



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 5, 2023 – 11:38 PM EST

PDB ID : 1M90  
Title : Co-crystal structure of CCA-Phe-caproic acid-biotin and sparsomycin bound to the 50S ribosomal subunit  
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2002-07-26  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

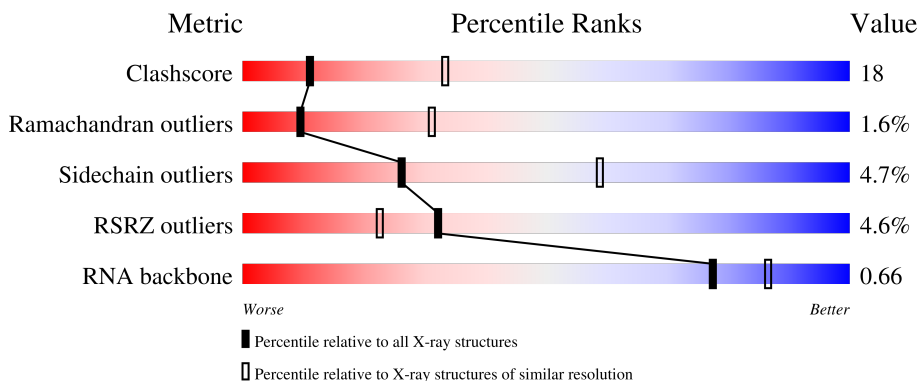
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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




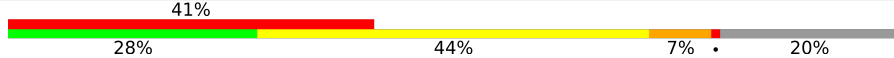
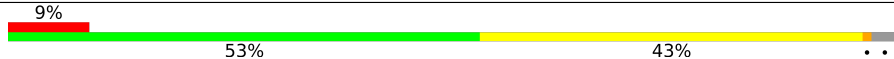
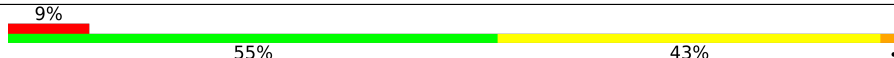
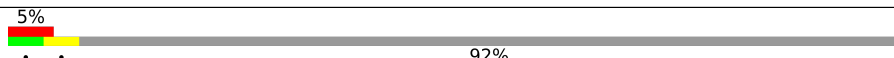
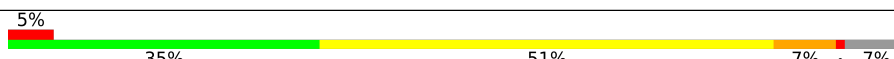
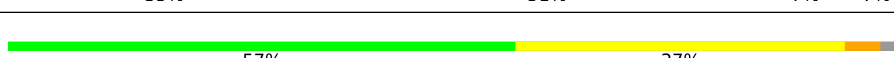
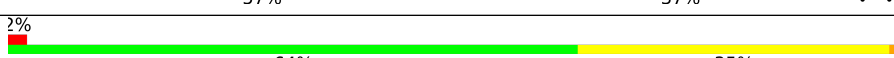
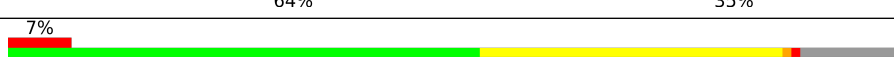
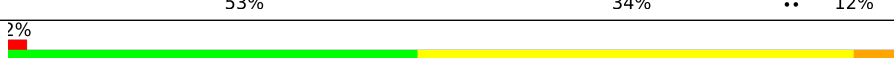








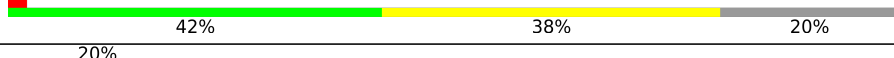
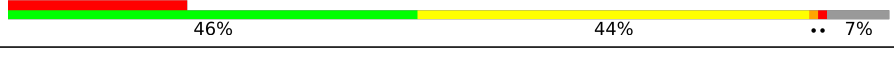
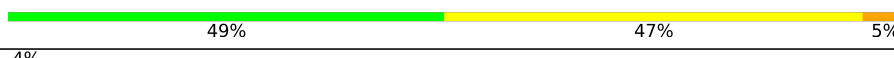
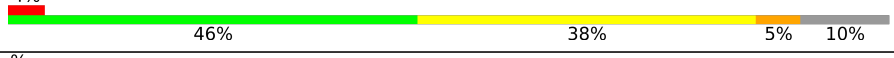
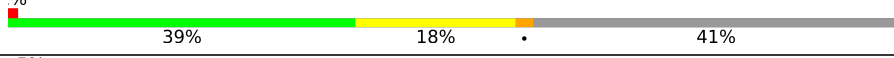


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	2922	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 30%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey;"></div> </div>
2	B	122	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 49%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div>
3	5	3	<div style="display: flex; align-items: center;"> <div style="width: 67%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: red;"></div> </div>
4	C	239	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div>
5	D	337	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange;"></div> </div>

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Mol	Chain	Length	Quality of chain
6	E	246	
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	
30	3	48	

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Mol	Chain	Length	Quality of chain
31	4	92	 % 61% 35%

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	A	8024	-	-	-	X
33	NA	A	8352	-	-	-	X
33	NA	A	8384	-	-	-	X
33	NA	A	8385	-	-	-	X
33	NA	B	8351	-	-	-	X
33	NA	S	8386	-	-	-	X
33	NA	T	8312	-	-	-	X

## 2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 98611 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	2754	59017	26346	10878	19048	2745	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	conflict	GB 3377779

- Molecule 2 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	122	2600	1160	472	847	121	0	0	0

- Molecule 3 is a RNA chain called CCA.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	237	1754	1072	352	325	5	0	0	0

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	337	2624	1616	493	510	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	246	1858	1131	344	382	1	0	0	0

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	H	119	885	552	141	191	1	0	0	0

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	J	156	1215	766	233	212	4	0	0	0

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	142	1119	696	199	221	3	0	0	0

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	L	132	993	609	189	191	4	0	0	0

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	M	145	1114	668	222	224		0	0	0

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	N	194	1605	988	346	266	5	0	0	0

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	O	186	1444	895	262	285	2	0	0	0

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	P	115	864	529	161	174		0	0	0

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	Q	143	1133	680	230	223		0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	conflict	UNP P14119

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	119	Total	C	N	O	0	0	0
			949	568	180	201			

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L30.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	X	154	1195	737	209	243	6	0	0	0

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	Z	142	1130	686	228	216		0	0	0

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	1	73	563	359	111	86	7	0	0	0

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	2	56	430	258	86	82	4	0	0	0

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	3	46	393	238	86	68	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	deletion	UNP P22452

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	111	Total	Mg	0	0
			111	111		
32	B	1	Total	Mg	0	0
			1	1		
32	5	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	L	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	1	1	Total	Mg	0	0
			1	1		
32	4	1	Total	Mg	0	0
			1	1		

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	A	73	Total	Na	0	0
			73	73		
33	B	2	Total	Na	0	0
			2	2		
33	C	1	Total	Na	0	0
			1	1		
33	E	1	Total	Na	0	0
			1	1		
33	J	1	Total	Na	0	0
			1	1		
33	K	1	Total	Na	0	0
			1	1		
33	M	1	Total	Na	0	0
			1	1		
33	N	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	R	1	Total 1	Na 1	0	0
33	S	2	Total 2	Na 2	0	0
33	T	1	Total 1	Na 1	0	0
33	U	1	Total 1	Na 1	0	0

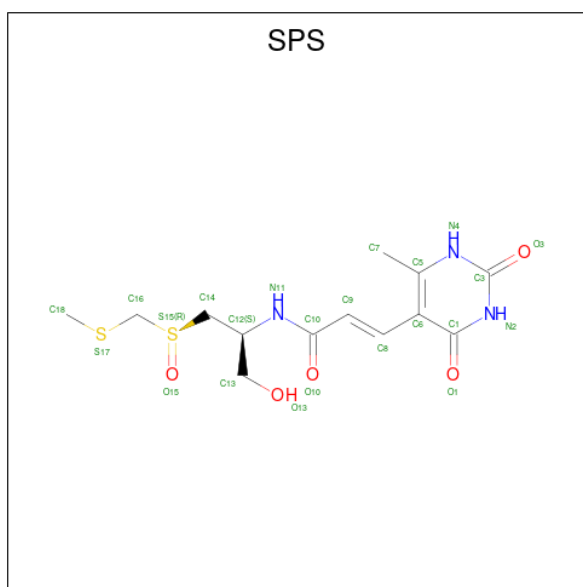
- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	2	Total 2	K 2	0	0

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

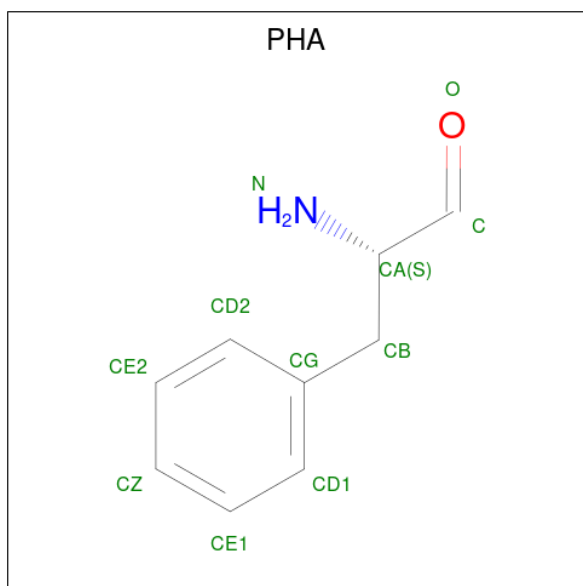
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	10	Total 10	Cl 10	0	0
35	C	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	3	Total 3	Cl 3	0	0
35	M	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	P	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	Z	1	Total 1	Cl 1	0	0
35	4	1	Total 1	Cl 1	0	0

- Molecule 36 is SPARSOMYCIN (three-letter code: SPS) (formula: C<sub>13</sub>H<sub>19</sub>N<sub>3</sub>O<sub>5</sub>S<sub>2</sub>).



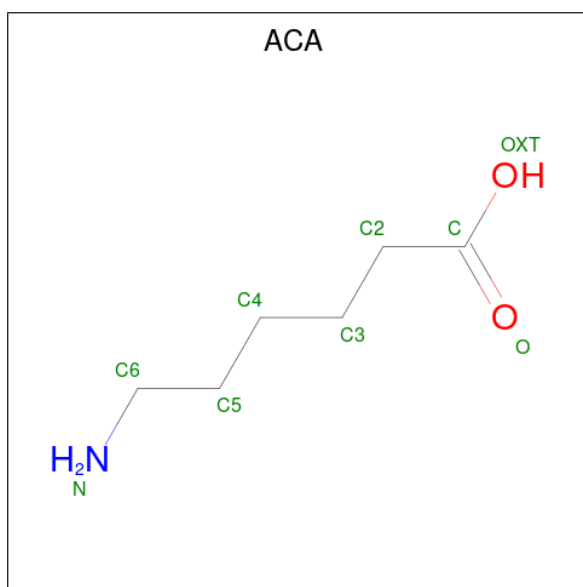
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
36	5	1	23	13	3	5	2	0	0

- Molecule 37 is PHENYLALANINAL (three-letter code: PHA) (formula:  $C_9H_{11}NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
37	5	1	11	9	1	1	0	0

- Molecule 38 is 6-AMINOHEXANOIC ACID (three-letter code: ACA) (formula:  $C_6H_{13}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	5	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	P	1	Total	Cd	0	0
			1	1		
39	V	1	Total	Cd	0	0
			1	1		
39	1	1	Total	Cd	0	0
			1	1		
39	2	1	Total	Cd	0	0
			1	1		
39	4	1	Total	Cd	0	0
			1	1		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	5920	Total	O	0	0
			5920	5920		
40	B	136	Total	O	0	0
			136	136		
40	5	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	C	119	Total 119	O 119	0	0
40	D	142	Total 142	O 142	0	0
40	E	172	Total 172	O 172	0	0
40	F	51	Total 51	O 51	0	0
40	G	44	Total 44	O 44	0	0
40	H	28	Total 28	O 28	0	0
40	I	21	Total 21	O 21	0	0
40	J	75	Total 75	O 75	0	0
40	K	56	Total 56	O 56	0	0
40	L	61	Total 61	O 61	0	0
40	M	86	Total 86	O 86	0	0
40	N	125	Total 125	O 125	0	0
40	O	69	Total 69	O 69	0	0
40	P	43	Total 43	O 43	0	0
40	Q	67	Total 67	O 67	0	0
40	R	49	Total 49	O 49	0	0
40	S	83	Total 83	O 83	0	0
40	T	35	Total 35	O 35	0	0
40	U	37	Total 37	O 37	0	0
40	V	24	Total 24	O 24	0	0
40	W	16	Total 16	O 16	0	0

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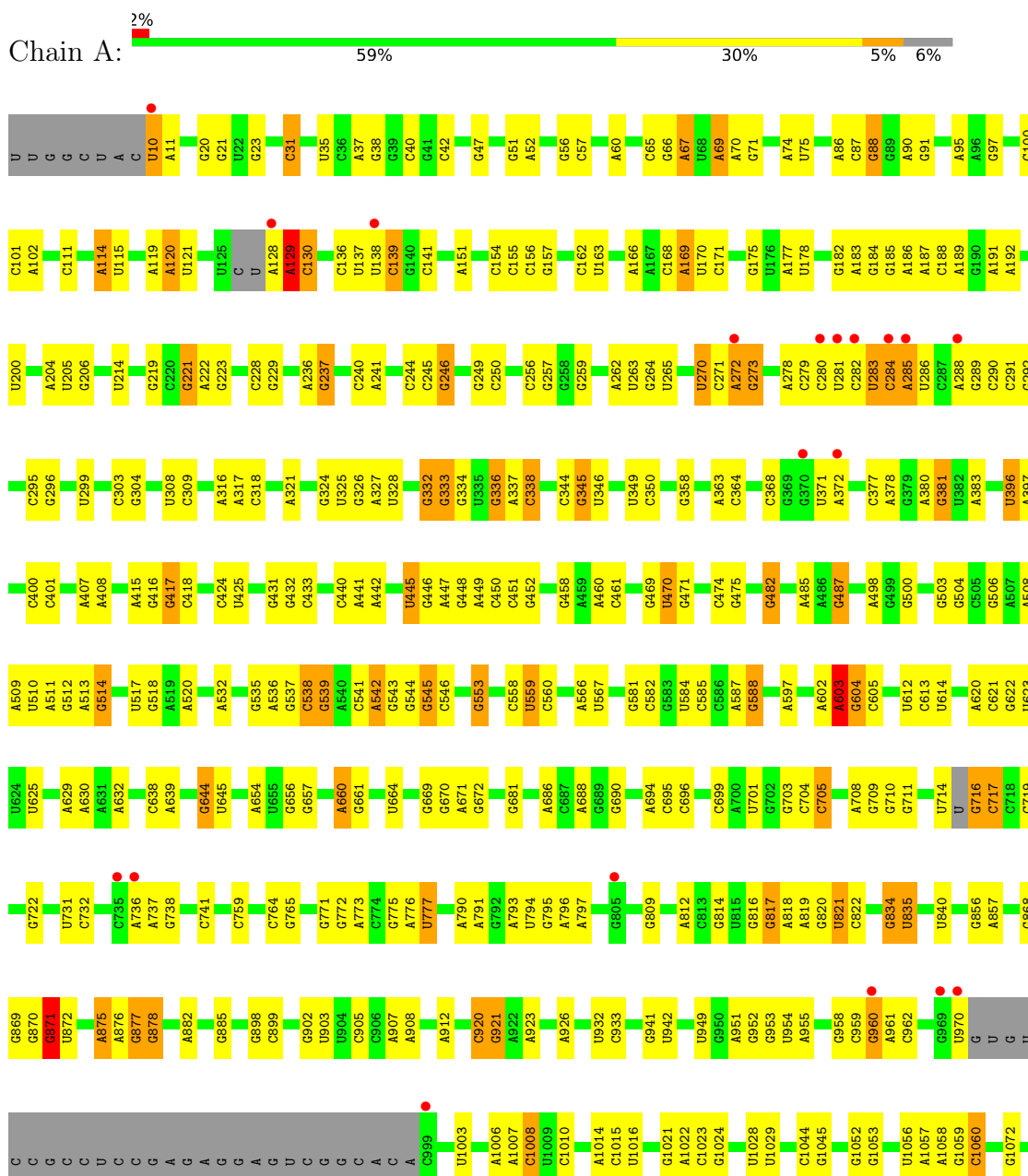
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
40	X	71	Total O 71 71	0	0
40	Y	31	Total O 31 31	0	0
40	Z	92	Total O 92 92	0	0
40	1	36	Total O 36 36	0	0
40	2	55	Total O 55 55	0	0
40	3	40	Total O 40 40	0	0
40	4	73	Total O 73 73	0	0

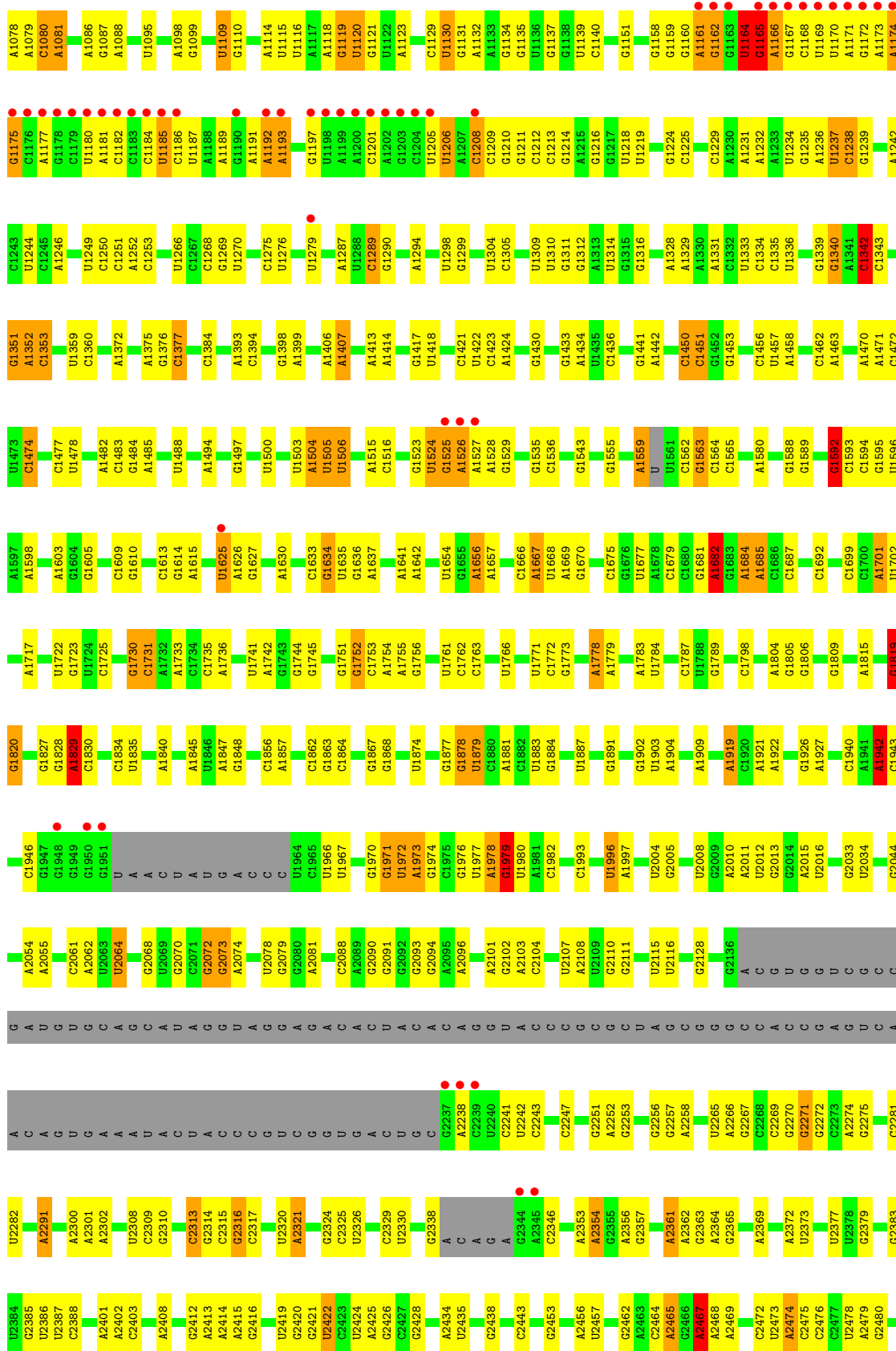
### 3 Residue-property plots [i](#)

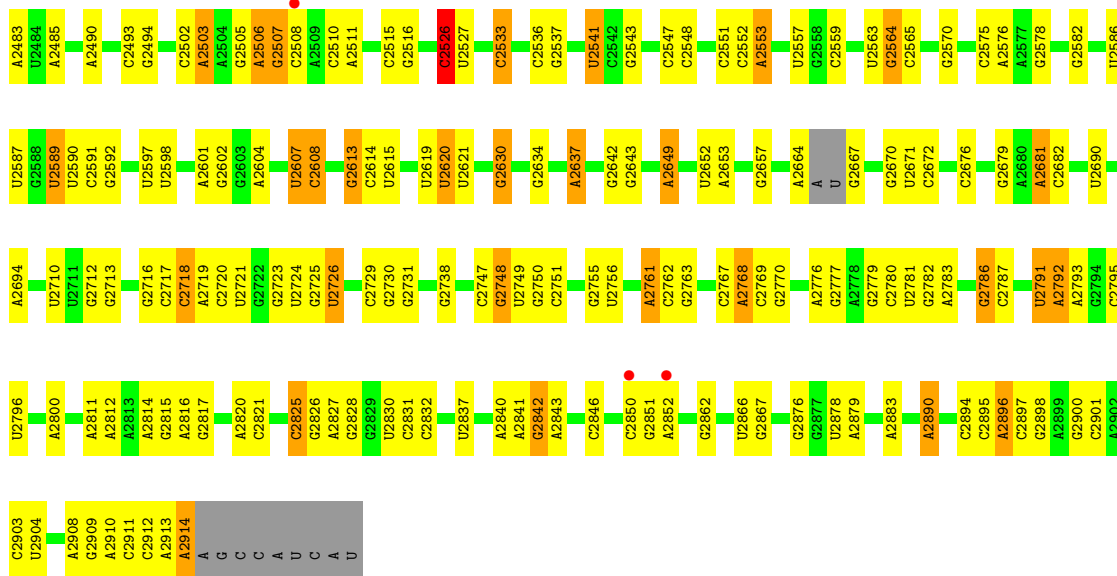
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S RRNA

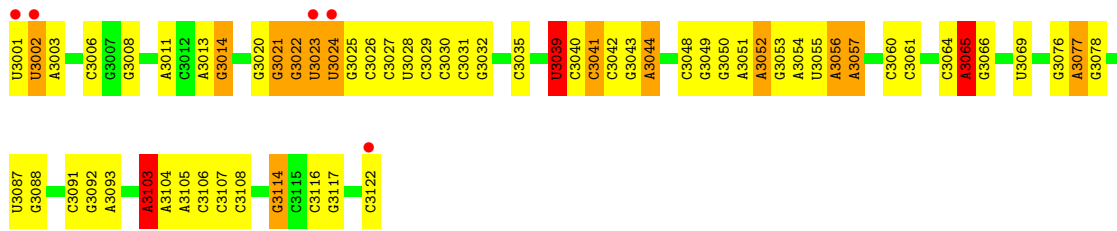








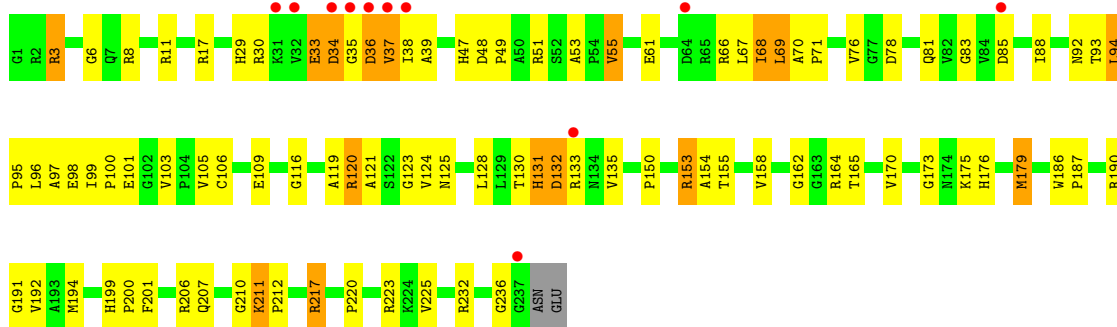
• Molecule 2: 5S RRNA



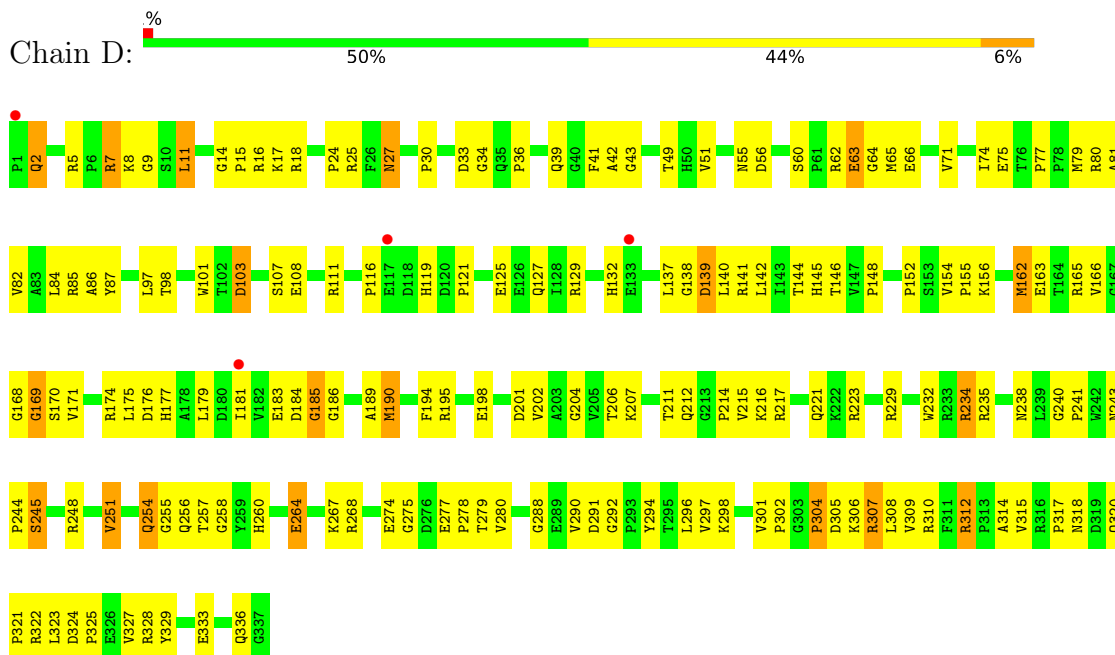
• Molecule 3: CCA



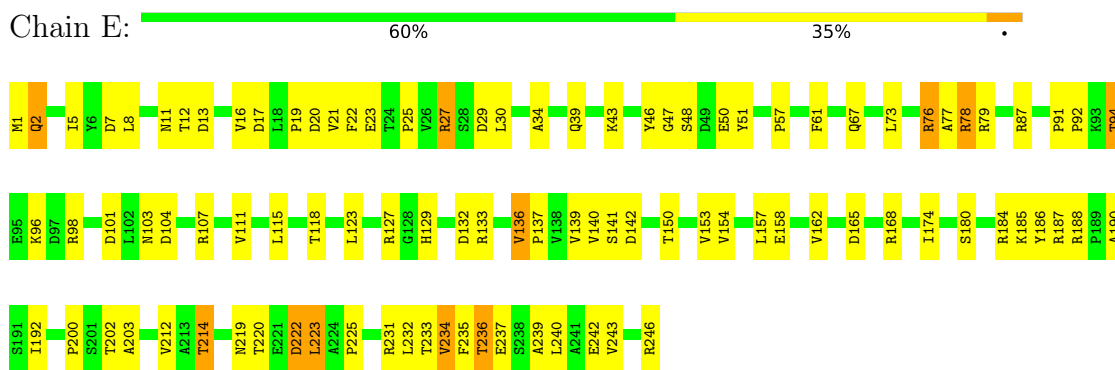
• Molecule 4: RIBOSOMAL PROTEIN L2



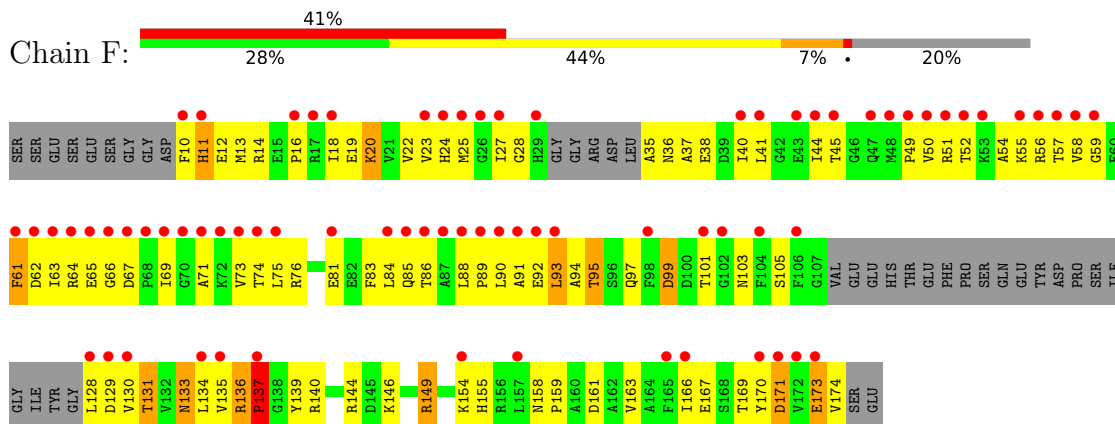
● Molecule 5: RIBOSOMAL PROTEIN L3



● Molecule 6: RIBOSOMAL PROTEIN L4

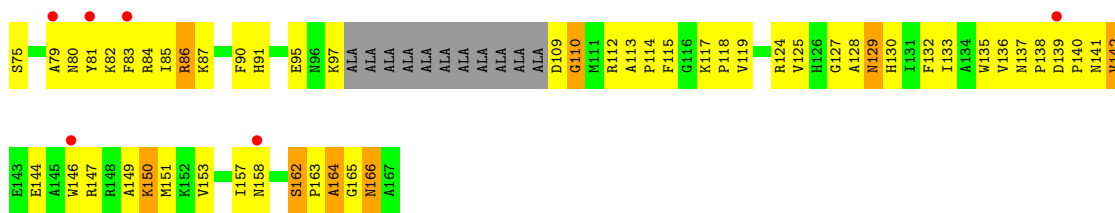


● Molecule 7: RIBOSOMAL PROTEIN L5



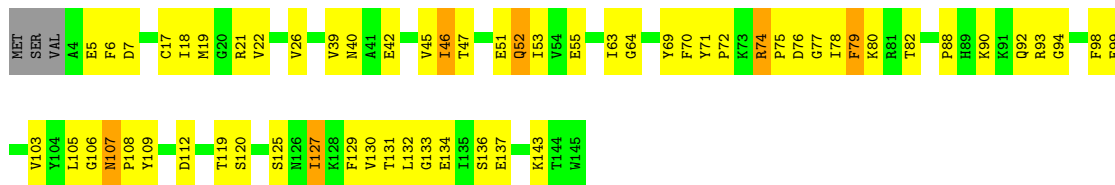
● Molecule 8: RIBOSOMAL PROTEIN L6





● Molecule 12: RIBOSOMAL PROTEIN L13

Chain K: 57% 37%



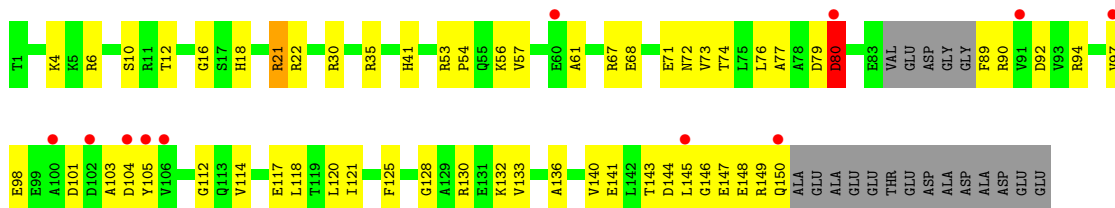
● Molecule 13: RIBOSOMAL PROTEIN L14

Chain L: 2% 64% 35%



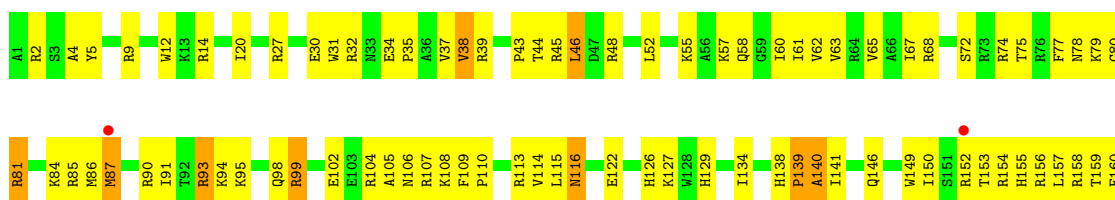
● Molecule 14: RIBOSOMAL PROTEIN L15

Chain M: 7% 53% 34% 12%



● Molecule 15: RIBOSOMAL PROTEIN L15E

Chain N: 2% 46% 49% 5%





- Molecule 16: RIBOSOMAL PROTEIN L18



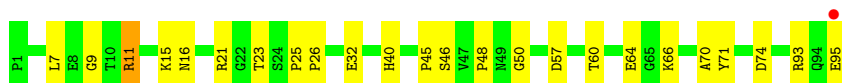
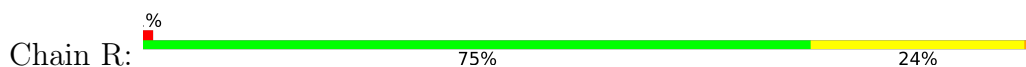
- Molecule 17: RIBOSOMAL PROTEIN L18E



- Molecule 18: RIBOSOMAL PROTEIN L19E

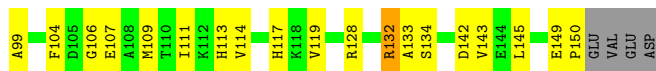


- Molecule 19: RIBOSOMAL PROTEIN L21E



- Molecule 20: RIBOSOMAL PROTEIN L22

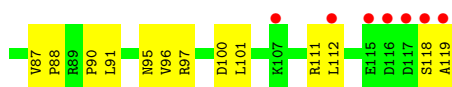
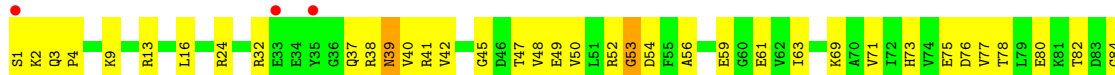




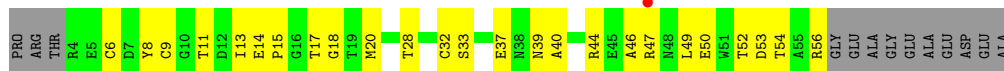
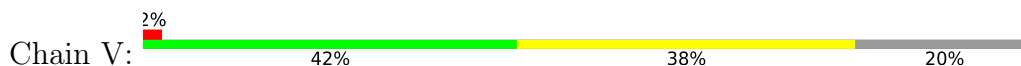
- Molecule 21: RIBOSOMAL PROTEIN L23



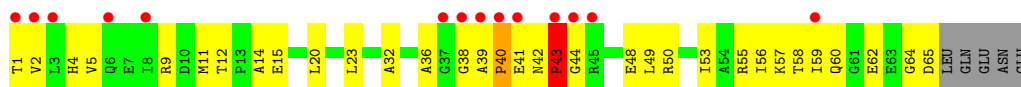
- Molecule 22: RIBOSOMAL PROTEIN L24



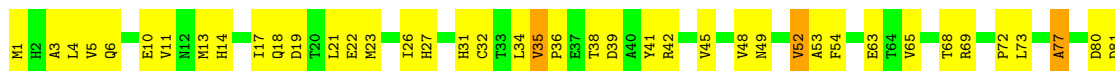
- Molecule 23: RIBOSOMAL PROTEIN L24E



- Molecule 24: RIBOSOMAL PROTEIN L29



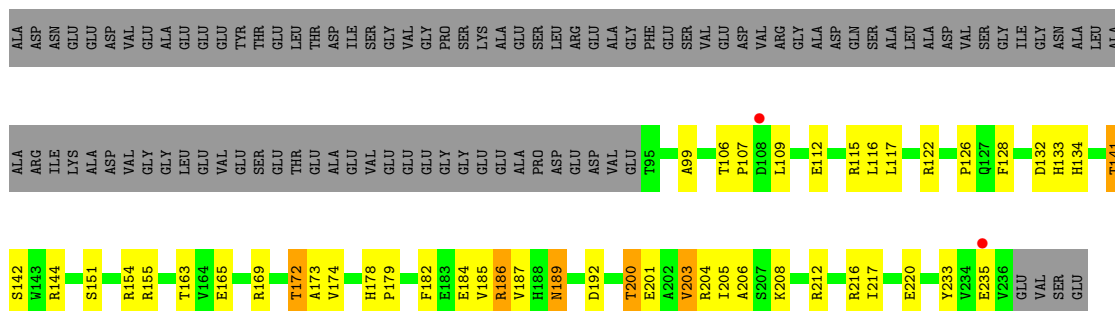
- Molecule 25: RIBOSOMAL PROTEIN L30



- Molecule 26: RIBOSOMAL PROTEIN L31E



- Molecule 27: RIBOSOMAL PROTEIN L32E



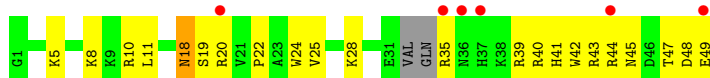
- Molecule 28: RIBOSOMAL PROTEIN L37Ae



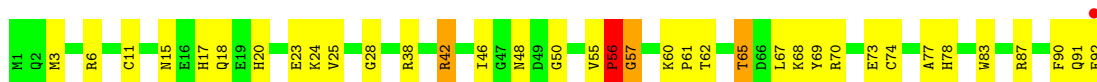
- Molecule 29: RIBOSOMAL PROTEIN L37E



- Molecule 30: RIBOSOMAL PROTEIN L39E



- Molecule 31: RIBOSOMAL PROTEIN L44E





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.66Å 299.77Å 573.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 49.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.3 (20.00-2.80) 94.4 (49.96-2.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.181 , 0.222 0.180 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.1	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	98611	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CD, SPS, K, ACA, PHA, NA, CL, MG

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	0.42	1/66076 (0.0%)	0.70	27/103052 (0.0%)
2	B	0.50	0/2905	0.79	4/4528 (0.1%)
3	5	0.74	0/65	1.17	1/99 (1.0%)
4	C	0.34	0/1787	0.66	0/2409
5	D	0.34	0/2689	0.65	0/3652
6	E	0.40	0/1883	0.66	0/2551
7	F	0.33	0/1111	0.60	0/1498
8	G	0.34	0/1382	0.59	0/1880
9	H	0.33	0/896	0.58	0/1219
10	I	0.27	0/241	0.47	0/324
11	J	0.39	0/1246	0.75	2/1686 (0.1%)
12	K	0.37	0/1135	0.61	0/1530
13	L	0.35	0/1003	0.67	0/1351
14	M	0.34	0/1126	0.67	0/1504
15	N	0.41	0/1633	0.70	1/2180 (0.0%)
16	O	0.31	0/1473	0.64	0/1999
17	P	0.38	0/873	0.63	0/1181
18	Q	0.37	0/1143	0.56	0/1521
19	R	0.38	0/748	0.67	0/1005
20	S	0.38	0/1172	0.67	0/1578
21	T	0.34	0/648	0.60	0/875
22	U	0.32	0/957	0.63	0/1289
23	V	0.35	0/417	0.57	0/562
24	W	0.32	0/502	0.56	0/675
25	X	0.36	0/1218	0.64	0/1655
26	Y	0.36	0/664	0.61	0/895
27	Z	0.39	0/1146	0.67	0/1536
28	1	0.39	0/575	0.71	0/763
29	2	0.44	0/437	0.67	0/578
30	3	0.34	0/398	0.56	0/527
31	4	0.40	0/771	0.62	0/1024
All	All	0.41	1/98320 (0.0%)	0.69	35/147126 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	58
2	B	0	3
All	All	1	61

