



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:58 AM GMT

PDB ID : 3CCL  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation U2535C. Density for Anisomycin is visible but not included in model.  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-26  
Resolution : 2.90 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

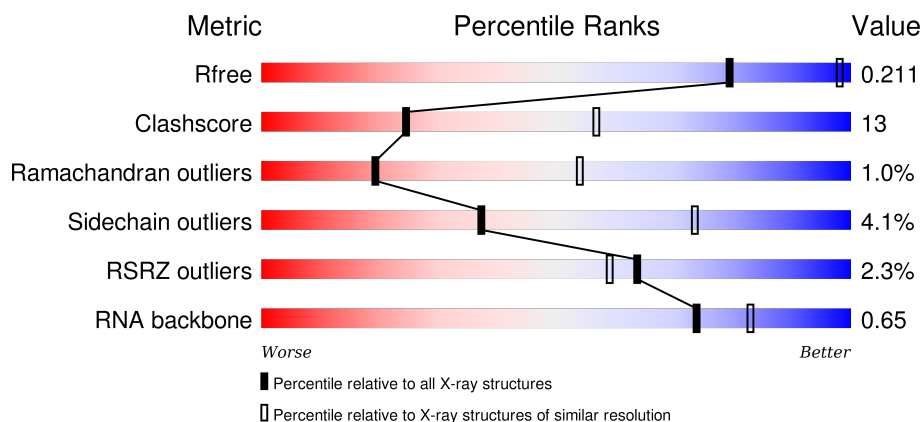
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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.





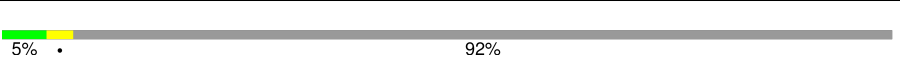
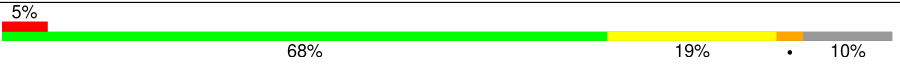
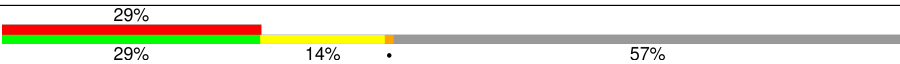

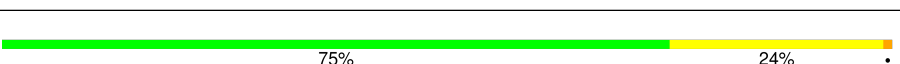
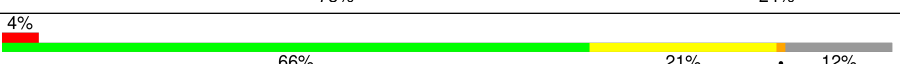
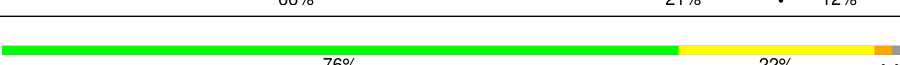
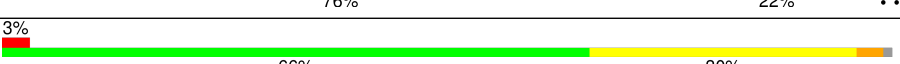
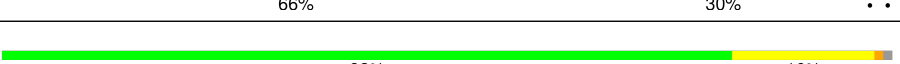
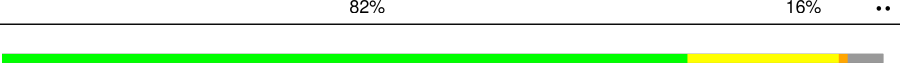

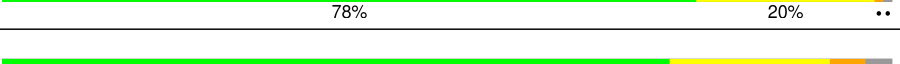



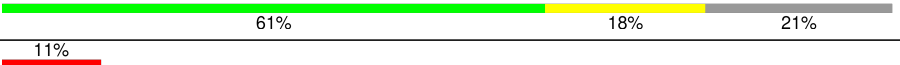

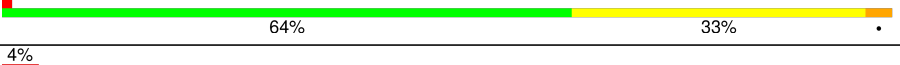
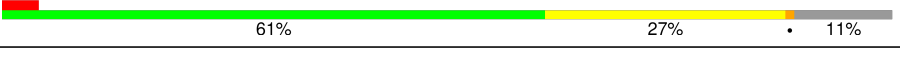
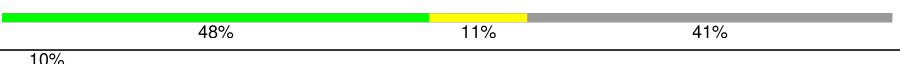
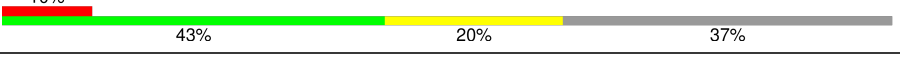
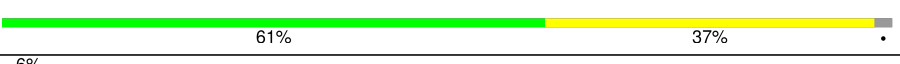

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>2%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
2	B	338	<div> <div>66%</div> <div>31%</div> <div>•</div> </div>
3	C	246	<div> <div>72%</div> <div>24%</div> <div>•</div> </div>
4	D	177	<div> <div>18%</div> <div>45%</div> <div>32%</div> <div>•</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	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	8008	-	-	-	X
32	MG	0	8009	-	-	-	X
32	MG	0	8041	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8084	-	-	-	X
32	MG	A	8051	-	-	-	X
33	K	0	8402	-	-	-	X
34	NA	0	8507	-	-	-	X
34	NA	0	8508	-	-	-	X
34	NA	0	8512	-	-	-	X
34	NA	0	8517	-	-	-	X
34	NA	0	8522	-	-	-	X
34	NA	0	8527	-	-	-	X
34	NA	0	8528	-	-	-	X
34	NA	0	8530	-	-	-	X
34	NA	0	8534	-	-	-	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	8559	-	-	-	X
34	NA	0	8562	-	-	-	X
34	NA	0	8563	-	-	-	X
34	NA	0	8564	-	-	-	X
34	NA	0	8565	-	-	-	X
34	NA	0	8568	-	-	-	X
34	NA	0	8569	-	-	-	X
34	NA	9	8572	-	-	-	X
36	SR	0	8903	-	-	-	X
36	SR	0	8904	-	-	-	X
36	SR	0	8947	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	SR	B	8987	-	-	-	X

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99122 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
			59020	26349	10874	19052	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	87	Total	Mg	0	0
			87	87		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	9	1	Total	Mg	0	0
			1	1		

- 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	67	Total Na 67 67	0	0
34	J	1	Total Na 1 1	0	0
34	Q	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	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	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
35	Y	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	93	Total 93	Sr 93	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
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	5929	Total 5929	O 5929	0	0
38	9	147	Total 147	O 147	0	0
38	A	116	Total 116	O 116	0	0
38	B	141	Total 141	O 141	0	0
38	C	170	Total 170	O 170	0	0
38	D	44	Total 44	O 44	0	0
38	E	45	Total 45	O 45	0	0
38	F	27	Total 27	O 27	0	0
38	G	19	Total 19	O 19	0	0
38	H	63	Total 63	O 63	0	0
38	I	8	Total 8	O 8	0	0
38	J	53	Total 53	O 53	0	0
38	K	56	Total 56	O 56	0	0
38	L	85	Total 85	O 85	0	0
38	M	123	Total 123	O 123	0	0
38	N	55	Total 55	O 55	0	0
38	O	43	Total 43	O 43	0	0
38	P	67	Total 67	O 67	0	0
38	Q	50	Total 50	O 50	0	0
38	R	85	Total 85	O 85	0	0
38	S	33	Total 33	O 33	0	0
38	T	34	Total 34	O 34	0	0

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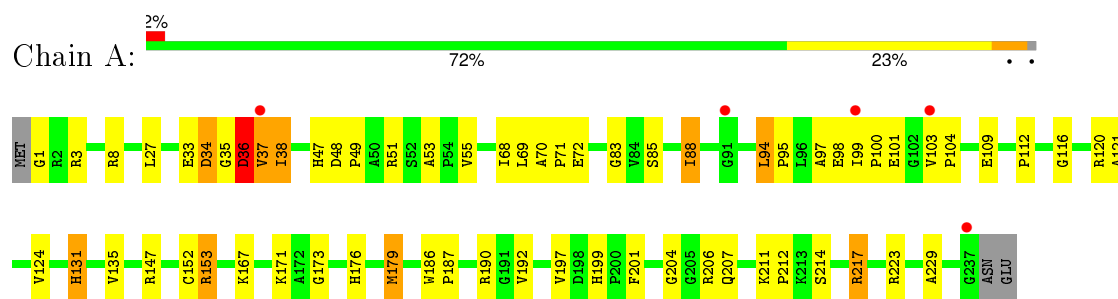
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	U	27	Total 27	O 27	0	0
38	V	13	Total 13	O 13	0	0
38	W	69	Total 69	O 69	0	0
38	X	25	Total 25	O 25	0	0
38	Y	95	Total 95	O 95	0	0
38	Z	26	Total 26	O 26	0	0
38	1	63	Total 63	O 63	0	0
38	2	50	Total 50	O 50	0	0
38	3	62	Total 62	O 62	0	0

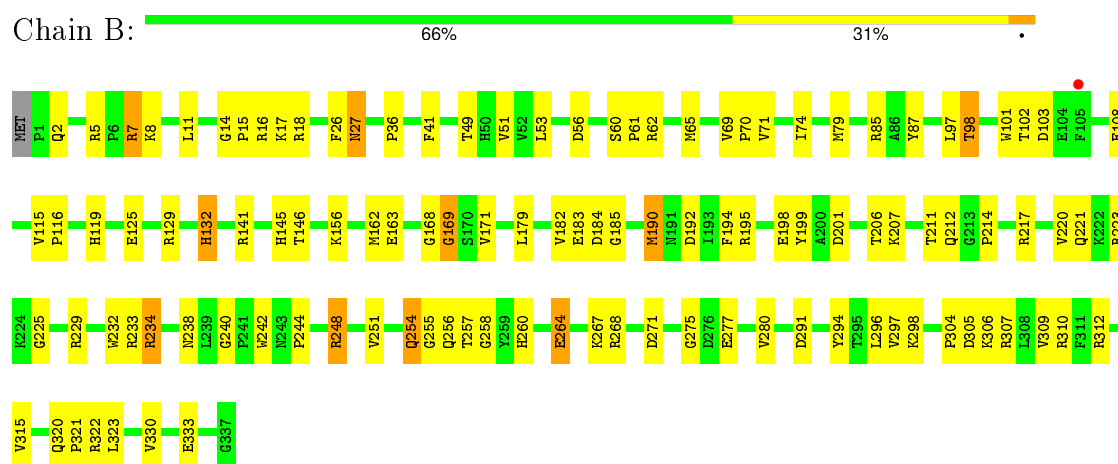
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

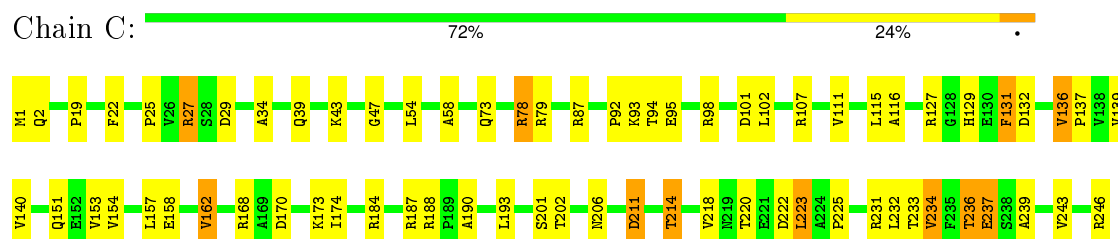
- Molecule 1: 50S ribosomal protein L2P



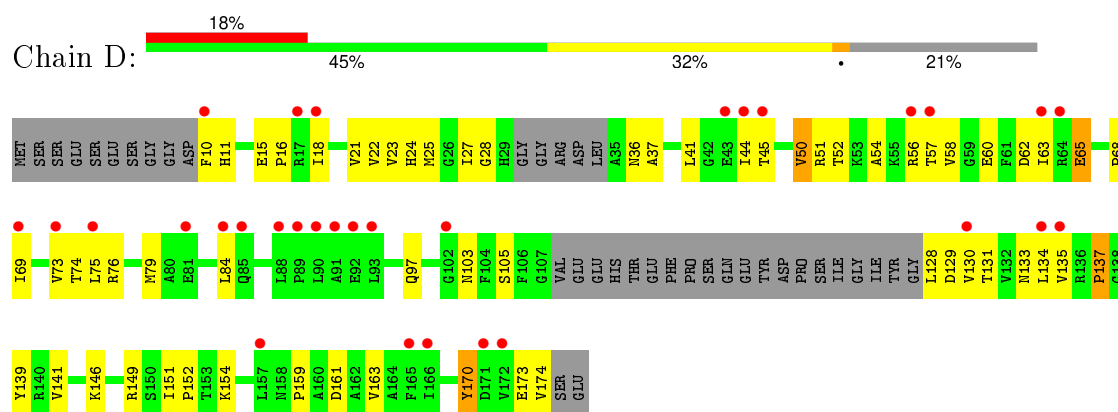
- Molecule 2: 50S ribosomal protein L3P



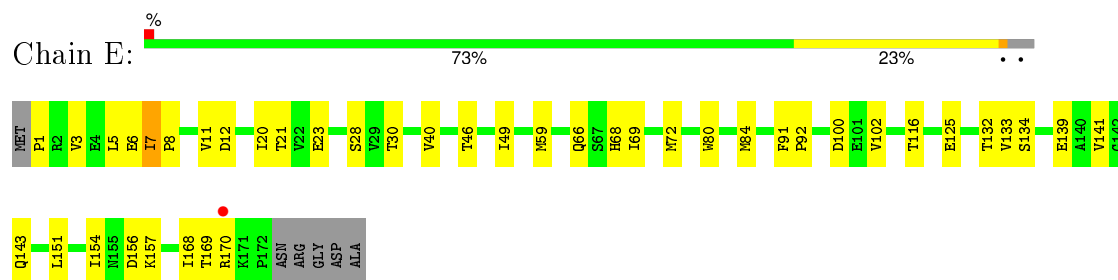
- Molecule 3: 50S ribosomal protein L4P



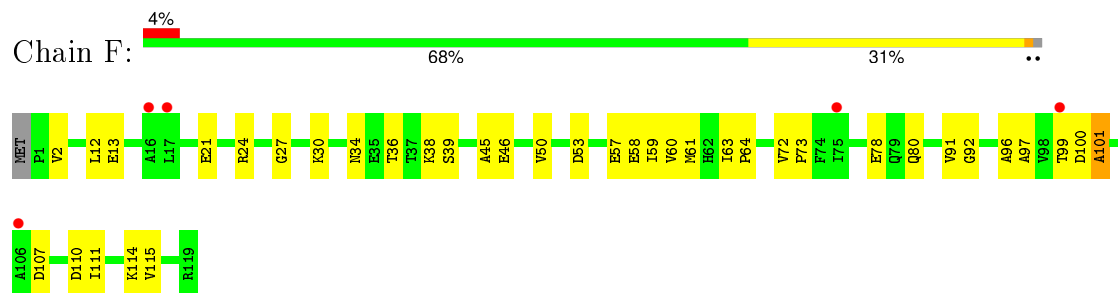
- Molecule 4: 50S ribosomal protein L5P



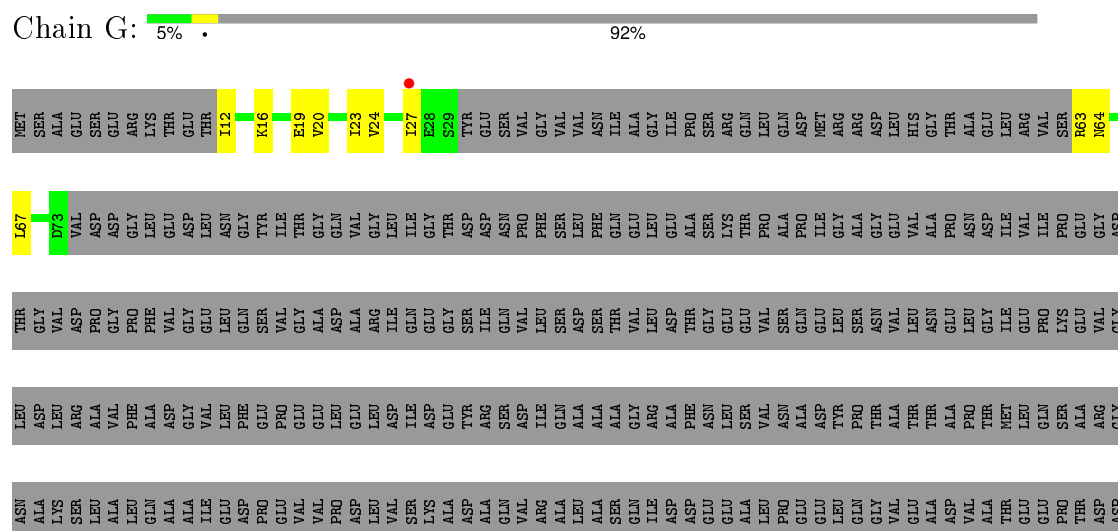
- Molecule 5: 50S ribosomal protein L6P



- Molecule 6: 50S ribosomal protein L7Ae

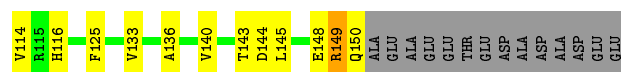


- Molecule 7: 50S ribosomal protein L10E



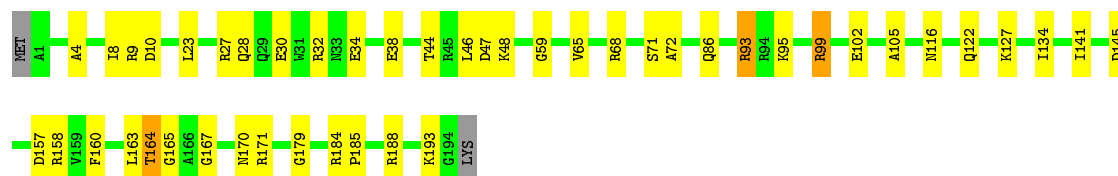






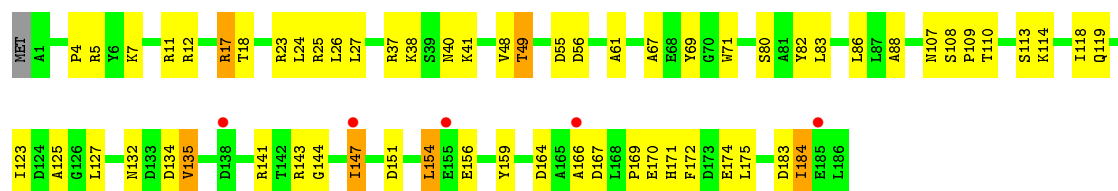
- Molecule 13: 50S ribosomal protein L15e

Chain M: 76% 22% ..



- Molecule 14: 50S ribosomal protein L18P

Chain N: 3% 66% 30% ..



- Molecule 15: 50S ribosomal protein L18e

Chain O: 82% 16% ..



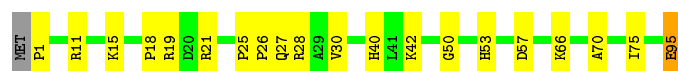
- Molecule 16: 50S ribosomal protein L19e

Chain P: 77% 17% ..



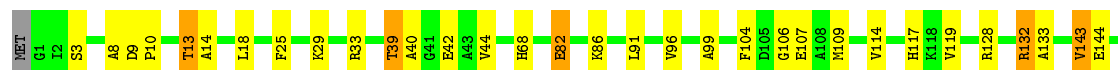
- Molecule 17: 50S ribosomal protein L21e

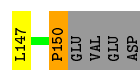
Chain Q: 78% 20% ..



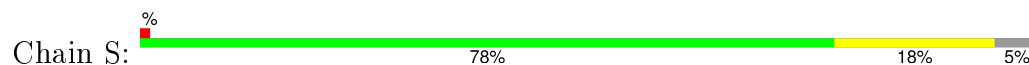
- Molecule 18: 50S ribosomal protein L22P

Chain R: 75% 18% ..

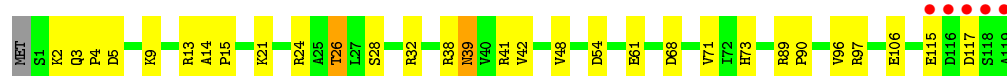
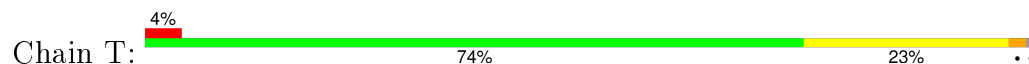




- Molecule 19: 50S ribosomal protein L23P



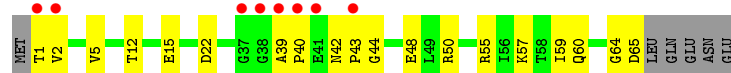
- Molecule 20: 50S ribosomal protein L24P



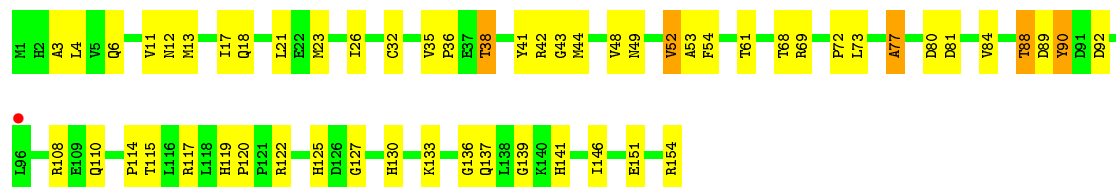
- Molecule 21: 50S ribosomal protein L24e



- Molecule 22: 50S ribosomal protein L29P



- Molecule 23: 50S ribosomal protein L30P

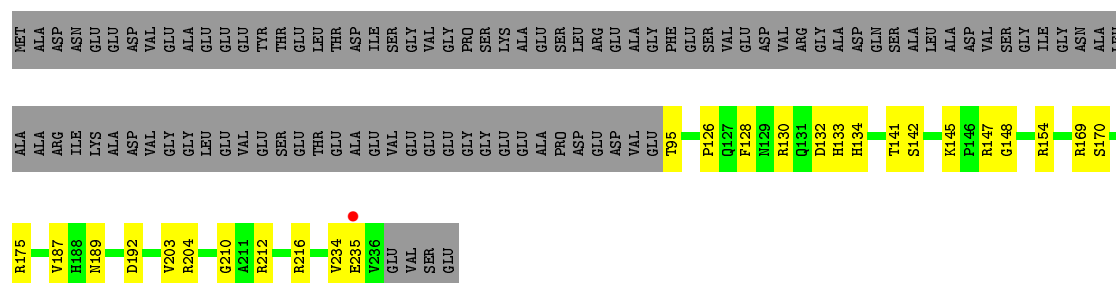


- Molecule 24: 50S ribosomal protein L31e

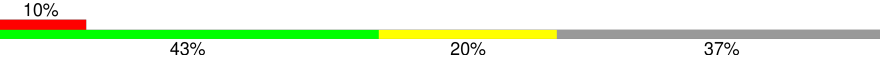


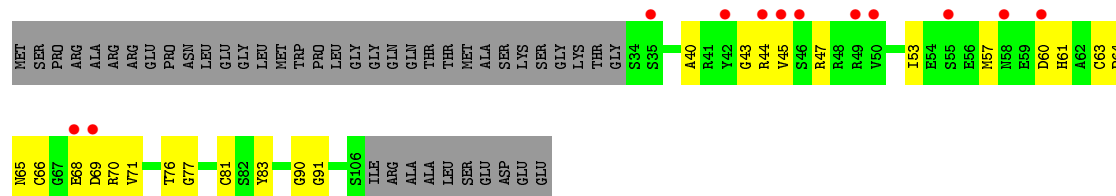
- Molecule 25: 50S ribosomal protein L32e

Chain Y: 



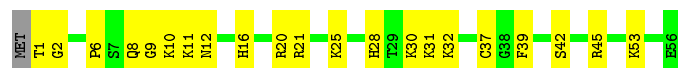
- Molecule 26: 50S ribosomal protein L37Ae

Chain Z: 



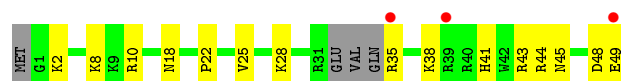
- Molecule 27: 50S ribosomal protein L37e

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: 



C1554	G1441	G1351	C1245	G1168	C1068	U	C880	A790	G684	C583	C491	A378	G289	C200	U107
G1555	A1442	C1353	A1246	U1169	C1069	C	G885	A791	C685	U584	C492	G379	C290	C200	U108
A1559	U1446	U1358	U1249	A1171	A1070	G	A886	G792	A886	U584	G496	A380	C291	U210	C111
U	U1447	U1359	C1250	G1172	G1071	A	G887	G800	A887	G588	A497	G381	G292	U211	G112
C1562	C1450	C1360	C1268	A1174	A1078	G	U888	U801	G689	G604	A498	U382	C295	U212	A113
A1573	C1451	C1366	G1269	G1175	A1079	A	G889	A807	G690	C605	G499	A383	G296	U214	A114
G1586	U1461	A1372	C1273	U1180	A1081	G	C899	A808	A694	C613	U392	U396	G297	G219	A119
U1587	C1462	G1373	A1278	A1181	C1080	A	U903	A809	A695	U614	G503	A397	C298	C220	A120
G1588	U1474	C1374	U1279	C1182	A1088	U	U904	G812	G697	U615	G504	U397	U299	U211	U121
G1589	C1474	A1375	A1280	C1183	C1097	C	C905	C813	A698	U616	C505	A397	G302	G222	U125
C1592	C1477	G1376	C1287	C1184	A1097	G	A912	U815	C699	U619	A507	U398	C303	G223	G
C1593	U1478	G1377	U1288	U1185	G1099	C	G920	U816	A700	A620	A508	U399	G304	U224	C
C1594	C1482	G1378	U1289	U1187	A1099	A	G921	G817	G702	C621	A509	A407	A306	G225	U
G1595	A1482	U1380	G1290	U1188	C1104	C	A922	G820	C704	U623	U510	A408	G307	G228	A128
U1596	C1483	A1381	A1291	G1189	U1109	A	A923	U821	C705	U624	A511	A409	U308	G229	C130
A1597	G1484	G1382	C1294	U1110	G1110	C999	A926	U822	G709	U625	G512	G417	C309	A236	A131
A1598	U1485	U1383	A1295	U1115	U1115	C1000	U932	U823	G710	U626	G513	A418	U312	G237	U134
C1603	A1486	C1384	A1296	U1116	U1116	U1001	U932	U824	G711	G627	G514	A419	U313	G237	G135
G1604	U1487	G1385	U1297	U1117	U1117	G1002	U932	U825	C712	A628	G515	C421	U316	A241	C136
G1605	U1488	G1386	U1297	U1118	U1118	C	A939	U826	C713	A629	G516	A423	U317	A241	U137
C1607	C1495	G1387	U1298	U1119	A1113	A1006	A939	U827	U713	A632	G517	A424	U318	A243	U138
U1603	U1503	G1391	G1299	U1120	G1119	A1007	G940	U834	U714	A633	U522	C424	U319	C244	C139
C1613	A1504	A1392	A1300	U1121	U1120	C1008	G941	U835	U	C633	C523	C440	G320	G249	C141
G1614	U1505	C1393	U1304	C1201	U1121	U1009	U942	U836	C716	G634	A524	C441	A329	C250	A145
A1615	U1506	C1394	C1305	C1202	G1127	C1010	A943	G836	C717	A635	A532	C442	C330	C251	A145
A1616	C1396	G1395	U1306	G1203	U1128	A1014	G944	U840	C718	G636	A532	C442	C330	C252	A151
C1617	C1396	C1397	A1307	U1205	C1129	C1015	U945	A841	G724	C638	G535	U445	G333	A255	A151
G1622	C1513	G1398	A1308	U1206	U1130	U1016	U947	U842	C725	A639	A536	A446	G336	C256	C154
A1624	U1515	C1400	G1312	A1207	U1131	U1016	G948	A843	U734	U645	A538	A447	G337	G257	C155
U1625	C1520	A1407	A1321	C1208	G1135	A1020	U949	U846	U735	U645	A539	A448	G338	G258	C156
A1626	A1522	U1408	G1322	G1211	U1136	C1025	G950	G847	A736	U645	A540	A449	G339	G259	G157
G1627	G1523	G1409	G1322	C1212	U1137	U1026	A951	C848	A737	G652	C541	C451	A347	A159	A159
A1630	U1524	U1409	G1322	G1216	U1138	U1028	G958	C853	G738	U653	A542	G452	C342	C162	C162
A1631	G1525	A1413	G1325	G1221	C1140	C1044	C959	C854	C741	U655	G544	U457	C344	U163	U163
A1632	A1526	A1414	A1328	U1149	U1149	G1045	G960	U857	G744	U656	G545	A458	A347	U265	A166
C1633	A1527	G1415	A1328	A1150	A1150	G1045	A961	U858	G745	C658	G553	A460	A351	G289	A167
G1636	A1528	U1419	G1331	G1151	G1151	G1052	C962	C849	G746	A659	C558	C461	A352	U270	C168
U1637	G1529	U1419	G1332	A1154	A1154	G1053	C963	U861	G747	A660	U559	A466	A352	A272	A177
G1637	U1535	U1422	U1333	G1155	G1155	G1054	G968	A867	C749	G661	U560	G467	G358	G273	U178
A1641	C1536	C1423	C1334	G1159	G1159	U1056	U970	G869	A750	G669	G564	U468	C363	U277	G182
A1642	C1537	A1424	G1339	G1160	G1160	A1057	G	G870	C759	A671	G567	U470	U364	U278	G185
C1644	U1539	C1426	G1340	A1161	A1161	A1058	U	U872	C764	G672	G568	G482	U366	G279	A186
U1645	C1545	G1430	A1342	G1162	G1162	C1060	U	U875	G765	C677	A569	C483	U367	U281	A187
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A1653	G1552	A1434	G1344	G1164	U1164	G1063	C	U877	U776	G681	C571	A485	G369	U283	A189
U1654	C1553	C1436	U1350	G1167	G1167	U1066	C	A878	U777	A682	G579	A486	G370	C284	G190
						A1067	C	C879		G683	A580	U488	A372	U286	A192

