	U2133	U2016	A1927	A1845	A1755	A1664
A2908	G2810	G2630	G2524	G2438	C2347	C	C	G2134	U2017	A1931	U1846	G1756	G1665
G2909	A2811	G2723	G2525	C2439	C2348	C	C	A2135	A2022	G1932	A1847	A1759	C1666
A2913	A2813	G2726	G2526	C2443	A2353	C	C	G2136	C2026	C1936	C1841	A1766	A1667
A2914	A2814	A2635	U2527	U2444	A2354	C	C	A	U2027	C1940	A1845	A1767	U1668
A	G	A2636	U2527	U2445	G2359	C	C	C	U2032	A1941	U1846	A1768	C1675
C	C	C2533	C2534	G2446	G2360	C	C	G	C2033	A1942	G1848	C1762	G1676
C	C	U2535	U2535	G2453	A2361	C	C	C	U2034	C1943	U1850	C1763	U1677
A	A	G2537	G2537	G2456	A2362	A	A	U	A2039	G1946	A1852	A1769	C1679
C	C	C2541	U2541	U2457	G2363	C	C	C	A2039	G1947	A1853	U1766	A1681
A	A	G2542	G2542	U2461	A2364	C	C	C	G2044	G1948	A1854	A1767	C1680
U	U	G2543	G2543	G2462	A2367	A	A	C	G2050	U	C1855	A1768	G1681
G2754	C2654	G2544	G2544	G2462	A2369	C	C	A	A2054	A	A1856	C1769	C1682
G2755	C2654	C2547	C2547	A2465	G2371	G	G	U	U2064	A	A1857	U1770	A1682
U2756	C2654	G2548	G2548	A2467	A2372	U	U	C	C2065	A	A1858	C1769	C1680
A2664	A	C2552	C2552	A2468	G2373	G	G	C	U2065	U	C1861	C1769	C1681
A	A	A2553	A2553	C2472	G2374	C	C	A	C2065	U	C1862	U1770	A1682

• Molecule 31: 5S RIBOSOMAL RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.76 Å   299.27 Å   574.37 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	49.99 – 2.80 85.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.99-2.80) 93.0 (85.47-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.179   ,   0.223 0.172   ,   0.211	Depositor DCC
$R_{free}$ test set	4353 reflections (1.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 69.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 667168 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, 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	0/1786	0.65	0/2408
2	B	0.33	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.63	0/2552
4	D	0.32	0/1111	0.55	0/1498
5	E	0.32	0/1382	0.58	0/1880
6	F	0.33	0/901	0.57	0/1224
7	G	0.30	0/241	0.48	0/324
8	H	0.33	0/1302	0.61	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.36	0/1136	0.59	0/1530
11	K	0.35	0/1004	0.67	0/1351
12	L	0.32	0/1130	0.63	0/1509
13	M	0.34	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.62	0/1999
15	O	0.33	0/874	0.58	0/1181
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.34	0/749	0.66	0/1005
18	R	1.26	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.33	0/648	0.57	0/875
20	T	0.33	0/958	0.64	1/1289 (0.1%)
21	U	0.34	0/417	0.57	0/562
22	V	0.31	0/502	0.51	0/675
23	W	0.34	0/1219	0.62	0/1655
24	X	0.34	0/664	0.60	0/895
25	Y	0.36	0/1146	0.63	0/1536
26	Z	0.35	0/584	0.59	0/781
27	1	0.39	0/438	0.61	0/578
28	2	0.34	0/401	0.59	0/529
29	3	0.37	0/771	0.57	0/1024
30	0	0.37	0/65953	0.69	16/102860 (0.0%)
31	9	0.31	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98697 (0.0%)	0.67	24/147579 (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
18	R	1	0
23	W	0	1
30	0	1	34
31	9	0	3
All	All	2	38

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.61	2.88	1.50
18	R	150	PRO	CA-C	-17.92	1.17	1.52
18	R	150	PRO	CG-CD	13.88	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.29	1.66	1.47
18	R	150	PRO	N-CD	10.71	1.62	1.47
18	R	150	PRO	CA-CB	7.49	1.68	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.50	55.74	112.00
18	R	150	PRO	N-CA-C	-19.33	61.84	112.10
18	R	150	PRO	CA-N-CD	12.33	128.96	111.70
18	R	150	PRO	N-CA-CB	10.99	116.49	103.30
30	0	2482	C	C2'-C3'-O3'	9.28	129.92	109.50
18	R	150	PRO	CA-C-O	-8.60	99.56	120.20
30	0	1942	A	C5'-C4'-C3'	6.99	127.19	116.00
30	0	1120	U	C5'-C4'-C3'	-6.55	105.51	116.00
30	0	871	G	C5'-C4'-O4'	-6.46	101.35	109.10
18	R	150	PRO	CA-CB-CG	-6.22	92.19	104.00
30	0	1504	A	C1'-O4'-C4'	-6.12	105.00	109.90
31	9	39	U	N1-C1'-C2'	5.91	121.68	114.00
30	0	1592	G	N9-C1'-C2'	5.58	121.26	114.00
30	0	1504	A	N9-C1'-C2'	5.43	121.06	114.00
30	0	2316	G	C5'-C4'-C3'	-5.42	107.33	116.00
30	0	2467	A	C1'-O4'-C4'	-5.41	105.58	109.90
20	T	52	ARG	N-CA-C	5.27	125.23	111.00
30	0	2726	U	N1-C1'-C2'	5.25	120.82	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1878	G	N9-C1'-C2'	-5.20	106.29	112.00
30	0	2482	C	C4'-C3'-O3'	5.19	123.38	113.00
30	0	841	A	C1'-O4'-C4'	-5.16	105.77	109.90
30	0	1942	A	C1'-O4'-C4'	-5.06	105.85	109.90
30	0	1829	A	N9-C1'-C2'	-5.05	106.44	112.00
30	0	2313	C	O4'-C4'-C3'	-5.01	98.99	104.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA
30	0	2482	C	C3'

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1300	G	Sidechain
30	0	1309	U	Sidechain
30	0	1417	G	Sidechain
30	0	1592	G	Sidechain
30	0	1771	U	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1861	C	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1970	G	Sidechain
30	0	1972	U	Sidechain
30	0	1979	G	Sidechain
30	0	221	G	Sidechain
30	0	2412	G	Sidechain
30	0	246	G	Sidechain
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2524	G	Sidechain
30	0	2552	C	Sidechain
30	0	2607	U	Sidechain
30	0	2673	U	Sidechain
30	0	2842	G	Sidechain
30	0	396	U	Sidechain

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Mol	Chain	Res	Type	Group
30	0	458	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	795	G	Sidechain
30	0	817	G	Sidechain
30	0	888	U	Sidechain
30	0	900	U	Sidechain
31	9	39	U	Sidechain
31	9	65	A	Sidechain
31	9	87	U	Sidechain
23	W	90	TYR	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	1753	0	1766	71	0
2	B	2625	0	2533	100	0
3	C	1860	0	1813	58	0
4	D	1094	0	1085	44	0
5	E	1357	0	1266	32	0
6	F	890	0	843	30	0
7	G	240	0	231	9	0
8	H	1282	0	1292	33	0
9	I	519	0	500	23	0
10	J	1120	0	1098	38	0
11	K	994	0	1027	35	0
12	L	1118	0	1076	28	0
13	M	1558	0	1573	45	0
14	N	1445	0	1401	57	0
15	O	865	0	873	19	0
16	P	1136	0	1123	18	0
17	Q	735	0	729	16	0
18	R	1149	0	1122	38	0
19	S	641	0	605	16	0
20	T	950	0	924	22	0
21	U	410	0	364	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	V	499	0	511	14	0
23	W	1196	0	1137	48	0
24	X	654	0	653	16	0
25	Y	1130	0	1133	38	0
26	Z	573	0	531	21	0
27	1	431	0	426	23	0
28	2	396	0	413	14	0
29	3	755	0	728	25	0
30	0	59017	0	29810	1217	0
31	9	2599	0	1325	89	0
32	0	84	0	0	0	0
32	9	2	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	9	0	0	1	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	3	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	92	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	J	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5933	0	0	188	0
38	1	56	0	0	4	0
38	2	38	0	0	0	0
38	3	65	0	0	4	0
38	9	144	0	0	9	0
38	A	110	0	0	6	0
38	B	144	0	0	18	0
38	C	178	0	0	14	0
38	D	45	0	0	3	0
38	E	43	0	0	2	0
38	F	27	0	0	2	0
38	G	17	0	0	0	0
38	H	69	0	0	8	0
38	I	6	0	0	0	0
38	J	53	0	0	2	0
38	K	56	0	0	3	0
38	L	92	0	0	6	0
38	M	129	0	0	4	0
38	N	63	0	0	6	0
38	O	40	0	0	2	0
38	P	66	0	0	1	0
38	Q	46	0	0	1	0
38	R	76	0	0	2	0
38	S	39	0	0	4	0
38	T	35	0	0	3	0
38	U	28	0	0	3	0
38	V	13	0	0	0	0
38	W	69	0	0	5	0
38	X	27	0	0	2	0
38	Y	91	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Z	25	0	0	3	0
All	All	99119	0	59911	2035	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 14.