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2474	A	C5-C6	-5.43	1.36	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-17.46	66.80	105.20
1	A	1164	U	OP2-P-O3'	-16.54	68.82	105.20
1	A	1563	G	C2'-C3'-O3'	9.62	130.67	109.50
1	A	1979	G	C2'-C3'-O3'	7.74	126.52	109.50
1	A	1942	A	C5'-C4'-C3'	7.39	127.82	116.00
2	B	3039	U	N1-C1'-C2'	7.36	123.57	114.00
3	5	9076	A	C2'-C3'-O3'	7.35	125.67	109.50
1	A	871	G	C5'-C4'-O4'	-7.05	100.64	109.10
1	A	2313	C	C5'-C4'-O4'	6.71	117.15	109.10
1	A	1504	A	C1'-O4'-C4'	-6.30	104.86	109.90
11	J	74	ASN	N-CA-C	-6.27	94.08	111.00
1	A	1819	G	C5'-C4'-C3'	6.09	125.75	116.00
1	A	1165	G	OP1-P-OP2	5.94	128.51	119.60
2	B	3103	A	C5'-C4'-O4'	5.90	116.17	109.10
1	A	1592	G	N9-C1'-C2'	5.88	121.64	114.00
1	A	2467	A	C1'-O4'-C4'	-5.68	105.36	109.90
1	A	1559	A	C2'-C3'-O3'	5.66	122.75	113.70
1	A	1504	A	N9-C1'-C2'	5.64	121.34	114.00
1	A	206	G	C5'-C4'-C3'	-5.54	107.13	116.00
1	A	1942	A	C5'-C4'-O4'	5.51	115.71	109.10
1	A	2316	G	C5'-C4'-C3'	-5.45	107.28	116.00
1	A	1942	A	C1'-O4'-C4'	-5.41	105.57	109.90
1	A	1120	U	C5'-C4'-C3'	-5.40	107.36	116.00
1	A	2726	U	N1-C1'-C2'	5.39	121.01	114.00
1	A	1942	A	C4'-C3'-C2'	-5.27	97.33	102.60
1	A	129	A	C2'-C3'-O3'	5.25	122.11	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3021	G	C5'-C4'-O4'	5.25	115.40	109.10
1	A	2291	A	N9-C1'-C2'	5.23	120.80	114.00
1	A	2475	C	O5'-P-OP1	5.17	116.91	110.70
1	A	2313	C	C5'-C4'-C3'	5.16	124.26	116.00
1	A	535	G	N9-C1'-C2'	5.15	120.70	114.00
2	B	3103	A	C4'-C3'-C2'	-5.07	97.53	102.60
15	N	139	PRO	N-CA-C	-5.07	98.92	112.10
11	J	110	GLY	N-CA-C	-5.03	100.53	113.10
1	A	603	A	N9-C1'-C2'	5.01	120.52	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

All (61) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1078	A	Sidechain
1	A	1340	G	Sidechain
1	A	1342	C	Sidechain
1	A	1351	G	Sidechain
1	A	1359	U	Sidechain
1	A	1417	G	Sidechain
1	A	1430	G	Sidechain
1	A	1458	A	Sidechain
1	A	1682	A	Sidechain
1	A	1809	G	Sidechain
1	A	1819	G	Sidechain
1	A	1829	A	Sidechain
1	A	1848	G	Sidechain
1	A	1863	G	Sidechain
1	A	1867	G	Sidechain
1	A	1877	G	Sidechain
1	A	1878	G	Sidechain
1	A	1970	G	Sidechain
1	A	1972	U	Sidechain
1	A	1978	A	Sidechain
1	A	1979	G	Sidechain
1	A	1993	C	Sidechain
1	A	221	G	Sidechain
1	A	2316	G	Sidechain