C2672	A2766	C2672	A2483	G2385	C2309	C	U	G2082	C	G1752	G1655
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U2690	A2773	C2591	C2494	C2403	A2321	A	U	A2096	G1971	C1767	U1668
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G2694	A2777	U2595	C2502	G2412	U2330	U	A	A2104	A1978	U1771	A1682
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C2716	A2799	C2644	U2537	A2456	G2359	C	C	C	A1941	U1835	A1732
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G2718	A2801	C2646	G2542	U2461	A2361	C	C	C	A2039	U1838	C1734
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U2720	A2803	A2649	U2544	A2465	A2363	C	C	C	G2044	A1840	A1736
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C2722	A2805	C2652	C2548	A2467	A2365	C	C	C	A2055	U1846	U1740
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G2763	A2846	C2692	U2599	U2488	A2405	C	C	C	C		
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G2769	A2852	C2698	U2605	U2494	A2411	C	C	C	C		
C2770	A2853	U2699	C2606	U2495	A2412	C	C	C	C		
U2771	A2854	C2700	U2607	U2496	A2413	C	C	C	C		
G2772	A2855	U2701	U2608	U2497	A2414	C	C	C	C		
C2773	A2856	C2702	C2609	U2498	A2415	C	C	C	C		
U2774	A2857	U2703	U2610	U2499	A2416	C	C	C	C		
G2775	A2858	C2704	U2611	U2500	A2417	C	C	C	C		
C2776	A2859	U2705	U2612	U2501	A2418	C	C	C	C		
U2777	A2860	C2706	A2513	U2502	A2419	C	C	C	C		
G2778	A2861	U2707	U2514	U2503	A2420	C	C	C	C		
C2779	A2862	C2708	A2515	U2504	A2421	C	C	C	C		
U2780	A2863	U2709	U2516	U2505	A2422	C	C	C	C		
G2781	A2864	C2710	U2517	U2506	A2423	C	C	C	C		
C2782	A2865	U2711	U2518	U2507	A2424	C	C	C	C		
U2783	A2866	C2712	U2519	U2508	A2425	C	C	C	C		
G2784	A2867	U2713	U2520	U2509	A2426	C	C	C	C		
C2785	A2868	C2714	U2521	U2510	A2427	C	C	C	C		
U2786	A2869	U2715	U2522	U2511	A2428	C	C	C	C		
G2787	A2870	C2716	U2523	U2512	A2429	C	C	C	C		
C2788	A2871	U2717	U2524	U2513	A2430	C	C	C	C		
U2789	A2872	C2718	U2525	U2514	A2431	C	C	C	C		
G2790	A2873	U2719	U2526	U2515	A2432	C	C	C	C		
C2791	A2874	C2720	U2527	U2516	A2433	C	C	C	C		
U2792	A2875	U2721	U2528	U2517	A2434	C	C	C	C		
G2793	A2876	C2722	U2529	U2518	A2435	C	C	C	C		
C2794	A2877	U2723	U2530	U2519	A2436	C	C	C	C		
U2795	A2878	C2724	U2531	U2520	A2437	C	C	C	C		
G2796	A2879	U2725	U2532	U2521	A2438	C	C	C	C		
C2797	A2880	C2726	U2533	U2522	A2439	C	C	C	C		
U2798	A2881	U2727	U2534	U2523	A2440	C	C	C	C		
G2799	A2882	C2728	U2535	U2524	A2441	C	C	C	C		
C2800	A2883	U2729	U2536	U2525	A2442	C	C	C	C		
U2801	A2884	C2730	U2537	U2526	A2443	C	C	C	C		
G2802	A2885	U2731	U2538	U2527	A2444	C	C	C	C		
C2803	A2886	C2732	U2539	U2528	A2445	C	C	C	C		
U2804	A2887	U2733	U2540	U2529	A2446	C	C	C	C		
G2805	A2888	C2734	U2541	U2530	A2447	C	C	C	C		
C2806	A2889	U2735	U2542	U2531	A2448	C	C	C	C		
U2807	A2890	C2736	U2543	U2532	A2449	C	C	C	C		
G2808	A2891	U2737	U2544	U2533	A2450	C	C	C	C		
C2809	A2892	C2738	U2545	U2534	A2451	C	C	C	C		
U2810	A2893	U2739	U2546	U2535	A2452	C	C	C	C		
G2811	A2894	C2740	U2547	U2536	A2453						



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	213.16Å 300.03Å 576.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 2.90 85.91 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.98-2.90) 92.3 (85.91-2.41)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.171 , 0.220 0.167 , 0.211	Depositor DCC
$R_{free}$ test set	3946 reflections (1.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	57.0	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 81.4	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 667133 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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	0.32	0/1786	0.64	0/2408
2	B	0.32	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.63	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.33	0/1382	0.56	0/1880
6	F	0.34	0/901	0.58	0/1224
7	G	0.31	0/241	0.49	0/324
8	H	0.33	0/1302	0.63	0/1743
9	I	0.29	0/526	0.51	0/716
10	J	0.36	0/1136	0.60	0/1530
11	K	0.35	0/1004	0.67	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.35	0/1582	0.61	0/2116
14	N	0.30	0/1474	0.62	0/1999
15	O	0.34	0/874	0.59	0/1181
16	P	0.32	0/1147	0.51	0/1528
17	Q	0.33	0/749	0.65	0/1005
18	R	1.26	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.32	0/648	0.55	0/875
20	T	0.33	0/958	0.64	0/1289
21	U	0.33	0/417	0.59	0/562
22	V	0.33	0/502	0.52	0/675
23	W	0.34	0/1219	0.63	0/1655
24	X	0.35	0/664	0.60	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.37	0/584	0.60	0/781
27	1	0.39	0/438	0.59	0/578
28	2	0.34	0/401	0.60	0/529
29	3	0.36	0/771	0.55	0/1024
30	0	0.37	0/65957	0.68	13/102867 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98701 (0.0%)	0.67	20/147586 (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	0	28
31	9	0	1
All	All	1	30

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.29	2.86	1.50
18	R	150	PRO	CA-C	-18.25	1.16	1.52
18	R	150	PRO	CG-CD	13.93	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.37	1.66	1.47
18	R	150	PRO	N-CD	10.73	1.62	1.47
18	R	150	PRO	CA-CB	7.62	1.68	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.83	112.00
18	R	150	PRO	N-CA-C	-19.40	61.65	112.10
18	R	150	PRO	CA-N-CD	12.30	128.92	111.70
18	R	150	PRO	N-CA-CB	10.97	116.46	103.30
18	R	150	PRO	CA-C-O	-8.51	99.79	120.20
30	0	1120	U	C5'-C4'-C3'	-6.39	105.78	116.00
30	0	1942	A	C5'-C4'-C3'	6.16	125.85	116.00
18	R	150	PRO	CA-CB-CG	-6.09	92.42	104.00
30	0	1592	G	N9-C1'-C2'	5.90	121.67	114.00
30	0	1504	A	C1'-O4'-C4'	-5.90	105.18	109.90
31	9	39	U	N1-C1'-C2'	5.83	121.57	114.00
30	0	871	G	C5'-C4'-O4'	-5.67	102.30	109.10
30	0	2316	G	C5'-C4'-C3'	-5.59	107.06	116.00
30	0	1504	A	N9-C1'-C2'	5.50	121.15	114.00
30	0	841	A	C1'-O4'-C4'	-5.46	105.53	109.90
30	0	2313	C	C5'-C4'-O4'	5.29	115.45	109.10
30	0	2726	U	N1-C1'-C2'	5.25	120.83	114.00
30	0	1165	G	C1'-O4'-C4'	-5.21	105.73	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2291	A	N9-C1'-C2'	5.20	120.75	114.00
30	0	2301	A	N9-C1'-C2'	5.11	120.65	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	131	A	Sidechain
30	0	1430	G	Sidechain
30	0	1592	G	Sidechain
30	0	1829	A	Sidechain
30	0	1848	G	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1970	G	Sidechain
30	0	220	C	Sidechain
30	0	2301	A	Sidechain
30	0	2412	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	333	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	888	U	Sidechain
31	9	39	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	63	0
2	B	2625	0	2533	89	0
3	C	1860	0	1813	59	0
4	D	1094	0	1085	45	0
5	E	1357	0	1266	29	0
6	F	890	0	843	26	0
7	G	240	0	231	8	0
8	H	1282	0	1292	33	0
9	I	519	0	500	23	0
10	J	1120	0	1098	32	0
11	K	994	0	1027	32	0
12	L	1118	0	1076	29	0
13	M	1558	0	1573	42	0
14	N	1445	0	1401	51	0
15	O	865	0	873	18	0
16	P	1136	0	1123	24	0
17	Q	735	0	729	21	0
18	R	1149	0	1122	37	0
19	S	641	0	605	10	0
20	T	950	0	924	21	0
21	U	410	0	364	8	0
22	V	499	0	511	17	0
23	W	1196	0	1137	56	0
24	X	654	0	653	18	0
25	Y	1130	0	1133	23	0
26	Z	573	0	532	15	0
27	1	431	0	426	23	0
28	2	396	0	413	15	0
29	3	755	0	728	18	0
30	0	59020	0	29811	1159	0
31	9	2599	0	1325	100	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	67	0	0	0	0
34	9	2	0	0	0	0
34	C	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	10	0	0	4	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	2	0
35	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	93	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	3	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	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	5929	0	0	185	0
38	1	63	0	0	4	0
38	2	50	0	0	1	0
38	3	62	0	0	3	0
38	9	147	0	0	7	0
38	A	116	0	0	5	0
38	B	141	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	C	170	0	0	13	0
38	D	44	0	0	3	0
38	E	45	0	0	2	0
38	F	27	0	0	2	0
38	G	19	0	0	1	0
38	H	63	0	0	7	0
38	I	8	0	0	3	0
38	J	53	0	0	1	0
38	K	56	0	0	5	0
38	L	85	0	0	6	0
38	M	123	0	0	2	0
38	N	55	0	0	5	0
38	O	43	0	0	3	0
38	P	67	0	0	2	0
38	Q	50	0	0	3	0
38	R	85	0	0	1	0
38	S	33	0	0	2	0
38	T	34	0	0	2	0
38	U	27	0	0	2	0
38	V	13	0	0	2	0
38	W	69	0	0	4	0
38	X	25	0	0	2	0
38	Y	95	0	0	5	0
38	Z	26	0	0	3	0
All	All	99122	0	59913	1941	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 13.