All (2035) 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.43
30:0:1160:G:C5'	30:0:1161:A:H5'	1.74	1.16
31:9:56:A:H2'	31:9:57:A:H5''	1.20	1.16
30:0:1160:G:H5'	30:0:1161:A:C5'	1.77	1.14
14:N:37:ARG:NH1	31:9:6:C:H5''	1.62	1.14
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.32	1.10
15:O:3:THR:HG22	30:0:656:G:H5'	1.30	1.10
31:9:76:G:H3'	31:9:77:A:H5''	1.32	1.09
30:0:871:G:C8	30:0:871:G:H5'	1.87	1.08
10:J:82:THR:HG23	30:0:1242:A:H5'	1.37	1.07
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.06
30:0:381:G:H5''	38:0:4318:HOH:O	1.55	1.05
30:0:545:G:H8	30:0:545:G:H5'	1.19	1.04
30:0:871:G:H8	30:0:871:G:H5'	1.18	1.03
13:M:171:ARG:HD3	30:0:156:C:H5''	1.41	1.01
30:0:2717:C:C2'	30:0:2718:C:H5''	1.90	1.01
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.78	0.98
30:0:1118:A:H3'	30:0:1118:A:H8	1.28	0.98
30:0:1187:U:HO2'	30:0:1189:A:H2	1.00	0.97
30:0:2717:C:H2'	30:0:2718:C:H5''	1.44	0.97
4:D:154:LYS:HD2	4:D:154:LYS:H	1.28	0.97
30:0:1666:C:O2'	30:0:1667:A:H5''	1.65	0.96
16:P:115:SER:H	16:P:118:GLN:HE21	1.11	0.95
30:0:1603:A:H5'	30:0:1605:G:O4'	1.67	0.95
2:B:238:ASN:HD22	2:B:240:GLY:H	1.15	0.94
31:9:56:A:C2'	31:9:57:A:H5''	1.96	0.94
30:0:1474:C:H6	30:0:1474:C:H5'	1.32	0.94
30:0:1701:A:H4'	30:0:1702:U:H5''	1.47	0.94
15:O:3:THR:CG2	30:0:656:G:H5'	1.96	0.94
11:K:10:GLN:H	11:K:10:GLN:HE21	1.03	0.94
22:V:1:THR:HB	30:0:93:C:H5''	1.49	0.93
30:0:1372:A:H3'	38:0:7212:HOH:O	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:164:THR:HG22	13:M:167:GLY:H	1.31	0.93
30:0:1118:A:H3'	30:0:1118:A:C8	2.03	0.93
3:C:236:THR:HG22	3:C:239:ALA:H	1.35	0.92
30:0:542:A:H5'	30:0:542:A:H8	1.35	0.91
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.13	0.91
30:0:545:G:C8	30:0:545:G:H5'	2.06	0.90
30:0:1701:A:H5'	38:0:6304:HOH:O	1.70	0.90
30:0:1835:U:H5	30:0:1840:A:N7	1.69	0.90
30:0:1166:A:H61	30:0:1180:U:H3	1.15	0.90
31:9:29:C:H2'	31:9:30:C:H5'	1.55	0.89
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.89
30:0:1160:G:H5'	30:0:1161:A:H5'	0.90	0.89
30:0:182:G:H5'	38:0:5167:HOH:O	1.71	0.89
30:0:541:C:H2'	30:0:542:A:H5''	1.55	0.89
30:0:541:C:C2'	30:0:542:A:H5''	2.03	0.89
30:0:871:G:C5'	30:0:871:G:H8	1.87	0.88
30:0:506:G:H22	30:0:509:A:C5'	1.85	0.88
30:0:2291:A:C8	30:0:2309:C:H5'	2.09	0.87
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.21	0.87
30:0:2783:A:H3'	38:0:5241:HOH:O	1.75	0.87
30:0:1118:A:H62	30:0:1244:U:H3	1.21	0.86
30:0:2908:A:H2'	30:0:2909:G:O4'	1.74	0.86
30:0:1474:C:C6	30:0:1474:C:H5'	2.11	0.86
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.57	0.86
30:0:282:C:H1'	30:0:368:C:N4	1.90	0.86
30:0:282:C:O2'	30:0:283:U:H5'	1.76	0.86
30:0:1116:U:HO2'	30:0:1118:A:H2	0.86	0.85
14:N:113:SER:HB2	38:N:8855:HOH:O	1.75	0.85
30:0:2586:U:H3	30:0:2592:G:H22	1.22	0.85
30:0:2506:A:HO2'	30:0:2507:G:H8	0.90	0.85
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.58	0.85
30:0:1165:G:H1'	30:0:1174:A:H1'	1.60	0.83
30:0:1666:C:C2'	30:0:1667:A:H5''	2.08	0.83
30:0:558:C:C2'	30:0:559:U:H5''	2.08	0.83
11:K:39:GLY:HA2	38:0:5229:HOH:O	1.79	0.83
30:0:1183:C:H2'	38:0:6261:HOH:O	1.77	0.83
30:0:541:C:H2'	30:0:542:A:C5'	2.08	0.83
28:2:41:HIS:H	28:2:45:ASN:HD22	1.25	0.83
30:0:2896:A:H5''	38:0:6117:HOH:O	1.77	0.83
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.58	0.83
30:0:1878:G:H1'	38:0:6139:HOH:O	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1189:A:H1'	30:0:1209:C:O4'	1.79	0.82
30:0:2812:A:H2	30:0:2814:A:H62	1.22	0.82
31:9:23:U:O2'	31:9:24:U:H4'	1.78	0.82
30:0:1184:C:H1'	38:0:7491:HOH:O	1.80	0.82
30:0:1116:U:O2'	30:0:1118:A:H2	1.63	0.82
30:0:1116:U:H3	30:0:1246:A:H62	1.27	0.81
30:0:1206:U:H6	30:0:1206:U:H5'	1.44	0.81
30:0:69:A:H5'	30:0:69:A:C8	2.15	0.81
1:A:199:HIS:HD2	1:A:201:PHE:H	1.28	0.81
8:H:30:LYS:H	8:H:62:HIS:HD2	1.28	0.81
30:0:1634:G:H3'	38:0:3895:HOH:O	1.79	0.81
30:0:396:U:H1'	38:0:7650:HOH:O	1.80	0.81
1:A:223:ARG:HH12	30:0:2270:G:H4'	1.46	0.81
31:9:49:G:H5''	38:9:9087:HOH:O	1.80	0.81
30:0:2502:C:C2'	30:0:2503:A:H5'	2.11	0.81
30:0:2005:G:H3'	30:0:2005:G:OP2	1.82	0.80
30:0:1300:G:H1'	38:0:4687:HOH:O	1.81	0.80
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.64	0.80
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.63	0.80
30:0:1119:G:N2	30:0:1246:A:C2	2.49	0.80
30:0:1667:A:H8	30:0:1667:A:H5'	1.47	0.80
30:0:1120:U:H5'	30:0:1121:G:OP2	1.82	0.80
23:W:88:THR:HB	38:W:6679:HOH:O	1.81	0.80
30:0:1666:C:H2'	30:0:1667:A:H5'	1.63	0.80
31:9:14:G:H5'	31:9:14:G:H8	1.48	0.79
30:0:1205:U:H2'	30:0:1206:U:C5'	2.12	0.79
30:0:506:G:H22	30:0:509:A:H5''	1.48	0.79
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.63	0.79
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.27	0.79
30:0:380:A:H2'	38:0:7250:HOH:O	1.83	0.79
30:0:1666:C:H2'	30:0:1667:A:C5'	2.12	0.79
30:0:877:G:H5'	30:0:878:G:OP1	1.83	0.79
30:0:2637:A:H5'	38:0:9273:HOH:O	1.83	0.79
8:H:168:VAL:HG13	38:H:8556:HOH:O	1.83	0.78
30:0:2506:A:O2'	30:0:2507:G:H8	1.65	0.78
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.47	0.78
30:0:69:A:H5'	30:0:69:A:H8	1.49	0.78
30:0:2502:C:H2'	30:0:2503:A:H5'	1.64	0.78
30:0:2004:U:H4'	38:0:5316:HOH:O	1.84	0.78
30:0:2769:C:C2'	30:0:2770:G:H5'	2.14	0.78
30:0:1183:C:N4	30:0:1184:C:H41	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:603:A:H5''	30:0:604:G:OP1	1.84	0.78
30:0:1278:A:H4'	30:0:1279:U:C4	2.19	0.78
30:0:31:C:H2'	38:0:7711:HOH:O	1.84	0.78
3:C:1:MET:HG2	3:C:2:GLN:H	1.48	0.78
30:0:2748:G:H1'	38:0:7918:HOH:O	1.84	0.78
30:0:2756:U:H3	30:0:2896:A:H2	1.31	0.78
30:0:2748:G:H5'	38:0:7565:HOH:O	1.82	0.78
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.66	0.78
30:0:236:A:H4'	30:0:237:G:H5'	1.66	0.78
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.78
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.18	0.77
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.65	0.77
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.83	0.77
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.48	0.77
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.67	0.77
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.65	0.77
30:0:1180:U:H1'	38:0:3238:HOH:O	1.85	0.76
4:D:25:MET:HE2	4:D:41:LEU:HG	1.65	0.76
38:C:8665:HOH:O	30:0:2100:A:H5'	1.85	0.76
30:0:283:U:H5	30:0:284:C:N3	1.83	0.76
30:0:558:C:O2'	30:0:559:U:H5''	1.85	0.76
30:0:1603:A:H5''	30:0:1605:G:H5'	1.67	0.76
20:T:61:GLU:HG2	38:T:3851:HOH:O	1.84	0.76
30:0:1641:A:H2'	30:0:1642:A:H5'	1.64	0.76
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.66	0.76
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.67	0.76
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.67	0.76
30:0:1201:C:H5''	38:0:6251:HOH:O	1.84	0.76
25:Y:200:THR:HG22	25:Y:201:GLU:HG3	1.66	0.76
30:0:1189:A:H3'	38:0:7703:HOH:O	1.85	0.76
30:0:130:C:H2'	38:0:3163:HOH:O	1.85	0.75
30:0:1973:A:H8	30:0:1973:A:H5'	1.51	0.75
30:0:2768:A:O2'	30:0:2769:C:H5'	1.86	0.75
30:0:1118:A:C8	30:0:1118:A:C3'	2.68	0.75
22:V:1:THR:HG23	22:V:2:VAL:H	1.50	0.75
30:0:31:C:H4'	38:0:7449:HOH:O	1.86	0.75
30:0:2717:C:O2'	30:0:2718:C:H5''	1.86	0.75
30:0:2638:G:H5'	38:0:4938:HOH:O	1.86	0.75
2:B:206:THR:HG21	30:0:2716:G:H5''	1.69	0.75
30:0:2578:G:H5'	30:0:2578:G:H8	1.52	0.74
30:0:506:G:H22	30:0:509:A:H5'	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2507:G:H2'	30:0:2510:C:H42	1.52	0.74
30:0:567:U:H5''	38:0:6425:HOH:O	1.86	0.74
30:0:1175:G:H1'	30:0:1193:A:H2'	1.68	0.74
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.49	0.74
2:B:162:MET:HG3	2:B:310:ARG:NH1	2.02	0.74
30:0:255:A:H2'	30:0:256:C:H6	1.51	0.74
14:N:37:ARG:HH12	31:9:6:C:H5''	1.49	0.74
30:0:2768:A:H5''	38:0:4425:HOH:O	1.88	0.74
30:0:871:G:C8	30:0:871:G:C5'	2.64	0.74
30:0:1172:G:H5''	38:0:7282:HOH:O	1.87	0.74
31:9:92:G:H2'	31:9:93:A:C8	2.23	0.73
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.28	0.73
30:0:2748:G:H2'	38:0:7565:HOH:O	1.88	0.73
30:0:619:U:H3'	38:0:3286:HOH:O	1.88	0.73
30:0:564:G:H1'	38:0:6331:HOH:O	1.88	0.73
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.68	0.73
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.03	0.73
10:J:47:THR:HB	38:0:4845:HOH:O	1.89	0.73
30:0:558:C:H2'	30:0:559:U:C5'	2.17	0.73
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.87	0.73
30:0:2769:C:O2'	30:0:2770:G:H5'	1.89	0.73
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.69	0.73
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.68	0.73
30:0:1441:G:O2'	30:0:1442:A:H5'	1.88	0.73
30:0:281:U:H2'	30:0:282:C:O4'	1.89	0.73
31:9:20:G:O2'	31:9:21:G:H5'	1.89	0.73
1:A:199:HIS:CD2	1:A:201:PHE:H	2.05	0.73
14:N:144:GLY:O	14:N:147:ILE:HG22	1.88	0.72
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.55	0.72
21:U:14:GLU:O	21:U:17:THR:HB	1.90	0.72
30:0:1183:C:H42	30:0:1184:C:H41	1.37	0.72
38:Y:8907:HOH:O	30:0:1330:A:H5''	1.89	0.72
30:0:1666:C:C2'	30:0:1667:A:C5'	2.67	0.72
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.72	0.72
18:R:128:ARG:NH2	30:0:2054:A:N3	2.38	0.72
30:0:2498:C:O2'	30:0:2499:U:H5'	1.90	0.71
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.56	0.71
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.04	0.71
16:P:117:SER:HB3	30:0:1593:C:OP1	1.90	0.71
31:9:2:U:OP2	31:9:3:A:H5'	1.91	0.71
26:Z:34:SER:N	30:0:797:A:H5'	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1632:A:H2'	30:0:1633:C:H5'	1.72	0.71
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.55	0.71
30:0:1182:C:H1'	30:0:1192:A:H8	1.54	0.71
30:0:544:G:H2'	30:0:545:G:H5''	1.73	0.71
30:0:1947:G:H2'	30:0:1948:G:H8	1.55	0.71
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.73	0.71
11:K:10:GLN:N	11:K:10:GLN:HE21	1.85	0.70
30:0:960:G:H3'	30:0:960:G:N3	2.05	0.70
3:C:139:VAL:HG13	38:C:8650:HOH:O	1.90	0.70
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.72	0.70
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.73	0.70
30:0:1172:G:H1'	38:0:4982:HOH:O	1.91	0.70
13:M:171:ARG:CD	30:0:156:C:H5''	2.19	0.70
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.56	0.70
30:0:1701:A:H4'	30:0:1702:U:C5'	2.20	0.70
30:0:2768:A:H2'	30:0:2769:C:O4'	1.91	0.70
29:3:73:GLU:HB3	38:3:9049:HOH:O	1.91	0.70
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.73	0.69
30:0:1525:G:H5'	30:0:1526:A:OP2	1.92	0.69
30:0:827:A:H1'	38:0:6233:HOH:O	1.92	0.69
15:O:3:THR:HG22	30:0:656:G:C5'	2.15	0.69
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.22	0.69
30:0:1701:A:H5''	30:0:1702:U:H3'	1.73	0.69
30:0:558:C:H2'	30:0:559:U:H5''	1.72	0.69
30:0:870:G:C2'	30:0:871:G:H5''	2.21	0.69
30:0:2717:C:H2'	30:0:2718:C:C5'	2.19	0.69
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.75	0.69
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.39	0.69
30:0:1058:A:H2'	30:0:1060:C:H5''	1.73	0.69
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.57	0.69
30:0:1819:G:H2'	30:0:1820:G:H4'	1.73	0.68
13:M:164:THR:HG22	13:M:167:GLY:N	2.08	0.68
30:0:271:C:H41	30:0:378:A:H2	1.41	0.68
12:L:133:VAL:HA	38:L:8878:HOH:O	1.93	0.68
23:W:26:ILE:HB	38:W:5420:HOH:O	1.92	0.68
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.18	0.68
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.75	0.68
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.76	0.68
30:0:1741:U:H5'	30:0:1742:A:OP1	1.94	0.68
30:0:1679:C:H5'	38:0:9321:HOH:O	1.92	0.68
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1730:G:H5'	30:0:1731:C:C5	2.29	0.68
18:R:150:PRO:O	18:R:150:PRO:CG	2.41	0.68
30:0:255:A:H2'	30:0:256:C:C6	2.29	0.68
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.05	0.67
30:0:2256:G:O2'	30:0:2257:G:H5'	1.94	0.67
2:B:162:MET:HG3	2:B:310:ARG:HH11	1.60	0.67
30:0:2769:C:H2'	30:0:2770:G:H5'	1.75	0.67
30:0:2635:A:O2'	30:0:2636:C:H5'	1.94	0.67
23:W:61:THR:HG23	23:W:151:GLU:HG3	1.76	0.67
30:0:1377:C:H6	30:0:1377:C:H5'	1.59	0.67
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.77	0.67
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.93	0.67
35:0:8813:CL:CL	38:0:4687:HOH:O	2.50	0.67
31:9:39:U:H1'	31:9:44:A:H61	1.60	0.67
30:0:2827:A:H2'	30:0:2828:G:O4'	1.94	0.67
30:0:2135:A:O2'	30:0:2136:G:H5'	1.95	0.67
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.59	0.67
10:J:127:ILE:HG22	35:J:8801:CL:CL	2.31	0.67
12:L:6:ARG:HD3	30:0:1299:G:O6	1.95	0.67
30:0:1189:A:H1'	30:0:1209:C:C1'	2.25	0.66
3:C:27:ARG:NH2	30:0:657:G:OP1	2.28	0.66
3:C:174:ILE:CD1	30:0:338:C:H4'	2.25	0.66
30:0:185:G:H4'	30:0:186:A:OP1	1.94	0.66
31:9:14:G:H5'	31:9:14:G:C8	2.29	0.66
9:I:110:ASP:O	30:0:1163:G:H5'	1.96	0.66
30:0:544:G:C2'	30:0:545:G:H5''	2.25	0.66
30:0:2102:G:C2	30:0:2103:A:C6	2.82	0.66
30:0:1562:C:O2	30:0:1562:C:H2'	1.94	0.66
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.78	0.66
30:0:1205:U:H2'	30:0:1206:U:H5'	1.76	0.66
5:E:143:GLN:NE2	30:0:2779:G:H21	1.93	0.66
30:0:1205:U:H2'	30:0:1206:U:H5''	1.76	0.66
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.78	0.66
10:J:82:THR:CG2	30:0:1242:A:H5'	2.22	0.66
10:J:107:ASN:HD22	10:J:109:TYR:H	1.43	0.66
30:0:2756:U:N3	30:0:2896:A:C2	2.63	0.66
30:0:2787:C:H5	38:0:4636:HOH:O	1.79	0.66
38:B:9099:HOH:O	30:0:2672:C:H1'	1.96	0.66
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.78	0.66
30:0:1171:A:H2'	30:0:1172:G:H5'	1.78	0.65
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2426:G:H1'	38:0:6110:HOH:O	1.95	0.65
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.78	0.65
31:9:76:G:H3'	31:9:77:A:C5'	2.20	0.65
30:0:1159:G:H21	30:0:1189:A:H8	1.43	0.65
12:L:136:ALA:HB3	38:L:8878:HOH:O	1.96	0.65
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.77	0.65
31:9:54:A:O2'	31:9:55:U:H5'	1.97	0.65
16:P:115:SER:H	16:P:118:GLN:NE2	1.89	0.65
30:0:1835:U:C5	30:0:1840:A:N7	2.58	0.65
3:C:174:ILE:HD11	30:0:338:C:H4'	1.78	0.65
30:0:2420:G:O2'	30:0:2421:G:H5'	1.97	0.65
30:0:2795:C:O2'	30:0:2796:U:H5'	1.97	0.65
30:0:138:U:H5''	30:0:139:C:OP2	1.96	0.65
30:0:1947:G:H2'	30:0:1948:G:C8	2.31	0.65
30:0:308:U:H5'	30:0:309:C:OP1	1.96	0.65
14:N:11:ARG:HD3	31:9:114:G:O6	1.97	0.65
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.12	0.65
30:0:2769:C:H2'	30:0:2770:G:C5'	2.26	0.65
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.12	0.64
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.78	0.64
2:B:211:THR:HG23	30:0:2840:A:OP1	1.96	0.64
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.80	0.64
30:0:1165:G:N2	30:0:1173:A:H5''	2.13	0.64
25:Y:204:ARG:HH22	30:0:553:G:P	2.21	0.64
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.97	0.64
30:0:1632:A:C2'	30:0:1633:C:H5'	2.27	0.64
27:1:1:THR:HA	38:0:9354:HOH:O	1.98	0.64
30:0:542:A:H5'	30:0:542:A:C8	2.25	0.64
30:0:2505:G:O2'	30:0:2506:A:H5'	1.97	0.64
30:0:559:U:H5'	30:0:559:U:H6	1.61	0.64
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.28	0.64
30:0:671:A:O2'	30:0:672:G:H2'	1.98	0.64
30:0:1206:U:H2'	30:0:1207:A:O4'	1.96	0.64
1:A:191:GLY:HA2	1:A:194:MET:CE	2.28	0.64
14:N:37:ARG:NH1	31:9:6:C:C5'	2.50	0.63
24:X:25:ARG:HD2	38:X:5356:HOH:O	1.98	0.63
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.32	0.63
30:0:1537:C:H1'	38:0:6614:HOH:O	1.97	0.63
4:D:25:MET:CE	4:D:37:ALA:HB1	2.28	0.63
30:0:272:A:H3'	38:0:7553:HOH:O	1.96	0.63
31:9:39:U:HO2'	31:9:42:C:H5	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2526:C:O2'	30:0:2527:U:H5'	1.98	0.63
1:A:35:GLY:O	1:A:36:ASP:HB3	1.99	0.63
30:0:2659:U:H5''	38:0:4129:HOH:O	1.98	0.63
30:0:2241:C:O2'	30:0:2242:U:H5'	1.98	0.63
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.81	0.63
10:J:107:ASN:ND2	10:J:109:TYR:H	1.96	0.63
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.13	0.63
8:H:165:ARG:HD2	38:H:8578:HOH:O	1.98	0.63
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.80	0.63
30:0:1174:A:C5	30:0:1201:C:H4'	2.33	0.63
12:L:41:HIS:HD2	30:0:926:A:O2'	1.82	0.63
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.34	0.63
21:U:9:CYS:HA	21:U:52:THR:HG23	1.81	0.63
30:0:2010:A:H2'	38:0:5975:HOH:O	1.98	0.63
16:P:59:ARG:HH22	16:P:66:GLN:NE2	1.96	0.63
30:0:2894:C:O2'	30:0:2895:C:H5'	1.98	0.63
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.81	0.63
30:0:613:C:H2'	30:0:614:U:H6	1.63	0.63
30:0:1342:C:C2'	30:0:1343:C:H5'	2.28	0.63
30:0:1165:G:H21	30:0:1173:A:H5''	1.63	0.63
30:0:1187:U:O2'	30:0:1189:A:H2	1.75	0.63
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.80	0.63
30:0:441:A:H1'	30:0:442:A:N7	2.14	0.62
23:W:88:THR:HG22	23:W:89:ASP:H	1.64	0.62
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.80	0.62
30:0:2111:G:H1'	38:0:9050:HOH:O	1.98	0.62
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.80	0.62
30:0:281:U:O2'	30:0:282:C:H5'	1.99	0.62
30:0:1119:G:H22	30:0:1246:A:H2	1.36	0.62
30:0:2756:U:N3	30:0:2896:A:H2	1.95	0.62
2:B:258:GLY:H	2:B:260:HIS:CE1	2.17	0.62
30:0:482:G:H4'	30:0:508:A:N1	2.15	0.62
30:0:2851:G:O2'	30:0:2852:A:H5'	2.00	0.62
28:2:41:HIS:HD2	28:2:44:ARG:H	1.47	0.62
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.15	0.62
31:9:76:G:C3'	31:9:77:A:H5''	2.20	0.62
4:D:154:LYS:HD2	4:D:154:LYS:N	2.09	0.62
30:0:1603:A:C5'	30:0:1605:G:H5'	2.29	0.62
30:0:280:C:H2'	30:0:281:U:O4'	2.00	0.62
30:0:2256:G:C2'	30:0:2257:G:H5'	2.30	0.62
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.00	0.62
30:0:2524:G:H21	30:0:2526:C:N4	1.98	0.61
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.82	0.61
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.15	0.61
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.65	0.61
30:0:1667:A:C8	30:0:1667:A:H5'	2.33	0.61
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.30	0.61
14:N:80:SER:HB2	38:N:8836:HOH:O	1.99	0.61
31:9:7:G:H5'	38:9:9097:HOH:O	2.00	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.27	0.61
30:0:2507:G:H2'	30:0:2510:C:N4	2.15	0.61
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.40	0.61
29:3:48:ASN:HD21	30:0:2468:A:H61	1.48	0.61
30:0:1477:C:H5'	30:0:1868:G:C5'	2.30	0.61
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.01	0.61
30:0:2563:U:H2'	30:0:2565:C:O5'	2.00	0.61
30:0:125:U:H2'	38:0:3765:HOH:O	1.99	0.61
1:A:51:ARG:HB2	38:A:9061:HOH:O	1.99	0.61
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.30	0.61
30:0:2300:A:H4'	30:0:2301:A:O5'	2.01	0.61
30:0:812:A:H1'	38:0:3959:HOH:O	2.00	0.61
30:0:1741:U:O2'	30:0:2723:G:H4'	2.00	0.61
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.65	0.61
2:B:238:ASN:HD22	2:B:240:GLY:N	1.92	0.61
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.81	0.61
2:B:145:HIS:HD2	2:B:146:THR:O	1.83	0.61
3:C:184:ARG:NH2	30:0:450:C:OP1	2.30	0.61
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.01	0.61
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.82	0.61
30:0:1132:A:N6	30:0:1229:C:H2'	2.16	0.61
30:0:2781:U:H2'	30:0:2782:G:H5'	1.82	0.61
30:0:285:A:H2'	30:0:286:U:O4'	2.00	0.61
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.14	0.61
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.82	0.61
31:9:95:C:O2'	31:9:96:C:H5'	2.01	0.61
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.65	0.60
30:0:2320:U:H4'	30:0:2321:A:O4'	2.01	0.60
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.83	0.60
31:9:75:G:H1	31:9:106:U:H3	1.49	0.60
11:K:10:GLN:H	11:K:10:GLN:NE2	1.87	0.60
30:0:299:U:H5'	38:0:7361:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.82	0.60
30:0:2781:U:C2'	30:0:2782:G:H5'	2.31	0.60
6:F:91:VAL:HG12	6:F:92:GLY:N	2.17	0.60
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.16	0.60
30:0:1641:A:C2'	30:0:1642:A:H5'	2.30	0.60
30:0:1819:G:H5'	38:0:4715:HOH:O	2.01	0.60
30:0:1528:A:H2'	30:0:1529:G:O4'	2.01	0.60
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.64	0.60
30:0:1972:U:H2'	30:0:1973:A:C5'	2.31	0.60
4:D:103:ASN:ND2	4:D:134:LEU:H	1.99	0.60
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.98	0.60
31:9:55:U:H4'	31:9:56:A:C8	2.36	0.60
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.82	0.60
28:2:38:LYS:HE3	38:0:4230:HOH:O	2.02	0.60
30:0:123:U:H5'	38:0:6683:HOH:O	2.01	0.60
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.83	0.60
3:C:214:THR:HG23	38:C:8639:HOH:O	2.01	0.60
10:J:90:LYS:HB2	35:J:8802:CL:CL	2.38	0.60
30:0:1730:G:H5''	30:0:1731:C:H6	1.67	0.60
22:V:39:ALA:N	22:V:40:PRO:HD2	2.16	0.60
23:W:80:ASP:O	23:W:84:VAL:HG23	2.02	0.60
30:0:2252:A:C5	30:0:2253:G:H1'	2.37	0.60
30:0:510:U:H6	38:0:7463:HOH:O	1.85	0.60
30:0:2505:G:C2'	30:0:2506:A:H5'	2.32	0.60
27:1:28:HIS:HE1	30:0:776:A:OP1	1.85	0.60
3:C:236:THR:HG22	3:C:239:ALA:N	2.13	0.59
1:A:211:LYS:HB2	38:A:9075:HOH:O	2.02	0.59
30:0:960:G:N3	30:0:960:G:C2'	2.64	0.59
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.36	0.59
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.31	0.59
25:Y:212:ARG:HD2	38:Y:8896:HOH:O	2.00	0.59
30:0:2878:U:H2'	30:0:2879:A:O4'	2.01	0.59
31:9:91:C:H2'	31:9:92:G:O4'	2.02	0.59
30:0:272:A:H5'	30:0:273:G:OP2	2.02	0.59
30:0:681:G:N3	30:0:681:G:H5'	2.17	0.59
30:0:1667:A:H2'	30:0:1668:U:C6	2.37	0.59
30:0:1730:G:C5'	30:0:1731:C:C6	2.85	0.59
30:0:204:A:H2'	30:0:205:U:H5'	1.84	0.59
30:0:249:G:O2'	30:0:250:C:H5'	2.03	0.59
18:R:117:HIS:HD2	30:0:20:G:H21	1.51	0.59
7:G:12:ILE:HG23	38:0:5471:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:39:THR:HG23	18:R:107:GLU:O	2.02	0.59
30:0:515:C:H5''	38:0:5654:HOH:O	2.02	0.59
30:0:1878:G:O2'	30:0:1879:U:C6	2.54	0.59
30:0:848:C:H5'	38:0:7295:HOH:O	2.02	0.59
30:0:961:A:H4'	38:0:6802:HOH:O	2.01	0.59
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.03	0.59
30:0:1165:G:H4'	30:0:1174:A:O2'	2.03	0.59
26:Z:34:SER:HB2	38:Z:8715:HOH:O	2.02	0.59
30:0:2670:G:O2'	30:0:2671:U:H5'	2.02	0.59
3:C:236:THR:HA	38:C:8653:HOH:O	2.01	0.59
30:0:853:C:H3'	38:0:4553:HOH:O	2.03	0.59
31:9:52:A:O2'	31:9:53:G:H5'	2.03	0.59
6:F:58:GLU:CD	13:M:27:ARG:HH22	2.05	0.59
30:0:1163:G:H1	30:0:1184:C:N4	2.01	0.59
3:C:1:MET:HG2	3:C:2:GLN:N	2.18	0.59
19:S:43:GLU:HB3	38:S:8997:HOH:O	2.02	0.59
31:9:22:G:H5'	31:9:23:U:OP1	2.03	0.58
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.03	0.58
30:0:316:A:N3	30:0:336:G:O2'	2.34	0.58
4:D:57:THR:HG23	4:D:63:ILE:HA	1.84	0.58
30:0:2649:A:H5'	30:0:2649:A:H8	1.68	0.58
30:0:2718:C:H6	30:0:2718:C:H5'	1.68	0.58
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.85	0.58
30:0:204:A:C2'	30:0:205:U:H5'	2.32	0.58
30:0:1834:C:H2'	30:0:1840:A:N6	2.17	0.58
30:0:283:U:C5	30:0:284:C:N3	2.70	0.58
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.32	0.58
28:2:10:ARG:NH2	30:0:121:U:OP2	2.34	0.58
30:0:2251:G:H2'	30:0:2252:A:C8	2.39	0.58
30:0:485:A:N3	30:0:487:G:H5''	2.18	0.58
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.86	0.58
30:0:2643:G:H5''	38:0:3928:HOH:O	2.04	0.58
30:0:12:U:H2'	30:0:13:G:H5'	1.84	0.58
5:E:111:LYS:HE3	30:0:2690:U:H4'	1.85	0.58
30:0:558:C:H2'	30:0:559:U:H5'	1.84	0.58
4:D:25:MET:HE1	4:D:37:ALA:HB1	1.84	0.58
30:0:2064:U:H5'	30:0:2652:U:O3'	2.04	0.58
30:0:1189:A:O2'	30:0:1208:C:H2'	2.03	0.58
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.30	0.58
31:9:1:U:O3'	31:9:3:A:H5''	2.03	0.58
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.86	0.58
30:0:541:C:H2'	30:0:542:A:H5'	1.85	0.58
30:0:1942:A:H3'	38:0:7371:HOH:O	2.03	0.58
30:0:214:U:H5'	38:0:6160:HOH:O	2.03	0.58
30:0:318:U:H5'	30:0:339:A:C2	2.39	0.58
31:9:39:U:H1'	31:9:44:A:N6	2.19	0.58
30:0:119:A:H2'	30:0:120:A:H5''	1.84	0.58
2:B:41:PHE:HB3	2:B:190:MET:HE1	1.85	0.58
30:0:1181:A:C2'	30:0:1182:C:H5'	2.34	0.58
30:0:559:U:C5	30:0:560:U:C5	2.92	0.58
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.34	0.58
30:0:304:G:H1'	30:0:347:A:N6	2.18	0.58
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.37	0.57
25:Y:174:VAL:HG23	25:Y:177:LYS:HD2	1.85	0.57
30:0:1603:A:H5'	30:0:1605:G:C4'	2.34	0.57
2:B:125:GLU:O	2:B:129:ARG:HG3	2.04	0.57
5:E:100:ASP:HB2	38:E:2789:HOH:O	2.03	0.57
30:0:1524:U:OP1	30:0:1524:U:H4'	2.04	0.57
14:N:37:ARG:HH11	31:9:6:C:H5''	1.64	0.57
16:P:64:GLU:HG2	38:P:168:HOH:O	2.03	0.57
15:O:25:VAL:HG12	30:0:709:G:O2'	2.04	0.57
1:A:179:MET:HG2	1:A:186:TRP:CB	2.35	0.57
3:C:236:THR:HG21	38:C:8577:HOH:O	2.03	0.57
31:9:52:A:H2'	31:9:53:G:O4'	2.04	0.57
22:V:55:ARG:O	22:V:59:ILE:HG12	2.05	0.57
30:0:1249:U:H2'	30:0:1250:C:C6	2.39	0.57
30:0:2832:C:H5	38:0:7237:HOH:O	1.87	0.57
30:0:1377:C:H5'	30:0:1377:C:C6	2.40	0.57
2:B:41:PHE:HA	2:B:79:MET:HE2	1.86	0.57
30:0:2361:A:H8	30:0:2361:A:H5'	1.70	0.57
27:1:25:LYS:HD2	28:2:49:GLU:H	1.69	0.57
30:0:558:C:C2'	30:0:559:U:C5'	2.77	0.57
7:G:20:VAL:O	7:G:24:VAL:HG23	2.05	0.57
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.85	0.57
30:0:2478:U:O2'	30:0:2479:A:H5'	2.04	0.57
1:A:36:ASP:O	1:A:38:ILE:N	2.38	0.57
25:Y:115:ARG:HH21	30:0:1266:U:H4'	1.70	0.57
30:0:2102:G:H1'	30:0:2103:A:N7	2.20	0.57
5:E:149:GLU:HG3	5:E:167:TYR:HA	1.84	0.57
30:0:1116:U:O2'	30:0:1118:A:C2	2.46	0.57
17:Q:25:PRO:HB2	38:9:9078:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1183:C:N3	30:0:1184:C:C5	2.73	0.56
30:0:960:G:C3'	30:0:960:G:N3	2.68	0.56
23:W:13:MET:HE3	23:W:18:GLN:HA	1.87	0.56
30:0:1200:A:H3'	38:0:5763:HOH:O	2.05	0.56
30:0:567:U:H5''	38:0:5297:HOH:O	2.05	0.56
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.39	0.56
18:R:9:ASP:O	18:R:13:THR:HB	2.05	0.56
30:0:2256:G:H2'	30:0:2257:G:C5'	2.35	0.56
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.05	0.56
12:L:41:HIS:CD2	30:0:926:A:O2'	2.58	0.56
27:1:10:LYS:HG3	38:1:8979:HOH:O	2.04	0.56
30:0:1160:G:H2'	38:0:5641:HOH:O	2.04	0.56
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.88	0.56
30:0:1398:G:O2'	30:0:1399:A:H5'	2.06	0.56
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.71	0.56
30:0:1730:G:H5''	30:0:1731:C:C6	2.41	0.56
30:0:2679:G:H2'	30:0:2681:A:OP2	2.06	0.56
30:0:65:C:O2'	30:0:66:G:H5'	2.05	0.56
30:0:185:G:H4'	30:0:186:A:H4'	1.86	0.56
30:0:2505:G:H2'	30:0:2506:A:H5'	1.87	0.56
30:0:2509:A:OP2	30:0:2510:C:H5	1.89	0.56
30:0:559:U:H5'	30:0:559:U:C6	2.40	0.56
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.39	0.56
30:0:952:G:H4'	38:0:4035:HOH:O	2.06	0.56
30:0:1778:A:H2'	30:0:1779:A:H5'	1.87	0.56
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.88	0.56
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.06	0.56
30:0:856:G:C8	38:0:5439:HOH:O	2.52	0.56
5:E:154:ILE:HD11	5:E:157:LYS:HE2	1.87	0.56
30:0:1819:G:H2'	30:0:1820:G:C4'	2.36	0.56
30:0:73:U:O2'	30:0:74:G:H5'	2.05	0.56
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.86	0.56
30:0:1044:C:H5''	38:0:9026:HOH:O	2.05	0.56
8:H:30:LYS:H	8:H:62:HIS:CD2	2.16	0.56
30:0:567:U:C5'	38:0:6425:HOH:O	2.49	0.56
1:A:48:ASP:HB3	38:A:9061:HOH:O	2.06	0.56
30:0:2353:A:H4'	30:0:2354:A:O5'	2.06	0.56
25:Y:141:THR:HG23	38:Y:8883:HOH:O	2.05	0.56
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.89	0.56
30:0:282:C:O2'	30:0:283:U:C5'	2.52	0.56
23:W:84:VAL:HG12	38:W:6679:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:42:ASN:HB3	38:0:7451:HOH:O	2.06	0.56
30:0:1615:A:H5'	38:0:4186:HOH:O	2.04	0.56
30:0:2316:G:H4'	38:0:6110:HOH:O	2.06	0.55
30:0:2089:A:O2'	30:0:2090:G:H5'	2.06	0.55
30:0:2372:A:H2'	30:0:2373:U:C6	2.41	0.55
30:0:999:C:O2'	30:0:1000:C:H5'	2.07	0.55
30:0:1625:U:H3'	30:0:1625:U:H6	1.70	0.55
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.95	0.55
1:A:51:ARG:NH1	1:A:120:ARG:O	2.39	0.55
3:C:25:PRO:HG2	38:C:8523:HOH:O	2.06	0.55
30:0:1205:U:C2'	30:0:1206:U:C5'	2.84	0.55
1:A:223:ARG:HD2	30:0:2272:G:OP1	2.06	0.55
30:0:1167:G:H2'	30:0:1168:C:O4'	2.07	0.55
13:M:188:ARG:HD3	30:0:155:C:OP2	2.05	0.55
4:D:159:PRO:O	4:D:163:VAL:HG23	2.06	0.55
30:0:1181:A:H2'	30:0:1182:C:H5'	1.87	0.55
30:0:1175:G:H1'	30:0:1193:A:C2'	2.34	0.55
30:0:2649:A:C8	30:0:2649:A:H5'	2.42	0.55
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.88	0.55
30:0:10:U:O4	30:0:532:A:OP2	2.23	0.55
27:1:16:HIS:HD2	30:0:470:U:O2'	1.88	0.55
30:0:1474:C:C5'	30:0:1474:C:H6	2.12	0.55
30:0:1527:A:H1'	30:0:1528:A:C8	2.42	0.55
30:0:2330:U:H4'	30:0:2331:C:OP1	2.06	0.55
2:B:244:PRO:HB3	30:0:1234:U:N3	2.21	0.55
24:X:30:MET:HG2	30:0:1384:C:H5'	1.88	0.55
30:0:821:U:H2'	30:0:822:C:H6	1.71	0.55
7:G:64:ASN:N	7:G:64:ASN:HD22	2.04	0.55
31:9:1:U:H5''	31:9:3:A:OP1	2.06	0.55
30:0:2238:A:O2'	30:0:2239:C:H5'	2.07	0.55
30:0:1406:A:H4'	30:0:1407:A:H5''	1.87	0.55
30:0:2344:G:H2'	30:0:2344:G:N3	2.21	0.55
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.16	0.55
4:D:103:ASN:HD22	4:D:134:LEU:H	1.54	0.55
30:0:941:G:C5	30:0:942:U:C4	2.95	0.55
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.86	0.55
30:0:1321:A:H2'	30:0:1322:G:C8	2.41	0.55
25:Y:235:GLU:H	25:Y:235:GLU:CD	2.09	0.55
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.86	0.55
30:0:2851:G:C2'	30:0:2852:A:H5'	2.36	0.55
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ASP:O	2:B:306:LYS:HB2	2.07	0.55
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.88	0.55
30:0:2472:C:O2'	30:0:2634:G:H4'	2.07	0.55
30:0:1202:A:H2'	30:0:1203:G:O4'	2.07	0.55
18:R:99:ALA:HB1	18:R:109:MET:CE	2.35	0.55
30:0:1393:A:H2'	30:0:1394:C:C6	2.42	0.55
30:0:2414:A:H2'	30:0:2415:A:C8	2.41	0.55
23:W:154:ARG:NH1	30:0:588:G:O6	2.39	0.55
30:0:1193:A:C2	30:0:1194:A:N6	2.75	0.54
30:0:1589:G:N2	30:0:1605:G:H1'	2.21	0.54
30:0:396:U:O2'	30:0:418:C:H4'	2.07	0.54
30:0:960:G:H2'	30:0:960:G:N3	2.20	0.54
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.06	0.54
18:R:39:THR:HG22	18:R:42:GLU:H	1.72	0.54
30:0:90:A:H2'	30:0:91:G:O4'	2.07	0.54
31:9:49:G:H2'	31:9:50:G:O4'	2.07	0.54
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.88	0.54
30:0:2432:C:O2'	30:0:2433:A:H5'	2.07	0.54
30:0:1130:U:H2'	30:0:1131:G:O4'	2.07	0.54
20:T:2:LYS:HG2	30:0:447:A:OP1	2.07	0.54
30:0:595:U:H2'	30:0:596:C:H6	1.72	0.54
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.47	0.54
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.40	0.54
30:0:128:A:O2'	30:0:129:A:H5'	2.07	0.54
14:N:141:ARG:HH21	31:9:48:C:H4'	1.72	0.54
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.90	0.54
30:0:1080:C:H4'	30:0:1081:A:OP1	2.07	0.54
12:L:18:HIS:HD2	30:0:902:G:N7	2.05	0.54
30:0:1909:A:N1	30:0:2128:G:H1'	2.23	0.54
2:B:62:ARG:HA	2:B:65:MET:CE	2.38	0.54
31:9:36:C:C5	31:9:37:C:C5	2.95	0.54
21:U:50:GLU:HB2	30:0:2866:U:C5	2.42	0.54
10:J:74:ARG:HH11	10:J:74:ARG:HB3	1.72	0.54
30:0:794:U:H3	30:0:819:A:H61	1.55	0.54
30:0:522:U:O2'	30:0:1366:C:H5'	2.07	0.54
31:9:49:G:O2'	31:9:50:G:H5'	2.08	0.54
30:0:1279:U:O2	30:0:1279:U:H2'	2.07	0.54
3:C:76:ARG:HG2	3:C:78:ARG:NH1	2.21	0.54
30:0:1972:U:H2'	30:0:1973:A:H5'	1.89	0.54
1:A:97:ALA:HA	1:A:131:HIS:HE2	1.73	0.54
1:A:36:ASP:HB2	1:A:85:SER:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:64:THR:O	23:W:68:THR:HG22	2.07	0.54
24:X:43:VAL:HG12	24:X:44:ASP:N	2.23	0.54
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.90	0.54
27:1:20:ARG:HG2	30:0:111:C:O2'	2.08	0.54
30:0:694:A:H2'	30:0:695:C:H5'	1.90	0.54
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.89	0.54
18:R:98:ASN:HD21	30:0:500:G:H21	1.54	0.54
2:B:212:GLN:HA	30:0:1733:A:H4'	1.89	0.54
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.41	0.54
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.40	0.54
30:0:1819:G:H2'	30:0:1820:G:C5'	2.38	0.54
30:0:1730:G:H5'	30:0:1731:C:H5	1.72	0.54
30:0:2419:U:H5''	30:0:2420:G:H5'	1.89	0.54
27:1:9:GLY:HA2	30:0:1687:C:O2	2.08	0.54
9:I:120:ALA:O	9:I:124:VAL:HG23	2.08	0.54
21:U:52:THR:HG22	21:U:54:THR:H	1.73	0.54
30:0:1947:G:N2	30:0:1966:U:C2	2.76	0.54
30:0:952:G:N3	30:0:2302:A:H2'	2.23	0.54
7:G:16:LYS:O	7:G:20:VAL:HG23	2.07	0.54
30:0:1484:G:H2'	38:0:9107:HOH:O	2.08	0.54
3:C:132:ASP:HB3	38:C:8566:HOH:O	2.09	0.54
30:0:1158:G:O2'	30:0:1159:G:H5'	2.09	0.53
30:0:1209:C:H2'	30:0:1210:G:H8	1.71	0.53
15:O:37:ARG:HD2	30:0:656:G:OP2	2.08	0.53