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Mol	Chain	Res	Type	Group
1	A	246	G	Sidechain
1	A	2465	A	Sidechain
1	A	2493	C	Sidechain
1	A	2503	A	Sidechain
1	A	2506	A	Sidechain
1	A	2526	C	Sidechain
1	A	2541	U	Sidechain
1	A	2543	G	Sidechain
1	A	2551	C	Sidechain
1	A	2552	C	Sidechain
1	A	2557	U	Sidechain
1	A	2564	G	Sidechain
1	A	2582	G	Sidechain
1	A	2607	U	Sidechain
1	A	2615	U	Sidechain
1	A	2620	U	Sidechain
1	A	2630	G	Sidechain
1	A	2637	A	Sidechain
1	A	270	U	Sidechain
1	A	2793	A	Sidechain
1	A	2842	G	Sidechain
1	A	332	G	Sidechain
1	A	333	G	Sidechain
1	A	396	U	Sidechain
1	A	445	U	Sidechain
1	A	458	G	Sidechain
1	A	460	A	Sidechain
1	A	469	G	Sidechain
1	A	470	U	Sidechain
1	A	471	G	Sidechain
1	A	482	G	Sidechain
1	A	518	G	Sidechain
1	A	722	G	Sidechain
1	A	817	G	Sidechain
2	B	3039	U	Sidechain
2	B	3065	A	Sidechain
2	B	3087	U	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	59017	0	29805	894	0
2	B	2600	0	1326	73	0
3	5	59	0	34	2	0
4	C	1754	0	1763	129	0
5	D	2624	0	2533	176	0
6	E	1858	0	1816	114	0
7	F	1094	0	1085	127	0
8	G	1357	0	1266	77	0
9	H	885	0	854	62	0
10	I	240	0	231	21	0
11	J	1215	0	1215	152	0
12	K	1119	0	1098	67	0
13	L	993	0	1027	55	0
14	M	1114	0	1072	61	0
15	N	1605	0	1676	159	0
16	O	1444	0	1401	128	0
17	P	864	0	873	41	0
18	Q	1133	0	1127	49	0
19	R	734	0	728	21	0
20	S	1149	0	1122	65	0
21	T	641	0	605	19	0
22	U	949	0	923	48	0
23	V	410	0	364	32	0
24	W	499	0	511	34	0
25	X	1195	0	1137	101	0
26	Y	654	0	653	47	0
27	Z	1130	0	1133	61	0
28	1	563	0	597	59	0
29	2	430	0	426	24	0
30	3	393	0	406	28	0
31	4	755	0	728	36	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	5	1	0	0	0	0
32	A	111	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	73	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	1	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	T	1	0	0	0	0
33	U	1	0	0	0	0
34	A	2	0	0	0	0
35	4	1	0	0	0	0
35	A	10	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	1	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	P	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	5	23	0	19	4	0
37	5	11	0	8	0	0
38	5	8	0	6	0	0
39	1	1	0	0	0	0
39	2	1	0	0	0	0
39	4	1	0	0	0	0
39	P	1	0	0	0	0
39	V	1	0	0	0	0
40	1	36	0	0	8	0
40	2	55	0	0	3	0
40	3	40	0	0	4	0
40	4	73	0	0	10	0
40	5	1	0	0	0	0
40	A	5920	0	0	193	0
40	B	136	0	0	11	0
40	C	119	0	0	23	0
40	D	142	0	0	30	0
40	E	172	0	0	27	0
40	F	51	0	0	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	G	44	0	0	8	0
40	H	28	0	0	8	0
40	I	21	0	0	6	0
40	J	75	0	0	23	0
40	K	56	0	0	5	0
40	L	61	0	0	16	0
40	M	86	0	0	19	0
40	N	125	0	0	21	0
40	O	69	0	0	17	0
40	P	43	0	0	7	0
40	Q	67	0	0	1	0
40	R	49	0	0	3	0
40	S	83	0	0	11	0
40	T	35	0	0	5	0
40	U	37	0	0	4	0
40	V	24	0	0	5	0
40	W	16	0	0	2	0
40	X	71	0	0	12	0
40	Y	31	0	0	5	0
40	Z	92	0	0	14	0
All	All	98611	0	59568	2699	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (2699) 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)
6:E:236:THR:HG22	6:E:239:ALA:H	1.04	1.16
1:A:1160:G:H5'	1:A:1161:A:H5'	1.22	1.15
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.63	1.13
11:J:45:GLN:HB3	11:J:163:PRO:HD2	1.30	1.12
24:W:12:THR:HG22	24:W:15:GLU:HG3	1.31	1.12
11:J:162:SER:HB2	11:J:163:PRO:HD3	1.31	1.10
1:A:1134:G:H4'	11:J:151:MET:HE1	1.33	1.09
1:A:156:C:H5''	15:N:171:ARG:HD3	1.36	1.08
1:A:1242:A:H5'	12:K:82:THR:HG23	1.39	1.04
26:Y:37:LEU:HD13	26:Y:85:VAL:HG21	1.35	1.03
7:F:134:LEU:HD11	7:F:166:ILE:HD11	1.38	1.02
2:B:3006:C:H5''	16:O:37:ARG:NH1	1.75	1.01
22:U:71:VAL:HG11	22:U:90:PRO:HB3	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:G:H4'	40:A:6940:HOH:O	1.60	0.99
13:L:10:GLN:NE2	13:L:10:GLN:H	1.60	0.99
11:J:86:ARG:HH11	11:J:133:ILE:HG13	0.83	0.99
11:J:26:LYS:HD2	11:J:28:ILE:HD12	1.44	0.98
11:J:29:ALA:HB3	11:J:65:ARG:HH12	1.26	0.98
1:A:542:A:H5'	1:A:542:A:H8	1.29	0.98
1:A:870:G:H2'	1:A:871:G:H5''	1.44	0.97
1:A:1751:G:H2'	1:A:1752:G:H5''	1.45	0.97
13:L:81:ARG:HB2	13:L:87:ARG:HH11	1.28	0.97
11:J:86:ARG:HH11	11:J:133:ILE:CG1	1.78	0.97
40:A:3981:HOH:O	15:N:146:GLN:HG2	1.61	0.97
5:D:140:LEU:HA	40:D:8574:HOH:O	1.63	0.97
20:S:99:ALA:HB1	20:S:109:MET:HE1	1.46	0.97
15:N:52:LEU:HD11	40:N:8617:HOH:O	1.64	0.96
16:O:83:LEU:HD13	16:O:175:LEU:HD23	1.45	0.95
13:L:29:LEU:HB3	13:L:55:VAL:HG11	1.47	0.95
2:B:3056:A:H2'	2:B:3057:A:H5''	1.48	0.95
6:E:5:ILE:HD11	6:E:16:VAL:HG23	1.48	0.95
28:1:10:ARG:HA	40:1:8415:HOH:O	1.67	0.95
2:B:3076:G:H3'	2:B:3077:A:H5''	1.47	0.94
15:N:164:THR:HG22	15:N:167:GLY:H	1.29	0.94
5:D:264:GLU:HG2	5:D:267:LYS:HE2	1.50	0.94
12:K:76:ASP:HA	40:K:5907:HOH:O	1.69	0.93
16:O:144:GLY:O	16:O:147:ILE:HG22	1.67	0.93
6:E:132:ASP:HB3	40:E:8363:HOH:O	1.66	0.93
6:E:115:LEU:HD13	6:E:223:LEU:HD21	1.49	0.93
1:A:856:G:H2'	40:A:4944:HOH:O	1.69	0.93
6:E:115:LEU:HD21	6:E:243:VAL:HG13	1.51	0.93
16:O:47:LEU:HD11	16:O:127:LEU:HD21	1.51	0.93
25:X:88:THR:HB	40:X:6679:HOH:O	1.69	0.93
4:C:211:LYS:HB3	4:C:212:PRO:HD2	1.51	0.91
18:Q:115:SER:H	18:Q:118:GLN:HE21	1.08	0.91
11:J:162:SER:HB2	11:J:163:PRO:CD	2.00	0.91
6:E:236:THR:HG22	6:E:239:ALA:N	1.84	0.91
1:A:1165:G:H4'	1:A:1174:A:O2'	1.71	0.91
1:A:1474:C:H6	1:A:1474:C:H5'	1.35	0.90
1:A:541:C:H2'	1:A:542:A:H5''	1.53	0.90
15:N:106:ASN:ND2	35:N:8518:CL:CL	2.41	0.90
7:F:25:MET:HE2	7:F:41:LEU:HG	1.53	0.90
13:L:10:GLN:HE21	13:L:10:GLN:N	1.68	0.90
25:X:6:GLN:HB2	25:X:26:ILE:HD12	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:137:GLN:HE21	25:X:141:HIS:HE1	1.15	0.90
1:A:871:G:H5'	1:A:871:G:C8	2.06	0.90
11:J:55:GLN:HE21	11:J:124:ARG:HE	1.19	0.90
27:Z:200:THR:HG22	27:Z:201:GLU:HG3	1.54	0.90
5:D:62:ARG:HA	5:D:65:MET:HE3	1.54	0.89
1:A:1667:A:H5'	1:A:1667:A:H8	1.36	0.89
25:X:88:THR:HG23	25:X:110:GLN:HE21	1.37	0.89
5:D:86:ALA:HA	40:D:8574:HOH:O	1.71	0.88
28:1:58:GLY:HA3	40:1:8437:HOH:O	1.72	0.88
25:X:88:THR:HG22	25:X:89:ASP:H	1.37	0.88
28:1:38:LYS:HE2	28:1:45:LYS:HE2	1.53	0.88
1:A:21:G:H5'	20:S:2:ILE:HA	1.56	0.88
7:F:64:ARG:HG2	7:F:67:ASP:HB3	1.56	0.88
1:A:2812:A:H2	1:A:2814:A:H62	1.21	0.87
1:A:1835:U:H5	1:A:1840:A:N7	1.72	0.87
25:X:21:LEU:HD13	25:X:26:ILE:HD11	1.54	0.87
1:A:2717:C:C2'	1:A:2718:C:H5''	2.05	0.87
8:G:20:ILE:HD11	8:G:40:VAL:HG11	1.57	0.87
6:E:2:GLN:HB3	40:E:8336:HOH:O	1.75	0.87
40:A:3296:HOH:O	15:N:189:VAL:HG21	1.73	0.86
28:1:38:LYS:HG2	28:1:45:LYS:HG2	1.55	0.86
1:A:2586:U:H3	1:A:2592:G:H22	1.23	0.86
15:N:106:ASN:HD22	15:N:114:VAL:HG23	1.39	0.86
1:A:871:G:H5'	1:A:871:G:H8	1.39	0.86
25:X:68:THR:HG23	25:X:69:ARG:HG2	1.57	0.86
18:Q:115:SER:OG	18:Q:118:GLN:HG3	1.75	0.86
13:L:10:GLN:H	13:L:10:GLN:HE21	0.90	0.86
16:O:87:LEU:HD12	16:O:186:LEU:HD21	1.55	0.86
40:A:5806:HOH:O	7:F:99:ASP:HA	1.75	0.86
7:F:105:SER:HB2	7:F:131:THR:HG23	1.56	0.85
16:O:113:SER:HB2	40:O:8561:HOH:O	1.75	0.85
20:S:8:ALA:HB1	20:S:13:THR:HG21	1.59	0.85
2:B:3006:C:H5''	16:O:37:ARG:HH12	1.41	0.85
21:T:43:GLU:HB3	40:T:8344:HOH:O	1.75	0.85
5:D:212:GLN:HB2	5:D:257:THR:HG21	1.58	0.85
1:A:1166:A:H1'	1:A:1192:A:C2	2.12	0.85
15:N:102:GLU:OE1	15:N:164:THR:HG21	1.77	0.85
13:L:81:ARG:HB2	13:L:87:ARG:NH1	1.92	0.84
20:S:18:LEU:HD12	20:S:143:VAL:HG11	1.58	0.84
7:F:154:LYS:H	7:F:154:LYS:HD2	1.41	0.84
15:N:35:PRO:HG2	15:N:38:VAL:HG23	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:62:THR:HB	40:4:8550:HOH:O	1.76	0.84
6:E:1:MET:HG2	6:E:2:GLN:H	1.41	0.84
1:A:2506:A:HO2'	1:A:2507:G:H8	0.87	0.84
5:D:321:PRO:HA	40:D:8652:HOH:O	1.78	0.84
1:A:645:U:OP2	14:M:4:LYS:HE2	1.77	0.84
14:M:133:VAL:HA	40:M:8574:HOH:O	1.76	0.84
14:M:79:ASP:HB3	40:M:8559:HOH:O	1.78	0.83
1:A:962:C:H1'	16:O:5:ARG:NH1	1.93	0.83
1:A:381:G:H5''	40:A:3830:HOH:O	1.77	0.83
1:A:1625:U:H4'	40:A:4182:HOH:O	1.76	0.83
1:A:1116:U:H3	1:A:1246:A:H62	1.26	0.83
1:A:1184:C:H1'	40:A:6979:HOH:O	1.77	0.83
21:T:57:THR:HG22	21:T:59:ASP:H	1.43	0.83
11:J:139:ASP:N	11:J:140:PRO:HD3	1.94	0.83
7:F:25:MET:HE1	7:F:37:ALA:HB1	1.59	0.83
1:A:1701:A:H5'	40:A:5794:HOH:O	1.80	0.82
5:D:238:ASN:HD22	5:D:240:GLY:H	1.23	0.82
14:M:68:GLU:HA	40:M:8542:HOH:O	1.79	0.82
1:A:1116:U:O2'	1:A:1118:A:H2	1.62	0.82
1:A:2717:C:H2'	1:A:2718:C:H5''	1.60	0.82
8:G:81:GLU:HG2	8:G:134:SER:HB3	1.61	0.82
7:F:146:LYS:NZ	16:O:107:ASN:HD21	1.77	0.82
11:J:27:LYS:H	11:J:58:HIS:HD2	1.27	0.82
6:E:242:GLU:HG3	40:E:8380:HOH:O	1.79	0.82
1:A:2780:C:H1'	8:G:143:GLN:HE21	1.44	0.81
31:4:25:VAL:HG22	31:4:68:LYS:HG3	1.60	0.81
1:A:1116:U:HO2'	1:A:1118:A:H2	0.81	0.81
1:A:2526:C:O2'	1:A:2527:U:H5'	1.80	0.81
13:L:39:GLY:HA2	40:L:4183:HOH:O	1.80	0.81
1:A:711:G:H1'	40:A:6602:HOH:O	1.80	0.81
1:A:2506:A:O2'	1:A:2507:G:H8	1.63	0.81
16:O:49:THR:HG22	16:O:56:ASP:HB2	1.63	0.81
6:E:127:ARG:NH2	6:E:225:PRO:HG2	1.96	0.81
11:J:4:ALA:HB3	40:J:8367:HOH:O	1.80	0.81
11:J:59:ASN:H	11:J:59:ASN:HD22	1.27	0.81
25:X:65:VAL:HA	25:X:68:THR:HG22	1.62	0.81
8:G:15:GLN:HG3	8:G:20:ILE:HG12	1.62	0.80
31:4:70:ARG:HG2	31:4:77:ALA:HB2	1.63	0.80
7:F:27:ILE:HG22	7:F:28:GLY:H	1.46	0.80
25:X:88:THR:HG23	25:X:110:GLN:NE2	1.96	0.80
1:A:506:G:H22	1:A:509:A:C5'	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:62:PRO:HG3	13:L:65:ARG:HH21	1.47	0.80
24:W:1:THR:HG23	24:W:2:VAL:H	1.46	0.80
4:C:88:ILE:HD13	4:C:100:PRO:HD3	1.64	0.80
6:E:78:ARG:HG3	6:E:78:ARG:HH11	1.47	0.80
6:E:236:THR:HG21	40:E:8372:HOH:O	1.82	0.80
11:J:165:GLY:HA3	40:J:8396:HOH:O	1.80	0.80
7:F:20:LYS:HA	7:F:75:LEU:O	1.82	0.80
40:A:6283:HOH:O	16:O:4:PRO:HD2	1.82	0.80
2:B:3023:U:H5''	2:B:3024:U:OP2	1.81	0.80
4:C:100:PRO:HG2	4:C:103:VAL:HG21	1.63	0.80
1:A:541:C:C2'	1:A:542:A:H5''	2.10	0.80
1:A:544:G:H2'	1:A:545:G:H5''	1.63	0.80
30:3:39:ARG:HG2	40:3:3143:HOH:O	1.81	0.79
1:A:545:G:H5'	1:A:545:G:H8	1.47	0.79
25:X:4:LEU:HD22	25:X:52:VAL:HG21	1.62	0.79
1:A:272:A:H3'	40:A:7046:HOH:O	1.81	0.79
1:A:1701:A:H4'	1:A:1702:U:H5''	1.62	0.79
17:P:96:VAL:HA	40:P:4258:HOH:O	1.81	0.79
1:A:870:G:C2'	1:A:871:G:H5''	2.12	0.79
1:A:2004:U:H4'	40:A:4823:HOH:O	1.80	0.79
1:A:2890:A:H1'	23:V:56:ARG:NH2	1.98	0.79
1:A:288:A:H61	1:A:364:C:H42	1.31	0.79
11:J:49:VAL:O	11:J:157:ILE:HG23	1.82	0.79
1:A:536:A:H3'	40:A:4563:HOH:O	1.82	0.79
4:C:35:GLY:O	4:C:36:ASP:HB3	1.82	0.79
25:X:72:PRO:HG2	25:X:77:ALA:HB3	1.65	0.79
1:A:2716:G:H5''	5:D:206:THR:HG21	1.66	0.78
8:G:97:VAL:HG12	40:G:4191:HOH:O	1.82	0.78
11:J:150:LYS:HE2	40:J:8383:HOH:O	1.82	0.78
31:4:70:ARG:HD3	40:4:8539:HOH:O	1.83	0.78
1:A:657:G:OP1	6:E:27:ARG:NH2	2.17	0.78
11:J:14:TYR:H	11:J:91:HIS:CE1	2.01	0.78
28:1:46:LYS:HD3	28:1:59:HIS:HB2	1.64	0.78
1:A:2533:C:H6	1:A:2533:C:H5'	1.47	0.78
24:W:12:THR:HG22	24:W:15:GLU:CG	2.12	0.78
1:A:1160:G:C5'	1:A:1161:A:H5'	2.11	0.78
11:J:55:GLN:NE2	11:J:124:ARG:HE	1.80	0.78
27:Z:185:VAL:HG12	40:Z:8565:HOH:O	1.84	0.78
11:J:59:ASN:HD22	11:J:59:ASN:N	1.81	0.78
15:N:35:PRO:CG	15:N:38:VAL:HG23	2.14	0.77
40:A:4376:HOH:O	15:N:14:ARG:HG2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:192:VAL:HB	40:C:8592:HOH:O	1.82	0.77
6:E:139:VAL:HG13	40:E:8450:HOH:O	1.83	0.77
5:D:201:ASP:HB2	5:D:312:ARG:HD2	1.65	0.77
11:J:2:PRO:HB2	40:J:8367:HOH:O	1.84	0.77
40:A:4465:HOH:O	2:B:3103:A:H4'	1.84	0.77
6:E:236:THR:CG2	6:E:239:ALA:H	1.93	0.77
9:H:58:GLU:HA	9:H:61:MET:HE2	1.65	0.77
1:A:1372:A:H3'	40:A:6696:HOH:O	1.83	0.77
6:E:5:ILE:HD11	6:E:16:VAL:CG2	2.14	0.77
1:A:21:G:C5'	20:S:2:ILE:HA	2.14	0.77
1:A:289:G:H22	1:A:363:A:H2	1.32	0.77
1:A:1450:C:H4'	1:A:1451:C:OP2	1.85	0.77
20:S:39:THR:HG22	20:S:42:GLU:H	1.49	0.77
29:2:8:GLN:HE22	29:2:11:LYS:NZ	1.82	0.77
5:D:7:ARG:HG2	5:D:7:ARG:HH11	1.50	0.77
15:N:138:HIS:ND1	15:N:139:PRO:O	2.18	0.77
24:W:42:ASN:HB3	40:W:7247:HOH:O	1.84	0.77
28:1:61:GLY:HA3	40:1:8426:HOH:O	1.83	0.77
13:L:74:VAL:HG11	13:L:113:ILE:HG12	1.66	0.76
28:1:40:PRO:HD3	28:1:47:LEU:HD11	1.65	0.76
5:D:41:PHE:HB3	5:D:190:MET:HE3	1.67	0.76
7:F:64:ARG:CG	7:F:67:ASP:HB3	2.15	0.76
16:O:7:LYS:HE3	19:R:21:ARG:O	1.84	0.76
20:S:18:LEU:HG	20:S:91:LEU:HD13	1.65	0.76
15:N:139:PRO:O	15:N:140:ALA:HB3	1.86	0.76
18:Q:115:SER:H	18:Q:118:GLN:NE2	1.83	0.76
6:E:236:THR:HA	40:E:8453:HOH:O	1.86	0.76
9:H:96:ALA:HA	40:H:3111:HOH:O	1.84	0.76
11:J:162:SER:CB	11:J:163:PRO:HD3	2.14	0.76
17:P:47:ARG:HH11	17:P:47:ARG:HG3	1.50	0.76
6:E:104:ASP:HA	6:E:107:ARG:HH12	1.50	0.76
14:M:67:ARG:O	14:M:71:GLU:HG3	1.85	0.76
22:U:9:LYS:HE3	22:U:13:ARG:NH1	2.01	0.76
1:A:2054:A:N3	20:S:128:ARG:NH2	2.34	0.76
1:A:2768:A:H2'	1:A:2769:C:O4'	1.86	0.76
15:N:87:MET:HG2	31:4:46:ILE:HG21	1.68	0.76
1:A:1164:U:C4'	1:A:1165:G:OP1	2.33	0.76
1:A:1164:U:H3	1:A:1192:A:H2	1.30	0.76
6:E:236:THR:H	6:E:239:ALA:HB3	1.51	0.76
1:A:31:C:H2'	40:A:7207:HOH:O	1.86	0.75
4:C:69:LEU:HD21	4:C:120:ARG:HB3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:41:THR:HA	40:J:8394:HOH:O	1.83	0.75
1:A:1634:G:H3'	40:A:3404:HOH:O	1.85	0.75
1:A:1751:G:C2'	1:A:1752:G:H5''	2.16	0.75
1:A:1244:U:OP1	12:K:18:ILE:HD13	1.87	0.75
20:S:111:ILE:HG23	20:S:145:LEU:HD11	1.68	0.75
14:M:148:GLU:HA	40:M:8573:HOH:O	1.85	0.75
40:A:4057:HOH:O	11:J:151:MET:HE2	1.87	0.75
2:B:3006:C:OP1	16:O:37:ARG:NH1	2.20	0.75
27:Z:187:VAL:HG23	27:Z:192:ASP:HB2	1.66	0.75
1:A:284:C:H4'	1:A:285:A:O5'	1.85	0.74
28:1:37:HIS:HB2	28:1:47:LEU:HB2	1.69	0.74
15:N:172:GLY:O	15:N:183:VAL:HG11	1.87	0.74
24:W:39:ALA:N	24:W:40:PRO:HD2	2.03	0.74
40:A:3236:HOH:O	15:N:157:LEU:HD11	1.88	0.74
1:A:346:U:H4'	40:A:6357:HOH:O	1.86	0.74
16:O:23:ARG:HD3	40:O:8548:HOH:O	1.86	0.74
1:A:1118:A:H8	1:A:1118:A:H3'	1.52	0.74
1:A:1118:A:H3'	1:A:1118:A:C8	2.22	0.74
8:G:23:GLU:HG2	8:G:28:SER:HB3	1.69	0.74
1:A:560:C:H42	1:A:597:A:H61	1.35	0.74
12:K:45:VAL:HG23	12:K:130:VAL:O	1.87	0.74
26:Y:78:GLU:HG2	26:Y:79:GLU:H	1.53	0.74
25:X:137:GLN:HE21	25:X:141:HIS:CE1	2.03	0.74
1:A:1603:A:H5'	1:A:1605:G:O4'	1.88	0.74
2:B:3056:A:C2'	2:B:3057:A:H5''	2.18	0.74
18:Q:59:ARG:NH2	18:Q:66:GLN:HE22	1.85	0.74
1:A:2291:A:C8	1:A:2309:C:H5'	2.23	0.73
11:J:137:ASN:O	11:J:139:ASP:N	2.21	0.73
25:X:122:ARG:HH21	25:X:154:ARG:HD2	1.52	0.73
1:A:1329:A:H2	40:A:4198:HOH:O	1.70	0.73
40:A:5309:HOH:O	15:N:170:CYS:SG	2.45	0.73
1:A:877:G:H5'	1:A:878:G:OP1	1.89	0.73
1:A:1191:A:H3'	1:A:1192:A:H5''	1.69	0.73
1:A:2710:U:H1'	40:A:7141:HOH:O	1.88	0.73
2:B:3029:C:H2'	2:B:3030:C:H5'	1.70	0.73
7:F:146:LYS:HZ1	16:O:107:ASN:HD21	1.36	0.73
12:K:107:ASN:ND2	12:K:109:TYR:H	1.86	0.73
6:E:214:THR:HG21	40:E:8400:HOH:O	1.89	0.73
25:X:88:THR:HG22	25:X:89:ASP:N	2.04	0.73
8:G:166:VAL:HG12	40:G:3134:HOH:O	1.89	0.73
9:H:63:ILE:HB	9:H:64:PRO:HD3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:99:ALA:HB1	20:S:109:MET:CE	2.18	0.73
1:A:871:G:H8	1:A:871:G:C5'	2.02	0.72
22:U:47:THR:HB	22:U:100:ASP:HB3	1.71	0.72
1:A:1666:C:O2'	1:A:1667:A:H5''	1.89	0.72
1:A:542:A:H5'	1:A:542:A:C8	2.19	0.72
31:4:73:GLU:HB3	40:4:8561:HOH:O	1.90	0.72
16:O:164:ASP:CG	16:O:167:ASP:HA	2.10	0.72
1:A:282:C:H1'	1:A:368:C:N4	2.04	0.72
26:Y:71:ARG:HB3	26:Y:88:GLU:OE1	1.90	0.72
1:A:2270:G:H4'	4:C:223:ARG:HH12	1.55	0.72
4:C:105:VAL:HG11	4:C:154:ALA:HB1	1.72	0.72
7:F:88:LEU:HB2	7:F:89:PRO:HD3	1.72	0.72
10:I:12:ILE:N	10:I:13:PRO:HD3	2.03	0.72
15:N:34:GLU:HB3	15:N:35:PRO:HD2	1.71	0.72
15:N:87:MET:HB3	31:4:46:ILE:HD13	1.69	0.72
16:O:48:VAL:CG1	16:O:55:ASP:HB3	2.20	0.72
28:1:49:ARG:HD2	40:1:8428:HOH:O	1.89	0.72
40:A:3066:HOH:O	15:N:152:ARG:HG3	1.89	0.72
8:G:69:ILE:HA	8:G:72:MET:CE	2.20	0.72
1:A:2908:A:H2'	1:A:2909:G:O4'	1.90	0.72
7:F:54:ALA:HB2	7:F:69:ILE:HD12	1.71	0.72
1:A:214:U:H5'	40:A:5654:HOH:O	1.89	0.71
22:U:32:ARG:NH1	22:U:38:ARG:HH12	1.88	0.71
14:M:143:THR:HG22	14:M:144:ASP:N	2.05	0.71
16:O:80:SER:HB2	40:O:8536:HOH:O	1.89	0.71
11:J:140:PRO:HB3	40:J:8381:HOH:O	1.90	0.71
1:A:1119:G:H2'	12:K:52:GLN:NE2	2.06	0.71
4:C:96:LEU:HD22	4:C:128:LEU:HD13	1.73	0.71
11:J:84:ARG:NH2	11:J:135:TRP:HH2	1.89	0.71
16:O:164:ASP:OD2	16:O:167:ASP:HA	1.90	0.71
1:A:2094:G:H4'	5:D:245:SER:HB3	1.71	0.71
4:C:170:VAL:HG22	28:1:22:ILE:HG23	1.71	0.71
1:A:1160:G:H5'	1:A:1161:A:C5'	2.11	0.71
9:H:91:VAL:HG12	9:H:92:GLY:N	2.06	0.71
25:X:122:ARG:HG2	25:X:122:ARG:HH11	1.55	0.71
27:Z:189:ASN:HA	27:Z:217:ILE:HD11	1.73	0.70
1:A:1679:C:H5'	40:A:8834:HOH:O	1.90	0.70
9:H:50:VAL:HG13	9:H:60:VAL:HG11	1.72	0.70
22:U:61:GLU:HG3	40:U:3851:HOH:O	1.91	0.70
5:D:62:ARG:HA	5:D:65:MET:CE	2.21	0.70
22:U:41:ARG:HG2	22:U:41:ARG:HH11	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1667:A:H5'	1:A:1667:A:C8	2.24	0.70
9:H:53:ASP:OD1	9:H:80:GLN:HB2	1.92	0.70
11:J:141:ASN:HA	40:J:8369:HOH:O	1.90	0.70
20:S:106:GLY:HA2	20:S:109:MET:HE3	1.73	0.70
27:Z:187:VAL:HG23	27:Z:192:ASP:CB	2.21	0.70
30:3:41:HIS:H	30:3:45:ASN:HD22	1.37	0.70
1:A:1165:G:OP1	1:A:1165:G:H3'	1.90	0.70
11:J:130:HIS:CD2	11:J:133:ILE:HD11	2.26	0.70
20:S:18:LEU:HD12	20:S:143:VAL:CG1	2.20	0.70
1:A:506:G:H22	1:A:509:A:H5'	1.57	0.70
1:A:2414:A:H2'	1:A:2415:A:C8	2.26	0.70
5:D:36:PRO:HA	5:D:168:GLY:CA	2.21	0.70
1:A:1187:U:HO2'	1:A:1189:A:H2	1.39	0.70
5:D:307:ARG:HH11	5:D:307:ARG:HB2	1.55	0.70
1:A:1505:U:H6	1:A:1505:U:H5'	1.56	0.70
1:A:2426:G:H1'	40:A:5606:HOH:O	1.90	0.70
20:S:18:LEU:HB2	20:S:143:VAL:HG12	1.72	0.70
23:V:9:CYS:HA	23:V:52:THR:HG23	1.72	0.70
25:X:149:LEU:HG	25:X:153:MET:HE2	1.72	0.70
40:A:6934:HOH:O	22:U:9:LYS:HB2	1.90	0.70
11:J:142:VAL:HG13	40:J:8381:HOH:O	1.91	0.70
13:L:74:VAL:CG1	13:L:113:ILE:HG12	2.22	0.70
15:N:52:LEU:HD13	15:N:116:ASN:HB3	1.74	0.70
1:A:470:U:O2'	29:2:16:HIS:HD2	1.74	0.69
6:E:200:PRO:HB3	6:E:212:VAL:HG23	1.74	0.69
1:A:1206:U:H6	1:A:1206:U:H5'	1.55	0.69
40:A:7100:HOH:O	28:1:31:ILE:HG13	1.92	0.69
12:K:103:VAL:HG12	40:K:5907:HOH:O	1.91	0.69
5:D:162:MET:HE3	5:D:308:LEU:HD21	1.74	0.69
1:A:281:U:H2'	1:A:282:C:O4'	1.92	0.69
1:A:559:U:H6	1:A:559:U:H5'	1.57	0.69
5:D:329:TYR:CE2	23:V:15:PRO:HG2	2.27	0.69
22:U:9:LYS:HE3	22:U:13:ARG:HH11	1.58	0.69
1:A:182:G:H5'	40:A:4672:HOH:O	1.92	0.69
5:D:254:GLN:HG2	5:D:255:GLY:N	2.07	0.69
11:J:53:PRO:HG3	11:J:127:GLY:H	1.57	0.69
4:C:55:VAL:HG22	4:C:68:ILE:O	1.92	0.69
11:J:5:MET:HG3	40:J:8367:HOH:O	1.92	0.69
1:A:1119:G:H22	1:A:1246:A:H2	1.41	0.69
1:A:2896:A:H5''	40:A:5613:HOH:O	1.91	0.69
10:I:23:ILE:HD13	10:I:67:LEU:HD23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:91:VAL:HG12	9:H:92:GLY:H	1.58	0.69
13:L:14:LYS:HB2	13:L:45:PRO:HG2	1.74	0.69
25:X:21:LEU:HD22	25:X:26:ILE:CD1	2.23	0.69
28:1:39:CYS:HA	28:1:47:LEU:HD11	1.75	0.69
1:A:111:C:O2'	29:2:20:ARG:HG2	1.93	0.69
40:A:4349:HOH:O	12:K:47:THR:HB	1.92	0.69
11:J:26:LYS:HG2	11:J:28:ILE:H	1.58	0.69
11:J:33:MET:HB2	11:J:83:PHE:HB3	1.75	0.69
15:N:139:PRO:O	15:N:140:ALA:CB	2.39	0.69
6:E:180:SER:HB2	40:E:8447:HOH:O	1.93	0.68
14:M:133:VAL:HB	40:M:8558:HOH:O	1.92	0.68
1:A:2346:C:O2'	7:F:52:THR:HG21	1.94	0.68
13:L:22:ASP:HB2	40:L:5264:HOH:O	1.92	0.68
27:Z:133:HIS:HD2	40:Z:8577:HOH:O	1.76	0.68
28:1:38:LYS:HE2	28:1:45:LYS:CE	2.22	0.68
5:D:179:LEU:O	5:D:183:GLU:HG2	1.94	0.68
5:D:238:ASN:HD22	5:D:240:GLY:N	1.91	0.68
12:K:74:ARG:HB3	12:K:74:ARG:HH11	1.56	0.68
15:N:87:MET:HB3	31:4:46:ILE:HG21	1.73	0.68
1:A:1209:C:H4'	40:A:4796:HOH:O	1.93	0.68
13:L:32:ILE:HD11	13:L:56:SER:HB3	1.76	0.68
13:L:81:ARG:HD3	13:L:87:ARG:NH1	2.08	0.68
15:N:164:THR:HG23	15:N:165:SER:N	2.08	0.68
20:S:39:THR:HG23	20:S:107:GLU:O	1.94	0.68
25:X:13:MET:HE3	25:X:17:ILE:HG22	1.76	0.68
1:A:1185:U:H2'	1:A:1186:C:C6	2.28	0.68
2:B:3014:G:H5'	2:B:3014:G:H8	1.57	0.68
40:B:4707:HOH:O	16:O:147:ILE:HB	1.94	0.68
8:G:69:ILE:HA	8:G:72:MET:HE3	1.76	0.68
1:A:1170:U:O2'	1:A:1172:G:N7	2.24	0.68
1:A:2676:C:H4'	12:K:70:PHE:CE1	2.29	0.68
4:C:131:HIS:O	4:C:132:ASP:HB2	1.93	0.68
1:A:541:C:H2'	1:A:542:A:C5'	2.24	0.68
4:C:199:HIS:HD2	4:C:201:PHE:H	1.42	0.68
1:A:338:C:H5''	40:E:8420:HOH:O	1.93	0.68
1:A:871:G:C8	1:A:871:G:C5'	2.77	0.68
1:A:1209:C:H2'	1:A:1210:G:H8	1.57	0.68
1:A:1641:A:H2'	1:A:1642:A:H5'	1.75	0.68
12:K:93:ARG:HB3	12:K:93:ARG:HH11	1.57	0.68
1:A:1441:G:H1'	40:A:7283:HOH:O	1.92	0.68
4:C:191:GLY:HA2	4:C:194:MET:CE	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:14:GLU:O	23:V:17:THR:HB	1.94	0.68
8:G:68:HIS:O	8:G:72:MET:HG3	1.95	0.67
16:O:71:TRP:CE3	16:O:175:LEU:HD22	2.29	0.67
26:Y:72:VAL:HG22	26:Y:85:VAL:HG12	1.75	0.67
1:A:175:G:H2'	15:N:192:ALA:HB3	1.75	0.67
1:A:962:C:H1'	16:O:5:ARG:HH12	1.58	0.67
7:F:54:ALA:CB	7:F:69:ILE:HD12	2.24	0.67
11:J:57:ARG:HG3	40:J:8355:HOH:O	1.94	0.67
1:A:506:G:H22	1:A:509:A:H5''	1.60	0.67
1:A:553:G:P	27:Z:204:ARG:HH22	2.18	0.67
1:A:1119:G:N2	1:A:1246:A:C2	2.58	0.67
40:A:3269:HOH:O	22:U:9:LYS:HD3	1.94	0.67
7:F:174:VAL:HG13	40:F:6555:HOH:O	1.93	0.67
6:E:140:VAL:HB	40:E:8453:HOH:O	1.94	0.67
40:A:3356:HOH:O	11:J:11:LYS:HE2	1.93	0.67
21:T:57:THR:HG22	21:T:59:ASP:N	2.08	0.67
7:F:44:ILE:HG12	7:F:83:PHE:HE1	1.59	0.67
11:J:47:GLU:HB3	11:J:133:ILE:HD13	1.77	0.67
13:L:62:PRO:HG3	13:L:65:ARG:NH2	2.09	0.67
25:X:6:GLN:HB2	25:X:26:ILE:CD1	2.25	0.67
26:Y:15:ARG:HB3	26:Y:15:ARG:HH11	1.60	0.67
5:D:145:HIS:HD2	5:D:146:THR:O	1.75	0.67
7:F:99:ASP:HB2	7:F:103:ASN:HB2	1.77	0.67
26:Y:12:ILE:HD12	26:Y:36:HIS:ND1	2.10	0.67
31:4:65:THR:HG23	31:4:67:LEU:HG	1.77	0.67
1:A:183:A:H5'	15:N:157:LEU:HD12	1.76	0.66
5:D:51:VAL:CG2	5:D:327:VAL:HG13	2.25	0.66
1:A:200:U:H2'	40:A:9956:HOH:O	1.95	0.66
40:A:7199:HOH:O	15:N:154:ARG:HB2	1.95	0.66
4:C:210:GLY:HA3	40:C:8585:HOH:O	1.93	0.66
5:D:214:PRO:HD2	40:D:8521:HOH:O	1.96	0.66
23:V:14:GLU:OE1	23:V:15:PRO:HD2	1.95	0.66
29:2:21:ARG:HD2	29:2:37:CYS:SG	2.36	0.66
31:4:60:LYS:HG3	31:4:61:PRO:HD2	1.76	0.66
1:A:396:U:H1'	40:A:7149:HOH:O	1.95	0.66
1:A:558:C:H2'	1:A:559:U:H5'	1.78	0.66
11:J:47:GLU:HB3	11:J:133:ILE:CD1	2.25	0.66
20:S:39:THR:HB	20:S:42:GLU:HG3	1.75	0.66
1:A:2878:U:H2'	1:A:2879:A:O4'	1.96	0.66
7:F:135:VAL:HG21	7:F:139:TYR:CD1	2.30	0.66
15:N:164:THR:HG22	15:N:167:GLY:N	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:G:C2'	1:A:545:G:H5''	2.25	0.66
7:F:23:VAL:HG23	7:F:23:VAL:O	1.96	0.66
1:A:2840:A:OP1	5:D:211:THR:HG23	1.96	0.66
11:J:31:PHE:HE2	11:J:87:LYS:O	1.78	0.66
20:S:18:LEU:HB2	20:S:143:VAL:CG1	2.26	0.66
1:A:2748:G:H2'	40:A:7058:HOH:O	1.95	0.66
8:G:20:ILE:CD1	8:G:40:VAL:HG11	2.25	0.66
9:H:39:SER:HB3	9:H:45:ALA:HB2	1.77	0.66
27:Z:141:THR:HG23	40:Z:8584:HOH:O	1.95	0.66
40:A:3193:HOH:O	15:N:79:LYS:HD3	1.96	0.66
2:B:3006:C:C5'	16:O:37:ARG:NH1	2.55	0.66
4:C:33:GLU:O	4:C:34:ASP:HB2	1.95	0.66
13:L:75:ARG:CZ	40:L:4172:HOH:O	2.43	0.66
25:X:21:LEU:HD21	25:X:48:VAL:HG11	1.76	0.66
1:A:2241:C:O2'	1:A:2242:U:H5'	1.96	0.66
4:C:95:PRO:HG2	4:C:98:GLU:HG2	1.78	0.66
13:L:82:ARG:NH2	13:L:115:ARG:HG2	2.11	0.66
25:X:21:LEU:HD21	25:X:48:VAL:CG1	2.26	0.66
1:A:1741:U:H5'	1:A:1742:A:OP1	1.96	0.65
7:F:57:THR:HG23	7:F:63:ILE:HG22	1.78	0.65
9:H:99:THR:HA	40:H:3461:HOH:O	1.96	0.65
11:J:3:GLY:HA2	11:J:57:ARG:HH12	1.59	0.65
18:Q:115:SER:N	18:Q:118:GLN:HE21	1.89	0.65
1:A:1119:G:H8	12:K:52:GLN:HE22	1.42	0.65
6:E:12:THR:HB	40:E:8443:HOH:O	1.96	0.65
24:W:55:ARG:O	24:W:59:ILE:HG12	1.96	0.65
7:F:135:VAL:HG22	7:F:136:ARG:H	1.60	0.65
16:O:183:ASP:OD2	16:O:186:LEU:HD12	1.95	0.65
7:F:64:ARG:CD	7:F:67:ASP:HB3	2.27	0.65
11:J:56:ILE:HG22	11:J:61:LEU:HD22	1.77	0.65
11:J:150:LYS:HB2	11:J:157:ILE:HD12	1.78	0.65
25:X:137:GLN:NE2	25:X:141:HIS:HE1	1.93	0.65
1:A:1835:U:C5	1:A:1840:A:N7	2.62	0.65
4:C:121:ALA:O	4:C:124:VAL:HG22	1.96	0.65
1:A:31:C:H4'	40:A:6934:HOH:O	1.96	0.65
2:B:3055:U:H4'	2:B:3056:A:C8	2.31	0.65
6:E:237:GLU:HB2	40:E:8429:HOH:O	1.96	0.65
8:G:11:VAL:HG12	8:G:12:ASP:N	2.11	0.65
1:A:299:U:H5'	40:A:6846:HOH:O	1.97	0.65
5:D:71:VAL:HG11	5:D:296:LEU:HB3	1.78	0.65
11:J:83:PHE:HZ	11:J:146:TRP:HE1	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:32:ARG:O	17:P:32:ARG:HD3	1.96	0.65
23:V:52:THR:HG22	23:V:54:THR:H	1.62	0.65
2:B:3041:C:O4'	7:F:50:VAL:HG23	1.97	0.65
5:D:103:ASP:HB2	40:D:8587:HOH:O	1.96	0.65
5:D:190:MET:HE1	5:D:194:PHE:CD1	2.32	0.65
8:G:132:THR:HB	40:G:2227:HOH:O	1.96	0.65
12:K:19:MET:HE3	12:K:132:LEU:HD11	1.78	0.65
15:N:114:VAL:HG21	15:N:159:THR:HG21	1.77	0.65
18:Q:143:ALA:HA	40:Q:2178:HOH:O	1.97	0.65
20:S:132:ARG:HG2	20:S:133:ALA:N	2.12	0.65
1:A:236:A:H4'	1:A:237:G:H5'	1.79	0.65
40:A:6388:HOH:O	15:N:178:LYS:HB2	1.96	0.65
7:F:35:ALA:N	40:F:5576:HOH:O	2.29	0.65
24:W:64:GLY:O	24:W:65:ASP:HB2	1.95	0.65
1:A:2630:G:O6	4:C:206:ARG:NH2	2.30	0.65
4:C:223:ARG:HG3	40:C:8599:HOH:O	1.97	0.65
9:H:110:GLU:HG2	40:H:6926:HOH:O	1.97	0.65
1:A:2505:G:O2'	1:A:2506:A:H5'	1.98	0.64
4:C:105:VAL:CG1	4:C:154:ALA:HB1	2.26	0.64
5:D:204:GLY:HA3	40:D:8648:HOH:O	1.95	0.64
6:E:47:GLY:HA2	6:E:92:PRO:HB2	1.78	0.64
6:E:76:ARG:HD2	40:E:8432:HOH:O	1.95	0.64
6:E:115:LEU:O	6:E:118:THR:HB	1.97	0.64
16:O:47:LEU:HD13	16:O:97:VAL:HG11	1.78	0.64
18:Q:10:ALA:HA	18:Q:13:VAL:HG12	1.79	0.64
1:A:603:A:H5''	1:A:604:G:OP1	1.97	0.64
1:A:1474:C:H5'	1:A:1474:C:C6	2.25	0.64
1:A:2783:A:H3'	40:A:4748:HOH:O	1.96	0.64
4:C:200:PRO:HG2	4:C:225:VAL:HG21	1.80	0.64
5:D:18:ARG:HG3	5:D:256:GLN:HG3	1.80	0.64
7:F:37:ALA:O	7:F:40:ILE:HG12	1.97	0.64
14:M:72:ASN:HB2	40:M:8584:HOH:O	1.97	0.64
15:N:186:SER:O	15:N:189:VAL:HG12	1.97	0.64
27:Z:189:ASN:HD22	27:Z:189:ASN:C	1.99	0.64
1:A:450:C:OP1	6:E:184:ARG:NH2	2.22	0.64
1:A:1172:G:H1'	40:A:4487:HOH:O	1.95	0.64
4:C:81:GLN:HB2	4:C:92:ASN:ND2	2.12	0.64
31:4:17:HIS:O	31:4:18:GLN:HG3	1.97	0.64
1:A:951:A:C2'	1:A:952:G:H5'	2.27	0.64
1:A:1118:A:H8	1:A:1119:G:H5''	1.60	0.64
1:A:1766:U:O2	1:A:1778:A:H5'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2827:A:H2'	1:A:2828:G:O4'	1.97	0.64
5:D:36:PRO:HA	5:D:168:GLY:HA3	1.80	0.64
7:F:97:GLN:HG2	7:F:97:GLN:O	1.98	0.64
14:M:145:LEU:O	14:M:148:GLU:HG3	1.96	0.64
16:O:155:GLU:O	16:O:156:GLU:HG3	1.98	0.64
16:O:86:LEU:HD12	16:O:125:ALA:HB2	1.80	0.64
24:W:49:LEU:O	24:W:53:ILE:HG13	1.98	0.64
25:X:4:LEU:HD22	25:X:52:VAL:CG2	2.28	0.64
9:H:50:VAL:CG1	9:H:60:VAL:HG11	2.26	0.64
13:L:34:VAL:HG22	13:L:47:ALA:HB2	1.77	0.64
15:N:12:TRP:CE2	15:N:20:ILE:HD11	2.33	0.64
1:A:338:C:H4'	6:E:174:ILE:CD1	2.27	0.64
1:A:2064:U:H4'	1:A:2653:A:OP1	1.98	0.64
5:D:275:GLY:O	5:D:291:ASP:HA	1.97	0.64
6:E:78:ARG:HG3	6:E:78:ARG:NH1	2.13	0.64
7:F:19:GLU:HG3	40:F:6165:HOH:O	1.98	0.64
1:A:820:G:O2'	1:A:856:G:H4'	1.98	0.64
4:C:37:VAL:HG22	40:C:8594:HOH:O	1.98	0.64
5:D:62:ARG:CA	5:D:65:MET:HE3	2.25	0.64
11:J:26:LYS:HD2	11:J:28:ILE:CD1	2.25	0.64
27:Z:186:ARG:HG2	27:Z:186:ARG:HH11	1.63	0.64
28:1:42:CYS:SG	28:1:44:PHE:HB2	2.37	0.64
1:A:2346:C:O5'	1:A:2346:C:H6	1.80	0.64
1:A:2717:C:O2'	1:A:2718:C:H5''	1.96	0.64
6:E:1:MET:HG2	6:E:2:GLN:N	2.11	0.64
22:U:9:LYS:CE	22:U:13:ARG:NH1	2.61	0.64
25:X:4:LEU:O	25:X:32:CYS:HA	1.98	0.64
12:K:52:GLN:HG3	12:K:53:ILE:N	2.13	0.63
15:N:60:ILE:C	15:N:61:ILE:HD12	2.19	0.63
24:W:12:THR:CG2	24:W:15:GLU:HG3	2.18	0.63
1:A:902:G:N7	14:M:18:HIS:HD2	1.96	0.63
1:A:1730:G:H5'	1:A:1731:C:C5	2.34	0.63
29:2:8:GLN:HE22	29:2:11:LYS:HZ2	1.44	0.63
30:3:35:ARG:HB2	40:3:2691:HOH:O	1.99	0.63
1:A:1234:U:N3	5:D:244:PRO:HB3	2.14	0.63
4:C:170:VAL:HG13	28:1:22:ILE:HG21	1.79	0.63
5:D:141:ARG:HG2	5:D:165:ARG:HA	1.80	0.63
9:H:50:VAL:HG21	9:H:63:ILE:HG21	1.80	0.63
10:I:12:ILE:HD12	40:I:692:HOH:O	1.98	0.63
14:M:53:ARG:NH2	14:M:57:VAL:HG12	2.13	0.63
27:Z:220:GLU:HG2	40:Z:8547:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:C:O2'	1:A:283:U:H5'	1.98	0.63
1:A:285:A:H2'	1:A:286:U:O4'	1.99	0.63
1:A:1080:C:H4'	1:A:1081:A:OP1	1.98	0.63
40:A:3162:HOH:O	17:P:3:THR:HG21	1.98	0.63
5:D:267:LYS:HD3	40:D:8524:HOH:O	1.98	0.63
1:A:20:G:H21	20:S:117:HIS:HD2	1.47	0.63
1:A:1973:A:H5'	1:A:1973:A:H8	1.63	0.63
6:E:104:ASP:HA	6:E:107:ARG:NH1	2.12	0.63
8:G:31:ARG:NH1	8:G:68:HIS:CG	2.67	0.63
21:T:51:GLN:HE21	21:T:53:ASN:HD21	1.45	0.63
11:J:48:LEU:HG	11:J:157:ILE:HG21	1.80	0.63
1:A:2533:C:H5'	1:A:2533:C:C6	2.32	0.63
7:F:51:ARG:HD3	40:F:7636:HOH:O	1.99	0.63
8:G:172:PRO:HB3	40:G:6931:HOH:O	1.99	0.63
11:J:3:GLY:HA2	11:J:57:ARG:NH1	2.13	0.63
15:N:169:ARG:HD2	40:N:8590:HOH:O	1.99	0.63
26:Y:76:ARG:HH11	26:Y:76:ARG:HG3	1.63	0.63
4:C:105:VAL:HG13	4:C:155:THR:O	1.99	0.63
9:H:19:ALA:O	9:H:22:VAL:HG22	1.99	0.63
12:K:107:ASN:HD21	12:K:109:TYR:HB2	1.64	0.63
20:S:39:THR:HB	20:S:42:GLU:CG	2.28	0.63
25:X:21:LEU:HB3	25:X:26:ILE:HG12	1.81	0.63
1:A:738:G:H3'	40:A:6557:HOH:O	1.99	0.63
4:C:192:VAL:HG13	40:C:8557:HOH:O	1.96	0.63
7:F:41:LEU:HA	7:F:44:ILE:HG22	1.80	0.63
8:G:100:ASP:HB2	40:G:2789:HOH:O	1.99	0.63
11:J:45:GLN:HG3	11:J:135:TRP:NE1	2.14	0.63
21:T:81:ILE:HG23	40:T:8336:HOH:O	1.99	0.63
30:3:41:HIS:N	30:3:45:ASN:HD22	1.95	0.63
2:B:3069:U:OP1	16:O:4:PRO:HG3	1.99	0.62
7:F:99:ASP:CB	7:F:103:ASN:H	2.12	0.62
15:N:37:VAL:CG1	15:N:63:VAL:HG11	2.29	0.62
20:S:9:ASP:O	20:S:13:THR:HB	1.99	0.62
1:A:2862:G:H4'	5:D:336:GLN:O	1.98	0.62
2:B:3054:A:O2'	2:B:3055:U:H5'	1.99	0.62
11:J:139:ASP:H	11:J:140:PRO:HD3	1.63	0.62
26:Y:31:ILE:O	26:Y:35:GLU:HG3	1.99	0.62
5:D:41:PHE:CD1	5:D:79:MET:HE2	2.34	0.62
11:J:27:LYS:N	11:J:58:HIS:HD2	1.95	0.62
16:O:154:LEU:O	16:O:155:GLU:HB3	2.00	0.62
1:A:2769:C:H2'	1:A:2770:G:O4'	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:64:ASN:HD22	10:I:64:ASN:N	1.96	0.62
11:J:69:ASN:O	11:J:72:VAL:HG12	1.98	0.62
14:M:148:GLU:HG2	40:M:8551:HOH:O	2.00	0.62
25:X:149:LEU:HG	25:X:153:MET:CE	2.29	0.62
1:A:281:U:H3'	40:A:6714:HOH:O	2.00	0.62
1:A:1134:G:H4'	11:J:151:MET:CE	2.21	0.62
1:A:1189:A:H3'	40:A:7200:HOH:O	1.99	0.62
1:A:2679:G:H2'	1:A:2681:A:OP2	2.00	0.62
1:A:1053:G:OP1	11:J:12:PRO:HG3	1.98	0.62
7:F:69:ILE:HG22	7:F:69:ILE:O	1.99	0.62
11:J:127:GLY:O	11:J:128:ALA:HB3	2.00	0.62
40:L:408:HOH:O	23:V:37:GLU:HB3	2.00	0.62
15:N:63:VAL:HG21	15:N:109:PHE:CE1	2.35	0.62
21:T:23:LYS:HE2	40:T:8330:HOH:O	1.98	0.62
1:A:1787:C:OP1	18:Q:68:LYS:HE2	2.00	0.62
1:A:1819:G:H2'	1:A:1820:G:H4'	1.82	0.62
4:C:199:HIS:CD2	4:C:201:PHE:H	2.17	0.62
8:G:84:MET:HE1	8:G:148:ILE:HD12	1.81	0.62
1:A:2508:C:H2'	40:A:6265:HOH:O	2.00	0.62
1:A:2830:U:H3'	40:A:4744:HOH:O	1.98	0.62
6:E:27:ARG:HG3	6:E:29:ASP:OD1	2.00	0.62
4:C:36:ASP:OD2	4:C:85:ASP:HB2	1.98	0.62
15:N:104:ARG:O	15:N:108:LYS:HE2	1.99	0.62
25:X:21:LEU:HD22	25:X:26:ILE:HD11	1.81	0.62
1:A:558:C:O2'	1:A:559:U:H5''	1.99	0.61
1:A:1213:C:O2'	1:A:1214:G:H5'	2.00	0.61
1:A:2503:A:OP1	11:J:147:ARG:NH2	2.33	0.61
4:C:153:ARG:HB2	4:C:153:ARG:HH11	1.64	0.61
1:A:1377:C:H6	1:A:1377:C:H5'	1.65	0.61
1:A:2456:A:H5'	40:A:5213:HOH:O	2.00	0.61
1:A:2690:U:O2'	8:G:111:LYS:HE3	2.00	0.61
40:A:6967:HOH:O	5:D:211:THR:HG21	1.98	0.61
15:N:61:ILE:HG13	40:N:8624:HOH:O	2.00	0.61
23:V:52:THR:HG22	23:V:54:THR:N	2.15	0.61
1:A:1666:C:H2'	1:A:1667:A:H5'	1.81	0.61
1:A:2420:G:O2'	1:A:2421:G:H5'	2.00	0.61
7:F:27:ILE:HG22	7:F:28:GLY:N	2.16	0.61
15:N:77:PHE:HD2	40:N:8527:HOH:O	1.83	0.61
11:J:85:ILE:HB	11:J:132:PHE:CE2	2.35	0.61
13:L:29:LEU:HB3	13:L:55:VAL:CG1	2.26	0.61
1:A:1058:A:H2'	1:A:1060:C:H5''	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1771:U:H4'	28:1:20:LEU:HD21	1.81	0.61
9:H:2:VAL:HG22	9:H:57:GLU:OE1	2.00	0.61
17:P:42:GLU:HB2	40:P:2176:HOH:O	1.98	0.61
1:A:1615:A:H4'	40:A:5402:HOH:O	2.01	0.61
40:A:8627:HOH:O	6:E:103:ASN:HB3	2.00	0.61
8:G:3:VAL:HG22	8:G:49:ILE:HB	1.83	0.61
11:J:44:ALA:HA	11:J:163:PRO:O	2.00	0.61
21:T:33:SER:OG	21:T:36:GLU:HG3	2.01	0.61
25:X:106:THR:OG1	25:X:109:GLU:HG3	2.00	0.61
1:A:1329:A:C2	40:A:4198:HOH:O	2.50	0.61
14:M:136:ALA:HB3	40:M:8574:HOH:O	2.00	0.61
27:Z:187:VAL:CG2	27:Z:192:ASP:HB2	2.29	0.61
1:A:2578:G:H5'	1:A:2578:G:H8	1.65	0.61
1:A:2756:U:H3	1:A:2896:A:H2	1.48	0.61
40:A:5046:HOH:O	15:N:58:GLN:HG3	2.00	0.61
7:F:38:GLU:HB3	7:F:49:PRO:HG2	1.82	0.61
10:I:12:ILE:HA	40:I:4499:HOH:O	1.99	0.61
40:A:4038:HOH:O	15:N:94:LYS:HE3	1.99	0.61
2:B:3048:C:H4'	16:O:141:ARG:HH21	1.65	0.61
16:O:157:PRO:HA	40:O:8526:HOH:O	1.99	0.61
27:Z:200:THR:HG22	27:Z:201:GLU:CG	2.30	0.61
1:A:2547:C:OP2	5:D:5:ARG:NH1	2.34	0.61
7:F:136:ARG:HD2	7:F:155:HIS:O	2.00	0.61
16:O:169:PRO:O	16:O:172:PHE:HB3	2.01	0.61
20:S:25:PHE:CE2	20:S:29:LYS:HE2	2.36	0.61
20:S:111:ILE:HG23	20:S:145:LEU:CD1	2.31	0.61
1:A:710:G:OP1	17:P:24:ALA:HB3	2.01	0.60
1:A:2256:G:H2'	1:A:2257:G:H5'	1.83	0.60
40:A:5644:HOH:O	30:3:20:ARG:HB3	2.00	0.60
8:G:15:GLN:NE2	8:G:40:VAL:O	2.33	0.60
11:J:166:ASN:N	11:J:166:ASN:HD22	1.97	0.60
24:W:44:GLY:O	24:W:48:GLU:HG2	2.01	0.60
1:A:1328:A:OP1	27:Z:169:ARG:HD2	2.02	0.60
1:A:1684:A:H1'	30:3:43:ARG:HH22	1.66	0.60
2:B:3039:U:H1'	2:B:3044:A:H61	1.65	0.60
6:E:162:VAL:HG12	6:E:192:ILE:HD11	1.83	0.60
7:F:95:THR:O	7:F:97:GLN:N	2.30	0.60
7:F:146:LYS:NZ	16:O:107:ASN:ND2	2.49	0.60
15:N:87:MET:CB	31:4:46:ILE:HG21	2.30	0.60
1:A:282:C:H1'	1:A:368:C:H42	1.65	0.60
1:A:1187:U:O2'	1:A:1189:A:H2	1.85	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:5036:HOH:O	5:D:298:LYS:HD3	2.01	0.60
4:C:190:ARG:NH2	4:C:207:GLN:OE1	2.35	0.60
4:C:191:GLY:HA2	4:C:194:MET:HE2	1.82	0.60
6:E:162:VAL:HG13	6:E:232:LEU:HD21	1.83	0.60
8:G:6:GLU:HA	8:G:46:THR:HG22	1.84	0.60
11:J:46:VAL:O	11:J:146:TRP:HH2	1.84	0.60
40:L:1387:HOH:O	23:V:20:MET:HE3	2.00	0.60
17:P:113:VAL:O	17:P:114:ILE:HD13	2.01	0.60
22:U:24:ARG:HH21	22:U:39:ASN:HD22	1.49	0.60
1:A:289:G:N2	1:A:363:A:H2	1.97	0.60
2:B:3026:C:H2'	2:B:3027:C:C6	2.36	0.60
10:I:12:ILE:N	10:I:13:PRO:CD	2.65	0.60
15:N:57:LYS:HE2	15:N:140:ALA:O	2.00	0.60
2:B:3055:U:H4'	2:B:3056:A:H8	1.65	0.60
5:D:154:VAL:HG12	5:D:156:LYS:HG2	1.83	0.60
7:F:25:MET:CE	7:F:37:ALA:HB1	2.31	0.60
11:J:84:ARG:CZ	11:J:135:TRP:HH2	2.14	0.60
16:O:71:TRP:HE3	16:O:175:LEU:HD22	1.66	0.60
18:Q:13:VAL:HG21	18:Q:41:ARG:HG2	1.84	0.60
20:S:119:VAL:O	20:S:119:VAL:HG12	2.00	0.60
24:W:56:ILE:O	24:W:60:GLN:HG3	2.02	0.60
1:A:1615:A:H5'	40:A:3695:HOH:O	2.02	0.60
1:A:2851:G:O2'	1:A:2852:A:H5'	2.01	0.60
5:D:42:ALA:HB1	5:D:308:LEU:HD11	1.83	0.60
13:L:74:VAL:HG13	13:L:113:ILE:HG23	1.82	0.60
20:S:17:MET:HE1	20:S:19:ARG:NH2	2.16	0.60
25:X:122:ARG:NH2	25:X:154:ARG:HD2	2.16	0.60
28:1:28:ASP:O	28:1:31:ILE:HG22	2.02	0.60
1:A:69:A:H5'	1:A:69:A:C8	2.37	0.60
4:C:93:THR:HG23	4:C:154:ALA:O	2.02	0.60
1:A:1119:G:H2'	12:K:52:GLN:HE22	1.66	0.60
1:A:1314:U:H2'	40:A:5390:HOH:O	2.02	0.60
4:C:211:LYS:HB3	4:C:212:PRO:CD	2.28	0.60
11:J:59:ASN:H	11:J:59:ASN:ND2	2.00	0.60
11:J:136:VAL:HG22	11:J:137:ASN:O	2.01	0.60
1:A:793:A:H5''	18:Q:83:LYS:HG2	1.84	0.60
1:A:1086:A:C6	25:X:11:VAL:HG11	2.36	0.60
1:A:558:C:H2'	1:A:559:U:C5'	2.32	0.59
1:A:1701:A:H4'	1:A:1702:U:C5'	2.31	0.59
7:F:19:GLU:O	7:F:20:LYS:HG2	2.02	0.59
13:L:115:ARG:HG3	13:L:116:GLU:N	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:120:LEU:HD12	14:M:133:VAL:HG21	1.84	0.59
20:S:39:THR:HB	20:S:42:GLU:CD	2.22	0.59
1:A:280:C:H2'	1:A:281:U:O4'	2.03	0.59
1:A:1182:C:H1'	1:A:1192:A:H8	1.67	0.59
11:J:75:SER:HB3	11:J:79:ALA:HB1	1.84	0.59
25:X:154:ARG:C	40:X:4276:HOH:O	2.39	0.59
16:O:159:TYR:HB3	16:O:162:ASP:HB2	1.84	0.59
26:Y:25:ARG:HG2	40:Y:5356:HOH:O	2.03	0.59
1:A:2815:G:OP2	12:K:99:GLU:HG2	2.03	0.59
15:N:52:LEU:HD21	40:N:8617:HOH:O	2.02	0.59
18:Q:105:LEU:HD21	18:Q:137:LEU:HD21	1.85	0.59
1:A:188:C:H5''	15:N:163:LEU:HD21	1.84	0.59
1:A:1299:G:O6	14:M:6:ARG:HD3	2.03	0.59
1:A:1594:C:OP2	18:Q:120:ARG:HD2	2.02	0.59
1:A:2502:C:H4'	11:J:151:MET:HG2	1.85	0.59
40:A:3495:HOH:O	22:U:82:THR:HA	2.01	0.59
11:J:139:ASP:HA	40:J:8373:HOH:O	2.02	0.59
1:A:681:G:H5'	1:A:681:G:N3	2.18	0.59
5:D:162:MET:CE	5:D:308:LEU:HD21	2.32	0.59
9:H:47:LEU:HB2	9:H:108:LEU:HD11	1.85	0.59
11:J:75:SER:O	11:J:79:ALA:HB2	2.02	0.59
16:O:47:LEU:HD12	16:O:92:ALA:HB1	1.84	0.59
26:Y:43:VAL:HG12	26:Y:44:ASP:N	2.16	0.59
1:A:371:U:H2'	1:A:372:A:H8	1.67	0.59
1:A:1654:U:H2'	4:C:47:HIS:HD2	1.67	0.59
4:C:132:ASP:OD1	4:C:133:ARG:N	2.34	0.59
5:D:55:ASN:HB3	5:D:63:GLU:HA	1.84	0.59
6:E:118:THR:O	6:E:136:VAL:HG13	2.02	0.59
8:G:23:GLU:HG2	8:G:28:SER:CB	2.33	0.59
17:P:39:THR:O	17:P:115:ARG:NH2	2.36	0.59
20:S:132:ARG:CZ	40:S:8582:HOH:O	2.49	0.59
1:A:538:C:OP2	27:Z:134:HIS:HE1	1.86	0.59
4:C:232:ARG:NH2	4:C:236:GLY:O	2.29	0.59
10:I:12:ILE:HG22	10:I:12:ILE:O	2.03	0.59
13:L:34:VAL:CG2	13:L:47:ALA:HB2	2.31	0.59
24:W:39:ALA:C	24:W:41:GLU:H	2.06	0.59
28:1:26:VAL:O	28:1:30:GLU:HG3	2.03	0.59
10:I:12:ILE:HG13	40:I:6833:HOH:O	2.02	0.59
11:J:55:GLN:HE22	11:J:91:HIS:CD2	2.20	0.59
11:J:136:VAL:HG23	40:J:8345:HOH:O	2.02	0.59
27:Z:189:ASN:ND2	27:Z:192:ASP:H	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1266:U:H4'	27:Z:115:ARG:HH21	1.66	0.59
6:E:168:ARG:NH2	6:E:190:ALA:O	2.35	0.59
13:L:106:GLY:HA3	40:L:5264:HOH:O	2.02	0.59
25:X:38:THR:HG22	40:X:3580:HOH:O	2.02	0.59
26:Y:25:ARG:HD2	40:Y:3861:HOH:O	2.03	0.59
26:Y:43:VAL:CG1	26:Y:47:ALA:HB3	2.32	0.59
1:A:431:G:P	15:N:48:ARG:HH12	2.26	0.58
1:A:2256:G:H2'	1:A:2257:G:C5'	2.33	0.58
2:B:3044:A:O4'	7:F:76:ARG:NE	2.36	0.58
6:E:76:ARG:HD3	40:E:8366:HOH:O	2.03	0.58
6:E:200:PRO:HB3	6:E:212:VAL:CG2	2.32	0.58
11:J:118:PRO:HD2	40:J:8341:HOH:O	2.01	0.58
15:N:74:ARG:HH11	15:N:74:ARG:HG3	1.68	0.58
24:W:58:THR:O	24:W:62:GLU:HG3	2.03	0.58
27:Z:117:LEU:HD12	27:Z:174:VAL:CG1	2.33	0.58
1:A:119:A:H2'	1:A:120:A:H5''	1.84	0.58
2:B:3092:G:H2'	2:B:3093:A:C8	2.38	0.58
7:F:55:LYS:HA	40:F:6752:HOH:O	2.02	0.58
15:N:48:ARG:NH2	40:N:8563:HOH:O	2.33	0.58
16:O:62:HIS:HB3	16:O:65:ASP:OD1	2.03	0.58
16:O:151:ASP:O	16:O:154:LEU:HB2	2.03	0.58
28:1:19:GLY:O	28:1:23:ARG:HG2	2.03	0.58
1:A:2672:C:H1'	40:D:8629:HOH:O	2.04	0.58
1:A:2694:A:H4'	8:G:91:PHE:CE1	2.37	0.58
5:D:195:ARG:HG2	5:D:323:LEU:HD22	1.84	0.58
7:F:166:ILE:HD12	40:F:6326:HOH:O	2.04	0.58
12:K:131:THR:HG22	12:K:133:GLY:N	2.18	0.58
30:3:40:ARG:HA	30:3:45:ASN:ND2	2.18	0.58
1:A:69:A:H5'	1:A:69:A:H8	1.68	0.58
1:A:272:A:H5'	1:A:273:G:OP2	2.03	0.58
1:A:2320:U:H4'	1:A:2321:A:O4'	2.03	0.58
1:A:2548:C:OP2	5:D:5:ARG:NH2	2.36	0.58
5:D:217:ARG:HG3	5:D:257:THR:HG22	1.84	0.58
5:D:314:ALA:HB3	5:D:317:PRO:HG3	1.85	0.58
7:F:25:MET:CE	7:F:41:LEU:HG	2.28	0.58
7:F:23:VAL:HG22	7:F:73:VAL:HB	1.86	0.58
7:F:86:THR:O	7:F:90:LEU:HG	2.04	0.58
23:V:46:ALA:HB1	23:V:52:THR:HG21	1.86	0.58
1:A:138:U:H5''	1:A:139:C:OP2	2.04	0.58
1:A:2081:A:H4'	12:K:69:TYR:CE1	2.39	0.58
5:D:175:LEU:HD23	5:D:175:LEU:C	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:103:THR:HA	18:Q:106:ARG:NH1	2.18	0.58
29:2:28:HIS:CD2	29:2:30:LYS:HB2	2.38	0.58
1:A:447:A:O2'	1:A:448:G:H5'	2.04	0.58
15:N:79:LYS:HD2	40:N:8556:HOH:O	2.02	0.58
16:O:78:MET:HB2	16:O:79:PRO:HD3	1.85	0.58
1:A:1351:G:OP1	6:E:96:LYS:NZ	2.32	0.58
1:A:2604:A:H5'	40:A:5307:HOH:O	2.04	0.58
8:G:137:ASP:OD1	8:G:139:GLU:HB2	2.04	0.58
11:J:71:TYR:C	11:J:73:GLN:H	2.07	0.58
16:O:61:ALA:HB3	16:O:88:ALA:HB2	1.86	0.58
19:R:64:GLU:HG3	19:R:74:ASP:OD2	2.04	0.58
27:Z:151:SER:HB3	27:Z:154:ARG:HB3	1.85	0.58
28:1:30:GLU:HA	28:1:33:HIS:HB3	1.84	0.58
1:A:1118:A:H62	1:A:1244:U:H3	1.50	0.58
1:A:2780:C:H1'	8:G:143:GLN:NE2	2.17	0.58
9:H:58:GLU:OE1	15:N:27:ARG:NH2	2.32	0.58
22:U:69:LYS:O	22:U:71:VAL:HG23	2.04	0.58
1:A:2453:G:H5'	40:A:4206:HOH:O	2.04	0.57
5:D:258:GLY:H	5:D:260:HIS:CE1	2.22	0.57
15:N:61:ILE:HA	40:N:8624:HOH:O	2.04	0.57
15:N:87:MET:CB	31:4:46:ILE:HD13	2.33	0.57
15:N:87:MET:CG	31:4:46:ILE:HG21	2.33	0.57
25:X:141:HIS:HB2	25:X:146:ILE:HG12	1.85	0.57
1:A:709:G:O2'	17:P:25:VAL:HG12	2.03	0.57
1:A:1162:G:H2'	40:A:6094:HOH:O	2.05	0.57
1:A:1441:G:O2'	1:A:1442:A:H5'	2.04	0.57
1:A:1972:U:H2'	1:A:1973:A:H5'	1.86	0.57
1:A:2769:C:O2'	1:A:2770:G:H5'	2.04	0.57
5:D:108:GLU:HB3	5:D:111:ARG:HD2	1.86	0.57
15:N:45:ARG:CZ	15:N:48:ARG:HG3	2.34	0.57
1:A:1123:A:C6	1:A:1238:C:H5'	2.39	0.57
1:A:1197:G:N2	40:A:5746:HOH:O	2.37	0.57
12:K:19:MET:CE	12:K:132:LEU:HD11	2.35	0.57
14:M:143:THR:CG2	14:M:144:ASP:N	2.67	0.57
1:A:2270:G:H4'	4:C:223:ARG:NH1	2.20	0.57
2:B:3013:A:O2'	2:B:3014:G:H5''	2.04	0.57
2:B:3026:C:H2'	2:B:3027:C:H6	1.69	0.57
17:P:105:ASN:HD21	17:P:109:SER:H	1.52	0.57
20:S:106:GLY:HA2	20:S:109:MET:CE	2.33	0.57
25:X:13:MET:HE1	25:X:18:GLN:HA	1.86	0.57
1:A:1118:A:C8	1:A:1119:G:H5''	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:U:H2'	1:A:1334:C:C6	2.39	0.57
1:A:2721:U:H4'	13:L:87:ARG:HG3	1.86	0.57
2:B:3041:C:C6	7:F:50:VAL:HG21	2.38	0.57
4:C:51:ARG:NH1	4:C:120:ARG:O	2.38	0.57
4:C:94:LEU:HG	4:C:99:ILE:HD11	1.86	0.57
8:G:7:ILE:HD11	8:G:11:VAL:C	2.24	0.57
11:J:35:ASN:ND2	11:J:80:ASN:HA	2.18	0.57
13:L:45:PRO:HB2	40:L:7169:HOH:O	2.04	0.57
13:L:74:VAL:HG12	13:L:75:ARG:HG3	1.85	0.57
1:A:584:U:H3'	40:A:5609:HOH:O	2.03	0.57
1:A:2769:C:C2'	1:A:2770:G:H5'	2.35	0.57
7:F:101:THR:HG22	40:F:7400:HOH:O	2.04	0.57
12:K:130:VAL:HG12	12:K:131:THR:N	2.19	0.57
24:W:39:ALA:N	24:W:40:PRO:CD	2.67	0.57
25:X:108:ARG:HG3	40:X:3483:HOH:O	2.04	0.57
30:3:22:PRO:HG2	30:3:25:VAL:HG23	1.87	0.57
7:F:105:SER:CB	7:F:131:THR:HG23	2.31	0.57
8:G:31:ARG:HH12	8:G:68:HIS:CE1	2.23	0.57
11:J:28:ILE:HA	11:J:62:GLU:OE1	2.05	0.57
15:N:38:VAL:C	15:N:63:VAL:HG13	2.25	0.57
16:O:86:LEU:O	16:O:90:LEU:HG	2.05	0.57
26:Y:74:ALA:HB2	26:Y:85:VAL:HG13	1.85	0.57
1:A:130:C:H2'	40:A:9668:HOH:O	2.05	0.57
1:A:621:C:H5'	27:Z:132:ASP:OD2	2.05	0.57