All (1941) 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'	1.77	1.12
30:0:871:G:C8	30:0:871:G:H5'	1.84	1.11
30:0:871:G:H8	30:0:871:G:H5'	1.09	1.10
31:9:56:A:H2'	31:9:57:A:H5''	1.31	1.10
14:N:37:ARG:NH1	31:9:6:C:H5''	1.63	1.09
30:0:1160:G:H5'	30:0:1161:A:C5'	1.82	1.09
13:M:171:ARG:HD3	30:0:156:C:H5''	1.33	1.09
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:76:G:H3'	31:9:77:A:H5''	1.36	1.06
30:0:545:G:H8	30:0:545:G:H5'	1.19	1.06
30:0:1205:U:H2'	30:0:1206:U:H5''	1.32	1.04
30:0:1160:G:H5'	30:0:1161:A:H5'	1.03	1.02
30:0:1701:A:H4'	30:0:1702:U:H5''	1.42	1.01
15:O:3:THR:HG22	30:0:656:G:H5'	1.41	1.01
10:J:82:THR:HG23	30:0:1242:A:H5'	1.39	1.01
30:0:2717:C:C2'	30:0:2718:C:H5''	1.92	0.99
30:0:1979:G:H2'	38:0:3301:HOH:O	1.61	0.98
31:9:29:C:H2'	31:9:30:C:H5'	1.44	0.98
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.46	0.97
11:K:10:GLN:H	11:K:10:GLN:HE21	0.95	0.95
30:0:182:G:H5'	38:0:5168:HOH:O	1.67	0.95
30:0:1666:C:O2'	30:0:1667:A:H5''	1.67	0.94
30:0:1118:A:H3'	30:0:1118:A:H8	1.30	0.94
30:0:2717:C:H2'	30:0:2718:C:H5''	1.50	0.94
30:0:381:G:H5''	38:0:4330:HOH:O	1.67	0.93
30:0:1187:U:HO2'	30:0:1189:A:H2	1.01	0.93
30:0:1205:U:H2'	30:0:1206:U:C5'	1.99	0.93
30:0:1118:A:H3'	30:0:1118:A:C8	2.03	0.93
30:0:1603:A:H5'	30:0:1605:G:O4'	1.67	0.92
30:0:1634:G:H3'	38:0:3907:HOH:O	1.70	0.91
30:0:282:C:H1'	30:0:368:C:N4	1.84	0.91
16:P:115:SER:H	16:P:118:GLN:HE21	1.03	0.91
10:J:52:GLN:NE2	30:0:1119:G:H2'	1.85	0.91
30:0:271:C:H41	30:0:378:A:H2	1.17	0.90
2:B:162:MET:SD	2:B:310:ARG:HD3	2.11	0.90
30:0:559:U:H5'	30:0:559:U:H6	1.35	0.90
30:0:545:G:C8	30:0:545:G:H5'	2.05	0.90
30:0:871:G:H8	30:0:871:G:C5'	1.85	0.90
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.20	0.90
30:0:542:A:H5'	30:0:542:A:H8	1.36	0.90
31:9:14:G:H5'	31:9:14:G:H8	1.37	0.90
31:9:56:A:C2'	31:9:57:A:H5''	2.03	0.89
26:Z:70:ARG:HD3	26:Z:83:TYR:HB2	1.55	0.89
30:0:1119:G:H22	30:0:1246:A:H2	1.20	0.89
30:0:870:G:H2'	30:0:871:G:H5''	1.53	0.89
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.17	0.88
30:0:1632:A:H2'	30:0:1633:C:H5'	1.56	0.88
30:0:2508:C:H2'	38:0:6764:HOH:O	1.73	0.87
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:558:C:C2'	30:0:559:U:H5''	2.05	0.86
30:0:1205:U:C2'	30:0:1206:U:H5''	2.05	0.86
30:0:506:G:H22	30:0:509:A:H5'	1.40	0.86
30:0:1184:C:H1'	38:0:7480:HOH:O	1.74	0.86
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.73	0.86
30:0:2507:G:H2'	30:0:2510:C:H42	1.41	0.86
30:0:541:C:C2'	30:0:542:A:H5''	2.06	0.86
30:0:2908:A:H2'	30:0:2909:G:O4'	1.76	0.86
30:0:1189:A:H1'	30:0:1209:C:O4'	1.76	0.85
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.58	0.85
30:0:1183:C:H2'	38:0:6249:HOH:O	1.76	0.85
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.58	0.85
30:0:1667:A:H8	30:0:1667:A:H5'	1.41	0.85
16:P:117:SER:HB3	30:0:1593:C:OP1	1.75	0.85
30:0:2717:C:O2'	30:0:2718:C:H5''	1.77	0.85
30:0:541:C:H2'	30:0:542:A:H5''	1.58	0.85
30:0:2586:U:H3	30:0:2592:G:H22	1.22	0.84
30:0:2291:A:C8	30:0:2309:C:H5'	2.12	0.84
2:B:238:ASN:HD22	2:B:240:GLY:H	1.24	0.84
38:O:7674:HOH:O	30:0:653:U:H5''	1.77	0.84
30:0:1206:U:H6	30:0:1206:U:H5'	1.41	0.84
30:0:2710:U:H1'	38:0:7632:HOH:O	1.77	0.84
30:0:2506:A:HO2'	30:0:2507:G:H8	1.21	0.84
31:9:2:U:OP2	31:9:3:A:H5'	1.78	0.84
30:0:1474:C:H6	30:0:1474:C:H5'	1.43	0.83
30:0:558:C:O2'	30:0:559:U:H5''	1.78	0.83
30:0:1474:C:C6	30:0:1474:C:H5'	2.13	0.83
18:R:29:LYS:HE2	30:0:524:A:C5'	2.08	0.83
4:D:154:LYS:HD2	4:D:154:LYS:H	1.43	0.83
30:0:506:G:H22	30:0:509:A:C5'	1.92	0.83
30:0:877:G:H5'	30:0:878:G:OP1	1.79	0.83
30:0:1119:G:N2	30:0:1246:A:C2	2.46	0.82
30:0:1116:U:O2'	30:0:1118:A:H2	1.62	0.82
14:N:37:ARG:HH12	31:9:6:C:H5''	1.43	0.82
18:R:29:LYS:HE2	30:0:524:A:H5''	1.59	0.82
30:0:1116:U:H3	30:0:1246:A:H62	1.24	0.82
30:0:283:U:H5	30:0:284:C:N3	1.78	0.81
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.27	0.81
30:0:69:A:H5'	30:0:69:A:C8	2.15	0.81
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.62	0.81
30:0:1878:G:H1'	38:0:6126:HOH:O	1.77	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2852:A:H5'	38:0:5244:HOH:O	1.80	0.81
15:O:3:THR:CG2	30:0:656:G:H5'	2.10	0.81
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.63	0.81
30:0:541:C:H2'	30:0:542:A:C5'	2.11	0.81
30:0:2529:G:H3'	38:0:7197:HOH:O	1.80	0.80
30:0:2506:A:O2'	30:0:2507:G:H8	1.64	0.79
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.62	0.79
11:K:10:GLN:H	11:K:10:GLN:NE2	1.79	0.79
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.63	0.79
30:0:2502:C:C2'	30:0:2503:A:H5'	2.13	0.78
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.65	0.78
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.64	0.78
11:K:39:GLY:HA2	38:0:5232:HOH:O	1.83	0.78
30:0:2578:G:H5'	30:0:2578:G:H8	1.48	0.78
30:0:1632:A:C2'	30:0:1633:C:H5'	2.13	0.78
30:0:2256:G:O2'	30:0:2257:G:H5'	1.82	0.78
3:C:236:THR:HG22	3:C:239:ALA:H	1.46	0.78
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.66	0.78
30:0:282:C:O2'	30:0:283:U:H5'	1.84	0.78
14:N:113:SER:HB2	38:N:8849:HOH:O	1.84	0.77
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.67	0.77
30:0:2526:C:H5'	30:0:2526:C:C6	2.19	0.77
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.65	0.77
30:0:1300:G:H1'	38:0:4694:HOH:O	1.83	0.77
30:0:2635:A:O2'	30:0:2636:C:H5'	1.84	0.77
13:M:164:THR:HG22	13:M:167:GLY:H	1.50	0.77
30:0:272:A:H3'	38:0:7542:HOH:O	1.84	0.77
31:9:14:G:H5'	31:9:14:G:C8	2.19	0.77
30:0:2502:C:H2'	30:0:2503:A:H5'	1.65	0.77
30:0:2608:C:H3'	38:0:7824:HOH:O	1.85	0.77
30:0:396:U:H1'	38:0:7640:HOH:O	1.85	0.77
30:0:69:A:H5'	30:0:69:A:H8	1.50	0.76
2:B:179:LEU:O	2:B:183:GLU:HG2	1.84	0.76
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.67	0.76
30:0:1701:A:H5'	38:0:6290:HOH:O	1.83	0.76
30:0:1118:A:H62	30:0:1244:U:H3	1.31	0.76
30:0:2783:A:H3'	38:0:5242:HOH:O	1.83	0.76
30:0:2812:A:H2	30:0:2814:A:H62	1.31	0.76
30:0:2679:G:H2'	30:0:2681:A:OP2	1.86	0.76
31:9:54:A:O2'	31:9:55:U:H5'	1.85	0.76
30:0:1372:A:H3'	38:0:7202:HOH:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2403:C:H5'	38:0:6033:HOH:O	1.84	0.76
22:V:1:THR:HB	30:0:93:C:H5''	1.68	0.76
30:0:192:A:H5'	38:0:7655:HOH:O	1.85	0.76
30:0:1603:A:H5''	30:0:1605:G:H5'	1.68	0.75
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.69	0.75
6:F:91:VAL:HG12	6:F:92:GLY:H	1.52	0.75
10:J:74:ARG:HB3	10:J:74:ARG:HH11	1.51	0.75
30:0:1172:G:H5''	38:0:7271:HOH:O	1.85	0.75
30:0:1116:U:HO2'	30:0:1118:A:H2	0.79	0.74
30:0:558:C:H2'	30:0:559:U:C5'	2.17	0.74
30:0:1701:A:H4'	30:0:1702:U:C5'	2.15	0.74
3:C:1:MET:HG2	3:C:2:GLN:H	1.51	0.74
30:0:2748:G:H5'	38:0:7554:HOH:O	1.87	0.74
30:0:2768:A:O2'	30:0:2769:C:H5'	1.87	0.74
30:0:2420:G:O2'	30:0:2421:G:H5'	1.86	0.74
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.69	0.74
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.70	0.74
30:0:2717:C:H2'	30:0:2718:C:C5'	2.18	0.74
3:C:127:ARG:NH2	3:C:225:PRO:HG2	2.03	0.74
30:0:2404:G:H5''	38:0:5222:HOH:O	1.88	0.74
18:R:25:PHE:CE2	18:R:29:LYS:HE3	2.23	0.73
11:K:10:GLN:N	11:K:10:GLN:HE21	1.79	0.73
35:0:8812:CL:CL	38:0:5135:HOH:O	2.41	0.73
30:0:1666:C:H2'	30:0:1667:A:H5'	1.70	0.73
22:V:1:THR:HG23	22:V:2:VAL:H	1.53	0.73
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.54	0.73
29:3:65:THR:HG22	29:3:67:LEU:HG	1.69	0.73
1:A:211:LYS:HB2	38:A:9082:HOH:O	1.87	0.73
30:0:2004:U:H4'	38:0:5316:HOH:O	1.88	0.73
30:0:138:U:H5''	30:0:139:C:OP2	1.88	0.73
15:O:42:GLU:HB2	38:O:2176:HOH:O	1.87	0.73
30:0:2896:A:H5''	38:0:6105:HOH:O	1.87	0.73
15:O:47:ARG:HG3	15:O:47:ARG:HH11	1.53	0.73
38:Z:8707:HOH:O	30:0:1886:A:H4'	1.89	0.73
3:C:139:VAL:HG13	38:C:8644:HOH:O	1.88	0.73
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.71	0.73
30:0:1666:C:C2'	30:0:1667:A:H5''	2.19	0.72
30:0:1641:A:H2'	30:0:1642:A:H5'	1.71	0.72
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.88	0.72
30:0:2765:C:H4'	38:0:5531:HOH:O	1.88	0.72
30:0:870:G:C2'	30:0:871:G:H5''	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:50:ARG:NH1	30:0:56:G:H5''	2.04	0.72
30:0:1118:A:C8	30:0:1118:A:C3'	2.69	0.72
30:0:2256:G:C2'	30:0:2257:G:H5'	2.18	0.72
28:2:41:HIS:H	28:2:45:ASN:HD22	1.35	0.72
30:0:827:A:H1'	38:0:6220:HOH:O	1.88	0.72
30:0:468:U:H3'	38:0:7580:HOH:O	1.89	0.72
30:0:871:G:C8	30:0:871:G:C5'	2.64	0.72
30:0:1187:U:O2'	30:0:1189:A:H2	1.71	0.72
30:0:2769:C:C2'	30:0:2770:G:H5'	2.20	0.72
22:V:50:ARG:HH12	30:0:56:G:H5''	1.55	0.72
30:0:1201:C:H5''	38:0:6238:HOH:O	1.89	0.72
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.24	0.72
20:T:9:LYS:HE2	20:T:13:ARG:NH1	2.04	0.72
1:A:135:VAL:HG11	1:A:147:ARG:NH2	2.04	0.71
35:0:8813:CL:CL	38:0:4694:HOH:O	2.45	0.71
30:0:1183:C:N4	30:0:1184:C:H41	1.87	0.71
10:J:52:GLN:HE22	30:0:1119:G:H2'	1.55	0.71
31:9:29:C:C2'	31:9:30:C:H5'	2.18	0.71
30:0:1525:G:H5'	30:0:1526:A:OP2	1.91	0.71
30:0:2491:G:H1'	38:0:6878:HOH:O	1.89	0.71
30:0:1189:A:H3'	38:0:7693:HOH:O	1.90	0.71
30:0:1741:U:H5'	30:0:1742:A:OP1	1.90	0.71
30:0:2372:A:H2'	30:0:2373:U:H6	1.56	0.70
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.21	0.70
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.92	0.70
2:B:307:ARG:HG3	2:B:307:ARG:HH11	1.57	0.70
2:B:206:THR:HG21	30:0:2716:G:H5''	1.73	0.70
31:9:20:G:O2'	31:9:21:G:H5'	1.91	0.70
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.57	0.70
30:0:2659:U:H5''	38:0:4138:HOH:O	1.92	0.70
30:0:2637:A:H5'	38:0:9281:HOH:O	1.92	0.70
31:9:92:G:H2'	31:9:93:A:C8	2.27	0.70
30:0:567:U:H5''	38:0:5297:HOH:O	1.92	0.70
30:0:1973:A:H5'	30:0:1973:A:H8	1.57	0.69
30:0:1835:U:C5	30:0:1840:A:N7	2.59	0.69
30:0:1750:C:H5''	38:0:3676:HOH:O	1.91	0.69
30:0:544:G:H2'	30:0:545:G:H5''	1.74	0.69
30:0:380:A:H2'	38:0:7240:HOH:O	1.92	0.69
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.75	0.69
24:X:71:ARG:HD3	38:X:2171:HOH:O	1.91	0.69
30:0:2010:A:H2'	38:0:5965:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:12:ILE:HG23	38:0:5468:HOH:O	1.93	0.69
30:0:281:U:O2'	30:0:282:C:H5'	1.93	0.69
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.23	0.69
16:P:115:SER:H	16:P:118:GLN:NE2	1.85	0.69
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.75	0.69
23:W:72:PRO:HG2	23:W:77:ALA:HB3	1.73	0.69
30:0:1441:G:O2'	30:0:1442:A:H5'	1.91	0.69
1:A:51:ARG:HB2	38:A:9066:HOH:O	1.91	0.69
30:0:2251:G:H2'	30:0:2252:A:C8	2.28	0.69
30:0:1377:C:H6	30:0:1377:C:H5'	1.58	0.69
27:1:25:LYS:HD2	28:2:49:GLU:H	1.58	0.68
30:0:1666:C:H2'	30:0:1667:A:C5'	2.22	0.68
8:H:59:GLN:HE21	8:H:129:ARG:NE	1.91	0.68
30:0:2111:G:H1'	38:0:9053:HOH:O	1.92	0.68
30:0:2768:A:H2'	30:0:2769:C:O4'	1.93	0.68
30:0:2563:U:H2'	30:0:2565:C:O5'	1.94	0.68
30:0:1183:C:H42	30:0:1184:C:H41	1.42	0.68
13:M:23:LEU:HD13	13:M:27:ARG:HH21	1.57	0.68
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.75	0.68
3:C:174:ILE:HD11	30:0:338:C:H4'	1.75	0.68
12:L:133:VAL:HA	38:L:8874:HOH:O	1.92	0.68
30:0:1603:A:C5'	30:0:1605:G:H5'	2.23	0.68
6:F:91:VAL:HG12	6:F:92:GLY:N	2.09	0.68
14:N:141:ARG:HH21	31:9:48:C:H4'	1.58	0.68
30:0:2453:G:H3'	38:0:5927:HOH:O	1.94	0.68
14:N:80:SER:HB2	38:N:8830:HOH:O	1.93	0.68
30:0:558:C:H2'	30:0:559:U:H5''	1.72	0.67
30:0:2256:G:H2'	30:0:2257:G:C5'	2.23	0.67
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.76	0.67
31:9:39:U:H1'	31:9:44:A:H61	1.59	0.67
31:9:23:U:O2'	31:9:24:U:H4'	1.94	0.67
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.75	0.67
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.60	0.67
18:R:150:PRO:O	18:R:150:PRO:CG	2.41	0.67
1:A:36:ASP:HB2	1:A:85:SER:H	1.60	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.28	0.67
30:0:1730:G:H5'	30:0:1731:C:C5	2.30	0.67
30:0:285:A:H2'	30:0:286:U:O4'	1.95	0.67
30:0:1834:C:H2'	30:0:1840:A:N6	2.09	0.66
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.77	0.66
23:W:88:THR:HG22	23:W:89:ASP:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.76	0.66
30:0:2509:A:OP2	30:0:2510:C:H5	1.78	0.66
30:0:2237:G:H1'	38:0:4866:HOH:O	1.94	0.66
30:0:853:C:H3'	38:0:4563:HOH:O	1.95	0.66
30:0:125:U:H2'	38:0:3776:HOH:O	1.94	0.66
30:0:2256:G:H2'	30:0:2257:G:H5'	1.77	0.66
30:0:2372:A:H2'	30:0:2373:U:C6	2.30	0.66
30:0:1524:U:OP1	30:0:1524:U:H4'	1.95	0.66
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.76	0.66
30:0:1120:U:H5'	30:0:1121:G:OP2	1.95	0.66
21:U:14:GLU:O	21:U:17:THR:HB	1.95	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.42	0.66
31:9:22:G:H5'	31:9:23:U:OP1	1.94	0.66
30:0:1667:A:C8	30:0:1667:A:H5'	2.29	0.66
30:0:31:C:H2'	38:0:7702:HOH:O	1.95	0.66
30:0:2836:G:H1'	38:0:6850:HOH:O	1.95	0.66
30:0:2498:C:O2'	30:0:2499:U:H5'	1.94	0.66
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.76	0.66
10:J:82:THR:CG2	30:0:1242:A:H5'	2.21	0.66
23:W:26:ILE:HB	38:W:5420:HOH:O	1.95	0.66
30:0:2320:U:H4'	30:0:2321:A:O4'	1.95	0.66
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.31	0.66
8:H:29:SER:HA	8:H:62:HIS:HD2	1.60	0.66
30:0:544:G:C2'	30:0:545:G:H5''	2.26	0.66
30:0:283:U:C5	30:0:284:C:N3	2.63	0.66
30:0:2505:G:C2'	30:0:2506:A:H5'	2.25	0.66
30:0:2505:G:O2'	30:0:2506:A:H5'	1.95	0.66
30:0:1562:C:O2	30:0:1562:C:H2'	1.95	0.66
30:0:1819:G:H2'	30:0:1820:G:H4'	1.76	0.66
30:0:2748:G:H1'	38:0:7914:HOH:O	1.95	0.65
30:0:485:A:N3	30:0:487:G:H5''	2.10	0.65
30:0:2795:C:O2'	30:0:2796:U:H5'	1.96	0.65
13:M:171:ARG:CD	30:0:156:C:H5''	2.18	0.65
1:A:35:GLY:O	1:A:36:ASP:HB3	1.96	0.65
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.62	0.65
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.78	0.65
13:M:102:GLU:OE1	13:M:164:THR:HG21	1.96	0.65
30:0:1477:C:H5'	30:0:1868:G:C5'	2.26	0.65
30:0:1666:C:C2'	30:0:1667:A:C5'	2.74	0.65
30:0:2766:A:H5'	38:0:9565:HOH:O	1.97	0.65
30:0:836:G:H5''	38:0:9288:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:74:ARG:O	10:J:78:ILE:HG12	1.97	0.65
29:3:48:ASN:HD21	30:0:2468:A:H61	1.43	0.65
30:0:558:C:C2'	30:0:559:U:C5'	2.75	0.64
30:0:960:G:H3'	30:0:960:G:N3	2.12	0.64
30:0:1741:U:O2'	30:0:2723:G:H4'	1.97	0.64
30:0:1183:C:O2	30:0:1183:C:H2'	1.95	0.64
30:0:1279:U:O2	30:0:1279:U:H2'	1.95	0.64
30:0:281:U:H2'	30:0:282:C:O4'	1.96	0.64
31:9:31:C:H1'	38:9:9014:HOH:O	1.96	0.64
18:R:29:LYS:HE2	30:0:524:A:H5'	1.79	0.64
19:S:43:GLU:HB3	38:S:8991:HOH:O	1.97	0.64
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.10	0.64
10:J:107:ASN:ND2	10:J:109:TYR:H	1.96	0.64
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.80	0.64
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.63	0.64
30:0:814:G:H4'	38:0:3141:HOH:O	1.98	0.64
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.79	0.64
30:0:564:G:H1'	38:0:6317:HOH:O	1.97	0.64
29:3:73:GLU:HB3	38:3:9049:HOH:O	1.97	0.64
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.80	0.64
30:0:2481:G:H5''	38:0:4558:HOH:O	1.97	0.64
30:0:1701:A:H5''	30:0:1702:U:H3'	1.80	0.64
30:0:2827:A:H2'	30:0:2828:G:O4'	1.98	0.64
14:N:37:ARG:NH1	31:9:6:C:C5'	2.52	0.63
18:R:9:ASP:O	18:R:13:THR:HB	1.98	0.63
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.27	0.63
30:0:1058:A:H2'	30:0:1060:C:H5''	1.78	0.63
14:N:11:ARG:HD3	31:9:114:G:O6	1.99	0.63
30:0:12:U:H2'	30:0:13:G:H5'	1.80	0.63
3:C:184:ARG:NH2	30:0:450:C:OP1	2.32	0.63
12:L:41:HIS:HD2	30:0:926:A:O2'	1.80	0.63
38:I:1549:HOH:O	30:0:1180:U:H1'	1.97	0.63
18:R:117:HIS:HD2	30:0:20:G:H21	1.45	0.63
23:W:6:GLN:CB	23:W:26:ILE:HD11	2.28	0.63
3:C:140:VAL:HB	38:C:8647:HOH:O	1.99	0.63
30:0:2768:A:H5''	38:0:4438:HOH:O	1.98	0.63
30:0:1243:C:H3'	38:0:4848:HOH:O	1.99	0.63
30:0:2509:A:H2'	30:0:2510:C:O4'	1.99	0.62
30:0:1166:A:OP1	30:0:1174:A:H4'	1.99	0.62
30:0:671:A:O2'	30:0:672:G:H2'	1.99	0.62
30:0:1185:U:H5'	38:0:7480:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2426:G:H1'	38:0:6098:HOH:O	1.99	0.62
30:0:2781:U:H2'	30:0:2782:G:H5'	1.79	0.62
31:9:114:G:H2'	31:9:115:C:C6	2.35	0.62
30:0:848:C:H5'	38:0:7283:HOH:O	1.99	0.62
27:1:8:GLN:HE22	27:1:11:LYS:NZ	1.97	0.62
31:9:49:G:O2'	31:9:50:G:H5'	1.99	0.62
30:0:1527:A:H1'	30:0:1528:A:C8	2.34	0.62
30:0:371:U:H2'	30:0:372:A:H8	1.65	0.62
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.80	0.62
30:0:559:U:H5'	30:0:559:U:C6	2.26	0.62
12:L:136:ALA:HB3	38:L:8874:HOH:O	2.00	0.62
31:9:39:U:H3'	31:9:40:C:H5''	1.82	0.62
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.82	0.62
30:0:2316:G:H4'	38:0:6098:HOH:O	2.00	0.62
26:Z:66:CYS:SG	26:Z:68:GLU:HB2	2.39	0.62
30:0:1398:G:O2'	30:0:1399:A:H5'	2.00	0.62
2:B:156:LYS:HB3	30:0:2846:C:H4'	1.81	0.62
27:1:28:HIS:HE1	30:0:776:A:OP1	1.83	0.62
30:0:378:A:H1'	38:0:3510:HOH:O	1.98	0.62
30:0:542:A:H5'	30:0:542:A:C8	2.25	0.62
30:0:2748:G:H2'	38:0:7554:HOH:O	1.98	0.62
30:0:1278:A:H4'	30:0:1279:U:C4	2.34	0.62
30:0:681:G:N3	30:0:681:G:H5'	2.15	0.62
30:0:1603:A:H5'	30:0:1605:G:C4'	2.30	0.61
30:0:2597:U:H2'	30:0:2598:U:H5'	1.81	0.61
38:B:9095:HOH:O	30:0:2672:C:H1'	2.00	0.61
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.81	0.61
30:0:1185:U:H2'	30:0:1186:C:C6	2.35	0.61
30:0:2781:U:C2'	30:0:2782:G:H5'	2.30	0.61
30:0:128:A:O2'	30:0:129:A:H5'	2.00	0.61
30:0:2300:A:H4'	30:0:2301:A:O5'	2.01	0.61
30:0:2851:G:O2'	30:0:2852:A:H5'	2.00	0.61
30:0:2769:C:H2'	30:0:2770:G:H5'	1.82	0.61
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.65	0.61
30:0:2252:A:C5	30:0:2253:G:H1'	2.34	0.61
30:0:1342:C:C2'	30:0:1343:C:H5'	2.30	0.61
9:I:110:ASP:O	30:0:1163:G:H5'	2.01	0.61
30:0:138:U:OP2	30:0:139:C:H5	1.83	0.61
30:0:1166:A:H61	30:0:1180:U:H3	1.46	0.61
23:W:81:ASP:OD1	23:W:92:ASP:HB2	1.99	0.61
30:0:558:C:H2'	30:0:559:U:H5'	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:308:U:H5'	30:0:309:C:OP1	1.99	0.61
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.98	0.61
30:0:2507:G:H2'	30:0:2510:C:N4	2.12	0.61
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.83	0.61
30:0:255:A:H2'	30:0:256:C:H6	1.64	0.61
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.00	0.61
30:0:2894:C:O2'	30:0:2895:C:H5'	2.01	0.61
23:W:61:THR:HG23	23:W:151:GLU:HG3	1.83	0.61
13:M:164:THR:HG22	13:M:167:GLY:N	2.15	0.61
31:9:1:U:O3'	31:9:3:A:H5''	2.01	0.61
30:0:1171:A:H2'	30:0:1172:G:H5'	1.81	0.61
30:0:2419:U:H5''	30:0:2420:G:H5'	1.83	0.61
30:0:1878:G:O2'	30:0:1879:U:C6	2.52	0.60
28:2:41:HIS:HD2	28:2:44:ARG:H	1.49	0.60
30:0:2718:C:H6	30:0:2718:C:H5'	1.66	0.60
13:M:145:ASP:HB2	38:M:8862:HOH:O	1.99	0.60
2:B:294:TYR:HE2	38:B:9111:HOH:O	1.84	0.60
30:0:2344:G:H2'	30:0:2344:G:N3	2.16	0.60
5:E:8:PRO:HB2	5:E:11:VAL:HG23	1.81	0.60
2:B:264:GLU:HG2	2:B:267:LYS:HE2	1.83	0.60
31:9:49:G:H2'	31:9:50:G:O4'	2.01	0.60
18:R:128:ARG:NH2	30:0:2054:A:N3	2.49	0.60
30:0:2616:G:H1'	38:0:9433:HOH:O	2.00	0.60
30:0:1174:A:C5	30:0:1201:C:H4'	2.36	0.60
30:0:1192:A:H3'	30:0:1193:A:H5'	1.83	0.60
30:0:1080:C:H4'	30:0:1081:A:OP1	2.01	0.60
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.94	0.60
23:W:48:VAL:HG12	23:W:52:VAL:HB	1.83	0.60
30:0:1972:U:H2'	30:0:1973:A:C5'	2.31	0.60
30:0:1730:G:H5''	30:0:1731:C:H6	1.65	0.60
30:0:1766:U:O2	30:0:1778:A:H5'	2.01	0.60
4:D:103:ASN:ND2	4:D:134:LEU:H	1.99	0.60
4:D:58:VAL:HB	4:D:62:ASP:HB2	1.83	0.60
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.83	0.60
1:A:199:HIS:CD2	1:A:201:PHE:H	2.19	0.60
18:R:39:THR:HG22	18:R:42:GLU:H	1.67	0.60
27:1:10:LYS:HG3	38:1:8981:HOH:O	2.01	0.60
30:0:2900:G:H2'	30:0:2901:C:O4'	2.01	0.60
2:B:62:ARG:HA	2:B:65:MET:CE	2.32	0.60
30:0:1182:C:H1'	30:0:1192:A:H8	1.67	0.60
17:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.67	0.60
30:0:1119:G:N2	30:0:1246:A:H2	1.92	0.60
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.42	0.60
1:A:48:ASP:HB3	38:A:9066:HOH:O	2.02	0.60
30:0:1730:G:H5''	30:0:1731:C:C6	2.37	0.60
2:B:41:PHE:HB3	2:B:190:MET:HE1	1.83	0.60
30:0:1116:U:O2'	30:0:1118:A:C2	2.46	0.59
30:0:1528:A:H2'	30:0:1529:G:O4'	2.02	0.59
30:0:515:C:H5''	38:0:5654:HOH:O	2.01	0.59
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.50	0.59
31:9:64:C:C2'	31:9:65:A:H5'	2.32	0.59
30:0:2505:G:H2'	30:0:2506:A:H5'	1.84	0.59
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.02	0.59
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.83	0.59
30:0:1641:A:C2'	30:0:1642:A:H5'	2.32	0.59
30:0:659:A:H5''	38:0:7111:HOH:O	2.03	0.59
30:0:2637:A:H4'	38:0:6071:HOH:O	2.02	0.59
30:0:2472:C:O2'	30:0:2634:G:H4'	2.03	0.59
30:0:1189:A:O2'	30:0:1208:C:H2'	2.03	0.59
31:9:49:G:H5''	38:9:9092:HOH:O	2.02	0.59
31:9:64:C:H2'	31:9:65:A:H5'	1.84	0.59
30:0:1189:A:H1'	30:0:1209:C:C1'	2.32	0.59
31:9:54:A:C2'	31:9:55:U:H5'	2.32	0.59
1:A:36:ASP:CB	1:A:85:SER:H	2.16	0.59
12:L:41:HIS:CD2	30:0:926:A:O2'	2.56	0.59
30:0:2613:G:O2'	30:0:2614:C:H5'	2.03	0.59
22:V:39:ALA:N	22:V:40:PRO:HD2	2.17	0.59
24:X:43:VAL:HG12	24:X:44:ASP:H	1.66	0.59
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.18	0.59
27:1:9:GLY:HA2	30:0:1687:C:O2	2.03	0.59
5:E:84:MET:HG2	5:E:168:ILE:HA	1.85	0.59
5:E:143:GLN:NE2	30:0:2779:G:H21	2.00	0.59
30:0:960:G:N3	30:0:960:G:C2'	2.65	0.59
30:0:2089:A:O2'	30:0:2090:G:H5'	2.03	0.59
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	1.84	0.59
30:0:583:C:H2'	30:0:584:U:H6	1.68	0.59
30:0:2802:C:H2'	30:0:2803:C:H6	1.68	0.59
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.84	0.59
30:0:1200:A:H3'	38:0:5763:HOH:O	2.03	0.58
31:9:76:G:C3'	31:9:77:A:H5''	2.24	0.58
23:W:139:GLY:O	23:W:141:HIS:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:13:MET:HE1	23:W:18:GLN:HA	1.83	0.58
31:9:1:U:H4'	31:9:3:A:OP1	2.03	0.58
30:0:2526:C:H5'	30:0:2526:C:H6	1.64	0.58
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.38	0.58
30:0:807:A:O2'	30:0:808:A:H5'	2.03	0.58
31:9:2:U:H4'	38:9:9104:HOH:O	2.02	0.58
30:0:1730:G:C5'	30:0:1731:C:C6	2.86	0.58
30:0:1942:A:O2'	30:0:1943:C:H5'	2.02	0.58
30:0:1183:C:N3	30:0:1184:C:C5	2.72	0.58
30:0:2421:G:H1'	38:0:7033:HOH:O	2.03	0.58
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.18	0.58
23:W:44:MET:CE	30:0:944:G:H21	2.16	0.58
8:H:168:VAL:HG13	38:H:210:HOH:O	2.03	0.58
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.85	0.58
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.68	0.58
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.84	0.58
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.84	0.58
30:0:90:A:H2'	30:0:91:G:O4'	2.02	0.58
30:0:1187:U:H2'	38:0:6907:HOH:O	2.04	0.58
30:0:1175:G:H1'	30:0:1193:A:H2'	1.84	0.58
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.85	0.58
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.04	0.58
30:0:644:G:N3	30:0:644:G:H5'	2.19	0.58
14:N:37:ARG:HH11	31:9:6:C:H5"	1.65	0.58
3:C:174:ILE:CD1	30:0:338:C:H4'	2.33	0.58
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.84	0.58
30:0:1174:A:C6	30:0:1201:C:H4'	2.39	0.58
21:U:17:THR:HG22	21:U:18:GLY:N	2.19	0.58
8:H:174:LEU:HA	38:H:220:HOH:O	2.02	0.58
9:I:126:THR:O	9:I:130:LEU:HG	2.03	0.58
2:B:258:GLY:H	2:B:260:HIS:CE1	2.21	0.58
31:9:107:C:O2'	31:9:108:C:H5'	2.04	0.57
21:U:6:CYS:HB2	21:U:32:CYS:HB3	1.85	0.57
30:0:2712:G:H5'	38:0:5232:HOH:O	2.03	0.57
30:0:2769:C:O2'	30:0:2770:G:H5'	2.04	0.57
2:B:98:THR:HG22	30:0:2820:A:OP1	2.04	0.57
30:0:2589:U:H2'	30:0:2590:U:C6	2.39	0.57
30:0:952:G:N3	30:0:2302:A:H2'	2.19	0.57
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.20	0.57
31:9:29:C:H2'	31:9:30:C:C5'	2.28	0.57
30:0:2756:U:H3	30:0:2896:A:H2	1.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:420:U:H2'	30:0:421:C:C6	2.39	0.57
30:0:272:A:H5'	30:0:273:G:OP2	2.03	0.57
30:0:541:C:H2'	30:0:542:A:H5'	1.86	0.57
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.19	0.57
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.34	0.57
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.68	0.57
14:N:7:LYS:HE3	17:Q:21:ARG:O	2.04	0.57
4:D:52:THR:HG21	30:0:2346:C:O2'	2.04	0.57
30:0:185:G:H4'	30:0:186:A:OP1	2.05	0.57
30:0:280:C:H2'	30:0:281:U:O4'	2.04	0.57
30:0:559:U:H6	30:0:559:U:C5'	2.12	0.57
17:Q:27:GLN:HE21	31:9:8:G:H4'	1.70	0.57
17:Q:18:PRO:O	17:Q:21:ARG:HB2	2.03	0.57
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.04	0.57
30:0:2135:A:O2'	30:0:2136:G:H5'	2.04	0.57
18:R:39:THR:HG23	18:R:107:GLU:O	2.04	0.57
30:0:2787:C:H5	38:0:4643:HOH:O	1.86	0.57
30:0:2604:A:H5'	38:0:5798:HOH:O	2.04	0.57
13:M:28:GLN:O	13:M:32:ARG:HG3	2.04	0.57
30:0:10:U:O4	30:0:532:A:OP2	2.23	0.57
30:0:1171:A:C2'	30:0:1172:G:H5'	2.35	0.57
30:0:1377:C:H5'	30:0:1377:C:C6	2.40	0.57
1:A:36:ASP:O	1:A:38:ILE:N	2.38	0.57
30:0:1942:A:H3'	38:0:7360:HOH:O	2.03	0.57
12:L:4:LYS:HE2	30:0:645:U:OP2	2.05	0.57
31:9:75:G:H1	31:9:106:U:H3	1.53	0.57
30:0:1016:U:H1'	38:0:3667:HOH:O	2.04	0.57
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.86	0.57
31:9:39:U:H1'	31:9:44:A:N6	2.19	0.57
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.87	0.57
3:C:188:ARG:HD3	38:C:8559:HOH:O	2.04	0.57
2:B:264:GLU:HG2	2:B:267:LYS:CE	2.35	0.57
30:0:960:G:H2'	30:0:960:G:N3	2.20	0.57
30:0:228:C:H2'	30:0:229:G:H5'	1.86	0.57
30:0:2559:C:H4'	38:0:7268:HOH:O	2.05	0.57
30:0:2488:A:H1'	38:0:9096:HOH:O	2.03	0.57
10:J:127:ILE:HG22	35:J:8801:CL:CL	2.42	0.57
30:0:2005:G:OP2	30:0:2005:G:H3'	2.05	0.57
3:C:1:MET:HG2	3:C:2:GLN:N	2.19	0.56
1:A:99:ILE:O	1:A:131:HIS:HE1	1.88	0.56
30:0:941:G:C5	30:0:942:U:C4	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1304:U:H2'	30:0:1305:C:C6	2.40	0.56
30:0:711:G:H1'	38:0:7108:HOH:O	2.04	0.56
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.35	0.56
30:0:2578:G:C8	30:0:2578:G:H5'	2.36	0.56
30:0:1838:U:O2'	30:0:2644:C:H5'	2.05	0.56
30:0:1632:A:C3'	30:0:1633:C:H5'	2.35	0.56
29:3:70:ARG:HB3	38:3:9059:HOH:O	2.04	0.56
12:L:143:THR:HG22	12:L:144:ASP:N	2.20	0.56
30:0:734:U:O2'	30:0:736:A:N7	2.39	0.56
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.05	0.56
30:0:1474:C:C5'	30:0:1474:C:H6	2.15	0.56
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.86	0.56
30:0:1947:G:N2	30:0:1966:U:C2	2.73	0.56
11:K:66:ARG:HH22	30:0:1994:A:P	2.29	0.56
2:B:125:GLU:O	2:B:129:ARG:HG3	2.06	0.56
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.69	0.56
20:T:2:LYS:HG2	30:0:447:A:OP1	2.05	0.56
30:0:506:G:N2	30:0:509:A:H5'	2.18	0.56
30:0:31:C:H4'	38:0:7437:HOH:O	2.06	0.56
27:1:42:SER:HB2	38:1:8956:HOH:O	2.05	0.56
16:P:143:ALA:HA	38:P:192:HOH:O	2.04	0.56
30:0:1209:C:H2'	30:0:1210:G:H8	1.70	0.56
31:9:13:A:O2'	31:9:14:G:H5''	2.06	0.56
30:0:2032:U:H2'	30:0:2033:G:C5'	2.36	0.56
30:0:368:C:H2'	30:0:369:G:H5'	1.88	0.56
30:0:363:C:O2'	30:0:364:U:H5'	2.06	0.56
30:0:876:A:N3	30:0:876:A:H2'	2.21	0.56
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.71	0.56
1:A:199:HIS:HD2	1:A:201:PHE:H	1.54	0.56
27:1:16:HIS:HD2	30:0:470:U:O2'	1.88	0.56
30:0:1972:U:H2'	30:0:1973:A:H5''	1.87	0.55
30:0:119:A:H2'	30:0:120:A:H5''	1.87	0.55
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.70	0.55
9:I:120:ALA:O	9:I:124:VAL:HG23	2.06	0.55
30:0:1904:A:H2'	30:0:1905:U:O4'	2.05	0.55
4:D:25:MET:CE	4:D:37:ALA:HB1	2.35	0.55
10:J:107:ASN:C	10:J:107:ASN:HD22	2.09	0.55
10:J:107:ASN:HD22	10:J:109:TYR:H	1.54	0.55
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.69	0.55
30:0:2064:U:H5'	30:0:2652:U:H4'	1.88	0.55
25:Y:212:ARG:HD2	38:Y:8900:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:10:ARG:NH2	30:0:121:U:OP2	2.35	0.55
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.06	0.55
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.89	0.55
30:0:821:U:H3'	38:0:3780:HOH:O	2.07	0.55
30:0:2781:U:H2'	30:0:2782:G:C5'	2.36	0.55
4:D:159:PRO:O	4:D:163:VAL:HG23	2.05	0.55
30:0:396:U:O2'	30:0:418:C:H4'	2.07	0.55
14:N:132:ASN:HD22	30:0:2413:A:H4'	1.72	0.55
16:P:7:LYS:HD3	16:P:21:VAL:HG22	1.87	0.55
30:0:2254:G:H1'	38:0:5546:HOH:O	2.07	0.55
30:0:407:A:H5'	38:0:6032:HOH:O	2.06	0.55
30:0:2840:A:H3'	38:0:7659:HOH:O	2.05	0.55
30:0:168:C:O5'	30:0:168:C:H6	1.89	0.55
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.88	0.55
30:0:1060:C:H6	30:0:1060:C:H5'	1.72	0.55
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.06	0.55
9:I:130:LEU:HD22	30:0:1167:G:H4'	1.89	0.55
30:0:711:G:C2	30:0:718:C:C2	2.95	0.55
30:0:660:A:H4'	30:0:661:G:O5'	2.07	0.55
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.88	0.55
29:3:15:ASN:O	30:0:2408:A:H4'	2.06	0.55
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.89	0.55
30:0:1596:U:H2'	30:0:1598:A:OP2	2.07	0.55
30:0:1132:A:N6	30:0:1229:C:H2'	2.22	0.55
3:C:132:ASP:HB3	38:C:8560:HOH:O	2.06	0.55
31:9:55:U:H4'	31:9:56:A:C8	2.42	0.55
30:0:2510:C:H5'	30:0:2511:A:OP2	2.07	0.55
31:9:24:U:H3'	31:9:25:G:C5'	2.37	0.55
27:1:1:THR:HA	38:1:8958:HOH:O	2.06	0.55
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.89	0.55
4:D:65:GLU:HA	38:D:6752:HOH:O	2.05	0.55
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.89	0.55
7:G:64:ASN:N	7:G:64:ASN:HD22	2.04	0.55
30:0:1538:C:O2'	30:0:1539:U:H5'	2.06	0.55
2:B:145:HIS:HD2	2:B:146:THR:O	1.90	0.55
7:G:23:ILE:O	7:G:27:ILE:HG13	2.06	0.55
13:M:95:LYS:HE2	30:0:157:G:H4'	1.89	0.55
2:B:102:THR:HG23	2:B:182:VAL:HG12	1.90	0.54
12:L:150:GLN:HB3	38:L:8869:HOH:O	2.06	0.54
1:A:121:ALA:O	1:A:124:VAL:HG22	2.07	0.54
30:0:2577:A:H8	38:0:9602:HOH:O	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.38	0.54
30:0:2083:A:H3'	38:0:7590:HOH:O	2.07	0.54
30:0:1523:G:C5	30:0:1524:U:C4	2.96	0.54
30:0:2878:U:H2'	30:0:2879:A:O4'	2.06	0.54
30:0:1154:A:H2'	30:0:1155:G:C8	2.42	0.54
30:0:1291:A:H2	38:0:5300:HOH:O	1.89	0.54
31:9:59:C:H6	31:9:59:C:O5'	1.90	0.54
2:B:27:ASN:H	2:B:27:ASN:HD22	1.56	0.54
30:0:2256:G:C2'	30:0:2257:G:C5'	2.84	0.54
30:0:1202:A:H2'	30:0:1203:G:O4'	2.07	0.54
26:Z:40:ALA:HA	30:0:1773:G:C8	2.42	0.54
30:0:292:G:H2'	30:0:358:G:N2	2.23	0.54
30:0:812:A:H1'	38:0:3969:HOH:O	2.06	0.54
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.38	0.54
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.89	0.54
31:9:52:A:O2'	31:9:53:G:H5'	2.08	0.54
30:0:241:A:C2	30:0:378:A:H4'	2.42	0.54
5:E:143:GLN:NE2	30:0:2780:C:H1'	2.22	0.54
30:0:1477:C:H5'	30:0:1868:G:H5'	1.89	0.54
3:C:154:VAL:O	3:C:158:GLU:HG3	2.07	0.54
30:0:282:C:H1'	30:0:368:C:H41	1.72	0.54
17:Q:27:GLN:HE21	31:9:8:G:C5'	2.20	0.54
30:0:1342:C:O2'	30:0:1343:C:H5'	2.07	0.54