31:9:39:U:H3'	31:9:40:C:H5''	1.91	0.53
30:0:1307:A:H2'	30:0:1308:A:C8	2.43	0.53
30:0:807:A:O2'	30:0:808:A:H5'	2.08	0.53
6:F:57:GLU:O	6:F:61:MET:HG3	2.08	0.53
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.73	0.53
30:0:1514:C:O2'	30:0:1515:A:H5'	2.09	0.53
22:V:64:GLY:O	22:V:65:ASP:HB2	2.08	0.53
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.09	0.53
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.44	0.53
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.72	0.53
6:F:101:ALA:HA	38:F:5413:HOH:O	2.09	0.53
2:B:265:LEU:HD21	2:B:316:ARG:HD3	1.90	0.53
30:0:876:A:N3	30:0:876:A:H2'	2.24	0.53
30:0:1174:A:C6	30:0:1201:C:H4'	2.44	0.53
23:W:115:THR:HG23	38:W:5420:HOH:O	2.08	0.53
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.23	0.53
21:U:37:GLU:HB3	38:U:408:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1202:A:C2'	30:0:1203:G:H5'	2.39	0.53
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.24	0.53
30:0:625:U:H5''	30:0:1044:C:N4	2.24	0.53
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.38	0.53
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.39	0.53
30:0:39:G:N2	30:0:444:C:C2	2.77	0.53
30:0:2121:G:O2'	30:0:2122:C:H5'	2.08	0.53
31:9:55:U:H4'	31:9:56:A:H8	1.72	0.53
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.44	0.53
30:0:1342:C:O2'	30:0:1343:C:H5'	2.08	0.53
10:J:74:ARG:O	10:J:78:ILE:HG12	2.08	0.53
30:0:2598:U:O2	30:0:2600:A:H8	1.92	0.53
8:H:170:ARG:HD2	38:H:8536:HOH:O	2.08	0.53
3:C:43:LYS:HG2	30:0:449:A:N7	2.24	0.53
30:0:1878:G:O2'	30:0:1879:U:P	2.67	0.53
30:0:1060:C:H6	30:0:1060:C:H5'	1.73	0.53
1:A:191:GLY:HA2	1:A:194:MET:HE3	1.90	0.53
1:A:121:ALA:O	1:A:124:VAL:HG22	2.08	0.53
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.44	0.53
30:0:1925:G:O2'	30:0:1926:G:H5'	2.09	0.53
18:R:29:LYS:HE2	30:0:524:A:H5'	1.91	0.53
30:0:1183:C:O2	30:0:1183:C:H2'	2.08	0.53
30:0:1185:U:H5'	38:0:7491:HOH:O	2.08	0.53
30:0:1181:A:N1	30:0:1192:A:O2'	2.39	0.53
23:W:21:LEU:O	23:W:26:ILE:HG23	2.09	0.53
30:0:2812:A:C2	30:0:2814:A:N6	2.67	0.53
30:0:2578:G:C8	30:0:2578:G:H5'	2.40	0.53
30:0:2781:U:H2'	30:0:2782:G:C5'	2.38	0.53
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.39	0.53
20:T:38:ARG:NH1	38:0:6714:HOH:O	2.41	0.53
25:Y:133:HIS:HD2	38:Y:8876:HOH:O	1.91	0.53
30:0:364:U:H2'	30:0:365:G:O4'	2.09	0.53
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.38	0.52
30:0:138:U:OP2	30:0:139:C:H5	1.92	0.52
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.06	0.52
11:K:66:ARG:HH22	30:0:1994:A:P	2.32	0.52
30:0:814:G:H4'	38:0:3135:HOH:O	2.09	0.52
30:0:277:U:O2'	30:0:278:A:H5'	2.09	0.52
4:D:154:LYS:H	4:D:154:LYS:CD	2.11	0.52
30:0:1120:U:C5'	30:0:1121:G:OP2	2.56	0.52
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2256:G:H2'	30:0:2257:G:H5'	1.89	0.52
23:W:44:MET:CE	30:0:944:G:H21	2.22	0.52
3:C:95:GLU:HG3	38:C:8680:HOH:O	2.09	0.52
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.90	0.52
2:B:85:ARG:NH1	38:B:9099:HOH:O	2.42	0.52
30:0:2010:A:C2'	38:0:5975:HOH:O	2.54	0.52
30:0:2252:A:H2'	30:0:2253:G:H5'	1.90	0.52
30:0:1131:G:C6	30:0:1230:A:C4	2.98	0.52
30:0:136:C:H2'	30:0:137:U:O4'	2.08	0.52
30:0:1714:C:O2'	30:0:1715:C:H5'	2.08	0.52
30:0:545:G:H8	30:0:545:G:C5'	2.06	0.52
30:0:1171:A:C2'	30:0:1172:G:H5'	2.39	0.52
5:E:69:ILE:HA	5:E:72:MET:CE	2.39	0.52
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.91	0.52
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.09	0.52
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.92	0.52
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.91	0.52
30:0:1787:C:H4'	30:0:2883:A:O4'	2.10	0.52
31:9:64:C:C2'	31:9:65:A:H5'	2.39	0.52
12:L:134:GLU:HG3	38:L:8861:HOH:O	2.09	0.52
8:H:30:LYS:N	8:H:62:HIS:HD2	2.02	0.52
5:E:9:GLU:HA	38:E:5240:HOH:O	2.08	0.52
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.92	0.52
30:0:1205:U:C2'	30:0:1206:U:H5''	2.37	0.52
30:0:1206:U:C5'	30:0:1206:U:H6	2.19	0.52
31:9:13:A:O2'	31:9:14:G:H5''	2.09	0.52
30:0:256:C:H2'	30:0:257:G:O4'	2.10	0.52
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.09	0.52
30:0:1268:C:O2'	30:0:1269:G:H5'	2.09	0.52
22:V:44:GLY:HA3	30:0:92:G:H4'	1.92	0.52
30:0:2281:C:C2'	30:0:2282:U:H5'	2.39	0.52
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.09	0.52
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.74	0.52
30:0:1342:C:H2'	30:0:1343:C:H5'	1.92	0.52
31:9:12:C:H5'	31:9:70:U:O4'	2.09	0.52
26:Z:40:ALA:HA	30:0:1773:G:C8	2.45	0.52
30:0:228:C:H2'	30:0:229:G:H5'	1.91	0.52
30:0:1339:G:C6	30:0:1340:G:N1	2.78	0.52
30:0:1187:U:H2'	38:0:6927:HOH:O	2.10	0.52
22:V:1:THR:CB	30:0:93:C:H5''	2.32	0.52
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:603:A:H1'	30:0:605:C:C2	2.45	0.52
30:0:319:A:H4'	30:0:338:C:C4	2.45	0.52
30:0:2102:G:N3	30:0:2103:A:C5	2.78	0.52
30:0:1130:U:H5'	38:0:7694:HOH:O	2.08	0.52
30:0:1636:G:O2'	30:0:1637:A:H5'	2.09	0.52
30:0:2493:C:O2	30:0:2493:C:H2'	2.09	0.52
3:C:140:VAL:HB	38:C:8653:HOH:O	2.09	0.52
30:0:369:G:H2'	30:0:370:G:H8	1.75	0.52
5:E:69:ILE:HA	5:E:72:MET:HE3	1.91	0.52
6:F:91:VAL:HG11	30:0:262:A:OP2	2.10	0.52
17:Q:95:GLU:HA	30:0:949:U:H4'	1.90	0.52
13:M:179:GLY:O	30:0:399:C:H5'	2.10	0.52
24:X:78:GLU:HG2	24:X:79:GLU:H	1.75	0.52
30:0:1087:G:H4'	30:0:1088:A:OP1	2.10	0.52
20:T:9:LYS:HB2	38:0:7449:HOH:O	2.10	0.52
30:0:1182:C:C1'	30:0:1192:A:H8	2.22	0.51
30:0:1205:U:H5	38:0:4440:HOH:O	1.94	0.51
30:0:541:C:C2'	30:0:542:A:C5'	2.76	0.51
1:A:99:ILE:O	1:A:131:HIS:HE1	1.93	0.51
30:0:1406:A:H5'	30:0:1407:A:C8	2.45	0.51
30:0:1081:A:H5''	38:0:3155:HOH:O	2.09	0.51
26:Z:57:MET:HE3	38:0:6301:HOH:O	2.10	0.51
2:B:294:TYR:HE2	38:B:9114:HOH:O	1.93	0.51
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.91	0.51
30:0:2511:A:H2'	30:0:2512:U:O4'	2.09	0.51
10:J:107:ASN:HD22	10:J:107:ASN:C	2.11	0.51
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.40	0.51
30:0:2064:U:H4'	30:0:2653:A:OP1	2.10	0.51
30:0:2415:A:H2'	30:0:2416:G:H5'	1.92	0.51
30:0:669:G:O2'	30:0:670:G:H5'	2.10	0.51
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.75	0.51
30:0:1595:G:O2'	30:0:1596:U:H5'	2.10	0.51
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.93	0.51
3:C:233:THR:HG22	3:C:234:VAL:H	1.75	0.51
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.11	0.51
13:M:163:LEU:HD21	30:0:188:C:H5''	1.91	0.51
5:E:11:VAL:HG12	5:E:12:ASP:N	2.26	0.51
30:0:2637:A:H4'	38:0:4938:HOH:O	2.10	0.51
30:0:2102:G:N2	30:0:2103:A:C6	2.78	0.51
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.10	0.51
30:0:856:G:H2'	38:0:5439:HOH:O	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.91	0.51
31:9:31:C:H2'	31:9:32:G:O4'	2.11	0.51
6:F:96:ALA:HA	38:F:3111:HOH:O	2.09	0.51
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.11	0.51
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.11	0.51
30:0:2372:A:H2'	30:0:2373:U:H6	1.74	0.51
30:0:264:G:H1'	30:0:265:U:H5	1.76	0.51
30:0:644:G:N3	30:0:644:G:H5'	2.25	0.51
4:D:141:VAL:HG21	31:9:57:A:H8	1.76	0.51
30:0:1119:G:N2	30:0:1246:A:H2	2.01	0.51
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.91	0.51
30:0:1766:U:O2	30:0:1778:A:H5'	2.10	0.51
3:C:233:THR:HG22	3:C:234:VAL:N	2.25	0.51
2:B:98:THR:HG22	30:0:2820:A:OP1	2.10	0.51
30:0:1838:U:O2'	30:0:2644:C:H5'	2.10	0.51
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.46	0.51
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.93	0.51
8:H:66:GLU:HA	38:H:8576:HOH:O	2.10	0.51
18:R:150:PRO:CG	18:R:150:PRO:CB	2.88	0.51
30:0:69:A:H8	30:0:69:A:C5'	2.23	0.51
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.93	0.51
30:0:200:C:H2'	38:0:3443:HOH:O	2.10	0.51
30:0:1506:U:H6	30:0:1506:U:H5'	1.75	0.51
30:0:1972:U:H2'	30:0:1973:A:H5''	1.92	0.51
4:D:76:ARG:NE	31:9:44:A:O4'	2.44	0.51
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.93	0.51
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.91	0.51
1:A:109:GLU:HG2	1:A:116:GLY:N	2.26	0.51
8:H:5:PRO:HD2	8:H:8:MET:SD	2.50	0.51
30:0:1166:A:P	30:0:1174:A:H4'	2.51	0.51
30:0:162:C:H2'	30:0:163:U:H5'	1.93	0.51
3:C:168:ARG:NH2	3:C:190:ALA:O	2.44	0.51
5:E:84:MET:HG2	5:E:168:ILE:HA	1.92	0.51
30:0:1163:G:C2	30:0:1184:C:N3	2.79	0.51
30:0:1165:G:N2	30:0:1173:A:C5'	2.74	0.51
30:0:1589:G:H22	30:0:1605:G:H1'	1.76	0.51
30:0:255:A:C5	30:0:256:C:C5	2.99	0.51
6:F:48:VAL:HG23	6:F:74:PHE:HB3	1.92	0.51
1:A:33:GLU:CD	1:A:33:GLU:H	2.15	0.51
30:0:816:G:C6	30:0:817:G:N1	2.79	0.51
23:W:139:GLY:O	23:W:141:HIS:HD2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:506:G:N2	30:0:509:A:H5''	2.22	0.51
30:0:1878:G:C1'	38:0:6139:HOH:O	2.45	0.51
30:0:1477:C:O2'	30:0:1478:U:H5'	2.10	0.51
6:F:48:VAL:CG2	6:F:74:PHE:HB3	2.42	0.51
30:0:2438:G:H2'	30:0:2439:C:O4'	2.11	0.51
30:0:2900:G:H2'	30:0:2901:C:O4'	2.11	0.51
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.51
14:N:110:THR:HB	14:N:113:SER:OG	2.11	0.50
31:9:114:G:H2'	31:9:115:C:C6	2.46	0.50
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.41	0.50
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.11	0.50
29:3:70:ARG:HB3	38:3:9062:HOH:O	2.10	0.50
21:U:33:SER:O	21:U:37:GLU:HG3	2.10	0.50
27:1:42:SER:HB2	38:1:8956:HOH:O	2.12	0.50
3:C:206:ASN:HB2	30:0:329:A:OP2	2.11	0.50
11:K:8:VAL:HG13	11:K:80:ILE:HG22	1.93	0.50
30:0:1373:G:H1'	38:0:6157:HOH:O	2.10	0.50
9:I:126:THR:O	9:I:130:LEU:HG	2.12	0.50
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.93	0.50
30:0:2526:C:H5'	30:0:2526:C:C6	2.46	0.50
27:1:21:ARG:HD2	27:1:39:PHE:HB2	1.94	0.50
30:0:1586:G:O2'	30:0:1587:U:H5'	2.10	0.50
19:S:76:GLU:HB3	38:S:8999:HOH:O	2.11	0.50
19:S:37:VAL:O	19:S:41:VAL:HG23	2.12	0.50
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.93	0.50
30:0:2587:OMU:H2'	30:0:2589:U:H5''	1.93	0.50
30:0:1730:G:C5'	30:0:1731:C:C5	2.93	0.50
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.42	0.50
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.93	0.50
20:T:26:THR:HA	20:T:39:ASN:HB3	1.92	0.50
30:0:291:C:H2'	30:0:292:G:O4'	2.11	0.50
30:0:1903:U:O2'	30:0:1904:A:N7	2.43	0.50
30:0:1202:A:O2'	30:0:1203:G:H5'	2.12	0.50
30:0:369:G:O2'	30:0:370:G:H5'	2.12	0.50
30:0:2510:C:H5'	30:0:2511:A:OP2	2.11	0.50
1:A:212:PRO:HB2	38:A:9024:HOH:O	2.11	0.50
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.92	0.50
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.93	0.50
3:C:79:ARG:O	3:C:87:ARG:HG2	2.12	0.50
30:0:2445:U:H2'	30:0:2446:G:C8	2.46	0.50
7:G:23:ILE:O	7:G:27:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:GLY:HA3	38:B:9031:HOH:O	2.12	0.50
30:0:407:A:H3'	38:0:4459:HOH:O	2.11	0.50
30:0:1137:G:H1'	38:0:3879:HOH:O	2.11	0.50
14:N:114:LYS:O	14:N:118:ILE:HG13	2.11	0.50
30:0:1206:U:C6	30:0:1206:U:H5'	2.35	0.50
14:N:37:ARG:NH1	31:9:6:C:OP1	2.43	0.50
30:0:2502:C:H2'	30:0:2503:A:C5'	2.39	0.50
30:0:1972:U:C2'	30:0:1973:A:H5''	2.41	0.50
8:H:48:VAL:HA	8:H:170:ARG:O	2.12	0.50
30:0:407:A:H2'	30:0:408:A:C8	2.47	0.50
30:0:1921:A:O2'	30:0:1922:A:H5'	2.12	0.50
30:0:1020:A:H1'	38:0:7252:HOH:O	2.10	0.50
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.92	0.50
30:0:1066:U:H2'	30:0:1067:A:C8	2.47	0.50
2:B:51:VAL:CG2	2:B:327:VAL:HG13	2.41	0.50
30:0:1588:G:C6	30:0:1589:G:C6	3.00	0.50
2:B:17:LYS:O	2:B:260:HIS:HD2	1.94	0.50
30:0:815:U:O2'	30:0:1598:A:H4'	2.12	0.50
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.93	0.50
30:0:292:G:H2'	30:0:358:G:N2	2.26	0.50
4:D:52:THR:HG21	30:0:2346:C:O2'	2.12	0.50
29:3:3:MET:O	29:3:90:PHE:HA	2.11	0.50
30:0:2026:C:O2'	30:0:2027:U:H5'	2.11	0.50
30:0:1183:C:H42	30:0:1184:C:N4	2.07	0.50
30:0:1207:A:C8	30:0:1208:C:C5	3.00	0.50
30:0:2768:A:H3'	38:0:4425:HOH:O	2.10	0.50
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.93	0.50
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.50
1:A:109:GLU:HG2	1:A:116:GLY:H	1.77	0.50
30:0:2825:C:H4'	30:0:2826:G:O5'	2.12	0.50
4:D:141:VAL:HG21	31:9:57:A:C8	2.46	0.49
30:0:541:C:O2'	30:0:542:A:H5''	2.12	0.49
8:H:59:GLN:HG2	8:H:129:ARG:HG2	1.92	0.49
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.94	0.49
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.39	0.49
30:0:1343:C:H2'	30:0:1344:G:O5'	2.12	0.49
30:0:2064:U:H5'	30:0:2652:U:H4'	1.93	0.49
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.11	0.49
31:9:64:C:H2'	31:9:65:A:H5'	1.94	0.49
13:M:66:SER:HB3	13:M:128:TRP:CD1	2.47	0.49
12:L:143:THR:HG22	12:L:144:ASP:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:131:THR:HB	10:J:134:GLU:HG3	1.94	0.49
30:0:2384:U:H5''	38:0:3492:HOH:O	2.12	0.49
13:M:80:GLY:O	13:M:81:ARG:HD3	2.12	0.49
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.47	0.49
29:3:38:ARG:HD2	30:0:396:U:OP2	2.13	0.49
30:0:2269:C:C2'	30:0:2270:G:H5'	2.42	0.49
30:0:1926:G:H2'	30:0:1927:A:C8	2.47	0.49
30:0:2697:A:H2'	30:0:2698:G:O4'	2.12	0.49
30:0:2608:C:H3'	38:0:7829:HOH:O	2.11	0.49
30:0:24:G:N2	30:0:518:G:H1'	2.27	0.49
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.22	0.49
5:E:80:TRP:O	5:E:134:SER:HA	2.13	0.49
30:0:1505:U:H1'	38:0:7609:HOH:O	2.13	0.49
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.12	0.49
30:0:1289:C:O2'	30:0:1290:G:H5'	2.12	0.49
23:W:24:LEU:O	23:W:26:ILE:HG22	2.13	0.49
31:9:23:U:C2'	31:9:24:U:H4'	2.42	0.49
30:0:827:A:H2'	30:0:828:G:O4'	2.12	0.49
30:0:440:C:H2'	30:0:441:A:C8	2.48	0.49
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.94	0.49
30:0:1768:C:H2'	30:0:1769:C:O4'	2.13	0.49
30:0:2607:U:H4'	38:0:9440:HOH:O	2.12	0.49
30:0:711:G:C2	30:0:718:C:C2	3.00	0.49
30:0:2846:C:H4'	38:0:5089:HOH:O	2.12	0.49
20:T:52:ARG:O	30:0:317:A:OP1	2.29	0.49
2:B:297:VAL:HB	38:B:9071:HOH:O	2.12	0.49
30:0:1592:G:H2'	30:0:1593:C:C6	2.48	0.49
4:D:23:VAL:HG22	4:D:73:VAL:HB	1.94	0.49
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.60	0.49
30:0:513:A:N3	38:0:3658:HOH:O	2.34	0.49
31:9:60:C:O2'	31:9:61:C:H5'	2.12	0.49
2:B:267:LYS:HD3	38:0:9562:HOH:O	2.11	0.49
17:Q:19:ARG:HH21	31:9:11:A:P	2.36	0.49
30:0:1157:C:O2'	30:0:1158:G:H5'	2.13	0.49
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.10	0.49
30:0:2506:A:N6	30:0:2511:A:O2'	2.42	0.49
30:0:523:C:H2'	30:0:524:A:C8	2.48	0.49
6:F:39:SER:OG	6:F:45:ALA:HB2	2.12	0.49
12:L:14:GLY:O	30:0:1295:G:H5''	2.13	0.49
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.13	0.49
30:0:1185:U:H2'	30:0:1186:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2712:G:H5'	38:0:5229:HOH:O	2.12	0.49
8:H:69:ARG:HD3	38:H:8576:HOH:O	2.11	0.49
20:T:68:ASP:HB2	38:0:5666:HOH:O	2.12	0.49
31:9:29:C:H2'	31:9:30:C:C5'	2.37	0.49
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.95	0.49
2:B:254:GLN:HG2	2:B:255:GLY:N	2.27	0.49
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.77	0.49
30:0:483:C:C4	30:0:484:A:C6	3.01	0.49
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.99	0.49
30:0:447:A:O2'	30:0:448:G:H5'	2.13	0.49
2:B:215:VAL:HA	2:B:220:VAL:HG22	1.95	0.49
31:9:35:C:H5''	38:9:9074:HOH:O	2.12	0.49
30:0:1160:G:H5'	30:0:1161:A:C4'	2.42	0.49
30:0:1173:A:H2	38:0:6300:HOH:O	1.95	0.49
30:0:255:A:C5	30:0:256:C:C4	3.01	0.49
21:U:52:THR:O	21:U:56:ARG:HG2	2.12	0.49
11:K:87:ARG:NH2	30:0:2720:C:O2	2.45	0.49
30:0:951:A:O2'	30:0:952:G:H5'	2.13	0.49
30:0:2281:C:H2'	30:0:2282:U:H5'	1.95	0.49
30:0:1762:C:H2'	30:0:1763:C:H6	1.78	0.49
30:0:78:G:C6	30:0:79:G:C6	3.01	0.49
30:0:343:C:O2'	30:0:344:C:H5'	2.12	0.49
30:0:2401:A:H2'	30:0:2402:A:C8	2.48	0.49
23:W:4:LEU:O	23:W:32:CYS:HA	2.13	0.48
2:B:36:PRO:HG3	2:B:169:GLY:H	1.78	0.48
30:0:120:A:H2'	30:0:120:A:N3	2.28	0.48
2:B:256:GLN:HG2	38:B:9120:HOH:O	2.12	0.48
30:0:2324:G:N2	30:0:2377:U:H1'	2.28	0.48
30:0:583:C:H2'	30:0:584:U:H6	1.78	0.48
3:C:63:SER:OG	30:0:2101:A:H2'	2.13	0.48
30:0:308:U:C4	30:0:342:C:H1'	2.48	0.48
27:1:16:HIS:CD2	30:0:470:U:O2'	2.65	0.48
30:0:807:A:C6	30:0:808:A:C6	3.01	0.48
30:0:2598:U:O2	30:0:2600:A:C8	2.66	0.48
13:M:81:ARG:HG3	13:M:85:ARG:HB2	1.95	0.48
30:0:1016:U:H1'	38:0:3657:HOH:O	2.13	0.48
30:0:660:A:H4'	30:0:661:G:O5'	2.14	0.48
30:0:2897:C:O2'	30:0:2898:G:H5'	2.13	0.48
30:0:1657:A:H2'	30:0:1658:A:C8	2.48	0.48
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.33	0.48
30:0:629:A:C2	30:0:2074:A:C2	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:57:THR:HG22	19:S:59:ASP:H	1.78	0.48
30:0:2269:C:H2'	30:0:2270:G:H5'	1.95	0.48
30:0:1973:A:H5'	30:0:1973:A:C8	2.39	0.48
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.95	0.48
30:0:304:G:H1'	30:0:347:A:H61	1.78	0.48
1:A:186:TRP:CG	1:A:187:PRO:HA	2.48	0.48
30:0:1067:A:H5'	38:0:4348:HOH:O	2.11	0.48
30:0:2435:U:H1'	38:0:5442:HOH:O	2.13	0.48
30:0:1226:G:H5'	38:0:4532:HOH:O	2.13	0.48
10:J:41:ALA:HB3	38:J:5907:HOH:O	2.12	0.48
30:0:2783:A:H2'	30:0:2784:A:C8	2.49	0.48
31:9:1:U:O3'	31:9:3:A:C5'	2.61	0.48
14:N:147:ILE:HD12	38:9:9087:HOH:O	2.12	0.48
2:B:51:VAL:HG23	2:B:329:TYR:O	2.13	0.48
30:0:2756:U:C2	30:0:2896:A:H2	2.31	0.48
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.29	0.48
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.96	0.48
30:0:1615:A:C5'	38:0:4186:HOH:O	2.62	0.48
30:0:1515:A:H2'	30:0:1516:U:C6	2.48	0.48
30:0:366:U:H2'	30:0:367:G:O4'	2.14	0.48
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.44	0.48
19:S:33:SER:O	19:S:37:VAL:HG23	2.12	0.48
30:0:2826:G:C6	30:0:2913:A:N6	2.82	0.48
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.95	0.48
3:C:218:VAL:HG12	38:C:8627:HOH:O	2.13	0.48
31:9:107:C:O2'	31:9:108:C:H5'	2.13	0.48
30:0:734:U:O2'	30:0:736:A:N7	2.41	0.48
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.39	0.48
10:J:47:THR:HG21	30:0:1244:U:H2'	1.96	0.48
30:0:1666:C:HO2'	30:0:1667:A:H5''	1.73	0.48
3:C:132:ASP:HB2	3:C:161:ASP:HB3	1.94	0.48
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.49	0.48
30:0:1451:C:H5'	30:0:1505:U:C5	2.48	0.48
18:R:33:ARG:NH1	38:R:8945:HOH:O	2.46	0.48
15:O:39:THR:O	15:O:115:ARG:NH2	2.46	0.48
27:1:45:ARG:HB3	38:1:8965:HOH:O	2.13	0.48
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.96	0.48
30:0:101:C:H2'	30:0:102:A:H8	1.79	0.48
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.60	0.48
30:0:1298:U:H2'	30:0:1299:G:C8	2.49	0.48
30:0:2104:C:O2	30:0:2485:A:N1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:482:G:O4'	30:0:511:A:C2	2.66	0.48
30:0:2689:A:H2'	30:0:2690:U:H5'	1.95	0.48
30:0:2613:G:O2'	30:0:2614:C:H5'	2.13	0.48
30:0:652:G:H8	38:0:3013:HOH:O	1.97	0.48
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.46	0.48
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.78	0.48
30:0:1188:A:C6	30:0:1189:A:C6	3.02	0.48
30:0:545:G:C8	30:0:545:G:C5'	2.89	0.48
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.62	0.48
30:0:1603:A:C5'	30:0:1605:G:O4'	2.51	0.48
30:0:559:U:C3'	30:0:559:U:C6	2.97	0.48
30:0:877:G:C5'	30:0:878:G:OP1	2.58	0.48
19:S:57:THR:HG22	19:S:59:ASP:N	2.29	0.48
31:9:108:C:H2'	31:9:109:G:C8	2.49	0.48
9:I:78:ALA:HB1	9:I:93:ALA:HB1	1.95	0.48
30:0:1381:A:N3	30:0:1382:G:H1'	2.29	0.48
30:0:2456:A:H2'	30:0:2457:U:C6	2.49	0.48
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.96	0.48
30:0:466:A:H2'	30:0:467:G:O4'	2.14	0.48
31:9:3:A:OP2	31:9:25:G:N2	2.47	0.48
2:B:72:THR:HB	38:B:9071:HOH:O	2.12	0.48
30:0:64:G:H2'	30:0:65:C:O4'	2.14	0.48
10:J:42:GLU:O	10:J:131:THR:HG23	2.14	0.48
30:0:912:A:C4	30:0:1294:A:C2	3.01	0.48
27:1:45:ARG:NH2	38:1:8973:HOH:O	2.42	0.48
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.96	0.48
30:0:2336:G:H1'	38:0:6316:HOH:O	2.14	0.48
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.79	0.48
30:0:2385:G:H2'	30:0:2386:U:C6	2.49	0.48
30:0:1163:G:N1	30:0:1184:C:N4	2.62	0.47
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.95	0.47
2:B:79:MET:HE1	38:B:9091:HOH:O	2.13	0.47
30:0:228:C:C2'	30:0:229:G:H5'	2.44	0.47
1:A:95:PRO:HA	1:A:153:ARG:HA	1.96	0.47
30:0:1135:G:H5'	38:0:5943:HOH:O	2.12	0.47
4:D:62:ASP:HA	38:D:4233:HOH:O	2.14	0.47
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.28	0.47
30:0:724:G:O2'	30:0:725:C:H5'	2.14	0.47
14:N:4:PRO:HB2	30:0:1010:C:H4'	1.95	0.47
30:0:2781:U:O2'	30:0:2782:G:H5'	2.14	0.47
3:C:78:ARG:HH11	3:C:78:ARG:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2072:G:C6	30:0:2533:C:H1'	2.49	0.47
30:0:1138:G:H4'	38:0:5714:HOH:O	2.12	0.47
1:A:206:ARG:NH2	30:0:2630:G:O6	2.47	0.47
30:0:179:C:H5''	38:0:9308:HOH:O	2.13	0.47
11:K:18:ILE:HG22	11:K:93:ASN:HB2	1.95	0.47
30:0:1189:A:H1'	30:0:1209:C:H1'	1.96	0.47
30:0:602:A:O2'	30:0:605:C:H4'	2.13	0.47
30:0:1592:G:H2'	30:0:1593:C:H6	1.78	0.47
30:0:876:A:N3	30:0:876:A:C2'	2.77	0.47
30:0:1755:A:H2'	30:0:1756:G:O4'	2.14	0.47
30:0:2534:C:H2'	30:0:2535:U:C6	2.50	0.47
30:0:1790:C:H2'	30:0:1791:U:H6	1.79	0.47
30:0:951:A:C2'	30:0:952:G:H5'	2.44	0.47
20:T:54:ASP:OD2	30:0:316:A:H5'	2.14	0.47
27:1:37:CYS:SG	27:1:39:PHE:HB2	2.54	0.47
30:0:111:C:O2'	30:0:112:G:H5'	2.14	0.47
30:0:2589:U:H2'	30:0:2590:U:C6	2.49	0.47
30:0:497:A:H2'	30:0:498:A:C5'	2.45	0.47
30:0:790:A:H2'	30:0:791:A:O4'	2.14	0.47
17:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.14	0.47
30:0:247:A:H2'	38:0:3924:HOH:O	2.14	0.47
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.95	0.47
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.96	0.47
30:0:42:C:H1'	38:0:4679:HOH:O	2.14	0.47
30:0:1163:G:N2	38:0:4729:HOH:O	2.47	0.47
30:0:1183:C:C2	30:0:1184:C:C5	3.02	0.47
30:0:283:U:H5	30:0:284:C:C4	2.32	0.47
7:G:12:ILE:HG12	38:0:5471:HOH:O	2.14	0.47
18:R:29:LYS:HE2	30:0:524:A:C5'	2.44	0.47
19:S:77:VAL:O	19:S:80:ARG:HG2	2.14	0.47
31:9:61:C:H2'	31:9:62:A:H8	1.79	0.47
30:0:920:C:H4'	30:0:921:G:C2	2.49	0.47
13:M:95:LYS:HE2	30:0:157:G:H4'	1.96	0.47
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.40	0.47
18:R:132:ARG:HG2	18:R:133:ALA:N	2.28	0.47
30:0:1166:A:C6	30:0:1181:A:C2	3.03	0.47
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.12	0.47
31:9:39:U:C2'	31:9:40:C:OP1	2.63	0.47
30:0:821:U:H2'	30:0:822:C:C6	2.50	0.47
13:M:30:GLU:O	13:M:34:GLU:HG3	2.15	0.47
2:B:62:ARG:HA	2:B:65:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.95	0.47
30:0:2802:C:H2'	30:0:2803:C:C6	2.49	0.47
30:0:517:U:H1'	38:0:7599:HOH:O	2.14	0.47
30:0:1386:G:O2'	30:0:1387:G:H5'	2.14	0.47
16:P:91:LYS:O	16:P:95:GLU:HG3	2.15	0.47
30:0:2387:U:H2'	30:0:2388:C:C6	2.49	0.47
30:0:1664:A:H8	30:0:1664:A:OP1	1.96	0.47
13:M:164:THR:HB	38:M:8819:HOH:O	2.15	0.47
13:M:9:ARG:HD2	30:0:380:A:OP2	2.15	0.47
30:0:1592:G:O2'	30:0:1593:C:O4'	2.32	0.47
26:Z:34:SER:N	30:0:796:A:HO2'	2.13	0.47
30:0:1058:A:H2'	30:0:1060:C:C5'	2.42	0.47
30:0:1741:U:C4	30:0:2033:G:C8	3.02	0.47
30:0:2032:U:H2'	30:0:2033:G:C5'	2.45	0.47
30:0:2133:U:H4'	30:0:2134:G:H5'	1.95	0.47
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.15	0.47
22:V:44:GLY:O	22:V:48:GLU:HG2	2.14	0.47
3:C:118:THR:O	3:C:136:VAL:HG13	2.13	0.47
30:0:1495:C:H1'	30:0:1573:A:H1'	1.97	0.47
30:0:711:G:H1'	38:0:7120:HOH:O	2.13	0.47
30:0:737:A:H2'	30:0:738:G:O4'	2.15	0.47
4:D:36:ASN:HA	38:D:7500:HOH:O	2.15	0.47
30:0:1214:G:H4'	38:0:4752:HOH:O	2.14	0.47
30:0:2842:G:H2'	30:0:2843:A:H5'	1.96	0.47
30:0:932:U:H2'	30:0:933:C:C6	2.49	0.47
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.14	0.47
30:0:1823:G:O2'	30:0:1824:C:H5'	2.15	0.47
30:0:1165:G:O3'	30:0:1174:A:H4'	2.14	0.47
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.42	0.47
30:0:1878:G:O2'	30:0:1879:U:H6	1.98	0.47
30:0:1592:G:O2'	30:0:1593:C:O5'	2.32	0.47
30:0:2361:A:H2'	30:0:2362:A:O4'	2.14	0.47
26:Z:57:MET:SD	26:Z:73:ARG:HD2	2.55	0.47
1:A:33:GLU:O	1:A:34:ASP:HB2	2.15	0.47
30:0:940:G:C5	30:0:1027:G:C2	3.03	0.47
30:0:1291:A:H2	38:0:5300:HOH:O	1.97	0.47
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.15	0.47
30:0:1029:U:O2'	30:0:1273:C:OP1	2.30	0.47
30:0:396:U:HO2'	30:0:397:A:P	2.38	0.47
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.79	0.47
30:0:734:U:H1'	30:0:737:A:N6	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:101:C:H2'	30:0:102:A:C8	2.50	0.47
30:0:2326:C:H4'	30:0:2412:G:C4'	2.45	0.47
31:9:1:U:H4'	31:9:3:A:OP1	2.15	0.47
10:J:76:ASP:HA	38:J:5907:HOH:O	2.14	0.47
30:0:1221:G:H8	38:0:6005:HOH:O	1.97	0.47
30:0:1422:U:H2'	30:0:1423:C:C6	2.49	0.47
30:0:445:U:H2'	30:0:446:G:H8	1.80	0.47
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.97	0.46
24:X:43:VAL:HG12	24:X:44:ASP:H	1.79	0.46
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.48	0.46
30:0:2866:U:H4'	30:0:2867:G:H5'	1.97	0.46
21:U:6:CYS:HA	21:U:13:ILE:HD11	1.97	0.46
9:I:101:LYS:O	9:I:105:GLU:HG3	2.15	0.46
8:H:31:ILE:HG23	38:H:8576:HOH:O	2.15	0.46
10:J:63:ILE:HD11	30:0:1236:A:C8	2.50	0.46
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.96	0.46
21:U:9:CYS:HA	21:U:52:THR:CG2	2.44	0.46
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.98	0.46
27:1:25:LYS:HD2	28:2:49:GLU:N	2.30	0.46
14:N:4:PRO:HG3	31:9:69:U:OP1	2.15	0.46
30:0:690:G:H4'	30:0:741:C:O2	2.15	0.46
30:0:953:G:H4'	30:0:954:U:OP1	2.15	0.46
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.50	0.46
30:0:151:A:C2	30:0:152:A:C2	3.04	0.46
30:0:2314:G:C2'	30:0:2315:C:H5'	2.45	0.46
23:W:5:VAL:HG11	23:W:153:MET:CE	2.45	0.46
30:0:2004:U:H2'	30:0:2005:G:OP1	2.14	0.46
30:0:255:A:C4	30:0:256:C:C6	3.02	0.46
30:0:1477:C:H5'	30:0:1868:G:H5''	1.97	0.46
14:N:169:PRO:O	14:N:172:PHE:HB3	2.16	0.46
15:O:39:THR:HB	38:0:4618:HOH:O	2.14	0.46
13:M:28:GLN:O	13:M:32:ARG:HG3	2.15	0.46
20:T:12:ARG:NH1	38:T:3035:HOH:O	2.49	0.46
23:W:88:THR:HG22	23:W:89:ASP:N	2.29	0.46
3:C:64:GLY:O	30:0:2100:A:H4'	2.15	0.46
30:0:1198:U:C6	30:0:1200:A:OP2	2.69	0.46
30:0:2329:C:O2'	30:0:2330:U:H5'	2.15	0.46
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.98	0.46
30:0:307:G:H3'	38:0:6714:HOH:O	2.15	0.46
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.48	0.46
30:0:1856:C:H5'	30:0:1858:A:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2515:C:H2'	30:0:2516:G:O4'	2.15	0.46
14:N:154:LEU:C	14:N:156:GLU:H	2.17	0.46
30:0:426:G:H2'	30:0:427:C:O4'	2.16	0.46
4:D:82:GLU:HA	4:D:85:GLN:HE21	1.81	0.46
30:0:1634:G:C3'	38:0:3895:HOH:O	2.51	0.46
30:0:2600:A:H2'	30:0:2601:A:O4'	2.15	0.46
30:0:137:U:OP1	30:0:259:G:O2'	2.30	0.46
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.50	0.46
25:Y:148:GLY:HA3	30:0:622:G:P	2.56	0.46
30:0:834:G:H4'	30:0:835:U:OP2	2.15	0.46
30:0:861:A:H4'	30:0:1697:G:H4'	1.98	0.46
30:0:1503:U:H2'	30:0:1504:A:O4'	2.15	0.46
30:0:17:G:H2'	30:0:18:C:C6	2.51	0.46
30:0:177:A:H2'	30:0:178:U:O4'	2.15	0.46
26:Z:45:VAL:HG12	38:Z:8713:HOH:O	2.15	0.46
5:E:133:VAL:HG12	5:E:141:VAL:HG13	1.98	0.46
30:0:645:U:O2	30:0:761:A:H2	1.97	0.46
30:0:1166:A:N6	30:0:1180:U:H3	1.97	0.46
30:0:1181:A:H2'	30:0:1182:C:C5'	2.45	0.46
30:0:1204:C:H2'	30:0:1205:U:O4'	2.15	0.46
30:0:2291:A:N9	30:0:2309:C:H5'	2.30	0.46
1:A:199:HIS:HE1	30:0:1881:A:OP1	1.98	0.46
30:0:1973:A:H2'	30:0:1974:G:O4'	2.16	0.46
10:J:19:MET:HE1	10:J:79:PHE:HA	1.98	0.46
30:0:1562:C:O2	30:0:1562:C:C2'	2.61	0.46
14:N:11:ARG:NH1	31:9:8:G:O6	2.49	0.46
30:0:2071:C:H5'	38:0:9527:HOH:O	2.16	0.46
2:B:27:ASN:HD21	30:0:2807:U:P	2.38	0.46
30:0:1419:U:H2'	30:0:1685:A:C2	2.51	0.46
14:N:171:HIS:CE1	38:N:8862:HOH:O	2.68	0.46
30:0:2754:G:H2'	30:0:2755:G:O4'	2.16	0.46
30:0:2765:C:H2'	30:0:2766:A:C8	2.50	0.46
30:0:1202:A:H2'	30:0:1203:G:C5'	2.45	0.46
30:0:1942:A:O2'	30:0:1943:C:H5'	2.16	0.46
30:0:905:C:H3'	38:0:5195:HOH:O	2.15	0.46
30:0:1926:G:H2'	30:0:1927:A:H8	1.80	0.46
20:T:111:ARG:HB3	20:T:119:ALA:HB2	1.98	0.46
30:0:2569:A:H2'	30:0:2570:G:O5'	2.16	0.46
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.97	0.46
30:0:2269:C:H2'	30:0:2270:G:C5'	2.46	0.46
2:B:205:VAL:O	2:B:307:ARG:NE	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2840:A:H3'	38:0:7669:HOH:O	2.15	0.46
30:0:365:G:C6	30:0:366:U:C4	3.04	0.46
1:A:29:HIS:HB2	1:A:153:ARG:HH12	1.80	0.46
30:0:834:G:H3'	30:0:835:U:H4'	1.97	0.46
4:D:131:THR:HG21	30:0:2348:C:H1'	1.97	0.46
30:0:2371:G:H5'	38:0:5018:HOH:O	2.15	0.46
30:0:2245:C:H6	30:0:2245:C:O5'	1.99	0.46
30:0:1244:U:H4'	30:0:1246:A:O4'	2.16	0.46
1:A:211:LYS:HG2	38:0:7054:HOH:O	2.16	0.46
30:0:2895:C:H2'	38:0:9570:HOH:O	2.15	0.46
2:B:234:ARG:HD3	30:0:1734:C:OP1	2.15	0.46
30:0:1321:A:H2'	30:0:1322:G:H8	1.80	0.46
30:0:807:A:H2'	30:0:808:A:C8	2.50	0.46
27:1:46:ARG:HA	38:0:3021:HOH:O	2.15	0.46
30:0:2710:U:O2'	30:0:2711:U:H5'	2.16	0.46
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.98	0.46
2:B:275:GLY:O	2:B:291:ASP:HA	2.16	0.46
31:9:23:U:HO2'	31:9:24:U:H4'	1.77	0.46
5:E:68:HIS:O	5:E:72:MET:HG3	2.15	0.46
12:L:39:GLU:HG2	30:0:926:A:C4'	2.46	0.46
30:0:2433:A:H2'	30:0:2434:A:C8	2.50	0.46
30:0:1902:G:H2'	30:0:1903:U:O4'	2.16	0.46
30:0:1904:A:H2'	30:0:1905:U:O4'	2.16	0.46
2:B:254:GLN:HG3	38:0:9698:HOH:O	2.14	0.46
30:0:106:A:H2'	30:0:107:U:O4'	2.16	0.46
8:H:91:ARG:O	30:0:1003:U:H4'	2.16	0.46
30:0:324:G:O2'	30:0:325:U:H5'	2.16	0.46
25:Y:107:PRO:HB3	25:Y:182:PHE:CD2	2.51	0.46
30:0:2512:U:H4'	30:0:2514:U:O4	2.16	0.45
24:X:76:ARG:NH1	24:X:76:ARG:HG3	2.27	0.45
12:L:57:VAL:HG12	12:L:57:VAL:O	2.16	0.45
30:0:2301:A:H5''	30:0:2302:A:H5'	1.98	0.45
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.98	0.45
30:0:2345:A:H3'	30:0:2346:C:C6	2.50	0.45
31:9:108:C:H2'	31:9:109:G:H8	1.81	0.45
30:0:1213:C:O2'	30:0:1214:G:H5'	2.16	0.45
6:F:21:GLU:O	6:F:24:ARG:HG2	2.16	0.45
29:3:34:LYS:HE2	38:0:4426:HOH:O	2.16	0.45
8:H:141:CYS:HB2	38:H:8540:HOH:O	2.17	0.45
30:0:192:A:H5'	38:0:7665:HOH:O	2.15	0.45
30:0:2505:G:H2'	30:0:2506:A:C5'	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.80	0.45
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.03	0.45
30:0:271:C:C2	30:0:273:G:O4'	2.69	0.45
7:G:16:LYS:HE2	7:G:63:ARG:NH1	2.31	0.45
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.46	0.45
30:0:2408:A:H2	38:0:3102:HOH:O	1.98	0.45
30:0:1398:G:H2'	30:0:1399:A:C8	2.51	0.45
19:S:45:TYR:O	19:S:80:ARG:NH2	2.49	0.45
30:0:2880:A:H2'	30:0:2881:C:H5'	1.99	0.45
2:B:10:SER:HB2	30:0:2714:U:H4'	1.96	0.45
29:3:22:VAL:HG11	29:3:67:LEU:HD13	1.98	0.45
30:0:1183:C:H1'	30:0:1192:A:N6	2.31	0.45
30:0:484:A:N1	30:0:506:G:H4'	2.31	0.45
30:0:2896:A:N3	30:0:2896:A:H2'	2.31	0.45
14:N:1:ALA:HB2	31:9:14:G:O2'	2.17	0.45
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.45
13:M:24:GLN:NE2	13:M:27:ARG:HH11	2.15	0.45
31:9:59:C:H6	31:9:59:C:O5'	1.99	0.45
30:0:661:G:C5	30:0:686:A:C2	3.05	0.45
30:0:2765:C:H2'	30:0:2766:A:H8	1.82	0.45
14:N:160:SER:HB3	31:9:51:A:H5'	1.97	0.45
30:0:803:C:O2'	30:0:804:C:H5'	2.17	0.45
18:R:71:LYS:HE2	30:0:2831:C:O3'	2.17	0.45
30:0:1544:U:H2'	30:0:1545:C:C6	2.52	0.45
2:B:198:GLU:HA	38:B:9121:HOH:O	2.16	0.45
30:0:1730:G:C5'	30:0:1731:C:H6	2.27	0.45
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.51	0.45
31:9:34:A:H2'	31:9:35:C:O4'	2.17	0.45
30:0:1790:C:H2'	30:0:1791:U:C6	2.51	0.45
30:0:587:A:H5''	38:0:7309:HOH:O	2.17	0.45
30:0:958:G:O2'	30:0:959:C:H5'	2.16	0.45
26:Z:76:THR:HG21	30:0:1652:C:H4'	1.98	0.45
19:S:11:THR:H	19:S:14:ALA:HB3	1.81	0.45
12:L:148:GLU:HA	38:L:8877:HOH:O	2.16	0.45
23:W:130:HIS:O	23:W:136:GLY:HA3	2.16	0.45
30:0:1622:G:H2'	30:0:1623:C:H5'	1.99	0.45
30:0:368:C:H2'	30:0:369:G:H5'	1.98	0.45
30:0:2748:G:C2'	38:0:7565:HOH:O	2.57	0.45
30:0:1771:U:O2'	30:0:1773:G:N7	2.48	0.45
30:0:1596:U:H2'	30:0:1598:A:OP2	2.15	0.45
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2326:C:H4'	30:0:2412:G:H4'	1.99	0.45
30:0:958:G:H2'	30:0:959:C:C6	2.52	0.45
30:0:1521:C:H2'	30:0:1522:A:H8	1.82	0.45
30:0:1626:A:H2'	30:0:1627:G:C5'	2.46	0.45
30:0:1186:C:N4	30:0:1187:U:C4	2.84	0.45
30:0:1190:G:H2'	38:0:4061:HOH:O	2.16	0.45
24:X:74:ALA:HB2	24:X:85:VAL:HG13	1.99	0.45
31:9:3:A:H2	31:9:21:G:N3	2.15	0.45
11:K:41:LYS:O	11:K:42:ASN:HB2	2.17	0.45
10:J:19:MET:CE	10:J:132:LEU:HD11	2.46	0.45
30:0:2102:G:C2	30:0:2104:C:C4	3.05	0.45