1:A:1189:A:H1'	1:A:1209:C:O4'	2.04	0.57
40:A:3488:HOH:O	31:4:57:GLY:HA2	2.04	0.57
2:B:3029:C:C2'	2:B:3030:C:H5'	2.35	0.57
4:C:66:ARG:HB2	4:C:66:ARG:HH11	1.69	0.57
11:J:46:VAL:HG12	11:J:146:TRP:HZ3	1.70	0.57
14:M:114:VAL:HG11	40:M:8574:HOH:O	2.03	0.57
28:1:11:THR:OG1	28:1:23:ARG:HB2	2.04	0.57
1:A:88:G:H5'	1:A:88:G:H8	1.70	0.57
1:A:1119:G:H8	12:K:52:GLN:NE2	2.03	0.57
1:A:1834:C:H2'	1:A:1840:A:N6	2.20	0.57
1:A:2815:G:N7	12:K:80:LYS:NZ	2.53	0.57
4:C:36:ASP:O	4:C:38:ILE:N	2.38	0.57
25:X:65:VAL:HA	25:X:68:THR:CG2	2.32	0.57
1:A:2265:U:H2'	1:A:2266:A:C8	2.40	0.56
7:F:44:ILE:HG23	7:F:45:THR:HG23	1.86	0.56
11:J:139:ASP:N	11:J:140:PRO:CD	2.67	0.56
15:N:134:ILE:HG23	15:N:141:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:21:SER:OG	17:P:106:PRO:HB2	2.05	0.56
28:1:30:GLU:HA	28:1:33:HIS:CB	2.35	0.56
1:A:121:U:OP2	30:3:10:ARG:NH2	2.38	0.56
1:A:449:A:N7	6:E:43:LYS:HG2	2.20	0.56
1:A:1189:A:H1'	1:A:1209:C:C1'	2.34	0.56
1:A:1500:U:P	18:Q:41:ARG:HH22	2.28	0.56
1:A:1667:A:H2'	1:A:1668:U:C6	2.41	0.56
1:A:2718:C:H6	1:A:2718:C:H5'	1.70	0.56
2:B:3014:G:H5'	2:B:3014:G:C8	2.40	0.56
6:E:142:ASP:OD1	6:E:237:GLU:HB3	2.04	0.56
7:F:36:ASN:HA	40:F:7500:HOH:O	2.04	0.56
1:A:407:A:H5'	40:A:5538:HOH:O	2.06	0.56
1:A:1159:G:H21	1:A:1189:A:H8	1.52	0.56
1:A:1333:U:H2'	1:A:1334:C:H6	1.70	0.56
1:A:2607:U:H4'	40:A:8949:HOH:O	2.05	0.56
5:D:305:ASP:O	5:D:306:LYS:HB2	2.06	0.56
5:D:307:ARG:HH11	5:D:307:ARG:CB	2.17	0.56
6:E:127:ARG:HG2	6:E:127:ARG:HH11	1.70	0.56
8:G:31:ARG:HH12	8:G:68:HIS:CG	2.22	0.56
8:G:79:GLY:HA3	40:G:7046:HOH:O	2.05	0.56
15:N:98:GLN:O	15:N:102:GLU:HG3	2.05	0.56
15:N:157:LEU:HB3	15:N:160:PHE:HD1	1.70	0.56
25:X:81:ASP:OD1	25:X:92:ASP:HB2	2.05	0.56
1:A:2729:C:O2'	1:A:2730:G:H5'	2.06	0.56
4:C:105:VAL:HG12	4:C:106:CYS:N	2.20	0.56
8:G:7:ILE:HG22	8:G:45:ASP:O	2.06	0.56
12:K:46:ILE:HA	40:K:1123:HOH:O	2.05	0.56
15:N:37:VAL:HG13	15:N:63:VAL:HG11	1.86	0.56
15:N:99:ARG:HD2	15:N:167:GLY:HA2	1.86	0.56
1:A:21:G:H4'	20:S:2:ILE:HG22	1.88	0.56
3:5:9076:A:H5''	36:5:9080:SPS:C8	2.35	0.56
5:D:66:GLU:OE1	5:D:328:ARG:HD2	2.05	0.56
7:F:95:THR:C	7:F:97:GLN:H	2.09	0.56
7:F:135:VAL:HG22	7:F:136:ARG:N	2.20	0.56
12:K:45:VAL:HG21	12:K:129:PHE:CD1	2.41	0.56
1:A:694:A:N3	40:A:3329:HOH:O	2.33	0.56
1:A:775:G:OP1	29:2:16:HIS:HE1	1.89	0.56
40:B:4707:HOH:O	16:O:147:ILE:HD12	2.04	0.56
9:H:50:VAL:CG2	9:H:63:ILE:HG21	2.34	0.56
11:J:14:TYR:N	11:J:91:HIS:CE1	2.71	0.56
12:K:74:ARG:HH11	12:K:74:ARG:CB	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:99:GLU:HA	40:K:7377:HOH:O	2.05	0.56
16:O:32:PRO:HD2	16:O:99:GLU:O	2.06	0.56
16:O:154:LEU:HG	16:O:155:GLU:H	1.69	0.56
25:X:65:VAL:CA	25:X:68:THR:HG22	2.35	0.56
1:A:1008:C:H5''	11:J:16:ARG:HH12	1.70	0.56
1:A:1130:U:H2'	1:A:1131:G:O4'	2.06	0.56
1:A:2890:A:H1'	23:V:56:ARG:HH21	1.70	0.56
4:C:192:VAL:HG12	4:C:207:GLN:HB3	1.87	0.56
9:H:21:GLU:O	9:H:24:ARG:HG3	2.04	0.56
13:L:55:VAL:HG12	13:L:56:SER:N	2.21	0.56
26:Y:9:VAL:HG22	26:Y:88:GLU:OE2	2.05	0.56
1:A:500:G:H21	20:S:98:ASN:HD21	1.52	0.56
1:A:1778:A:H2'	1:A:1779:A:H5'	1.88	0.56
1:A:2502:C:C2'	1:A:2503:A:H5'	2.36	0.56
1:A:2676:C:H4'	12:K:70:PHE:HE1	1.69	0.56
4:C:76:VAL:HG23	28:1:63:LYS:HB3	1.87	0.56
11:J:166:ASN:N	11:J:166:ASN:ND2	2.53	0.56
25:X:80:ASP:O	25:X:84:VAL:HG23	2.05	0.56
27:Z:107:PRO:HB3	27:Z:182:PHE:CD2	2.41	0.56
1:A:567:U:H5''	40:X:5817:HOH:O	2.05	0.56
25:X:41:TYR:O	25:X:45:VAL:HG13	2.06	0.56
27:Z:235:GLU:H	27:Z:235:GLU:CD	2.08	0.56
30:3:18:ASN:HD21	30:3:40:ARG:H	1.52	0.56
1:A:1636:G:O2'	1:A:1637:A:H5'	2.05	0.56
1:A:2310:G:OP2	11:J:114:PRO:HD2	2.05	0.56
16:O:11:ARG:NH2	40:O:8520:HOH:O	2.38	0.56
22:U:53:GLY:HA3	40:U:6384:HOH:O	2.06	0.56
25:X:108:ARG:HE	25:X:114:PRO:HG3	1.71	0.56
25:X:126:ASP:HB3	25:X:135:GLY:O	2.06	0.56
1:A:545:G:H5'	1:A:545:G:C8	2.35	0.55
1:A:1118:A:C8	1:A:1118:A:C3'	2.86	0.55
1:A:1209:C:H2'	1:A:1210:G:C8	2.41	0.55
4:C:101:GLU:OE2	4:C:131:HIS:HB2	2.06	0.55
7:F:38:GLU:OE2	7:F:51:ARG:CZ	2.54	0.55
7:F:93:LEU:HB3	7:F:97:GLN:OE1	2.06	0.55
16:O:38:LYS:HD2	16:O:114:LYS:HE3	1.88	0.55
25:X:90:TYR:N	25:X:90:TYR:CD1	2.74	0.55
40:A:5786:HOH:O	17:P:7:LEU:HD22	2.05	0.55
40:A:6970:HOH:O	6:E:188:ARG:CD	2.53	0.55
7:F:99:ASP:HB3	7:F:103:ASN:H	1.71	0.55
15:N:183:VAL:HG12	15:N:184:ARG:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:1:THR:HA	40:2:435:HOH:O	2.07	0.55
1:A:820:G:H5'	1:A:821:U:H5'	1.88	0.55
1:A:2301:A:H5''	1:A:2302:A:H5'	1.87	0.55
1:A:2363:G:O3'	19:R:11:ARG:NH1	2.40	0.55
2:B:3020:G:H3'	40:B:2984:HOH:O	2.06	0.55
5:D:141:ARG:HD2	5:D:163:GLU:OE2	2.06	0.55
8:G:15:GLN:HG2	8:G:19:ASP:O	2.07	0.55
1:A:95:A:H5''	1:A:97:G:O4'	2.06	0.55
1:A:157:G:H4'	15:N:95:LYS:HE3	1.89	0.55
1:A:899:C:H5'	40:A:9712:HOH:O	2.07	0.55
1:A:2502:C:C4'	11:J:151:MET:HG2	2.36	0.55
4:C:88:ILE:HD13	4:C:100:PRO:CD	2.36	0.55
5:D:74:ILE:HD13	5:D:309:VAL:HG21	1.87	0.55
8:G:9:GLU:HG3	8:G:10:ASP:N	2.21	0.55
28:1:38:LYS:HG3	40:1:8429:HOH:O	2.05	0.55
1:A:182:G:O3'	15:N:157:LEU:HD13	2.06	0.55
1:A:1120:U:H5'	1:A:1121:G:OP2	2.06	0.55
3:5:9076:A:H5''	36:5:9080:SPS:C6	2.36	0.55
12:K:74:ARG:O	12:K:78:ILE:HG12	2.06	0.55
17:P:87:THR:O	17:P:91:GLN:HG3	2.05	0.55
25:X:122:ARG:CZ	40:X:5817:HOH:O	2.55	0.55
1:A:485:A:N3	1:A:487:G:H5''	2.22	0.55
1:A:797:A:C4'	28:1:10:ARG:N	2.70	0.55
1:A:926:A:O2'	14:M:41:HIS:HD2	1.90	0.55
4:C:100:PRO:HG2	4:C:103:VAL:CG2	2.35	0.55
6:E:185:LYS:HD3	6:E:186:TYR:CE1	2.42	0.55
6:E:246:ARG:NE	40:E:8423:HOH:O	2.40	0.55
6:E:246:ARG:NH2	40:E:8423:HOH:O	2.39	0.55
7:F:58:VAL:HG12	7:F:59:GLY:N	2.21	0.55
11:J:27:LYS:H	11:J:58:HIS:CD2	2.16	0.55
1:A:400:C:O2'	1:A:401:C:H5'	2.06	0.55
1:A:1996:U:O2'	1:A:1997:A:H5'	2.06	0.55
40:A:9456:HOH:O	26:Y:23:HIS:HD2	1.90	0.55
2:B:3039:U:H1'	2:B:3044:A:N6	2.21	0.55
7:F:50:VAL:O	7:F:71:ALA:HA	2.06	0.55
7:F:163:VAL:HA	40:F:6326:HOH:O	2.06	0.55
1:A:474:C:O3'	6:E:73:LEU:HD21	2.07	0.55
1:A:2468:A:H61	31:4:48:ASN:HD21	1.54	0.55
4:C:8:ARG:HG2	40:C:8552:HOH:O	2.06	0.55
7:F:10:PHE:CG	7:F:11:HIS:N	2.74	0.55
11:J:117:LYS:HB2	40:J:8341:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:100:ALA:O	16:O:129:ILE:HG23	2.07	0.55
24:W:4:HIS:HB3	40:W:6622:HOH:O	2.06	0.55
1:A:1132:A:N6	1:A:1229:C:H2'	2.22	0.55
1:A:1972:U:H2'	1:A:1973:A:C5'	2.37	0.55
1:A:2570:G:H5''	40:A:4427:HOH:O	2.07	0.55
4:C:191:GLY:HA2	4:C:194:MET:HE3	1.88	0.55
18:Q:16:VAL:HG12	18:Q:17:GLY:N	2.22	0.55
23:V:52:THR:CG2	23:V:54:THR:HB	2.37	0.55
25:X:35:VAL:HG23	25:X:41:TYR:CD2	2.42	0.55
5:D:36:PRO:HA	5:D:168:GLY:HA2	1.88	0.55
6:E:107:ARG:NE	40:E:8459:HOH:O	2.11	0.55
18:Q:38:GLU:HA	18:Q:41:ARG:NH1	2.22	0.55
18:Q:105:LEU:CD2	18:Q:137:LEU:HD21	2.37	0.55
28:1:53:GLY:HA2	28:1:67:GLY:O	2.07	0.55
1:A:316:A:H5'	22:U:54:ASP:OD2	2.06	0.54
1:A:415:A:O2'	1:A:416:G:H5'	2.07	0.54
1:A:1940:C:H4'	40:A:6857:HOH:O	2.07	0.54
9:H:58:GLU:CD	15:N:27:ARG:HH22	2.09	0.54
11:J:75:SER:C	11:J:79:ALA:HB2	2.28	0.54
25:X:88:THR:CG2	25:X:89:ASP:H	2.16	0.54
25:X:90:TYR:CE2	25:X:99:ALA:HB2	2.42	0.54
26:Y:18:ARG:NH1	40:Y:4132:HOH:O	2.40	0.54
1:A:317:A:H5''	22:U:52:ARG:HD2	1.88	0.54
1:A:558:C:C2'	1:A:559:U:H5''	2.37	0.54
1:A:2506:A:O2'	1:A:2507:G:O5'	2.25	0.54
4:C:109:GLU:HG2	4:C:116:GLY:N	2.22	0.54
5:D:2:GLN:HA	40:D:8615:HOH:O	2.06	0.54
9:H:101:ALA:HB2	9:H:108:LEU:CD2	2.37	0.54
9:H:107:VAL:O	9:H:111:ILE:HG13	2.06	0.54
10:I:12:ILE:HB	40:I:4714:HOH:O	2.06	0.54
14:M:143:THR:HG22	14:M:144:ASP:H	1.73	0.54
1:A:259:G:H21	15:N:58:GLN:NE2	2.05	0.54
15:N:43:PRO:HG3	15:N:62:VAL:HG21	1.90	0.54
27:Z:212:ARG:HD2	40:Z:8596:HOH:O	2.07	0.54
28:1:62:TYR:CE2	28:1:64:ILE:HG23	2.42	0.54
1:A:2064:U:H5'	1:A:2652:U:O3'	2.08	0.54
4:C:109:GLU:HG2	4:C:116:GLY:H	1.73	0.54
5:D:195:ARG:NH1	5:D:324:ASP:OD1	2.40	0.54
16:O:90:LEU:HB2	16:O:186:LEU:HD22	1.88	0.54
1:A:244:C:OP2	9:H:38:LYS:HE3	2.08	0.54
1:A:470:U:O2'	29:2:16:HIS:CD2	2.59	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1477:C:H5'	1:A:1868:G:C5'	2.37	0.54
1:A:1753:C:O2	5:D:229:ARG:NH2	2.39	0.54
1:A:2281:C:C2'	1:A:2282:U:H5'	2.36	0.54
1:A:2419:U:H5''	1:A:2420:G:H5'	1.90	0.54
16:O:87:LEU:CD1	16:O:186:LEU:HD21	2.32	0.54
16:O:110:THR:HB	16:O:113:SER:OG	2.08	0.54
25:X:4:LEU:HD23	25:X:54:PHE:HB3	1.88	0.54
1:A:281:U:O2'	1:A:282:C:H5'	2.08	0.54
1:A:316:A:N3	1:A:336:G:O2'	2.40	0.54
1:A:1342:C:O2'	1:A:1343:C:H5'	2.07	0.54
1:A:2300:A:H4'	1:A:2301:A:O5'	2.08	0.54
15:N:61:ILE:HD12	15:N:61:ILE:N	2.23	0.54
25:X:110:GLN:NE2	25:X:110:GLN:HA	2.23	0.54
30:3:22:PRO:HG2	30:3:25:VAL:CG2	2.37	0.54
1:A:656:G:OP2	17:P:37:ARG:HD2	2.07	0.54
1:A:960:G:H2'	1:A:960:G:N3	2.23	0.54
1:A:1164:U:H4'	1:A:1165:G:OP1	2.07	0.54
1:A:1181:A:H2'	1:A:1182:C:O4'	2.07	0.54
1:A:1878:G:H1'	40:A:5635:HOH:O	2.06	0.54
2:B:3028:U:H2'	2:B:3029:C:C6	2.43	0.54
4:C:88:ILE:HG22	4:C:88:ILE:O	2.08	0.54
4:C:212:PRO:HB2	40:C:8561:HOH:O	2.06	0.54
6:E:13:ASP:OD1	6:E:13:ASP:O	2.25	0.54
8:G:101:GLU:HB2	8:G:116:THR:O	2.08	0.54
1:A:2587:U:H2'	1:A:2589:U:H5''	1.90	0.54
6:E:25:PRO:HG2	40:E:8324:HOH:O	2.08	0.54
9:H:16:ALA:HA	9:H:111:ILE:HD13	1.90	0.54
11:J:84:ARG:CZ	11:J:135:TRP:CH2	2.91	0.54
15:N:84:LYS:HE2	40:N:8577:HOH:O	2.08	0.54
17:P:14:LEU:CD2	17:P:102:ILE:HD11	2.38	0.54
1:A:183:A:C5'	15:N:157:LEU:HD12	2.38	0.54
1:A:2438:G:H5'	40:A:5683:HOH:O	2.07	0.54
2:B:3002:U:OP2	2:B:3002:U:H4'	2.08	0.54
8:G:22:VAL:O	8:G:28:SER:HA	2.08	0.54
1:A:1528:A:H2'	1:A:1529:G:O4'	2.08	0.54
1:A:2795:C:O2'	1:A:2796:U:H5'	2.07	0.54
9:H:99:THR:O	9:H:99:THR:HG23	2.07	0.54
12:K:133:GLY:O	12:K:137:GLU:HG3	2.07	0.54
16:O:12:ARG:HD3	16:O:18:THR:OG1	2.08	0.54
16:O:37:ARG:NE	40:O:8534:HOH:O	2.41	0.54
1:A:175:G:C2'	15:N:192:ALA:HB3	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:A:OP2	17:P:38:ARG:HD3	2.08	0.53
1:A:2361:A:H5'	1:A:2361:A:H8	1.73	0.53
1:A:2434:A:O3'	31:4:28:GLY:HA3	2.09	0.53
1:A:2473:U:O3'	1:A:2474:A:H3'	2.07	0.53
6:E:129:HIS:HD2	6:E:165:ASP:OD2	1.91	0.53
11:J:31:PHE:CD2	11:J:85:ILE:HG23	2.43	0.53
22:U:73:HIS:CD2	22:U:88:PRO:HG3	2.42	0.53
24:W:39:ALA:O	24:W:41:GLU:N	2.41	0.53
27:Z:112:GLU:CD	27:Z:115:ARG:NH1	2.61	0.53
27:Z:117:LEU:HD12	27:Z:174:VAL:HG11	1.91	0.53
31:4:11:CYS:HB2	31:4:20:HIS:CE1	2.43	0.53
4:C:94:LEU:N	4:C:94:LEU:HD23	2.23	0.53
7:F:94:ALA:O	7:F:95:THR:O	2.26	0.53
9:H:58:GLU:HG3	9:H:61:MET:HE1	1.91	0.53
14:M:125:PHE:CZ	14:M:140:VAL:HG13	2.44	0.53
15:N:81:ARG:O	15:N:86:MET:HE2	2.08	0.53
22:U:32:ARG:NH1	22:U:38:ARG:NH1	2.56	0.53
25:X:21:LEU:CD1	25:X:26:ILE:HD11	2.35	0.53
26:Y:75:ALA:O	26:Y:83:ALA:HA	2.08	0.53
1:A:1596:U:H2'	1:A:1598:A:OP2	2.08	0.53
1:A:2897:C:H2'	1:A:2898:G:H8	1.72	0.53
5:D:185:GLY:HA2	40:D:8628:HOH:O	2.08	0.53
5:D:248:ARG:O	5:D:251:VAL:CG1	2.57	0.53
8:G:31:ARG:HH12	8:G:68:HIS:CD2	2.26	0.53
16:O:49:THR:CG2	16:O:56:ASP:HB2	2.36	0.53
1:A:2694:A:H4'	8:G:91:PHE:HE1	1.74	0.53
40:A:6970:HOH:O	6:E:188:ARG:HD2	2.08	0.53
40:A:9798:HOH:O	13:L:9:THR:HA	2.07	0.53
5:D:268:ARG:NE	40:D:8602:HOH:O	2.40	0.53
10:I:23:ILE:O	10:I:27:ILE:HG13	2.08	0.53
15:N:182:LYS:HB2	15:N:194:ALA:HB2	1.91	0.53
16:O:139:TRP:HA	16:O:139:TRP:CE3	2.43	0.53
25:X:125:HIS:CD2	25:X:127:GLY:H	2.26	0.53
26:Y:78:GLU:CG	26:Y:79:GLU:H	2.20	0.53
1:A:656:G:H5'	17:P:3:THR:CG2	2.38	0.53
1:A:1167:G:O2'	1:A:1168:C:H5'	2.08	0.53
1:A:1887:U:OP1	28:1:21:LYS:HE3	2.09	0.53
5:D:297:VAL:HB	40:D:8600:HOH:O	2.08	0.53
5:D:314:ALA:CB	5:D:317:PRO:HG3	2.39	0.53
27:Z:184:GLU:OE1	27:Z:204:ARG:NH1	2.41	0.53
29:2:28:HIS:CE1	29:2:31:LYS:HE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:82:VAL:O	5:D:82:VAL:HG12	2.08	0.53
8:G:69:ILE:HA	8:G:72:MET:HE2	1.89	0.53
9:H:113:ASP:O	9:H:117:GLU:HG3	2.08	0.53
24:W:64:GLY:O	24:W:65:ASP:CB	2.57	0.53
1:A:65:C:O2'	1:A:66:G:H5'	2.08	0.53
1:A:1559:A:H1'	40:A:5381:HOH:O	2.08	0.53
40:A:9693:HOH:O	15:N:9:ARG:HG3	2.08	0.53
5:D:138:GLY:O	5:D:139:ASP:O	2.26	0.53
8:G:145:ALA:HB1	8:G:168:ILE:CD1	2.39	0.53
12:K:107:ASN:C	12:K:107:ASN:HD22	2.11	0.53
13:L:87:ARG:CZ	40:L:4854:HOH:O	2.56	0.53
15:N:164:THR:CG2	15:N:165:SER:N	2.72	0.53
18:Q:131:PHE:CD1	18:Q:137:LEU:HD13	2.43	0.53
23:V:13:ILE:HG12	23:V:32:CYS:HB3	1.90	0.53
25:X:19:ASP:O	25:X:23:MET:HG3	2.08	0.53
27:Z:112:GLU:OE2	27:Z:115:ARG:NH1	2.41	0.53
1:A:263:U:O4'	9:H:59:ILE:HD13	2.09	0.53
5:D:30:PRO:HB2	5:D:39:GLN:NE2	2.23	0.53
8:G:93:MET:HE1	8:G:165:GLY:N	2.24	0.53
11:J:53:PRO:HA	11:J:125:VAL:O	2.09	0.53
15:N:72:SER:HB2	15:N:93:ARG:HG2	1.91	0.53
8:G:49:ILE:HD11	8:G:69:ILE:HD12	1.91	0.53
14:M:6:ARG:NH2	40:M:8547:HOH:O	2.41	0.53
1:A:1377:C:H5'	1:A:1377:C:C6	2.44	0.53
1:A:1393:A:H2'	1:A:1394:C:C6	2.44	0.53
2:B:3039:U:H3'	2:B:3040:C:H5''	1.91	0.53
4:C:128:LEU:HG	40:C:8574:HOH:O	2.09	0.53
5:D:329:TYR:HE2	23:V:15:PRO:HG2	1.73	0.53
6:E:235:PHE:HE2	6:E:243:VAL:HG21	1.74	0.53
14:M:143:THR:HG22	14:M:145:LEU:H	1.74	0.53
16:O:64:SER:C	16:O:66:LEU:H	2.13	0.53
16:O:171:HIS:CE1	40:O:8568:HOH:O	2.62	0.53
31:4:55:VAL:HB	31:4:56:PRO:HD2	1.90	0.53
1:A:1677:U:OP2	30:3:8:LYS:NZ	2.42	0.52
1:A:1741:U:O2'	1:A:2723:G:H4'	2.09	0.52
1:A:2608:C:H2'	40:A:3086:HOH:O	2.08	0.52
1:A:2781:U:H1'	8:G:139:GLU:OE2	2.08	0.52
40:A:4082:HOH:O	6:E:50:GLU:HG2	2.07	0.52
4:C:123:GLY:HA3	4:C:162:GLY:HA2	1.91	0.52
6:E:107:ARG:NH2	40:E:8459:HOH:O	2.42	0.52
6:E:233:THR:HG22	6:E:234:VAL:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:31:PHE:HA	11:J:85:ILE:CG2	2.39	0.52
11:J:58:HIS:HA	11:J:61:LEU:HD23	1.92	0.52
12:K:52:GLN:HG3	12:K:53:ILE:H	1.73	0.52
12:K:107:ASN:HD22	12:K:109:TYR:H	1.57	0.52
16:O:154:LEU:HG	16:O:155:GLU:N	2.23	0.52
18:Q:120:ARG:NH2	18:Q:123:TYR:CD2	2.77	0.52
23:V:47:ARG:HG3	40:V:4381:HOH:O	2.08	0.52
1:A:1847:A:OP1	4:C:175:LYS:HG3	2.09	0.52
5:D:27:ASN:HD22	5:D:27:ASN:H	1.55	0.52
6:E:219:ASN:O	6:E:222:ASP:OD1	2.26	0.52
27:Z:106:THR:HG23	27:Z:107:PRO:HD2	1.91	0.52
1:A:396:U:O2'	1:A:418:C:H4'	2.10	0.52
1:A:1086:A:N6	25:X:11:VAL:HG11	2.25	0.52
1:A:2837:U:H1'	5:D:307:ARG:HH12	1.73	0.52
40:A:8909:HOH:O	15:N:94:LYS:HE2	2.09	0.52
5:D:307:ARG:HH11	5:D:307:ARG:CG	2.22	0.52
6:E:111:VAL:HB	40:E:8323:HOH:O	2.09	0.52
14:M:148:GLU:HB2	40:M:8593:HOH:O	2.09	0.52
18:Q:80:ARG:HG2	18:Q:87:ARG:CZ	2.39	0.52
18:Q:91:LYS:O	18:Q:95:GLU:HG3	2.08	0.52
26:Y:30:MET:HE1	26:Y:58:ALA:HB3	1.91	0.52
26:Y:76:ARG:O	26:Y:77:PHE:HB3	2.09	0.52
1:A:660:A:H4'	1:A:661:G:O5'	2.10	0.52
2:B:3049:G:H5''	40:B:4707:HOH:O	2.09	0.52
8:G:21:THR:HG23	8:G:30:THR:OG1	2.10	0.52
8:G:77:THR:OG1	8:G:78:GLU:N	2.42	0.52
8:G:81:GLU:HG2	8:G:134:SER:CB	2.34	0.52
15:N:173:LEU:HD23	15:N:183:VAL:HG12	1.91	0.52
21:T:29:ASP:OD1	21:T:31:ARG:HG3	2.08	0.52
23:V:9:CYS:CA	23:V:52:THR:HG23	2.39	0.52
1:A:1168:C:H2'	1:A:1169:U:O4'	2.09	0.52
1:A:2256:G:C2'	1:A:2257:G:H5'	2.39	0.52
40:A:9479:HOH:O	25:X:10:GLU:HG2	2.08	0.52
15:N:114:VAL:HG21	15:N:159:THR:CG2	2.39	0.52
16:O:152:GLU:C	16:O:154:LEU:H	2.11	0.52
18:Q:98:ILE:HD12	18:Q:102:ARG:NE	2.25	0.52
28:1:11:THR:CG2	28:1:23:ARG:HB2	2.39	0.52
1:A:256:C:H2'	1:A:257:G:O4'	2.10	0.52
1:A:1189:A:O2'	1:A:1208:C:H2'	2.10	0.52
1:A:1299:G:N2	40:A:4198:HOH:O	2.42	0.52
1:A:1593:C:OP1	18:Q:117:SER:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2111:G:H1'	40:A:8563:HOH:O	2.09	0.52
1:A:2361:A:H2'	1:A:2362:A:C8	2.44	0.52
4:C:192:VAL:CG1	4:C:207:GLN:HB3	2.40	0.52
7:F:22:VAL:HG22	7:F:74:THR:HG22	1.91	0.52
7:F:140:ARG:O	7:F:144:ARG:HG2	2.09	0.52
11:J:13:ALA:HA	11:J:91:HIS:CE1	2.45	0.52
20:S:132:ARG:NH2	40:S:8582:HOH:O	2.43	0.52
25:X:38:THR:O	25:X:42:ARG:HB2	2.10	0.52
29:2:25:LYS:HE2	40:2:7213:HOH:O	2.08	0.52
1:A:602:A:O2'	1:A:605:C:H4'	2.09	0.52
1:A:951:A:O2'	1:A:952:G:H5'	2.09	0.52
1:A:1353:C:P	40:A:4194:HOH:O	2.66	0.52
4:C:165:THR:HG22	40:C:8615:HOH:O	2.09	0.52
4:C:220:PRO:HD2	4:C:223:ARG:HD3	1.92	0.52
7:F:11:HIS:C	7:F:13:MET:H	2.13	0.52
17:P:47:ARG:HG3	17:P:47:ARG:NH1	2.23	0.52
18:Q:38:GLU:HA	18:Q:41:ARG:HH11	1.75	0.52
22:U:41:ARG:HG2	22:U:41:ARG:NH1	2.25	0.52
1:A:1120:U:C6	1:A:1120:U:H5''	2.45	0.52
1:A:1701:A:H5''	1:A:1702:U:H3'	1.92	0.52
1:A:2502:C:H2'	1:A:2503:A:H5'	1.91	0.52
12:K:131:THR:HG22	12:K:134:GLU:H	1.75	0.52
26:Y:66:THR:HG23	26:Y:67:PRO:HD2	1.91	0.52
1:A:447:A:OP1	22:U:2:LYS:HG2	2.10	0.52
1:A:2443:C:H3'	40:A:9983:HOH:O	2.09	0.52
5:D:168:GLY:N	5:D:174:ARG:HD3	2.24	0.52
7:F:103:ASN:ND2	7:F:134:LEU:H	2.07	0.52
9:H:46:GLU:O	9:H:73:PRO:HD2	2.09	0.52
14:M:61:ALA:HA	40:M:8564:HOH:O	2.09	0.52
26:Y:78:GLU:HG2	26:Y:79:GLU:N	2.24	0.52
1:A:283:U:H5''	1:A:284:C:P	2.50	0.52
1:A:661:G:C5	1:A:686:A:C2	2.98	0.52
1:A:1151:G:OP1	10:I:63:ARG:NH1	2.43	0.52
1:A:1189:A:H1'	1:A:1209:C:H1'	1.92	0.52
1:A:1250:C:O2'	1:A:1251:C:H5'	2.09	0.52
1:A:2251:G:H2'	1:A:2252:A:C8	2.45	0.52
9:H:46:GLU:N	40:H:3461:HOH:O	2.43	0.52
15:N:30:GLU:O	15:N:34:GLU:HG3	2.09	0.52
21:T:8:PRO:HD2	24:W:32:ALA:HA	1.91	0.52
25:X:38:THR:HG22	25:X:39:ASP:H	1.75	0.52
1:A:21:G:H5''	20:S:1:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:U:O4'	6:E:202:THR:HG22	2.10	0.51
1:A:407:A:H2'	1:A:408:A:C8	2.45	0.51
1:A:1787:C:H4'	1:A:2883:A:O4'	2.10	0.51
1:A:1874:U:H2'	4:C:120:ARG:HG3	1.92	0.51
1:A:2894:C:O2'	1:A:2895:C:H5'	2.09	0.51
5:D:212:GLN:OE1	5:D:216:LYS:HD3	2.10	0.51
7:F:41:LEU:HA	7:F:44:ILE:CG2	2.39	0.51
7:F:94:ALA:HB3	7:F:174:VAL:HA	1.92	0.51
7:F:99:ASP:CB	7:F:103:ASN:HB2	2.39	0.51
1:A:290:C:O2'	1:A:291:C:H5'	2.10	0.51
1:A:380:A:OP2	15:N:9:ARG:HD2	2.09	0.51
1:A:417:G:P	40:A:6928:HOH:O	2.67	0.51
1:A:1484:G:H2'	40:A:8618:HOH:O	2.10	0.51
2:B:3042:C:H2'	40:B:6700:HOH:O	2.10	0.51
4:C:105:VAL:HG11	4:C:154:ALA:CB	2.40	0.51
5:D:139:ASP:HB2	5:D:165:ARG:HE	1.75	0.51
7:F:10:PHE:CD1	7:F:11:HIS:N	2.78	0.51
7:F:67:ASP:O	7:F:69:ILE:HG13	2.10	0.51
11:J:35:ASN:ND2	11:J:79:ALA:O	2.43	0.51
12:K:45:VAL:HG22	12:K:46:ILE:N	2.24	0.51
22:U:63:ILE:HD11	22:U:75:GLU:HB2	1.92	0.51
25:X:108:ARG:NH2	40:X:2359:HOH:O	2.44	0.51
1:A:136:C:H2'	1:A:137:U:O4'	2.10	0.51
1:A:558:C:C2'	1:A:559:U:C5'	2.88	0.51
4:C:211:LYS:HD3	40:C:8608:HOH:O	2.10	0.51
5:D:16:ARG:NE	40:D:8550:HOH:O	2.30	0.51
7:F:99:ASP:O	7:F:159:PRO:HG3	2.09	0.51
11:J:45:GLN:HB3	11:J:163:PRO:CD	2.21	0.51
16:O:170:GLU:O	16:O:174:GLU:HG3	2.10	0.51
22:U:111:ARG:HB3	22:U:119:ALA:HB2	1.92	0.51
23:V:47:ARG:CG	40:V:4381:HOH:O	2.58	0.51
25:X:21:LEU:HD22	25:X:26:ILE:HD13	1.93	0.51
25:X:84:VAL:HG12	40:X:6679:HOH:O	2.09	0.51
27:Z:144:ARG:CZ	40:Z:8608:HOH:O	2.58	0.51
1:A:1304:U:H2'	1:A:1305:C:C6	2.46	0.51
1:A:1515:A:H2'	1:A:1516:C:C6	2.45	0.51
1:A:2832:C:H5	40:A:6721:HOH:O	1.92	0.51
11:J:59:ASN:N	11:J:59:ASN:ND2	2.54	0.51
14:M:143:THR:CG2	14:M:144:ASP:H	2.22	0.51
16:O:48:VAL:HG11	16:O:55:ASP:HB3	1.90	0.51
1:A:1641:A:C2'	1:A:1642:A:H5'	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:A:6934:HOH:O	22:U:9:LYS:HD2	2.10	0.51
5:D:280:VAL:HG13	5:D:333:GLU:O	2.10	0.51
14:M:73:VAL:HG11	14:M:118:LEU:HD21	1.91	0.51
30:3:41:HIS:H	30:3:45:ASN:ND2	2.06	0.51
1:A:101:C:H2'	1:A:102:A:H8	1.75	0.51
1:A:714:U:H3'	40:A:6455:HOH:O	2.11	0.51
1:A:2717:C:H2'	1:A:2718:C:C5'	2.35	0.51
40:A:6536:HOH:O	4:C:211:LYS:HG2	2.10	0.51
2:B:3035:C:H5''	40:B:4078:HOH:O	2.11	0.51
4:C:125:ASN:HB3	4:C:158:VAL:HG12	1.91	0.51
12:K:90:LYS:HB2	35:K:8502:CL:CL	2.48	0.51
13:L:125:ALA:C	13:L:127:ALA:H	2.14	0.51
15:N:182:LYS:HD2	15:N:193:LYS:HB2	1.91	0.51
17:P:26:TRP:HB2	40:P:3062:HOH:O	2.11	0.51
1:A:155:C:OP2	15:N:188:ARG:HD3	2.11	0.51
1:A:588:G:O6	25:X:154:ARG:NH1	2.44	0.51
1:A:1342:C:C2'	1:A:1343:C:H5'	2.41	0.51
2:B:3027:C:H1'	40:B:2772:HOH:O	2.10	0.51
2:B:3049:G:H2'	2:B:3050:G:O4'	2.11	0.51
9:H:99:THR:O	9:H:100:ASP:HB2	2.10	0.51
14:M:30:ARG:NH2	40:M:8521:HOH:O	2.31	0.51
15:N:5:TYR:HE2	15:N:46:LEU:HD13	1.76	0.51
15:N:80:GLY:O	15:N:81:ARG:HD3	2.11	0.51
16:O:143:ARG:HA	16:O:172:PHE:CD2	2.45	0.51
16:O:182:GLY:O	16:O:183:ASP:O	2.28	0.51
21:T:73:ASP:OD1	21:T:76:GLU:HG3	2.11	0.51
25:X:38:THR:HG22	25:X:39:ASP:N	2.25	0.51
26:Y:74:ALA:CB	26:Y:85:VAL:HG22	2.40	0.51
1:A:380:A:H5''	15:N:48:ARG:NH2	2.25	0.51
40:A:9207:HOH:O	5:D:254:GLN:HG3	2.09	0.51
2:B:3006:C:C5'	16:O:37:ARG:HH12	2.18	0.51
12:K:39:VAL:HG12	12:K:40:ASN:ND2	2.26	0.51
15:N:107:ARG:NH1	40:N:8578:HOH:O	2.42	0.51
16:O:141:ARG:HB3	40:O:8571:HOH:O	2.10	0.51
20:S:96:VAL:HG13	20:S:106:GLY:HA3	1.92	0.51
22:U:41:ARG:NH1	22:U:42:VAL:O	2.43	0.51
25:X:21:LEU:HB3	25:X:26:ILE:CG1	2.41	0.51
29:2:8:GLN:HE22	29:2:11:LYS:HZ1	1.59	0.51
1:A:1525:G:H5'	1:A:1526:A:OP2	2.11	0.51
1:A:2866:U:H4'	1:A:2867:G:H5'	1.92	0.51
6:E:16:VAL:HG12	6:E:17:ASP:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:167:GLU:OE2	7:F:173:GLU:HG2	2.10	0.51
15:N:157:LEU:HD23	40:N:8629:HOH:O	2.10	0.51
16:O:47:LEU:CD1	16:O:97:VAL:HG11	2.40	0.51
17:P:14:LEU:HD23	17:P:102:ILE:HD11	1.92	0.51
1:A:818:A:O2'	28:1:13:ARG:HD3	2.11	0.51
1:A:1130:U:H5'	40:A:7191:HOH:O	2.10	0.51
1:A:1500:U:OP2	18:Q:41:ARG:NH2	2.43	0.51
1:A:1733:A:H4'	5:D:212:GLN:HA	1.91	0.51
1:A:2898:G:H4'	5:D:288:GLY:HA2	1.93	0.51
2:B:3049:G:O2'	2:B:3050:G:H5'	2.11	0.51
5:D:16:ARG:NH2	40:D:8550:HOH:O	2.36	0.51
5:D:85:ARG:NH1	40:D:8629:HOH:O	2.44	0.51
7:F:57:THR:HG23	7:F:63:ILE:CB	2.41	0.51
8:G:118:ILE:HG23	8:G:144:THR:HG21	1.93	0.51
23:V:11:THR:HG22	23:V:53:ASP:OD2	2.11	0.51
29:2:10:LYS:HG3	40:2:2979:HOH:O	2.10	0.51
5:D:156:LYS:HE3	40:D:8625:HOH:O	2.11	0.50
15:N:63:VAL:HG21	15:N:109:PHE:CZ	2.46	0.50
16:O:180:LEU:O	16:O:181:ASP:HB3	2.11	0.50
27:Z:216:ARG:HD3	40:Z:8564:HOH:O	2.11	0.50
28:1:46:LYS:NZ	40:1:8439:HOH:O	2.43	0.50
1:A:2314:G:C2'	1:A:2315:C:H5'	2.41	0.50
8:G:24:GLY:HA3	8:G:76:VAL:HB	1.93	0.50
9:H:111:ILE:O	9:H:115:VAL:HG23	2.10	0.50
12:K:131:THR:HG22	12:K:133:GLY:H	1.75	0.50
14:M:104:ASP:HB3	40:M:8564:HOH:O	2.12	0.50
16:O:23:ARG:NH1	40:O:8548:HOH:O	2.44	0.50
16:O:73:ALA:HB2	16:O:163:PHE:CZ	2.47	0.50
16:O:159:TYR:HE2	16:O:163:PHE:HE2	1.60	0.50
31:4:3:MET:O	31:4:90:PHE:HA	2.11	0.50
1:A:475:G:OP1	6:E:73:LEU:HD22	2.11	0.50
1:A:1007:A:H2'	11:J:19:TYR:CZ	2.46	0.50
1:A:1471:A:H2'	1:A:1472:C:C6	2.46	0.50
1:A:1592:G:O2'	1:A:1593:C:O4'	2.28	0.50
40:A:3574:HOH:O	5:D:27:ASN:HB2	2.10	0.50
5:D:198:GLU:HB3	40:D:8590:HOH:O	2.11	0.50
11:J:47:GLU:HG2	11:J:133:ILE:HD12	1.92	0.50
12:K:75:PRO:HG2	12:K:105:LEU:HD21	1.93	0.50
13:L:87:ARG:NE	40:L:4854:HOH:O	2.44	0.50
15:N:113:ARG:NH2	15:N:156:ARG:HG2	2.27	0.50
18:Q:103:THR:O	18:Q:107:GLU:HG3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:U:H2'	1:A:372:A:C8	2.45	0.50
1:A:777:U:O2'	29:2:11:LYS:HG2	2.12	0.50
1:A:1450:C:C4'	1:A:1451:C:OP2	2.59	0.50
1:A:2428:G:N7	31:4:60:LYS:NZ	2.57	0.50
1:A:2670:G:O2'	1:A:2671:U:H5'	2.11	0.50
2:B:3030:C:OP1	7:F:137:PRO:O	2.29	0.50
4:C:125:ASN:CB	4:C:158:VAL:HG12	2.42	0.50
4:C:164:ARG:NE	40:C:8586:HOH:O	2.44	0.50
5:D:14:GLY:HA2	5:D:15:PRO:C	2.31	0.50
5:D:140:LEU:HD23	40:D:8574:HOH:O	2.12	0.50
6:E:153:VAL:O	6:E:157:LEU:HG	2.11	0.50
9:H:80:GLN:HB3	40:H:2563:HOH:O	2.12	0.50
10:I:20:VAL:O	10:I:24:VAL:HG23	2.12	0.50
11:J:47:GLU:CB	11:J:133:ILE:HD13	2.41	0.50
11:J:144:GLU:OE1	11:J:144:GLU:HA	2.11	0.50
11:J:150:LYS:HG2	40:J:8383:HOH:O	2.12	0.50
20:S:33:ARG:NH1	40:S:8541:HOH:O	2.45	0.50
25:X:125:HIS:HE1	40:X:3071:HOH:O	1.94	0.50
40:A:6218:HOH:O	27:Z:165:GLU:HB3	2.11	0.50
40:A:7074:HOH:O	31:4:60:LYS:HG3	2.10	0.50
5:D:279:THR:OG1	5:D:290:VAL:HB	2.12	0.50
11:J:39:GLY:O	11:J:41:THR:N	2.45	0.50
15:N:185:PRO:HG2	15:N:189:VAL:HG11	1.93	0.50
17:P:25:VAL:HG23	17:P:26:TRP:N	2.26	0.50
22:U:49:GLU:OE2	22:U:97:ARG:HD2	2.12	0.50
25:X:130:HIS:O	25:X:136:GLY:HA3	2.12	0.50
30:3:48:ASP:O	30:3:49:GLU:HB2	2.12	0.50
1:A:710:G:P	17:P:24:ALA:HB3	2.52	0.50
1:A:949:U:O2'	19:R:40:HIS:HE1	1.94	0.50
1:A:1180:U:H2'	1:A:1181:A:O4'	2.11	0.50
5:D:24:PRO:CG	5:D:204:GLY:HA2	2.42	0.50
15:N:55:LYS:HB2	15:N:60:ILE:CD1	2.41	0.50
19:R:40:HIS:HD2	19:R:60:THR:OG1	1.94	0.50
25:X:31:HIS:HB3	40:X:5420:HOH:O	2.11	0.50
27:Z:186:ARG:HG2	27:Z:186:ARG:NH1	2.26	0.50
1:A:814:G:H4'	40:A:9641:HOH:O	2.11	0.50
1:A:1527:A:H1'	1:A:1528:A:C8	2.46	0.50
1:A:2269:C:C2'	1:A:2270:G:H5'	2.41	0.50
1:A:2387:U:H2'	1:A:2388:C:C6	2.46	0.50
4:C:186:TRP:CG	4:C:187:PRO:HA	2.47	0.50
6:E:140:VAL:HG12	6:E:141:SER:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:11:HIS:O	7:F:12:GLU:HB3	2.11	0.50
15:N:74:ARG:HG3	15:N:74:ARG:NH1	2.27	0.50
15:N:134:ILE:CG2	15:N:141:ILE:HD13	2.41	0.50
15:N:169:ARG:NH1	40:N:8572:HOH:O	2.44	0.50
23:V:52:THR:HG22	23:V:54:THR:HB	1.94	0.50
1:A:101:C:H2'	1:A:102:A:C8	2.47	0.50
1:A:776:A:OP1	29:2:28:HIS:HE1	1.95	0.50
1:A:1205:U:C2'	1:A:1206:U:H5''	2.41	0.50
4:C:153:ARG:HD3	40:C:8532:HOH:O	2.10	0.50
8:G:132:THR:O	8:G:132:THR:HG23	2.11	0.50
13:L:82:ARG:HH21	13:L:115:ARG:HG2	1.77	0.50
16:O:11:ARG:HG3	16:O:14:ARG:NH1	2.26	0.50
27:Z:144:ARG:NE	40:Z:8608:HOH:O	2.44	0.50
1:A:2004:U:O2	1:A:2004:U:H2'	2.11	0.50
40:A:5707:HOH:O	30:3:44:ARG:HG2	2.11	0.50
5:D:144:THR:HG22	5:D:145:HIS:N	2.27	0.50
6:E:129:HIS:CE1	6:E:231:ARG:HA	2.47	0.50
7:F:49:PRO:HG3	40:F:5828:HOH:O	2.12	0.50
7:F:149:ARG:NH1	40:F:3066:HOH:O	2.24	0.50
8:G:152:THR:HG21	8:G:165:GLY:HA2	1.93	0.50
11:J:95:GLU:HB3	11:J:119:VAL:HG11	1.94	0.50
16:O:184:ILE:HG22	16:O:185:GLU:N	2.26	0.50
21:T:11:THR:H	21:T:14:ALA:HB3	1.77	0.50
28:1:30:GLU:O	28:1:33:HIS:HB3	2.12	0.50
1:A:383:A:H4'	40:A:4846:HOH:O	2.12	0.49
1:A:812:A:H1'	40:A:3466:HOH:O	2.11	0.49
1:A:1173:A:H2'	40:A:3860:HOH:O	2.12	0.49
1:A:1819:G:H5'	40:A:4224:HOH:O	2.12	0.49
1:A:2768:A:O2'	1:A:2769:C:H5'	2.11	0.49
4:C:53:ALA:HB3	40:C:8603:HOH:O	2.12	0.49
5:D:43:GLY:O	5:D:308:LEU:HD12	2.12	0.49
5:D:51:VAL:HG23	5:D:329:TYR:O	2.12	0.49
5:D:132:HIS:HB2	5:D:137:LEU:HD22	1.94	0.49
5:D:336:GLN:NE2	40:D:8523:HOH:O	2.45	0.49
7:F:23:VAL:HG21	7:F:45:THR:HG21	1.94	0.49
12:K:42:GLU:O	12:K:131:THR:HG23	2.11	0.49
15:N:155:HIS:CE1	15:N:158:ARG:HE	2.30	0.49
25:X:22:GLU:HG2	25:X:27:HIS:CD2	2.47	0.49
1:A:1003:U:O2'	11:J:90:PHE:HE1	1.95	0.49
1:A:1236:A:H2'	1:A:1237:U:O4'	2.13	0.49
1:A:1730:G:C5'	1:A:1731:C:C6	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2589:U:H2'	1:A:2590:U:C6	2.47	0.49
1:A:2896:A:H2'	1:A:2896:A:N3	2.27	0.49
4:C:192:VAL:HG12	4:C:192:VAL:O	2.11	0.49
5:D:27:ASN:HB3	40:D:8622:HOH:O	2.13	0.49
7:F:99:ASP:HB2	7:F:103:ASN:H	1.77	0.49
9:H:79:GLN:HB2	9:H:82:ASP:OD2	2.13	0.49
10:I:64:ASN:N	10:I:64:ASN:ND2	2.60	0.49
25:X:139:GLY:O	25:X:141:HIS:HD2	1.95	0.49
1:A:74:A:H2'	1:A:75:U:C6	2.47	0.49
1:A:1098:A:H2'	1:A:1099:G:O4'	2.12	0.49
1:A:1268:C:O2'	1:A:1269:G:H5'	2.11	0.49
1:A:1717:A:H5''	18:Q:54:LYS:HB2	1.95	0.49
1:A:2010:A:H2'	40:A:5474:HOH:O	2.13	0.49
1:A:2420:G:H4'	40:A:3605:HOH:O	2.12	0.49
1:A:2613:G:O2'	1:A:2614:C:H5'	2.12	0.49
15:N:87:MET:HB2	15:N:91:ILE:HD11	1.94	0.49
16:O:77:ASN:OD1	16:O:80:SER:HB2	2.12	0.49
17:P:26:TRP:N	40:P:3062:HOH:O	2.44	0.49
25:X:6:GLN:CB	25:X:26:ILE:HD12	2.34	0.49
1:A:349:U:O2'	1:A:350:C:H5'	2.12	0.49
1:A:432:G:O2'	1:A:433:C:H5'	2.12	0.49
1:A:542:A:H2'	1:A:543:G:O4'	2.12	0.49
1:A:1535:G:H2'	1:A:1536:C:C6	2.47	0.49
1:A:1942:A:O2'	1:A:1943:C:H5'	2.13	0.49
1:A:2619:U:H2'	1:A:2620:U:C6	2.47	0.49
4:C:173:GLY:O	4:C:176:HIS:HB3	2.12	0.49
7:F:93:LEU:HG	40:F:3862:HOH:O	2.11	0.49
8:G:11:VAL:CG1	8:G:12:ASP:N	2.75	0.49
14:M:57:VAL:HG12	14:M:57:VAL:O	2.13	0.49
15:N:172:GLY:C	15:N:183:VAL:HG11	2.33	0.49
1:A:926:A:O2'	14:M:41:HIS:CD2	2.65	0.49
4:C:94:LEU:HG	4:C:99:ILE:CD1	2.42	0.49
4:C:164:ARG:HB2	28:1:68:CYS:SG	2.52	0.49
5:D:7:ARG:HH11	5:D:7:ARG:CG	2.20	0.49
8:G:7:ILE:HD11	8:G:11:VAL:O	2.12	0.49
11:J:129:ASN:HD22	11:J:129:ASN:N	2.10	0.49
14:M:97:VAL:HG12	14:M:98:GLU:O	2.13	0.49
25:X:13:MET:CE	25:X:17:ILE:HG22	2.42	0.49
4:C:153:ARG:HH11	4:C:153:ARG:CB	2.25	0.49
7:F:23:VAL:HG23	7:F:41:LEU:HD22	1.94	0.49
7:F:27:ILE:HD11	7:F:37:ALA:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:45:GLN:HE21	11:J:135:TRP:HE1	1.60	0.49
13:L:34:VAL:HB	40:L:7169:HOH:O	2.13	0.49
16:O:15:GLU:HB2	16:O:17:ARG:HG3	1.94	0.49
20:S:113:HIS:O	20:S:145:LEU:HD12	2.12	0.49
31:4:48:ASN:ND2	31:4:50:GLY:H	2.10	0.49
1:A:559:U:H2'	1:A:560:C:O4'	2.13	0.49
1:A:703:G:O2'	1:A:704:C:H5'	2.13	0.49
1:A:821:U:H2'	1:A:822:C:H6	1.76	0.49
1:A:1168:C:H5	40:A:7011:HOH:O	1.96	0.49
1:A:2353:A:H4'	1:A:2354:A:O5'	2.12	0.49
1:A:2365:G:H4'	19:R:45:PRO:O	2.12	0.49
7:F:158:ASN:HB2	7:F:161:ASP:OD2	2.12	0.49
8:G:116:THR:HG22	8:G:151:LEU:HD22	1.94	0.49
20:S:44:VAL:O	20:S:48:GLU:HG3	2.12	0.49
22:U:78:THR:HB	22:U:87:VAL:O	2.13	0.49
27:Z:144:ARG:NH1	40:Z:8571:HOH:O	2.37	0.49
28:1:22:ILE:O	28:1:26:VAL:HG23	2.11	0.49
1:A:1056:U:H2'	1:A:1057:A:O4'	2.13	0.49
4:C:36:ASP:HA	4:C:83:GLY:HA3	1.95	0.49
5:D:84:LEU:O	5:D:84:LEU:HD13	2.12	0.49
7:F:59:GLY:C	7:F:61:PHE:H	2.16	0.49
1:A:875:A:C2	4:C:194:MET:SD	3.06	0.49
1:A:1656:A:H2'	1:A:1657:A:O4'	2.13	0.49
1:A:1730:G:H5'	1:A:1731:C:C6	2.48	0.49
1:A:1735:C:O2'	1:A:1736:A:H5'	2.12	0.49
1:A:1926:G:H2'	1:A:1927:A:C8	2.48	0.49
8:G:126:ILE:HB	8:G:131:LEU:HD23	1.94	0.49
11:J:65:ARG:HB3	40:J:8385:HOH:O	2.12	0.49
16:O:43:VAL:HG11	16:O:81:ALA:HA	1.94	0.49
21:T:81:ILE:HG12	40:T:8336:HOH:O	2.11	0.49
22:U:49:GLU:HB3	22:U:59:GLU:CG	2.43	0.49
25:X:1:MET:HB2	25:X:103:GLU:HG2	1.95	0.49
25:X:3:ALA:O	25:X:54:PHE:HA	2.13	0.49
30:3:40:ARG:HG3	30:3:45:ASN:CB	2.43	0.49
1:A:377:C:H5	40:A:9819:HOH:O	1.95	0.49
1:A:514:G:OP1	1:A:514:G:H2'	2.12	0.49
1:A:920:C:H5''	1:A:921:G:O5'	2.13	0.49
1:A:2073:G:OP2	1:A:2490:A:H5'	2.13	0.49
1:A:2274:A:H1'	15:N:86:MET:HE1	1.95	0.49
2:B:3064:C:H2'	2:B:3065:A:H5'	1.95	0.49
5:D:223:ARG:HG3	5:D:232:TRP:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:127:ARG:HG2	6:E:127:ARG:NH1	2.28	0.49
8:G:5:LEU:HD21	8:G:66:GLN:HG3	1.93	0.49
8:G:92:PRO:HB2	40:G:4917:HOH:O	2.12	0.49
11:J:75:SER:HB3	11:J:79:ALA:CB	2.43	0.49
15:N:65:VAL:HG21	15:N:105:ALA:HB2	1.94	0.49
15:N:154:ARG:HG3	40:N:8614:HOH:O	2.12	0.49
16:O:58:LEU:HD12	16:O:58:LEU:N	2.28	0.49
20:S:82:GLU:O	20:S:86:LYS:HG3	2.12	0.49
31:4:15:ASN:ND2	40:4:8547:HOH:O	2.46	0.49
1:A:1003:U:O2	11:J:90:PHE:CZ	2.65	0.48
1:A:1119:G:C8	12:K:52:GLN:NE2	2.81	0.48
4:C:39:ALA:O	4:C:61:GLU:HG3	2.13	0.48
17:P:38:ARG:NH1	40:P:7674:HOH:O	2.46	0.48
25:X:122:ARG:HG2	25:X:152:ALA:O	2.11	0.48
27:Z:106:THR:CG2	27:Z:107:PRO:HD2	2.43	0.48
1:A:816:G:C6	1:A:817:G:N1	2.81	0.48
2:B:3076:G:C3'	2:B:3077:A:H5''	2.32	0.48
4:C:97:ALA:HB2	4:C:150:PRO:HB2	1.95	0.48
5:D:217:ARG:HG3	5:D:257:THR:CG2	2.42	0.48
16:O:163:PHE:HE1	16:O:171:HIS:HD1	1.61	0.48
19:R:11:ARG:HD3	40:R:5620:HOH:O	2.12	0.48
20:S:132:ARG:NH1	40:S:8582:HOH:O	2.45	0.48
1:A:1137:G:H1'	40:A:3388:HOH:O	2.12	0.48
1:A:1211:G:O2'	1:A:1212:C:H5'	2.13	0.48
1:A:1699:C:H4'	40:A:5952:HOH:O	2.13	0.48
1:A:2361:A:H5''	40:A:8523:HOH:O	2.13	0.48
5:D:268:ARG:NH2	5:D:325:PRO:HG3	2.28	0.48
5:D:305:ASP:O	5:D:306:LYS:CB	2.61	0.48
14:M:73:VAL:HG23	14:M:74:THR:N	2.28	0.48
25:X:119:HIS:HD2	25:X:120:PRO:O	1.96	0.48
26:Y:43:VAL:CG1	26:Y:44:ASP:N	2.75	0.48
29:2:25:LYS:HG3	30:3:49:GLU:H	1.76	0.48
1:A:538:C:H5''	1:A:539:G:C8	2.48	0.48
1:A:625:U:H5''	1:A:1044:C:N4	2.28	0.48
40:B:7568:HOH:O	16:O:107:ASN:HB3	2.13	0.48
6:E:133:ARG:HD2	40:E:8409:HOH:O	2.13	0.48
15:N:104:ARG:O	15:N:108:LYS:HG2	2.13	0.48
20:S:34:GLU:HG2	20:S:46:TYR:OH	2.12	0.48
28:1:56:MET:HA	28:1:62:TYR:O	2.13	0.48
1:A:482:G:H4'	1:A:508:A:N1	2.29	0.48
1:A:553:G:H5'	40:A:3009:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1505:U:H5'	1:A:1505:U:C6	2.44	0.48
1:A:2385:G:H2'	1:A:2386:U:C6	2.48	0.48
40:A:4595:HOH:O	5:D:216:LYS:HA	2.13	0.48
5:D:74:ILE:HG13	40:D:8600:HOH:O	2.12	0.48
5:D:168:GLY:H	5:D:174:ARG:HD3	1.79	0.48
7:F:81:GLU:O	7:F:85:GLN:HG3	2.13	0.48
11:J:157:ILE:CG2	11:J:158:ASN:N	2.76	0.48
20:S:104:PHE:HB2	20:S:109:MET:HE1	1.95	0.48
26:Y:30:MET:HE1	26:Y:55:ASN:HA	1.95	0.48
31:4:87:ARG:HG3	40:4:8573:HOH:O	2.13	0.48
1:A:790:A:H2'	1:A:791:A:O4'	2.14	0.48
1:A:1139:U:H2'	1:A:1140:C:C6	2.49	0.48
2:B:3001:U:O3'	2:B:3003:A:H5''	2.14	0.48
4:C:211:LYS:NZ	40:C:8573:HOH:O	2.47	0.48
7:F:146:LYS:HZ1	16:O:107:ASN:ND2	2.08	0.48
7:F:170:TYR:O	7:F:171:ASP:HB3	2.12	0.48
8:G:32:ARG:O	8:G:33:LEU:HD23	2.12	0.48
9:H:36:THR:HG23	9:H:97:ALA:HB2	1.95	0.48
10:I:27:ILE:HD12	10:I:70:ALA:HB1	1.96	0.48
11:J:13:ALA:HA	11:J:91:HIS:HE1	1.78	0.48
11:J:81:TYR:CD1	11:J:81:TYR:C	2.86	0.48
13:L:65:ARG:HD3	40:L:5358:HOH:O	2.14	0.48
15:N:67:ILE:CD1	15:N:104:ARG:HD2	2.43	0.48
15:N:149:TRP:O	15:N:152:ARG:HG2	2.14	0.48
17:P:112:ARG:HA	40:P:1484:HOH:O	2.11	0.48
21:T:57:THR:CG2	21:T:58:MET:N	2.77	0.48
27:Z:115:ARG:NE	40:Z:8553:HOH:O	2.47	0.48
30:3:19:SER:HB3	40:3:4479:HOH:O	2.13	0.48
1:A:954:U:O2'	1:A:955:A:H5'	2.13	0.48
1:A:1384:C:H5'	26:Y:30:MET:HG2	1.96	0.48
1:A:1497:G:H4'	1:A:1627:G:O2'	2.13	0.48
1:A:1666:C:H2'	1:A:1667:A:C5'	2.43	0.48
1:A:2090:G:H2'	1:A:2091:G:C8	2.48	0.48
40:A:6916:HOH:O	22:U:2:LYS:HE2	2.13	0.48
40:A:8832:HOH:O	28:1:16:PRO:HG3	2.14	0.48
4:C:48:ASP:HB3	40:C:8603:HOH:O	2.12	0.48
7:F:65:GLU:HG3	40:F:6752:HOH:O	2.12	0.48
8:G:31:ARG:NH1	40:G:5919:HOH:O	2.45	0.48
9:H:46:GLU:OE1	9:H:100:ASP:HA	2.14	0.48
16:O:21:HIS:HB2	40:O:8533:HOH:O	2.14	0.48
22:U:1:SER:N	40:U:5837:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1268:C:H2'	1:A:1269:G:H8	1.79	0.48
1:A:1603:A:H5''	1:A:1605:G:H5'	1.95	0.48
1:A:2435:U:H1'	40:A:4946:HOH:O	2.14	0.48
1:A:2821:C:H4'	5:D:116:PRO:HB3	1.95	0.48
5:D:320:GLN:HG3	5:D:321:PRO:HD2	1.95	0.48
6:E:16:VAL:HG12	6:E:17:ASP:H	1.79	0.48
9:H:47:LEU:HD22	9:H:108:LEU:CD1	2.44	0.48
10:I:63:ARG:N	40:I:2569:HOH:O	2.47	0.48
11:J:147:ARG:HA	11:J:150:LYS:NZ	2.29	0.48
13:L:10:GLN:NE2	13:L:10:GLN:N	2.43	0.48
13:L:58:THR:HG22	13:L:59:LYS:HG3	1.95	0.48
14:M:53:ARG:NH2	14:M:57:VAL:CG1	2.77	0.48
18:Q:10:ALA:HA	18:Q:13:VAL:CG1	2.43	0.48
18:Q:134:VAL:O	18:Q:137:LEU:HB3	2.13	0.48
19:R:25:PRO:HB2	40:R:4350:HOH:O	2.13	0.48
1:A:120:A:H2'	1:A:120:A:N3	2.29	0.48
1:A:1423:C:O2'	1:A:1424:A:H5'	2.14	0.48
1:A:1614:G:H2'	40:A:4142:HOH:O	2.12	0.48
1:A:1878:G:O2'	1:A:1879:U:P	2.71	0.48
1:A:2064:U:H5'	1:A:2652:U:H4'	1.95	0.48
1:A:2326:U:H4'	1:A:2412:G:H4'	1.96	0.48
1:A:2712:G:O2'	1:A:2713:G:H5'	2.14	0.48
2:B:3042:C:O2	7:F:76:ARG:NH1	2.47	0.48
2:B:3107:C:H5	40:B:3167:HOH:O	1.97	0.48
6:E:107:ARG:NH1	6:E:107:ARG:HB3	2.29	0.48
6:E:150:THR:HA	6:E:203:ALA:O	2.12	0.48
7:F:23:VAL:O	7:F:23:VAL:CG2	2.61	0.48
7:F:57:THR:HG23	7:F:63:ILE:CG2	2.42	0.48
31:4:65:THR:HB	31:4:83:TRP:H	1.78	0.48
1:A:644:G:N3	1:A:644:G:H5'	2.27	0.48
1:A:1015:C:H2'	1:A:1016:U:H6	1.79	0.48
1:A:1023:C:O2'	1:A:1024:G:H5'	2.14	0.48
1:A:1654:U:H2'	4:C:47:HIS:CD2	2.47	0.48
1:A:1666:C:C2'	1:A:1667:A:C5'	2.92	0.48
1:A:1909:A:N1	1:A:2128:G:H1'	2.28	0.48
1:A:2054:A:H2	20:S:128:ARG:HH22	1.58	0.48
1:A:2269:C:H2'	1:A:2270:G:H5'	1.94	0.48
2:B:3056:A:H1'	7:F:14:ARG:HG2	1.96	0.48
5:D:16:ARG:NH1	40:D:8611:HOH:O	2.46	0.48
5:D:248:ARG:O	5:D:251:VAL:HG12	2.13	0.48
16:O:47:LEU:HD12	16:O:92:ALA:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:154:LEU:O	16:O:155:GLU:CB	2.62	0.48
16:O:163:PHE:HA	40:O:8519:HOH:O	2.13	0.48
29:2:25:LYS:HG2	29:2:25:LYS:O	2.14	0.48
1:A:2274:A:O2'	1:A:2275:G:H5'	2.13	0.47
1:A:2896:A:OP1	26:Y:15:ARG:NH1	2.47	0.47
40:A:6056:HOH:O	28:1:22:ILE:HG13	2.14	0.47
9:H:22:VAL:HG21	9:H:104:ALA:HB2	1.96	0.47
23:V:17:THR:HG22	23:V:18:GLY:N	2.29	0.47
1:A:177:A:H2'	1:A:178:U:O4'	2.14	0.47
1:A:1762:C:H2'	1:A:1763:C:H6	1.79	0.47
2:B:3023:U:C5'	2:B:3024:U:OP2	2.57	0.47
6:E:246:ARG:HB3	6:E:246:ARG:NH1	2.28	0.47
7:F:18:ILE:HG12	7:F:134:LEU:CD2	2.44	0.47
7:F:58:VAL:CG1	7:F:59:GLY:N	2.76	0.47
11:J:130:HIS:CG	11:J:133:ILE:HD11	2.48	0.47
16:O:89:GLY:O	16:O:92:ALA:HB3	2.14	0.47
1:A:1151:G:OP1	10:I:16:LYS:NZ	2.45	0.47
1:A:1406:A:H4'	1:A:1407:A:H5''	1.96	0.47
1:A:1462:C:H2'	1:A:1463:A:C8	2.50	0.47
1:A:1669:A:H2'	1:A:1670:G:C8	2.49	0.47
1:A:2004:U:H2'	1:A:2005:G:OP1	2.14	0.47
5:D:132:HIS:CE1	5:D:171:VAL:HG21	2.50	0.47
7:F:159:PRO:O	7:F:163:VAL:HG23	2.14	0.47
8:G:86:VAL:CG1	8:G:129:GLU:HA	2.44	0.47
11:J:163:PRO:HG2	40:J:8340:HOH:O	2.13	0.47
15:N:31:TRP:HA	15:N:34:GLU:HG3	1.95	0.47
19:R:93:ARG:HH11	19:R:93:ARG:HG3	1.79	0.47
22:U:101:LEU:HD13	22:U:112:LEU:HD11	1.96	0.47
23:V:33:SER:O	23:V:37:GLU:HG3	2.15	0.47
1:A:128:A:H3'	1:A:128:A:C8	2.49	0.47
1:A:154:C:P	15:N:188:ARG:HH12	2.37	0.47
1:A:1060:C:H6	1:A:1060:C:H5'	1.80	0.47
1:A:1187:U:H2'	40:A:6408:HOH:O	2.13	0.47
1:A:2266:A:OP2	15:N:90:ARG:NH2	2.47	0.47
1:A:2281:C:H2'	1:A:2282:U:H5'	1.96	0.47
1:A:2403:C:H3'	40:A:4729:HOH:O	2.15	0.47
1:A:2649:A:H5'	1:A:2649:A:H8	1.78	0.47
8:G:126:ILE:HB	8:G:131:LEU:CD2	2.44	0.47
14:M:149:ARG:O	14:M:150:GLN:HB2	2.15	0.47
15:N:114:VAL:HB	15:N:159:THR:HG23	1.96	0.47
15:N:122:GLU:OE2	15:N:127:LYS:HE2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:73:ALA:N	40:O:8568:HOH:O	2.47	0.47
20:S:39:THR:CG2	20:S:42:GLU:HG3	2.44	0.47
21:T:6:LYS:HB2	21:T:27:ALA:O	2.14	0.47
1:A:182:G:O3'	15:N:157:LEU:CD1	2.62	0.47
1:A:656:G:H5'	17:P:3:THR:HG22	1.96	0.47
1:A:1010:C:H4'	16:O:4:PRO:HB2	1.97	0.47
1:A:2443:C:O3'	14:M:56:LYS:HE3	2.15	0.47
1:A:2730:G:O2'	1:A:2731:G:H5'	2.14	0.47
5:D:41:PHE:HA	5:D:79:MET:HE2	1.95	0.47
5:D:56:ASP:OD1	5:D:322:ARG:HB3	2.13	0.47
5:D:207:LYS:HG2	5:D:304:PRO:HB3	1.96	0.47
6:E:214:THR:HG23	40:E:8437:HOH:O	2.14	0.47
11:J:35:ASN:HD21	11:J:80:ASN:HA	1.79	0.47
15:N:99:ARG:CD	15:N:167:GLY:HA2	2.45	0.47
16:O:71:TRP:N	40:O:8539:HOH:O	2.46	0.47
27:Z:107:PRO:HB3	27:Z:182:PHE:CE2	2.49	0.47
1:A:794:U:H3	1:A:819:A:H61	1.63	0.47
1:A:1123:A:C2	1:A:1129:C:H4'	2.49	0.47
1:A:2094:G:C4'	5:D:245:SER:HB3	2.41	0.47
4:C:51:ARG:HB2	40:C:8603:HOH:O	2.14	0.47
4:C:194:MET:CE	4:C:199:HIS:HB2	2.45	0.47
7:F:41:LEU:CA	7:F:44:ILE:HG22	2.44	0.47
7:F:65:GLU:HA	40:F:6752:HOH:O	2.13	0.47
11:J:139:ASP:HB2	40:J:8348:HOH:O	2.15	0.47
12:K:19:MET:HE2	12:K:79:PHE:HA	1.97	0.47
12:K:77:GLY:O	12:K:78:ILE:C	2.53	0.47
19:R:32:GLU:HA	19:R:71:TYR:OH	2.15	0.47
19:R:93:ARG:HG3	19:R:93:ARG:NH1	2.30	0.47
26:Y:21:PRO:HG2	26:Y:24:LYS:HD3	1.95	0.47
1:A:669:G:O2'	1:A:670:G:H5'	2.15	0.47
1:A:797:A:O4'	28:1:10:ARG:N	2.48	0.47
1:A:1015:C:H2'	1:A:1016:U:C6	2.50	0.47
2:B:3031:C:H2'	2:B:3032:G:O4'	2.15	0.47
2:B:3051:A:H5'	16:O:160:SER:HB3	1.97	0.47
4:C:51:ARG:NH2	4:C:69:LEU:HD13	2.29	0.47
4:C:217:ARG:HH11	4:C:217:ARG:CG	2.28	0.47
7:F:154:LYS:H	7:F:154:LYS:CD	2.15	0.47
8:G:107:PHE:CE2	8:G:108:LEU:HD13	2.50	0.47
11:J:14:TYR:N	11:J:91:HIS:HE1	2.12	0.47
11:J:127:GLY:O	11:J:128:ALA:CB	2.63	0.47
13:L:28:GLU:OE2	13:L:58:THR:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:72:ASN:O	14:M:76:LEU:HG	2.14	0.47
16:O:73:ALA:HB1	16:O:74:PRO:CD	2.45	0.47
16:O:139:TRP:HA	16:O:139:TRP:HE3	1.80	0.47
20:S:39:THR:CB	20:S:42:GLU:HG3	2.45	0.47
27:Z:154:ARG:NH1	27:Z:155:ARG:HG3	2.30	0.47
31:4:69:TYR:HB2	31:4:78:HIS:CE1	2.50	0.47
1:A:424:C:H2'	1:A:425:U:C6	2.50	0.47
1:A:2842:G:H2'	1:A:2843:A:H5'	1.96	0.47
4:C:70:ALA:HA	4:C:71:PRO:HD3	1.76	0.47
6:E:61:PHE:HB3	40:E:8446:HOH:O	2.14	0.47
11:J:26:LYS:HA	11:J:58:HIS:CD2	2.49	0.47
11:J:85:ILE:HB	11:J:132:PHE:HE2	1.80	0.47
11:J:150:LYS:HA	11:J:153:VAL:HG22	1.96	0.47
14:M:101:ASP:C	14:M:103:ALA:H	2.18	0.47
17:P:77:ALA:HB1	17:P:98:LEU:HD12	1.97	0.47
18:Q:13:VAL:HG13	18:Q:14:LEU:N	2.30	0.47
27:Z:187:VAL:HB	40:Z:8565:HOH:O	2.14	0.47
1:A:797:A:H4'	28:1:10:ARG:N	2.28	0.47
1:A:2563:U:H2'	1:A:2565:C:O5'	2.14	0.47
40:A:6970:HOH:O	6:E:188:ARG:HD3	2.15	0.47
6:E:234:VAL:O	6:E:234:VAL:HG22	2.15	0.47
9:H:26:THR:HB	9:H:102:GLY:HA3	1.97	0.47
11:J:31:PHE:HD2	11:J:85:ILE:O	1.97	0.47
22:U:75:GLU:O	22:U:76:ASP:HB2	2.13	0.47
1:A:1331:A:OP2	27:Z:142:SER:OG	2.31	0.47
1:A:2472:C:O2'	1:A:2634:G:H4'	2.14	0.47
4:C:95:PRO:HA	4:C:153:ARG:HA	1.97	0.47
17:P:96:VAL:HG13	17:P:100:GLN:HB2	1.97	0.47
22:U:38:ARG:HH11	22:U:38:ARG:HG3	1.79	0.47
26:Y:41:PHE:O	26:Y:43:VAL:HG23	2.14	0.47
1:A:816:G:H5'	1:A:1598:A:H4'	1.96	0.46
1:A:1192:A:H3'	1:A:1193:A:H5'	1.96	0.46
1:A:1864:C:OP1	15:N:75:THR:HG23	2.16	0.46
6:E:246:ARG:CZ	40:E:8423:HOH:O	2.63	0.46
18:Q:59:ARG:HH22	18:Q:66:GLN:HE22	1.59	0.46
1:A:629:A:H2'	1:A:630:A:O4'	2.15	0.46
1:A:1418:U:OP1	30:3:42:TRP:HB3	2.15	0.46
1:A:1730:G:C5'	1:A:1731:C:H6	2.27	0.46
1:A:2724:U:H2'	1:A:2725:G:O4'	2.15	0.46
1:A:2768:A:H3'	40:A:3940:HOH:O	2.15	0.46
1:A:2812:A:C2	1:A:2814:A:N6	2.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:110:GLU:O	9:H:114:LYS:HG3	2.14	0.46
11:J:147:ARG:HA	11:J:150:LYS:HZ2	1.79	0.46
21:T:51:GLN:HE21	21:T:53:ASN:ND2	2.12	0.46
27:Z:178:HIS:CG	27:Z:179:PRO:HD2	2.51	0.46
1:A:1503:U:H2'	1:A:1504:A:O4'	2.16	0.46
1:A:1789:G:O6	18:Q:73:HIS:HE1	1.98	0.46
1:A:2464:C:H5''	1:A:2465:A:OP1	2.15	0.46
2:B:3088:G:OP1	25:X:130:HIS:NE2	2.45	0.46
5:D:7:ARG:HG2	5:D:7:ARG:NH1	2.26	0.46
11:J:109:ASP:HB2	40:J:8347:HOH:O	2.15	0.46
15:N:115:LEU:HD13	15:N:116:ASN:HB2	1.98	0.46
22:U:49:GLU:OE2	22:U:97:ARG:NH1	2.40	0.46
26:Y:30:MET:CE	26:Y:58:ALA:HB3	2.46	0.46
26:Y:37:LEU:HD21	26:Y:72:VAL:HG11	1.98	0.46
1:A:1235:G:C1'	12:K:63:ILE:HG23	2.45	0.46
