Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 04:55 PM EDT

PDB ID	:	1NJI
Title	:	Structure of chloramphenicol bound to the 50S ribosomal subunit
Authors	:	Hansen, J.L.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2002-12-31
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

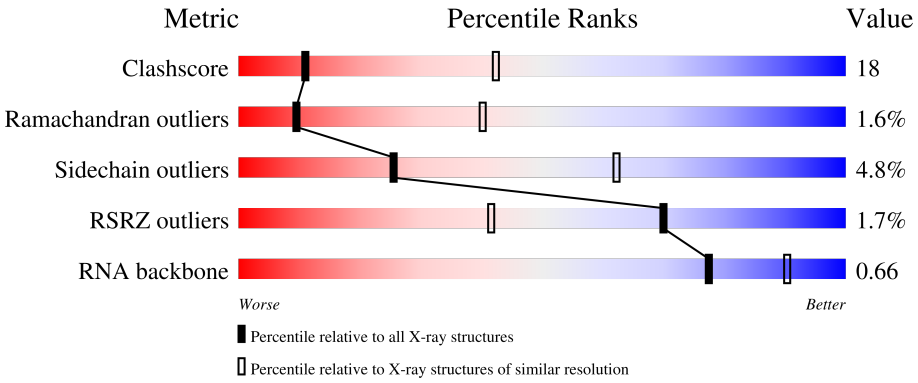
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.00 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	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	57% 31% 6% • 6%
2	B	122	5% 56% 30% 11% •
3	C	239	54% 39% 6% •
4	D	337	51% 44% 5%
5	E	246	57% 38% 5%

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Mol	Chain	Length	Quality of chain
6	F	176	18% 28% 43% 7% 20%
7	G	177	2% 60% 36%
8	H	119	2% 56% 42%
9	I	348	% 92%
10	J	167	% 35% 51% 6% 7%
11	K	145	58% 35% 5%
12	L	132	66% 33%
13	M	164	4% 50% 37% 12%
14	N	194	42% 53% 6%
15	O	186	2% 42% 52% 6%
16	P	115	73% 26%
17	Q	148	68% 28%
18	R	95	% 77% 20%
19	S	154	66% 29%
20	T	84	71% 24%
21	U	119	3% 59% 38%
22	V	66	48% 32% 20%
23	W	70	6% 50% 40% 7%
24	X	154	50% 46%
25	Y	91	2% 45% 41% 10%
26	Z	240	% 41% 15% 41%
27	1	73	38% 56% 5%
28	2	56	66% 34%
29	3	48	2% 48% 46%
30	4	92	62% 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
31	MG	A	8049	-	-	-	X
33	NA	A	8371	-	-	-	X
33	NA	A	8376	-	-	-	X
33	NA	A	8377	-	-	-	X
33	NA	A	8382	-	-	-	X
33	NA	A	8384	-	-	-	X

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 98536 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 ribosomal RNA.

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

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

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 protein called 50S ribosomal protein L2P.

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

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	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	SEE REMARK 999	UNP P20279
D	310	ARG	PHE	SEE REMARK 999	UNP P20279

- Molecule 5 is a protein called 50S ribosomal protein L4E.

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

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 9 is a protein called Acidic ribosomal protein P0 homolog.

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

- Molecule 10 is a protein called 50S ribosomal protein L10e.

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

- Molecule 11 is a protein called 50S ribosomal protein L13P.

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

- Molecule 12 is a protein called 50S ribosomal protein L14P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15P.

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

- Molecule 14 is a protein called 50S ribosomal protein L15E.

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

- Molecule 15 is a protein called 50S ribosomal protein L18P.

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

- Molecule 16 is a protein called 50S ribosomal protein L18E.

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

- Molecule 17 is a protein called 50S ribosomal protein L19E.

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

- Molecule 18 is a protein called 50S ribosomal protein L21e.

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

- Molecule 19 is a protein called 50S ribosomal protein L22P.

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

- Molecule 20 is a protein called 50S ribosomal protein L23P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24E.

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

- Molecule 23 is a protein called 50S ribosomal protein L29P.

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

- Molecule 24 is a protein called 50S ribosomal protein L30P.

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

- Molecule 25 is a protein called 50S ribosomal protein L31E.

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

- Molecule 26 is a protein called 50S ribosomal protein L32E.

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

- Molecule 27 is a protein called 50S ribosomal protein L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	A	109	Total	Mg	0	0
			109	109		
31	B	1	Total	Mg	0	0
			1	1		
31	C	1	Total	Mg	0	0
			1	1		
31	D	1	Total	Mg	0	0
			1	1		
31	L	1	Total	Mg	0	0
			1	1		
31	U	1	Total	Mg	0	0
			1	1		
31	Z	1	Total	Mg	0	0
			1	1		
31	1	1	Total	Mg	0	0
			1	1		
31	4	1	Total	Mg	0	0
			1	1		

- Molecule 32 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	71	Total Na 71 71	0	0
33	B	2	Total Na 2 2	0	0
33	C	1	Total Na 1 1	0	0
33	E	1	Total Na 1 1	0	0
33	J	2	Total Na 2 2	0	0
33	K	1	Total Na 1 1	0	0
33	M	1	Total Na 1 1	0	0
33	N	1	Total Na 1 1	0	0
33	R	1	Total Na 1 1	0	0
33	S	2	Total Na 2 2	0	0
33	T	1	Total Na 1 1	0	0
33	U	1	Total Na 1 1	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	9	Total Cl 9 9	0	0
34	C	1	Total Cl 1 1	0	0
34	D	1	Total Cl 1 1	0	0
34	K	3	Total Cl 3 3	0	0