30:0:441:A:H1'	30:0:442:A:N7	2.23	0.54
31:9:3:A:H2	31:9:21:G:N3	2.06	0.54
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.08	0.54
12:L:73:VAL:HG21	12:L:116:HIS:CE1	2.42	0.54
25:Y:204:ARG:HH22	30:0:553:G:P	2.31	0.54
3:C:218:VAL:HG12	38:C:8620:HOH:O	2.07	0.54
7:G:16:LYS:O	7:G:20:VAL:HG23	2.08	0.54
18:R:68:HIS:O	30:0:2842:G:H5'	2.08	0.54
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.88	0.54
12:L:143:THR:HG22	12:L:144:ASP:H	1.71	0.54
1:A:112:PRO:HD3	1:A:152:CYS:SG	2.48	0.54
19:S:33:SER:O	19:S:37:VAL:HG23	2.07	0.54
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.90	0.54
18:R:132:ARG:HG2	18:R:133:ALA:N	2.23	0.53
4:D:105:SER:OG	30:0:2338:G:H1'	2.07	0.53
18:R:150:PRO:CG	18:R:150:PRO:CB	2.86	0.53
3:C:236:THR:HA	38:C:8647:HOH:O	2.08	0.53
10:J:39:VAL:HG13	10:J:106:GLY:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:73:ASP:HA	15:O:92:VAL:O	2.08	0.53
13:M:30:GLU:O	13:M:34:GLU:HG3	2.09	0.53
8:H:26:ILE:HA	8:H:123:ILE:HG21	1.90	0.53
30:0:2670:G:O2'	30:0:2671:U:H5'	2.07	0.53
30:0:1819:G:H2'	30:0:1820:G:C4'	2.39	0.53
30:0:1586:G:O2'	30:0:1587:U:H5'	2.08	0.53
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.91	0.53
2:B:307:ARG:HG3	2:B:307:ARG:NH1	2.23	0.53
30:0:2064:U:H5'	30:0:2652:U:O3'	2.08	0.53
30:0:2842:G:H2'	30:0:2843:A:H5'	1.90	0.53
30:0:488:U:H2'	38:0:4019:HOH:O	2.08	0.53
30:0:136:C:H2'	30:0:137:U:O4'	2.08	0.53
30:0:1919:A:H4'	38:0:4862:HOH:O	2.07	0.53
30:0:1373:G:H1'	38:0:6143:HOH:O	2.08	0.53
30:0:1592:G:H2'	30:0:1593:C:H6	1.72	0.53
30:0:1339:G:C6	30:0:1340:G:N1	2.77	0.53
30:0:1205:U:C2'	30:0:1206:U:C5'	2.76	0.53
23:W:125:HIS:HE1	38:W:3071:HOH:O	1.91	0.53
14:N:144:GLY:O	14:N:147:ILE:HG23	2.08	0.53
30:0:1451:C:H5'	30:0:1505:U:C5	2.43	0.53
31:9:24:U:H3'	31:9:25:G:H5'	1.91	0.53
30:0:2502:C:H2'	30:0:2503:A:C5'	2.37	0.53
18:R:99:ALA:HB1	18:R:109:MET:CE	2.37	0.53
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.43	0.53
30:0:544:G:C3'	30:0:545:G:H5"	2.39	0.53
4:D:154:LYS:HD2	4:D:154:LYS:N	2.16	0.53
30:0:2769:C:H2'	30:0:2770:G:C5'	2.39	0.53
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.44	0.53
1:A:135:VAL:HG21	1:A:147:ARG:HB3	1.91	0.53
30:0:2250:G:H2'	30:0:2251:G:O4'	2.09	0.53
30:0:920:C:H5"	30:0:921:G:O5'	2.09	0.53
22:V:55:ARG:O	22:V:59:ILE:HG12	2.09	0.53
30:0:1135:G:H5'	38:0:5935:HOH:O	2.07	0.53
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.74	0.53
30:0:635:A:H2'	30:0:636:G:H5"	1.90	0.53
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.74	0.53
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.91	0.53
30:0:510:U:H6	38:0:7450:HOH:O	1.92	0.53
30:0:299:U:H5'	38:0:7349:HOH:O	2.08	0.53
30:0:282:C:O2'	30:0:283:U:C5'	2.56	0.53
30:0:1166:A:P	30:0:1174:A:H4'	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:108:HIS:H	9:I:109:PRO:HD2	1.74	0.53
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.57	0.53
30:0:820:G:H3'	38:0:3058:HOH:O	2.08	0.53
30:0:513:A:N3	38:0:3668:HOH:O	2.34	0.53
30:0:1066:U:H2'	30:0:1067:A:C8	2.42	0.53
23:W:154:ARG:NH1	30:0:588:G:O6	2.42	0.53
30:0:284:C:C6	30:0:284:C:OP2	2.62	0.52
27:1:16:HIS:HE1	30:0:775:G:OP1	1.92	0.52
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.52
30:0:958:G:H2'	30:0:959:C:C6	2.43	0.52
30:0:1819:G:H2'	30:0:1820:G:C5'	2.39	0.52
5:E:11:VAL:HG12	5:E:12:ASP:N	2.24	0.52
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.90	0.52
2:B:254:GLN:HG2	2:B:255:GLY:N	2.24	0.52
31:9:91:C:H2'	31:9:92:G:O4'	2.09	0.52
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.91	0.52
10:J:41:ALA:HB3	38:J:5907:HOH:O	2.09	0.52
30:0:1787:C:H4'	30:0:2883:A:O4'	2.09	0.52
30:0:2356:A:H5'	38:0:5644:HOH:O	2.09	0.52
25:Y:216:ARG:HD2	38:Y:8870:HOH:O	2.08	0.52
30:0:255:A:H2'	30:0:256:C:C6	2.45	0.52
30:0:920:C:H4'	30:0:921:G:C2	2.44	0.52
5:E:6:GLU:HG2	5:E:46:THR:HG22	1.92	0.52
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.09	0.52
30:0:1268:C:O2'	30:0:1269:G:H5'	2.08	0.52
14:N:5:ARG:NH1	30:0:1010:C:OP1	2.42	0.52
30:0:2291:A:N9	30:0:2309:C:H5'	2.25	0.52
2:B:36:PRO:HG3	2:B:169:GLY:H	1.75	0.52
30:0:1181:A:N1	30:0:1192:A:O2'	2.43	0.52
13:M:158:ARG:HB2	13:M:163:LEU:HB2	1.91	0.52
30:0:2263:G:H1'	38:0:6631:HOH:O	2.09	0.52
30:0:1515:A:H2'	30:0:1516:U:C6	2.44	0.52
30:0:1624:A:H5'	30:0:1626:A:O4'	2.09	0.52
30:0:2478:U:O2'	30:0:2479:A:H5'	2.09	0.52
15:O:32:ARG:HD3	15:O:32:ARG:O	2.09	0.52
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.44	0.52
30:0:120:A:H2'	30:0:120:A:N3	2.25	0.52
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.91	0.52
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.91	0.52
30:0:1314:U:H2'	38:0:5880:HOH:O	2.09	0.52
30:0:1342:C:H2'	30:0:1343:C:H5'	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2445:U:H2'	30:0:2446:G:H8	1.75	0.52
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.92	0.52
30:0:2103:A:H2'	30:0:2104:C:H5'	1.92	0.52
30:0:2756:U:N3	30:0:2896:A:H2	2.08	0.52
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.44	0.52
30:0:1972:U:C2'	30:0:1973:A:H5''	2.39	0.52
30:0:1679:C:H5'	38:0:9331:HOH:O	2.10	0.52
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.10	0.52
31:9:45:A:H2'	31:9:46:C:H6	1.75	0.52
30:0:2359:G:H3'	38:0:5698:HOH:O	2.10	0.52
30:0:1170:U:H2'	30:0:1172:G:OP2	2.09	0.52
30:0:2769:C:H2'	30:0:2770:G:O4'	2.09	0.52
30:0:2756:U:N3	30:0:2896:A:C2	2.74	0.52
30:0:1730:G:C5'	30:0:1731:C:C5	2.93	0.52
30:0:2326:C:H4'	30:0:2412:G:H4'	1.92	0.52
22:V:64:GLY:O	22:V:65:ASP:HB2	2.09	0.52
6:F:21:GLU:O	6:F:24:ARG:HG2	2.09	0.52
30:0:694:A:H2'	30:0:695:C:H5'	1.90	0.52
17:Q:19:ARG:HH21	31:9:11:A:P	2.33	0.52
30:0:2764:C:O2'	30:0:2765:C:H5'	2.09	0.52
30:0:567:U:H5''	38:0:6408:HOH:O	2.08	0.52
2:B:79:MET:HE1	38:B:9089:HOH:O	2.09	0.52
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.91	0.52
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.91	0.52
3:C:43:LYS:HG2	30:0:449:A:N7	2.25	0.52
14:N:37:ARG:HD3	35:N:8807:CL:CL	2.47	0.51
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.10	0.51
30:0:541:C:O2'	30:0:542:A:H5''	2.10	0.51
30:0:613:C:H2'	30:0:614:U:H6	1.74	0.51
30:0:2524:G:H21	30:0:2526:C:N4	2.08	0.51
30:0:1477:C:O2'	30:0:1478:U:H5'	2.10	0.51
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.40	0.51
30:0:497:A:H2'	30:0:498:A:C5'	2.40	0.51
13:M:188:ARG:NH1	30:0:154:C:H3'	2.24	0.51
30:0:619:U:H3'	38:0:3289:HOH:O	2.09	0.51
30:0:2105:C:H2'	30:0:2106:C:C6	2.45	0.51
16:P:115:SER:OG	16:P:118:GLN:HG3	2.10	0.51
31:9:2:U:C4'	38:9:9104:HOH:O	2.57	0.51
30:0:2768:A:N3	30:0:2768:A:H3'	2.25	0.51
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.40	0.51
13:M:188:ARG:HD3	30:0:155:C:OP2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:65:C:O2'	30:0:66:G:H5'	2.10	0.51
30:0:2269:C:C2'	30:0:2270:G:H5'	2.40	0.51
30:0:506:G:H22	30:0:509:A:H5''	1.73	0.51
30:0:1592:G:H2'	30:0:1593:C:C6	2.45	0.51
30:0:1878:G:C1'	38:0:6126:HOH:O	2.44	0.51
30:0:812:A:H2'	30:0:813:C:C6	2.45	0.51
30:0:1131:G:C6	30:0:1230:A:C4	2.99	0.51
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.91	0.51
13:M:179:GLY:O	30:0:399:C:H5'	2.10	0.51
12:L:61:ALA:HB2	12:L:105:TYR:CE2	2.45	0.51
26:Z:57:MET:HE3	38:0:6288:HOH:O	2.09	0.51
30:0:447:A:O2'	30:0:448:G:H5'	2.11	0.51
19:S:11:THR:H	19:S:14:ALA:HB3	1.75	0.51
30:0:1447:U:H3'	30:0:1506:U:O2	2.11	0.51
3:C:153:VAL:O	3:C:157:LEU:HG	2.10	0.51
30:0:1029:U:O2'	30:0:1273:C:OP1	2.25	0.51
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.26	0.51
30:0:2717:C:C2'	30:0:2718:C:C5'	2.75	0.51
30:0:1730:G:H5'	30:0:1731:C:H5	1.74	0.51
30:0:256:C:H2'	30:0:257:G:O4'	2.10	0.51
30:0:1080:C:O5'	30:0:1080:C:H6	1.94	0.51
30:0:512:G:O3'	30:0:513:A:H8	1.92	0.51
30:0:2445:U:H2'	30:0:2446:G:C8	2.46	0.51
31:9:12:C:H5'	31:9:70:U:O4'	2.11	0.51
30:0:445:U:H2'	30:0:446:G:H8	1.75	0.51
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.76	0.51
23:W:125:HIS:CD2	23:W:127:GLY:H	2.29	0.51
30:0:228:C:C2'	30:0:229:G:H5'	2.41	0.51
12:L:149:ARG:O	12:L:150:GLN:HB2	2.10	0.51
30:0:690:G:H4'	30:0:741:C:O2	2.11	0.51
30:0:318:U:H5'	30:0:339:A:C2	2.46	0.51
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.93	0.51
12:L:14:GLY:O	30:0:1295:G:H5''	2.10	0.51
30:0:1535:G:H2'	30:0:1536:C:C6	2.46	0.51
30:0:545:G:H8	30:0:545:G:C5'	2.06	0.51
23:W:139:GLY:O	23:W:141:HIS:CD2	2.64	0.51
4:D:25:MET:HE2	4:D:41:LEU:HG	1.92	0.51
30:0:1973:A:H2'	30:0:1974:G:O4'	2.10	0.51
30:0:1015:C:H2'	30:0:1016:U:H6	1.75	0.51
18:R:18:LEU:HB2	18:R:143:VAL:HG13	1.91	0.51
30:0:1422:U:H2'	30:0:1423:C:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2401:A:H2'	30:0:2402:A:C8	2.46	0.51
31:9:1:U:O3'	31:9:3:A:C5'	2.58	0.51
2:B:234:ARG:HG3	30:0:1735:C:OP2	2.11	0.51
28:2:35:ARG:HB2	38:2:2691:HOH:O	2.09	0.51
6:F:101:ALA:HA	38:F:5413:HOH:O	2.10	0.51
30:0:968:G:C2	30:0:1001:U:O2	2.63	0.51
30:0:1160:G:H5'	30:0:1161:A:H5'	1.84	0.51
30:0:1183:C:C2	30:0:1184:C:C5	2.99	0.51
30:0:483:C:C4	30:0:484:A:C6	2.99	0.51
27:1:25:LYS:HD2	28:2:49:GLU:N	2.23	0.51
2:B:85:ARG:NH1	38:B:9095:HOH:O	2.44	0.51
16:P:1:THR:O	30:0:1396:C:H1'	2.11	0.51
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.93	0.51
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.45	0.51
2:B:41:PHE:HA	2:B:79:MET:HE2	1.91	0.51
30:0:2326:C:H4'	30:0:2412:G:C4'	2.41	0.51
30:0:407:A:H3'	38:0:4473:HOH:O	2.10	0.50
30:0:1268:C:H2'	30:0:1269:G:H8	1.76	0.50
30:0:101:C:H2'	30:0:102:A:H8	1.76	0.50
30:0:1139:U:H2'	30:0:1140:C:C6	2.46	0.50
3:C:95:GLU:HG3	38:C:8672:HOH:O	2.12	0.50
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.92	0.50
30:0:2754:G:H2'	30:0:2755:G:O4'	2.11	0.50
14:N:4:PRO:HG3	31:9:69:U:OP1	2.11	0.50
3:C:236:THR:HG22	3:C:239:ALA:N	2.20	0.50
30:0:1193:A:C2	30:0:1194:A:N6	2.79	0.50
1:A:51:ARG:NH1	1:A:120:ARG:O	2.44	0.50
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.58	0.50
30:0:951:A:C2'	30:0:952:G:H5'	2.41	0.50
9:I:95:LEU:HD22	9:I:99:GLN:HB3	1.93	0.50
8:H:69:ARG:HD3	38:H:229:HOH:O	2.11	0.50
30:0:1739:G:O2'	30:0:1740:U:H5'	2.11	0.50
30:0:1160:G:H5'	30:0:1161:A:C4'	2.40	0.50
31:9:76:G:H3'	31:9:77:A:C5'	2.24	0.50
30:0:1878:G:O2'	30:0:1879:U:H6	1.95	0.50
2:B:62:ARG:HA	2:B:65:MET:HE2	1.93	0.50
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.08	0.50
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.93	0.50
2:B:214:PRO:HD2	38:B:8990:HOH:O	2.11	0.50
27:1:2:GLY:O	27:1:6:PRO:HG2	2.11	0.50
30:0:899:C:H5'	38:0:3209:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1183:C:O2	30:0:1183:C:C2'	2.60	0.50
30:0:1118:A:H8	30:0:1119:G:H5''	1.75	0.50
30:0:271:C:C2	30:0:273:G:O4'	2.64	0.50
30:0:1878:G:O2'	30:0:1879:U:P	2.70	0.50
30:0:960:G:C3'	30:0:960:G:N3	2.74	0.50
30:0:185:G:H4'	30:0:186:A:H4'	1.93	0.50
12:L:143:THR:HG21	38:L:8838:HOH:O	2.10	0.50
30:0:737:A:H2'	30:0:738:G:O4'	2.10	0.50
30:0:2269:C:H2'	30:0:2270:G:H5'	1.93	0.50
2:B:305:ASP:O	2:B:306:LYS:HB2	2.12	0.50
30:0:700:A:H5''	30:0:701:U:H5'	1.93	0.50
29:3:29:ARG:NH2	30:0:1925:G:H5'	2.26	0.50
14:N:37:ARG:NH1	31:9:6:C:OP1	2.44	0.50
2:B:310:ARG:HB3	38:B:9109:HOH:O	2.11	0.50
2:B:217:ARG:CG	2:B:257:THR:HG22	2.38	0.50
30:0:661:G:C5	30:0:686:A:C2	3.00	0.50
3:C:214:THR:HG23	38:C:8633:HOH:O	2.11	0.50
20:T:54:ASP:OD2	30:0:316:A:H5'	2.11	0.50
12:L:27:ARG:HH21	12:L:30:ARG:HG2	1.77	0.50
8:H:170:ARG:HD2	38:H:190:HOH:O	2.11	0.50
30:0:1289:C:O2'	30:0:1290:G:H5'	2.12	0.50
31:9:5:G:O2'	31:9:6:C:H5'	2.11	0.50
30:0:1244:U:H4'	30:0:1246:A:O4'	2.11	0.50
30:0:1181:A:H2'	30:0:1182:C:H5'	1.94	0.50
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.45	0.50
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.93	0.50
30:0:440:C:H2'	30:0:441:A:C8	2.47	0.50
7:G:20:VAL:O	7:G:24:VAL:HG23	2.12	0.50
30:0:947:U:H2'	30:0:948:G:C8	2.47	0.50
19:S:77:VAL:O	19:S:80:ARG:HG2	2.12	0.50
30:0:2276:U:H2'	30:0:2277:U:C6	2.46	0.50
31:9:95:C:O2'	31:9:96:C:H5'	2.12	0.50
30:0:1166:A:C6	30:0:1181:A:C2	2.99	0.50
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.42	0.50
30:0:137:U:OP1	30:0:259:G:O2'	2.30	0.50
18:R:33:ARG:NH1	38:R:8950:HOH:O	2.45	0.50
20:T:28:SER:O	20:T:32:ARG:HG3	2.11	0.50
30:0:2511:A:H4'	38:0:5478:HOH:O	2.12	0.50
1:A:171:LYS:HB2	30:0:820:G:C5	2.47	0.50
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.92	0.50
30:0:1056:U:H2'	30:0:1057:A:O4'	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:GLY:O	2:B:291:ASP:HA	2.12	0.50
30:0:1185:U:H2'	30:0:1186:C:H6	1.77	0.50
15:O:37:ARG:HD2	30:0:656:G:OP2	2.12	0.50
30:0:182:G:H5''	38:0:3733:HOH:O	2.12	0.50
30:0:541:C:C2'	30:0:542:A:C5'	2.78	0.50
30:0:877:G:C5'	30:0:878:G:OP1	2.57	0.50
30:0:2010:A:C2'	38:0:5965:HOH:O	2.55	0.50
24:X:61:ARG:HH12	24:X:67:PRO:HD3	1.77	0.50
23:W:80:ASP:O	23:W:84:VAL:HG23	2.10	0.50
30:0:816:G:C6	30:0:817:G:N1	2.80	0.50
14:N:110:THR:HB	14:N:113:SER:OG	2.12	0.49
30:0:1743:G:N7	38:0:9265:HOH:O	2.35	0.49
30:0:1211:G:H2'	30:0:1212:C:H6	1.77	0.49
30:0:1588:G:C6	30:0:1589:G:N1	2.81	0.49
30:0:509:A:H2'	38:0:7099:HOH:O	2.11	0.49
2:B:212:GLN:HA	30:0:1733:A:H4'	1.93	0.49
30:0:1972:U:H2'	30:0:1973:A:H5'	1.93	0.49
30:0:2414:A:H2'	30:0:2415:A:C8	2.47	0.49
30:0:364:U:H2'	30:0:365:G:O4'	2.12	0.49
30:0:1657:A:H2'	30:0:1658:A:C8	2.47	0.49
30:0:2851:G:C2'	30:0:2852:A:H5'	2.43	0.49
22:V:1:THR:CB	30:0:93:C:H5''	2.40	0.49
31:9:59:C:H2'	31:9:60:C:C6	2.47	0.49
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.11	0.49
28:2:38:LYS:HE3	38:0:4239:HOH:O	2.12	0.49
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.93	0.49
20:T:5:ASP:O	20:T:9:LYS:HB2	2.13	0.49
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.93	0.49
30:0:1903:U:O2'	30:0:1904:A:N7	2.42	0.49
30:0:1856:C:H5'	30:0:1858:A:O4'	2.12	0.49
14:N:154:LEU:C	14:N:156:GLU:H	2.14	0.49
5:E:5:LEU:HD21	5:E:66:GLN:HG3	1.93	0.49
5:E:133:VAL:HG12	5:E:141:VAL:HG13	1.94	0.49
30:0:1625:U:H3'	30:0:1625:U:H6	1.75	0.49
30:0:669:G:O2'	30:0:670:G:H5'	2.12	0.49
30:0:1838:U:H3'	38:0:5533:HOH:O	2.12	0.49
11:K:27:ARG:HD2	38:K:3442:HOH:O	2.11	0.49
30:0:1762:C:H2'	30:0:1763:C:H6	1.77	0.49
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.45	0.49
30:0:1790:C:H2'	30:0:1791:U:H6	1.76	0.49
18:R:40:ALA:O	18:R:44:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:63:GLU:HG2	38:K:6344:HOH:O	2.11	0.49
30:0:2709:G:N2	38:0:7632:HOH:O	2.46	0.49
30:0:1545:C:H2'	30:0:1546:G:O4'	2.12	0.49
30:0:1940:C:H4'	38:0:7360:HOH:O	2.12	0.49
30:0:407:A:H2'	30:0:408:A:C8	2.48	0.49
30:0:1503:U:H2'	30:0:1504:A:O4'	2.11	0.49
6:F:58:GLU:HB3	13:M:8:ILE:HG23	1.95	0.49
30:0:2493:C:O2	30:0:2493:C:H2'	2.11	0.49
2:B:238:ASN:HD22	2:B:240:GLY:N	2.02	0.49
30:0:2345:A:H3'	30:0:2346:C:C6	2.47	0.49
14:N:169:PRO:O	14:N:172:PHE:HB3	2.13	0.49
30:0:876:A:N3	30:0:876:A:C2'	2.76	0.49
30:0:2435:U:H1'	38:0:5440:HOH:O	2.13	0.49
1:A:33:GLU:CD	1:A:33:GLU:H	2.15	0.49
30:0:2271:G:N3	30:0:2271:G:H2'	2.27	0.49
31:9:3:A:C2	31:9:21:G:N3	2.81	0.49
31:9:3:A:N6	31:9:22:G:H1'	2.28	0.49
4:D:103:ASN:ND2	4:D:133:ASN:HA	2.27	0.49
30:0:1391:G:H2'	30:0:1392:A:H5'	1.95	0.49
30:0:702:G:O2'	30:0:703:G:H5'	2.13	0.49
3:C:78:ARG:HH11	3:C:78:ARG:HG3	1.78	0.49
8:H:30:LYS:H	8:H:62:HIS:CD2	2.30	0.49
30:0:951:A:O2'	30:0:952:G:H5'	2.13	0.49
30:0:2880:A:H2'	30:0:2881:C:H5'	1.95	0.49
2:B:244:PRO:HB3	30:0:1234:U:N3	2.27	0.49
24:X:30:MET:HG2	30:0:1384:C:H5'	1.94	0.49
30:0:1149:U:H5''	30:0:1151:G:O4'	2.13	0.49
1:A:186:TRP:CG	1:A:187:PRO:HA	2.48	0.49
15:O:25:VAL:HG12	30:0:709:G:O2'	2.11	0.49
3:C:162:VAL:HG22	3:C:232:LEU:HD21	1.94	0.49
30:0:2649:A:H5'	30:0:2649:A:H8	1.77	0.49
30:0:2908:A:O5'	30:0:2908:A:H8	1.94	0.49
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.23	0.49
2:B:41:PHE:HB3	2:B:190:MET:CE	2.43	0.49
30:0:2802:C:H2'	30:0:2803:C:C6	2.46	0.49
30:0:815:U:O2'	30:0:1598:A:H4'	2.12	0.49
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.95	0.49
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.12	0.49
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.94	0.49
30:0:2387:U:H2'	30:0:2388:C:C6	2.48	0.49
30:0:297:U:H2'	30:0:298:C:C6	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:56:A:C3'	31:9:57:A:H5''	2.43	0.48
30:0:1118:A:C8	30:0:1119:G:H5''	2.47	0.48
24:X:85:VAL:HG12	24:X:86:GLU:N	2.28	0.48
31:9:63:C:O2'	31:9:64:C:H5'	2.13	0.48
30:0:2353:A:H4'	30:0:2354:A:O5'	2.13	0.48
30:0:1159:G:H1	30:0:1208:C:H42	1.61	0.48
31:9:2:U:P	31:9:3:A:H5'	2.53	0.48
30:0:2420:G:H2'	30:0:2421:G:C8	2.48	0.48
4:D:62:ASP:HA	38:D:4233:HOH:O	2.14	0.48
30:0:2697:A:H2'	30:0:2698:G:O4'	2.13	0.48
30:0:2335:C:H2'	30:0:2336:G:C8	2.48	0.48
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.95	0.48
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.95	0.48
30:0:1181:A:C2'	30:0:1182:C:H5'	2.43	0.48
30:0:1477:C:H5'	30:0:1868:G:H5''	1.94	0.48
30:0:2781:U:O2'	30:0:2782:G:H5'	2.13	0.48
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.28	0.48
23:W:38:THR:O	23:W:42:ARG:HB2	2.13	0.48
9:I:78:ALA:HB1	9:I:93:ALA:HB1	1.95	0.48
30:0:1119:G:N2	30:0:1246:A:N1	2.61	0.48
22:V:12:THR:HG22	22:V:15:GLU:CG	2.39	0.48
17:Q:50:GLY:HA2	38:0:6033:HOH:O	2.12	0.48
30:0:1419:U:H2'	30:0:1685:A:C2	2.48	0.48
30:0:947:U:H2'	30:0:948:G:H8	1.78	0.48
17:Q:1:PRO:HA	30:0:2299:G:O6	2.13	0.48
30:0:2419:U:H5''	30:0:2420:G:C5'	2.42	0.48
23:W:90:TYR:N	23:W:90:TYR:CD1	2.80	0.48
30:0:1523:G:H2'	30:0:1524:U:C6	2.48	0.48
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.95	0.48
9:I:87:PRO:HB3	38:I:6825:HOH:O	2.13	0.48
30:0:2842:G:C2'	30:0:2843:A:H5'	2.43	0.48
8:H:34:HIS:HD2	8:H:90:LEU:O	1.96	0.48
30:0:1221:G:C8	38:0:5995:HOH:O	2.55	0.48
10:J:130:VAL:HG12	10:J:131:THR:N	2.28	0.48
2:B:18:ARG:HE	2:B:256:GLN:NE2	2.11	0.48
30:0:2825:C:H4'	30:0:2826:G:O5'	2.13	0.48
4:D:170:TYR:CD1	4:D:170:TYR:N	2.81	0.48
30:0:2134:G:C6	30:0:2258:A:C8	3.02	0.48
30:0:1206:U:C5'	30:0:1206:U:H6	2.18	0.48
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.39	0.48
2:B:17:LYS:O	2:B:260:HIS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:ARG:HD3	38:0:3517:HOH:O	2.14	0.48
30:0:1513:C:O2'	30:0:1514:C:H5'	2.13	0.48
30:0:482:G:H4'	30:0:508:A:N1	2.29	0.48
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.95	0.48
13:M:167:GLY:O	13:M:171:ARG:HG3	2.13	0.48
30:0:2896:A:N3	30:0:2896:A:H2'	2.29	0.48
30:0:2335:C:H2'	30:0:2336:G:H8	1.77	0.48
20:T:68:ASP:HB2	38:0:5667:HOH:O	2.12	0.48
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.95	0.48
10:J:74:ARG:CB	10:J:74:ARG:HH11	2.25	0.48
1:A:36:ASP:HA	1:A:83:GLY:HA3	1.96	0.48
30:0:2598:U:O2	30:0:2600:A:H8	1.97	0.48
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.78	0.48
30:0:535:G:C6	30:0:2064:U:C5	3.01	0.48
7:G:19:GLU:O	7:G:23:ILE:HG13	2.14	0.48
16:P:13:VAL:HG21	16:P:41:ARG:HG2	1.96	0.48
30:0:2001:G:O2'	30:0:2002:C:H5'	2.13	0.48
13:M:164:THR:HG23	13:M:165:GLY:N	2.29	0.48
30:0:2506:A:N6	30:0:2511:A:O2'	2.46	0.48
6:F:91:VAL:CG1	6:F:92:GLY:H	2.25	0.48
30:0:130:C:H2'	38:0:3167:HOH:O	2.14	0.48
30:0:2587:OMU:H5	38:0:7497:HOH:O	2.12	0.48
30:0:2415:A:H2'	30:0:2416:G:H5'	1.96	0.48
30:0:2649:A:H5'	30:0:2649:A:C8	2.49	0.48
29:3:91:GLN:O	29:3:92:GLU:HB2	2.14	0.48
30:0:1562:C:O2	30:0:1562:C:C2'	2.62	0.48
13:M:163:LEU:HD21	30:0:188:C:H5''	1.96	0.48
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.95	0.48
14:N:119:GLN:O	14:N:123:ILE:HG13	2.14	0.48
23:W:23:MET:O	30:0:1025:C:H5'	2.14	0.48
18:R:14:ALA:HB3	18:R:147:LEU:HB2	1.96	0.48
30:0:834:G:H4'	30:0:835:U:OP2	2.13	0.48
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.78	0.48
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.73	0.48
14:N:11:ARG:NH1	31:9:8:G:O6	2.47	0.47
1:A:212:PRO:HA	30:0:1943:C:O4'	2.14	0.47
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.95	0.47
12:L:22:ARG:HG2	38:0:9996:HOH:O	2.14	0.47
11:K:118:ALA:HA	11:K:125:ALA:HB2	1.95	0.47
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.95	0.47
30:0:1209:C:O2'	30:0:1210:G:H5'	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:4:LEU:HD22	23:W:52:VAL:CG2	2.44	0.47
30:0:1947:G:N2	30:0:1966:U:N3	2.61	0.47
30:0:821:U:H2'	30:0:822:C:H6	1.79	0.47
30:0:1130:U:H2'	30:0:1131:G:O4'	2.13	0.47
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.96	0.47
25:Y:210:GLY:N	30:0:1313:A:H5''	2.29	0.47
30:0:1161:A:O5'	30:0:1161:A:H8	1.96	0.47
30:0:523:C:H2'	30:0:524:A:C8	2.50	0.47
23:W:119:HIS:HE1	38:0:9557:HOH:O	1.97	0.47
2:B:62:ARG:HA	2:B:65:MET:HE3	1.95	0.47
30:0:407:A:H8	38:0:4473:HOH:O	1.98	0.47
3:C:246:ARG:NE	38:C:8620:HOH:O	2.40	0.47
2:B:5:ARG:HD2	2:B:8:LYS:NZ	2.30	0.47
30:0:2334:C:O2'	30:0:2335:C:H5'	2.14	0.47
18:R:114:VAL:HA	18:R:144:GLU:O	2.14	0.47
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.14	0.47
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.14	0.47
3:C:19:PRO:HG2	3:C:22:PHE:CE1	2.49	0.47
23:W:4:LEU:CD2	23:W:54:PHE:HB3	2.39	0.47
30:0:567:U:C5'	38:0:6408:HOH:O	2.63	0.47
31:9:47:A:C2	31:9:48:C:C2	3.02	0.47
30:0:2589:U:H2'	30:0:2590:U:H6	1.77	0.47
30:0:920:C:H5'	30:0:921:G:C4	2.49	0.47
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.11	0.47
30:0:1762:C:H2'	30:0:1763:C:C6	2.50	0.47
1:A:33:GLU:O	1:A:34:ASP:HB2	2.14	0.47
3:C:22:PHE:HA	3:C:116:ALA:HA	1.96	0.47
30:0:1768:C:H2'	30:0:1769:C:O4'	2.14	0.47
5:E:21:THR:HG23	5:E:30:THR:OG1	2.14	0.47
3:C:233:THR:HG22	3:C:234:VAL:N	2.29	0.47
30:0:2112:A:H2'	30:0:2113:G:C8	2.49	0.47
30:0:823:U:H3'	38:0:4459:HOH:O	2.14	0.47
30:0:2420:G:H2'	30:0:2421:G:H8	1.79	0.47
31:9:114:G:H2'	31:9:115:C:H6	1.78	0.47
30:0:1343:C:H2'	30:0:1344:G:O5'	2.15	0.47
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.48	0.47
3:C:136:VAL:HG22	3:C:137:PRO:HA	1.97	0.47
30:0:1589:G:N2	30:0:1605:G:H1'	2.29	0.47
30:0:523:C:H2'	30:0:524:A:H8	1.80	0.47
23:W:115:THR:HG23	38:W:5420:HOH:O	2.15	0.47
23:W:52:VAL:HG22	23:W:53:ALA:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2587:OMU:H6	30:0:2587:OMU:O5'	2.14	0.47
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.47
14:N:132:ASN:O	14:N:135:VAL:HG12	2.15	0.47
1:A:171:LYS:HB2	30:0:820:G:C6	2.50	0.47
8:H:66:GLU:HA	38:H:229:HOH:O	2.13	0.47
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.49	0.47
30:0:1615:A:H5'	38:0:4194:HOH:O	2.14	0.47
10:J:90:LYS:HB2	35:J:8802:CL:CL	2.52	0.47
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.80	0.47
30:0:1450:C:H5''	38:0:9621:HOH:O	2.15	0.47
23:W:125:HIS:HD2	23:W:127:GLY:H	1.62	0.47
30:0:2526:C:C6	30:0:2526:C:C5'	2.95	0.47
30:0:2637:A:C5'	38:0:4941:HOH:O	2.62	0.47
30:0:308:U:C4	30:0:342:C:H1'	2.49	0.47
30:0:101:C:H2'	30:0:102:A:C8	2.50	0.47
10:J:131:THR:HB	10:J:134:GLU:HG3	1.96	0.47
30:0:2691:A:H5'	30:0:2693:U:H1'	1.96	0.47
30:0:312:U:C2	30:0:320:G:N2	2.83	0.47
1:A:8:ARG:HG2	38:A:9016:HOH:O	2.14	0.47
30:0:222:A:H2'	30:0:223:G:O4'	2.14	0.47
29:3:3:MET:O	29:3:90:PHE:HA	2.15	0.47
30:0:2506:A:O2'	30:0:2507:G:C8	2.50	0.47
31:9:1:U:C4'	31:9:3:A:OP1	2.62	0.47
6:F:91:VAL:HG11	30:0:262:A:OP2	2.14	0.47
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.80	0.47
30:0:2269:C:H2'	30:0:2270:G:C5'	2.45	0.47
30:0:2241:C:O2'	30:0:2242:U:H5'	2.15	0.47
30:0:1682:A:H5''	38:0:9463:HOH:O	2.14	0.47
8:H:54:VAL:HG13	8:H:162:PRO:HG3	1.97	0.47
30:0:251:C:H2'	30:0:252:C:H6	1.80	0.47
30:0:304:G:H1'	30:0:347:A:N6	2.29	0.47
30:0:625:U:H5''	30:0:1044:C:N4	2.30	0.47
30:0:545:G:C8	30:0:545:G:C5'	2.88	0.47
30:0:1667:A:H2'	30:0:1668:U:C6	2.50	0.47
30:0:1632:A:H2'	30:0:1633:C:C5'	2.39	0.47
30:0:1165:G:H4'	30:0:1174:A:O2'	2.15	0.47
31:9:42:C:H5'	31:9:43:G:OP2	2.15	0.47
30:0:2000:G:O2'	30:0:2001:G:H5'	2.15	0.47
30:0:685:C:O2	30:0:748:C:H4'	2.15	0.47
2:B:132:HIS:NE2	2:B:171:VAL:HG23	2.28	0.47
30:0:629:A:C2	30:0:2074:A:C2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:9:ARG:HD2	30:0:380:A:OP2	2.15	0.47
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.30	0.47
30:0:1167:G:H2'	30:0:1168:C:O4'	2.15	0.47
1:A:223:ARG:NH1	30:0:2270:G:H4'	2.30	0.47
10:J:36:VAL:HG12	10:J:37:ALA:N	2.30	0.47
10:J:42:GLU:O	10:J:131:THR:HG23	2.15	0.47
12:L:67:ARG:HB2	12:L:112:GLY:HA3	1.96	0.47
30:0:264:G:H1'	30:0:265:U:H5	1.80	0.47
30:0:295:C:H2'	30:0:296:G:O4'	2.15	0.47
30:0:638:C:H2'	30:0:639:A:C8	2.50	0.47
30:0:2073:G:OP2	30:0:2490:A:H5'	2.15	0.47
4:D:141:VAL:HG21	31:9:57:A:H8	1.80	0.46
31:9:3:A:OP2	31:9:25:G:N2	2.47	0.46
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.14	0.46
30:0:677:C:O2'	30:0:678:G:H5'	2.15	0.46
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.97	0.46
30:0:1321:A:H2'	30:0:1322:G:C8	2.50	0.46
31:9:7:G:H5'	38:9:9100:HOH:O	2.16	0.46
11:K:41:LYS:O	11:K:42:ASN:HB2	2.15	0.46
2:B:298:LYS:HG2	38:0:5531:HOH:O	2.15	0.46
30:0:1180:U:O2'	30:0:1181:A:H5'	2.15	0.46
23:W:119:HIS:HD2	23:W:120:PRO:O	1.98	0.46
1:A:53:ALA:HB3	38:A:9066:HOH:O	2.15	0.46
30:0:853:C:H2'	30:0:854:G:O4'	2.15	0.46
30:0:1477:C:C5'	30:0:1868:G:H5''	2.45	0.46
30:0:1805:G:H2'	30:0:1806:G:H8	1.79	0.46
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.51	0.46
31:9:45:A:C5	31:9:46:C:C5	3.02	0.46
25:Y:210:GLY:H	30:0:1313:A:H5''	1.80	0.46
17:Q:75:ILE:HB	38:Q:6286:HOH:O	2.15	0.46
30:0:2566:A:C2	30:0:2696:G:O4'	2.68	0.46
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.41	0.46
29:3:38:ARG:HB3	29:3:42:ARG:HH12	1.81	0.46
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.95	0.46
30:0:319:A:H4'	30:0:338:C:C4	2.50	0.46
30:0:255:A:C5	30:0:256:C:C5	3.02	0.46
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.97	0.46
8:H:5:PRO:HD2	8:H:8:MET:SD	2.55	0.46
14:N:17:ARG:HB3	14:N:17:ARG:HH11	1.80	0.46
30:0:2249:G:C2	30:0:2253:G:C6	3.04	0.46
30:0:2250:G:C2	30:0:2251:G:H1'	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:27:GLN:HE21	31:9:8:G:H5''	1.80	0.46
20:T:26:THR:HA	20:T:39:ASN:HB3	1.97	0.46
31:9:65:A:N6	31:9:112:U:C6	2.83	0.46
1:A:204:GLY:N	30:0:2634:G:OP2	2.47	0.46
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.97	0.46
30:0:1139:U:H2'	30:0:1140:C:H6	1.80	0.46
29:3:29:ARG:NH2	30:0:1925:G:C5'	2.79	0.46
30:0:1925:G:O2'	30:0:1926:G:H5'	2.16	0.46
3:C:19:PRO:HG2	3:C:22:PHE:CD1	2.51	0.46
8:H:99:ARG:NH1	30:0:1055:G:OP2	2.47	0.46
30:0:2831:C:C2'	30:0:2832:C:H5'	2.45	0.46
30:0:800:G:H2'	30:0:801:U:C6	2.50	0.46
9:I:107:LYS:HB3	9:I:110:ASP:HB2	1.97	0.46
31:9:55:U:H4'	31:9:56:A:H8	1.80	0.46
30:0:369:G:H2'	30:0:370:G:H8	1.81	0.46
8:H:31:ILE:HG23	38:H:229:HOH:O	2.15	0.46
30:0:1393:A:H2'	30:0:1394:C:C6	2.51	0.46
3:C:206:ASN:HB2	30:0:329:A:OP2	2.16	0.46
12:L:6:ARG:HD3	30:0:1299:G:O6	2.15	0.46
30:0:2869:G:H2'	30:0:2870:C:C6	2.50	0.46
30:0:1641:A:H2'	30:0:1642:A:C5'	2.44	0.46
13:M:27:ARG:HH12	13:M:44:THR:CG2	2.28	0.46
21:U:44:ARG:HB3	38:U:3805:HOH:O	2.15	0.46
30:0:255:A:C4	30:0:256:C:C6	3.04	0.46
30:0:1942:A:H4'	38:0:9046:HOH:O	2.16	0.46
30:0:736:A:H2'	30:0:737:A:O4'	2.16	0.46
30:0:365:G:C6	30:0:366:U:C4	3.04	0.46
30:0:1211:G:H2'	30:0:1212:C:C6	2.50	0.46
30:0:2826:G:C6	30:0:2913:A:N6	2.84	0.46
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.75	0.46
16:P:120:ARG:NH1	30:0:1594:C:C5	2.84	0.46
6:F:96:ALA:HA	38:F:3111:HOH:O	2.15	0.46
30:0:158:A:H3'	38:0:7573:HOH:O	2.15	0.46
30:0:622:G:O2'	30:0:623:U:H5'	2.15	0.46
30:0:2895:C:H2'	38:0:9573:HOH:O	2.15	0.46
30:0:2379:G:N7	30:0:2408:A:N1	2.64	0.46
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.98	0.46
30:0:2594:C:O2'	30:0:2595:U:H5'	2.16	0.46
30:0:2433:A:H2'	30:0:2434:A:C8	2.50	0.46
13:M:184:ARG:HG3	13:M:185:PRO:HA	1.98	0.46
12:L:18:HIS:HB2	30:0:903:U:O4	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:451:C:O2'	30:0:452:G:H5'	2.16	0.46
30:0:1603:A:H5''	30:0:1604:G:H3'	1.98	0.46
13:M:27:ARG:NH1	13:M:44:THR:CG2	2.78	0.46
26:Z:76:THR:HG21	30:0:1652:C:H4'	1.96	0.46
30:0:1825:U:O2'	30:0:1826:C:H5'	2.15	0.46
30:0:1015:C:O5'	30:0:1015:C:H6	1.98	0.46
30:0:366:U:H2'	30:0:367:G:O4'	2.16	0.46
31:9:45:A:H2'	31:9:46:C:C6	2.51	0.46
30:0:1506:U:H6	30:0:1506:U:H5'	1.81	0.46
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.30	0.46
30:0:466:A:H2'	30:0:467:G:O4'	2.15	0.46
23:W:21:LEU:O	23:W:26:ILE:HG23	2.16	0.46
30:0:1180:U:H2'	30:0:1181:A:O4'	2.16	0.46
30:0:1684:A:O2'	30:0:1685:A:H5''	2.16	0.46
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.16	0.46
4:D:103:ASN:HD22	4:D:134:LEU:H	1.60	0.46
30:0:1774:G:H1'	38:0:4551:HOH:O	2.14	0.46
31:9:52:A:H2'	31:9:53:G:O4'	2.16	0.46
30:0:958:G:O2'	30:0:959:C:H5'	2.15	0.46
16:P:120:ARG:NH2	16:P:123:TYR:CD2	2.83	0.46
30:0:2361:A:H2'	30:0:2362:A:C8	2.49	0.46
8:H:165:ARG:HD2	38:H:231:HOH:O	2.16	0.46
30:0:1714:C:O2'	30:0:1715:C:H5'	2.16	0.46
30:0:1622:G:H2'	30:0:1623:C:H5'	1.98	0.46
15:O:24:ALA:HB3	30:0:710:G:OP1	2.16	0.46
30:0:1165:G:H1'	30:0:1174:A:H1'	1.97	0.45
30:0:1202:A:O2'	30:0:1203:G:H5'	2.16	0.45
30:0:1523:G:C6	30:0:1524:U:C4	3.04	0.45
30:0:1278:A:H2'	30:0:1280:A:C8	2.51	0.45
15:O:63:LYS:NZ	30:0:659:A:N7	2.53	0.45
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.16	0.45
30:0:735:C:C5	30:0:736:A:N3	2.84	0.45
30:0:2355:G:H5''	30:0:2356:A:OP2	2.16	0.45
30:0:2869:G:H2'	30:0:2870:C:H6	1.81	0.45
16:P:40:VAL:O	16:P:44:VAL:HG23	2.17	0.45
30:0:417:G:P	38:0:7432:HOH:O	2.74	0.45
30:0:271:C:N4	30:0:378:A:C2	2.71	0.45
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.51	0.45
24:X:43:VAL:HG12	24:X:44:ASP:N	2.30	0.45
31:9:106:U:O2'	31:9:107:C:H5'	2.15	0.45
30:0:711:G:O2'	30:0:712:C:H5'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:NH2	30:0:1853:C:O2'	2.49	0.45
30:0:64:G:H2'	30:0:65:C:O4'	2.16	0.45
30:0:24:G:N2	30:0:518:G:H1'	2.31	0.45
3:C:79:ARG:O	3:C:87:ARG:HG2	2.16	0.45
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.31	0.45
30:0:496:G:H3'	38:0:7681:HOH:O	2.15	0.45
30:0:236:A:H4'	30:0:237:G:OP1	2.15	0.45
20:T:38:ARG:NH1	38:0:6693:HOH:O	2.42	0.45
9:I:114:TYR:N	9:I:114:TYR:CD1	2.84	0.45
2:B:26:PHE:HE1	38:B:9109:HOH:O	1.99	0.45
30:0:1201:C:H2'	30:0:1202:A:H5'	1.98	0.45
21:U:17:THR:CG2	21:U:18:GLY:N	2.79	0.45
30:0:2467:A:O2'	30:0:2468:A:H2'	2.17	0.45
20:T:21:LYS:HA	20:T:24:ARG:HG3	1.99	0.45
30:0:2092:G:H2'	30:0:2613:G:OP1	2.16	0.45
15:O:25:VAL:HG23	15:O:26:TRP:N	2.31	0.45
4:D:170:TYR:HD1	4:D:170:TYR:N	2.14	0.45
3:C:233:THR:HG22	3:C:234:VAL:H	1.81	0.45
30:0:105:G:O2'	30:0:106:A:H5'	2.16	0.45