1:A:2720:C:O2	13:L:87:ARG:NH2	2.49	0.46
1:A:2769:C:H2'	1:A:2770:G:C5'	2.45	0.46
2:B:3092:G:C6	2:B:3093:A:C6	3.04	0.46
7:F:19:GLU:O	7:F:133:ASN:HB3	2.15	0.46
11:J:71:TYR:C	11:J:73:GLN:N	2.67	0.46
1:A:544:G:H2'	1:A:545:G:C5'	2.40	0.46
1:A:1555:G:H4'	1:A:1630:A:H2	1.81	0.46
1:A:1862:C:H1'	40:A:6727:HOH:O	2.15	0.46
8:G:11:VAL:HG13	8:G:23:GLU:O	2.14	0.46
16:O:93:GLN:HG2	40:O:8559:HOH:O	2.15	0.46
23:V:49:LEU:HD11	40:V:3805:HOH:O	2.16	0.46
24:W:57:LYS:HA	24:W:60:GLN:HE21	1.80	0.46
1:A:581:G:H5'	40:A:7202:HOH:O	2.16	0.46
1:A:2072:G:C6	1:A:2533:C:H1'	2.51	0.46
5:D:75:GLU:C	5:D:77:PRO:HD3	2.36	0.46
7:F:86:THR:C	7:F:89:PRO:HD2	2.35	0.46
13:L:98:VAL:HG13	13:L:99:ASP:N	2.30	0.46
14:M:54:PRO:HG2	14:M:57:VAL:CG2	2.46	0.46
15:N:78:ASN:C	15:N:79:LYS:HG2	2.36	0.46
28:1:42:CYS:SG	28:1:43:GLY:N	2.89	0.46
28:1:58:GLY:CA	40:1:8437:HOH:O	2.45	0.46
30:3:18:ASN:ND2	30:3:40:ARG:H	2.14	0.46
1:A:1666:C:C2'	1:A:1667:A:H5''	2.45	0.46
2:B:3078:G:N2	2:B:3103:A:OP2	2.45	0.46
9:H:48:VAL:HG23	9:H:74:PHE:CB	2.46	0.46
15:N:87:MET:HE2	40:N:8593:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:184:ILE:HG22	16:O:185:GLU:HG3	1.96	0.46
20:S:119:VAL:O	20:S:119:VAL:CG1	2.63	0.46
24:W:11:MET:HB3	24:W:15:GLU:HB2	1.97	0.46
1:A:2338:G:H2'	7:F:129:ASP:OD1	2.15	0.46
40:C:8610:HOH:O	28:1:75:ALA:HB3	2.16	0.46
8:G:95:VAL:O	8:G:126:ILE:HD13	2.15	0.46
18:Q:14:LEU:HD13	18:Q:51:ALA:HB2	1.97	0.46
20:S:114:VAL:O	20:S:114:VAL:HG13	2.15	0.46
26:Y:26:ALA:HB1	26:Y:59:TRP:CE2	2.50	0.46
1:A:130:C:H5'	40:A:4731:HOH:O	2.14	0.46
1:A:283:U:H5	1:A:284:C:N4	2.14	0.46
1:A:1667:A:H2'	1:A:1668:U:H6	1.80	0.46
1:A:1919:A:H4'	40:A:4363:HOH:O	2.16	0.46
1:A:2597:U:H2'	1:A:2598:U:H5'	1.98	0.46
5:D:119:HIS:O	5:D:121:PRO:HD3	2.16	0.46
6:E:20:ASP:O	6:E:23:GLU:HB2	2.15	0.46
8:G:101:GLU:OE2	8:G:115:ARG:NH1	2.48	0.46
9:H:48:VAL:CG2	9:H:74:PHE:HB3	2.45	0.46
9:H:91:VAL:CG1	9:H:92:GLY:N	2.76	0.46
12:K:93:ARG:HB3	12:K:93:ARG:NH1	2.30	0.46
14:M:130:ARG:HA	40:M:8558:HOH:O	2.15	0.46
19:R:32:GLU:O	19:R:93:ARG:NH2	2.49	0.46
20:S:68:HIS:CG	20:S:76:ASP:HB2	2.51	0.46
21:T:10:VAL:HG11	24:W:36:ALA:HA	1.98	0.46
1:A:37:A:H2'	1:A:38:G:C8	2.51	0.46
1:A:764:C:H2'	1:A:765:G:O4'	2.16	0.46
1:A:1506:U:H6	1:A:1506:U:H5'	1.80	0.46
1:A:1682:A:H5''	40:A:8964:HOH:O	2.15	0.46
1:A:1687:C:O2	29:2:9:GLY:HA2	2.16	0.46
22:U:80:GLU:OE2	22:U:84:GLY:HA2	2.16	0.46
23:V:39:ASN:ND2	23:V:44:ARG:HH11	2.14	0.46
27:Z:144:ARG:NH2	40:Z:8608:HOH:O	2.48	0.46
28:1:29:VAL:O	28:1:33:HIS:HB2	2.15	0.46
28:1:57:CYS:SG	28:1:59:HIS:HB3	2.55	0.46
1:A:170:U:H2'	1:A:171:C:H5'	1.98	0.45
1:A:241:A:C2	1:A:378:A:H4'	2.51	0.45
1:A:834:G:H3'	1:A:835:U:H4'	1.98	0.45
1:A:2506:A:H1'	40:A:5568:HOH:O	2.16	0.45
40:A:9048:HOH:O	18:Q:81:LYS:HG2	2.15	0.45
4:C:199:HIS:HD2	4:C:201:PHE:HB2	1.80	0.45
5:D:41:PHE:CE1	5:D:79:MET:HG3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:241:PRO:HD2	40:D:8650:HOH:O	2.15	0.45
5:D:301:VAL:HG13	5:D:302:PRO:HD2	1.97	0.45
18:Q:131:PHE:CE1	18:Q:137:LEU:HD13	2.51	0.45
1:A:736:A:H2'	1:A:737:A:O4'	2.16	0.45
1:A:2078:U:O2'	1:A:2079:G:H5'	2.16	0.45
1:A:2780:C:H2'	1:A:2781:U:C6	2.51	0.45
5:D:152:PRO:HD2	40:D:8626:HOH:O	2.16	0.45
7:F:86:THR:HG23	40:F:7477:HOH:O	2.16	0.45
9:H:28:ALA:HB3	9:H:99:THR:O	2.15	0.45
11:J:112:ARG:O	11:J:113:ALA:C	2.54	0.45
17:P:32:ARG:HE	17:P:35:LYS:HD2	1.81	0.45
20:S:25:PHE:CE2	20:S:29:LYS:CE	3.00	0.45
26:Y:70:ILE:O	26:Y:70:ILE:HG23	2.16	0.45
1:A:51:G:O2'	1:A:52:A:H5'	2.16	0.45
1:A:184:G:H5''	15:N:153:THR:HG22	1.98	0.45
1:A:1783:A:O2'	1:A:1784:U:H5'	2.16	0.45
1:A:2507:G:H2'	1:A:2510:C:H42	1.81	0.45
36:5:9080:SPS:O1	36:5:9080:SPS:H91	2.16	0.45
4:C:8:ARG:NH1	40:C:8552:HOH:O	2.48	0.45
5:D:129:ARG:NH2	5:D:176:ASP:OD1	2.47	0.45
5:D:304:PRO:HD2	5:D:307:ARG:HD2	1.98	0.45
15:N:153:THR:O	15:N:156:ARG:HG3	2.16	0.45
16:O:61:ALA:CB	16:O:88:ALA:HB2	2.47	0.45
25:X:122:ARG:HH22	25:X:154:ARG:C	2.20	0.45
30:3:40:ARG:HA	30:3:45:ASN:HD22	1.79	0.45
31:4:6:ARG:NE	40:4:8524:HOH:O	2.48	0.45
1:A:249:G:O2'	1:A:250:C:H5'	2.16	0.45
1:A:566:A:H2'	1:A:567:U:O4'	2.16	0.45
1:A:1119:G:N2	1:A:1246:A:H2	2.09	0.45
1:A:1352:A:N1	6:E:48:SER:HB3	2.30	0.45
1:A:1819:G:H2'	1:A:1820:G:C4'	2.47	0.45
1:A:2243:C:H5''	40:A:3263:HOH:O	2.16	0.45
1:A:2649:A:H5'	1:A:2649:A:C8	2.52	0.45
1:A:2831:C:H2'	1:A:2832:C:H5'	1.99	0.45
4:C:34:ASP:OD1	4:C:35:GLY:N	2.46	0.45
4:C:55:VAL:HG13	4:C:67:LEU:HD22	1.98	0.45
4:C:194:MET:HE1	4:C:199:HIS:HB2	1.98	0.45
5:D:7:ARG:HD3	5:D:9:GLY:O	2.16	0.45
6:E:39:GLN:O	6:E:43:LYS:HD3	2.17	0.45
12:K:51:GLU:O	12:K:55:GLU:HG3	2.16	0.45
18:Q:16:VAL:CG1	18:Q:17:GLY:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:9:VAL:HG13	26:Y:88:GLU:OE1	2.16	0.45
1:A:56:G:H5''	24:W:50:ARG:NH1	2.32	0.45
1:A:558:C:H5'	40:A:4774:HOH:O	2.16	0.45
1:A:1028:U:H1'	40:A:3159:HOH:O	2.17	0.45
1:A:1562:C:H42	1:A:2738:G:H1	1.64	0.45
1:A:2791:U:H1'	1:A:2792:A:H5''	1.99	0.45
5:D:24:PRO:HG2	5:D:204:GLY:HA2	1.97	0.45
5:D:81:ALA:O	5:D:186:GLY:HA3	2.17	0.45
6:E:34:ALA:HB3	6:E:220:THR:HG21	1.99	0.45
7:F:94:ALA:HB3	7:F:174:VAL:CA	2.47	0.45
14:M:73:VAL:HG23	14:M:74:THR:H	1.81	0.45
14:M:90:ARG:NH2	14:M:121:ILE:HD11	2.31	0.45
25:X:13:MET:HE3	25:X:17:ILE:CG2	2.44	0.45
25:X:122:ARG:CG	25:X:152:ALA:O	2.64	0.45
28:1:13:ARG:NH1	28:1:14:PHE:CE2	2.85	0.45
28:1:56:MET:HE2	28:1:63:LYS:HG3	1.99	0.45
1:A:321:A:H1'	40:A:6543:HOH:O	2.17	0.45
1:A:2265:U:H2'	1:A:2266:A:H8	1.81	0.45
40:A:3203:HOH:O	8:G:143:GLN:HG2	2.17	0.45
2:B:3092:G:H22	11:J:52:LYS:NZ	2.15	0.45
4:C:179:MET:HG2	4:C:186:TRP:CB	2.47	0.45
5:D:7:ARG:NH1	5:D:11:LEU:HD22	2.31	0.45
9:H:41:GLU:OE2	15:N:2:ARG:HB2	2.16	0.45
10:I:67:LEU:O	10:I:71:LEU:HG	2.16	0.45
11:J:132:PHE:O	11:J:133:ILE:HD13	2.17	0.45
40:L:7438:HOH:O	23:V:20:MET:HE1	2.17	0.45
16:O:163:PHE:O	16:O:164:ASP:O	2.34	0.45
18:Q:16:VAL:CG1	18:Q:20:ARG:HB2	2.47	0.45
25:X:125:HIS:HD2	25:X:127:GLY:H	1.64	0.45
27:Z:122:ARG:NH2	40:Z:8535:HOH:O	2.48	0.45
1:A:20:G:H1'	20:S:5:SER:HB3	1.98	0.45
1:A:795:G:N3	1:A:817:G:C2	2.85	0.45
1:A:951:A:H2'	1:A:952:G:H5'	1.97	0.45
1:A:2372:A:H2'	1:A:2373:U:C6	2.52	0.45
1:A:2478:U:O2'	1:A:2479:A:H5'	2.17	0.45
1:A:2904:U:H4'	26:Y:8:ARG:NH1	2.32	0.45
4:C:99:ILE:O	4:C:131:HIS:CE1	2.70	0.45
5:D:202:VAL:HG11	5:D:301:VAL:HG13	1.99	0.45
11:J:157:ILE:HG22	11:J:158:ASN:N	2.31	0.45
15:N:52:LEU:HD13	15:N:116:ASN:CB	2.46	0.45
26:Y:8:ARG:NH1	40:Y:2479:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:2:25:LYS:HD2	30:3:48:ASP:HA	1.97	0.45
1:A:1205:U:H2'	1:A:1206:U:C5'	2.47	0.45
1:A:2005:G:H3'	1:A:2005:G:OP2	2.17	0.45
1:A:2421:G:H3'	1:A:2422:U:H5''	1.98	0.45
4:C:81:GLN:HB2	4:C:92:ASN:HD22	1.80	0.45
5:D:55:ASN:HB3	5:D:64:GLY:H	1.82	0.45
6:E:107:ARG:O	6:E:111:VAL:HG23	2.17	0.45
7:F:99:ASP:HB2	7:F:103:ASN:CB	2.46	0.45
1:A:168:C:O2'	1:A:169:A:H5'	2.17	0.45
1:A:2274:A:H1'	15:N:86:MET:SD	2.57	0.45
4:C:179:MET:HG2	4:C:186:TRP:CG	2.51	0.45
6:E:123:LEU:HA	6:E:123:LEU:HD23	1.85	0.45
14:M:53:ARG:HH22	14:M:57:VAL:HG12	1.78	0.45
15:N:87:MET:H	15:N:87:MET:HG3	1.26	0.45
21:T:37:VAL:O	21:T:41:VAL:HG23	2.16	0.45
25:X:38:THR:HB	40:X:5390:HOH:O	2.16	0.45
1:A:338:C:H4'	6:E:174:ILE:HD11	1.98	0.45
1:A:613:C:H2'	1:A:614:U:H6	1.82	0.45
1:A:1191:A:C3'	1:A:1192:A:H5''	2.43	0.45
1:A:1565:C:O4'	1:A:2738:G:H1'	2.17	0.45
2:B:3064:C:C2'	2:B:3065:A:H5'	2.47	0.45
6:E:19:PRO:HG2	6:E:22:PHE:CD1	2.52	0.45
7:F:91:ALA:HB1	40:F:5198:HOH:O	2.17	0.45
8:G:145:ALA:HB1	8:G:168:ILE:HD11	1.99	0.45
9:H:56:PRO:CG	15:N:44:THR:HA	2.46	0.45
9:H:117:GLU:C	9:H:119:ARG:H	2.20	0.45
10:I:69:ARG:NH1	40:I:3513:HOH:O	2.50	0.45
15:N:138:HIS:C	15:N:139:PRO:O	2.48	0.45
16:O:34:LEU:HA	16:O:47:LEU:HD23	1.99	0.45
26:Y:37:LEU:CD1	26:Y:85:VAL:HG21	2.24	0.45
29:2:21:ARG:HD2	29:2:39:PHE:HB2	1.98	0.45
31:4:87:ARG:NH1	40:4:8525:HOH:O	2.49	0.45
1:A:440:C:H2'	1:A:441:A:C8	2.52	0.44
1:A:2456:A:H2'	1:A:2457:U:C6	2.52	0.44
14:M:92:ASP:OD1	14:M:94:ARG:HB2	2.17	0.44
15:N:81:ARG:HG3	15:N:85:ARG:HB2	1.99	0.44
19:R:66:LYS:HB2	19:R:70:ALA:O	2.17	0.44
20:S:29:LYS:HD3	40:S:8530:HOH:O	2.18	0.44
27:Z:154:ARG:HH12	27:Z:155:ARG:HG3	1.82	0.44
28:1:30:GLU:HB3	28:1:34:LYS:HE3	1.99	0.44
28:1:31:ILE:HG23	28:1:32:LYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:73:GLU:HB2	40:4:8527:HOH:O	2.16	0.44
1:A:88:G:N7	30:3:28:LYS:HD2	2.31	0.44
1:A:517:U:H1'	40:A:7095:HOH:O	2.17	0.44
1:A:716:G:C2'	1:A:717:C:O5'	2.65	0.44
1:A:797:A:H5'	28:1:10:ARG:HG2	1.99	0.44
1:A:1634:G:H2'	1:A:1635:U:C6	2.52	0.44
1:A:1641:A:H2'	1:A:1642:A:C5'	2.46	0.44
6:E:5:ILE:CD1	6:E:16:VAL:HG23	2.35	0.44
6:E:236:THR:HG22	6:E:239:ALA:CB	2.47	0.44
7:F:10:PHE:CE1	7:F:11:HIS:HB3	2.52	0.44
11:J:112:ARG:HB3	40:J:8395:HOH:O	2.17	0.44
12:K:39:VAL:CG1	12:K:107:ASN:HB2	2.47	0.44
14:M:77:ALA:HB3	40:M:8530:HOH:O	2.16	0.44
22:U:38:ARG:NH1	22:U:38:ARG:HG3	2.31	0.44
25:X:34:LEU:CD1	25:X:100:LEU:HD13	2.47	0.44
30:3:40:ARG:HD2	30:3:47:THR:HG22	1.99	0.44
1:A:1269:G:H2'	1:A:1270:U:C6	2.53	0.44
1:A:1681:G:H5''	1:A:1682:A:H5'	1.99	0.44
1:A:2326:U:H4'	1:A:2412:G:C4'	2.47	0.44
4:C:69:LEU:CD2	4:C:120:ARG:HB3	2.43	0.44
4:C:192:VAL:CG1	4:C:192:VAL:O	2.65	0.44
5:D:127:GLN:HG3	40:D:8636:HOH:O	2.16	0.44
9:H:28:ALA:CB	9:H:99:THR:HG23	2.47	0.44
13:L:78:LYS:HA	13:L:79:PRO:HD3	1.87	0.44
29:2:8:GLN:NE2	29:2:11:LYS:NZ	2.60	0.44
1:A:960:G:N3	1:A:960:G:C2'	2.80	0.44
1:A:1592:G:HO2'	1:A:1593:C:C5'	2.30	0.44
1:A:2104:C:O2	1:A:2485:A:N1	2.51	0.44
1:A:2415:A:N3	16:O:26:LEU:HD13	2.32	0.44
1:A:2748:G:H5'	40:A:7058:HOH:O	2.18	0.44
40:A:5137:HOH:O	18:Q:55:LYS:HA	2.17	0.44
2:B:3003:A:H2	2:B:3021:G:N3	2.15	0.44
12:K:75:PRO:HG2	12:K:105:LEU:CD2	2.47	0.44
14:M:67:ARG:HB2	14:M:112:GLY:HA3	1.99	0.44
14:M:125:PHE:CE1	14:M:140:VAL:HG13	2.53	0.44
15:N:108:LYS:HE3	40:N:8615:HOH:O	2.17	0.44
20:S:47:LEU:O	20:S:51:ILE:HG13	2.18	0.44
26:Y:76:ARG:HG3	26:Y:76:ARG:NH1	2.31	0.44
27:Z:189:ASN:CA	27:Z:217:ILE:HD11	2.46	0.44
31:4:70:ARG:NH1	40:4:8539:HOH:O	2.46	0.44
1:A:716:G:H2'	1:A:717:C:O5'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1450:C:O2'	1:A:1494:A:H5'	2.17	0.44
1:A:1921:A:C6	1:A:1922:A:C2	3.05	0.44
5:D:175:LEU:HD23	5:D:175:LEU:O	2.17	0.44
6:E:27:ARG:HG2	6:E:30:LEU:HG	1.98	0.44
7:F:56:ARG:N	40:F:6752:HOH:O	2.51	0.44
7:F:59:GLY:O	7:F:61:PHE:N	2.39	0.44
13:L:72:VAL:HG11	13:L:121:PHE:CD1	2.52	0.44
14:M:121:ILE:HG12	14:M:141:GLU:HB2	1.99	0.44
15:N:78:ASN:O	15:N:79:LYS:HG2	2.18	0.44
16:O:42:HIS:CG	16:O:62:HIS:HE1	2.35	0.44
22:U:45:GLY:C	40:U:3851:HOH:O	2.55	0.44
22:U:73:HIS:CD2	22:U:88:PRO:CG	3.00	0.44
23:V:20:MET:CG	23:V:28:THR:HG23	2.48	0.44
27:Z:126:PRO:HG2	27:Z:128:PHE:CE1	2.53	0.44
27:Z:189:ASN:C	27:Z:189:ASN:ND2	2.70	0.44
1:A:278:A:H2'	1:A:279:C:O4'	2.18	0.44
1:A:333:G:O2'	1:A:334:G:H5'	2.18	0.44
1:A:441:A:H1'	1:A:442:A:N7	2.32	0.44
1:A:2252:A:C5	1:A:2253:G:H1'	2.52	0.44
4:C:33:GLU:H	4:C:33:GLU:CD	2.21	0.44
6:E:214:THR:HB	40:E:8326:HOH:O	2.18	0.44
8:G:84:MET:HE3	8:G:148:ILE:HG21	1.99	0.44
9:H:21:GLU:O	9:H:24:ARG:CG	2.66	0.44
11:J:56:ILE:HG21	11:J:61:LEU:HD13	2.00	0.44
12:K:74:ARG:NH1	12:K:76:ASP:HB2	2.33	0.44
14:M:12:THR:HG21	14:M:16:GLY:O	2.17	0.44
15:N:37:VAL:HG21	15:N:108:LYS:CG	2.48	0.44
17:P:35:LYS:HD3	40:P:3360:HOH:O	2.17	0.44
1:A:587:A:H5''	40:A:6797:HOH:O	2.17	0.44
1:A:1021:G:O2'	1:A:1022:A:H5'	2.18	0.44
1:A:1966:U:H2'	1:A:1967:U:C6	2.52	0.44
4:C:81:GLN:CB	4:C:92:ASN:ND2	2.80	0.44
4:C:170:VAL:HG13	28:1:22:ILE:CG2	2.46	0.44
5:D:168:GLY:O	5:D:169:GLY:O	2.36	0.44
14:M:89:PHE:N	40:M:8572:HOH:O	2.50	0.44
23:V:44:ARG:HB3	40:V:3805:HOH:O	2.18	0.44
25:X:107:LEU:O	25:X:112:LEU:HB2	2.17	0.44
25:X:122:ARG:NH2	40:X:4276:HOH:O	2.44	0.44
27:Z:109:LEU:HA	40:Z:8566:HOH:O	2.18	0.44
1:A:303:C:H2'	1:A:304:G:O4'	2.18	0.44
1:A:581:G:O2'	1:A:582:C:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2385:G:H2'	1:A:2386:U:H6	1.83	0.44
1:A:2767:C:OP1	5:D:318:ASN:ND2	2.51	0.44
40:A:3265:HOH:O	15:N:108:LYS:HD2	2.18	0.44
9:H:22:VAL:CG2	9:H:104:ALA:HB2	2.47	0.44
11:J:55:GLN:HE21	11:J:124:ARG:NE	2.01	0.44
11:J:163:PRO:O	11:J:164:ALA:HB2	2.18	0.44
12:K:75:PRO:HD3	12:K:136:SER:OG	2.17	0.44
13:L:132:VAL:C	40:L:3160:HOH:O	2.55	0.44
16:O:37:ARG:NH2	40:O:8534:HOH:O	2.49	0.44
16:O:67:ALA:HA	16:O:71:TRP:H	1.82	0.44
17:P:81:PHE:N	17:P:81:PHE:CD1	2.85	0.44
22:U:3:GLN:HA	22:U:4:PRO:HD3	1.85	0.44
28:1:34:LYS:HE2	40:1:8425:HOH:O	2.17	0.44
1:A:475:G:H5'	6:E:73:LEU:HD23	2.00	0.44
1:A:638:C:H2'	1:A:639:A:C8	2.53	0.44
1:A:1902:G:H2'	1:A:1903:U:O4'	2.18	0.44
1:A:2506:A:C1'	40:A:5568:HOH:O	2.66	0.44
2:B:3008:G:O6	16:O:11:ARG:NH1	2.51	0.44
2:B:3022:G:N7	2:B:3055:U:O2'	2.35	0.44
5:D:63:GLU:O	5:D:63:GLU:HG3	2.17	0.44
5:D:232:TRP:CD1	5:D:235:ARG:HD2	2.52	0.44
13:L:109:LEU:HD13	13:L:113:ILE:HD11	2.00	0.44
19:R:25:PRO:HA	19:R:26:PRO:HD3	1.86	0.44
20:S:4:TYR:N	40:S:8546:HOH:O	2.51	0.44
22:U:50:VAL:HG12	22:U:56:ALA:HA	2.00	0.44
1:A:262:A:OP2	9:H:91:VAL:HG11	2.18	0.43
1:A:603:A:H4'	1:A:604:G:O5'	2.18	0.43
1:A:941:G:O2'	1:A:942:U:H5'	2.17	0.43
1:A:1249:U:H2'	1:A:1250:C:C6	2.53	0.43
1:A:1592:G:O2'	1:A:1593:C:O5'	2.31	0.43
1:A:2015:A:H2'	1:A:2016:U:O4'	2.18	0.43
1:A:2415:A:C2	16:O:25:ARG:HB3	2.53	0.43
5:D:177:HIS:O	5:D:181:ILE:HG13	2.17	0.43
5:D:279:THR:CG2	5:D:280:VAL:N	2.80	0.43
5:D:312:ARG:HD3	5:D:315:VAL:HG13	1.99	0.43
8:G:34:TRP:O	12:K:127:ILE:HD11	2.18	0.43
8:G:84:MET:HB2	8:G:131:LEU:HB2	2.00	0.43
9:H:34:ASN:HA	15:N:4:ALA:HB2	2.00	0.43
12:K:17:CYS:HA	12:K:119:THR:O	2.18	0.43
12:K:63:ILE:HG22	12:K:64:GLY:N	2.31	0.43
24:W:23:LEU:HD12	24:W:56:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:U:H1'	40:A:3234:HOH:O	2.17	0.43
1:A:1730:G:H5'	1:A:1731:C:H5	1.81	0.43
1:A:1752:G:H2'	40:A:7066:HOH:O	2.19	0.43
1:A:2324:G:N2	1:A:2377:U:H1'	2.33	0.43
40:A:8971:HOH:O	20:S:83:LYS:HD3	2.18	0.43
5:D:51:VAL:HG21	5:D:327:VAL:HG13	1.99	0.43
6:E:77:ALA:O	6:E:78:ARG:HG3	2.18	0.43
11:J:1:LYS:N	40:J:8371:HOH:O	2.51	0.43
11:J:83:PHE:HE1	11:J:146:TRP:CZ2	2.36	0.43
12:K:80:LYS:HE2	12:K:98:PHE:CZ	2.53	0.43
13:L:22:ASP:C	13:L:22:ASP:OD1	2.57	0.43
15:N:95:LYS:HG2	15:N:99:ARG:HB3	2.00	0.43
18:Q:7:LYS:HD2	18:Q:21:VAL:CG2	2.46	0.43
22:U:37:GLN:OE1	22:U:118:SER:HA	2.17	0.43
24:W:5:VAL:CG1	24:W:9:ARG:NH1	2.81	0.43
28:1:25:ARG:O	28:1:29:VAL:HG23	2.19	0.43
1:A:156:C:H5''	15:N:171:ARG:CD	2.26	0.43
1:A:695:C:H2'	1:A:696:C:C6	2.53	0.43
1:A:1182:C:H1'	1:A:1192:A:C8	2.50	0.43
1:A:1523:G:H2'	1:A:1524:U:C6	2.53	0.43
1:A:1857:A:N6	1:A:2247:C:H1'	2.33	0.43
2:B:3060:C:O2'	2:B:3061:C:H5'	2.17	0.43
5:D:60:SER:C	5:D:62:ARG:H	2.20	0.43
5:D:80:ARG:HD3	40:D:8601:HOH:O	2.18	0.43
5:D:87:TYR:OH	5:D:163:GLU:OE2	2.25	0.43
6:E:154:VAL:O	6:E:158:GLU:HG3	2.18	0.43
7:F:23:VAL:HG12	7:F:130:VAL:HG22	2.00	0.43
8:G:83:GLY:O	8:G:169:THR:N	2.39	0.43
8:G:133:VAL:HG12	8:G:141:VAL:HG13	2.00	0.43
14:M:54:PRO:HG2	14:M:57:VAL:HG21	1.99	0.43
14:M:80:ASP:HB2	14:M:90:ARG:O	2.18	0.43
15:N:38:VAL:O	15:N:38:VAL:HG12	2.17	0.43
16:O:161:GLY:O	16:O:162:ASP:C	2.56	0.43
31:4:74:CYS:N	40:4:8561:HOH:O	2.51	0.43
1:A:289:G:O2'	1:A:290:C:H5'	2.18	0.43
1:A:795:G:H1'	1:A:817:G:N2	2.33	0.43
1:A:1158:G:O2'	1:A:1159:G:H5'	2.17	0.43
1:A:1375:A:C2'	1:A:1376:G:H5'	2.48	0.43
5:D:7:ARG:CD	5:D:9:GLY:O	2.66	0.43
5:D:154:VAL:HA	5:D:155:PRO:HD3	1.84	0.43
6:E:7:ASP:OD1	6:E:11:ASN:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:140:VAL:CG1	6:E:141:SER:N	2.82	0.43
7:F:144:ARG:NH2	40:F:3839:HOH:O	2.45	0.43
11:J:86:ARG:HD3	11:J:130:HIS:HD2	1.83	0.43
23:V:6:CYS:C	23:V:8:TYR:H	2.20	0.43
25:X:4:LEU:HD23	25:X:4:LEU:HA	1.84	0.43
25:X:21:LEU:CD2	25:X:48:VAL:HG11	2.47	0.43
1:A:67:A:H5'	1:A:69:A:C8	2.53	0.43
1:A:128:A:O2'	1:A:129:A:H5'	2.18	0.43
1:A:324:G:O2'	1:A:325:U:H5'	2.19	0.43
1:A:1470:A:OP1	15:N:93:ARG:HD2	2.18	0.43
1:A:2061:C:C2'	1:A:2062:A:H5'	2.49	0.43
4:C:35:GLY:O	4:C:36:ASP:CB	2.60	0.43
4:C:130:THR:HG22	4:C:131:HIS:O	2.17	0.43
5:D:274:GLU:HA	5:D:292:GLY:O	2.18	0.43
6:E:1:MET:HG2	6:E:2:GLN:NE2	2.33	0.43
7:F:67:ASP:OD2	7:F:69:ILE:HD11	2.19	0.43
12:K:22:VAL:O	12:K:26:VAL:HG23	2.18	0.43
13:L:28:GLU:HB3	13:L:59:LYS:HB2	2.00	0.43
16:O:24:LEU:HD13	19:R:26:PRO:HB3	2.00	0.43
16:O:37:ARG:CZ	40:O:8534:HOH:O	2.66	0.43
20:S:59:PHE:CZ	20:S:79:ARG:HB2	2.54	0.43
24:W:12:THR:HG23	24:W:14:ALA:H	1.83	0.43
26:Y:34:ARG:NH1	26:Y:48:VAL:O	2.50	0.43
1:A:612:U:H2'	1:A:613:C:C6	2.54	0.43
1:A:671:A:O2'	1:A:672:G:H2'	2.19	0.43
1:A:2776:A:H2'	1:A:2777:G:O4'	2.18	0.43
5:D:125:GLU:O	5:D:129:ARG:HG3	2.18	0.43
7:F:95:THR:C	7:F:97:GLN:N	2.71	0.43
10:I:63:ARG:O	10:I:67:LEU:HG	2.18	0.43
11:J:47:GLU:CB	11:J:133:ILE:CD1	2.95	0.43
13:L:4:LEU:HD22	13:L:116:GLU:HB3	2.01	0.43
18:Q:10:ALA:CA	18:Q:13:VAL:HG12	2.46	0.43
21:T:51:GLN:NE2	21:T:53:ASN:HD21	2.12	0.43
22:U:77:VAL:HG11	22:U:91:LEU:HD11	1.99	0.43
24:W:38:GLY:C	24:W:40:PRO:HD2	2.38	0.43
28:1:10:ARG:HG3	28:1:11:THR:N	2.34	0.43
1:A:796:A:HO2'	28:1:10:ARG:N	2.16	0.43
1:A:1287:A:O4'	25:X:117:ARG:HD3	2.17	0.43
1:A:1413:A:H2'	1:A:1414:A:O4'	2.19	0.43
1:A:2044:G:OP1	26:Y:23:HIS:HE1	2.00	0.43
1:A:2115:U:H2'	1:A:2116:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2274:A:N3	15:N:86:MET:CE	2.82	0.43
1:A:2413:A:N7	16:O:109:PRO:HB3	2.34	0.43
40:A:4896:HOH:O	28:1:13:ARG:NH1	2.51	0.43
7:F:64:ARG:HG2	7:F:66:GLY:O	2.19	0.43
13:L:101:ASN:O	13:L:102:GLU:HB2	2.19	0.43
26:Y:27:ASP:OD2	26:Y:27:ASP:N	2.52	0.43
26:Y:43:VAL:HG12	26:Y:47:ALA:HB3	2.00	0.43
27:Z:187:VAL:HB	27:Z:203:VAL:HG22	2.01	0.43
1:A:737:A:H2'	1:A:738:G:O4'	2.18	0.43
1:A:1109:U:O4	12:K:21:ARG:HA	2.19	0.43
1:A:1191:A:N1	1:A:1206:U:O4	2.52	0.43
5:D:142:LEU:HG	5:D:166:VAL:CG2	2.49	0.43
7:F:62:ASP:HA	40:F:4233:HOH:O	2.19	0.43
8:G:112:ALA:HA	8:G:113:PRO:HD3	1.90	0.43
9:H:101:ALA:HB2	9:H:108:LEU:HD22	1.99	0.43
10:I:16:LYS:O	10:I:20:VAL:HG23	2.19	0.43
11:J:46:VAL:O	11:J:146:TRP:CH2	2.68	0.43
11:J:72:VAL:HG11	11:J:81:TYR:CZ	2.54	0.43
14:M:21:ARG:N	40:M:8531:HOH:O	2.51	0.43
17:P:26:TRP:HA	17:P:26:TRP:CE3	2.54	0.43
27:Z:117:LEU:HA	27:Z:174:VAL:HG11	2.00	0.43
1:A:189:A:OP1	15:N:171:ARG:NH2	2.52	0.43
1:A:903:U:O4	14:M:18:HIS:HB2	2.18	0.43
1:A:970:U:H2'	40:A:5838:HOH:O	2.19	0.43
1:A:1603:A:C5'	1:A:1605:G:H5'	2.49	0.43
1:A:1926:G:H2'	1:A:1927:A:H8	1.84	0.43
1:A:2356:A:H2'	1:A:2357:G:O4'	2.18	0.43
40:A:4243:HOH:O	16:O:21:HIS:HD2	2.01	0.43
4:C:30:ARG:HE	4:C:30:ARG:HB3	1.69	0.43
4:C:199:HIS:CD2	4:C:201:PHE:HB2	2.53	0.43
8:G:11:VAL:HG11	8:G:22:VAL:HG13	2.00	0.43
11:J:26:LYS:HG2	11:J:28:ILE:N	2.29	0.43
15:N:55:LYS:O	15:N:60:ILE:HD12	2.19	0.43
17:P:107:GLU:O	17:P:108:GLY:C	2.57	0.43
20:S:72:VAL:CG1	20:S:75:TRP:HB3	2.48	0.43
22:U:48:VAL:CG1	22:U:96:VAL:HG13	2.49	0.43
24:W:5:VAL:HG11	24:W:9:ARG:NH1	2.34	0.43
1:A:187:A:H3'	1:A:188:C:H6	1.83	0.43
1:A:245:C:H2'	1:A:246:G:H5'	2.01	0.43
1:A:283:U:H5''	1:A:284:C:OP2	2.19	0.43
1:A:291:C:H2'	1:A:292:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:C:H2'	1:A:345:G:O4'	2.18	0.43
1:A:958:G:H2'	1:A:959:C:C6	2.53	0.43
1:A:1175:G:H1'	1:A:1193:A:H2'	2.01	0.43
9:H:63:ILE:HB	9:H:64:PRO:CD	2.44	0.43
22:U:49:GLU:HB3	22:U:59:GLU:HG3	2.01	0.43
25:X:54:PHE:CZ	25:X:140:LYS:HB2	2.53	0.43
25:X:88:THR:CG2	25:X:110:GLN:NE2	2.75	0.43
25:X:142:ASP:HB3	25:X:145:GLY:H	1.82	0.43
1:A:35:U:H5'	6:E:47:GLY:O	2.19	0.42
1:A:289:G:N1	1:A:363:A:C2	2.85	0.42
1:A:559:U:H5'	1:A:559:U:C6	2.45	0.42
1:A:664:U:O4	1:A:681:G:H5''	2.18	0.42
1:A:912:A:C4	1:A:1294:A:C2	3.07	0.42
1:A:920:C:H4'	1:A:921:G:C2	2.54	0.42
1:A:1135:G:H5'	40:A:5445:HOH:O	2.19	0.42
1:A:1166:A:H61	1:A:1180:U:H3	1.67	0.42
1:A:1231:A:N3	1:A:2553:A:H5''	2.34	0.42
1:A:1314:U:H5''	1:A:1316:G:O4'	2.19	0.42
1:A:1588:G:C6	1:A:1589:G:N1	2.87	0.42
1:A:1684:A:O2'	1:A:1685:A:H5''	2.19	0.42
1:A:2401:A:H2'	1:A:2402:A:C8	2.55	0.42
1:A:2755:G:H1'	40:A:4197:HOH:O	2.19	0.42
7:F:23:VAL:HG21	7:F:45:THR:CG2	2.48	0.42
11:J:48:LEU:HD13	11:J:146:TRP:HB3	2.02	0.42
14:M:128:GLY:O	14:M:132:LYS:HG3	2.18	0.42
14:M:143:THR:HG21	40:M:8537:HOH:O	2.19	0.42
15:N:37:VAL:HG21	15:N:108:LYS:HG3	2.01	0.42
20:S:119:VAL:HG21	20:S:142:ASP:CG	2.39	0.42
1:A:240:C:H4'	15:N:146:GLN:NE2	2.34	0.42
1:A:485:A:O2'	1:A:487:G:H5'	2.19	0.42
1:A:694:A:H2'	1:A:695:C:H5'	2.01	0.42
1:A:710:G:N2	1:A:719:C:C2	2.88	0.42
1:A:1114:A:H2'	1:A:1115:U:H6	1.84	0.42
1:A:1309:U:O2'	1:A:1310:U:H5'	2.17	0.42
1:A:2088:C:H1'	1:A:2841:A:N1	2.35	0.42
1:A:2269:C:H2'	1:A:2270:G:C5'	2.49	0.42
1:A:2362:A:H2'	1:A:2363:G:C8	2.54	0.42
1:A:2712:G:H5'	40:L:4183:HOH:O	2.18	0.42
1:A:2781:U:C2'	1:A:2782:G:H5'	2.49	0.42
4:C:186:TRP:CD1	4:C:187:PRO:HA	2.54	0.42
8:G:108:LEU:HD11	8:G:164:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:67:ILE:HD13	15:N:104:ARG:HH11	1.84	0.42
17:P:96:VAL:CG1	17:P:100:GLN:HB2	2.49	0.42
18:Q:115:SER:O	18:Q:117:SER:N	2.52	0.42
20:S:119:VAL:HG11	40:S:8583:HOH:O	2.18	0.42
24:W:1:THR:HG23	24:W:2:VAL:N	2.23	0.42
1:A:585:C:H6	40:A:5609:HOH:O	2.01	0.42
1:A:1335:C:H2'	1:A:1336:U:C6	2.54	0.42
1:A:2787:C:H5	40:A:4147:HOH:O	2.01	0.42
2:B:3020:G:O2'	2:B:3021:G:H5'	2.19	0.42
7:F:84:LEU:C	7:F:86:THR:H	2.22	0.42
11:J:114:PRO:O	11:J:115:PHE:C	2.58	0.42
1:A:1206:U:H5'	1:A:1206:U:C6	2.45	0.42
1:A:1744:G:H2'	1:A:1745:G:H5'	2.00	0.42
1:A:1756:G:H1'	40:A:5773:HOH:O	2.19	0.42
1:A:1827:G:C6	1:A:1828:G:C6	3.08	0.42
1:A:2004:U:H5''	1:A:2005:G:C8	2.55	0.42
1:A:2911:C:H3'	40:A:5070:HOH:O	2.19	0.42
2:B:3014:G:O2'	16:O:1:ALA:HB2	2.20	0.42
2:B:3091:C:H2'	2:B:3092:G:O4'	2.18	0.42
2:B:3114:G:O6	16:O:11:ARG:HD3	2.19	0.42
4:C:211:LYS:CB	4:C:212:PRO:CD	2.98	0.42
5:D:254:GLN:HG2	5:D:255:GLY:H	1.82	0.42
6:E:79:ARG:O	6:E:87:ARG:HG2	2.20	0.42
9:H:28:ALA:HB3	9:H:99:THR:HG23	2.01	0.42
9:H:101:ALA:HA	40:H:5413:HOH:O	2.19	0.42
16:O:38:LYS:HE2	16:O:107:ASN:ND2	2.34	0.42
24:W:20:LEU:HD22	24:W:60:GLN:HE22	1.84	0.42
26:Y:71:ARG:HD3	40:Y:2171:HOH:O	2.19	0.42
29:2:28:HIS:CD2	29:2:31:LYS:HG3	2.55	0.42
1:A:10:U:O4	1:A:532:A:OP2	2.37	0.42
1:A:451:C:O2'	1:A:452:G:H5'	2.19	0.42
1:A:1819:G:H2'	1:A:1820:G:C5'	2.50	0.42
1:A:1881:A:OP1	4:C:199:HIS:HE1	2.01	0.42
1:A:2816:A:H5''	1:A:2817:G:H5'	2.02	0.42
1:A:2909:G:H2'	1:A:2910:A:H8	1.85	0.42
40:A:5758:HOH:O	23:V:56:ARG:HD3	2.19	0.42
40:A:9673:HOH:O	15:N:87:MET:HE3	2.18	0.42
5:D:51:VAL:HA	5:D:329:TYR:O	2.19	0.42
7:F:167:GLU:C	7:F:169:THR:H	2.23	0.42
12:K:131:THR:HB	12:K:134:GLU:HG3	2.00	0.42
16:O:182:GLY:N	40:O:8572:HOH:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:29:VAL:O	17:P:33:LEU:HG	2.20	0.42
23:V:37:GLU:O	23:V:40:ALA:HB3	2.19	0.42
1:A:182:G:H4'	15:N:157:LEU:HD13	2.01	0.42
1:A:1236:A:C8	12:K:63:ILE:HD11	2.55	0.42
1:A:1595:G:O2'	1:A:1596:U:H5'	2.20	0.42
1:A:2821:C:H4'	5:D:116:PRO:CB	2.50	0.42
1:A:2897:C:H2'	1:A:2898:G:C8	2.53	0.42
1:A:2900:G:H2'	1:A:2901:C:O4'	2.20	0.42
40:A:7227:HOH:O	6:E:94:THR:HG21	2.19	0.42
4:C:128:LEU:HD21	4:C:131:HIS:HE1	1.84	0.42
5:D:82:VAL:HG12	5:D:101:TRP:CE3	2.55	0.42
5:D:243:ASN:HA	5:D:244:PRO:C	2.39	0.42
6:E:107:ARG:HB3	6:E:107:ARG:CZ	2.49	0.42
6:E:236:THR:O	6:E:237:GLU:C	2.57	0.42
7:F:174:VAL:CG1	40:F:6555:HOH:O	2.59	0.42
8:G:31:ARG:NH1	8:G:68:HIS:ND1	2.67	0.42
11:J:1:LYS:N	40:J:8353:HOH:O	2.52	0.42
11:J:165:GLY:C	11:J:166:ASN:HD22	2.23	0.42
16:O:90:LEU:CB	16:O:186:LEU:HD22	2.49	0.42
16:O:108:SER:HA	16:O:109:PRO:HD3	1.78	0.42
17:P:59:VAL:HG23	17:P:111:VAL:HG23	2.01	0.42
20:S:39:THR:HB	20:S:42:GLU:OE1	2.20	0.42
25:X:146:ILE:HG22	25:X:147:ASP:N	2.33	0.42
1:A:23:G:H1'	1:A:520:A:N6	2.35	0.42
1:A:37:A:H2'	1:A:38:G:H8	1.84	0.42
1:A:709:G:O2'	17:P:25:VAL:CG1	2.67	0.42
1:A:771:G:OP2	15:N:79:LYS:HE3	2.19	0.42
1:A:907:A:H4'	1:A:1328:A:C2	2.55	0.42
1:A:932:U:H2'	1:A:933:C:C6	2.55	0.42
1:A:1116:U:O2'	1:A:1118:A:C2	2.49	0.42
1:A:1218:U:H2'	1:A:1219:U:C6	2.54	0.42
1:A:1504:A:H4'	1:A:1506:U:C5	2.55	0.42
1:A:1675:C:H5''	30:3:5:LYS:HD2	2.02	0.42
1:A:2271:G:H2'	1:A:2271:G:N3	2.34	0.42
1:A:2515:C:H2'	1:A:2516:G:O4'	2.20	0.42
4:C:66:ARG:HB2	4:C:66:ARG:NH1	2.34	0.42
4:C:175:LYS:HE2	40:C:8576:HOH:O	2.19	0.42
9:H:57:GLU:O	9:H:61:MET:HG3	2.20	0.42
11:J:149:ALA:C	11:J:151:MET:H	2.23	0.42
14:M:10:SER:O	14:M:12:THR:N	2.51	0.42
15:N:32:ARG:NH2	40:N:8597:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:159:THR:HA	40:N:8520:HOH:O	2.20	0.42
16:O:143:ARG:HH12	16:O:173:ASP:CG	2.19	0.42
20:S:68:HIS:CD2	20:S:76:ASP:HB2	2.54	0.42
21:T:76:GLU:HB3	40:T:8345:HOH:O	2.19	0.42
24:W:42:ASN:O	24:W:44:GLY:N	2.52	0.42
26:Y:15:ARG:HH11	26:Y:15:ARG:CB	2.30	0.42
27:Z:172:THR:HG22	27:Z:173:ALA:N	2.35	0.42
1:A:338:C:H4'	6:E:174:ILE:HD12	2.00	0.42
1:A:553:G:P	27:Z:204:ARG:NH2	2.91	0.42
1:A:1311:G:C2	1:A:1312:G:C8	3.08	0.42
1:A:2494:G:H4'	11:J:5:MET:SD	2.60	0.42
1:A:2820:A:H2'	1:A:2821:C:C6	2.55	0.42
1:A:2911:C:H2'	1:A:2912:C:C6	2.55	0.42
1:A:2912:C:H2'	1:A:2913:A:O4'	2.20	0.42
2:B:3056:A:C3'	2:B:3057:A:H5''	2.50	0.42
6:E:236:THR:C	40:E:8450:HOH:O	2.57	0.42
15:N:164:THR:HB	40:N:8520:HOH:O	2.19	0.42
16:O:154:LEU:CG	16:O:155:GLU:H	2.27	0.42
17:P:26:TRP:HA	17:P:26:TRP:HE3	1.84	0.42
20:S:82:GLU:HG3	20:S:83:LYS:N	2.34	0.42
25:X:122:ARG:HH11	25:X:122:ARG:CG	2.26	0.42
1:A:1289:C:O2'	1:A:1290:G:H5'	2.19	0.42
1:A:1805:G:O2'	1:A:1806:G:H5'	2.20	0.42
1:A:1972:U:C2'	1:A:1973:A:C5'	2.98	0.42
1:A:1976:G:O2'	1:A:1977:U:H5'	2.20	0.42
1:A:2383:G:N3	40:A:6217:HOH:O	2.36	0.42
1:A:2769:C:H2'	1:A:2770:G:H5'	2.02	0.42
5:D:25:ARG:HA	5:D:310:ARG:HH21	1.85	0.42
6:E:51:TYR:CE2	29:2:53:LYS:HB3	2.55	0.42
6:E:223:LEU:HD12	6:E:223:LEU:HA	1.86	0.42
7:F:51:ARG:HA	40:F:7636:HOH:O	2.20	0.42
12:K:39:VAL:HG11	12:K:107:ASN:HB2	2.02	0.42
15:N:122:GLU:HB2	15:N:126:HIS:O	2.20	0.42
16:O:63:SER:O	16:O:66:LEU:HB2	2.19	0.42
16:O:73:ALA:HB1	16:O:74:PRO:HD2	2.01	0.42
16:O:175:LEU:HD12	16:O:175:LEU:HA	1.87	0.42
25:X:139:GLY:O	25:X:141:HIS:CD2	2.72	0.42
31:4:91:GLN:O	31:4:92:GLU:HB2	2.19	0.42
1:A:40:C:H4'	40:A:6511:HOH:O	2.18	0.42
1:A:57:C:H5''	40:A:6270:HOH:O	2.19	0.42
1:A:138:U:OP2	1:A:139:C:H5	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1477:C:O2'	1:A:1478:U:H5'	2.20	0.42
1:A:1943:C:H4'	4:C:211:LYS:O	2.20	0.42
1:A:2421:G:H3'	1:A:2422:U:C5'	2.50	0.42
40:A:4038:HOH:O	15:N:94:LYS:CE	2.61	0.42
5:D:170:SER:O	5:D:174:ARG:HG2	2.20	0.42
6:E:115:LEU:CD2	6:E:243:VAL:HG13	2.37	0.42
15:N:67:ILE:HD13	15:N:104:ARG:NH1	2.35	0.42
17:P:14:LEU:HG	17:P:102:ILE:HD11	2.02	0.42
18:Q:10:ALA:O	18:Q:13:VAL:HG12	2.20	0.42
22:U:40:VAL:HG23	22:U:119:ALA:C	2.41	0.42
23:V:50:GLU:CD	40:V:7349:HOH:O	2.58	0.42
25:X:14:HIS:HB2	25:X:17:ILE:HG13	2.01	0.42
25:X:21:LEU:HD21	25:X:48:VAL:HG13	2.01	0.42
26:Y:74:ALA:HB1	26:Y:85:VAL:HG22	2.01	0.42
27:Z:205:ILE:O	27:Z:206:ALA:C	2.59	0.42
1:A:204:A:C2'	1:A:205:U:H5'	2.50	0.41
1:A:772:G:H2'	1:A:773:A:O4'	2.19	0.41
1:A:1114:A:H2'	1:A:1115:U:C6	2.55	0.41
1:A:1275:C:C2'	1:A:1276:U:H5'	2.50	0.41
1:A:1339:G:C6	1:A:1340:G:N1	2.87	0.41
1:A:1943:C:O4'	4:C:212:PRO:HA	2.19	0.41
1:A:2329:C:O2'	1:A:2330:U:H5'	2.20	0.41
40:A:5539:HOH:O	19:R:50:GLY:HA2	2.19	0.41
40:A:9494:HOH:O	14:M:22:ARG:HG2	2.20	0.41
4:C:39:ALA:HB3	4:C:61:GLU:OE2	2.20	0.41
5:D:49:THR:CG2	5:D:280:VAL:CG2	2.98	0.41
5:D:162:MET:HG3	5:D:310:ARG:CZ	2.50	0.41
7:F:93:LEU:HB2	40:F:5198:HOH:O	2.19	0.41
8:G:73:PHE:O	8:G:76:VAL:HG22	2.20	0.41
9:H:91:VAL:CG1	9:H:92:GLY:H	2.29	0.41
11:J:71:TYR:O	11:J:73:GLN:N	2.53	0.41
14:M:104:ASP:O	14:M:105:TYR:HB3	2.20	0.41
15:N:113:ARG:NH1	15:N:150:ILE:O	2.48	0.41
26:Y:15:ARG:HB3	26:Y:15:ARG:NH1	2.31	0.41
1:A:240:C:O2	1:A:240:C:H2'	2.21	0.41
1:A:941:G:C5	1:A:942:U:C4	3.08	0.41
1:A:1433:G:O2'	1:A:1434:A:H5'	2.20	0.41
1:A:2314:G:H2'	1:A:2315:C:H5'	2.02	0.41
1:A:2467:A:O2'	1:A:2468:A:H2'	2.20	0.41
1:A:2756:U:N3	1:A:2896:A:H2	2.15	0.41
2:B:3026:C:O2'	2:B:3027:C:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3048:C:H4'	16:O:141:ARG:NH2	2.35	0.41
7:F:99:ASP:HB2	7:F:103:ASN:CA	2.50	0.41
19:R:46:SER:O	19:R:48:PRO:HD3	2.19	0.41
28:1:33:HIS:HE1	28:1:49:ARG:NE	2.18	0.41
1:A:100:C:H4'	22:U:16:LEU:HB2	2.02	0.41
1:A:1252:A:H2'	1:A:1253:C:O4'	2.20	0.41
1:A:1434:A:H2'	1:A:1436:C:C5	2.55	0.41
1:A:2055:A:H5'	20:S:134:SER:HB2	2.02	0.41
1:A:2377:U:O5'	1:A:2377:U:H6	2.03	0.41
1:A:2424:U:H1'	19:R:7:LEU:HD12	2.02	0.41
5:D:17:LYS:O	5:D:260:HIS:HD2	2.03	0.41
6:E:21:VAL:C	6:E:23:GLU:H	2.23	0.41
6:E:57:PRO:HG2	6:E:73:LEU:HD13	2.01	0.41
15:N:39:ARG:HA	15:N:63:VAL:HG22	2.03	0.41
16:O:122:ALA:O	16:O:127:LEU:HB2	2.20	0.41
17:P:73:ASP:HA	17:P:92:VAL:O	2.21	0.41
19:R:23:THR:HA	40:R:4792:HOH:O	2.20	0.41
25:X:52:VAL:HG13	25:X:53:ALA:N	2.34	0.41
27:Z:112:GLU:OE1	27:Z:112:GLU:HA	2.21	0.41
27:Z:116:LEU:HA	27:Z:116:LEU:HD23	1.80	0.41
1:A:708:A:H2'	1:A:709:G:O4'	2.20	0.41
1:A:870:G:C3'	1:A:871:G:H5''	2.50	0.41
1:A:920:C:H5'	1:A:921:G:C4	2.56	0.41
1:A:1205:U:H2'	1:A:1206:U:H5''	2.01	0.41
1:A:1298:U:H2'	1:A:1299:G:C8	2.55	0.41
1:A:1845:A:OP2	4:C:190:ARG:NH1	2.52	0.41
1:A:2308:U:C5	1:A:2310:G:C8	3.08	0.41
1:A:2642:G:H2'	1:A:2643:G:O4'	2.20	0.41
1:A:2667:G:H1'	1:A:2914:A:N3	2.35	0.41
1:A:2825:C:H4'	1:A:2826:G:O5'	2.20	0.41
40:B:3472:HOH:O	16:O:41:LYS:HD3	2.19	0.41
5:D:62:ARG:CB	5:D:65:MET:HE3	2.50	0.41
5:D:215:VAL:HB	5:D:234:ARG:HH12	1.85	0.41
6:E:129:HIS:HE1	6:E:231:ARG:HA	1.85	0.41
10:I:71:LEU:C	10:I:73:ASP:H	2.23	0.41
11:J:26:LYS:CD	11:J:28:ILE:HB	2.51	0.41
11:J:86:ARG:H	11:J:86:ARG:HG2	1.54	0.41
12:K:39:VAL:HG13	12:K:106:GLY:O	2.19	0.41
13:L:6:ALA:HB3	13:L:116:GLU:HG2	2.03	0.41
13:L:99:ASP:OD1	13:L:101:ASN:N	2.52	0.41
15:N:108:LYS:N	15:N:108:LYS:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:165:SER:HB2	40:N:8549:HOH:O	2.20	0.41
16:O:127:LEU:HD12	16:O:127:LEU:HA	1.83	0.41
16:O:149:GLU:O	16:O:152:GLU:HB2	2.21	0.41
22:U:9:LYS:NZ	22:U:13:ARG:NH1	2.69	0.41
25:X:35:VAL:CG2	25:X:41:TYR:CD2	3.04	0.41
25:X:63:GLU:HG2	25:X:93:ILE:HG22	2.01	0.41
1:A:503:G:H2'	1:A:504:G:H8	1.85	0.41
1:A:513:A:N3	40:A:3173:HOH:O	2.36	0.41
1:A:622:G:O2'	1:A:623:U:H5'	2.20	0.41
1:A:870:G:OP2	4:C:3:ARG:HD3	2.19	0.41
1:A:1482:A:O2'	1:A:1483:C:H5'	2.21	0.41
1:A:1772:C:H5'	1:A:1773:G:C5	2.55	0.41
1:A:1878:G:O2'	1:A:1879:U:OP2	2.38	0.41
1:A:2070:G:H5''	40:A:3293:HOH:O	2.20	0.41
1:A:2786:G:H2'	40:A:6694:HOH:O	2.20	0.41
40:A:6141:HOH:O	11:J:150:LYS:NZ	2.50	0.41
2:B:3003:A:OP2	2:B:3025:G:N2	2.53	0.41
2:B:3013:A:H3'	2:B:3014:G:H5'	2.01	0.41
4:C:135:VAL:N	40:C:8593:HOH:O	2.52	0.41
5:D:221:GLN:HE22	13:L:42:ASN:HD22	1.68	0.41
7:F:92:GLU:O	7:F:93:LEU:O	2.38	0.41
9:H:21:GLU:HA	9:H:24:ARG:HE	1.85	0.41
11:J:68:ALA:HB2	11:J:149:ALA:HB2	2.01	0.41
13:L:90:PHE:CD1	13:L:90:PHE:N	2.89	0.41
14:M:144:ASP:HA	14:M:147:GLU:HG3	2.02	0.41
23:V:9:CYS:HA	23:V:52:THR:CG2	2.46	0.41
25:X:35:VAL:HA	25:X:36:PRO:HD3	1.80	0.41
26:Y:66:THR:HG22	26:Y:67:PRO:O	2.21	0.41
31:4:38:ARG:O	31:4:42:ARG:HB2	2.21	0.41
1:A:42:C:H1'	40:A:4191:HOH:O	2.21	0.41
1:A:90:A:H2'	1:A:91:G:O4'	2.21	0.41
1:A:1406:A:H4'	1:A:1407:A:C5'	2.50	0.41
1:A:1878:G:O2'	1:A:1879:U:C6	2.71	0.41
1:A:2575:C:H2'	1:A:2576:A:O4'	2.20	0.41
1:A:2780:C:H2'	1:A:2781:U:H6	1.86	0.41
40:A:8599:HOH:O	15:N:174:ARG:HG3	2.21	0.41
4:C:36:ASP:O	4:C:37:VAL:C	2.59	0.41
5:D:139:ASP:HB3	40:D:8546:HOH:O	2.20	0.41
5:D:277:GLU:N	5:D:278:PRO:HD2	2.35	0.41
6:E:115:LEU:HD12	6:E:115:LEU:HA	1.87	0.41
25:X:26:ILE:O	25:X:26:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:U:H1'	1:A:532:A:H62	1.86	0.41
1:A:162:C:H2'	1:A:163:U:H5'	2.03	0.41
1:A:690:G:H4'	1:A:741:C:O2	2.20	0.41
1:A:731:U:H2'	1:A:732:C:C6	2.55	0.41
1:A:1003:U:O2	11:J:90:PHE:HZ	2.03	0.41
1:A:1829:A:H2'	1:A:1830:C:H5'	2.03	0.41
1:A:2364:A:H5''	19:R:15:LYS:HD3	2.01	0.41
1:A:2559:C:H4'	40:A:6765:HOH:O	2.20	0.41
1:A:2591:C:H2'	1:A:2592:G:O4'	2.21	0.41
1:A:2846:C:H4'	40:A:4593:HOH:O	2.19	0.41
2:B:3040:C:N4	7:F:51:ARG:HB2	2.35	0.41
2:B:3104:A:O2'	2:B:3105:A:H5'	2.20	0.41
2:B:3107:C:H2'	2:B:3108:C:C6	2.55	0.41
36:5:9080:SPS:H71	36:5:9080:SPS:H81	1.82	0.41
5:D:60:SER:C	5:D:62:ARG:N	2.73	0.41
5:D:148:PRO:HD2	40:D:8575:HOH:O	2.21	0.41
5:D:189:ALA:HB1	40:D:8561:HOH:O	2.19	0.41
5:D:320:GLN:HG3	5:D:321:PRO:CD	2.50	0.41
11:J:48:LEU:CG	11:J:157:ILE:HG21	2.50	0.41
1:A:221:G:H2'	1:A:222:A:C8	2.55	0.41
1:A:396:U:OP2	31:4:38:ARG:NH1	2.47	0.41
1:A:542:A:C8	1:A:542:A:C5'	2.99	0.41
1:A:876:A:N3	1:A:876:A:H2'	2.36	0.41
1:A:1164:U:O4'	1:A:1165:G:OP1	2.38	0.41
1:A:1166:A:H1'	1:A:1192:A:N1	2.32	0.41
1:A:1609:C:H2'	1:A:1610:G:H8	1.86	0.41
1:A:1754:A:H2'	1:A:1755:A:O4'	2.20	0.41
1:A:2768:A:H5''	40:A:3940:HOH:O	2.21	0.41
1:A:2781:U:H2'	1:A:2782:G:H5'	2.03	0.41
4:C:48:ASP:HA	4:C:49:PRO:HD3	1.92	0.41
5:D:145:HIS:CD2	5:D:146:THR:O	2.65	0.41
7:F:57:THR:HG23	7:F:63:ILE:HA	2.03	0.41
7:F:95:THR:HG21	7:F:174:VAL:HG22	2.03	0.41
11:J:97:LYS:HD3	11:J:117:LYS:HE2	2.03	0.41
12:K:88:PRO:O	12:K:94:GLY:HA3	2.20	0.41
30:3:24:TRP:CD1	40:3:6863:HOH:O	2.73	0.41
31:4:23:GLU:HG2	31:4:24:LYS:N	2.36	0.41
1:A:1014:A:H2'	1:A:1015:C:H5'	2.03	0.41
1:A:1079:A:N1	1:A:2068:G:O2'	2.50	0.41
1:A:1095:U:O2	25:X:120:PRO:HG2	2.21	0.41
1:A:1174:A:C5	1:A:1201:C:H4'	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1299:G:H5'	40:A:3582:HOH:O	2.21	0.41
1:A:1421:C:O2'	1:A:1422:U:H5'	2.21	0.41
1:A:1804:A:H2'	1:A:1805:G:C8	2.55	0.41
1:A:2107:U:O2'	1:A:2108:A:H5'	2.21	0.41
1:A:2256:G:O2'	1:A:2257:G:H5'	2.20	0.41
1:A:2419:U:H5''	1:A:2420:G:C5'	2.50	0.41
1:A:2425:A:H2'	40:A:8743:HOH:O	2.20	0.41
1:A:2621:U:H5	40:A:9490:HOH:O	2.04	0.41
40:A:4388:HOH:O	15:N:174:ARG:HG2	2.20	0.41
4:C:29:HIS:HB2	4:C:153:ARG:HH12	1.86	0.41
4:C:66:ARG:NH1	4:C:66:ARG:CB	2.84	0.41
4:C:105:VAL:CG1	4:C:106:CYS:N	2.83	0.41
4:C:164:ARG:CZ	40:C:8586:HOH:O	2.69	0.41
5:D:7:ARG:CG	5:D:7:ARG:NH1	2.80	0.41
5:D:36:PRO:CA	5:D:168:GLY:HA3	2.48	0.41
5:D:238:ASN:ND2	5:D:240:GLY:N	2.66	0.41
9:H:58:GLU:HG3	9:H:61:MET:CE	2.50	0.41
12:K:6:PHE:HB3	12:K:109:TYR:OH	2.21	0.41
12:K:92:GLN:HB3	40:K:1405:HOH:O	2.20	0.41
12:K:130:VAL:CG1	12:K:131:THR:N	2.83	0.41
13:L:27:ARG:HD2	40:L:4747:HOH:O	2.21	0.41
13:L:49:LEU:HD21	13:L:74:VAL:O	2.20	0.41
16:O:38:LYS:HE3	16:O:38:LYS:HB2	1.70	0.41
16:O:154:LEU:CG	16:O:155:GLU:N	2.83	0.41
18:Q:41:ARG:O	18:Q:44:VAL:HB	2.20	0.41
20:S:29:LYS:HB3	40:S:8530:HOH:O	2.21	0.41
20:S:79:ARG:C	20:S:81:PRO:HD3	2.41	0.41
20:S:149:GLU:HA	20:S:150:PRO:HD3	1.93	0.41
24:W:39:ALA:C	24:W:41:GLU:N	2.74	0.41
25:X:5:VAL:O	25:X:52:VAL:HG22	2.21	0.41
27:Z:117:LEU:HD12	27:Z:174:VAL:HG13	2.02	0.41
28:1:39:CYS:HA	28:1:40:PRO:HD3	1.98	0.41
28:1:81:LYS:O	28:1:82:ALA:C	2.59	0.41
1:A:228:C:H2'	1:A:229:G:H5'	2.03	0.41
1:A:1453:G:N2	1:A:1675:C:C2	2.89	0.41
1:A:1543:G:N1	1:A:1641:A:OP2	2.43	0.41
1:A:2761:A:C4	1:A:2763:G:C8	3.09	0.41
4:C:150:PRO:HD3	40:C:8593:HOH:O	2.21	0.41
5:D:5:ARG:HD2	5:D:8:LYS:NZ	2.36	0.41
6:E:118:THR:CG2	6:E:137:PRO:HB3	2.50	0.41
9:H:78:GLU:HG3	40:H:5966:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:46:LEU:HG	40:N:8623:HOH:O	2.21	0.41
18:Q:37:ARG:O	18:Q:41:ARG:HG3	2.20	0.41
18:Q:94:TRP:CZ2	18:Q:98:ILE:HG13	2.56	0.41
18:Q:141:ILE:C	18:Q:143:ALA:H	2.24	0.41
22:U:52:ARG:HB2	22:U:95:ASN:HB3	2.03	0.41
24:W:1:THR:O	24:W:4:HIS:CE1	2.74	0.41
1:A:86:A:C2	30:3:25:VAL:HG13	2.57	0.40
1:A:445:U:H1'	40:A:6846:HOH:O	2.21	0.40
1:A:962:C:C1'	16:O:5:ARG:NH1	2.76	0.40
1:A:1456:C:H2'	1:A:1457:U:C6	2.56	0.40
1:A:1762:C:H2'	1:A:1763:C:C6	2.56	0.40
1:A:1946:C:H2'	1:A:1971:G:C8	2.56	0.40
1:A:2061:C:H2'	1:A:2062:A:H5'	2.03	0.40
1:A:2251:G:H2'	1:A:2252:A:H8	1.87	0.40
7:F:128:LEU:N	40:F:6007:HOH:O	2.53	0.40
8:G:162:PHE:CD1	8:G:162:PHE:N	2.88	0.40
16:O:22:GLN:HG2	16:O:26:LEU:HD22	2.03	0.40
24:W:20:LEU:HD22	24:W:60:GLN:NE2	2.36	0.40
1:A:326:G:O2'	1:A:327:A:H5'	2.20	0.40
1:A:545:G:H2'	1:A:546:C:O4'	2.21	0.40
1:A:644:G:H1'	40:A:5916:HOH:O	2.21	0.40
1:A:1173:A:H4'	1:A:1174:A:C8	2.56	0.40
1:A:1805:G:H2'	1:A:1806:G:H8	1.86	0.40
1:A:1883:U:O2'	1:A:1884:G:H5'	2.21	0.40
40:A:4136:HOH:O	4:C:6:GLY:HA3	2.21	0.40
40:A:6509:HOH:O	19:R:9:GLY:HA2	2.20	0.40
40:A:8731:HOH:O	4:C:11:ARG:HD3	2.22	0.40
2:B:3106:C:O2'	2:B:3107:C:H5'	2.22	0.40
5:D:279:THR:HG22	5:D:280:VAL:N	2.35	0.40
5:D:294:TYR:HE2	40:D:8645:HOH:O	2.04	0.40
7:F:49:PRO:HA	7:F:73:VAL:HG22	2.03	0.40
8:G:137:ASP:O	8:G:141:VAL:HG23	2.21	0.40
11:J:33:MET:SD	11:J:65:ARG:HD2	2.62	0.40
11:J:43:PRO:HD2	11:J:137:ASN:HA	2.03	0.40
15:N:74:ARG:HD3	15:N:91:ILE:HD12	2.02	0.40
15:N:169:ARG:NH2	40:N:8549:HOH:O	2.46	0.40
16:O:164:ASP:OD1	16:O:164:ASP:C	2.59	0.40
17:P:25:VAL:HG23	17:P:26:TRP:H	1.86	0.40
18:Q:2:ASP:C	18:Q:2:ASP:OD1	2.58	0.40
18:Q:98:ILE:HD13	18:Q:98:ILE:O	2.21	0.40
25:X:48:VAL:O	25:X:48:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:126:PRO:HG2	27:Z:128:PHE:CZ	2.55	0.40
27:Z:187:VAL:HB	27:Z:203:VAL:CG2	2.51	0.40
1:A:222:A:H2'	1:A:223:G:O4'	2.20	0.40
1:A:264:G:H1'	1:A:265:U:H5	1.86	0.40
1:A:295:C:H2'	1:A:296:G:O4'	2.20	0.40
1:A:450:C:H4'	6:E:46:TYR:CE1	2.56	0.40
1:A:704:C:H2'	1:A:705:C:H6	1.85	0.40
1:A:1343:C:C2'	27:Z:208:LYS:HZ1	2.32	0.40
1:A:1398:G:H2'	1:A:1399:A:C8	2.56	0.40
1:A:1761:U:H5'	18:Q:81:LYS:O	2.22	0.40
1:A:1773:G:C8	28:1:16:PRO:HA	2.56	0.40
1:A:2266:A:H2'	1:A:2267:G:C8	2.57	0.40
1:A:2812:A:H1'	40:A:5306:HOH:O	2.21	0.40
5:D:24:PRO:HG3	5:D:204:GLY:HA2	2.04	0.40
5:D:41:PHE:CZ	5:D:79:MET:HG3	2.56	0.40
5:D:258:GLY:N	5:D:260:HIS:CE1	2.88	0.40
6:E:98:ARG:NH1	40:E:8357:HOH:O	2.50	0.40
12:K:71:TYR:CD1	12:K:72:PRO:HD2	2.56	0.40
13:L:75:ARG:NH2	40:L:4172:HOH:O	2.54	0.40
15:N:67:ILE:HD11	15:N:104:ARG:HD2	2.02	0.40
15:N:98:GLN:HB2	15:N:129:HIS:NE2	2.36	0.40
16:O:67:ALA:HA	16:O:71:TRP:HB3	2.03	0.40
20:S:33:ARG:NH2	40:S:8530:HOH:O	2.40	0.40
22:U:48:VAL:HG13	22:U:96:VAL:HG13	2.04	0.40
27:Z:99:ALA:HB2	27:Z:233:TYR:CZ	2.56	0.40
30:3:11:LEU:HD23	30:3:11:LEU:HA	1.86	0.40
1:A:47:G:N3	1:A:114:A:C2	2.90	0.40
1:A:445:U:H2'	1:A:446:G:H8	1.86	0.40
1:A:1052:G:H2'	1:A:1052:G:N3	2.37	0.40
1:A:1224:G:H2'	1:A:1225:C:C6	2.56	0.40
1:A:1613:C:H2'	1:A:1614:G:O4'	2.21	0.40
1:A:1815:A:H4'	1:A:2751:C:O4'	2.22	0.40
1:A:2093:G:H5''	40:A:8989:HOH:O	2.21	0.40
1:A:2379:G:N7	1:A:2408:A:N1	2.69	0.40
1:A:2416:G:O2'	16:O:25:ARG:HG2	2.21	0.40
1:A:2890:A:C1'	23:V:56:ARG:NH2	2.77	0.40
40:A:3702:HOH:O	27:Z:186:ARG:HD2	2.21	0.40
2:B:3026:C:P	40:B:3472:HOH:O	2.80	0.40
2:B:3052:A:H2'	2:B:3053:G:O4'	2.22	0.40
2:B:3116:C:O2'	2:B:3117:G:H5'	2.21	0.40
6:E:76:ARG:HG2	6:E:78:ARG:NH1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:26:THR:HG21	9:H:103:ALA:CB	2.50	0.40
9:H:32:GLY:N	40:H:3111:HOH:O	2.53	0.40
11:J:65:ARG:CZ	40:J:8385:HOH:O	2.70	0.40
12:K:107:ASN:HD22	12:K:108:PRO:N	2.20	0.40
13:L:66:ARG:HG2	13:L:66:ARG:HH11	1.87	0.40
20:S:15:LYS:HE3	40:S:8577:HOH:O	2.22	0.40
24:W:42:ASN:N	24:W:43:PRO:HD3	2.36	0.40
1:A:332:G:O2'	1:A:333:G:H5'	2.22	0.40
1:A:512:G:O3'	1:A:513:A:H8	2.05	0.40
1:A:907:A:H2'	1:A:908:A:H8	1.86	0.40
1:A:1044:C:H5''	40:A:8542:HOH:O	2.21	0.40
1:A:1891:G:H1'	1:A:1972:U:C2	2.56	0.40
1:A:2325:C:H1'	40:A:3658:HOH:O	2.21	0.40
1:A:2657:G:OP1	5:D:17:LYS:HB2	2.22	0.40
1:A:2718:C:H5'	1:A:2718:C:C6	2.54	0.40
1:A:2779:G:H21	8:G:143:GLN:NE2	2.19	0.40
4:C:17:ARG:HD2	40:C:8542:HOH:O	2.22	0.40
12:K:45:VAL:CG2	12:K:46:ILE:N	2.85	0.40
14:M:146:GLY:C	14:M:148:GLU:H	2.25	0.40
20:S:61:GLN:NE2	40:S:8537:HOH:O	2.55	0.40
29:2:21:ARG:CD	29:2:37:CYS:SG	3.09	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	
4	C	235/239 (98%)	209 (89%)	21 (9%)	5 (2%)	7	23
5	D	335/337 (99%)	303 (90%)	25 (8%)	7 (2%)	7	23
6	E	244/246 (99%)	218 (89%)	25 (10%)	1 (0%)	34	66
7	F	134/176 (76%)	98 (73%)	28 (21%)	8 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	G	170/177 (96%)	159 (94%)	10 (6%)	1 (1%)	25	56
9	H	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	5	18
10	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	J	152/167 (91%)	133 (88%)	13 (9%)	6 (4%)	3	10
12	K	140/145 (97%)	126 (90%)	11 (8%)	3 (2%)	7	23
13	L	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	10	33
14	M	141/164 (86%)	120 (85%)	19 (14%)	2 (1%)	11	34
15	N	192/194 (99%)	174 (91%)	16 (8%)	2 (1%)	15	44
16	O	184/186 (99%)	167 (91%)	11 (6%)	6 (3%)	4	13
17	P	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
18	Q	141/148 (95%)	137 (97%)	3 (2%)	1 (1%)	22	53
19	R	93/95 (98%)	85 (91%)	8 (9%)	0	100	100
20	S	148/154 (96%)	140 (95%)	7 (5%)	1 (1%)	22	53
21	T	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
22	U	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	17	46
23	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	4	13
25	X	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	12	36
26	Y	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	5	19
27	Z	140/240 (58%)	139 (99%)	1 (1%)	0	100	100
28	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	11	34
29	2	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	85 (94%)	3 (3%)	2 (2%)	6	22
All	All	3633/4235 (86%)	3313 (91%)	262 (7%)	58 (2%)	9	31