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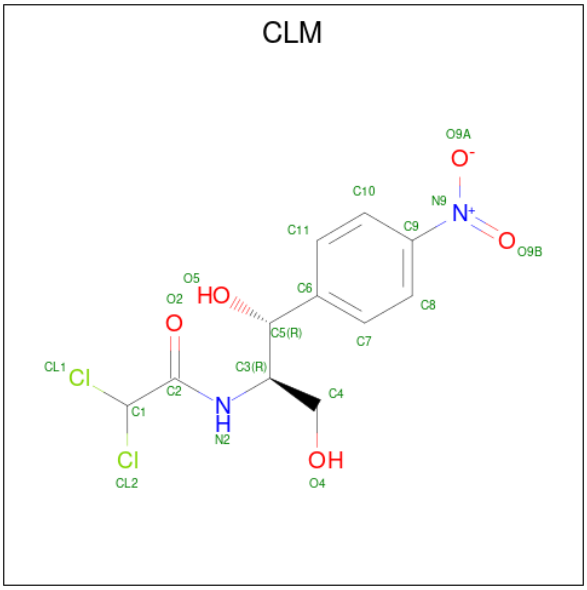
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	M	1	Total Cl 1 1	0	0
34	N	1	Total Cl 1 1	0	0
34	O	1	Total Cl 1 1	0	0
34	P	1	Total Cl 1 1	0	0
34	R	1	Total Cl 1 1	0	0
34	S	1	Total Cl 1 1	0	0
34	Z	1	Total Cl 1 1	0	0
34	4	1	Total Cl 1 1	0	0

- Molecule 35 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	1	Total C Cl N O 20 11 2 2 5	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	P	1	Total Cd 1 1	0	0
36	V	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	2	1	Total Cd 1 1	0	0
36	4	1	Total Cd 1 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	5906	Total O 5906 5906	0	0
37	B	143	Total O 143 143	0	0
37	C	123	Total O 123 123	0	0
37	D	147	Total O 147 147	0	0
37	E	167	Total O 167 167	0	0
37	F	50	Total O 50 50	0	0
37	G	45	Total O 45 45	0	0
37	H	29	Total O 29 29	0	0
37	I	21	Total O 21 21	0	0
37	J	76	Total O 76 76	0	0
37	K	54	Total O 54 54	0	0
37	L	61	Total O 61 61	0	0
37	M	78	Total O 78 78	0	0
37	N	125	Total O 125 125	0	0
37	O	69	Total O 69 69	0	0

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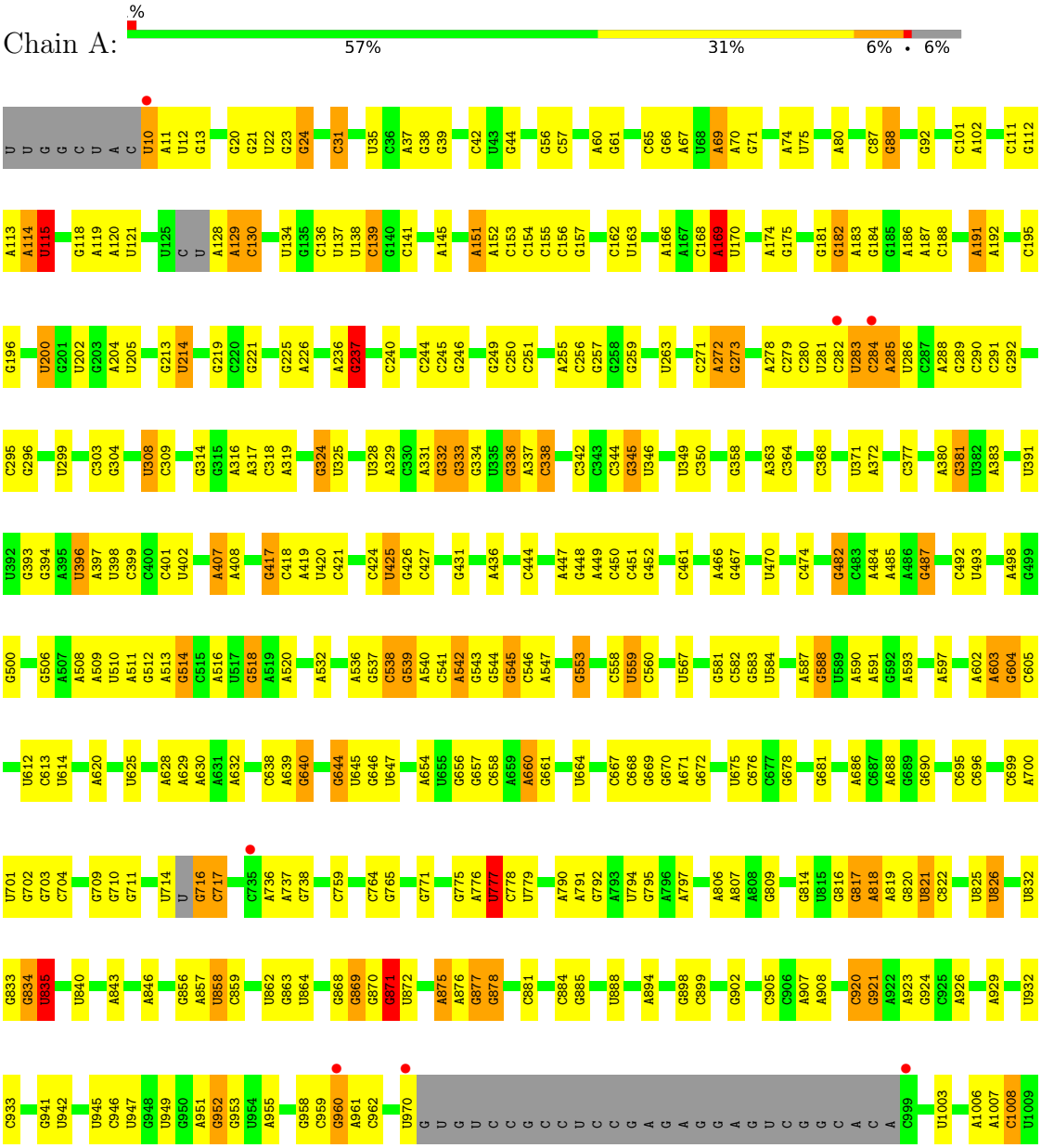
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	P	45	Total O 45 45	0	0
37	Q	73	Total O 73 73	0	0
37	R	53	Total O 53 53	0	0
37	S	85	Total O 85 85	0	0
37	T	35	Total O 35 35	0	0
37	U	40	Total O 40 40	0	0
37	V	28	Total O 28 28	0	0
37	W	17	Total O 17 17	0	0
37	X	69	Total O 69 69	0	0
37	Y	28	Total O 28 28	0	0
37	Z	98	Total O 98 98	0	0
37	1	37	Total O 37 37	0	0
37	2	54	Total O 54 54	0	0
37	3	43	Total O 43 43	0	0
37	4	68	Total O 68 68	0	0