30:0:1477:C:H5'	30:0:1868:G:H5'	1.96	0.45
18:R:39:THR:HB	18:R:42:GLU:HG3	1.99	0.45
13:M:24:GLN:HA	13:M:24:GLN:NE2	2.32	0.45
30:0:1008:C:O2'	30:0:1009:U:H5'	2.17	0.45
30:0:1762:C:O2'	30:0:1763:C:H5'	2.17	0.45
30:0:570:C:H6	30:0:570:C:O5'	2.00	0.45
30:0:1123:A:C2	30:0:1129:C:H4'	2.52	0.45
6:F:107:ASP:O	6:F:111:ILE:HG13	2.16	0.45
4:D:18:ILE:HD13	4:D:84:LEU:HD12	1.97	0.45
30:0:371:U:H2'	30:0:372:A:H8	1.82	0.45
30:0:48:A:N1	30:0:148:A:O2'	2.42	0.45
30:0:1588:G:C6	30:0:1589:G:N1	2.85	0.45
30:0:2769:C:H2'	30:0:2770:G:O4'	2.16	0.45
30:0:960:G:H8	38:0:5988:HOH:O	1.99	0.45
30:0:2691:A:H5'	30:0:2693:U:H1'	1.99	0.45
2:B:223:ARG:HG3	2:B:232:TRP:O	2.16	0.45
30:0:95:A:H5''	30:0:97:G:O4'	2.16	0.45
30:0:1149:U:H5''	30:0:1151:G:O4'	2.17	0.45
30:0:2729:C:O2'	30:0:2730:G:H5'	2.16	0.45
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.84	0.45
30:0:1931:A:H2'	30:0:1932:G:H5'	1.99	0.45
14:N:37:ARG:NH2	38:N:8834:HOH:O	2.48	0.45
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.44	0.45
24:X:72:VAL:HG22	24:X:85:VAL:HG12	1.99	0.45
30:0:559:U:H3'	30:0:559:U:C6	2.51	0.45
10:J:75:PRO:HD3	10:J:136:SER:OG	2.17	0.45
30:0:594:C:C4	30:0:595:U:C4	3.05	0.45
3:C:76:ARG:HH22	30:0:1363:G:P	2.40	0.45
30:0:2265:U:H2'	30:0:2266:A:C8	2.51	0.45
15:O:77:ALA:HA	15:O:96:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1154:A:H2'	30:0:1155:G:C8	2.52	0.45
1:A:210:GLY:HA3	38:0:5306:HOH:O	2.16	0.45
30:0:1434:A:H2'	30:0:1436:C:C5	2.51	0.45
8:H:174:LEU:HA	38:H:8567:HOH:O	2.17	0.45
12:L:80:ASP:HB2	12:L:90:ARG:O	2.17	0.45
30:0:2553:A:H2'	30:0:2553:A:N3	2.31	0.45
30:0:254:C:O2	30:0:254:C:H2'	2.15	0.45
30:0:1278:A:H4'	30:0:1279:U:N3	2.32	0.45
30:0:657:G:H2'	30:0:658:C:C6	2.52	0.45
30:0:407:A:H8	38:0:4459:HOH:O	2.00	0.45
30:0:2092:G:H2'	30:0:2613:G:OP1	2.16	0.45
30:0:1576:G:H2'	30:0:1577:U:O4'	2.17	0.45
2:B:229:ARG:HD2	38:0:9112:HOH:O	2.17	0.45
30:0:2106:C:H5'	30:0:2284:G:H21	1.81	0.45
30:0:1444:G:O2'	30:0:1445:G:H5'	2.17	0.45
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.78	0.45
30:0:1245:C:O5'	30:0:1245:C:H6	1.99	0.45
30:0:1878:G:H5'	38:0:4371:HOH:O	2.18	0.44
38:Y:8907:HOH:O	30:0:1330:A:C5'	2.54	0.44
30:0:2672:C:O2'	30:0:2673:U:H5'	2.17	0.44
15:O:24:ALA:HB3	30:0:710:G:OP1	2.17	0.44
30:0:111:C:C2'	30:0:112:G:H5'	2.48	0.44
30:0:2072:G:H3'	30:0:2073:G:C5'	2.48	0.44
13:M:182:LYS:HE2	30:0:392:U:O2'	2.17	0.44
9:I:84:SER:HB3	9:I:92:VAL:CG2	2.47	0.44
30:0:1413:A:H2'	30:0:1414:A:O4'	2.17	0.44
30:0:2566:A:C2	30:0:2696:G:O4'	2.70	0.44
12:L:92:ASP:HA	12:L:121:ILE:HB	1.98	0.44
30:0:1457:U:H5	38:0:7895:HOH:O	2.00	0.44
30:0:1165:G:H21	30:0:1173:A:C5'	2.27	0.44
30:0:2717:C:C2'	30:0:2718:C:C5'	2.78	0.44
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.82	0.44
15:O:25:VAL:CG1	30:0:710:G:H5'	2.48	0.44
30:0:941:G:C6	30:0:942:U:C4	3.06	0.44
9:I:93:ALA:HB3	9:I:132:VAL:HG22	1.99	0.44
30:0:1453:G:N2	30:0:1675:C:C2	2.86	0.44
30:0:2487:C:H5	38:0:4897:HOH:O	2.01	0.44
29:3:91:GLN:O	29:3:92:GLU:HB2	2.18	0.44
30:0:1184:C:O2'	30:0:1185:U:OP2	2.33	0.44
3:C:2:GLN:HB3	38:C:8588:HOH:O	2.17	0.44
30:0:1972:U:C2'	30:0:1973:A:C5'	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:ARG:HB3	38:B:9112:HOH:O	2.18	0.44
30:0:2134:G:C6	30:0:2258:A:C8	3.06	0.44
31:9:52:A:C2'	31:9:53:G:H5'	2.48	0.44
6:F:58:GLU:HA	6:F:61:MET:HG3	2.00	0.44
4:D:135:VAL:HG22	4:D:136:ARG:H	1.82	0.44
2:B:16:ARG:NH2	38:B:9020:HOH:O	2.42	0.44
3:C:107:ARG:O	3:C:111:VAL:HG23	2.17	0.44
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.99	0.44
30:0:1976:G:O2'	30:0:1977:U:H5'	2.18	0.44
30:0:1739:G:O2'	30:0:1740:U:H5'	2.17	0.44
10:J:47:THR:HG22	10:J:48:GLY:N	2.32	0.44
30:0:1589:G:C2	30:0:1605:G:N3	2.86	0.44
30:0:1940:C:H4'	38:0:7371:HOH:O	2.17	0.44
31:9:3:A:N6	31:9:22:G:H1'	2.32	0.44
30:0:69:A:C8	30:0:69:A:C5'	2.95	0.44
20:T:62:VAL:N	38:T:3851:HOH:O	2.51	0.44
30:0:1406:A:H4'	30:0:1407:A:C5'	2.48	0.44
30:0:488:U:H2'	38:0:4010:HOH:O	2.18	0.44
30:0:1850:U:H2'	30:0:1851:G:H8	1.82	0.44
30:0:962:C:H2'	30:0:963:C:H5'	2.00	0.44
6:F:46:GLU:OE2	6:F:100:ASP:HA	2.17	0.44
16:P:115:SER:OG	16:P:118:GLN:HG3	2.17	0.44
30:0:2498:C:C2'	30:0:2499:U:H5'	2.47	0.44
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.33	0.44
2:B:41:PHE:HB3	2:B:190:MET:CE	2.45	0.44
6:F:48:VAL:HG23	6:F:74:PHE:CB	2.46	0.44
12:L:34:GLY:HA2	38:0:5421:HOH:O	2.17	0.44
23:W:23:MET:O	30:0:1025:C:H5'	2.17	0.44
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.99	0.44
30:0:1783:A:O2'	30:0:1784:U:H5'	2.17	0.44
6:F:59:ILE:CD1	30:0:263:U:C2	3.01	0.44
26:Z:44:ARG:HB2	30:0:1886:A:O2'	2.17	0.44
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.49	0.44
30:0:646:G:H2'	30:0:647:U:C6	2.53	0.44
13:M:75:ARG:HH11	30:0:1864:C:H5	1.61	0.44
14:N:132:ASN:O	14:N:135:VAL:HG12	2.17	0.44
30:0:1588:G:C5	30:0:1589:G:C6	3.06	0.44
30:0:2256:G:C2'	30:0:2257:G:C5'	2.96	0.44
15:O:25:VAL:HG23	15:O:26:TRP:N	2.33	0.44
9:I:102:GLN:HA	9:I:105:GLU:OE2	2.18	0.44
30:0:1520:G:H2'	30:0:1521:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1497:G:H4'	30:0:1627:G:O2'	2.18	0.44
30:0:1683:G:C2	30:0:1693:A:O4'	2.71	0.44
13:M:164:THR:HG23	13:M:165:GLY:N	2.33	0.44
30:0:2421:G:H3'	30:0:2422:U:C5'	2.47	0.44
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.47	0.44
3:C:184:ARG:HD2	30:0:1306:U:OP1	2.18	0.44
29:3:11:CYS:HB2	29:3:20:HIS:HE1	1.82	0.44
30:0:629:A:H2'	30:0:630:A:O4'	2.18	0.44
30:0:920:C:H5''	30:0:921:G:O5'	2.17	0.44
30:0:932:U:H2'	30:0:933:C:H6	1.83	0.44
30:0:1624:A:H5'	30:0:1626:A:O4'	2.17	0.44
14:N:109:PRO:HB3	30:0:2413:A:N7	2.33	0.44
30:0:1021:G:O2'	30:0:1022:A:H5'	2.17	0.44
12:L:89:PHE:N	38:L:8876:HOH:O	2.50	0.44
9:I:69:PRO:HA	30:0:1164:U:OP1	2.18	0.44
23:W:125:HIS:HB2	23:W:137:GLN:HG2	1.99	0.44
30:0:2506:A:C4	38:0:6073:HOH:O	2.70	0.44
28:2:41:HIS:CD2	28:2:44:ARG:H	2.33	0.44
1:A:53:ALA:HB3	38:A:9061:HOH:O	2.18	0.44
30:0:538:C:H5''	30:0:539:G:C8	2.53	0.44
2:B:243:ASN:HA	2:B:244:PRO:C	2.37	0.44
2:B:5:ARG:HD2	2:B:8:LYS:NZ	2.33	0.44
30:0:1762:C:H2'	30:0:1763:C:C6	2.53	0.44
30:0:1218:U:H2'	30:0:1219:U:C6	2.52	0.44
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.48	0.44
14:N:23:ARG:NH1	38:N:8865:HOH:O	2.51	0.44
30:0:1350:U:H4'	38:0:5132:HOH:O	2.17	0.44
30:0:823:U:H3'	38:0:4445:HOH:O	2.18	0.44
15:O:32:ARG:HD3	15:O:32:ARG:O	2.18	0.44
30:0:1702:U:H1'	38:0:5781:HOH:O	2.18	0.44
30:0:1477:C:C5'	30:0:1868:G:H5''	2.47	0.44
6:F:91:VAL:CG1	6:F:92:GLY:N	2.79	0.44
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.53	0.44
29:3:70:ARG:HD3	38:3:9062:HOH:O	2.18	0.44
30:0:523:C:H2'	30:0:524:A:H8	1.83	0.44
29:3:3:MET:HG3	29:3:4:PRO:HD2	1.99	0.44
31:9:59:C:H2'	31:9:60:C:C6	2.53	0.44
30:0:1015:C:H2'	30:0:1016:U:H6	1.83	0.44
30:0:1544:U:H2'	30:0:1545:C:H6	1.83	0.44
38:Z:8706:HOH:O	30:0:1886:A:H4'	2.18	0.44
30:0:113:A:OP2	30:0:114:A:H2'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:165:GLU:HB3	38:Y:8888:HOH:O	2.17	0.44
3:C:153:VAL:O	3:C:157:LEU:HG	2.17	0.44
1:A:105:VAL:HG12	1:A:106:CYS:N	2.31	0.43
30:0:2252:A:C2'	30:0:2253:G:H5'	2.47	0.43
30:0:2642:G:H2'	30:0:2643:G:O4'	2.18	0.43
30:0:212:A:O4'	30:0:214:U:C6	2.71	0.43
2:B:8:LYS:HG3	2:B:220:VAL:HG12	2.00	0.43
30:0:861:A:C4'	30:0:1697:G:H4'	2.48	0.43
30:0:1520:G:C6	30:0:1521:C:C4	3.06	0.43
14:N:132:ASN:HD22	30:0:2413:A:H4'	1.83	0.43
30:0:2777:G:O2'	30:0:2778:A:H5'	2.18	0.43
23:W:43:GLY:HA3	30:0:945:U:O2'	2.18	0.43
25:Y:152:LYS:HB3	25:Y:160:LYS:HG3	2.00	0.43
30:0:1427:A:H61	30:0:1440:U:H1'	1.82	0.43
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.53	0.43
14:N:42:HIS:HB3	14:N:62:HIS:CE1	2.53	0.43
30:0:1192:A:H3'	30:0:1193:A:H5'	1.99	0.43
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.99	0.43
30:0:1878:G:O2'	30:0:1879:U:OP2	2.36	0.43
30:0:2133:U:H4'	30:0:2134:G:C5'	2.47	0.43
12:L:33:ALA:HB2	30:0:165:A:H5''	2.00	0.43
30:0:2816:A:H5''	30:0:2817:G:H5'	2.00	0.43
30:0:2375:A:H2'	30:0:2376:C:C6	2.53	0.43
30:0:349:U:O2'	30:0:350:G:H5'	2.18	0.43
30:0:2087:C:O2'	30:0:2088:C:H5'	2.18	0.43
12:L:18:HIS:HE1	30:0:901:G:OP2	2.00	0.43
30:0:1014:A:H2'	30:0:1015:C:H5'	2.00	0.43
30:0:1850:U:H2'	30:0:1851:G:C8	2.52	0.43
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.18	0.43
30:0:1681:G:H5''	30:0:1682:A:H5'	2.00	0.43
30:0:684:G:H2'	30:0:685:C:C6	2.54	0.43
30:0:1705:C:H2'	30:0:1706:G:O4'	2.18	0.43
4:D:138:GLY:N	38:D:7597:HOH:O	2.51	0.43
2:B:177:HIS:O	2:B:181:ILE:HG13	2.19	0.43
30:0:1815:A:H4'	30:0:2751:C:O4'	2.19	0.43
3:C:170:ASP:OD2	30:0:330:C:H5	2.02	0.43
5:E:90:HIS:CE1	30:0:2694:A:H5''	2.53	0.43
30:0:1625:U:H3'	30:0:1625:U:C6	2.52	0.43
4:D:58:VAL:HB	4:D:62:ASP:HB2	1.99	0.43
2:B:10:SER:O	2:B:16:ARG:NH1	2.48	0.43
30:0:945:U:H2'	30:0:946:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2791:U:H1'	30:0:2792:A:H5''	2.00	0.43
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.99	0.43
1:A:173:GLY:O	1:A:176:HIS:HB3	2.18	0.43
30:0:423:A:C5	30:0:424:C:C5	3.07	0.43
30:0:700:A:H5''	30:0:701:U:H5'	2.00	0.43
30:0:1463:U:H2'	30:0:1464:C:C6	2.54	0.43
30:0:2271:G:N3	30:0:2271:G:H2'	2.33	0.43
4:D:25:MET:SD	4:D:40:ILE:HD11	2.59	0.43
3:C:240:LEU:HB2	38:C:8650:HOH:O	2.18	0.43
30:0:2421:G:H3'	30:0:2422:U:H5''	2.01	0.43
2:B:62:ARG:HA	2:B:65:MET:HE2	2.00	0.43
3:C:39:GLN:O	3:C:43:LYS:HD3	2.18	0.43
30:0:398:U:H2'	30:0:399:C:C6	2.54	0.43
9:I:108:HIS:H	9:I:109:PRO:HD2	1.83	0.43
2:B:248:ARG:NH2	38:B:8994:HOH:O	2.51	0.43
30:0:2809:G:H2'	30:0:2810:G:O4'	2.19	0.43
30:0:899:C:H5'	38:0:3205:HOH:O	2.18	0.43
30:0:638:C:H2'	30:0:639:A:C8	2.54	0.43
29:3:48:ASN:ND2	29:3:50:GLY:H	2.16	0.43
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.48	0.43
30:0:1333:U:H2'	30:0:1334:C:H6	1.84	0.43
30:0:1761:U:H2'	30:0:1762:C:C6	2.54	0.43
30:0:1706:G:C6	30:0:1707:G:C6	3.06	0.43
30:0:1400:C:O2'	30:0:1401:G:H5'	2.19	0.43
30:0:1042:U:O2'	30:0:1043:C:H5'	2.18	0.43
30:0:1409:G:C2	30:0:1410:G:C8	3.07	0.43
20:T:28:SER:O	20:T:32:ARG:HG3	2.18	0.43
30:0:170:U:H2'	30:0:171:C:H5'	1.99	0.43
22:V:29:ASN:O	22:V:33:VAL:HG23	2.19	0.43
31:9:28:U:H5	38:9:9019:HOH:O	2.02	0.43
11:K:55:VAL:HG12	11:K:56:SER:N	2.34	0.43
3:C:93:LYS:O	3:C:98:ARG:NH2	2.51	0.43
30:0:1773:G:N2	30:0:1774:G:C8	2.86	0.43
30:0:1838:U:H3'	38:0:5534:HOH:O	2.19	0.43
19:S:57:THR:C	19:S:59:ASP:H	2.22	0.43
31:9:73:A:N1	31:9:108:C:O2	2.52	0.43
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.49	0.43
12:L:145:LEU:O	12:L:148:GLU:HG3	2.19	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.34	0.43
29:3:30:GLN:NE2	38:3:9042:HOH:O	2.51	0.43
14:N:65:ASP:HB3	38:N:8824:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1118:A:H8	30:0:1119:G:H5''	1.83	0.43
30:0:1170:U:O2'	30:0:1172:G:N7	2.45	0.43
26:Z:61:HIS:O	26:Z:69:ASP:HA	2.19	0.43
30:0:907:A:H4'	30:0:1328:A:C2	2.53	0.43
1:A:194:MET:SD	30:0:875:A:C2	3.12	0.43
22:V:39:ALA:N	22:V:40:PRO:CD	2.80	0.43
30:0:111:C:H2'	30:0:112:G:C5'	2.48	0.43
30:0:2597:U:H2'	30:0:2598:U:H5'	2.00	0.43
30:0:106:A:O2'	30:0:107:U:H5'	2.19	0.43
30:0:1622:G:C2'	30:0:1623:C:H5'	2.48	0.43
9:I:84:SER:HB3	9:I:92:VAL:HG21	1.99	0.43
15:O:38:ARG:HD3	30:0:654:A:OP2	2.19	0.43
25:Y:158:LYS:HD3	38:0:6305:HOH:O	2.18	0.43
30:0:2616:G:H1'	38:0:9424:HOH:O	2.18	0.43
28:2:28:LYS:O	30:0:87:C:H2'	2.19	0.43
13:M:49:ALA:C	13:M:54:TYR:HB3	2.39	0.43
13:M:171:ARG:NH2	30:0:189:A:OP1	2.52	0.43
30:0:2004:U:H2'	30:0:2004:U:O2	2.19	0.43
30:0:191:A:C4	30:0:237:G:N7	2.87	0.43
30:0:613:C:H2'	30:0:614:U:C6	2.50	0.43
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.33	0.43
4:D:23:VAL:HG23	4:D:23:VAL:O	2.19	0.43
25:Y:107:PRO:HB3	25:Y:182:PHE:CE2	2.54	0.43
30:0:1311:G:C2	30:0:1312:G:C8	3.06	0.43
30:0:289:G:O2'	30:0:290:C:H5'	2.19	0.43
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.34	0.43
30:0:1074:G:H4'	30:0:1260:G:C6	2.54	0.43
18:R:82:GLU:O	18:R:86:LYS:HG3	2.19	0.43
8:H:122:LYS:HB2	8:H:122:LYS:HE3	1.89	0.43
30:0:2506:A:O2'	30:0:2507:G:P	2.77	0.43
28:2:41:HIS:HE1	30:0:1439:C:OP1	2.02	0.43
30:0:69:A:H2'	30:0:70:A:OP2	2.18	0.43
30:0:1170:U:H1'	30:0:1172:G:N7	2.34	0.43
30:0:1525:G:OP1	30:0:1525:G:H4'	2.19	0.43
30:0:2102:G:C2	30:0:2103:A:N6	2.87	0.43
30:0:2134:G:N2	30:0:2242:U:C2	2.87	0.43
30:0:1343:C:C2'	30:0:1344:G:O5'	2.66	0.43
30:0:2253:G:H2'	30:0:2254:G:H8	1.84	0.43
30:0:305:A:C5	30:0:329:A:C2	3.07	0.43
30:0:1503:U:H3'	30:0:1503:U:H6	1.84	0.43
30:0:2379:G:N7	30:0:2408:A:N1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:ARG:NE	38:B:9020:HOH:O	2.38	0.43
22:V:4:HIS:HB3	38:0:7000:HOH:O	2.19	0.43
6:F:37:THR:O	6:F:41:GLU:HG3	2.19	0.43
18:R:47:LEU:HB2	18:R:89:LEU:HD21	2.01	0.43
2:B:154:VAL:HG12	2:B:156:LYS:HG2	2.01	0.43
30:0:168:C:H6	30:0:168:C:O5'	2.01	0.43
30:0:2638:G:H1'	38:0:7780:HOH:O	2.19	0.42
30:0:2769:C:C2'	30:0:2770:G:C5'	2.87	0.42
2:B:162:MET:SD	2:B:310:ARG:HD3	2.59	0.42
3:C:129:HIS:CE1	3:C:232:LEU:H	2.37	0.42
21:U:17:THR:CG2	21:U:18:GLY:N	2.81	0.42
29:3:69:TYR:CZ	29:3:80:ARG:HD2	2.54	0.42
30:0:694:A:C2'	30:0:695:C:H5'	2.49	0.42
30:0:1041:U:H4'	30:0:1295:G:H5'	2.01	0.42
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.54	0.42
1:A:175:LYS:HG3	30:0:1847:A:OP1	2.19	0.42
25:Y:146:PRO:O	25:Y:154:ARG:HG3	2.19	0.42
2:B:314:ALA:HB3	2:B:317:PRO:HG3	2.01	0.42
30:0:503:G:H2'	30:0:504:G:H8	1.84	0.42
30:0:134:U:C2	30:0:145:A:C2	3.07	0.42
30:0:2274:A:O2'	30:0:2275:G:H5'	2.19	0.42
10:J:88:PRO:HD3	30:0:1104:C:H4'	2.00	0.42
2:B:171:VAL:O	2:B:175:LEU:HB2	2.19	0.42
7:G:67:LEU:O	7:G:71:LEU:HG	2.18	0.42
30:0:1206:U:C3'	30:0:1206:U:C6	3.03	0.42
31:9:1:U:C4'	31:9:3:A:OP1	2.67	0.42
31:9:3:A:H1'	38:9:9036:HOH:O	2.18	0.42
30:0:1438:G:HO2'	30:0:1684:A:H2	1.67	0.42
30:0:2252:A:H2'	30:0:2253:G:C5'	2.49	0.42
30:0:2039:A:H4'	30:0:2760:C:O2'	2.19	0.42
4:D:63:ILE:HG13	4:D:64:ARG:N	2.34	0.42
3:C:218:VAL:N	38:C:8627:HOH:O	2.51	0.42
6:F:46:GLU:CD	6:F:100:ASP:HA	2.39	0.42
2:B:216:LYS:HA	38:0:5091:HOH:O	2.20	0.42
30:0:1211:G:H2'	30:0:1212:C:C6	2.54	0.42
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.01	0.42
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.85	0.42
30:0:2543:G:H2'	30:0:2544:G:O4'	2.18	0.42
30:0:2011:A:H4'	30:0:2012:U:O5'	2.19	0.42
30:0:1759:A:N3	30:0:1818:C:H2'	2.34	0.42
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:284:C:H4'	30:0:285:A:H8	1.84	0.42
23:W:119:HIS:CG	38:0:5297:HOH:O	2.71	0.42
30:0:1654:U:H5'	38:0:7446:HOH:O	2.18	0.42
12:L:120:LEU:HD12	12:L:133:VAL:HG21	2.01	0.42
30:0:820:G:O2'	30:0:856:G:H4'	2.20	0.42
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.49	0.42
14:N:139:TRP:HA	14:N:139:TRP:HE3	1.83	0.42
30:0:152:A:O2'	30:0:153:C:H5'	2.18	0.42
30:0:99:A:C8	30:0:100:C:C5	3.07	0.42
12:L:73:VAL:HG11	12:L:118:LEU:HD21	2.01	0.42
30:0:2758:G:H2'	30:0:2759:C:C6	2.54	0.42
30:0:1202:A:H2'	30:0:1203:G:H5'	2.00	0.42
2:B:74:ILE:HG13	38:B:9071:HOH:O	2.20	0.42
30:0:1632:A:C3'	30:0:1633:C:H5'	2.50	0.42
31:9:39:U:O2'	31:9:42:C:C5	2.72	0.42
25:Y:184:GLU:OE2	25:Y:204:ARG:HD2	2.20	0.42
3:C:46:TYR:CE1	30:0:450:C:H4'	2.54	0.42
30:0:154:C:H2'	30:0:155:C:H6	1.84	0.42
20:T:21:LYS:HA	20:T:24:ARG:HG3	2.01	0.42
30:0:2105:C:O2'	30:0:2284:G:N2	2.53	0.42
30:0:413:G:H2'	30:0:414:C:C6	2.54	0.42
30:0:1574:C:H6	30:0:1574:C:O5'	2.02	0.42
30:0:1161:A:O5'	30:0:1161:A:H8	2.02	0.42
30:0:1119:G:N2	30:0:1246:A:N1	2.67	0.42
30:0:1246:A:C4	30:0:1248:A:C8	3.08	0.42
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.52	0.42
29:3:69:TYR:O	29:3:77:ALA:HA	2.19	0.42
30:0:1615:A:H4'	38:0:5897:HOH:O	2.17	0.42
27:1:16:HIS:HE1	30:0:775:G:OP1	2.02	0.42
30:0:2842:G:C2'	30:0:2843:A:H5'	2.49	0.42
30:0:17:G:H2'	30:0:18:C:H6	1.83	0.42
30:0:677:C:P	38:0:7159:HOH:O	2.76	0.42
16:P:94:TRP:CZ2	16:P:98:ILE:HG13	2.55	0.42
30:0:947:U:O2'	30:0:948:G:H5'	2.20	0.42
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.55	0.42
2:B:307:ARG:HB3	38:B:9117:HOH:O	2.20	0.42
31:9:92:G:C6	31:9:93:A:C6	3.08	0.42
30:0:2094:G:O6	30:0:2649:A:H2	2.01	0.42
30:0:2090:G:H2'	30:0:2091:G:C8	2.53	0.42
30:0:2820:A:H2'	30:0:2821:C:C6	2.54	0.42
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:ARG:NH2	38:0:7159:HOH:O	2.53	0.42
30:0:47:G:N3	30:0:114:A:C2	2.88	0.42
30:0:1760:G:H5'	30:0:1818:C:O2'	2.19	0.42
14:N:119:GLN:O	14:N:123:ILE:HG13	2.19	0.42
30:0:764:C:H2'	30:0:765:G:O4'	2.19	0.42
30:0:1309:U:O2'	30:0:1310:U:H5'	2.20	0.42
30:0:1746:A:O4'	30:0:1747:A:C2	2.72	0.42
14:N:151:ASP:OD1	14:N:166:ALA:HA	2.19	0.42
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.91	0.42
2:B:60:SER:HA	2:B:61:PRO:HD3	1.89	0.42
30:0:1183:C:H41	30:0:1192:A:P	2.43	0.42
1:A:212:PRO:HA	30:0:1943:C:O4'	2.20	0.42
2:B:26:PHE:HE1	38:B:9112:HOH:O	2.02	0.42
30:0:1441:G:H1'	38:0:7786:HOH:O	2.19	0.42
3:C:46:TYR:CE2	3:C:98:ARG:NH1	2.87	0.42
5:E:91:PHE:HE1	30:0:2694:A:C4'	2.31	0.42
30:0:2653:A:H2'	30:0:2654:C:C6	2.55	0.42
7:G:64:ASN:N	7:G:64:ASN:ND2	2.67	0.42
31:9:65:A:N6	31:9:112:U:C6	2.88	0.42
30:0:23:G:C6	30:0:24:G:N1	2.88	0.42
19:S:57:THR:HG23	38:S:8982:HOH:O	2.19	0.42
29:3:65:THR:CG2	29:3:67:LEU:HG	2.50	0.42
30:0:1211:G:H2'	30:0:1212:C:H6	1.84	0.42
30:0:2594:C:O2'	30:0:2595:U:H5'	2.20	0.42
30:0:699:C:H6	30:0:744:G:O4'	2.03	0.42
30:0:295:C:H2'	30:0:296:G:O4'	2.19	0.42
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.20	0.42
31:9:42:C:H5'	31:9:43:G:OP2	2.19	0.42
2:B:211:THR:HG21	38:0:7480:HOH:O	2.19	0.42
1:A:36:ASP:CB	1:A:85:SER:H	2.33	0.42
30:0:2064:U:H2'	30:0:2065:C:H6	1.85	0.42
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.55	0.42
14:N:22:GLN:HA	14:N:25:ARG:CZ	2.50	0.42
30:0:2819:C:H2'	30:0:2820:A:C8	2.54	0.42
30:0:2105:C:H2'	30:0:2106:C:C6	2.55	0.42
2:B:132:HIS:CE1	2:B:171:VAL:HG23	2.55	0.42
20:T:77:VAL:HG11	20:T:91:LEU:HD11	2.02	0.42
30:0:1139:U:H2'	30:0:1140:C:C6	2.55	0.42
11:K:89:LYS:HE2	21:U:19:THR:HG21	2.02	0.42
30:0:40:C:H4'	38:0:7030:HOH:O	2.20	0.42
30:0:542:A:H1'	38:0:4680:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.35	0.42
30:0:2354:A:C2	30:0:2367:A:C8	3.08	0.42
14:N:61:ALA:CB	14:N:88:ALA:HB2	2.49	0.42
2:B:141:ARG:HG2	2:B:165:ARG:HA	2.02	0.42
30:0:2415:A:C2'	30:0:2416:G:H5'	2.49	0.42
30:0:595:U:H2'	30:0:596:C:C6	2.54	0.42
30:0:128:A:H3'	30:0:128:A:C8	2.55	0.42
30:0:1902:G:N2	30:0:1936:C:C2	2.88	0.42
30:0:2824:C:O3'	30:0:2825:C:H6	2.02	0.42
2:B:5:ARG:NH1	30:0:2547:C:OP2	2.53	0.42
30:0:860:U:H2'	30:0:861:A:C8	2.54	0.42
14:N:108:SER:HA	14:N:109:PRO:HD3	1.74	0.42
27:1:12:ASN:O	30:0:1415:G:H5'	2.20	0.42
13:M:167:GLY:O	13:M:171:ARG:HG3	2.20	0.42
1:A:88:ILE:HG22	1:A:88:ILE:O	2.19	0.42
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.42
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.84	0.42
30:0:920:C:H5'	30:0:921:G:C4	2.55	0.42
30:0:2379:G:H5'	30:0:2381:C:O4'	2.20	0.42
30:0:2691:A:OP1	30:0:2691:A:H8	2.03	0.42
30:0:1946:C:H2'	30:0:1971:G:C8	2.55	0.42
18:R:40:ALA:O	18:R:44:VAL:HG23	2.19	0.42
13:M:46:LEU:HG	38:M:8922:HOH:O	2.18	0.42
17:Q:86:VAL:HG13	17:Q:91:LEU:HD11	2.01	0.42
30:0:59:A:H5'	38:0:4331:HOH:O	2.20	0.42
30:0:851:C:O2	30:0:2022:A:H2	2.03	0.42
30:0:1825:U:O2'	30:0:1826:C:H5'	2.20	0.42
16:P:7:LYS:HD3	16:P:21:VAL:CG2	2.50	0.42
10:J:26:VAL:HG13	10:J:36:VAL:HG11	2.02	0.42
30:0:559:U:H2'	30:0:560:U:O4'	2.20	0.41
23:W:122:ARG:NH2	38:0:6425:HOH:O	2.53	0.41
30:0:441:A:H8	30:0:441:A:O5'	2.03	0.41
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.20	0.41
30:0:699:C:C6	30:0:744:G:C4	3.08	0.41
3:C:200:PRO:HB3	3:C:212:VAL:HG23	2.02	0.41
30:0:1788:U:C2	30:0:1805:G:N2	2.88	0.41
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.84	0.41
6:F:30:LYS:HE2	6:F:99:THR:HG21	2.01	0.41
16:P:81:LYS:HG2	38:0:9537:HOH:O	2.19	0.41
30:0:1425:G:O2'	30:0:1426:C:H5'	2.20	0.41
30:0:2718:C:H5'	30:0:2718:C:C6	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:28:HIS:HD2	27:1:30:LYS:H	1.66	0.41
30:0:1625:U:C3'	30:0:1625:U:C6	3.03	0.41
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.07	0.41
1:A:29:HIS:HB2	1:A:153:ARG:NH1	2.35	0.41
30:0:2754:G:C2'	30:0:2755:G:H5'	2.50	0.41
29:3:22:VAL:CG1	29:3:67:LEU:HD13	2.51	0.41
30:0:1706:G:C6	30:0:1707:G:N1	2.87	0.41
30:0:1788:U:O2'	30:0:1789:G:H5'	2.20	0.41
30:0:1481:G:H2'	30:0:1482:A:O4'	2.20	0.41
18:R:114:VAL:HA	18:R:144:GLU:O	2.20	0.41
10:J:45:VAL:HG11	10:J:121:LEU:HD22	2.02	0.41
30:0:2461:U:O2	30:0:2466:G:H1'	2.19	0.41
30:0:1163:G:H2'	30:0:1164:U:C5	2.54	0.41
30:0:2893:C:O2'	30:0:2894:C:H5'	2.19	0.41
30:0:1250:C:O2'	30:0:1251:C:H5'	2.20	0.41
30:0:1921:A:C6	30:0:1922:A:C2	3.09	0.41
30:0:2802:C:H2'	30:0:2803:C:H6	1.85	0.41
30:0:2325:U:O2'	30:0:2411:C:H1'	2.20	0.41
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.47	0.41
30:0:1511:U:O2'	30:0:1512:G:H5'	2.20	0.41
4:D:167:GLU:C	4:D:169:THR:H	2.24	0.41
30:0:2510:C:H42	30:0:2564:G:H22	1.68	0.41
30:0:567:U:O5'	30:0:567:U:H6	2.03	0.41
20:T:18:GLU:O	20:T:21:LYS:HG2	2.20	0.41
30:0:1855:G:H4'	30:0:1856:C:O5'	2.20	0.41
16:P:1:THR:O	30:0:1396:C:H1'	2.19	0.41
30:0:1304:U:H2'	30:0:1305:C:C6	2.56	0.41
2:B:95:ARG:HA	2:B:96:PRO:HD3	1.93	0.41
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.01	0.41
30:0:311:C:H2'	30:0:312:U:C6	2.55	0.41
30:0:2359:G:H3'	38:0:5696:HOH:O	2.21	0.41
1:A:23:TYR:HB2	30:0:1872:C:C5	2.55	0.41
5:E:118:ILE:HG23	5:E:144:THR:HG21	2.01	0.41
2:B:57:GLU:HA	2:B:58:PRO:HD2	1.91	0.41
30:0:1175:G:H1'	30:0:1193:A:C8	2.55	0.41
30:0:1183:C:N3	30:0:1184:C:N4	2.68	0.41
14:N:37:ARG:HD3	35:N:8807:CL:CL	2.57	0.41
30:0:1118:A:C8	30:0:1119:G:H5''	2.55	0.41
30:0:1700:C:H5''	30:0:1701:A:OP2	2.19	0.41
23:W:139:GLY:O	23:W:141:HIS:CD2	2.72	0.41
30:0:2727:A:C6	30:0:2756:U:C2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:19:PRO:HG2	3:C:22:PHE:CD1	2.56	0.41
30:0:241:A:C2	30:0:378:A:H4'	2.56	0.41
30:0:2255:A:N1	30:0:2256:G:C4	2.88	0.41
27:1:25:LYS:HE3	38:0:7430:HOH:O	2.20	0.41
30:0:699:C:C2	30:0:744:G:C2	3.08	0.41
15:O:21:SER:OG	15:O:106:PRO:HB2	2.20	0.41
4:D:55:LYS:HB2	38:0:6341:HOH:O	2.20	0.41
5:E:95:VAL:HG11	5:E:131:LEU:HD11	2.02	0.41
30:0:1180:U:O2'	30:0:1181:A:H5'	2.20	0.41
30:0:2564:G:OP2	30:0:2565:C:H5''	2.21	0.41
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.35	0.41
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	2.03	0.41
30:0:1845:A:O2'	30:0:1846:U:H5'	2.19	0.41
30:0:861:A:H4'	30:0:1697:G:C4'	2.51	0.41
30:0:571:C:H6	30:0:571:C:O5'	2.04	0.41
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.41
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.56	0.41
1:A:164:ARG:NE	38:0:5420:HOH:O	2.54	0.41
16:P:134:VAL:O	16:P:137:LEU:HB3	2.21	0.41
1:A:123:GLY:HA3	1:A:162:GLY:HA2	2.03	0.41
30:0:1361:C:H2'	30:0:1362:U:C6	2.55	0.41
25:Y:216:ARG:HD2	38:Y:8866:HOH:O	2.19	0.41
31:9:2:U:P	31:9:3:A:H5'	2.61	0.41
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.33	0.41
20:T:9:LYS:HD2	38:0:7449:HOH:O	2.20	0.41
30:0:553:G:O4'	30:0:1325:G:H5'	2.21	0.41
30:0:1523:G:C6	30:0:1524:U:O4	2.74	0.41
30:0:2329:C:H2'	30:0:2330:U:C6	2.56	0.41
38:C:8571:HOH:O	20:T:2:LYS:HE2	2.19	0.41
17:Q:15:LYS:HB3	17:Q:15:LYS:HE2	1.82	0.41
30:0:2587:OMU:O3'	30:0:2587:OMU:HM22	2.21	0.41
2:B:119:HIS:O	2:B:121:PRO:HD3	2.20	0.41
30:0:2248:C:H3'	38:0:5454:HOH:O	2.20	0.41
30:0:1594:C:O2'	30:0:1607:A:H4'	2.20	0.41
30:0:1565:C:H2'	30:0:1566:C:C6	2.56	0.41
30:0:2276:U:H2'	30:0:2277:U:C6	2.56	0.41
13:M:184:ARG:HG3	13:M:185:PRO:HA	2.03	0.41
3:C:154:VAL:O	3:C:158:GLU:HG3	2.20	0.41
30:0:2584:G:H4'	38:0:7141:HOH:O	2.20	0.41
9:I:87:PRO:HG2	30:0:1181:A:H4'	2.03	0.41
30:0:1193:A:H2	30:0:1194:A:N6	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:41:HIS:HB3	28:2:44:ARG:HB2	2.03	0.41
2:B:262:ARG:HG3	30:0:2716:G:H5'	2.02	0.41
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.21	0.41
25:Y:117:LEU:HB2	25:Y:174:VAL:HG21	2.02	0.41
30:0:2089:A:C2'	30:0:2090:G:H5'	2.50	0.41
19:S:80:ARG:NH1	38:S:8999:HOH:O	2.54	0.41
30:0:407:A:H5'	38:0:6043:HOH:O	2.19	0.41
18:R:114:VAL:HG13	18:R:114:VAL:O	2.20	0.41
6:F:14:ASP:O	6:F:18:GLU:HG3	2.20	0.41
13:M:169:ARG:NH2	38:M:8849:HOH:O	2.49	0.41
30:0:1829:A:H2'	30:0:1830:C:H5'	2.03	0.41
30:0:1364:G:H1'	38:0:4805:HOH:O	2.21	0.41
30:0:1098:A:H2'	30:0:1099:G:O4'	2.20	0.41
30:0:2115:U:H2'	30:0:2116:U:C6	2.56	0.41
30:0:11:A:N3	30:0:11:A:H2'	2.36	0.41
30:0:1185:U:C5'	38:0:7491:HOH:O	2.67	0.41
30:0:1191:A:C2	30:0:1207:A:C2	3.08	0.41
30:0:1207:A:N6	38:0:5641:HOH:O	2.53	0.41
30:0:1209:C:O2'	30:0:1210:G:H5'	2.21	0.41
31:9:57:A:N6	38:9:9060:HOH:O	2.53	0.41
30:0:1840:A:H4'	30:0:1841:C:O5'	2.21	0.41
30:0:506:G:N2	30:0:509:A:C5'	2.69	0.41
30:0:506:G:N2	30:0:509:A:H5'	2.28	0.41
25:Y:144:ARG:NH2	38:Y:8907:HOH:O	2.54	0.41
21:U:46:ALA:HB1	21:U:52:THR:HG21	2.03	0.41
1:A:105:VAL:HG11	1:A:154:ALA:CB	2.49	0.41
30:0:1889:C:H2'	30:0:1890:U:O4'	2.21	0.41
9:I:73:LEU:HD12	9:I:107:LYS:HZ1	1.84	0.41
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.36	0.41
24:X:30:MET:HE1	24:X:58:ALA:HB3	2.02	0.41
2:B:53:LEU:HD11	2:B:327:VAL:HG22	2.02	0.41
19:S:57:THR:CG2	19:S:58:MET:N	2.83	0.41
18:R:119:VAL:HG12	18:R:119:VAL:O	2.21	0.41
30:0:2073:G:OP2	30:0:2490:A:H5'	2.21	0.41
30:0:1504:A:H5'	38:0:4416:HOH:O	2.21	0.41
29:3:15:ASN:O	30:0:2408:A:H4'	2.20	0.41
30:0:1626:A:H2'	30:0:1627:G:H5'	2.02	0.41
30:0:1976:G:O2'	30:0:1977:U:C5'	2.69	0.41
30:0:424:C:H2'	30:0:425:U:C6	2.56	0.41
20:T:16:LEU:HB2	30:0:100:C:H4'	2.03	0.41
30:0:1482:A:O2'	30:0:1483:C:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:CZ	38:0:5420:HOH:O	2.68	0.41
30:0:393:G:C6	30:0:394:G:C6	3.08	0.41
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.21	0.41
8:H:34:HIS:HD2	8:H:90:LEU:O	2.03	0.41
11:K:63:GLU:HG2	38:K:6344:HOH:O	2.20	0.41
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.20	0.41
19:S:42:GLU:HG2	19:S:49:VAL:HG23	2.02	0.41
30:0:697:G:H4'	30:0:730:G:O3'	2.21	0.41
30:0:1649:G:O2'	30:0:1650:C:H5'	2.21	0.41
30:0:196:G:H1'	30:0:198:A:N7	2.36	0.41
30:0:199:A:H8	38:0:6963:HOH:O	2.04	0.41
30:0:226:A:H1'	30:0:393:G:C5	2.56	0.41
5:E:21:THR:HG23	5:E:30:THR:OG1	2.21	0.41
5:E:23:GLU:HG2	5:E:28:SER:HB3	2.02	0.41
29:3:31:THR:O	30:0:1923:G:H4'	2.21	0.41
17:Q:47:VAL:HA	17:Q:48:PRO:HD3	1.81	0.41
38:X:2479:HOH:O	30:0:2904:U:H4'	2.20	0.41
26:Z:74:GLN:HB2	26:Z:78:ILE:HG22	2.03	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.39	0.41
3:C:19:PRO:HD2	3:C:240:LEU:HD11	2.02	0.41
30:0:2252:A:H2'	30:0:2253:G:O4'	2.21	0.41
29:3:6:ARG:HA	29:3:20:HIS:O	2.21	0.41
3:C:118:THR:CG2	3:C:137:PRO:HB3	2.50	0.41
30:0:2445:U:H2'	30:0:2446:G:H8	1.83	0.41
30:0:1495:C:OP2	30:0:1505:U:N3	2.53	0.41
30:0:2754:G:O2'	30:0:2755:G:H5'	2.21	0.41
14:N:42:HIS:CG	14:N:62:HIS:HE1	2.38	0.41
14:N:82:TYR:OH	14:N:176:ARG:NH1	2.54	0.41
25:Y:210:GLY:H	30:0:1313:A:H5''	1.85	0.41
11:K:4:LEU:HD22	11:K:116:GLU:HB3	2.02	0.41
18:R:80:TYR:O	30:0:2050:G:H5''	2.20	0.41
30:0:34:C:H1'	38:0:9175:HOH:O	2.19	0.41
30:0:1603:A:C5'	30:0:1605:G:C5'	2.98	0.40
30:0:397:A:O2'	30:0:417:G:N3	2.38	0.40
30:0:2135:A:O4'	30:0:2243:C:N4	2.54	0.40
6:F:48:VAL:HG12	6:F:97:ALA:CB	2.51	0.40
14:N:141:ARG:NH2	31:9:48:C:H4'	2.35	0.40
31:9:65:A:C2'	31:9:66:G:OP2	2.68	0.40
30:0:1015:C:H2'	30:0:1016:U:C6	2.56	0.40
30:0:682:A:H2'	30:0:683:G:O4'	2.20	0.40
11:K:1:MET:HE1	38:K:6646:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:118:LEU:O	6:F:119:ARG:HB3	2.21	0.40
31:9:81:C:C2'	31:9:82:U:H5'	2.51	0.40
30:0:2016:U:H2'	30:0:2017:U:O4'	2.20	0.40
30:0:1559:A:C1'	38:0:5876:HOH:O	2.68	0.40
30:0:542:A:H2'	30:0:543:G:O4'	2.21	0.40
30:0:67:A:H5''	30:0:69:A:C8	2.57	0.40
1:A:223:ARG:HB2	30:0:2272:G:H5'	2.03	0.40
10:J:127:ILE:CG2	35:J:8801:CL:CL	3.02	0.40
1:A:101:GLU:HG2	38:A:9034:HOH:O	2.20	0.40
2:B:321:PRO:HG3	38:B:9065:HOH:O	2.21	0.40
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.57	0.40
30:0:2314:G:H2'	30:0:2315:C:H5'	2.03	0.40
30:0:570:C:H2'	30:0:571:C:H5'	2.02	0.40
16:P:105:LEU:HD21	16:P:137:LEU:HD11	2.04	0.40
23:W:29:VAL:O	23:W:30:ASN:HB2	2.21	0.40
18:R:15:LYS:HE3	38:R:8976:HOH:O	2.21	0.40
30:0:81:G:N3	30:0:98:A:C2	2.89	0.40
8:H:49:GLN:HG3	8:H:140:TYR:CE2	2.56	0.40
12:L:50:GLY:C	30:0:2453:G:H4'	2.41	0.40
30:0:1896:G:C6	30:0:1897:U:C4	3.09	0.40
18:R:59:PHE:O	18:R:63:ASN:HB3	2.21	0.40
25:Y:122:ARG:NH2	38:Y:8833:HOH:O	2.54	0.40
23:W:125:HIS:NE2	30:0:1097:A:H5''	2.36	0.40
30:0:282:C:C2'	30:0:283:U:H5'	2.51	0.40
30:0:560:U:H2'	30:0:561:G:H8	1.86	0.40
20:T:9:LYS:HD3	38:0:3755:HOH:O	2.20	0.40
1:A:103:VAL:HA	1:A:104:PRO:HD3	1.92	0.40
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.21	0.40
21:U:49:LEU:HG	38:U:3805:HOH:O	2.21	0.40
25:Y:112:GLU:OE2	25:Y:115:ARG:NH1	2.55	0.40
30:0:1081:A:C6	30:0:1082:A:N1	2.89	0.40
30:0:2566:A:H2	30:0:2695:C:O2	2.03	0.40
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	2.04	0.40
30:0:574:G:O2'	30:0:575:A:H5'	2.21	0.40
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.85	0.40
30:0:1613:C:H2'	30:0:1614:G:O4'	2.21	0.40
31:9:110:G:C5	31:9:111:U:C5	3.09	0.40
38:M:8835:HOH:O	30:0:169:A:H5''	2.22	0.40
30:0:1375:A:C2'	30:0:1376:G:H5'	2.50	0.40
30:0:1160:G:O2'	30:0:1190:G:H1'	2.22	0.40
30:0:1117:A:C2	30:0:1244:U:C2	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:GLN:NE2	30:0:1119:G:H8	2.19	0.40
23:W:125:HIS:CD2	23:W:127:GLY:H	2.39	0.40
30:0:282:C:H1'	30:0:368:C:H41	1.78	0.40
30:0:2727:A:N1	30:0:2756:U:C2	2.90	0.40
31:9:3:A:H2'	38:9:9039:HOH:O	2.21	0.40
30:0:1268:C:H2'	30:0:1269:G:H8	1.87	0.40
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.56	0.40
18:R:113:HIS:O	18:R:145:LEU:HD12	2.20	0.40
30:0:2346:C:O5'	30:0:2346:C:H6	2.03	0.40
30:0:1294:A:H2'	30:0:1295:G:O4'	2.21	0.40
30:0:2266:A:H2'	30:0:2267:G:C8	2.57	0.40
30:0:372:A:H2'	30:0:373:G:C8	2.57	0.40
25:Y:130:ARG:HD2	38:Y:8850:HOH:O	2.19	0.40
30:0:502:A:H2'	30:0:503:G:O4'	2.21	0.40
30:0:1391:G:H2'	30:0:1392:A:H5'	2.03	0.40
30:0:1450:C:H4'	30:0:1493:A:C5	2.56	0.40
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.80	0.40
2:B:285:VAL:O	2:B:286:ASN:HB2	2.21	0.40
30:0:1201:C:H2'	30:0:1202:A:H5'	2.04	0.40
31:9:28:U:H2'	31:9:29:C:C6	2.56	0.40
30:0:2712:G:P	38:0:5229:HOH:O	2.80	0.40
2:B:215:VAL:HB	38:B:9085:HOH:O	2.21	0.40
13:M:193:LYS:HB3	30:0:392:U:C5'	2.52	0.40
12:L:30:ARG:NH2	38:L:8822:HOH:O	2.53	0.40
30:0:415:A:O2'	30:0:416:G:H5'	2.21	0.40
30:0:895:A:H2'	30:0:896:C:C6	2.56	0.40
30:0:800:G:H2'	30:0:801:U:C6	2.56	0.40
30:0:2290:U:H2'	38:0:7160:HOH:O	2.22	0.40
12:L:11:ARG:NH1	30:0:903:U:OP2	2.54	0.40
30:0:1970:G:H2'	30:0:1970:G:N3	2.36	0.40
30:0:1052:G:N3	30:0:1052:G:H2'	2.36	0.40
8:H:157:TYR:C	8:H:157:TYR:CD1	2.94	0.40
30:0:2728:C:H6	30:0:2728:C:O5'	2.04	0.40
14:N:17:ARG:HH11	14:N:17:ARG:HB3	1.86	0.40
30:0:713:U:H6	30:0:713:U:O5'	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	212 (90%)	19 (8%)	4 (2%)	11	36
2	B	335/338 (99%)	307 (92%)	24 (7%)	4 (1%)	16	47
3	C	244/246 (99%)	224 (92%)	20 (8%)	0	100	100
4	D	134/177 (76%)	110 (82%)	20 (15%)	4 (3%)	5	18
5	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
6	F	117/120 (98%)	106 (91%)	8 (7%)	3 (3%)	7	22
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	15	44
9	I	68/162 (42%)	52 (76%)	15 (22%)	1 (2%)	13	40
10	J	140/145 (97%)	129 (92%)	10 (7%)	1 (1%)	26	62
11	K	130/132 (98%)	122 (94%)	7 (5%)	1 (1%)	24	58
12	L	141/165 (86%)	128 (91%)	12 (8%)	1 (1%)	26	62
13	M	192/196 (98%)	184 (96%)	7 (4%)	1 (0%)	34	69
14	N	184/187 (98%)	168 (91%)	12 (6%)	4 (2%)	8	28
15	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
16	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
21	U	51/67 (76%)	47 (92%)	4 (8%)	0	100	100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100	100
23	W	152/154 (99%)	150 (99%)	0	2 (1%)	15	44
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	15	44
25	Y	140/241 (58%)	140 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	63 (89%)	7 (10%)	1 (1%)	14	42
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	17	50
All	All	3705/4472 (83%)	3453 (93%)	221 (6%)	31 (1%)	24	58