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	20	LYS
7	F	93	LEU
7	F	95	THR
7	F	173	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	H	101	ALA
11	J	162	SER
14	M	80	ASP
16	O	154	LEU
16	O	164	ASP
16	O	183	ASP
24	W	43	PRO
4	C	34	ASP
4	C	37	VAL
4	C	132	ASP
5	D	34	GLY
5	D	169	GLY
7	F	11	HIS
7	F	171	ASP
11	J	164	ALA
12	K	5	GLU
16	O	162	ASP
28	1	81	LYS
31	4	56	PRO
31	4	57	GLY
5	D	184	ASP
7	F	137	PRO
9	H	64	PRO
11	J	40	PRO
11	J	138	PRO
12	K	143	LYS
13	L	126	SER
15	N	140	ALA
16	O	65	ASP
16	O	181	ASP
25	X	49	ASN
25	X	77	ALA
26	Y	77	PHE
4	C	119	ALA
5	D	185	GLY
18	Q	116	SER
22	U	53	GLY
4	C	211	LYS
5	D	2	GLN
5	D	107	SER
9	H	61	MET
12	K	7	ASP

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Mol	Chain	Res	Type
14	M	21	ARG
20	S	81	PRO
6	E	8	LEU
13	L	119	GLN
24	W	40	PRO
11	J	72	VAL
7	F	16	PRO
8	G	44	GLY
26	Y	70	ILE
15	N	110	PRO
11	J	110	GLY