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.50	0.45
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.97	0.45
5:E:1:PRO:HG2	5:E:59:MET:SD	2.56	0.45
30:0:1883:U:C2'	30:0:1884:G:H5'	2.46	0.45
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.30	0.45
30:0:1909:A:N1	30:0:2128:G:H1'	2.31	0.45
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.80	0.45
31:9:2:U:OP2	31:9:2:U:H4'	2.16	0.45
30:0:1942:A:HO2'	30:0:1943:C:H5'	1.80	0.45
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.97	0.45
30:0:1015:C:H2'	30:0:1016:U:C6	2.51	0.45
30:0:210:U:H2'	30:0:211:U:C6	2.51	0.45
30:0:1834:C:H2'	30:0:1840:A:H62	1.82	0.45
3:C:236:THR:CG2	3:C:239:ALA:H	2.21	0.45
30:0:2895:C:O2'	30:0:2896:A:H5''	2.16	0.45
27:1:25:LYS:O	27:1:25:LYS:HG2	2.17	0.45
30:0:1268:C:H2'	30:0:1269:G:C8	2.52	0.45
30:0:1001:U:O2'	30:0:1002:G:H5'	2.17	0.45
30:0:1855:G:H4'	30:0:1856:C:O5'	2.16	0.45
30:0:843:A:C2	30:0:846:A:C8	3.04	0.45
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.98	0.45
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:141:VAL:HG21	31:9:57:A:C8	2.51	0.45
30:0:1634:G:C3'	38:0:3907:HOH:O	2.46	0.45
28:2:48:ASP:O	28:2:49:GLU:HB2	2.17	0.45
1:A:199:HIS:HD2	1:A:201:PHE:HB2	1.82	0.45
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.81	0.45
30:0:945:U:H2'	30:0:946:C:C6	2.52	0.45
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.52	0.45
30:0:682:A:H2'	30:0:683:G:O4'	2.16	0.45
30:0:2456:A:H5'	38:0:5702:HOH:O	2.17	0.45
30:0:423:A:C5	30:0:424:C:C5	3.05	0.45
25:Y:133:HIS:HD2	38:Y:8881:HOH:O	1.98	0.45
30:0:2314:G:C2'	30:0:2315:C:H5'	2.47	0.45
30:0:2664:A:H8	30:0:2664:A:OP1	1.99	0.45
30:0:1183:C:H42	30:0:1184:C:N4	2.10	0.45
30:0:2506:A:C4	38:0:6063:HOH:O	2.67	0.45
30:0:2681:A:H4'	30:0:2682:C:OP1	2.16	0.45
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.83	0.45
23:W:13:MET:CE	23:W:17:ILE:HG22	2.47	0.45
30:0:1624:A:H4'	30:0:1626:A:H5''	1.99	0.45
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.50	0.45
30:0:482:G:O4'	30:0:511:A:C2	2.69	0.45
30:0:73:U:O2'	30:0:74:G:H5'	2.17	0.45
30:0:1386:G:O2'	30:0:1387:G:H5'	2.17	0.45
30:0:1379:A:H1'	38:0:9695:HOH:O	2.16	0.45
14:N:40:ASN:ND2	31:9:28:U:H5''	2.31	0.45
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.99	0.45
30:0:670:G:H2'	30:0:671:A:C8	2.51	0.45
1:A:190:ARG:NH1	30:0:1845:A:OP2	2.49	0.45
30:0:1014:A:H2'	30:0:1015:C:H5'	1.99	0.45
12:L:61:ALA:HB2	12:L:105:TYR:CZ	2.52	0.45
30:0:1484:G:H2'	38:0:9106:HOH:O	2.17	0.45
2:B:223:ARG:HG3	2:B:232:TRP:O	2.17	0.45
30:0:2727:A:C6	30:0:2756:U:C2	3.05	0.45
30:0:2248:C:C4	30:0:2249:G:N7	2.85	0.45
30:0:1221:G:H8	38:0:5995:HOH:O	1.95	0.45
11:K:118:ALA:CA	11:K:125:ALA:HB2	2.47	0.45
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.16	0.45
30:0:1400:C:O2'	30:0:1401:G:H5'	2.17	0.45
25:Y:170:SER:OG	25:Y:175:ARG:HG3	2.16	0.45
5:E:154:ILE:HD11	5:E:157:LYS:NZ	2.32	0.45
30:0:1191:A:C2	30:0:1207:A:C2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1279:U:O2	30:0:1279:U:C2'	2.64	0.45
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.47	0.45
30:0:2819:C:H2'	30:0:2820:A:C8	2.51	0.45
30:0:441:A:H8	30:0:441:A:O5'	1.99	0.45
30:0:2002:C:H2'	30:0:2003:U:H5'	1.99	0.45
11:K:34:VAL:HB	38:K:7169:HOH:O	2.17	0.45
30:0:861:A:H4'	30:0:1697:G:H4'	1.99	0.45
30:0:1425:G:O2'	30:0:1426:C:H5'	2.17	0.45
30:0:1537:C:H1'	38:0:6597:HOH:O	2.16	0.45
27:1:20:ARG:HG2	30:0:111:C:O2'	2.17	0.45
24:X:74:ALA:HB2	24:X:85:VAL:HG13	2.00	0.44
30:0:2812:A:H1'	38:0:5796:HOH:O	2.17	0.44
31:9:39:U:HO2'	31:9:42:C:H5	1.65	0.44
30:0:128:A:H3'	30:0:128:A:C8	2.52	0.44
17:Q:42:LYS:HE2	30:0:952:G:OP1	2.18	0.44
30:0:1771:U:O2'	30:0:1773:G:N7	2.50	0.44
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.82	0.44
30:0:107:U:H2'	30:0:108:U:H5'	1.99	0.44
31:9:36:C:C5	31:9:37:C:C5	3.05	0.44
30:0:2072:G:C6	30:0:2533:C:H1'	2.52	0.44
12:L:36:ASP:HB2	38:L:8836:HOH:O	2.17	0.44
30:0:1333:U:H2'	30:0:1334:C:C6	2.52	0.44
30:0:2483:A:H4'	30:0:2484:U:OP2	2.17	0.44
30:0:368:C:C2'	30:0:369:G:H5'	2.47	0.44
30:0:506:G:N2	30:0:509:A:C5'	2.72	0.44
23:W:4:LEU:O	23:W:32:CYS:HA	2.17	0.44
20:T:9:LYS:HD2	38:0:3766:HOH:O	2.16	0.44
30:0:2689:A:H2'	30:0:2690:U:H5'	1.99	0.44
30:0:2329:C:O2'	30:0:2330:U:H5'	2.17	0.44
30:0:213:G:N2	30:0:225:G:H2'	2.32	0.44
6:F:30:LYS:HE2	6:F:99:THR:HG21	1.99	0.44
30:0:2543:G:H2'	30:0:2544:G:O4'	2.17	0.44
30:0:790:A:H1'	30:0:1710:A:H2'	1.99	0.44
30:0:905:C:H3'	38:0:5198:HOH:O	2.17	0.44
30:0:1759:A:N3	30:0:1818:C:H2'	2.33	0.44
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.80	0.44
13:M:164:THR:CG2	13:M:167:GLY:H	2.27	0.44
30:0:2511:A:H2'	30:0:2512:U:O4'	2.17	0.44
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.31	0.44
30:0:1545:C:H1'	30:0:1641:A:N6	2.33	0.44
20:T:9:LYS:HG3	38:0:7437:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:39:U:C2'	31:9:40:C:OP1	2.65	0.44
30:0:579:G:H2'	30:0:580:A:C8	2.52	0.44
30:0:1522:A:C2	30:0:1665:G:C6	3.05	0.44
30:0:343:C:O2'	30:0:344:C:H5'	2.17	0.44
13:M:86:GLN:NE2	30:0:2274:A:H1'	2.32	0.44
21:U:33:SER:O	21:U:37:GLU:HG3	2.16	0.44
30:0:281:U:H5	38:0:7606:HOH:O	2.01	0.44
3:C:236:THR:HG22	3:C:239:ALA:CB	2.47	0.44
30:0:1175:G:H8	30:0:1193:A:HO2'	1.64	0.44
2:B:320:GLN:NE2	2:B:321:PRO:HD2	2.29	0.44
1:A:223:ARG:HD2	30:0:2272:G:OP1	2.17	0.44
17:Q:95:GLU:HA	30:0:949:U:H4'	1.99	0.44
30:0:1622:G:C2'	30:0:1623:C:H5'	2.47	0.44
30:0:2775:A:C6	30:0:2799:A:C8	3.06	0.44
30:0:2239:C:H2'	30:0:2240:U:C6	2.53	0.44
30:0:2375:A:H2'	30:0:2376:C:C6	2.53	0.44
30:0:999:C:O2'	30:0:1000:C:H5'	2.18	0.44
1:A:109:GLU:HG2	1:A:116:GLY:N	2.33	0.44
5:E:169:THR:HG22	5:E:170:ARG:HG3	2.00	0.44
13:M:164:THR:HB	38:M:8819:HOH:O	2.18	0.44
14:N:141:ARG:NH2	31:9:48:C:H4'	2.27	0.44
6:F:57:GLU:O	6:F:61:MET:HG3	2.18	0.44
14:N:143:ARG:HE	14:N:143:ARG:HB3	1.61	0.44
30:0:2238:A:O2'	30:0:2239:C:H5'	2.17	0.44
2:B:211:THR:HG21	38:0:7469:HOH:O	2.17	0.44
30:0:249:G:O2'	30:0:250:C:H5'	2.17	0.44
25:Y:134:HIS:HE1	30:0:538:C:OP2	2.01	0.44
19:S:57:THR:HG22	19:S:58:MET:N	2.32	0.44
38:C:8546:HOH:O	30:0:457:U:H4'	2.17	0.44
30:0:2858:U:H2'	30:0:2859:C:O4'	2.16	0.44
31:9:1:U:H5''	31:9:3:A:OP1	2.18	0.44
30:0:2812:A:N7	38:0:7529:HOH:O	2.36	0.44
30:0:1973:A:H5'	30:0:1973:A:C8	2.44	0.44
11:K:87:ARG:NE	38:0:5721:HOH:O	2.50	0.44
30:0:1790:C:H2'	30:0:1791:U:C6	2.51	0.44
30:0:2800:A:H5'	30:0:2801:A:OP2	2.18	0.44
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.98	0.44
30:0:277:U:O2'	30:0:278:A:H5'	2.18	0.44
2:B:280:VAL:HG13	2:B:333:GLU:O	2.18	0.44
13:M:99:ARG:HH21	13:M:170:ASN:HD22	1.64	0.44
30:0:1593:C:H1'	38:0:6112:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1592:G:O2'	30:0:1593:C:O4'	2.33	0.44
23:W:122:ARG:NH2	38:0:5297:HOH:O	2.49	0.44
30:0:371:U:H2'	30:0:372:A:C8	2.48	0.44
30:0:2653:A:H2'	30:0:2654:C:C6	2.53	0.44
30:0:636:G:H1'	30:0:2058:G:C4	2.53	0.44
30:0:302:A:O2'	30:0:303:C:H5'	2.17	0.44
30:0:1950:G:H2'	30:0:1951:G:C8	2.53	0.44
4:D:57:THR:HG23	4:D:63:ILE:HA	2.00	0.44
30:0:1434:A:H2'	30:0:1436:C:C5	2.53	0.44
23:W:133:LYS:HG3	38:W:5904:HOH:O	2.18	0.44
7:G:63:ARG:N	38:G:2569:HOH:O	2.50	0.44
30:0:1191:A:H2	30:0:1206:U:H3	1.65	0.44
30:0:2718:C:H5'	30:0:2718:C:C6	2.50	0.44
30:0:2252:A:C6	30:0:2253:G:H1'	2.53	0.44
4:D:76:ARG:NE	31:9:44:A:O4'	2.51	0.44
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.98	0.44
30:0:291:C:H2'	30:0:292:G:O4'	2.18	0.44
18:R:132:ARG:NH2	30:0:2055:A:H4'	2.32	0.44
30:0:1067:A:H3'	38:0:4304:HOH:O	2.17	0.44
30:0:2831:C:H2'	30:0:2832:C:H5'	1.99	0.44
30:0:790:A:H2'	30:0:791:A:O4'	2.17	0.44
7:G:63:ARG:O	7:G:67:LEU:HG	2.17	0.44
30:0:289:G:O2'	30:0:290:C:H5'	2.17	0.44
30:0:1603:A:C5'	30:0:1605:G:C5'	2.95	0.44
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.43	0.44
30:0:1181:A:H2'	30:0:1182:C:C5'	2.48	0.44
30:0:1202:A:C2'	30:0:1203:G:H5'	2.48	0.44
30:0:567:U:O2'	30:0:568:G:H5'	2.17	0.44
30:0:2064:U:H4'	30:0:2653:A:OP1	2.17	0.44
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.82	0.44
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.99	0.44
30:0:1044:C:H5''	38:0:9029:HOH:O	2.18	0.44
25:Y:142:SER:OG	30:0:1331:G:OP2	2.32	0.44
30:0:699:C:H6	30:0:744:G:O4'	2.01	0.44
30:0:2264:A:H2'	30:0:2265:U:C6	2.53	0.44
14:N:164:ASP:OD1	14:N:167:ASP:HA	2.18	0.44
30:0:705:C:H2'	30:0:705:C:O2	2.17	0.44
30:0:1163:G:C2	30:0:1184:C:N3	2.86	0.43
28:2:41:HIS:CD2	28:2:44:ARG:H	2.33	0.43
30:0:2598:U:O2	30:0:2600:A:C8	2.71	0.43
30:0:129:A:H4'	30:0:130:C:OP1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ALA:HA	1:A:131:HIS:NE2	2.33	0.43
8:H:87:LYS:NZ	8:H:87:LYS:HB2	2.33	0.43
25:Y:141:THR:HG23	38:Y:8888:HOH:O	2.18	0.43
15:O:65:LEU:HD13	30:0:746:A:C6	2.53	0.43
30:0:47:G:N3	30:0:114:A:C2	2.86	0.43
30:0:1127:C:C5	30:0:1128:U:C4	3.06	0.43
3:C:168:ARG:NH2	3:C:190:ALA:O	2.51	0.43
30:0:825:U:H5''	30:0:826:U:OP1	2.18	0.43
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.45	0.43
30:0:1552:G:N2	30:0:1634:G:H1'	2.33	0.43
4:D:154:LYS:H	4:D:154:LYS:CD	2.24	0.43
6:F:91:VAL:CG1	6:F:92:GLY:N	2.78	0.43
30:0:2421:G:H3'	30:0:2422:U:C5'	2.47	0.43
18:R:104:PHE:HB3	18:R:109:MET:HE1	2.01	0.43
18:R:128:ARG:NH2	30:0:2054:A:C2	2.86	0.43
30:0:2488:A:H2'	30:0:2489:G:O4'	2.19	0.43
30:0:1947:G:H2'	30:0:1948:G:H8	1.82	0.43
30:0:2379:G:H5'	30:0:2381:C:O4'	2.18	0.43
30:0:677:C:P	38:0:7147:HOH:O	2.75	0.43
30:0:2566:A:H2	30:0:2695:C:O2	2.01	0.43
31:9:35:C:H5''	38:9:9080:HOH:O	2.17	0.43
30:0:134:U:C2	30:0:145:A:C2	3.07	0.43
14:N:114:LYS:O	14:N:118:ILE:HG13	2.18	0.43
30:0:1115:U:O2'	30:0:1116:U:H5'	2.18	0.43
30:0:484:A:N1	30:0:506:G:H4'	2.33	0.43
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.83	0.43
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.83	0.43
30:0:1762:C:O2'	30:0:1763:C:H5'	2.17	0.43
22:V:44:GLY:HA3	30:0:92:G:H4'	1.99	0.43
30:0:2607:U:H4'	38:0:9448:HOH:O	2.18	0.43
12:L:48:LYS:HE2	30:0:220:C:C2	2.53	0.43
5:E:80:TRP:O	5:E:134:SER:HA	2.18	0.43
9:I:111:LEU:CD2	30:0:1163:G:H4'	2.45	0.43
30:0:1700:C:H5''	30:0:1701:A:OP2	2.18	0.43
30:0:2256:G:H2'	30:0:2257:G:O5'	2.17	0.43
16:P:7:LYS:HG2	16:P:23:PHE:CE2	2.54	0.43
30:0:1395:C:H2'	30:0:1396:C:C6	2.53	0.43
31:9:34:A:H2'	31:9:35:C:O4'	2.18	0.43
30:0:17:G:H2'	30:0:18:C:H6	1.82	0.43
35:0:8814:CL:CL	38:0:7753:HOH:O	2.59	0.43
14:N:41:LYS:HD3	38:9:9063:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1245:C:O5'	30:0:1245:C:H6	2.01	0.43
30:0:559:U:H2'	30:0:560:U:O4'	2.18	0.43
30:0:2504:A:H2'	30:0:2505:G:H5'	2.00	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.96	0.43
8:H:61:ARG:HG3	38:0:4984:HOH:O	2.17	0.43
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.52	0.43
1:A:103:VAL:HA	1:A:104:PRO:HD3	1.83	0.43
1:A:95:PRO:HA	1:A:153:ARG:HA	1.99	0.43
24:X:15:ARG:HH22	30:0:2856:A:P	2.41	0.43
4:D:50:VAL:HG13	31:9:41:C:O4'	2.18	0.43
13:M:157:ASP:HB3	13:M:160:PHE:HD1	1.84	0.43
3:C:93:LYS:O	3:C:98:ARG:NH2	2.51	0.43
30:0:1896:G:C6	30:0:1897:U:C4	3.07	0.43
30:0:522:U:O2'	30:0:1366:C:H5'	2.18	0.43
11:K:115:ARG:HG3	11:K:116:GLU:N	2.34	0.43
6:F:59:ILE:HD13	30:0:263:U:O4'	2.18	0.43
2:B:271:ASP:HB3	2:B:296:LEU:HD12	1.99	0.43
2:B:198:GLU:HA	38:B:9119:HOH:O	2.19	0.43
1:A:55:VAL:HG23	1:A:68:ILE:O	2.19	0.43
30:0:1964:U:H2'	30:0:1964:U:O2	2.17	0.43
30:0:1187:U:C2	30:0:1189:A:OP2	2.72	0.43
30:0:1702:U:H5'	38:0:3432:HOH:O	2.18	0.43
31:9:28:U:H2'	31:9:29:C:C6	2.54	0.43
23:W:125:HIS:HB2	23:W:137:GLN:HG2	2.00	0.43
30:0:542:A:H2'	30:0:543:G:O4'	2.18	0.43
4:D:25:MET:CE	4:D:41:LEU:HG	2.47	0.43
12:L:39:GLU:HG2	30:0:926:A:C4'	2.48	0.43
25:Y:216:ARG:NH1	38:Y:8833:HOH:O	2.51	0.43
30:0:2070:G:H2'	30:0:2072:G:OP1	2.19	0.43
30:0:570:C:H2'	30:0:571:C:H5'	2.01	0.43
13:M:193:LYS:HB3	30:0:392:U:H4'	1.99	0.43
30:0:2437:A:H2'	30:0:2438:G:C8	2.54	0.43
30:0:2906:A:H5'	30:0:2907:C:O4'	2.19	0.43
14:N:151:ASP:OD1	14:N:166:ALA:HA	2.19	0.43
30:0:1063:G:H8	38:0:9865:HOH:O	2.01	0.43
30:0:1198:U:C6	30:0:1200:A:OP2	2.72	0.43
30:0:2587:OMU:H2'	30:0:2589:U:H5''	2.00	0.43
1:A:179:MET:HG2	1:A:186:TRP:CB	2.49	0.43
3:C:54:LEU:HD23	3:C:79:ARG:HG3	2.00	0.43
30:0:969:G:H1	30:0:999:C:H42	1.66	0.43
30:0:17:G:H2'	30:0:18:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.54	0.43
2:B:87:TYR:HD1	38:B:9041:HOH:O	2.01	0.43
30:0:243:A:H61	30:0:269:G:H1'	1.83	0.43
2:B:14:GLY:HA2	2:B:15:PRO:C	2.39	0.43
3:C:25:PRO:HG2	38:C:8523:HOH:O	2.18	0.43
30:0:37:A:H2'	30:0:38:G:C8	2.54	0.43
30:0:2115:U:H2'	30:0:2116:U:C6	2.53	0.43
30:0:1163:G:H1	30:0:1184:C:N4	2.16	0.43
30:0:1588:G:C6	30:0:1589:G:C6	3.07	0.43
2:B:297:VAL:HB	38:B:9070:HOH:O	2.19	0.43
23:W:13:MET:HE3	23:W:17:ILE:HG22	2.00	0.43
30:0:734:U:H2'	30:0:736:A:OP2	2.19	0.43
2:B:234:ARG:NH2	30:0:2039:A:OP2	2.51	0.43
30:0:947:U:O2'	30:0:948:G:H5'	2.19	0.43
30:0:2134:G:N2	30:0:2242:U:C2	2.87	0.43
30:0:886:A:OP2	30:0:2113:G:H5'	2.19	0.43
28:2:28:LYS:O	30:0:87:C:H2'	2.18	0.43
3:C:173:LYS:HE3	30:0:1311:G:O6	2.18	0.43
30:0:652:G:H8	38:0:3020:HOH:O	2.00	0.43
2:B:248:ARG:NH1	38:B:9080:HOH:O	2.50	0.43
16:P:133:SER:HA	38:0:3512:HOH:O	2.18	0.43
6:F:72:VAL:HA	6:F:73:PRO:HD3	1.85	0.43
4:D:10:PHE:CG	4:D:11:HIS:N	2.87	0.43
30:0:1553:C:H2'	30:0:1554:C:H6	1.84	0.43
14:N:108:SER:HA	14:N:109:PRO:HD3	1.78	0.43
30:0:1186:C:N4	30:0:1187:U:C4	2.87	0.43
31:9:1:U:O3'	31:9:3:A:OP1	2.36	0.43
30:0:129:A:O2'	30:0:131:A:OP1	2.36	0.43
30:0:1942:A:H2'	30:0:1943:C:H6	1.83	0.43
31:9:106:U:O5'	31:9:106:U:H6	2.01	0.43
30:0:735:C:C5	30:0:736:A:C2	3.06	0.43
30:0:297:U:H1'	38:0:3947:HOH:O	2.18	0.43
30:0:792:G:H4'	38:0:3424:HOH:O	2.19	0.43
3:C:170:ASP:OD2	30:0:330:C:H5	2.01	0.43
27:1:37:CYS:SG	27:1:39:PHE:HB2	2.59	0.43
13:M:171:ARG:NH2	30:0:189:A:OP1	2.51	0.43
30:0:2712:G:O2'	30:0:2713:G:H5'	2.19	0.43
30:0:2820:A:H2'	30:0:2821:C:C6	2.54	0.43
30:0:2842:G:H2'	30:0:2843:A:C5'	2.48	0.43
30:0:1883:U:O2'	30:0:1884:G:H5'	2.19	0.43
19:S:57:THR:C	19:S:59:ASP:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.34	0.43
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.54	0.43
30:0:282:C:O2'	30:0:283:U:C4'	2.67	0.42
23:W:21:LEU:HD21	23:W:48:VAL:CG1	2.46	0.42
3:C:236:THR:HG22	3:C:239:ALA:HB2	2.01	0.42
30:0:2783:A:H2'	30:0:2784:A:C8	2.54	0.42
30:0:2756:U:C2	30:0:2896:A:H2	2.37	0.42
27:1:28:HIS:HD2	27:1:30:LYS:H	1.66	0.42
5:E:69:ILE:HA	5:E:72:MET:CE	2.48	0.42
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.34	0.42
26:Z:47:ARG:NH1	38:Z:8704:HOH:O	2.50	0.42
30:0:305:A:C5	30:0:329:A:C2	3.07	0.42
30:0:212:A:O4'	30:0:214:U:C6	2.72	0.42
15:O:81:PHE:HB2	15:O:86:GLU:HB2	2.01	0.42
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.54	0.42
14:N:171:HIS:CE1	38:N:8855:HOH:O	2.72	0.42
14:N:23:ARG:O	14:N:27:LEU:HG	2.18	0.42
13:M:47:ASP:CG	13:M:48:LYS:N	2.72	0.42
21:U:4:ARG:N	38:U:5334:HOH:O	2.52	0.42
30:0:1965:C:O5'	30:0:1965:C:H6	2.02	0.42
30:0:1052:G:H2'	30:0:1052:G:N3	2.33	0.42
3:C:184:ARG:NH1	30:0:1306:U:OP1	2.51	0.42
30:0:128:A:O2'	30:0:129:A:C5'	2.67	0.42
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.53	0.42
30:0:834:G:H3'	30:0:835:U:H4'	2.01	0.42
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.33	0.42
30:0:1921:A:C6	30:0:1922:A:C2	3.08	0.42
30:0:2332:A:H3'	30:0:2333:G:H8	1.84	0.42
30:0:867:A:H2	30:0:880:C:O2	2.02	0.42
3:C:237:GLU:HA	38:C:8626:HOH:O	2.18	0.42
30:0:1706:G:C5	30:0:1707:G:C6	3.07	0.42
30:0:162:C:H2'	30:0:163:U:H5'	2.02	0.42
2:B:238:ASN:ND2	2:B:240:GLY:H	2.04	0.42
2:B:74:ILE:HG13	38:B:9070:HOH:O	2.17	0.42
30:0:31:C:C4'	38:0:7437:HOH:O	2.66	0.42
30:0:128:A:C8	30:0:128:A:C3'	3.02	0.42
19:S:57:THR:HG23	38:S:8979:HOH:O	2.19	0.42
14:N:164:ASP:CG	14:N:167:ASP:HA	2.39	0.42
30:0:2347:C:H2'	30:0:2348:C:H6	1.83	0.42
14:N:69:TYR:CE2	14:N:184:ILE:HD11	2.55	0.42
30:0:1249:U:H2'	30:0:1250:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:932:U:H1'	30:0:1296:A:H1'	2.00	0.42
30:0:1350:U:H4'	38:0:5134:HOH:O	2.18	0.42
30:0:1461:U:H2'	30:0:1462:C:C6	2.54	0.42
30:0:2121:G:O2'	30:0:2122:C:H5'	2.19	0.42
18:R:104:PHE:CB	18:R:109:MET:HE1	2.49	0.42
30:0:1741:U:C4	30:0:2033:G:C8	3.07	0.42
30:0:699:C:C2	30:0:744:G:C2	3.07	0.42
6:F:59:ILE:CD1	30:0:263:U:C2	3.02	0.42
29:3:11:CYS:HB2	29:3:20:HIS:HE1	1.85	0.42
15:O:105:ASN:HD21	15:O:109:SER:N	2.17	0.42
30:0:1613:C:H2'	30:0:1614:G:O4'	2.19	0.42
6:F:110:ASP:O	6:F:114:LYS:HG3	2.20	0.42
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.42
30:0:40:C:H6	30:0:40:C:O5'	2.02	0.42
23:W:4:LEU:HD23	23:W:4:LEU:HA	1.83	0.42
10:J:75:PRO:HD3	10:J:136:SER:OG	2.20	0.42
30:0:2032:U:O2'	30:0:2033:G:H5''	2.20	0.42
14:N:71:TRP:HB2	38:N:8833:HOH:O	2.19	0.42
18:R:3:SER:HB2	30:0:20:G:O3'	2.19	0.42
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.20	0.42
30:0:74:G:H2'	30:0:75:U:C6	2.54	0.42
30:0:2801:A:H2'	30:0:2801:A:N3	2.34	0.42
30:0:1020:A:H1'	38:0:7242:HOH:O	2.19	0.42
16:P:87:ARG:HG2	38:P:188:HOH:O	2.18	0.42
30:0:177:A:H2'	30:0:178:U:O4'	2.19	0.42
30:0:69:A:C8	30:0:69:A:C5'	2.96	0.42
30:0:1081:A:H5''	38:0:3159:HOH:O	2.19	0.42
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.55	0.42
30:0:2089:A:C2'	30:0:2090:G:H5'	2.49	0.42
30:0:2657:G:O2'	30:0:2842:G:N7	2.47	0.42
30:0:2754:G:C2'	30:0:2755:G:H5'	2.49	0.42
30:0:316:A:N3	30:0:336:G:O2'	2.46	0.42
30:0:1482:A:O2'	30:0:1483:C:H5'	2.20	0.42
30:0:1760:G:H5'	30:0:1818:C:O2'	2.20	0.42
30:0:1495:C:H1'	30:0:1573:A:H1'	2.02	0.42
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.19	0.42
24:X:78:GLU:HB3	38:X:5564:HOH:O	2.19	0.42
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.85	0.42
30:0:2523:U:O2'	30:0:2524:G:H5'	2.20	0.42
17:Q:28:ARG:HG2	38:Q:4350:HOH:O	2.20	0.42
30:0:1735:C:O2'	30:0:1736:A:H5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ASP:HB2	2:B:322:ARG:HE	1.85	0.42
4:D:18:ILE:HD13	4:D:84:LEU:HD12	2.01	0.42
30:0:2421:G:H3'	30:0:2422:U:H5''	2.02	0.42
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.84	0.42
28:2:41:HIS:HB3	28:2:44:ARG:HB2	2.02	0.42
30:0:1058:A:H2'	30:0:1060:C:C5'	2.48	0.42
30:0:2600:A:H2'	30:0:2601:A:O4'	2.19	0.42
30:0:583:C:H2'	30:0:584:U:C6	2.50	0.42
30:0:445:U:H2'	30:0:446:G:C8	2.54	0.42
11:K:29:LEU:HD22	11:K:55:VAL:HG11	2.02	0.42
30:0:2265:U:H2'	30:0:2266:A:C8	2.55	0.42
30:0:113:A:OP2	30:0:114:A:H2'	2.19	0.42
4:D:21:VAL:HA	4:D:131:THR:O	2.19	0.42
8:H:91:ARG:NH1	8:H:138:THR:OG1	2.50	0.42
30:0:2809:G:H2'	30:0:2810:G:O4'	2.20	0.42
18:R:82:GLU:O	18:R:86:LYS:HG3	2.19	0.42
14:N:37:ARG:NH2	38:N:8828:HOH:O	2.51	0.42
30:0:1603:A:H5'	30:0:1605:G:C5'	2.49	0.42
30:0:1878:G:O2'	30:0:1879:U:OP2	2.38	0.42
30:0:2255:A:O2'	30:0:2256:G:H5'	2.20	0.42
30:0:1562:C:N4	38:0:5872:HOH:O	2.52	0.42
14:N:159:TYR:HE1	31:9:50:G:H5''	1.85	0.42
19:S:37:VAL:O	19:S:41:VAL:HG23	2.20	0.42
16:P:13:VAL:HG13	16:P:14:LEU:N	2.35	0.42
9:I:114:TYR:N	9:I:114:TYR:HD1	2.17	0.42
30:0:1307:A:H2'	30:0:1308:A:C8	2.55	0.42
28:2:2:LYS:HG3	30:0:1486:A:C5	2.55	0.42
1:A:206:ARG:NH2	30:0:2630:G:O6	2.53	0.42
11:K:78:LYS:HA	11:K:79:PRO:HD3	1.94	0.42
6:F:107:ASP:O	6:F:111:ILE:HG13	2.19	0.42
6:F:111:ILE:O	6:F:115:VAL:HG23	2.20	0.42
20:T:41:ARG:NH1	20:T:42:VAL:O	2.53	0.42
30:0:1644:C:O2'	30:0:1645:U:H5'	2.19	0.42
30:0:2032:U:C2'	30:0:2033:G:C5'	2.98	0.42
30:0:1398:G:H2'	30:0:1399:A:C8	2.55	0.42
20:T:97:ARG:NH2	30:0:308:U:H5'	2.35	0.42
30:0:1788:U:C2	30:0:1805:G:N2	2.88	0.42
2:B:5:ARG:NH1	30:0:2547:C:OP2	2.53	0.42
2:B:18:ARG:HG3	2:B:256:GLN:HG3	2.01	0.42
3:C:111:VAL:HB	38:C:8522:HOH:O	2.20	0.42
8:H:12:ILE:HD12	8:H:57:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2461:U:O2	30:0:2466:G:H1'	2.19	0.42
30:0:912:A:C4	30:0:1294:A:C2	3.07	0.42
30:0:634:G:O2'	30:0:1358:A:OP1	2.35	0.42
30:0:2758:G:H2'	30:0:2759:C:C6	2.55	0.42
30:0:2553:A:H2'	30:0:2553:A:N3	2.34	0.42
18:R:9:ASP:HA	18:R:10:PRO:HD2	1.90	0.41
30:0:12:U:C2'	30:0:13:G:H5'	2.49	0.41
30:0:1942:A:C4'	38:0:9046:HOH:O	2.67	0.41
30:0:1845:A:O2'	30:0:1846:U:H5'	2.19	0.41
22:V:44:GLY:O	22:V:48:GLU:HG2	2.20	0.41
4:D:131:THR:HG21	30:0:2348:C:H1'	2.01	0.41
27:1:45:ARG:HB3	38:1:8967:HOH:O	2.20	0.41
23:W:11:VAL:O	23:W:12:ASN:HB2	2.20	0.41
6:F:38:LYS:HE3	30:0:244:C:OP2	2.20	0.41
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.43	0.41
30:0:2290:U:H2'	38:0:7148:HOH:O	2.19	0.41
31:9:5:G:C2'	31:9:6:C:H5'	2.49	0.41
23:W:125:HIS:CE1	30:0:1097:A:H5''	2.56	0.41
22:V:1:THR:HG23	22:V:2:VAL:HG23	2.02	0.41
29:3:70:ARG:HD3	38:3:9059:HOH:O	2.19	0.41
30:0:1598:A:N6	35:0:8815:CL:CL	2.90	0.41
30:0:488:U:C2'	38:0:4019:HOH:O	2.67	0.41
3:C:39:GLN:O	3:C:43:LYS:HD3	2.19	0.41
30:0:297:U:H2'	30:0:298:C:H6	1.83	0.41
24:X:34:ARG:NH1	24:X:48:VAL:O	2.51	0.41
30:0:351:A:O2'	30:0:352:A:H5'	2.20	0.41
4:D:151:ILE:HA	4:D:152:PRO:HD3	1.92	0.41
30:0:1636:G:O2'	30:0:1637:A:H5'	2.20	0.41
13:M:65:VAL:HG21	13:M:105:ALA:HB2	2.02	0.41
26:Z:63:CYS:HA	26:Z:64:PRO:HD3	1.91	0.41
4:D:76:ARG:NH1	31:9:42:C:O2	2.50	0.41
31:9:49:G:C2'	31:9:50:G:H5'	2.50	0.41
30:0:2090:G:H2'	30:0:2091:G:C8	2.55	0.41
30:0:941:G:C6	30:0:942:U:C4	3.08	0.41
24:X:22:ASN:HA	24:X:25:ARG:HG3	2.02	0.41
10:J:88:PRO:HD3	30:0:1104:C:H4'	2.01	0.41
30:0:383:A:H2'	30:0:384:G:O4'	2.19	0.41
30:0:2088:C:H1'	30:0:2841:A:N1	2.35	0.41
30:0:1375:A:C2'	30:0:1376:G:H5'	2.50	0.41
24:X:72:VAL:HG22	24:X:85:VAL:HG12	2.03	0.41
23:W:3:ALA:O	23:W:54:PHE:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:59:GLY:HA3	13:M:141:ILE:HD12	2.02	0.41
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.33	0.41
30:0:1625:U:H3'	30:0:1625:U:C6	2.54	0.41
30:0:1706:G:C6	30:0:1707:G:C6	3.09	0.41
1:A:167:LYS:HB2	26:Z:53:ILE:HD13	2.02	0.41
1:A:214:SER:HB2	38:0:4377:HOH:O	2.20	0.41
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.20	0.41
20:T:3:GLN:HA	20:T:4:PRO:HD3	1.85	0.41
30:0:1184:C:O2'	30:0:1185:U:OP2	2.35	0.41
30:0:69:A:H2'	30:0:70:A:OP2	2.20	0.41
30:0:2635:A:C2'	30:0:2636:C:H5'	2.50	0.41
12:L:114:VAL:HG11	38:L:8874:HOH:O	2.20	0.41
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.50	0.41
30:0:920:C:H4'	30:0:921:G:N2	2.35	0.41
29:3:28:GLY:HA3	30:0:2435:U:OP1	2.20	0.41
11:K:37:TYR:HB3	38:K:7169:HOH:O	2.20	0.41
23:W:43:GLY:HA3	30:0:945:U:O2'	2.20	0.41
30:0:423:A:C4	30:0:424:C:C6	3.09	0.41
30:0:2274:A:O2'	30:0:2275:G:H5'	2.20	0.41
15:O:21:SER:OG	15:O:106:PRO:HB2	2.20	0.41
30:0:1069:C:H2'	30:0:1070:A:O4'	2.21	0.41
30:0:2385:G:H2'	30:0:2386:U:C6	2.56	0.41
30:0:724:G:O2'	30:0:725:C:H5'	2.21	0.41
27:1:12:ASN:O	30:0:1415:G:H5'	2.20	0.41
30:0:2505:G:H2'	30:0:2506:A:C5'	2.48	0.41
30:0:2506:A:O2'	30:0:2507:G:P	2.79	0.41
30:0:1193:A:H2	30:0:1194:A:N6	2.16	0.41
10:J:19:MET:CE	10:J:132:LEU:HD11	2.51	0.41
30:0:1787:C:O2'	30:0:1788:U:H5'	2.20	0.41
30:0:1594:C:O2'	30:0:1607:A:H4'	2.20	0.41
30:0:307:G:H3'	38:0:6693:HOH:O	2.21	0.41
30:0:1483:C:O2'	30:0:1484:G:H5'	2.21	0.41
3:C:107:ARG:O	3:C:111:VAL:HG23	2.21	0.41
1:A:1:GLY:HA2	1:A:197:VAL:HG23	2.03	0.41
30:0:2777:G:O2'	30:0:2778:A:H5'	2.20	0.41
30:0:1413:A:H2'	30:0:1414:A:O4'	2.20	0.41
1:A:173:GLY:O	1:A:176:HIS:HB3	2.19	0.41
30:0:2281:C:C2'	30:0:2282:U:H5'	2.50	0.41
30:0:2032:U:H2'	30:0:2033:G:H5'	2.03	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.85	0.41
30:0:309:C:O2	30:0:309:C:H2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:736:A:H8	38:0:7219:HOH:O	2.03	0.41
30:0:1926:G:H2'	30:0:1927:A:H8	1.86	0.41
30:0:571:C:H6	30:0:571:C:O5'	2.04	0.41
3:C:101:ASP:HB2	30:0:750:A:O3'	2.21	0.41
30:0:2903:C:O2'	30:0:2904:U:H5'	2.21	0.41
30:0:1381:A:N3	30:0:1382:G:H1'	2.36	0.41
4:D:128:LEU:N	38:D:6007:HOH:O	2.53	0.41
30:0:459:A:H4'	38:0:9460:HOH:O	2.20	0.41
2:B:233:ARG:NH1	2:B:233:ARG:HG2	2.35	0.41
30:0:1926:G:H2'	30:0:1927:A:C8	2.55	0.41
9:I:101:LYS:O	9:I:105:GLU:HG3	2.20	0.41
30:0:764:C:H2'	30:0:765:G:O4'	2.20	0.41
30:0:1829:A:H2'	30:0:1830:C:H5'	2.03	0.41
30:0:962:C:H2'	30:0:963:C:H5'	2.03	0.41
30:0:1159:G:H2'	30:0:1160:G:O4'	2.21	0.41
30:0:1634:G:H2'	30:0:1635:U:C6	2.56	0.41
30:0:2506:A:O2'	30:0:2507:G:O5'	2.39	0.41
30:0:653:U:H2'	30:0:654:A:C8	2.55	0.41
29:3:38:ARG:NH1	30:0:396:U:C2	2.89	0.41
23:W:119:HIS:CG	38:0:5297:HOH:O	2.74	0.41
30:0:2316:G:H8	38:0:5663:HOH:O	2.03	0.41
27:1:28:HIS:O	27:1:32:LYS:N	2.48	0.41
5:E:7:ILE:HG13	5:E:11:VAL:HB	2.03	0.41
30:0:2354:A:C2	30:0:2367:A:C8	3.09	0.41
30:0:535:G:O6	30:0:2064:U:C6	2.74	0.41
5:E:68:HIS:CE1	38:E:5919:HOH:O	2.74	0.41
16:P:59:ARG:O	16:P:63:ARG:HG3	2.21	0.41
30:0:1626:A:H2'	30:0:1627:G:O4'	2.21	0.41
30:0:1625:U:C3'	30:0:1625:U:C6	3.04	0.41
30:0:1298:U:H2'	30:0:1299:G:C8	2.56	0.41
12:L:6:ARG:NH1	30:0:1299:G:N7	2.69	0.41
30:0:2314:G:H2'	30:0:2315:C:H5'	2.03	0.41
2:B:242:TRP:CZ2	30:0:2607:U:C4	3.08	0.41
30:0:243:A:H61	30:0:269:G:C1'	2.34	0.41
30:0:1520:G:C6	30:0:1521:C:C4	3.08	0.41
5:E:125:GLU:HB2	5:E:132:THR:HG23	2.03	0.41
2:B:60:SER:HA	2:B:61:PRO:HD3	1.87	0.41
14:N:82:TYR:CD2	14:N:82:TYR:C	2.93	0.41
22:V:5:VAL:HG23	38:V:2271:HOH:O	2.20	0.41
2:B:101:TRP:HB2	2:B:119:HIS:CD2	2.56	0.41
31:9:61:C:H2'	31:9:62:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:506:G:N1	30:0:509:A:OP2	2.54	0.41
30:0:2765:C:H2'	30:0:2766:A:C8	2.56	0.41
30:0:1903:U:O2'	30:0:1904:A:C8	2.72	0.41
30:0:694:A:C2'	30:0:695:C:H5'	2.51	0.41
18:R:18:LEU:HG	18:R:91:LEU:HD13	2.03	0.41
30:0:2754:G:O2'	30:0:2755:G:H5'	2.20	0.41
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.90	0.41
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.56	0.41
30:0:963:C:O2	30:0:1005:A:N1	2.54	0.41
30:0:491:C:O2'	30:0:492:C:H5'	2.21	0.41
2:B:225:GLY:HA3	38:B:9027:HOH:O	2.21	0.41
30:0:1871:U:O4'	30:0:1873:G:C8	2.74	0.41
30:0:1795:G:H2'	30:0:1796:A:O4'	2.21	0.41
30:0:615:G:H2'	30:0:616:U:C6	2.56	0.41
20:T:106:GLU:HG3	38:T:4913:HOH:O	2.21	0.41
30:0:1205:U:H2'	30:0:1206:U:H5'	1.94	0.40
30:0:1116:U:C2	30:0:1246:A:N6	2.89	0.40
30:0:2491:G:C1'	38:0:6878:HOH:O	2.58	0.40
9:I:112:LEU:HG	30:0:1162:G:O2'	2.21	0.40
22:V:39:ALA:N	22:V:40:PRO:CD	2.84	0.40
30:0:2112:A:H2'	30:0:2113:G:H8	1.85	0.40
30:0:304:G:H1'	30:0:347:A:H61	1.86	0.40
30:0:106:A:H2'	30:0:107:U:O4'	2.21	0.40
1:A:109:GLU:HG2	1:A:116:GLY:H	1.85	0.40
30:0:1375:A:H2'	30:0:1376:G:H5'	2.04	0.40
23:W:130:HIS:NE2	31:9:88:G:OP1	2.50	0.40
23:W:130:HIS:O	23:W:136:GLY:HA3	2.21	0.40
30:0:626:U:C4	30:0:627:G:C6	3.09	0.40
30:0:1555:G:H4'	30:0:1630:A:H2	1.86	0.40
3:C:131:PHE:CD2	3:C:131:PHE:N	2.89	0.40
8:H:157:TYR:CD1	8:H:157:TYR:C	2.94	0.40
15:O:38:ARG:NH1	38:O:7674:HOH:O	2.53	0.40
20:T:9:LYS:HE2	20:T:13:ARG:HH12	1.84	0.40
30:0:2564:G:OP2	30:0:2565:C:H5''	2.21	0.40
1:A:38:ILE:HA	1:A:38:ILE:HD13	1.88	0.40
1:A:88:ILE:HG22	1:A:88:ILE:O	2.21	0.40
30:0:1992:U:H2'	30:0:1994:A:OP2	2.20	0.40
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.83	0.40
30:0:423:A:H2'	30:0:424:C:H6	1.87	0.40
30:0:499:G:O2'	30:0:500:G:H5'	2.21	0.40
14:N:170:GLU:O	14:N:174:GLU:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.21	0.40
30:0:2614:C:O2'	30:0:2615:U:H5'	2.21	0.40
30:0:1947:G:H2'	30:0:1948:G:C8	2.56	0.40
30:0:821:U:H2'	30:0:822:C:C6	2.57	0.40
30:0:553:G:O4'	30:0:1325:G:H5'	2.22	0.40
30:0:1761:U:H2'	30:0:1762:C:C6	2.55	0.40
30:0:570:C:H6	30:0:570:C:O5'	2.04	0.40
27:1:21:ARG:HD2	27:1:39:PHE:HB2	2.04	0.40
25:Y:145:LYS:O	25:Y:147:ARG:HG2	2.21	0.40
3:C:193:LEU:HD12	3:C:211:ASP:O	2.21	0.40
3:C:102:LEU:HD12	3:C:102:LEU:HA	1.91	0.40
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.21	0.40
30:0:138:U:OP2	30:0:139:C:C5	2.70	0.40
30:0:2032:U:H2'	30:0:2033:G:H5''	2.03	0.40
4:D:22:VAL:HA	4:D:73:VAL:O	2.21	0.40
9:I:130:LEU:HA	38:I:6825:HOH:O	2.22	0.40
30:0:2135:A:O4'	30:0:2243:C:N4	2.54	0.40
30:0:1014:A:H5''	31:9:101:G:O2'	2.22	0.40
5:E:68:HIS:O	5:E:72:MET:HG3	2.22	0.40
18:R:18:LEU:HD12	18:R:143:VAL:HG11	2.03	0.40
4:D:23:VAL:HG12	4:D:130:VAL:HG22	2.03	0.40
18:R:114:VAL:HG13	18:R:114:VAL:O	2.22	0.40
25:Y:148:GLY:HA3	30:0:622:G:P	2.62	0.40
30:0:1311:G:C2	30:0:1312:G:C8	3.09	0.40
30:0:939:A:N1	30:0:1027:G:O2'	2.50	0.40
2:B:229:ARG:HD2	38:0:9111:HOH:O	2.20	0.40
30:0:503:G:H2'	30:0:504:G:H8	1.87	0.40
12:L:145:LEU:O	12:L:148:GLU:HG3	2.21	0.40
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.22	0.40
26:Z:45:VAL:HG12	38:Z:8713:HOH:O	2.21	0.40
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.85	0.40
30:0:2509:A:C2	30:0:2510:C:H1'	2.56	0.40
2:B:267:LYS:HD3	38:0:9565:HOH:O	2.22	0.40
30:0:1773:G:N2	30:0:1774:G:C8	2.90	0.40
30:0:812:A:H2'	30:0:813:C:O4'	2.21	0.40
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.86	0.40
30:0:695:C:H2'	30:0:696:C:C6	2.57	0.40
13:M:188:ARG:HH11	30:0:154:C:H3'	1.86	0.40
16:P:94:TRP:CZ2	16:P:98:ILE:HG13	2.57	0.40
30:0:214:U:H5'	38:0:6146:HOH:O	2.22	0.40
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2897:C:O2'	30:0:2898:G:H5'	2.22	0.40
30:0:1236:A:H2'	30:0:1237:U:O4'	2.22	0.40
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.85	0.40
30:0:2734:G:O2'	30:0:2735:U:H5'	2.22	0.40
27:1:53:LYS:HA	27:1:53:LYS:HD3	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	211 (90%)	18 (8%)	6 (3%)	7	26
2	B	335/338 (99%)	306 (91%)	25 (8%)	4 (1%)	16	48
3	C	244/246 (99%)	224 (92%)	19 (8%)	1 (0%)	39	74
4	D	134/177 (76%)	113 (84%)	16 (12%)	5 (4%)	4	17
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
6	F	117/120 (98%)	106 (91%)	8 (7%)	3 (3%)	7	26
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	147 (94%)	8 (5%)	1 (1%)	30	67
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	13	42
10	J	140/145 (97%)	130 (93%)	9 (6%)	1 (1%)	26	63
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	24	60
12	L	141/165 (86%)	125 (89%)	14 (10%)	2 (1%)	14	44
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	34	71
14	N	184/187 (98%)	169 (92%)	12 (6%)	3 (2%)	12	40
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	141 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	110 (94%)	7 (6%)	0	100	100
21	U	51/67 (76%)	45 (88%)	5 (10%)	1 (2%)	9	33
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	12	40
23	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	15	46
24	X	80/92 (87%)	75 (94%)	4 (5%)	1 (1%)	15	46
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
26	Z	71/116 (61%)	62 (87%)	7 (10%)	2 (3%)	6	24
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
All	All	3705/4472 (83%)	3447 (93%)	222 (6%)	36 (1%)	19	54