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	VAL
6	F	101	ALA
8	H	19	ARG
12	L	149	ARG
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
23	W	77	ALA
1	A	34	ASP
2	B	185	GLY
4	D	137	PRO
2	B	2	GLN
6	F	100	ASP
11	K	127	ALA
1	A	36	ASP
2	B	169	GLY
2	B	206	THR
4	D	27	ILE
4	D	56	ARG
4	D	65	GLU
6	F	61	MET
13	M	71	SER
14	N	139	TRP
23	W	49	ASN
24	X	70	ILE
26	Z	44	ARG
29	3	56	PRO
10	J	65	ASN
8	H	171	GLY
9	I	83	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	169 (94%)	10 (6%)	26	59
2	B	282/283 (100%)	267 (95%)	15 (5%)	28	61
3	C	193/193 (100%)	178 (92%)	15 (8%)	16	41
4	D	117/148 (79%)	112 (96%)	5 (4%)	35	70
5	E	152/156 (97%)	148 (97%)	4 (3%)	54	86
6	F	93/94 (99%)	92 (99%)	1 (1%)	80	95
7	G	27/282 (10%)	26 (96%)	1 (4%)	41	76
8	H	134/145 (92%)	130 (97%)	4 (3%)	48	82
9	I	58/130 (45%)	57 (98%)	1 (2%)	68	92
10	J	118/121 (98%)	108 (92%)	10 (8%)	13	36
11	K	106/106 (100%)	102 (96%)	4 (4%)	40	74
12	L	113/127 (89%)	108 (96%)	5 (4%)	35	69
13	M	158/160 (99%)	149 (94%)	9 (6%)	25	58
14	N	149/150 (99%)	141 (95%)	8 (5%)	27	60
15	O	93/94 (99%)	92 (99%)	1 (1%)	80	95
16	P	113/117 (97%)	111 (98%)	2 (2%)	66	91
17	Q	79/80 (99%)	75 (95%)	4 (5%)	29	63
18	R	117/122 (96%)	114 (97%)	3 (3%)	54	86
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	97 (92%)	8 (8%)	16	42
21	U	44/53 (83%)	43 (98%)	1 (2%)	58	88
22	V	51/57 (90%)	49 (96%)	2 (4%)	39	74
23	W	130/130 (100%)	126 (97%)	4 (3%)	47	81
24	X	66/74 (89%)	57 (86%)	9 (14%)	5	14
25	Y	120/196 (61%)	115 (96%)	5 (4%)	36	71
26	Z	60/94 (64%)	60 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	57	87
29	3	79/79 (100%)	77 (98%)	2 (2%)	55	86
All	All	3095/3646 (85%)	2961 (96%)	134 (4%)	35	70