### 5.3.2 Protein sidechains [i](#)

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	
4	C	179/181 (99%)	166 (93%)	13 (7%)	14	38
5	D	282/282 (100%)	264 (94%)	18 (6%)	17	45
6	E	193/193 (100%)	177 (92%)	16 (8%)	11	32
7	F	117/147 (80%)	109 (93%)	8 (7%)	16	42
8	G	152/155 (98%)	148 (97%)	4 (3%)	46	79
9	H	92/92 (100%)	91 (99%)	1 (1%)	73	92
10	I	27/283 (10%)	27 (100%)	0	100	100
11	J	122/122 (100%)	110 (90%)	12 (10%)	8	24
12	K	118/121 (98%)	109 (92%)	9 (8%)	13	36
13	L	106/106 (100%)	103 (97%)	3 (3%)	43	77
14	M	112/126 (89%)	109 (97%)	3 (3%)	44	78
15	N	166/166 (100%)	157 (95%)	9 (5%)	22	53
16	O	149/149 (100%)	144 (97%)	5 (3%)	37	71
17	P	93/93 (100%)	91 (98%)	2 (2%)	52	83
18	Q	113/116 (97%)	110 (97%)	3 (3%)	44	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	R	79/79 (100%)	75 (95%)	4 (5%)	24	55
20	S	117/121 (97%)	113 (97%)	4 (3%)	37	71
21	T	71/73 (97%)	71 (100%)	0	100	100
22	U	105/105 (100%)	104 (99%)	1 (1%)	76	93
23	V	44/52 (85%)	44 (100%)	0	100	100
24	W	51/56 (91%)	50 (98%)	1 (2%)	55	84
25	X	130/130 (100%)	123 (95%)	7 (5%)	22	53
26	Y	66/73 (90%)	62 (94%)	4 (6%)	18	48
27	Z	120/195 (62%)	113 (94%)	7 (6%)	20	50
28	1	56/56 (100%)	51 (91%)	5 (9%)	9	28
29	2	46/46 (100%)	46 (100%)	0	100	100
30	3	42/44 (96%)	41 (98%)	1 (2%)	49	81
31	4	79/79 (100%)	76 (96%)	3 (4%)	33	67
All	All	3027/3441 (88%)	2884 (95%)	143 (5%)	26	59

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	C	3	ARG
4	C	33	GLU
4	C	36	ASP
4	C	55	VAL
4	C	68	ILE
4	C	69	LEU
4	C	78	ASP
4	C	94	LEU
4	C	120	ARG
4	C	131	HIS
4	C	153	ARG
4	C	179	MET
4	C	217	ARG
5	D	7	ARG
5	D	11	LEU
5	D	27	ASN
5	D	33	ASP
5	D	63	GLU
5	D	97	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	D	98	THR
5	D	103	ASP
5	D	162	MET
5	D	190	MET
5	D	234	ARG
5	D	245	SER
5	D	251	VAL
5	D	254	GLN
5	D	264	GLU
5	D	304	PRO
5	D	307	ARG
5	D	312	ARG
6	E	2	GLN
6	E	27	ARG
6	E	67	GLN
6	E	76	ARG
6	E	78	ARG
6	E	91	PRO
6	E	94	THR
6	E	101	ASP
6	E	136	VAL
6	E	187	ARG
6	E	214	THR
6	E	222	ASP
6	E	223	LEU
6	E	234	VAL
6	E	236	THR
6	E	240	LEU
7	F	24	HIS
7	F	61	PHE
7	F	99	ASP
7	F	131	THR
7	F	133	ASN
7	F	136	ARG
7	F	137	PRO
7	F	149	ARG
8	G	7	ILE
8	G	54	ASP
8	G	102	VAL
8	G	164	ASP
9	H	1	PRO
11	J	1	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	J	30	GLN
11	J	59	ASN
11	J	61	LEU
11	J	72	VAL
11	J	73	GLN
11	J	82	LYS
11	J	86	ARG
11	J	129	ASN
11	J	142	VAL
11	J	150	LYS
11	J	166	ASN
12	K	46	ILE
12	K	52	GLN
12	K	74	ARG
12	K	79	PHE
12	K	107	ASN
12	K	112	ASP
12	K	120	SER
12	K	125	SER
12	K	127	ILE
13	L	7	ASP
13	L	10	GLN
13	L	98	VAL
14	M	35	ARG
14	M	80	ASP
14	M	117	GLU
15	N	38	VAL
15	N	46	LEU
15	N	68	ARG
15	N	81	ARG
15	N	87	MET
15	N	93	ARG
15	N	99	ARG
15	N	116	ASN
15	N	164	THR
16	O	26	LEU
16	O	127	LEU
16	O	128	ASP
16	O	152	GLU
16	O	163	PHE
17	P	3	THR
17	P	98	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	Q	52	LYS
18	Q	91	LYS
18	Q	98	ILE
19	R	11	ARG
19	R	16	ASN
19	R	57	ASP
19	R	95	GLU
20	S	13	THR
20	S	39	THR
20	S	82	GLU
20	S	132	ARG
22	U	39	ASN
24	W	43	PRO
25	X	35	VAL
25	X	52	VAL
25	X	73	LEU
25	X	122	ARG
25	X	142	ASP
25	X	146	ILE
25	X	154	ARG
26	Y	15	ARG
26	Y	27	ASP
26	Y	49	ARG
26	Y	72	VAL
27	Z	141	THR
27	Z	163	THR
27	Z	172	THR
27	Z	186	ARG
27	Z	189	ASN
27	Z	200	THR
27	Z	203	VAL
28	1	11	THR
28	1	42	CYS
28	1	44	PHE
28	1	49	ARG
28	1	64	ILE
30	3	18	ASN
31	4	42	ARG
31	4	56	PRO
31	4	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
4	C	47	HIS
4	C	92	ASN
4	C	127	GLN
4	C	199	HIS
5	D	27	ASN
5	D	145	HIS
5	D	238	ASN
5	D	256	GLN
5	D	260	HIS
5	D	332	ASN
6	E	2	GLN
6	E	39	GLN
6	E	129	HIS
6	E	163	HIS
7	F	103	ASN
7	F	133	ASN
8	G	106	ASN
8	G	143	GLN
10	I	17	GLN
10	I	64	ASN
11	J	8	ASN
11	J	35	ASN
11	J	55	GLN
11	J	58	HIS
11	J	59	ASN
11	J	69	ASN
11	J	74	ASN
11	J	80	ASN
11	J	91	HIS
11	J	129	ASN
11	J	130	HIS
11	J	137	ASN
11	J	166	ASN
12	K	52	GLN
12	K	107	ASN
12	K	126	ASN
13	L	10	GLN
13	L	42	ASN
14	M	18	HIS
14	M	41	HIS
14	M	42	ASN
14	M	116	HIS
15	N	26	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	N	58	GLN
15	N	89	ASN
15	N	176	GLN
16	O	107	ASN
16	O	153	GLN
17	P	53	GLN
18	Q	50	GLN
18	Q	66	GLN
18	Q	73	HIS
18	Q	118	GLN
19	R	16	ASN
19	R	40	HIS
20	S	61	GLN
20	S	94	ASN
20	S	98	ASN
20	S	113	HIS
20	S	117	HIS
20	S	122	GLN
21	T	53	ASN
22	U	39	ASN
22	U	43	ASN
22	U	73	HIS
23	V	39	ASN
23	V	48	ASN
24	W	60	GLN
25	X	27	HIS
25	X	87	HIS
25	X	110	GLN
25	X	119	HIS
25	X	125	HIS
25	X	141	HIS
26	Y	23	HIS
27	Z	133	HIS
27	Z	134	HIS
27	Z	149	GLN
27	Z	189	ASN
28	1	33	HIS
28	1	70	GLN
29	2	8	GLN
29	2	16	HIS
29	2	28	HIS
30	3	16	ASN

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Mol	Chain	Res	Type
30	3	18	ASN
30	3	41	HIS
30	3	45	ASN
31	4	30	GLN
31	4	48	ASN

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	237 (8%)	38 (1%)
2	B	121/122 (99%)	15 (12%)	3 (2%)
3	5	2/3 (66%)	1 (50%)	0
All	All	2870/3047 (94%)	253 (8%)	41 (1%)

All (253) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A
1	A	70	A
1	A	71	G
1	A	87	C
1	A	88	G
1	A	114	A
1	A	115	U
1	A	120	A
1	A	130	C
1	A	139	C
1	A	141	C
1	A	151	A
1	A	166	A
1	A	169	A
1	A	185	G
1	A	186	A
1	A	191	A
1	A	192	A
1	A	219	G
1	A	237	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	271	C
1	A	272	A
1	A	273	G
1	A	283	U
1	A	284	C
1	A	285	A
1	A	308	U
1	A	309	C
1	A	318	C
1	A	336	G
1	A	337	A
1	A	345	G
1	A	358	G
1	A	381	G
1	A	397	A
1	A	417	G
1	A	461	C
1	A	487	G
1	A	498	A
1	A	510	U
1	A	511	A
1	A	514	G
1	A	537	G
1	A	538	C
1	A	539	G
1	A	542	A
1	A	545	G
1	A	553	G
1	A	559	U
1	A	588	G
1	A	604	G
1	A	620	A
1	A	632	A
1	A	644	G
1	A	660	A
1	A	688	A
1	A	701	U
1	A	705	C
1	A	717	C
1	A	759	C
1	A	777	U
1	A	809	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	821	U
1	A	835	U
1	A	840	U
1	A	857	A
1	A	868	G
1	A	869	G
1	A	871	G
1	A	872	U
1	A	875	A
1	A	877	G
1	A	878	G
1	A	882	A
1	A	885	G
1	A	898	G
1	A	905	C
1	A	920	C
1	A	921	G
1	A	923	A
1	A	953	G
1	A	960	G
1	A	961	A
1	A	1006	A
1	A	1008	C
1	A	1029	U
1	A	1045	G
1	A	1059	G
1	A	1060	C
1	A	1072	G
1	A	1081	A
1	A	1087	G
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1130	U
1	A	1161	A
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1175	G
1	A	1177	A
1	A	1185	U
1	A	1192	A
1	A	1193	A
1	A	1206	U
1	A	1208	C
1	A	1216	G
1	A	1237	U
1	A	1238	C
1	A	1239	G
1	A	1279	U
1	A	1289	C
1	A	1342	C
1	A	1353	C
1	A	1360	C
1	A	1377	C
1	A	1407	A
1	A	1451	C
1	A	1474	C
1	A	1485	A
1	A	1488	U
1	A	1505	U
1	A	1506	U
1	A	1524	U
1	A	1525	G
1	A	1526	A
1	A	1564	C
1	A	1580	A
1	A	1592	G
1	A	1625	U
1	A	1626	A
1	A	1633	C
1	A	1634	G
1	A	1656	A
1	A	1667	A
1	A	1682	A
1	A	1684	A
1	A	1685	A
1	A	1692	C
1	A	1701	A
1	A	1722	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1752	G
1	A	1778	A
1	A	1798	C
1	A	1820	G
1	A	1829	A
1	A	1856	C
1	A	1879	U
1	A	1904	A
1	A	1919	A
1	A	1942	A
1	A	1971	G
1	A	1973	A
1	A	1974	G
1	A	1978	A
1	A	1979	G
1	A	1980	U
1	A	1982	C
1	A	1996	U
1	A	2008	U
1	A	2011	A
1	A	2012	U
1	A	2013	G
1	A	2033	G
1	A	2034	U
1	A	2064	U
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2096	A
1	A	2101	A
1	A	2102	G
1	A	2103	A
1	A	2110	G
1	A	2238	A
1	A	2258	A
1	A	2271	G
1	A	2272	G
1	A	2317	C
1	A	2321	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2422	U
1	A	2462	G
1	A	2469	A
1	A	2476	C
1	A	2480	G
1	A	2483	A
1	A	2507	G
1	A	2511	A
1	A	2533	C
1	A	2537	G
1	A	2541	U
1	A	2553	A
1	A	2564	G
1	A	2589	U
1	A	2601	A
1	A	2602	G
1	A	2608	C
1	A	2613	G
1	A	2637	A
1	A	2649	A
1	A	2664	A
1	A	2681	A
1	A	2682	C
1	A	2719	A
1	A	2726	U
1	A	2747	C
1	A	2748	G
1	A	2749	U
1	A	2750	G
1	A	2762	C
1	A	2768	A
1	A	2786	G
1	A	2792	A
1	A	2800	A
1	A	2811	A
1	A	2825	C
1	A	2850	C
1	A	2876	G
1	A	2890	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	2896	A
1	A	2903	C
1	A	2914	A
2	B	3002	U
2	B	3011	A
2	B	3014	G
2	B	3022	G
2	B	3024	U
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A
2	B	3056	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C
3	5	9076	A

All (41) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	10	U
1	A	69	A
1	A	129	A
1	A	284	C
1	A	338	C
1	A	603	A
1	A	644	G
1	A	699	C
1	A	716	G
1	A	834	G
1	A	857	A
1	A	871	G
1	A	877	G
1	A	1080	C
1	A	1164	U
1	A	1232	A
1	A	1237	U
1	A	1352	A
1	A	1377	C

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Mol	Chain	Res	Type
1	A	1450	C
1	A	1563	G
1	A	1667	A
1	A	1684	A
1	A	1692	C
1	A	1730	G
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2313	C
1	A	2467	A
1	A	2526	C
1	A	2536	C
1	A	2649	A
1	A	2718	C
1	A	2726	U
1	A	2761	A
1	A	2791	U
2	B	3023	U
2	B	3065	A
2	B	3103	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 237 ligands modelled in this entry, 234 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
38	ACA	5	9078	37	7,7,8	1.26	1 (14%)	6,6,8	0.86	0
36	SPS	5	9080	32	20,23,23	1.94	6 (30%)	18,30,30	2.98	5 (27%)
37	PHA	5	9077	38,3	10,11,11	0.77	0	10,13,13	0.90	1 (10%)

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
38	ACA	5	9078	37	-	1/4/5/6	-
36	SPS	5	9080	32	-	5/15/18/18	0/1/1/1
37	PHA	5	9077	38,3	-	2/5/6/6	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	9080	SPS	C6-C1	4.34	1.54	1.43
36	5	9080	SPS	C16-S17	-3.47	1.76	1.79
36	5	9080	SPS	C9-C10	-3.19	1.41	1.48
36	5	9080	SPS	C1-N2	2.93	1.38	1.33
36	5	9080	SPS	C5-N4	2.92	1.38	1.34
36	5	9080	SPS	O15-S15	-2.37	1.41	1.50
38	5	9078	ACA	C3-C2	-2.35	1.42	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	9080	SPS	C6-C1-N2	-9.15	118.02	124.40
36	5	9080	SPS	C3-N2-C1	6.86	120.94	115.14
37	5	9077	PHA	CB-CA-C	-2.64	106.52	111.47
36	5	9080	SPS	O15-S15-C16	2.55	109.50	106.47
36	5	9080	SPS	C9-C10-N11	2.23	118.85	114.56
36	5	9080	SPS	C6-C5-N4	-2.03	119.81	122.12

There are no chirality outliers.