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
6	F	101	ALA
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
1	A	27	LEU
8	H	19	ARG
1	A	34	ASP
10	J	65	ASN
23	W	49	ASN
23	W	77	ALA
26	Z	44	ARG
1	A	36	ASP
2	B	2	GLN
2	B	185	GLY
4	D	65	GLU
11	K	127	ALA
12	L	149	ARG

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Mol	Chain	Res	Type
13	M	71	SER
24	X	70	ILE
26	Z	65	ASN
2	B	184	ASP
4	D	56	ARG
6	F	100	ASP
12	L	82	ALA
21	U	55	ALA
22	V	43	PRO
1	A	69	LEU
3	C	201	SER
4	D	27	ILE
4	D	97	GLN
9	I	83	GLY
1	A	88	ILE
2	B	169	GLY
6	F	27	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%)	170 (95%)	9 (5%)	30	65
2	B	282/283 (100%)	263 (93%)	19 (7%)	20	50
3	C	193/193 (100%)	176 (91%)	17 (9%)	12	35
4	D	117/148 (79%)	110 (94%)	7 (6%)	24	57
5	E	152/156 (97%)	149 (98%)	3 (2%)	63	88
6	F	93/94 (99%)	91 (98%)	2 (2%)	60	88
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	129 (96%)	5 (4%)	41	77
9	I	58/130 (45%)	57 (98%)	1 (2%)	68	91
10	J	118/121 (98%)	110 (93%)	8 (7%)	20	49
11	K	106/106 (100%)	104 (98%)	2 (2%)	65	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	113/127 (89%)	110 (97%)	3 (3%)	52	84
13	M	158/160 (99%)	151 (96%)	7 (4%)	35	70
14	N	149/150 (99%)	142 (95%)	7 (5%)	32	68
15	O	93/94 (99%)	92 (99%)	1 (1%)	80	95
16	P	113/117 (97%)	111 (98%)	2 (2%)	66	90
17	Q	79/80 (99%)	76 (96%)	3 (4%)	40	76
18	R	117/122 (96%)	111 (95%)	6 (5%)	29	65
19	S	71/74 (96%)	70 (99%)	1 (1%)	74	93
20	T	105/106 (99%)	97 (92%)	8 (8%)	16	43
21	U	44/53 (83%)	43 (98%)	1 (2%)	58	87
22	V	51/57 (90%)	50 (98%)	1 (2%)	63	88
23	W	130/130 (100%)	126 (97%)	4 (3%)	47	82
24	X	66/74 (89%)	62 (94%)	4 (6%)	23	56
25	Y	120/196 (61%)	116 (97%)	4 (3%)	45	80
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	57	86
29	3	79/79 (100%)	78 (99%)	1 (1%)	76	94
All	All	3095/3646 (85%)	2968 (96%)	127 (4%)	37	73