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	30	ARG
1	A	36	ASP
1	A	68	ILE
1	A	69	LEU
1	A	94	LEU
1	A	131	HIS
1	A	153	ARG
1	A	179	MET
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	27	ASN
2	B	56	ASP
2	B	97	LEU
2	B	98	THR
2	B	132	HIS
2	B	149	ASP
2	B	162	MET
2	B	190	MET
2	B	234	ARG
2	B	254	GLN
2	B	257	THR
2	B	277	GLU
2	B	312	ARG
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	94	THR
3	C	115	LEU
3	C	136	VAL
3	C	151	GLN
3	C	162	VAL

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Mol	Chain	Res	Type
3	C	187	ARG
3	C	211	ASP
3	C	214	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	243	VAL
4	D	19	GLU
4	D	24	HIS
4	D	50	VAL
4	D	149	ARG
4	D	161	ASP
5	E	7	ILE
5	E	86	VAL
5	E	102	VAL
5	E	156	ASP
6	F	12	LEU
7	G	73	ASP
8	H	65	LEU
8	H	87	LYS
8	H	157	TYR
8	H	173	GLU
9	I	94	ASP
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	79	PHE
10	J	93	ARG
10	J	107	ASN
10	J	112	ASP
10	J	120	SER
10	J	127	ILE
10	J	131	THR
11	K	7	ASP
11	K	10	GLN
11	K	98	VAL
11	K	119	GLN
12	L	35	ARG
12	L	43	HIS
12	L	99	GLU
12	L	104	ASP
12	L	140	VAL