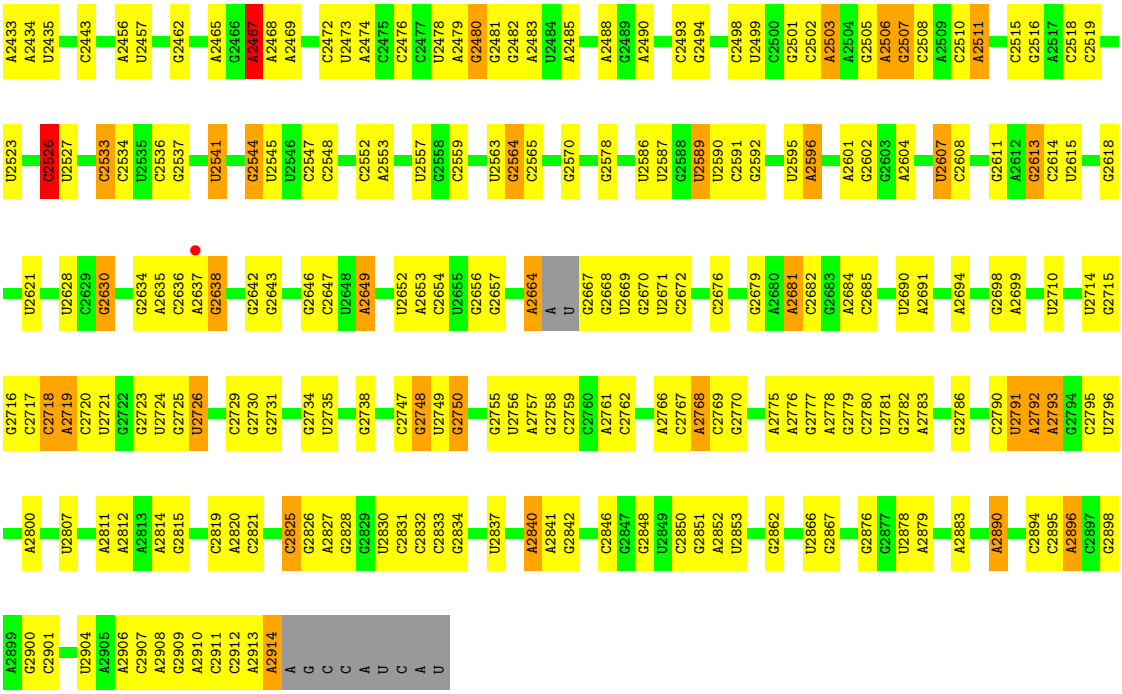
3 Residue-property plots (i)

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 ribosomal RNA

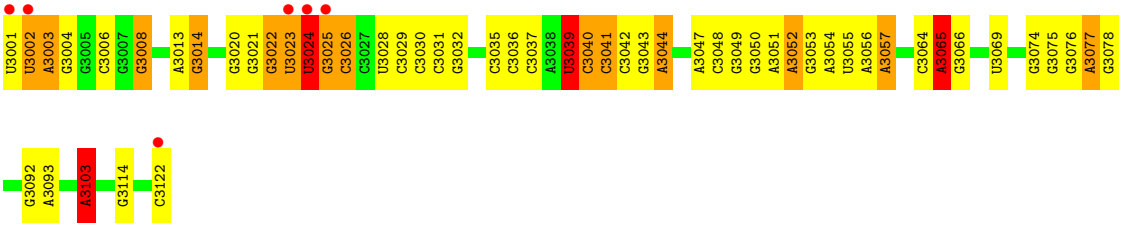
Chain A:





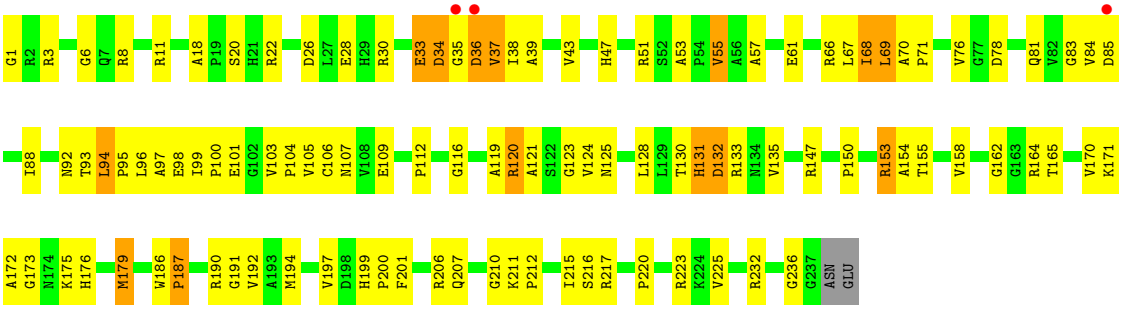
• Molecule 2: 5S ribosomal RNA

Chain B:



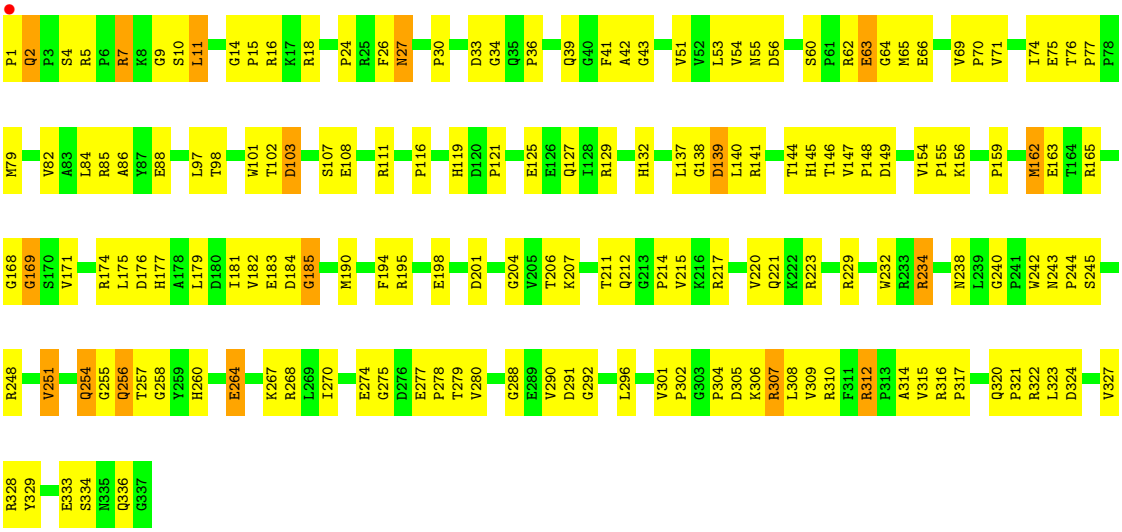
• Molecule 3: 50S ribosomal protein L2P

Chain C:



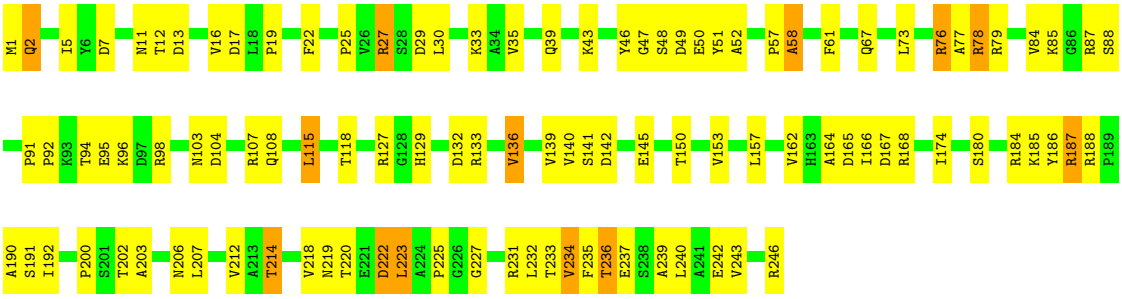
• Molecule 4: 50S ribosomal protein L3P

Chain D:



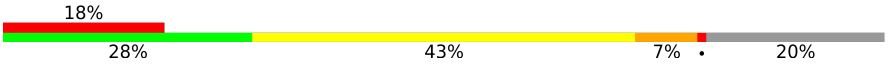
• Molecule 5: 50S ribosomal protein L4E

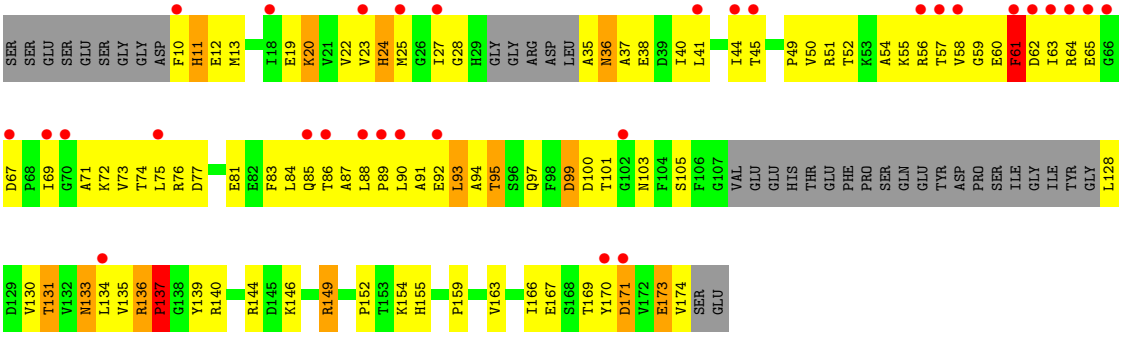
Chain E:



• Molecule 6: 50S ribosomal protein L5P

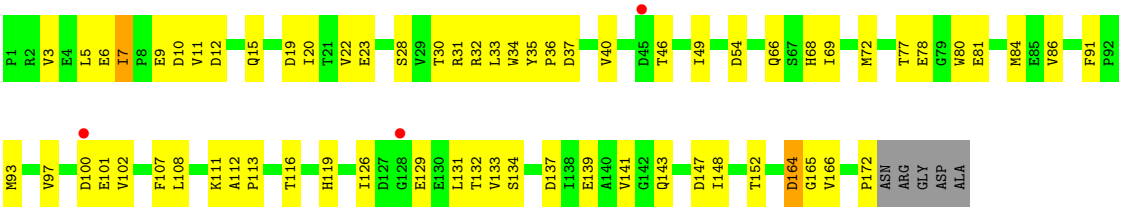
Chain F:





• Molecule 7: 50S ribosomal protein L6P

Chain G:

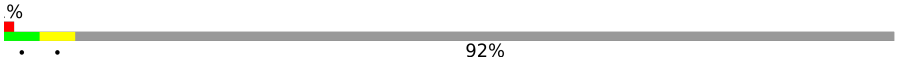


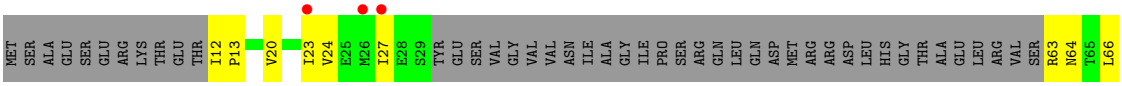
• Molecule 8: 50S ribosomal protein L7Ae