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	36	ASP
1	A	37	VAL
1	A	38	ILE
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	16	ARG
2	B	27	ASN

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Mol	Chain	Res	Type
2	B	49	THR
2	B	71	VAL
2	B	97	LEU
2	B	98	THR
2	B	103	ASP
2	B	108	GLU
2	B	132	HIS
2	B	190	MET
2	B	192	ASP
2	B	234	ARG
2	B	248	ARG
2	B	251	VAL
2	B	254	GLN
2	B	264	GLU
2	B	277	GLU
3	C	27	ARG
3	C	78	ARG
3	C	94	THR
3	C	131	PHE
3	C	136	VAL
3	C	151	GLN
3	C	162	VAL
3	C	187	ARG
3	C	202	THR
3	C	211	ASP
3	C	214	THR
3	C	222	ASP
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	237	GLU
3	C	243	VAL
4	D	24	HIS
4	D	36	ASN
4	D	50	VAL
4	D	137	PRO
4	D	149	ARG
4	D	161	ASP
4	D	170	TYR
5	E	7	ILE
5	E	102	VAL
5	E	156	ASP

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Mol	Chain	Res	Type
6	F	12	LEU
6	F	46	GLU
8	H	62	HIS
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
9	I	114	TYR
10	J	45	VAL
10	J	46	ILE
10	J	52	GLN
10	J	74	ARG
10	J	76	ASP
10	J	79	PHE
10	J	107	ASN
10	J	112	ASP
11	K	10	GLN
11	K	119	GLN
12	L	35	ARG
12	L	80	ASP
12	L	104	ASP
13	M	10	ASP
13	M	46	LEU
13	M	68	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
13	M	164	THR
14	N	17	ARG
14	N	26	LEU
14	N	49	THR
14	N	127	LEU
14	N	134	ASP
14	N	135	VAL
14	N	147	ILE
15	O	38	ARG
16	P	21	VAL
16	P	98	ILE
17	Q	11	ARG
17	Q	57	ASP
17	Q	95	GLU
18	R	13	THR

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Mol	Chain	Res	Type
18	R	39	THR
18	R	82	GLU
18	R	119	VAL
18	R	132	ARG
18	R	143	VAL
19	S	10	VAL
20	T	26	THR
20	T	39	ASN
20	T	48	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	22	ASP
23	W	38	THR
23	W	52	VAL
23	W	88	THR
23	W	146	ILE
24	X	27	ASP
24	X	46	ASP
24	X	79	GLU
24	X	82	GLU
25	Y	95	THR
25	Y	154	ARG
25	Y	189	ASN
25	Y	203	VAL
28	2	18	ASN
29	3	3	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS
2	B	2	GLN
2	B	27	ASN
2	B	145	HIS
2	B	238	ASN
2	B	256	GLN
2	B	260	HIS

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Mol	Chain	Res	Type
2	B	320	GLN
3	C	2	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
4	D	103	ASN
5	E	119	HIS
5	E	143	GLN
5	E	150	GLN
7	G	17	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
10	J	142	ASN
11	K	10	GLN
11	K	42	ASN
11	K	44	HIS
11	K	67	GLN
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	58	GLN
13	M	77	HIS
13	M	137	ASN
13	M	170	ASN
14	N	93	GLN
14	N	107	ASN
14	N	132	ASN
16	P	50	GLN
16	P	66	GLN
16	P	118	GLN
17	Q	27	GLN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS

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Mol	Chain	Res	Type
19	S	44	GLN
19	S	53	ASN
20	T	39	ASN
21	U	39	ASN
22	V	4	HIS
22	V	60	GLN
23	W	2	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	23	HIS
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
26	Z	61	HIS
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
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%)	242 (8%)	27 (0%)
31	9	121/122 (99%)	15 (12%)	1 (0%)
All	All	2866/3045 (94%)	257 (8%)	28 (0%)

All (257) 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

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Mol	Chain	Res	Type
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	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	186	A
30	0	187	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

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Mol	Chain	Res	Type
30	0	553	G
30	0	559	U
30	0	588	G
30	0	604	G
30	0	605	C
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	698	A
30	0	701	U
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	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

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Mol	Chain	Res	Type
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
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	1331	G
30	0	1342	C
30	0	1353	C
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1409	G
30	0	1474	C
30	0	1488	U
30	0	1505	U
30	0	1506	U
30	0	1524	U
30	0	1525	G
30	0	1526	A
30	0	1562	C

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Mol	Chain	Res	Type
30	0	1592	G
30	0	1617	C
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1731	C
30	0	1732	A
30	0	1752	G
30	0	1778	A
30	0	1779	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1968	A
30	0	1971	G
30	0	1973	A
30	0	1978	A
30	0	1979	G
30	0	1980	U
30	0	1996	U
30	0	2004	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G
30	0	2033	G

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Mol	Chain	Res	Type
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	2110	G
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2317	C
30	0	2321	A
30	0	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	2469	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2513	A
30	0	2526	C
30	0	2527	U
30	0	2533	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C