All (8) torsion outliers are listed below:

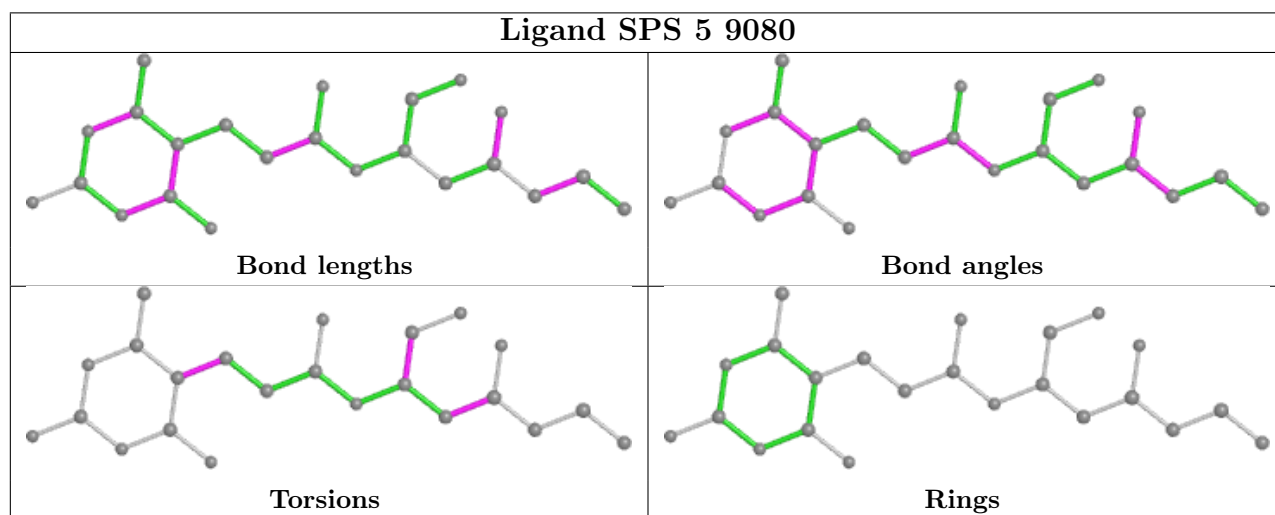
Mol	Chain	Res	Type	Atoms
36	5	9080	SPS	C5-C6-C8-C9
36	5	9080	SPS	N11-C12-C13-O13
36	5	9080	SPS	C14-C12-C13-O13
36	5	9080	SPS	C12-C14-S15-O15
36	5	9080	SPS	C12-C14-S15-C16
37	5	9077	PHA	CA-CB-CG-CD2
37	5	9077	PHA	CA-CB-CG-CD1
38	5	9078	ACA	C2-C3-C4-C5

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	9080	SPS	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2754/2922 (94%)	-0.03	73 (2%) 54 44	18, 43, 87, 135	0
2	B	122/122 (100%)	0.33	5 (4%) 37 27	35, 60, 87, 145	0
3	5	3/3 (100%)	-0.12	0 100 100	33, 33, 35, 36	0
4	C	237/239 (99%)	0.12	11 (4%) 32 22	24, 47, 79, 101	0
5	D	337/337 (100%)	-0.02	4 (1%) 79 73	25, 53, 79, 88	0
6	E	246/246 (100%)	-0.29	0 100 100	21, 42, 64, 75	0
7	F	140/176 (79%)	2.02	73 (52%) 0 0	51, 94, 112, 118	0
8	G	172/177 (97%)	0.92	16 (9%) 8 4	44, 67, 85, 92	0
9	H	119/119 (100%)	0.57	11 (9%) 9 5	45, 66, 91, 97	0
10	I	29/348 (8%)	2.37	18 (62%) 0 0	66, 85, 93, 96	0
11	J	156/167 (93%)	0.32	9 (5%) 23 15	34, 52, 77, 80	0
12	K	142/145 (97%)	-0.01	0 100 100	33, 49, 68, 86	0
13	L	132/132 (100%)	-0.11	2 (1%) 73 68	31, 50, 70, 80	0
14	M	145/164 (88%)	0.39	11 (7%) 13 7	20, 60, 98, 111	0
15	N	194/194 (100%)	-0.15	3 (1%) 73 68	28, 39, 58, 68	0
16	O	186/186 (100%)	0.53	20 (10%) 5 3	36, 59, 99, 111	0
17	P	115/115 (100%)	-0.06	1 (0%) 84 80	35, 49, 67, 77	0
18	Q	143/148 (96%)	0.11	1 (0%) 87 84	36, 52, 64, 74	0
19	R	95/95 (100%)	-0.12	1 (1%) 80 75	29, 40, 54, 70	0
20	S	150/154 (97%)	-0.24	0 100 100	29, 41, 61, 70	0
21	T	81/84 (96%)	0.08	2 (2%) 57 47	40, 54, 73, 80	0
22	U	119/119 (100%)	0.32	10 (8%) 11 5	36, 52, 76, 90	0
23	V	53/66 (80%)	0.19	1 (1%) 66 59	39, 53, 69, 77	0
24	W	65/70 (92%)	1.27	14 (21%) 0 0	49, 68, 105, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	154/154 (100%)	-0.26	0 100 100	32, 45, 63, 72	0
26	Y	82/91 (90%)	0.14	4 (4%) 29 20	40, 57, 79, 99	0
27	Z	142/240 (59%)	-0.10	2 (1%) 75 70	24, 41, 65, 82	0
28	1	73/73 (100%)	0.22	4 (5%) 25 16	46, 60, 71, 79	0
29	2	56/56 (100%)	-0.61	0 100 100	24, 29, 35, 43	0
30	3	46/48 (95%)	0.40	6 (13%) 3 2	31, 57, 84, 98	0
31	4	92/92 (100%)	0.08	1 (1%) 80 75	31, 51, 64, 78	0
All	All	6580/7282 (90%)	0.11	303 (4%) 32 22	18, 48, 88, 145	0

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	W	1	THR	10.6
2	B	3001	U	9.3
1	A	1172	G	6.7
1	A	1173	A	6.2
7	F	88	LEU	6.2
7	F	57	THR	5.9
16	O	166	ALA	5.9
1	A	1177	A	5.8
7	F	69	ILE	5.8
21	T	81	ILE	5.5
7	F	62	ASP	5.4
2	B	3023	U	5.4
16	O	186	LEU	5.4
7	F	63	ILE	5.3
5	D	1	PRO	5.3
7	F	18	ILE	5.2
1	A	1198	U	5.1
24	W	40	PRO	5.0
10	I	24	VAL	5.0
9	H	106	THR	4.8
7	F	90	LEU	4.7
1	A	2237	G	4.6
1	A	1169	U	4.6
8	G	45	ASP	4.6
7	F	10	PHE	4.6
24	W	39	ALA	4.6
16	O	162	ASP	4.5
7	F	27	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
7	F	56	ARG	4.4
10	I	23	ILE	4.4
24	W	43	PRO	4.3
7	F	66	GLY	4.2
1	A	735	C	4.2
10	I	27	ILE	4.2
1	A	1175	G	4.2
2	B	3002	U	4.2
1	A	1171	A	4.1
1	A	1525	G	4.0
1	A	1951	G	4.0
10	I	26	MET	4.0
1	A	1199	A	4.0
1	A	1181	A	3.9
1	A	1192	A	3.9
7	F	26	GLY	3.9
24	W	38	GLY	3.9
4	C	85	ASP	3.8
1	A	960	G	3.8
4	C	36	ASP	3.8
1	A	1950	G	3.8
28	I	22	ILE	3.8
1	A	1200	A	3.7
7	F	170	TYR	3.7
7	F	67	ASP	3.6
11	J	32	ASP	3.6
26	Y	80	GLU	3.6
14	M	104	ASP	3.6
1	A	970	U	3.6
7	F	58	VAL	3.6
7	F	44	ILE	3.6
16	O	165	ALA	3.6
7	F	84	LEU	3.5
1	A	282	C	3.5
7	F	92	GLU	3.5
1	A	285	A	3.5
16	O	143	ARG	3.5
7	F	102	GLY	3.5
7	F	104	PHE	3.5
10	I	65	THR	3.5
16	O	148	ALA	3.5
16	O	152	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
26	Y	88	GLU	3.4
7	F	17	ARG	3.4
7	F	165	PHE	3.4
1	A	2238	A	3.4
8	G	100	ASP	3.4
28	1	11	THR	3.4
1	A	1168	C	3.4
7	F	72	LYS	3.4
16	O	139	TRP	3.4
9	H	17	LEU	3.3
7	F	25	MET	3.3
7	F	24	HIS	3.3
14	M	102	ASP	3.3
7	F	166	ILE	3.3
14	M	100	ALA	3.3
4	C	35	GLY	3.3
7	F	51	ARG	3.3
24	W	41	GLU	3.3
7	F	64	ARG	3.3
1	A	1170	U	3.3
14	M	60	GLU	3.2
1	A	1182	C	3.2
1	A	1174	A	3.2
23	V	47	ARG	3.2
1	A	1201	C	3.2
7	F	85	GLN	3.2
19	R	95	GLU	3.2
2	B	3122	C	3.2
4	C	37	VAL	3.1
7	F	53	LYS	3.1
11	J	83	PHE	3.1
7	F	128	LEU	3.1
4	C	31	LYS	3.1
16	O	138	ASP	3.1
7	F	157	LEU	3.1
7	F	129	ASP	3.1
1	A	1167	G	3.1
22	U	119	ALA	3.1
7	F	75	LEU	3.1
1	A	1203	G	3.1
8	G	10	ASP	3.1
7	F	89	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
7	F	65	GLU	3.0
1	A	1190	G	3.0
1	A	372	A	3.0
8	G	28	SER	3.0
22	U	115	GLU	3.0
22	U	116	ASP	3.0
10	I	12	ILE	3.0
10	I	20	VAL	3.0
1	A	1185	U	3.0
7	F	73	VAL	3.0
4	C	32	VAL	3.0
16	O	145	ALA	3.0
8	G	122	THR	3.0
14	M	97	VAL	3.0
1	A	1162	G	3.0
1	A	1178	G	2.9
26	Y	74	ALA	2.9
14	M	105	TYR	2.9
1	A	1163	G	2.9
1	A	284	C	2.9
10	I	15	TRP	2.9
7	F	70	GLY	2.9
1	A	2345	A	2.9
7	F	130	VAL	2.9
1	A	1186	C	2.9
16	O	178	THR	2.9
7	F	45	THR	2.8
9	H	26	THR	2.8
27	Z	235	GLU	2.8
7	F	81	GLU	2.8
1	A	370	G	2.8
14	M	80	ASP	2.8
1	A	1166	A	2.8
1	A	1161	A	2.8
1	A	1202	A	2.8
10	I	13	PRO	2.8
10	I	71	LEU	2.8
22	U	117	ASP	2.7
1	A	138	U	2.7
10	I	66	LEU	2.7
16	O	159	TYR	2.7
1	A	1204	C	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	3024	U	2.7
7	F	87	ALA	2.7
1	A	128	A	2.6
7	F	86	THR	2.6
11	J	72	VAL	2.6
14	M	106	VAL	2.6
7	F	41	LEU	2.6
11	J	36	ASN	2.6
4	C	133	ARG	2.6
1	A	1184	C	2.6
7	F	55	LYS	2.6
7	F	106	PHE	2.6
7	F	29	HIS	2.6
9	H	119	ARG	2.6
24	W	2	VAL	2.6
8	G	42	VAL	2.6
5	D	117	GLU	2.6
7	F	68	PRO	2.6
9	H	103	ALA	2.6
28	1	44	PHE	2.6
13	L	119	GLN	2.5
9	H	108	LEU	2.5
1	A	1193	A	2.5
7	F	61	PHE	2.5
8	G	128	GLY	2.5
17	P	23	GLY	2.5
1	A	999	C	2.5
9	H	44	SER	2.5
18	Q	77	ALA	2.5
22	U	118	SER	2.5
24	W	37	GLY	2.5
7	F	47	GLN	2.5
16	O	150	TYR	2.5
8	G	154	ILE	2.5
1	A	1205	U	2.5
1	A	2344	G	2.5
8	G	82	TYR	2.5
16	O	140	GLN	2.5
1	A	2239	C	2.5
16	O	158	LEU	2.5
30	3	49	GLU	2.5
8	G	72	MET	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
10	I	72	ASP	2.5
7	F	135	VAL	2.4
7	F	172	VAL	2.4
4	C	237	GLY	2.4
7	F	71	ALA	2.4
1	A	736	A	2.4
1	A	1180	U	2.4
1	A	805	G	2.4
10	I	21	ASP	2.4
1	A	1527	A	2.4
7	F	49	PRO	2.4
10	I	16	LYS	2.4
5	D	133	GLU	2.4
24	W	6	GLN	2.4
7	F	98	PHE	2.4
11	J	81	TYR	2.4
1	A	969	G	2.4
1	A	1948	G	2.4
7	F	43	GLU	2.3
7	F	40	ILE	2.3
7	F	23	VAL	2.3
1	A	280	C	2.3
10	I	69	ARG	2.3
24	W	59	ILE	2.3
7	F	50	VAL	2.3
16	O	147	ILE	2.3
22	U	112	LEU	2.3
14	M	145	LEU	2.3
1	A	272	A	2.3
1	A	288	A	2.3
1	A	1208	C	2.3
7	F	134	LEU	2.3
24	W	3	LEU	2.3
24	W	44	GLY	2.3
7	F	154	LYS	2.3
15	N	152	ARG	2.2
9	H	19	ALA	2.2
11	J	146	TRP	2.2
16	O	137	ALA	2.2
28	1	38	LYS	2.2
1	A	2852	A	2.2
30	3	36	ASN	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
16	O	163	PHE	2.2
8	G	126	ILE	2.2
1	A	2850	C	2.2
22	U	107	LYS	2.2
7	F	91	ALA	2.2
16	O	179	LEU	2.2
14	M	91	VAL	2.2
11	J	158	ASN	2.2
27	Z	108	ASP	2.2
30	3	35	ARG	2.2
1	A	1165	G	2.2
1	A	1197	G	2.2
13	L	132	VAL	2.2
1	A	1176	C	2.2
9	H	99	THR	2.2
22	U	1	SER	2.2
10	I	73	ASP	2.2
1	A	1625	U	2.2
24	W	8	ILE	2.2
15	N	87	MET	2.2
1	A	1526	A	2.2
9	H	107	VAL	2.2
4	C	64	ASP	2.2
4	C	38	ILE	2.2
22	U	33	GLU	2.2
7	F	11	HIS	2.1
7	F	52	THR	2.1
7	F	93	LEU	2.1
7	F	171	ASP	2.1
21	T	70	GLU	2.1
8	G	22	VAL	2.1
11	J	139	ASP	2.1
7	F	16	PRO	2.1
4	C	34	ASP	2.1
10	I	17	GLN	2.1
11	J	79	ALA	2.1
7	F	59	GLY	2.1
1	A	1179	C	2.1
1	A	2508	C	2.1
24	W	45	ARG	2.1
7	F	74	THR	2.1
22	U	35	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	281	U	2.1
30	3	44	ARG	2.1
10	I	28	GLU	2.1
16	O	177	GLU	2.1
1	A	1183	C	2.1
5	D	181	ILE	2.1
8	G	121	ASP	2.1
7	F	48	MET	2.1
8	G	95	VAL	2.1
1	A	10	U	2.0
7	F	101	THR	2.0
15	N	194	ALA	2.0
7	F	137	PRO	2.0
8	G	27	GLY	2.0
8	G	88	TYR	2.0
9	H	22	VAL	2.0
14	M	150	GLN	2.0
30	3	37	HIS	2.0
1	A	1279	U	2.0
26	Y	7	GLU	2.0
31	4	92	GLU	2.0
7	F	173	GLU	2.0
30	3	20	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
33	NA	S	8386	1/1	0.37	0.92	91,91,91,91	0
33	NA	A	8384	1/1	0.38	0.81	75,75,75,75	0
32	MG	A	8024	1/1	0.48	1.23	89,89,89,89	0
39	CD	P	8405	1/1	0.56	0.14	174,174,174,174	0
33	NA	B	8351	1/1	0.59	0.53	78,78,78,78	0
33	NA	T	8312	1/1	0.67	0.65	79,79,79,79	0
33	NA	A	8385	1/1	0.68	0.41	50,50,50,50	0
33	NA	J	8322	1/1	0.70	0.31	61,61,61,61	0
33	NA	A	8307	1/1	0.70	0.27	46,46,46,46	0
33	NA	A	8324	1/1	0.71	0.17	55,55,55,55	0
32	MG	B	8095	1/1	0.71	0.18	70,70,70,70	0
33	NA	A	8368	1/1	0.73	0.20	56,56,56,56	0
32	MG	A	8113	1/1	0.74	0.20	43,43,43,43	0
33	NA	A	8329	1/1	0.75	0.23	54,54,54,54	0
33	NA	A	8311	1/1	0.76	0.29	55,55,55,55	0
33	NA	A	8352	1/1	0.76	0.41	71,71,71,71	0
38	ACA	5	9078	8/9	0.79	0.38	45,53,55,55	0
33	NA	A	8333	1/1	0.79	0.15	33,33,33,33	0
33	NA	B	8383	1/1	0.80	0.61	69,69,69,69	0
32	MG	A	8076	1/1	0.80	0.09	50,50,50,50	0
35	CL	O	8507	1/1	0.84	0.27	59,59,59,59	0
33	NA	A	8359	1/1	0.84	0.38	40,40,40,40	0
33	NA	A	8364	1/1	0.84	0.27	39,39,39,39	0
33	NA	A	8363	1/1	0.85	0.25	49,49,49,49	0
33	NA	A	8371	1/1	0.85	0.31	61,61,61,61	0
33	NA	A	8372	1/1	0.86	0.44	58,58,58,58	0
35	CL	K	8502	1/1	0.87	0.14	66,66,66,66	0
33	NA	A	8313	1/1	0.88	0.10	62,62,62,62	0
33	NA	A	8326	1/1	0.88	0.33	37,37,37,37	0
33	NA	M	8380	1/1	0.89	0.41	64,64,64,64	0
33	NA	A	8382	1/1	0.89	0.17	72,72,72,72	0
32	MG	A	8089	1/1	0.89	0.08	58,58,58,58	0
33	NA	A	8314	1/1	0.89	0.19	38,38,38,38	0
33	NA	A	8310	1/1	0.89	0.26	39,39,39,39	0
33	NA	A	8357	1/1	0.89	0.08	53,53,53,53	0
32	MG	I	8105	1/1	0.89	0.28	32,32,32,32	0
33	NA	E	8304	1/1	0.90	0.17	33,33,33,33	0
33	NA	A	8308	1/1	0.90	0.10	43,43,43,43	0
32	MG	A	8082	1/1	0.90	0.12	53,53,53,53	0
32	MG	A	8045	1/1	0.91	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	A	8369	1/1	0.91	0.14	49,49,49,49	0
34	K	A	8390	1/1	0.91	0.36	70,70,70,70	0
32	MG	A	8090	1/1	0.91	0.28	70,70,70,70	0
32	MG	A	8101	1/1	0.91	0.13	52,52,52,52	0
32	MG	A	8087	1/1	0.91	0.19	63,63,63,63	0
33	NA	A	8341	1/1	0.91	0.13	41,41,41,41	0
32	MG	A	8114	1/1	0.92	0.22	54,54,54,54	0
33	NA	A	8362	1/1	0.92	0.31	64,64,64,64	0
33	NA	A	8375	1/1	0.92	0.59	47,47,47,47	0
32	MG	A	8085	1/1	0.92	0.11	45,45,45,45	0
32	MG	A	8106	1/1	0.92	0.08	52,52,52,52	0
33	NA	A	8365	1/1	0.92	0.23	43,43,43,43	0
33	NA	A	8366	1/1	0.92	0.49	68,68,68,68	0
33	NA	A	8355	1/1	0.92	0.55	56,56,56,56	0
32	MG	A	8049	1/1	0.92	0.62	77,77,77,77	0
32	MG	A	8057	1/1	0.93	0.13	40,40,40,40	0
33	NA	A	8335	1/1	0.93	0.22	43,43,43,43	0
33	NA	A	8373	1/1	0.93	0.48	50,50,50,50	0
33	NA	N	8347	1/1	0.93	0.12	23,23,23,23	0
33	NA	A	8301	1/1	0.93	0.17	46,46,46,46	0
33	NA	A	8377	1/1	0.93	0.22	66,66,66,66	0
33	NA	U	8343	1/1	0.93	0.15	33,33,33,33	0
33	NA	A	8342	1/1	0.93	0.22	40,40,40,40	0
35	CL	A	8517	1/1	0.93	0.14	59,59,59,59	0
33	NA	A	8303	1/1	0.93	0.18	43,43,43,43	0
35	CL	K	8521	1/1	0.93	0.10	50,50,50,50	0
33	NA	A	8353	1/1	0.93	0.15	23,23,23,23	0
35	CL	Z	8520	1/1	0.93	0.12	42,42,42,42	0
32	MG	A	8050	1/1	0.93	0.15	64,64,64,64	0
33	NA	A	8332	1/1	0.93	0.14	29,29,29,29	0
32	MG	A	8111	1/1	0.94	0.10	51,51,51,51	0
32	MG	A	8047	1/1	0.94	0.15	66,66,66,66	0
32	MG	A	8066	1/1	0.94	0.23	84,84,84,84	0
33	NA	A	8319	1/1	0.94	0.10	36,36,36,36	0
32	MG	A	8070	1/1	0.94	0.15	47,47,47,47	0
32	MG	A	8027	1/1	0.94	0.08	49,49,49,49	0
35	CL	A	8511	1/1	0.94	0.11	48,48,48,48	0
32	MG	A	8094	1/1	0.94	0.04	63,63,63,63	0
35	CL	C	8509	1/1	0.94	0.19	56,56,56,56	0
32	MG	A	8046	1/1	0.94	0.08	47,47,47,47	0
33	NA	A	8305	1/1	0.94	0.13	35,35,35,35	0
32	MG	A	8103	1/1	0.94	0.18	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	C	8345	1/1	0.94	0.13	44,44,44,44	0
35	CL	4	8504	1/1	0.94	0.14	67,67,67,67	0
32	MG	A	8083	1/1	0.94	0.09	41,41,41,41	0
32	MG	A	8108	1/1	0.94	0.13	60,60,60,60	0
32	MG	A	8063	1/1	0.95	0.05	73,73,73,73	0
32	MG	A	8032	1/1	0.95	0.08	28,28,28,28	0
33	NA	A	8306	1/1	0.95	0.52	32,32,32,32	0
32	MG	A	8053	1/1	0.95	0.14	50,50,50,50	0
33	NA	S	8337	1/1	0.95	0.19	28,28,28,28	0
33	NA	A	8367	1/1	0.95	0.10	44,44,44,44	0
32	MG	A	8099	1/1	0.95	0.12	48,48,48,48	0
33	NA	A	8340	1/1	0.95	0.47	44,44,44,44	0
33	NA	A	8309	1/1	0.95	0.09	32,32,32,32	0
35	CL	A	8503	1/1	0.95	0.13	46,46,46,46	0
32	MG	A	8100	1/1	0.95	0.16	65,65,65,65	0
32	MG	A	8119	1/1	0.95	0.14	41,41,41,41	0
32	MG	A	8041	1/1	0.95	0.16	53,53,53,53	0
32	MG	U	8073	1/1	0.95	0.09	46,46,46,46	0
33	NA	A	8356	1/1	0.95	0.28	47,47,47,47	0
33	NA	A	8317	1/1	0.95	0.17	45,45,45,45	0
33	NA	A	8358	1/1	0.95	0.80	82,82,82,82	0
32	MG	A	8088	1/1	0.95	0.09	30,30,30,30	0
33	NA	A	8360	1/1	0.95	0.56	39,39,39,39	0
32	MG	A	8104	1/1	0.95	0.26	52,52,52,52	0
33	NA	A	8334	1/1	0.96	0.06	32,32,32,32	0
32	MG	L	8069	1/1	0.96	0.07	50,50,50,50	0
33	NA	A	8378	1/1	0.96	0.54	47,47,47,47	0
33	NA	A	8336	1/1	0.96	0.06	53,53,53,53	0
33	NA	A	8338	1/1	0.96	0.09	41,41,41,41	0
32	MG	A	8062	1/1	0.96	0.10	48,48,48,48	0
32	MG	A	8091	1/1	0.96	0.05	69,69,69,69	0
32	MG	A	8092	1/1	0.96	0.13	79,79,79,79	0
33	NA	A	8350	1/1	0.96	0.24	32,32,32,32	0
32	MG	A	8004	1/1	0.96	0.07	26,26,26,26	0
32	MG	A	8096	1/1	0.96	0.07	46,46,46,46	0
33	NA	K	8346	1/1	0.96	0.08	40,40,40,40	0
33	NA	A	8354	1/1	0.96	0.27	34,34,34,34	0
32	MG	A	8098	1/1	0.96	0.13	36,36,36,36	0
32	MG	A	8042	1/1	0.96	0.13	31,31,31,31	0
32	MG	A	8068	1/1	0.96	0.16	50,50,50,50	0
32	MG	A	8044	1/1	0.96	0.06	36,36,36,36	0
32	MG	A	8075	1/1	0.96	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8051	1/1	0.96	0.08	57,57,57,57	0
32	MG	A	8079	1/1	0.96	0.11	27,27,27,27	0
32	MG	A	8107	1/1	0.96	0.05	43,43,43,43	0
35	CL	A	8515	1/1	0.96	0.34	65,65,65,65	0
32	MG	A	8005	1/1	0.96	0.12	33,33,33,33	0
32	MG	A	8054	1/1	0.96	0.10	24,24,24,24	0
35	CL	K	8501	1/1	0.96	0.12	55,55,55,55	0
32	MG	A	8055	1/1	0.96	0.08	43,43,43,43	0
32	MG	A	8007	1/1	0.96	0.06	16,16,16,16	0
33	NA	A	8328	1/1	0.96	0.32	34,34,34,34	0
35	CL	P	8508	1/1	0.96	0.10	62,62,62,62	0
32	MG	A	8116	1/1	0.96	0.11	51,51,51,51	0
33	NA	A	8331	1/1	0.96	0.17	31,31,31,31	0
36	SPS	5	9080	23/23	0.96	0.21	30,33,47,49	0
37	PHA	5	9077	11/11	0.96	0.24	41,45,52,53	0
32	MG	A	8059	1/1	0.96	0.13	35,35,35,35	0
32	MG	A	8061	1/1	0.96	0.07	34,34,34,34	0
33	NA	A	8318	1/1	0.97	0.41	55,55,55,55	0
32	MG	A	8071	1/1	0.97	0.04	63,63,63,63	0
33	NA	A	8321	1/1	0.97	0.19	54,54,54,54	0
32	MG	5	8118	1/1	0.97	0.12	29,29,29,29	0
32	MG	A	8016	1/1	0.97	0.11	39,39,39,39	0
33	NA	A	8361	1/1	0.97	0.28	47,47,47,47	0
33	NA	R	8348	1/1	0.97	0.17	42,42,42,42	0
32	MG	A	8056	1/1	0.97	0.06	39,39,39,39	0
32	MG	Z	8109	1/1	0.97	0.07	33,33,33,33	0
32	MG	A	8033	1/1	0.97	0.10	28,28,28,28	0
32	MG	A	8081	1/1	0.97	0.12	43,43,43,43	0
33	NA	A	8302	1/1	0.97	0.14	46,46,46,46	0
32	MG	A	8058	1/1	0.97	0.11	37,37,37,37	0
35	CL	A	8505	1/1	0.97	0.16	49,49,49,49	0
32	MG	A	8037	1/1	0.97	0.05	34,34,34,34	0
35	CL	A	8512	1/1	0.97	0.09	47,47,47,47	0
35	CL	A	8514	1/1	0.97	0.12	46,46,46,46	0
32	MG	A	8040	1/1	0.97	0.12	53,53,53,53	0
35	CL	A	8516	1/1	0.97	0.13	56,56,56,56	0
33	NA	A	8370	1/1	0.97	0.41	57,57,57,57	0
32	MG	A	8022	1/1	0.97	0.12	40,40,40,40	0
33	NA	A	8339	1/1	0.97	0.14	22,22,22,22	0
32	MG	A	8008	1/1	0.97	0.05	35,35,35,35	0
32	MG	A	8064	1/1	0.97	0.14	31,31,31,31	0
32	MG	A	8052	1/1	0.97	0.06	40,40,40,40	0

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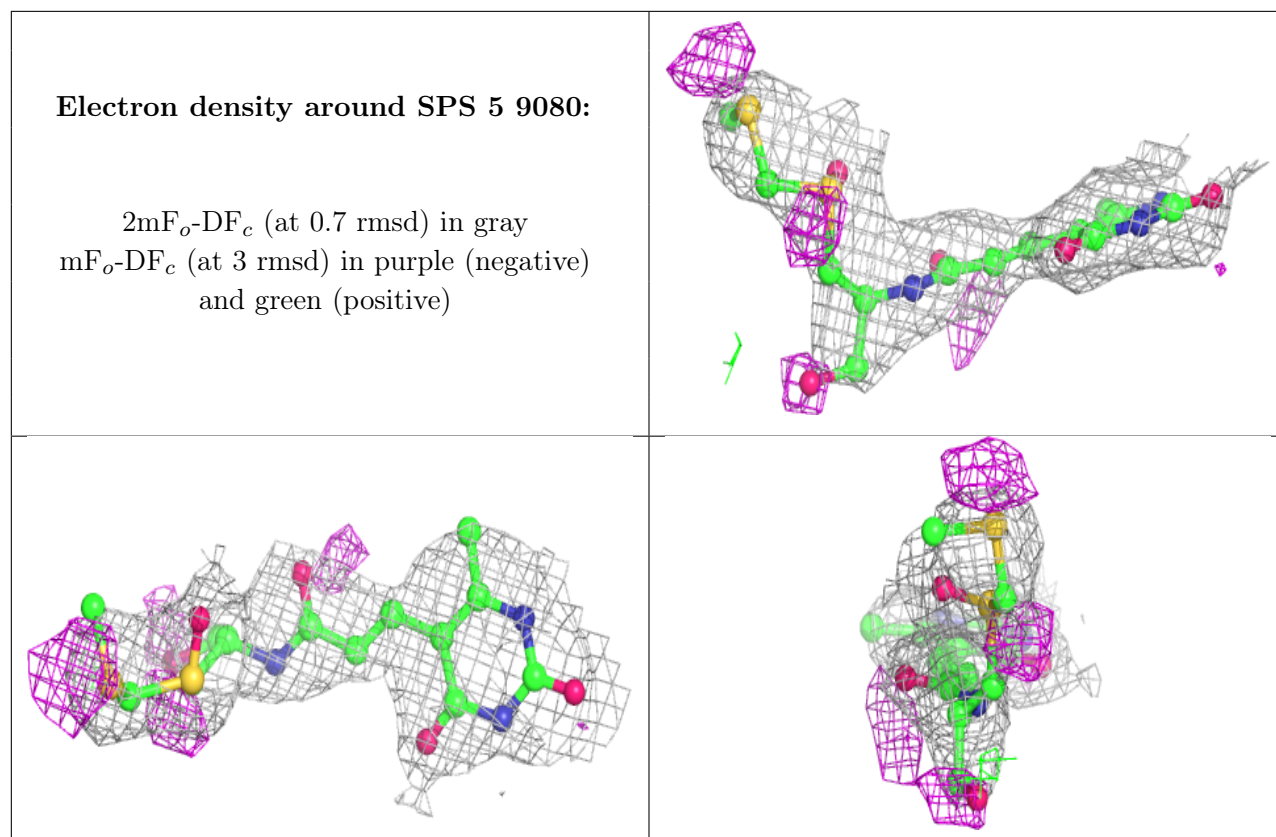
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	A	8349	1/1	0.97	0.14	41,41,41,41	0
33	NA	A	8379	1/1	0.97	0.12	45,45,45,45	0
32	MG	A	8067	1/1	0.97	0.12	43,43,43,43	0
32	MG	A	8043	1/1	0.97	0.08	39,39,39,39	0
32	MG	A	8117	1/1	0.97	0.08	25,25,25,25	0
33	NA	A	8316	1/1	0.97	0.20	40,40,40,40	0
32	MG	A	8013	1/1	0.97	0.17	32,32,32,32	0
32	MG	A	8035	1/1	0.98	0.03	52,52,52,52	0
32	MG	A	8036	1/1	0.98	0.05	32,32,32,32	0
32	MG	A	8021	1/1	0.98	0.11	33,33,33,33	0
32	MG	A	8038	1/1	0.98	0.09	27,27,27,27	0
32	MG	A	8110	1/1	0.98	0.11	35,35,35,35	0
32	MG	A	8011	1/1	0.98	0.09	26,26,26,26	0
32	MG	A	8112	1/1	0.98	0.17	28,28,28,28	0
32	MG	A	8023	1/1	0.98	0.06	39,39,39,39	0
32	MG	A	8001	1/1	0.98	0.07	27,27,27,27	0
32	MG	A	8115	1/1	0.98	0.06	42,42,42,42	0
33	NA	A	8374	1/1	0.98	0.67	53,53,53,53	0
35	CL	A	8513	1/1	0.98	0.11	50,50,50,50	0
32	MG	A	8093	1/1	0.98	0.08	49,49,49,49	0
33	NA	A	8376	1/1	0.98	0.14	47,47,47,47	0
32	MG	A	8072	1/1	0.98	0.10	56,56,56,56	0
32	MG	A	8025	1/1	0.98	0.07	40,40,40,40	0
35	CL	A	8522	1/1	0.98	0.16	55,55,55,55	0
32	MG	A	8097	1/1	0.98	0.17	28,28,28,28	0
35	CL	D	8519	1/1	0.98	0.11	40,40,40,40	0
33	NA	A	8381	1/1	0.98	0.23	44,44,44,44	0
32	MG	A	8015	1/1	0.98	0.09	29,29,29,29	0
33	NA	A	8320	1/1	0.98	0.11	38,38,38,38	0
35	CL	M	8510	1/1	0.98	0.16	47,47,47,47	0
35	CL	N	8518	1/1	0.98	0.12	39,39,39,39	0
32	MG	A	8029	1/1	0.98	0.08	41,41,41,41	0
32	MG	A	8006	1/1	0.98	0.04	30,30,30,30	0
35	CL	S	8506	1/1	0.98	0.11	46,46,46,46	0
32	MG	A	8019	1/1	0.98	0.04	29,29,29,29	0
33	NA	A	8327	1/1	0.98	0.12	41,41,41,41	0
32	MG	A	8102	1/1	0.98	0.12	45,45,45,45	0
32	MG	4	8078	1/1	0.98	0.04	41,41,41,41	0
33	NA	A	8330	1/1	0.98	0.22	34,34,34,34	0
32	MG	A	8048	1/1	0.98	0.16	58,58,58,58	0
32	MG	A	8018	1/1	0.99	0.09	31,31,31,31	0
32	MG	C	8065	1/1	0.99	0.11	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8077	1/1	0.99	0.06	27,27,27,27	0
32	MG	A	8030	1/1	0.99	0.10	32,32,32,32	0
32	MG	A	8080	1/1	0.99	0.05	36,36,36,36	0
33	NA	A	8325	1/1	0.99	0.36	50,50,50,50	0
32	MG	A	8031	1/1	0.99	0.05	27,27,27,27	0
32	MG	A	8060	1/1	0.99	0.18	42,42,42,42	0
32	MG	A	8003	1/1	0.99	0.12	26,26,26,26	0
32	MG	A	8084	1/1	0.99	0.05	40,40,40,40	0
32	MG	A	8012	1/1	0.99	0.09	28,28,28,28	0
32	MG	A	8086	1/1	0.99	0.17	45,45,45,45	0
32	MG	A	8034	1/1	0.99	0.07	33,33,33,33	0
32	MG	A	8002	1/1	0.99	0.06	28,28,28,28	0
32	MG	A	8014	1/1	0.99	0.06	25,25,25,25	0
32	MG	A	8009	1/1	0.99	0.04	26,26,26,26	0
32	MG	A	8010	1/1	0.99	0.09	35,35,35,35	0
32	MG	A	8039	1/1	0.99	0.08	42,42,42,42	0
32	MG	A	8026	1/1	0.99	0.07	26,26,26,26	0
32	MG	A	8017	1/1	0.99	0.03	19,19,19,19	0
33	NA	A	8315	1/1	0.99	0.10	32,32,32,32	0
32	MG	A	8074	1/1	0.99	0.03	29,29,29,29	0
33	NA	A	8344	1/1	0.99	0.05	25,25,25,25	0
34	K	A	8391	1/1	0.99	0.25	48,48,48,48	0
32	MG	A	8028	1/1	0.99	0.09	34,34,34,34	0
39	CD	1	8403	1/1	0.99	0.08	62,62,62,62	0
39	CD	2	8402	1/1	0.99	0.07	56,56,56,56	0
39	CD	4	8404	1/1	0.99	0.06	57,57,57,57	0
32	MG	A	8020	1/1	1.00	0.07	28,28,28,28	0
33	NA	A	8323	1/1	1.00	0.10	42,42,42,42	0
39	CD	V	8401	1/1	1.00	0.07	62,62,62,62	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.