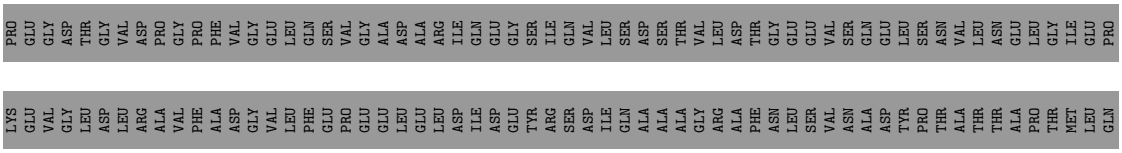
Chain H:

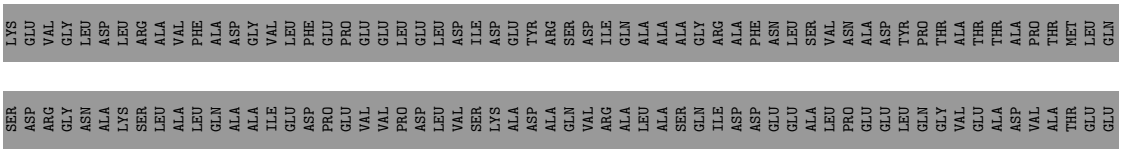
• Molecule 9: Acidic ribosomal protein P0 homolog

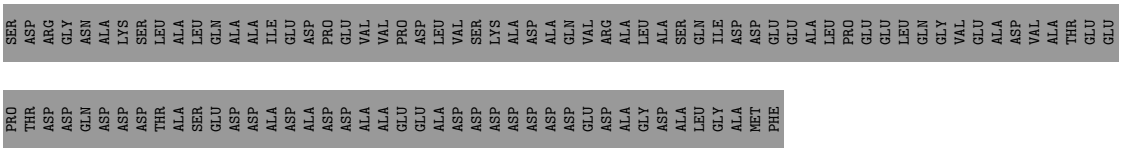
Chain I:





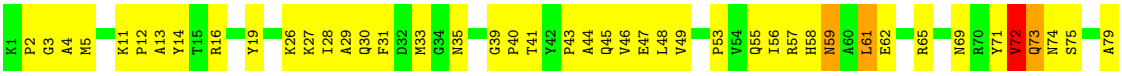






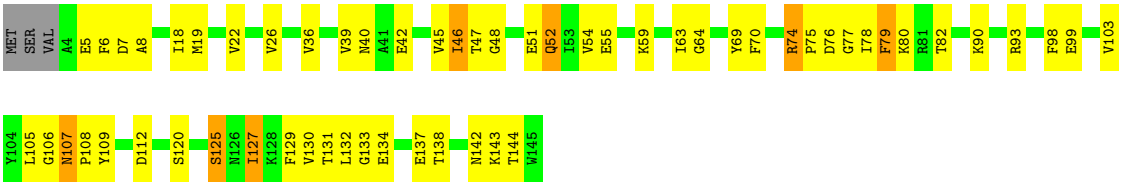
• Molecule 10: 50S ribosomal protein L10e

Chain J:



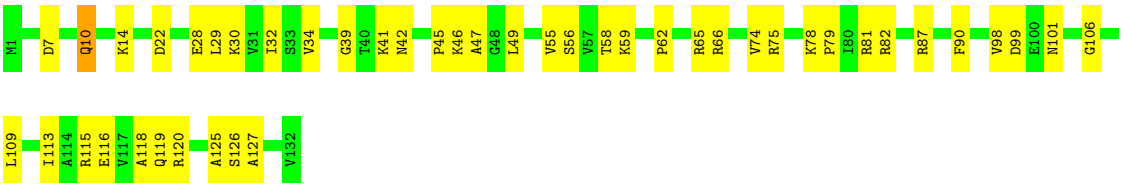
• Molecule 11: 50S ribosomal protein L13P

Chain K:



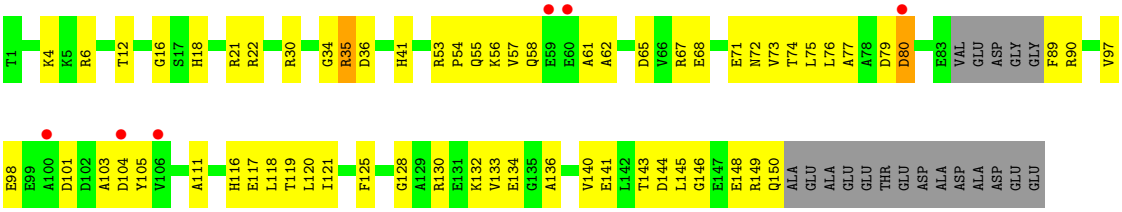
• Molecule 12: 50S ribosomal protein L14P

Chain L:



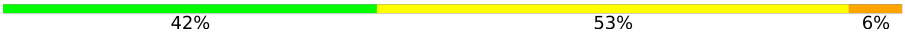
• Molecule 13: 50S ribosomal protein L15P

Chain M:



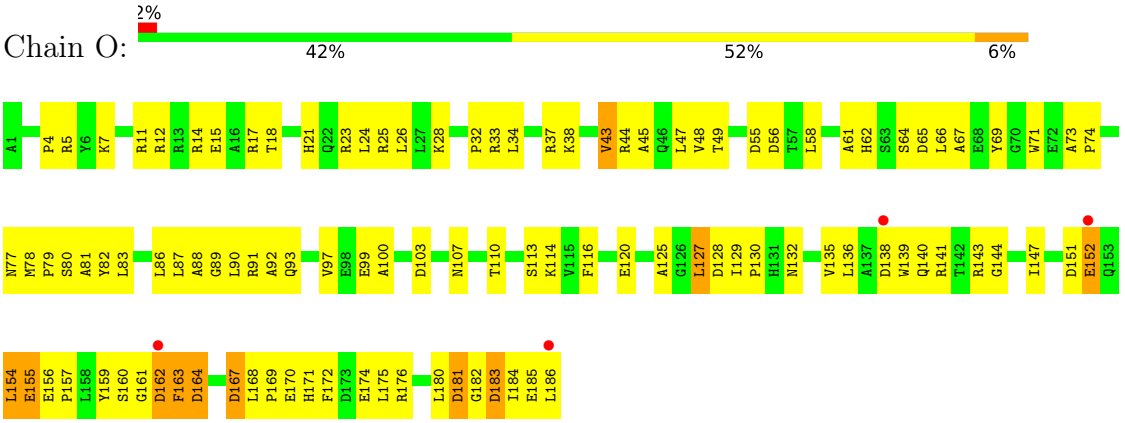
• Molecule 14: 50S ribosomal protein L15E

Chain N:



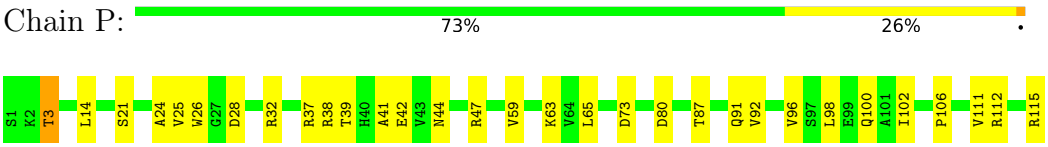
• Molecule 15: 50S ribosomal protein L18P

Chain O:



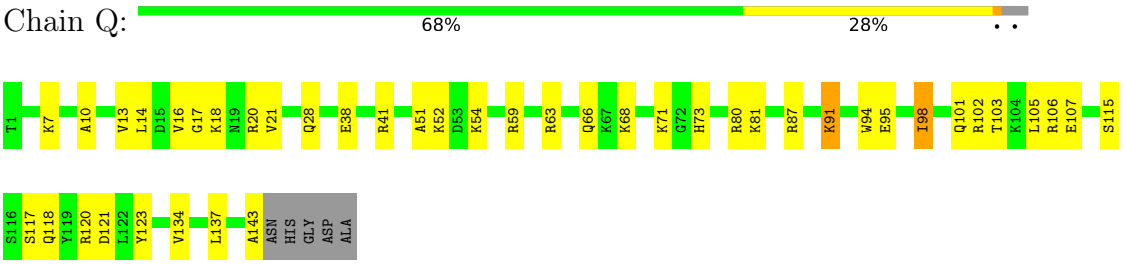
• Molecule 16: 50S ribosomal protein L18E

Chain P:



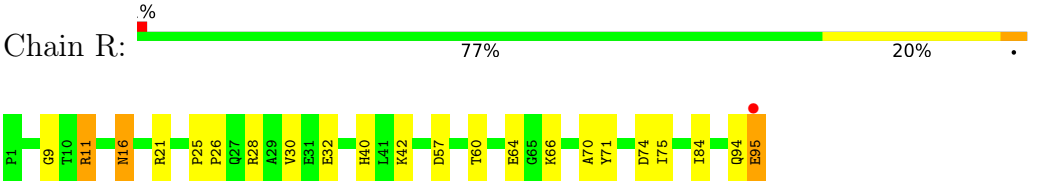
• Molecule 17: 50S ribosomal protein L19E

Chain Q:



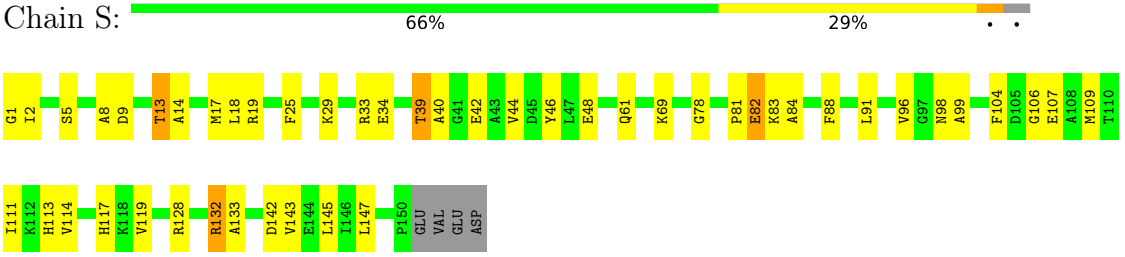
• Molecule 18: 50S ribosomal protein L21e

Chain R:



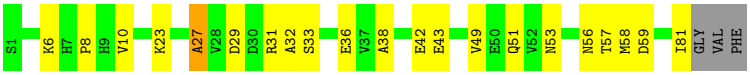
• Molecule 19: 50S ribosomal protein L22P

Chain S:

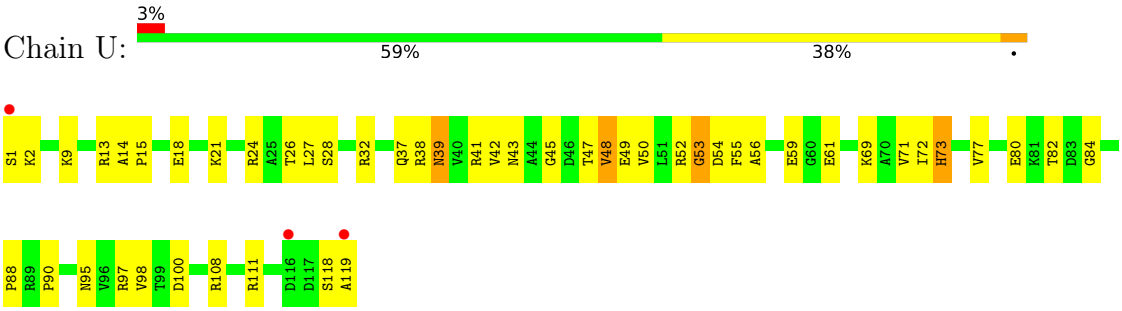


• Molecule 20: 50S ribosomal protein L23P

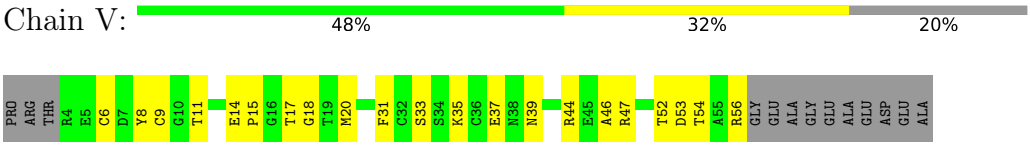
Chain T:



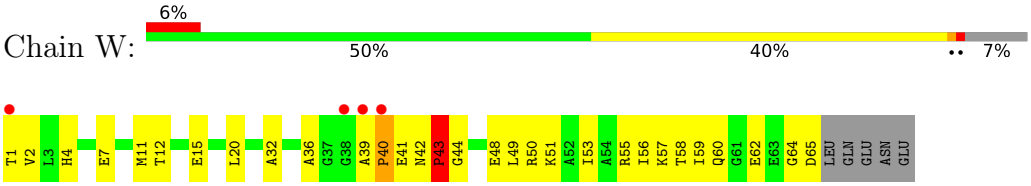
• Molecule 21: 50S ribosomal protein L24P



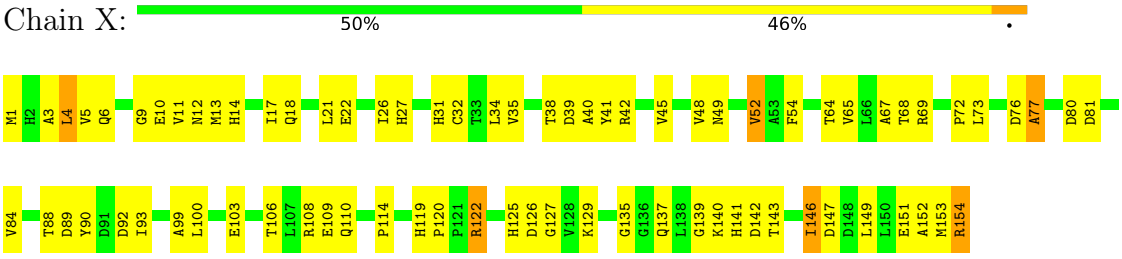
• Molecule 22: 50S ribosomal protein L24E



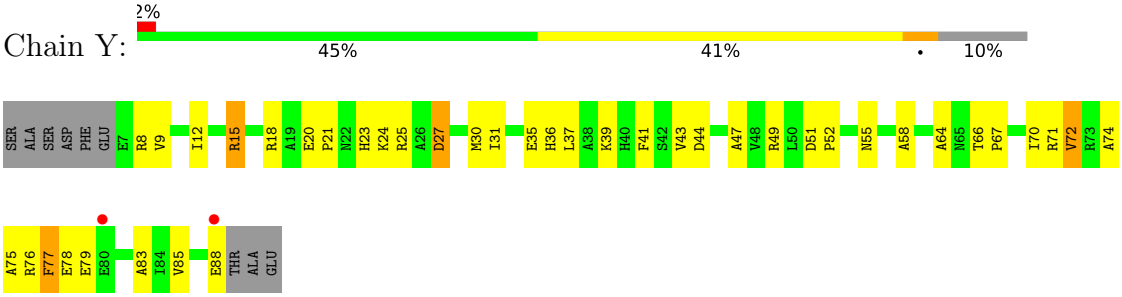
• Molecule 23: 50S ribosomal protein L29P



• Molecule 24: 50S ribosomal protein L30P

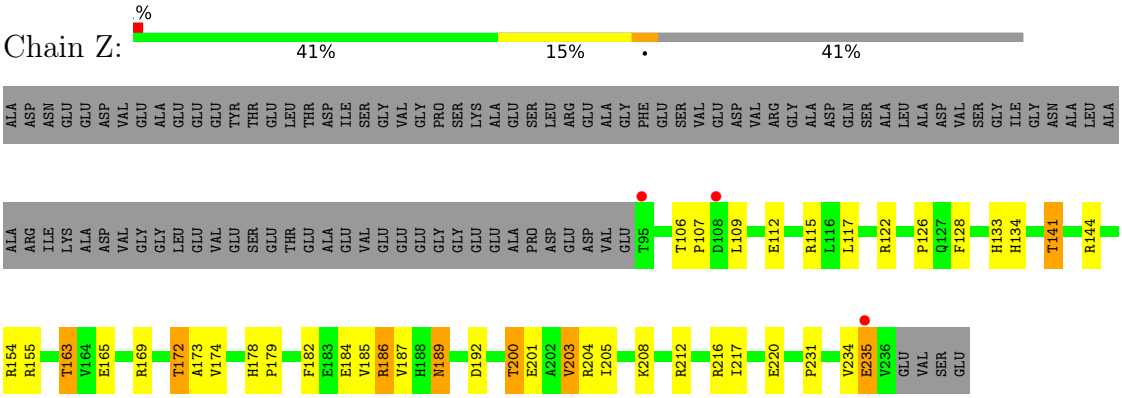


• Molecule 25: 50S ribosomal protein L31E



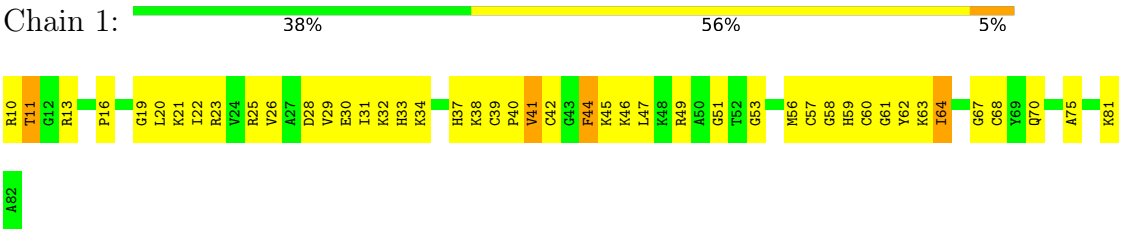
• Molecule 26: 50S ribosomal protein L32E