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Mol	Chain	Res	Type
13	M	10	ASP
13	M	46	LEU
13	M	68	ARG
13	M	81	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	145	ASP
13	M	164	THR
14	N	17	ARG
14	N	26	LEU
14	N	49	THR
14	N	56	ASP
14	N	134	ASP
14	N	135	VAL
14	N	173	ASP
14	N	177	GLU
15	O	28	ASP
16	P	91	LYS
16	P	98	ILE
17	Q	18	PRO
17	Q	20	ASP
17	Q	57	ASP
17	Q	95	GLU
18	R	39	THR
18	R	132	ARG
18	R	143	VAL
20	T	26	THR
20	T	39	ASN
20	T	71	VAL
20	T	73	HIS
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
20	T	117	ASP
21	U	47	ARG
22	V	12	THR
22	V	65	ASP
23	W	26	ILE
23	W	52	VAL
23	W	73	LEU
23	W	146	ILE

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Mol	Chain	Res	Type
24	X	15	ARG
24	X	27	ASP
24	X	44	ASP
24	X	46	ASP
24	X	49	ARG
24	X	52	PRO
24	X	72	VAL
24	X	82	GLU
24	X	88	GLU
25	Y	103	THR
25	Y	144	ARG
25	Y	189	ASN
25	Y	200	THR
25	Y	203	VAL
28	2	18	ASN
29	3	3	MET
29	3	56	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	85	GLN
4	D	103	ASN
5	E	90	HIS
5	E	119	HIS
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN

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Mol	Chain	Res	Type
8	H	62	HIS
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
11	K	67	GLN
11	K	119	GLN
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	58	GLN
13	M	137	ASN
13	M	170	ASN
14	N	107	ASN
14	N	132	ASN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
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	53	ASN
19	S	55	GLN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	60	GLN
23	W	12	ASN
23	W	14	HIS
23	W	27	HIS
23	W	28	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS

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Mol	Chain	Res	Type
24	X	23	HIS
24	X	36	HIS
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	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	20	HIS
29	3	48	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	236 (8%)	30 (1%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	254 (8%)	31 (1%)

All (254) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	130	C
30	0	141	C
30	0	151	A
30	0	166	A

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Mol	Chain	Res	Type
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
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	498	A
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
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	698	A

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Mol	Chain	Res	Type
30	0	701	U
30	0	702	G
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	884	C
30	0	885	G
30	0	898	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1088	A
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1137	G
30	0	1151	G

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Mol	Chain	Res	Type
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	1289	C
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1492	A
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1592	G
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

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Mol	Chain	Res	Type
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1732	A
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1965	C
30	0	1968	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1996	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	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	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G

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Mol	Chain	Res	Type
30	0	2291	A
30	0	2317	C
30	0	2321	A
30	0	2345	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	2465	A
30	0	2467	A
30	0	2476	C
30	0	2482	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2527	U
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2637	A
30	0	2649	A
30	0	2664	A
30	0	2676	C
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

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Mol	Chain	Res	Type
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2836	G
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	39	U
31	9	40	C
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

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	169	A
30	0	603	A
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A