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Mol	Chain	Res	Type
30	0	2613	G
30	0	2637	A
30	0	2638	G
30	0	2645	U
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2718	C
30	0	2719	A
30	0	2726	U
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	40	C
31	9	41	C
31	9	43	G
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 (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	604	G
30	0	644	G
30	0	681	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1080	C
30	0	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	1692	C
30	0	1979	G
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2649	A
30	0	2718	C
30	0	2726	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	1.01	1 (8%)	19,31,34	3.13	2 (10%)
30	OMG	0	2588	30	17,26,27	1.03	1 (5%)	21,38,41	2.51	3 (14%)
30	UR3	0	2619	30	12,22,23	0.76	0	16,32,35	0.75	0
30	PSU	0	2621	30	13,21,22	1.80	2 (15%)	18,30,33	6.12	4 (22%)
30	1MA	0	628	30	14,25,26	1.00	1 (7%)	15,37,40	1.09	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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.55	1.47	1.52
30	0	2587	OMU	C4-N3	2.43	1.37	1.33
30	0	2621	PSU	C4-N3	2.59	1.37	1.33
30	0	628	1MA	C6-N6	2.64	1.33	1.29
30	0	2588	OMG	C6-N1	3.14	1.38	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-21.50	114.61	128.33
30	0	2588	OMG	C5-C6-N1	-8.65	111.77	123.59
30	0	628	1MA	C2-N3-C4	-3.64	110.76	116.40
30	0	2587	OMU	C5-C4-N3	-3.28	114.70	123.12
30	0	2588	OMG	N3-C2-N1	-2.28	123.97	127.44
30	0	2621	PSU	C5-C1'-C2'	-2.21	111.59	115.52
30	0	2621	PSU	C6-N1-C2	2.69	119.79	115.47
30	0	2588	OMG	C6-N1-C2	6.60	125.11	115.94
30	0	2587	OMU	C4-N3-C2	13.01	127.03	114.14
30	0	2621	PSU	C4-N3-C2	13.70	127.09	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	3	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.39	5 (2%) 67 62	35, 59, 97, 117	0
2	B	337/338 (99%)	-0.59	1 (0%) 94 94	36, 60, 90, 100	0
3	C	246/246 (100%)	-0.57	0 100 100	30, 51, 75, 89	0
4	D	140/177 (79%)	1.10	31 (22%) 1 0	73, 108, 135, 146	0
5	E	172/178 (96%)	-0.51	1 (0%) 90 89	51, 74, 96, 104	0
6	F	119/120 (99%)	0.14	5 (4%) 40 33	55, 78, 111, 125	0
7	G	29/348 (8%)	0.50	1 (3%) 49 41	83, 103, 109, 112	0
8	H	160/177 (90%)	0.04	9 (5%) 28 21	50, 73, 106, 113	0
9	I	70/162 (43%)	3.19	47 (67%) 0 0	137, 156, 173, 174	0
10	J	142/145 (97%)	-0.56	1 (0%) 89 88	41, 58, 78, 97	0
11	K	132/132 (100%)	-0.71	0 100 100	40, 55, 79, 82	0
12	L	145/165 (87%)	0.08	7 (4%) 34 28	34, 73, 123, 136	0
13	M	194/196 (98%)	-0.70	0 100 100	35, 50, 66, 73	0
14	N	186/187 (99%)	-0.07	5 (2%) 58 52	52, 75, 123, 135	0
15	O	115/116 (99%)	-0.60	0 100 100	45, 61, 78, 84	0
16	P	143/149 (95%)	-0.63	0 100 100	46, 61, 77, 84	0
17	Q	95/96 (98%)	-0.60	0 100 100	44, 55, 71, 86	0
18	R	150/155 (96%)	-0.72	0 100 100	39, 52, 71, 86	0
19	S	81/85 (95%)	-0.50	1 (1%) 81 78	49, 65, 86, 98	0
20	T	119/120 (99%)	-0.34	5 (4%) 40 33	47, 62, 89, 123	0
21	U	53/67 (79%)	-0.62	0 100 100	48, 62, 79, 88	0
22	V	65/71 (91%)	0.71	8 (12%) 5 3	55, 80, 129, 134	0
23	W	154/154 (100%)	-0.52	1 (0%) 90 89	41, 57, 74, 88	0
24	X	82/92 (89%)	-0.18	4 (4%) 33 27	49, 67, 90, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.75	1 (0%) 89 88	31, 50, 73, 94	0
26	Z	73/116 (62%)	0.75	12 (16%) 2 1	63, 87, 101, 106	0
27	1	56/57 (98%)	-0.65	0 100 100	32, 39, 45, 53	0
28	2	46/50 (92%)	-0.11	3 (6%) 22 16	41, 69, 104, 115	0
29	3	92/92 (100%)	-0.37	0 100 100	44, 68, 81, 91	0
30	0	2749/2923 (94%)	-0.60	5 (0%) 95 95	28, 53, 96, 172	0
31	9	122/122 (100%)	-0.77	1 (0%) 87 86	45, 74, 96, 153	0
All	All	6646/7517 (88%)	-0.42	154 (2%) 64 59	28, 58, 108, 174	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	74	ILE	10.2
22	V	39	ALA	8.0
22	V	1	THR	7.8
26	Z	46	SER	7.7
4	D	63	ILE	7.6
9	I	70	THR	7.5
9	I	66	GLY	7.5
9	I	72	GLU	7.4
9	I	71	ALA	7.4
22	V	43	PRO	7.1
9	I	104	ALA	6.7
9	I	106	GLN	6.6
14	N	166	ALA	6.4
4	D	57	THR	6.0
9	I	100	VAL	5.9
22	V	40	PRO	5.9
9	I	80	PHE	5.5
26	Z	58	ASN	5.3
9	I	79	GLY	5.3
9	I	128	THR	5.2
4	D	85	GLN	5.1
9	I	108	HIS	5.0
4	D	134	LEU	4.9
26	Z	35	SER	4.9
9	I	132	VAL	4.9
9	I	113	SER	4.9
9	I	109	PRO	4.8
9	I	102	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
9	I	112	LEU	4.7
20	T	118	SER	4.6
26	Z	44	ARG	4.6
1	A	237	GLY	4.5
9	I	93	ALA	4.4
4	D	18	ILE	4.3
9	I	105	GLU	4.3
9	I	99	GLN	4.3
26	Z	45	VAL	4.3
4	D	90	LEU	4.2
9	I	76	ASP	4.1
9	I	69	PRO	4.0
19	S	81	ILE	3.9
14	N	155	GLU	3.9
9	I	97	VAL	3.9
9	I	83	GLY	3.8
9	I	92	VAL	3.8
9	I	110	ASP	3.8
9	I	86	GLU	3.8
20	T	116	ASP	3.8
26	Z	60	ASP	3.8
6	F	106	ALA	3.8
9	I	88	GLN	3.7
4	D	88	LEU	3.7
30	0	735	C	3.7
8	H	40	GLN	3.5
9	I	111	LEU	3.5
9	I	78	ALA	3.5
12	L	60	GLU	3.4
26	Z	50	VAL	3.4
9	I	82	THR	3.4
24	X	71	ARG	3.4
9	I	81	GLU	3.3
22	V	38	GLY	3.3
9	I	103	ILE	3.3
4	D	84	LEU	3.3
9	I	98	ASP	3.3
20	T	119	ALA	3.3
4	D	91	ALA	3.2
9	I	75	LYS	3.2
12	L	81	VAL	3.2
4	D	102	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
12	L	75	LEU	3.2
4	D	64	ARG	3.1
22	V	41	GLU	3.1
8	H	86	TYR	3.0
4	D	69	ILE	3.0
26	Z	69	ASP	3.0
28	2	49	GLU	3.0
25	Y	235	GLU	3.0
8	H	133	GLY	3.0
4	D	81	GLU	3.0
4	D	44	ILE	2.9
4	D	75	LEU	2.9
26	Z	49	ARG	2.9
4	D	92	GLU	2.9
4	D	17	ARG	2.9
4	D	93	LEU	2.8
22	V	37	GLY	2.8
31	9	1	U	2.8
4	D	45	THR	2.7
1	A	37	VAL	2.7
7	G	27	ILE	2.7
9	I	67	VAL	2.7
8	H	149	VAL	2.7
1	A	91	GLY	2.7
30	0	282	C	2.6
12	L	80	ASP	2.6
9	I	116	LEU	2.6
4	D	135	VAL	2.6
20	T	115	GLU	2.6
4	D	165	PHE	2.5
30	0	1198	U	2.5
9	I	84	SER	2.4
6	F	75	ILE	2.4
6	F	99	THR	2.4
9	I	94	ASP	2.4
4	D	157	LEU	2.4
4	D	89	PRO	2.4
6	F	17	LEU	2.4
30	0	1199	A	2.4
9	I	114	TYR	2.4
4	D	10	PHE	2.3
26	Z	42	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	99	ILE	2.3
4	D	172	VAL	2.3
9	I	118	ASN	2.3
9	I	73	LEU	2.3
20	T	117	ASP	2.3
4	D	166	ILE	2.3
9	I	91	PHE	2.3
9	I	127	CYS	2.3
4	D	130	VAL	2.3
14	N	138	ASP	2.3
30	0	1172	G	2.3
4	D	171	ASP	2.2
6	F	16	ALA	2.2
26	Z	68	GLU	2.2
8	H	37	GLY	2.2
28	2	39	ARG	2.2
10	J	70	PHE	2.2
2	B	105	PHE	2.2
22	V	2	VAL	2.2
28	2	35	ARG	2.2
24	X	85	VAL	2.2
23	W	96	LEU	2.2
26	Z	55	SER	2.2
8	H	39	LYS	2.2
8	H	76	LEU	2.2
8	H	158	ASN	2.1
14	N	185	GLU	2.1
1	A	103	VAL	2.1
12	L	76	LEU	2.1
24	X	7	GLU	2.1
8	H	35	LYS	2.1
4	D	56	ARG	2.1
9	I	125	GLY	2.1
9	I	133	THR	2.1
14	N	147	ILE	2.1
12	L	106	VAL	2.1
12	L	100	ALA	2.0
24	X	80	GLU	2.0
5	E	170	ARG	2.0
4	D	73	VAL	2.0
4	D	43	GLU	2.0
9	I	68	PRO	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	OMU	0	2587	21/22	0.99	0.13	-	40,43,46,49	0
30	1MA	0	628	23/24	0.99	0.15	-	35,38,38,39	0
30	OMG	0	2588	24/25	0.98	0.12	-	38,42,43,43	0
30	PSU	0	2621	20/21	0.99	0.14	-	35,38,47,48	0
30	UR3	0	2619	21/22	0.98	0.14	-	43,45,48,49	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	8565	1/1	0.94	0.93	67.70	68,68,68,68	0
34	NA	0	8562	1/1	0.55	0.80	63.04	74,74,74,74	0
34	NA	0	8564	1/1	0.96	0.42	34.64	81,81,81,81	0
34	NA	0	8547	1/1	0.93	0.60	26.69	54,54,54,54	0
34	NA	0	8522	1/1	0.54	0.39	21.22	83,83,83,83	0
34	NA	0	8568	1/1	0.97	0.50	18.72	50,50,50,50	0
34	NA	0	8512	1/1	0.99	0.42	15.04	56,56,56,56	0
34	NA	0	8542	1/1	0.96	0.39	14.61	66,66,66,66	0
34	NA	0	8555	1/1	0.64	0.49	14.54	51,51,51,51	0
34	NA	0	8553	1/1	0.99	0.36	13.94	68,68,68,68	0
34	NA	9	8572	1/1	0.72	0.34	13.34	111,111,111,111	0
36	SR	B	8987	1/1	0.67	0.49	13.33	200,200,200,200	0
34	NA	0	8563	1/1	0.71	0.36	11.31	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8528	1/1	0.85	0.29	10.62	58,58,58,58	0
36	SR	0	8903	1/1	0.99	0.18	8.43	58,58,58,58	0
34	NA	0	8530	1/1	0.91	0.28	6.97	55,55,55,55	0
34	NA	0	8556	1/1	0.96	0.40	6.75	49,49,49,49	0
34	NA	0	8517	1/1	0.99	0.20	6.69	36,36,36,36	0
34	NA	0	8552	1/1	1.00	0.29	6.17	72,72,72,72	0
32	MG	0	8047	1/1	0.99	0.28	5.86	65,65,65,65	0
34	NA	0	8527	1/1	0.87	0.23	5.38	71,71,71,71	0
36	SR	0	8947	1/1	0.82	0.27	5.32	200,200,200,200	0
34	NA	0	8508	1/1	0.98	0.18	5.08	39,39,39,39	0
34	NA	0	8559	1/1	0.90	0.14	4.95	76,76,76,76	0
32	MG	A	8051	1/1	0.88	0.41	4.92	72,72,72,72	0
32	MG	0	8041	1/1	0.98	0.20	4.74	31,31,31,31	0
33	K	0	8402	1/1	0.97	0.27	4.36	87,87,87,87	0
32	MG	0	8008	1/1	0.99	0.15	3.89	27,27,27,27	0
34	NA	0	8534	1/1	0.96	0.23	3.66	42,42,42,42	0
32	MG	0	8084	1/1	0.99	0.15	3.05	37,37,37,37	0
36	SR	0	8904	1/1	0.99	0.19	2.90	66,66,66,66	0
32	MG	0	8009	1/1	0.99	0.20	2.80	29,29,29,29	0
34	NA	0	8569	1/1	0.96	0.20	2.10	54,54,54,54	0
34	NA	0	8507	1/1	0.95	0.16	2.09	42,42,42,42	0
32	MG	0	8014	1/1	0.99	0.15	1.96	35,35,35,35	0
36	SR	0	8918	1/1	0.98	0.14	1.90	85,85,85,85	0
32	MG	0	8003	1/1	1.00	0.18	1.86	34,34,34,34	0
32	MG	0	8067	1/1	0.97	0.20	1.76	34,34,34,34	0
32	MG	0	8028	1/1	0.99	0.16	1.58	27,27,27,27	0
32	MG	0	8016	1/1	0.98	0.18	1.35	60,60,60,60	0
34	NA	0	8575	1/1	0.97	0.18	1.31	86,86,86,86	0
32	MG	0	8006	1/1	0.94	0.14	1.30	30,30,30,30	0
36	SR	A	8929	1/1	0.95	0.16	1.25	137,137,137,137	0
36	SR	0	8992	1/1	0.95	0.15	1.21	137,137,137,137	0
32	MG	0	8045	1/1	0.99	0.11	1.08	35,35,35,35	0
36	SR	R	8912	1/1	0.99	0.16	1.03	86,86,86,86	0
32	MG	0	8004	1/1	1.00	0.17	0.89	30,30,30,30	0
34	NA	0	8557	1/1	0.87	0.10	0.82	52,52,52,52	0
34	NA	0	8558	1/1	0.94	0.18	0.68	50,50,50,50	0
32	MG	0	8062	1/1	0.88	0.17	0.61	50,50,50,50	0
34	NA	0	8533	1/1	0.90	0.13	0.60	67,67,67,67	0
35	CL	0	8815	1/1	0.96	0.10	0.53	78,78,78,78	0
36	SR	0	8948	1/1	0.97	0.12	0.48	102,102,102,102	0
34	NA	0	8504	1/1	0.99	0.16	0.31	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8537	1/1	0.96	0.11	0.13	41,41,41,41	0
34	NA	0	8502	1/1	0.89	0.12	0.11	65,65,65,65	0
32	MG	0	8070	1/1	0.98	0.13	0.00	45,45,45,45	0
34	NA	C	8503	1/1	0.91	0.16	-0.06	44,44,44,44	0
34	NA	J	8538	1/1	0.85	0.16	-0.27	60,60,60,60	0
32	MG	0	8088	1/1	0.98	0.13	-0.28	42,42,42,42	0
34	NA	0	8523	1/1	0.98	0.12	-0.28	45,45,45,45	0
37	CD	U	8701	1/1	0.99	0.11	-0.30	72,72,72,72	0
33	K	0	8401	1/1	0.93	0.13	-0.31	74,74,74,74	0
36	SR	0	8972	1/1	0.96	0.14	-0.32	141,141,141,141	0
32	MG	0	8011	1/1	1.00	0.16	-0.36	33,33,33,33	0
35	CL	J	8821	1/1	0.99	0.13	-0.48	71,71,71,71	0
32	MG	0	8012	1/1	0.98	0.16	-0.56	25,25,25,25	0
32	MG	0	8043	1/1	0.96	0.10	-0.62	49,49,49,49	0
36	SR	3	8932	1/1	1.00	0.12	-0.62	79,79,79,79	0
34	NA	0	8515	1/1	0.96	0.14	-0.63	37,37,37,37	0
32	MG	K	8054	1/1	0.95	0.13	-0.80	50,50,50,50	0
32	MG	0	8050	1/1	0.98	0.12	-0.83	37,37,37,37	0
32	MG	B	8042	1/1	0.98	0.09	-0.84	50,50,50,50	0
35	CL	M	8818	1/1	0.98	0.10	-0.88	47,47,47,47	0
36	SR	0	8935	1/1	0.99	0.10	-0.89	80,80,80,80	0
32	MG	0	8021	1/1	0.96	0.10	-0.92	30,30,30,30	0
34	NA	M	8539	1/1	0.99	0.10	-1.02	34,34,34,34	0
36	SR	0	8936	1/1	0.98	0.10	-1.14	94,94,94,94	0
34	NA	0	8520	1/1	0.97	0.08	-1.21	53,53,53,53	0
36	SR	F	9005	1/1	0.98	0.07	-1.31	134,134,134,134	0
32	MG	0	8010	1/1	0.96	0.12	-1.31	35,35,35,35	0
37	CD	Z	8703	1/1	0.99	0.09	-1.34	91,91,91,91	0
37	CD	1	8702	1/1	0.99	0.10	-1.40	65,65,65,65	0
34	NA	R	8532	1/1	0.97	0.08	-1.44	46,46,46,46	0
34	NA	Q	8540	1/1	0.92	0.08	-1.49	60,60,60,60	0
35	CL	L	8810	1/1	0.96	0.08	-1.54	61,61,61,61	0
36	SR	0	8943	1/1	0.99	0.07	-1.64	117,117,117,117	0
37	CD	3	8704	1/1	1.00	0.07	-1.69	81,81,81,81	0
32	MG	0	8025	1/1	0.99	0.11	-1.85	35,35,35,35	0
36	SR	0	8969	1/1	0.97	0.10	-1.88	160,160,160,160	0
32	MG	T	8057	1/1	0.93	0.07	-1.89	65,65,65,65	0
32	MG	0	8058	1/1	0.99	0.08	-1.90	23,23,23,23	0
35	CL	O	8808	1/1	0.93	0.07	-1.99	81,81,81,81	0
36	SR	0	8975	1/1	0.97	0.07	-1.99	135,135,135,135	0
36	SR	A	8930	1/1	0.99	0.05	-2.05	104,104,104,104	0
36	SR	9	8978	1/1	0.99	0.07	-2.27	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8085	1/1	0.96	0.08	-2.52	73,73,73,73	0
32	MG	0	8052	1/1	0.93	0.07	-2.53	52,52,52,52	0
35	CL	0	8813	1/1	0.99	0.06	-2.78	61,61,61,61	0
36	SR	0	8985	1/1	0.89	0.06	-2.78	143,143,143,143	0
35	CL	0	8805	1/1	0.97	0.06	-2.83	67,67,67,67	0
36	SR	0	8949	1/1	0.97	0.09	-3.09	119,119,119,119	0
36	SR	0	8945	1/1	0.95	0.07	-3.28	112,112,112,112	0
32	MG	0	8001	1/1	0.97	0.09	-3.61	33,33,33,33	0
36	SR	0	8902	1/1	1.00	0.11	-3.64	66,66,66,66	0
35	CL	0	8812	1/1	0.97	0.06	-3.82	54,54,54,54	0
35	CL	3	8804	1/1	0.99	0.06	-3.88	67,67,67,67	0
34	NA	0	8519	1/1	0.92	0.12	-3.89	50,50,50,50	0
32	MG	0	8060	1/1	0.95	0.06	-3.96	61,61,61,61	0
32	MG	0	8002	1/1	0.99	0.07	-4.04	32,32,32,32	0
32	MG	Y	8086	1/1	0.98	0.05	-4.19	46,46,46,46	0
35	CL	B	8819	1/1	0.98	0.09	-4.22	54,54,54,54	0
36	SR	1	8913	1/1	1.00	0.09	-4.26	96,96,96,96	0
36	SR	0	8910	1/1	0.99	0.05	-4.51	101,101,101,101	0
32	MG	0	8065	1/1	0.99	0.06	-4.57	49,49,49,49	0
34	NA	0	8521	1/1	0.97	0.07	-4.60	65,65,65,65	0
32	MG	0	8034	1/1	0.99	0.07	-4.64	45,45,45,45	0
36	SR	0	8984	1/1	0.92	0.04	-5.67	123,123,123,123	0
32	MG	0	8075	1/1	0.90	0.03	-5.85	46,46,46,46	0
36	SR	0	8970	1/1	0.95	0.03	-6.52	128,128,128,128	0
32	MG	0	8044	1/1	0.98	0.05	-6.72	53,53,53,53	0
32	MG	0	8013	1/1	0.99	0.03	-8.68	30,30,30,30	0
32	MG	0	8040	1/1	0.98	0.16	-	96,96,96,96	0
36	SR	0	8921	1/1	0.97	0.12	-	92,92,92,92	0
36	SR	0	8942	1/1	0.92	0.08	-	133,133,133,133	0
36	SR	0	8923	1/1	0.98	0.10	-	116,116,116,116	0
36	SR	0	8946	1/1	0.94	0.23	-	122,122,122,122	0
35	CL	0	8814	1/1	0.98	0.10	-	60,60,60,60	0
36	SR	B	8950	1/1	0.98	0.17	-	132,132,132,132	0
36	SR	9	8980	1/1	0.76	0.15	-	200,200,200,200	0
34	NA	0	8571	1/1	0.85	0.09	-	77,77,77,77	0
32	MG	0	8005	1/1	0.99	0.17	-	33,33,33,33	0
32	MG	0	8055	1/1	0.98	0.20	-	46,46,46,46	0
36	SR	0	8924	1/1	0.94	0.16	-	135,135,135,135	0
32	MG	0	8063	1/1	0.96	0.17	-	71,71,71,71	0
36	SR	0	8988	1/1	0.78	0.13	-	173,173,173,173	0
36	SR	0	8920	1/1	0.98	0.05	-	134,134,134,134	0
34	NA	0	8511	1/1	0.96	0.13	-	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
32	MG	0	8090	1/1	0.93	0.33	-	62,62,62,62	0
36	SR	0	8996	1/1	0.84	1.02	-	200,200,200,200	0
36	SR	0	8994	1/1	0.40	0.98	-	200,200,200,200	0
36	SR	0	8939	1/1	0.94	0.04	-	160,160,160,160	0
32	MG	0	8015	1/1	0.99	0.17	-	36,36,36,36	0
36	SR	0	8953	1/1	0.98	0.08	-	157,157,157,157	0
32	MG	0	8048	1/1	0.95	0.20	-	26,26,26,26	0
36	SR	0	8906	1/1	1.00	0.21	-	60,60,60,60	0
36	SR	0	8928	1/1	0.88	0.06	-	135,135,135,135	0
36	SR	0	8993	1/1	0.78	0.09	-	182,182,182,182	0
32	MG	9	8074	1/1	0.96	0.11	-	77,77,77,77	0
32	MG	0	8089	1/1	0.58	0.12	-	57,57,57,57	0
36	SR	0	8997	1/1	0.72	0.47	-	200,200,200,200	0
36	SR	0	8941	1/1	0.95	0.13	-	116,116,116,116	0
32	MG	0	8061	1/1	0.96	0.21	-	30,30,30,30	0
36	SR	0	8979	1/1	0.90	0.20	-	198,198,198,198	0
36	SR	0	9004	1/1	0.98	0.64	-	200,200,200,200	0
32	MG	0	8017	1/1	0.99	0.22	-	25,25,25,25	0
34	NA	0	8506	1/1	0.81	0.25	-	68,68,68,68	0
34	NA	0	8549	1/1	0.97	0.28	-	58,58,58,58	0
32	MG	0	8072	1/1	0.91	0.10	-	53,53,53,53	0
34	NA	0	8501	1/1	0.98	0.22	-	44,44,44,44	0
32	MG	0	8053	1/1	0.98	0.04	-	59,59,59,59	0
36	SR	0	9002	1/1	0.97	0.08	-	184,184,184,184	0
36	SR	0	9006	1/1	0.11	1.24	-	200,200,200,200	0
35	CL	R	8806	1/1	0.97	0.13	-	52,52,52,52	0
36	SR	0	8926	1/1	0.98	0.10	-	127,127,127,127	0
34	NA	0	8548	1/1	0.90	0.16	-	55,55,55,55	0
36	SR	0	8995	1/1	0.96	0.17	-	140,140,140,140	0
32	MG	0	8081	1/1	0.85	0.19	-	74,74,74,74	0
35	CL	0	8811	1/1	0.92	0.11	-	68,68,68,68	0
36	SR	0	8964	1/1	0.98	0.10	-	139,139,139,139	0
32	MG	0	8046	1/1	0.97	0.13	-	41,41,41,41	0
36	SR	0	8960	1/1	0.92	0.05	-	150,150,150,150	0
36	SR	0	8911	1/1	0.97	0.08	-	85,85,85,85	0
34	NA	0	8505	1/1	0.80	1.03	-	49,49,49,49	0
35	CL	J	8802	1/1	0.97	0.09	-	76,76,76,76	0
34	NA	0	8536	1/1	0.94	0.08	-	65,65,65,65	0
35	CL	0	8816	1/1	0.97	0.18	-	85,85,85,85	0
32	MG	0	8091	1/1	0.77	0.06	-	62,62,62,62	0
36	SR	0	8973	1/1	0.98	0.07	-	137,137,137,137	0
36	SR	0	8956	1/1	0.94	0.09	-	155,155,155,155	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8983	1/1	0.91	0.45	-	195,195,195,195	0
34	NA	0	8570	1/1	0.71	0.13	-	60,60,60,60	0
36	SR	1	8952	1/1	0.99	0.13	-	91,91,91,91	0
36	SR	0	8914	1/1	1.00	0.27	-	110,110,110,110	0
35	CL	0	8817	1/1	0.99	0.10	-	65,65,65,65	0
36	SR	0	8931	1/1	0.98	0.09	-	117,117,117,117	0
34	NA	0	8524	1/1	0.95	0.18	-	58,58,58,58	0
32	MG	0	8037	1/1	0.74	0.33	-	90,90,90,90	0
34	NA	0	8560	1/1	0.78	0.37	-	83,83,83,83	0
34	NA	0	8566	1/1	0.93	0.25	-	60,60,60,60	0
32	MG	0	8069	1/1	0.99	0.17	-	72,72,72,72	0
32	MG	0	8082	1/1	0.90	0.28	-	69,69,69,69	0
34	NA	9	8543	1/1	0.96	0.18	-	49,49,49,49	0
36	SR	0	8963	1/1	0.97	0.04	-	134,134,134,134	0
32	MG	0	8035	1/1	0.94	0.14	-	68,68,68,68	0
36	SR	0	8967	1/1	0.97	0.08	-	132,132,132,132	0
32	MG	0	8022	1/1	0.99	0.11	-	32,32,32,32	0
36	SR	0	8927	1/1	0.87	0.06	-	151,151,151,151	0
36	SR	0	8966	1/1	0.94	0.08	-	111,111,111,111	0
36	SR	0	8922	1/1	0.42	0.22	-	170,170,170,170	0
36	SR	0	8981	1/1	0.98	0.16	-	153,153,153,153	0
34	NA	0	8516	1/1	0.96	0.12	-	42,42,42,42	0
32	MG	0	8026	1/1	0.98	0.07	-	37,37,37,37	0
32	MG	0	8030	1/1	0.98	0.48	-	69,69,69,69	0
34	NA	0	8551	1/1	0.97	0.24	-	59,59,59,59	0
36	SR	0	8958	1/1	0.92	0.11	-	123,123,123,123	0
36	SR	0	9008	1/1	0.99	0.14	-	89,89,89,89	0
36	SR	0	8938	1/1	0.77	0.13	-	192,192,192,192	0
32	MG	0	8064	1/1	0.96	0.15	-	37,37,37,37	0
36	SR	3	8999	1/1	0.99	0.04	-	106,106,106,106	0
32	MG	0	8049	1/1	0.98	0.38	-	68,68,68,68	0
36	SR	9	9003	1/1	0.97	0.01	-	170,170,170,170	0
36	SR	0	8965	1/1	0.98	0.05	-	124,124,124,124	0
36	SR	0	8991	1/1	0.58	0.09	-	197,197,197,197	0
36	SR	0	9001	1/1	0.71	0.10	-	173,173,173,173	0
34	NA	0	8531	1/1	0.94	0.11	-	44,44,44,44	0
36	SR	0	8998	1/1	0.89	0.13	-	175,175,175,175	0
32	MG	0	8038	1/1	0.93	0.10	-	75,75,75,75	0
34	NA	0	8526	1/1	0.96	0.05	-	57,57,57,57	0
35	CL	Y	8820	1/1	0.99	0.23	-	51,51,51,51	0
32	MG	0	8020	1/1	0.98	0.13	-	43,43,43,43	0
36	SR	0	8954	1/1	0.97	0.12	-	112,112,112,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	J	8801	1/1	0.96	0.17	-	79,79,79,79	0
32	MG	0	8073	1/1	0.99	0.07	-	83,83,83,83	0
36	SR	0	8917	1/1	0.95	0.13	-	111,111,111,111	0
32	MG	0	8092	1/1	0.96	0.26	-	67,67,67,67	0
32	MG	0	8066	1/1	0.92	0.15	-	76,76,76,76	0
32	MG	0	8077	1/1	0.88	0.07	-	49,49,49,49	0
32	MG	0	8039	1/1	0.96	0.25	-	77,77,77,77	0
36	SR	0	8901	1/1	0.98	0.10	-	85,85,85,85	0
36	SR	0	8944	1/1	0.80	0.12	-	182,182,182,182	0
32	MG	0	8083	1/1	0.92	0.11	-	73,73,73,73	0
32	MG	0	8023	1/1	0.99	0.14	-	32,32,32,32	0
36	SR	0	9000	1/1	0.99	0.12	-	177,177,177,177	0
34	NA	0	8525	1/1	0.78	0.19	-	78,78,78,78	0
34	NA	0	8541	1/1	0.92	0.22	-	69,69,69,69	0
36	SR	0	8962	1/1	0.93	0.05	-	175,175,175,175	0
36	SR	0	8959	1/1	0.81	0.20	-	174,174,174,174	0
36	SR	0	8905	1/1	0.99	0.28	-	68,68,68,68	0
32	MG	0	8079	1/1	0.96	0.10	-	55,55,55,55	0
36	SR	0	8955	1/1	0.97	0.16	-	200,200,200,200	0
32	MG	0	8080	1/1	0.99	0.36	-	69,69,69,69	0
36	SR	0	8908	1/1	0.96	0.10	-	110,110,110,110	0
37	CD	O	8705	1/1	1.00	0.07	-	94,94,94,94	0
32	MG	0	8059	1/1	0.91	0.06	-	59,59,59,59	0
32	MG	0	8027	1/1	0.99	0.09	-	49,49,49,49	0
34	NA	0	8535	1/1	0.94	0.25	-	53,53,53,53	0
34	NA	0	8546	1/1	0.60	1.30	-	112,112,112,112	0
32	MG	0	8007	1/1	0.95	0.20	-	38,38,38,38	0
32	MG	0	8068	1/1	0.99	0.09	-	54,54,54,54	0
34	NA	0	8574	1/1	0.90	0.38	-	55,55,55,55	0
36	SR	0	8937	1/1	0.97	0.21	-	115,115,115,115	0
36	SR	0	8957	1/1	0.86	0.10	-	196,196,196,196	0
32	MG	0	8087	1/1	0.91	0.08	-	47,47,47,47	0
36	SR	0	8933	1/1	0.97	0.17	-	150,150,150,150	0
36	SR	0	8974	1/1	0.93	0.13	-	149,149,149,149	0
34	NA	0	8544	1/1	0.84	0.20	-	75,75,75,75	0
36	SR	0	8925	1/1	1.00	0.12	-	91,91,91,91	0
32	MG	0	8019	1/1	0.99	0.18	-	27,27,27,27	0
32	MG	0	8076	1/1	0.98	0.07	-	42,42,42,42	0
36	SR	0	8907	1/1	1.00	0.14	-	56,56,56,56	0
32	MG	0	8024	1/1	0.96	0.13	-	55,55,55,55	0
32	MG	0	8078	1/1	0.97	0.32	-	61,61,61,61	0
34	NA	0	8518	1/1	0.71	0.47	-	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8514	1/1	0.96	0.59	-	48,48,48,48	0
36	SR	0	8934	1/1	0.99	0.11	-	130,130,130,130	0
32	MG	0	8031	1/1	0.97	0.39	-	72,72,72,72	0
35	CL	0	8822	1/1	0.98	0.55	-	106,106,106,106	0
36	SR	0	8916	1/1	0.99	0.06	-	113,113,113,113	0
36	SR	0	8982	1/1	0.75	1.20	-	200,200,200,200	0
34	NA	0	8509	1/1	0.92	0.15	-	69,69,69,69	0
32	MG	0	8032	1/1	0.98	0.05	-	46,46,46,46	0
36	SR	0	8989	1/1	0.92	0.13	-	185,185,185,185	0
32	MG	0	8071	1/1	0.89	0.19	-	71,71,71,71	0
36	SR	0	8971	1/1	0.95	0.07	-	180,180,180,180	0
36	SR	0	8919	1/1	0.61	0.13	-	192,192,192,192	0
32	MG	0	8093	1/1	0.98	0.08	-	35,35,35,35	0
36	SR	0	8951	1/1	0.88	0.07	-	142,142,142,142	0
32	MG	0	8056	1/1	0.98	0.11	-	51,51,51,51	0
32	MG	0	8018	1/1	0.99	0.19	-	46,46,46,46	0
36	SR	0	8976	1/1	0.81	0.25	-	200,200,200,200	0
36	SR	S	8961	1/1	0.93	0.10	-	122,122,122,122	0
32	MG	0	8033	1/1	0.98	0.09	-	49,49,49,49	0
36	SR	0	9007	1/1	0.89	1.35	-	200,200,200,200	0
35	CL	A	8809	1/1	0.94	0.09	-	74,74,74,74	0
36	SR	0	8968	1/1	0.90	0.08	-	165,165,165,165	0
34	NA	0	8529	1/1	0.93	0.05	-	45,45,45,45	0
36	SR	0	8940	1/1	0.99	0.08	-	93,93,93,93	0
34	NA	S	8510	1/1	0.91	0.06	-	49,49,49,49	0
35	CL	N	8807	1/1	0.97	0.10	-	71,71,71,71	0
36	SR	0	8990	1/1	0.99	0.10	-	137,137,137,137	0
34	NA	0	8554	1/1	0.97	0.89	-	78,78,78,78	0
35	CL	0	8803	1/1	0.97	0.08	-	62,62,62,62	0
34	NA	0	8561	1/1	0.91	0.50	-	78,78,78,78	0
34	NA	0	8513	1/1	0.97	0.13	-	58,58,58,58	0
36	SR	0	8986	1/1	0.61	0.17	-	200,200,200,200	0
34	NA	0	8545	1/1	0.95	0.14	-	41,41,41,41	0
32	MG	0	8036	1/1	0.83	0.09	-	50,50,50,50	0
34	NA	0	8573	1/1	0.95	0.26	-	77,77,77,77	0
34	NA	0	8567	1/1	0.94	0.21	-	80,80,80,80	0
36	SR	0	8909	1/1	0.98	0.14	-	85,85,85,85	0
36	SR	0	8915	1/1	0.91	0.09	-	131,131,131,131	0
32	MG	0	8029	1/1	0.97	0.17	-	48,48,48,48	0
34	NA	0	8550	1/1	0.82	0.52	-	61,61,61,61	0
36	SR	A	8977	1/1	0.87	0.06	-	161,161,161,161	0

## 6.5 Other polymers

There are no such residues in this entry.