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Mol	Chain	Res	Type
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	1165	G
30	0	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1377	C
30	0	1474	C
30	0	1506	U
30	0	1685	A
30	0	1692	C
30	0	1942	A
30	0	2467	A
30	0	2482	C
30	0	2526	C
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
30	0	2791	U
31	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
30	OMU	0	2587	30	12,22,23	0.96	1 (8%)	19,31,34	3.13	2 (10%)
30	OMG	0	2588	30	17,26,27	1.00	2 (11%)	21,38,41	2.53	3 (14%)
30	UR3	0	2619	30	12,22,23	0.74	0	16,32,35	0.75	0
30	PSU	0	2621	30	13,21,22	1.71	2 (15%)	18,30,33	6.12	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	1MA	0	628	30	14,25,26	0.96	1 (7%)	15,37,40	1.11	1 (6%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.17	1.47	1.52
30	0	2588	OMG	C8-N7	-2.04	1.30	1.34
30	0	2587	OMU	C4-N3	2.29	1.37	1.33
30	0	628	1MA	C6-N6	2.55	1.33	1.29
30	0	2621	PSU	C4-N3	2.55	1.37	1.33
30	0	2588	OMG	C6-N1	3.04	1.38	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-21.49	114.62	128.33
30	0	2588	OMG	C5-C6-N1	-8.68	111.72	123.59
30	0	628	1MA	C2-N3-C4	-3.67	110.72	116.40
30	0	2587	OMU	C5-C4-N3	-3.24	114.80	123.12
30	0	2588	OMG	N3-C2-N1	-2.26	124.00	127.44
30	0	2621	PSU	C6-N1-C2	2.76	119.91	115.47
30	0	2588	OMG	C6-N1-C2	6.67	125.19	115.94
30	0	2587	OMU	C4-N3-C2	12.99	127.00	114.14
30	0	2621	PSU	C4-N3-C2	13.78	127.16	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	237/240 (98%)	-0.57	6 (2%) 61 48	22, 48, 85, 107	0
2	B	337/338 (99%)	-0.76	0 100 100	24, 49, 78, 90	0
3	C	246/246 (100%)	-0.71	0 100 100	20, 40, 64, 79	0
4	D	140/177 (79%)	0.95	27 (19%) 2 1	61, 98, 123, 132	0
5	E	172/178 (96%)	-0.46	2 (1%) 81 73	43, 66, 86, 91	0
6	F	119/120 (99%)	0.00	3 (2%) 61 48	44, 67, 97, 113	0
7	G	29/348 (8%)	0.71	6 (20%) 1 1	77, 94, 103, 104	0
8	H	160/177 (90%)	0.36	16 (10%) 9 4	48, 69, 99, 104	0
9	I	70/162 (43%)	3.48	49 (70%) 0 0	128, 145, 162, 163	0
10	J	142/145 (97%)	-0.73	0 100 100	32, 47, 68, 90	0
11	K	132/132 (100%)	-0.92	0 100 100	30, 44, 67, 73	0
12	L	145/165 (87%)	-0.18	4 (2%) 56 44	25, 62, 112, 124	0
13	M	194/196 (98%)	-0.86	0 100 100	26, 39, 55, 63	0
14	N	186/187 (99%)	-0.30	3 (1%) 74 66	39, 63, 111, 120	0
15	O	115/116 (99%)	-0.74	0 100 100	33, 51, 68, 72	0
16	P	143/149 (95%)	-0.79	0 100 100	33, 49, 65, 73	0
17	Q	95/96 (98%)	-0.74	0 100 100	35, 45, 62, 79	0
18	R	150/155 (96%)	-0.85	0 100 100	27, 42, 62, 77	0
19	S	81/85 (95%)	-0.58	1 (1%) 81 73	38, 54, 74, 87	0
20	T	119/120 (99%)	-0.55	2 (1%) 73 63	37, 52, 80, 109	0
21	U	53/67 (79%)	-0.68	0 100 100	37, 50, 68, 78	0
22	V	65/71 (91%)	0.70	6 (9%) 11 5	47, 68, 117, 122	0
23	W	154/154 (100%)	-0.67	0 100 100	32, 47, 63, 77	0
24	X	82/92 (89%)	-0.46	2 (2%) 62 50	41, 57, 82, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.86	1 (0%) 89 84	21, 40, 63, 86	0
26	Z	73/116 (62%)	0.36	6 (8%) 14 7	53, 72, 85, 95	0
27	1	56/57 (98%)	-0.72	0 100 100	22, 28, 36, 44	0
28	2	46/50 (92%)	-0.35	2 (4%) 39 27	30, 56, 84, 98	0
29	3	92/92 (100%)	-0.54	0 100 100	33, 56, 68, 81	0
30	0	2749/2923 (94%)	-0.65	22 (0%) 87 81	19, 42, 86, 163	0
31	9	122/122 (100%)	-0.69	2 (1%) 74 66	34, 64, 87, 144	0
All	All	6646/7517 (88%)	-0.51	160 (2%) 62 50	19, 48, 97, 163	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	12.6
9	I	74	ILE	10.3
22	V	39	ALA	8.5
9	I	104	ALA	8.3
9	I	70	THR	8.2
4	D	63	ILE	7.9
9	I	128	THR	7.4
22	V	40	PRO	7.0
9	I	72	GLU	6.7
9	I	102	GLN	6.5
9	I	71	ALA	6.5
9	I	108	HIS	6.4
9	I	132	VAL	6.2
9	I	66	GLY	6.2
9	I	97	VAL	5.7
9	I	112	LEU	5.6
9	I	100	VAL	5.6
14	N	166	ALA	5.5
9	I	80	PHE	5.5
9	I	99	GLN	5.4
22	V	43	PRO	5.1
9	I	106	GLN	5.0
9	I	93	ALA	5.0
9	I	113	SER	4.9
1	A	237	GLY	4.9
9	I	109	PRO	4.7
9	I	98	ASP	4.7
9	I	88	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
9	I	116	LEU	4.6
31	9	1	U	4.4
22	V	41	GLU	4.4
9	I	91	PHE	4.2
9	I	92	VAL	4.2
4	D	57	THR	4.1
9	I	79	GLY	4.1
9	I	83	GLY	4.1
9	I	76	ASP	4.0
9	I	103	ILE	4.0
9	I	86	GLU	3.9
30	0	1172	G	3.9
4	D	85	GLN	3.9
4	D	64	ARG	3.8
9	I	110	ASP	3.8
9	I	105	GLU	3.7
12	L	80	ASP	3.7
26	Z	46	SER	3.7
4	D	90	LEU	3.6
8	H	40	GLN	3.6
22	V	38	GLY	3.5
24	X	80	GLU	3.5
9	I	111	LEU	3.4
9	I	78	ALA	3.4
30	0	1199	A	3.4
9	I	82	THR	3.4
9	I	69	PRO	3.3
9	I	133	THR	3.3
26	Z	35	SER	3.2
30	0	1198	U	3.2
8	H	77	ILE	3.2
8	H	169	GLU	3.2
4	D	18	ILE	3.2
9	I	67	VAL	3.1
26	Z	69	ASP	3.1
9	I	95	LEU	3.1
7	G	27	ILE	3.0
9	I	94	ASP	3.0
30	0	735	C	3.0
7	G	23	ILE	3.0
30	0	1202	A	3.0
4	D	40	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
12	L	81	VAL	2.9
4	D	89	PRO	2.9
8	H	37	GLY	2.9
9	I	73	LEU	2.8
26	Z	44	ARG	2.8
4	D	88	LEU	2.8
8	H	84	GLY	2.8
4	D	44	ILE	2.8
1	A	37	VAL	2.8
4	D	10	PHE	2.8
8	H	82	GLU	2.8
25	Y	235	GLU	2.8
8	H	86	TYR	2.8
9	I	81	GLU	2.8
4	D	170	TYR	2.7
30	0	282	C	2.7
6	F	106	ALA	2.7
24	X	88	GLU	2.7
4	D	92	GLU	2.7
8	H	76	LEU	2.7
8	H	39	LYS	2.7
9	I	117	THR	2.7
26	Z	58	ASN	2.6
7	G	26	MET	2.6
4	D	61	PHE	2.6
20	T	116	ASP	2.5
30	0	2237	G	2.5
9	I	118	ASN	2.5
4	D	73	VAL	2.5
30	0	970	U	2.5
9	I	84	SER	2.5
4	D	81	GLU	2.5
14	N	185	GLU	2.5
1	A	99	ILE	2.5
8	H	141	CYS	2.5
4	D	93	LEU	2.4
4	D	69	ILE	2.4
30	0	1173	A	2.4
30	0	1176	C	2.4
28	2	39	ARG	2.4
30	0	1171	A	2.4
31	9	24	U	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	75	LEU	2.3
26	Z	55	SER	2.3
12	L	60	GLU	2.3
30	0	2637	A	2.3
8	H	38	ARG	2.3
30	0	1165	G	2.3
30	0	1200	A	2.3
30	0	1203	G	2.3
19	S	81	ILE	2.3
9	I	75	LYS	2.3
4	D	171	ASP	2.3
9	I	126	THR	2.3
9	I	127	CYS	2.3
5	E	100	ASP	2.3
7	G	24	VAL	2.3
8	H	48	VAL	2.3
30	0	969	G	2.3
20	T	119	ALA	2.3
4	D	41	LEU	2.3
30	0	2508	C	2.3
8	H	85	ASP	2.2
30	0	1951	G	2.2
6	F	119	ARG	2.2
9	I	101	LYS	2.2
30	0	1177	A	2.2
8	H	174	LEU	2.2
12	L	75	LEU	2.2
4	D	84	LEU	2.2
8	H	90	LEU	2.2
4	D	70	GLY	2.2
30	0	1163	G	2.2
4	D	158	ASN	2.2
9	I	125	GLY	2.1
28	2	20	ARG	2.1
1	A	36	ASP	2.1
4	D	104	PHE	2.1
5	E	45	ASP	2.1
4	D	24	HIS	2.1
30	0	1197	G	2.1
7	G	72	ASP	2.1
8	H	68	SER	2.1
6	F	49	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
14	N	147	ILE	2.0
7	G	28	GLU	2.0
4	D	86	THR	2.0
1	A	236	GLY	2.0
30	0	960	G	2.0
1	A	35	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
30	OMG	0	2588	24/25	0.98	0.12	-	29,31,34,35	0
30	1MA	0	628	23/24	0.98	0.14	-	23,27,29,31	0
30	OMU	0	2587	21/22	0.99	0.11	-	29,31,32,35	0
30	UR3	0	2619	21/22	0.98	0.13	-	33,36,38,41	0
30	PSU	0	2621	20/21	0.98	0.14	-	22,26,37,37	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
34	NA	0	8562	1/1	0.82	0.66	177.83	78,78,78,78	0
36	SR	B	8987	1/1	0.90	0.90	39.67	200,200,200,200	0
34	NA	0	8565	1/1	0.80	0.38	38.65	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8563	1/1	0.85	0.64	30.12	74,74,74,74	0
36	SR	J	8986	1/1	0.80	0.80	28.73	200,200,200,200	0
34	NA	0	8555	1/1	0.90	0.58	25.17	54,54,54,54	0
34	NA	0	8535	1/1	0.82	0.24	23.76	47,47,47,47	0
34	NA	0	8512	1/1	0.86	0.37	21.49	50,50,50,50	0
34	NA	0	8522	1/1	0.86	0.42	21.34	73,73,73,73	0
34	NA	0	8542	1/1	0.84	0.39	19.78	48,48,48,48	0
34	NA	0	8564	1/1	0.90	0.27	18.08	61,61,61,61	0
34	NA	0	8560	1/1	0.85	0.38	16.21	74,74,74,74	0
34	NA	9	8572	1/1	0.29	0.33	13.21	93,93,93,93	0
34	NA	0	8552	1/1	0.94	0.33	10.66	56,56,56,56	0
34	NA	0	8559	1/1	0.93	0.18	10.03	73,73,73,73	0
34	NA	0	8547	1/1	0.97	0.25	9.33	43,43,43,43	0
34	NA	0	8556	1/1	0.98	0.56	9.17	44,44,44,44	0
34	NA	0	8553	1/1	0.95	0.31	9.03	68,68,68,68	0
36	SR	0	8992	1/1	0.99	0.24	7.19	136,136,136,136	0
34	NA	0	8567	1/1	0.94	0.26	6.91	77,77,77,77	0
34	NA	0	8569	1/1	0.91	0.28	6.72	65,65,65,65	0
33	K	0	8401	1/1	0.59	0.53	6.48	132,132,132,132	0
34	NA	0	8575	1/1	0.97	0.32	6.37	86,86,86,86	0
36	SR	0	8903	1/1	1.00	0.15	6.23	46,46,46,46	0
36	SR	0	8947	1/1	0.77	0.22	6.12	170,170,170,170	0
34	NA	0	8507	1/1	0.99	0.17	5.09	31,31,31,31	0
34	NA	0	8557	1/1	0.92	0.12	5.01	56,56,56,56	0
34	NA	0	8530	1/1	0.87	0.21	4.99	46,46,46,46	0
36	SR	0	9001	1/1	0.67	0.17	4.99	158,158,158,158	0
32	MG	A	8051	1/1	0.90	0.37	4.74	62,62,62,62	0
32	MG	0	8014	1/1	0.98	0.16	4.45	21,21,21,21	0
32	MG	0	8041	1/1	0.95	0.20	4.26	25,25,25,25	0
32	MG	0	8015	1/1	0.99	0.14	4.13	24,24,24,24	0
32	MG	0	8009	1/1	0.99	0.19	4.12	18,18,18,18	0
34	NA	0	8517	1/1	0.99	0.18	4.03	28,28,28,28	0
34	NA	0	8527	1/1	0.99	0.18	3.70	53,53,53,53	0
32	MG	0	8047	1/1	0.98	0.22	3.52	38,38,38,38	0
36	SR	0	8904	1/1	0.99	0.18	3.21	48,48,48,48	0
34	NA	0	8558	1/1	0.90	0.20	3.12	45,45,45,45	0
36	SR	0	8926	1/1	0.95	0.13	3.03	114,114,114,114	0
32	MG	0	8028	1/1	0.98	0.17	2.95	22,22,22,22	0
36	SR	0	8969	1/1	0.98	0.15	2.65	158,158,158,158	0
32	MG	0	8045	1/1	0.95	0.11	2.52	28,28,28,28	0
34	NA	0	8504	1/1	0.98	0.18	2.35	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8533	1/1	0.85	0.15	2.34	45,45,45,45	0
34	NA	0	8521	1/1	0.98	0.18	2.33	52,52,52,52	0
34	NA	0	8537	1/1	0.96	0.13	2.27	34,34,34,34	0
32	MG	0	8004	1/1	0.99	0.18	1.71	22,22,22,22	0
32	MG	0	8011	1/1	0.95	0.18	1.49	20,20,20,20	0
34	NA	0	8528	1/1	0.99	0.13	1.46	35,35,35,35	0
32	MG	0	8008	1/1	0.99	0.12	1.34	19,19,19,19	0
36	SR	R	8912	1/1	0.98	0.17	1.24	78,78,78,78	0
32	MG	0	8006	1/1	0.96	0.13	1.17	25,25,25,25	0
32	MG	0	8088	1/1	0.90	0.13	1.01	30,30,30,30	0
34	NA	0	8523	1/1	0.95	0.12	0.83	41,41,41,41	0
32	MG	0	8085	1/1	0.83	0.11	0.72	76,76,76,76	0
36	SR	0	8972	1/1	0.90	0.19	0.68	163,163,163,163	0
32	MG	0	8067	1/1	0.99	0.17	0.62	31,31,31,31	0
32	MG	0	8003	1/1	1.00	0.14	0.61	28,28,28,28	0
32	MG	0	8062	1/1	0.99	0.16	0.60	37,37,37,37	0
36	SR	3	8932	1/1	0.99	0.12	0.33	67,67,67,67	0
37	CD	1	8702	1/1	0.99	0.12	0.30	59,59,59,59	0
34	NA	0	8568	1/1	0.81	0.17	0.18	36,36,36,36	0
36	SR	0	8944	1/1	0.71	0.10	0.17	167,167,167,167	0
32	MG	0	8072	1/1	0.95	0.14	0.04	48,48,48,48	0
32	MG	0	8084	1/1	0.99	0.11	0.03	31,31,31,31	0
34	NA	0	8534	1/1	0.98	0.15	0.01	37,37,37,37	0
36	SR	0	8985	1/1	0.79	0.08	-0.39	115,115,115,115	0
32	MG	0	8012	1/1	0.99	0.16	-0.54	15,15,15,15	0
34	NA	M	8539	1/1	0.97	0.10	-0.67	26,26,26,26	0
32	MG	B	8042	1/1	0.98	0.08	-0.74	50,50,50,50	0
34	NA	J	8538	1/1	0.77	0.11	-0.93	51,51,51,51	0
32	MG	0	8058	1/1	0.98	0.09	-1.03	18,18,18,18	0
32	MG	0	8010	1/1	0.90	0.13	-1.08	44,44,44,44	0
34	NA	0	8520	1/1	0.85	0.09	-1.11	47,47,47,47	0
36	SR	A	8929	1/1	0.92	0.09	-1.17	123,123,123,123	0
32	MG	0	8001	1/1	0.97	0.10	-1.35	33,33,33,33	0
36	SR	0	8948	1/1	0.98	0.10	-1.45	94,94,94,94	0
36	SR	0	8922	1/1	0.82	0.13	-1.45	150,150,150,150	0
34	NA	0	8513	1/1	0.97	0.13	-1.52	42,42,42,42	0
34	NA	0	8571	1/1	0.85	0.07	-1.56	72,72,72,72	0
35	CL	J	8821	1/1	0.99	0.06	-1.60	60,60,60,60	0
35	CL	M	8818	1/1	0.99	0.08	-1.64	34,34,34,34	0
34	NA	Q	8540	1/1	0.95	0.07	-1.72	48,48,48,48	0
32	MG	B	8043	1/1	0.99	0.07	-1.72	38,38,38,38	0
37	CD	3	8704	1/1	1.00	0.06	-1.74	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
36	SR	0	8975	1/1	0.94	0.07	-1.74	124,124,124,124	0
37	CD	U	8701	1/1	1.00	0.07	-1.81	48,48,48,48	0
35	CL	O	8808	1/1	0.93	0.07	-1.88	58,58,58,58	0
34	NA	0	8515	1/1	0.92	0.09	-1.94	32,32,32,32	0
32	MG	T	8057	1/1	0.87	0.09	-1.98	59,59,59,59	0
32	MG	A	8050	1/1	0.99	0.10	-2.10	34,34,34,34	0
34	NA	0	8550	1/1	0.95	0.13	-2.16	51,51,51,51	0
35	CL	K	8812	1/1	0.99	0.07	-2.19	39,39,39,39	0
32	MG	0	8052	1/1	0.98	0.08	-2.21	39,39,39,39	0
36	SR	0	8943	1/1	0.99	0.05	-2.26	94,94,94,94	0
35	CL	3	8804	1/1	0.98	0.06	-2.28	57,57,57,57	0
37	CD	Z	8703	1/1	1.00	0.06	-2.45	79,79,79,79	0
36	SR	0	8902	1/1	0.99	0.13	-2.46	57,57,57,57	0
36	SR	0	8945	1/1	0.96	0.08	-2.46	97,97,97,97	0
36	SR	0	8962	1/1	0.92	0.12	-2.54	168,168,168,168	0
33	K	0	8402	1/1	0.96	0.10	-2.80	69,69,69,69	0
32	MG	0	8087	1/1	1.00	0.11	-2.89	29,29,29,29	0
36	SR	F	9005	1/1	0.99	0.04	-2.90	118,118,118,118	0
36	SR	0	8936	1/1	1.00	0.07	-2.92	84,84,84,84	0
36	SR	9	8978	1/1	0.95	0.07	-2.93	133,133,133,133	0
35	CL	0	8813	1/1	0.97	0.06	-3.23	49,49,49,49	0
32	MG	0	8065	1/1	0.99	0.08	-3.28	38,38,38,38	0
34	NA	0	8519	1/1	0.98	0.12	-3.32	37,37,37,37	0
35	CL	0	8815	1/1	0.94	0.06	-3.34	61,61,61,61	0
32	MG	0	8002	1/1	0.99	0.08	-3.95	25,25,25,25	0
36	SR	1	8913	1/1	0.99	0.08	-3.96	76,76,76,76	0
36	SR	0	8910	1/1	0.99	0.05	-4.14	93,93,93,93	0
32	MG	0	8044	1/1	0.80	0.07	-4.15	40,40,40,40	0
32	MG	0	8025	1/1	0.99	0.07	-4.17	22,22,22,22	0
35	CL	0	8805	1/1	0.97	0.05	-4.18	50,50,50,50	0
32	MG	0	8075	1/1	0.65	0.06	-4.18	45,45,45,45	0
36	SR	0	8970	1/1	0.94	0.04	-5.06	118,118,118,118	0
32	MG	Y	8086	1/1	0.95	0.07	-6.40	34,34,34,34	0
35	CL	B	8819	1/1	0.99	0.04	-7.76	44,44,44,44	0
36	SR	0	8949	1/1	0.97	0.05	-8.31	99,99,99,99	0
32	MG	0	8013	1/1	0.99	0.04	-9.34	22,22,22,22	0
32	MG	0	8034	1/1	0.98	0.03	-11.21	36,36,36,36	0
36	SR	0	8939	1/1	0.91	0.05	-	128,128,128,128	0
36	SR	0	8976	1/1	0.83	0.21	-	185,185,185,185	0
32	MG	0	8032	1/1	1.00	0.06	-	38,38,38,38	0
34	NA	0	8508	1/1	0.97	0.27	-	43,43,43,43	0
36	SR	0	8993	1/1	0.77	0.10	-	170,170,170,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8915	1/1	0.88	0.10	-	110,110,110,110	0
32	MG	0	8024	1/1	0.97	0.15	-	55,55,55,55	0
36	SR	0	8937	1/1	0.90	0.18	-	100,100,100,100	0
35	CL	J	8802	1/1	0.97	0.07	-	55,55,55,55	0
36	SR	0	8928	1/1	0.82	0.07	-	127,127,127,127	0
36	SR	0	8982	1/1	0.69	0.31	-	178,178,178,178	0
34	NA	0	8546	1/1	0.90	0.87	-	69,69,69,69	0
34	NA	0	8574	1/1	0.92	0.52	-	65,65,65,65	0
32	MG	0	8039	1/1	0.96	0.17	-	70,70,70,70	0
36	SR	0	8938	1/1	0.92	0.10	-	158,158,158,158	0
34	NA	0	8506	1/1	0.76	0.10	-	56,56,56,56	0
32	MG	0	8017	1/1	0.98	0.27	-	32,32,32,32	0
36	SR	0	8911	1/1	0.95	0.09	-	74,74,74,74	0
32	MG	0	8030	1/1	0.84	0.24	-	60,60,60,60	0
32	MG	0	8080	1/1	0.92	0.11	-	66,66,66,66	0
34	NA	0	8529	1/1	0.93	0.05	-	30,30,30,30	0
36	SR	0	8979	1/1	0.87	0.12	-	200,200,200,200	0
36	SR	0	9000	1/1	0.89	0.23	-	160,160,160,160	0
32	MG	0	8091	1/1	0.95	0.03	-	48,48,48,48	0
32	MG	0	8026	1/1	0.97	0.10	-	32,32,32,32	0
34	NA	0	8516	1/1	0.99	0.07	-	27,27,27,27	0
32	MG	0	8073	1/1	0.92	0.06	-	65,65,65,65	0
32	MG	9	8074	1/1	0.99	0.14	-	62,62,62,62	0
34	NA	S	8510	1/1	0.95	0.10	-	29,29,29,29	0
36	SR	0	8901	1/1	0.99	0.08	-	74,74,74,74	0
32	MG	0	8063	1/1	0.96	0.27	-	78,78,78,78	0
36	SR	0	8960	1/1	0.96	0.04	-	135,135,135,135	0
34	NA	0	8531	1/1	0.96	0.08	-	44,44,44,44	0
36	SR	0	8917	1/1	0.98	0.11	-	103,103,103,103	0
36	SR	0	8905	1/1	0.99	0.24	-	52,52,52,52	0
35	CL	A	8809	1/1	0.96	0.07	-	63,63,63,63	0
32	MG	0	8092	1/1	0.97	0.02	-	51,51,51,51	0
32	MG	0	8076	1/1	0.93	0.14	-	38,38,38,38	0
34	NA	0	8505	1/1	0.91	0.28	-	36,36,36,36	0
36	SR	0	8908	1/1	0.96	0.13	-	92,92,92,92	0
36	SR	0	8925	1/1	0.99	0.10	-	83,83,83,83	0
34	NA	0	8526	1/1	0.98	0.03	-	36,36,36,36	0
36	SR	0	8920	1/1	0.98	0.03	-	108,108,108,108	0
32	MG	0	8022	1/1	0.96	0.13	-	30,30,30,30	0
36	SR	0	8918	1/1	0.99	0.11	-	74,74,74,74	0
34	NA	0	8501	1/1	0.97	0.15	-	31,31,31,31	0
36	SR	0	8981	1/1	0.93	0.14	-	156,156,156,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8959	1/1	0.81	0.14	-	157,157,157,157	0
32	MG	0	8007	1/1	0.98	0.19	-	29,29,29,29	0
32	MG	9	8040	1/1	0.93	0.09	-	69,69,69,69	0
32	MG	0	8069	1/1	0.95	0.39	-	99,99,99,99	0
32	MG	0	8059	1/1	0.97	0.07	-	44,44,44,44	0
32	MG	0	8083	1/1	0.98	0.03	-	48,48,48,48	0
36	SR	0	8942	1/1	0.97	0.08	-	108,108,108,108	0
34	NA	0	8502	1/1	0.87	0.10	-	62,62,62,62	0
32	MG	0	8046	1/1	0.94	0.14	-	33,33,33,33	0
36	SR	0	8916	1/1	0.98	0.09	-	101,101,101,101	0
32	MG	0	8068	1/1	0.96	0.09	-	51,51,51,51	0
34	NA	0	8525	1/1	0.76	0.25	-	71,71,71,71	0
32	MG	0	8023	1/1	0.97	0.09	-	24,24,24,24	0
32	MG	0	8060	1/1	0.94	0.11	-	52,52,52,52	0
35	CL	0	8822	1/1	0.99	0.24	-	78,78,78,78	0
35	CL	0	8817	1/1	0.96	0.05	-	50,50,50,50	0
36	SR	0	8965	1/1	0.99	0.05	-	117,117,117,117	0
35	CL	R	8806	1/1	0.99	0.10	-	38,38,38,38	0
36	SR	0	9006	1/1	0.62	2.88	-	200,200,200,200	0
32	MG	0	8033	1/1	0.93	0.07	-	35,35,35,35	0
36	SR	0	8954	1/1	0.94	0.08	-	94,94,94,94	0
36	SR	0	8951	1/1	0.69	0.06	-	138,138,138,138	0
32	MG	0	8071	1/1	0.70	0.16	-	49,49,49,49	0
36	SR	0	8958	1/1	0.95	0.08	-	101,101,101,101	0
36	SR	0	8983	1/1	0.91	0.24	-	169,169,169,169	0
36	SR	0	8946	1/1	0.99	0.17	-	110,110,110,110	0
32	MG	0	8048	1/1	0.98	0.21	-	19,19,19,19	0
32	MG	0	8031	1/1	0.75	0.09	-	59,59,59,59	0
36	SR	0	8984	1/1	0.97	0.09	-	111,111,111,111	0
34	NA	0	8509	1/1	0.53	0.16	-	56,56,56,56	0
32	MG	0	8064	1/1	0.94	0.16	-	36,36,36,36	0
36	SR	A	8930	1/1	0.93	0.05	-	96,96,96,96	0
36	SR	0	9008	1/1	0.99	0.10	-	84,84,84,84	0
36	SR	0	8955	1/1	0.59	0.06	-	187,187,187,187	0
36	SR	0	9004	1/1	0.95	0.39	-	200,200,200,200	0
36	SR	0	8996	1/1	0.85	0.61	-	200,200,200,200	0
36	SR	0	8933	1/1	0.94	0.18	-	136,136,136,136	0
36	SR	S	8961	1/1	0.73	0.09	-	116,116,116,116	0
36	SR	0	8940	1/1	0.99	0.10	-	85,85,85,85	0
34	NA	R	8532	1/1	0.98	0.07	-	37,37,37,37	0
36	SR	0	8909	1/1	1.00	0.14	-	77,77,77,77	0
34	NA	9	8543	1/1	0.97	0.15	-	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8549	1/1	0.93	0.48	-	50,50,50,50	0
36	SR	0	8924	1/1	0.83	0.17	-	139,139,139,139	0
34	NA	0	8514	1/1	0.78	0.33	-	42,42,42,42	0
35	CL	J	8801	1/1	0.97	0.06	-	66,66,66,66	0
34	NA	0	8570	1/1	0.96	0.10	-	43,43,43,43	0
32	MG	0	8018	1/1	0.98	0.20	-	29,29,29,29	0
32	MG	0	8029	1/1	0.98	0.15	-	37,37,37,37	0
32	MG	0	8082	1/1	0.98	0.17	-	77,77,77,77	0
32	MG	0	8056	1/1	0.97	0.10	-	48,48,48,48	0
35	CL	0	8816	1/1	0.95	0.06	-	66,66,66,66	0
36	SR	0	8914	1/1	0.92	0.24	-	106,106,106,106	0
36	SR	0	8998	1/1	0.93	0.12	-	148,148,148,148	0
36	SR	0	8953	1/1	0.95	0.15	-	140,140,140,140	0
36	SR	0	8974	1/1	0.90	0.21	-	160,160,160,160	0
36	SR	0	8966	1/1	0.96	0.06	-	100,100,100,100	0
36	SR	0	8941	1/1	0.94	0.12	-	99,99,99,99	0
36	SR	0	8991	1/1	0.93	0.07	-	183,183,183,183	0
34	NA	C	8503	1/1	0.99	0.15	-	31,31,31,31	0
32	MG	0	8016	1/1	0.97	0.12	-	46,46,46,46	0
36	SR	1	8952	1/1	1.00	0.10	-	73,73,73,73	0
34	NA	0	8573	1/1	0.95	0.22	-	64,64,64,64	0
37	CD	O	8705	1/1	0.98	0.08	-	80,80,80,80	0
36	SR	0	8931	1/1	0.98	0.09	-	98,98,98,98	0
36	SR	0	8927	1/1	0.82	0.10	-	136,136,136,136	0
36	SR	0	8906	1/1	1.00	0.19	-	48,48,48,48	0
35	CL	L	8810	1/1	0.95	0.06	-	53,53,53,53	0
36	SR	0	8989	1/1	0.96	0.18	-	177,177,177,177	0
32	MG	0	8049	1/1	0.98	0.27	-	65,65,65,65	0
36	SR	0	8990	1/1	0.98	0.17	-	124,124,124,124	0
34	NA	0	8511	1/1	0.94	0.20	-	59,59,59,59	0
36	SR	9	9003	1/1	0.86	0.13	-	157,157,157,157	0
32	MG	0	8027	1/1	0.99	0.05	-	29,29,29,29	0
36	SR	0	8973	1/1	0.98	0.08	-	124,124,124,124	0
36	SR	0	8921	1/1	0.95	0.10	-	82,82,82,82	0
36	SR	0	8907	1/1	1.00	0.11	-	54,54,54,54	0
35	CL	Y	8820	1/1	0.97	0.07	-	35,35,35,35	0
36	SR	0	8968	1/1	0.87	0.09	-	165,165,165,165	0
36	SR	9	8980	1/1	0.95	0.11	-	168,168,168,168	0
32	MG	0	8021	1/1	0.97	0.07	-	29,29,29,29	0
32	MG	0	8089	1/1	0.96	0.10	-	43,43,43,43	0
36	SR	0	8994	1/1	0.73	0.38	-	200,200,200,200	0
34	NA	0	8554	1/1	0.98	0.39	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8967	1/1	0.97	0.03	-	127,127,127,127	0
36	SR	0	8971	1/1	0.92	0.04	-	150,150,150,150	0
36	SR	A	8977	1/1	0.77	0.11	-	159,159,159,159	0
32	MG	0	8061	1/1	0.98	0.21	-	22,22,22,22	0
32	MG	0	8093	1/1	0.98	0.09	-	29,29,29,29	0
32	MG	0	8078	1/1	0.87	0.35	-	50,50,50,50	0
36	SR	0	8963	1/1	0.90	0.05	-	167,167,167,167	0
32	MG	0	8081	1/1	0.96	0.16	-	64,64,64,64	0
36	SR	0	8956	1/1	0.93	0.07	-	130,130,130,130	0
32	MG	0	8005	1/1	0.98	0.22	-	31,31,31,31	0
32	MG	0	8019	1/1	1.00	0.18	-	24,24,24,24	0
32	MG	0	8055	1/1	0.99	0.15	-	35,35,35,35	0
34	NA	0	8548	1/1	0.87	0.20	-	56,56,56,56	0
36	SR	0	8934	1/1	0.98	0.09	-	104,104,104,104	0
34	NA	0	8536	1/1	0.98	0.15	-	47,47,47,47	0
34	NA	0	8541	1/1	0.97	0.20	-	53,53,53,53	0
34	NA	0	8544	1/1	0.77	0.14	-	60,60,60,60	0
32	MG	0	8066	1/1	0.92	0.18	-	44,44,44,44	0
34	NA	0	8545	1/1	0.98	0.13	-	38,38,38,38	0
32	MG	0	8020	1/1	0.95	0.13	-	37,37,37,37	0
35	CL	0	8814	1/1	0.96	0.10	-	48,48,48,48	0
36	SR	0	8935	1/1	0.99	0.10	-	73,73,73,73	0
36	SR	B	8950	1/1	0.87	0.13	-	121,121,121,121	0
32	MG	0	8035	1/1	0.94	0.10	-	49,49,49,49	0
34	NA	0	8566	1/1	0.91	0.32	-	43,43,43,43	0
36	SR	0	9007	1/1	0.96	0.43	-	187,187,187,187	0
32	MG	0	8036	1/1	0.90	0.09	-	33,33,33,33	0
36	SR	0	8923	1/1	0.98	0.04	-	104,104,104,104	0
36	SR	0	8995	1/1	0.86	0.15	-	133,133,133,133	0
34	NA	0	8524	1/1	0.97	0.20	-	39,39,39,39	0
32	MG	0	8038	1/1	0.68	0.18	-	65,65,65,65	0
36	SR	0	8919	1/1	0.67	0.12	-	159,159,159,159	0
36	SR	0	8964	1/1	0.96	0.08	-	118,118,118,118	0
36	SR	0	8997	1/1	0.75	0.34	-	196,196,196,196	0
32	MG	0	8037	1/1	0.90	0.20	-	92,92,92,92	0
32	MG	0	8053	1/1	0.91	0.06	-	52,52,52,52	0
32	MG	0	8070	1/1	0.97	0.18	-	45,45,45,45	0
35	CL	N	8807	1/1	0.97	0.07	-	57,57,57,57	0
35	CL	0	8811	1/1	0.98	0.11	-	62,62,62,62	0
35	CL	0	8803	1/1	0.96	0.09	-	46,46,46,46	0
32	MG	K	8054	1/1	0.98	0.07	-	34,34,34,34	0
36	SR	0	9002	1/1	0.95	0.13	-	173,173,173,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	H	8518	1/1	0.92	0.48	-	86,86,86,86	0
34	NA	0	8561	1/1	0.94	0.51	-	76,76,76,76	0
36	SR	0	8988	1/1	0.93	0.18	-	159,159,159,159	0
36	SR	3	8999	1/1	0.97	0.05	-	94,94,94,94	0
32	MG	0	8090	1/1	0.72	0.13	-	70,70,70,70	0
32	MG	0	8077	1/1	0.94	0.07	-	32,32,32,32	0
36	SR	0	8957	1/1	0.81	0.11	-	187,187,187,187	0
32	MG	0	8079	1/1	0.92	0.14	-	48,48,48,48	0
34	NA	0	8551	1/1	0.97	0.11	-	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.