Chain Z:



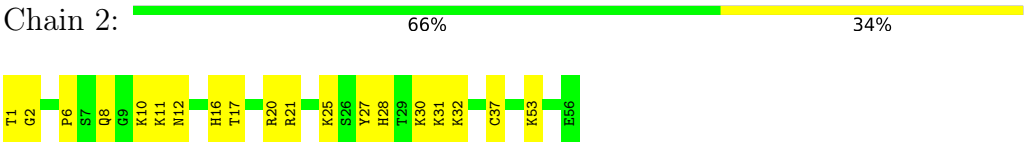
• Molecule 27: 50S ribosomal protein L37AE

Chain 1:



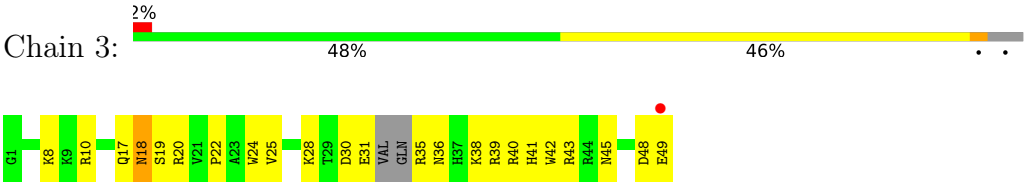
• Molecule 28: 50S ribosomal protein L37e

Chain 2:



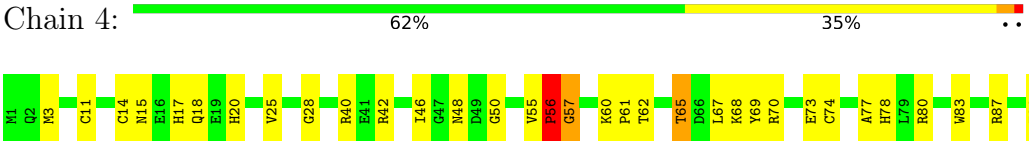
• Molecule 29: 50S ribosomal protein L39e

Chain 3:



• Molecule 30: 50S ribosomal protein L44E

Chain 4:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.72Å 299.75Å 573.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.96 – 2.87	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-3.00) 92.7 (49.96-2.87)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	0.25	Depositor
$< I/\sigma(I) >$ [1]	0.68 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.176 , 0.209 0.174 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 61.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	98536	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, CD, K, CL, CLM, NA

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	0.47	5/66076 (0.0%)	0.73	32/103052 (0.0%)
2	B	0.49	0/2905	0.77	4/4528 (0.1%)
3	C	0.44	0/1787	0.73	0/2409
4	D	0.41	0/2689	0.69	0/3652
5	E	0.46	0/1883	0.69	0/2551
6	F	0.35	0/1111	0.62	0/1498
7	G	0.40	0/1382	0.62	0/1880
8	H	0.37	0/896	0.59	0/1219
9	I	0.34	0/241	0.51	0/324
10	J	0.44	0/1246	0.77	1/1686 (0.1%)
11	K	0.44	0/1135	0.64	0/1530
12	L	0.42	0/1003	0.70	0/1351
13	M	0.40	0/1126	0.70	0/1504
14	N	0.47	0/1633	0.74	0/2180
15	O	0.35	0/1473	0.67	0/1999
16	P	0.40	0/873	0.67	0/1181
17	Q	0.41	0/1143	0.58	0/1521
18	R	0.46	0/748	0.73	0/1005
19	S	0.44	0/1172	0.71	0/1578
20	T	0.39	0/648	0.63	1/875 (0.1%)
21	U	0.39	0/957	0.68	0/1289
22	V	0.38	0/417	0.62	0/562
23	W	0.34	0/502	0.58	0/675
24	X	0.42	0/1218	0.69	0/1655
25	Y	0.41	0/664	0.64	0/895
26	Z	0.45	0/1146	0.68	0/1536
27	1	0.46	0/575	0.76	0/763
28	2	0.49	0/437	0.75	0/578
29	3	0.39	0/398	0.57	0/527
30	4	0.47	0/771	0.66	0/1024
All	All	0.46	5/98255 (0.0%)	0.71	38/147027 (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	90
2	B	1	3
All	All	2	93

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2097	G	O3'-P	8.81	1.71	1.61
1	A	2097	G	C3'-O3'	-7.93	1.31	1.42
1	A	2098	C	P-O5'	-7.79	1.51	1.59
1	A	1206	U	P-OP2	6.71	1.60	1.49
1	A	2098	C	P-OP1	-5.46	1.39	1.49

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1164	U	OP1-P-O3'	-18.95	63.51	105.20
1	A	1164	U	OP2-P-O3'	-17.97	65.67	105.20
1	A	1165	G	O5'-P-OP1	-14.27	92.85	105.70
2	B	3024	U	C2'-C3'-O3'	9.63	130.69	109.50
1	A	1563	G	C2'-C3'-O3'	9.41	130.20	109.50
1	A	1979	G	C2'-C3'-O3'	9.27	129.90	109.50
1	A	1165	G	O5'-P-OP2	-8.75	97.83	105.70
1	A	1942	A	C5'-C4'-C3'	8.47	129.56	116.00
2	B	3039	U	N1-C1'-C2'	7.03	123.14	114.00
1	A	1942	A	C5'-C4'-O4'	6.85	117.32	109.10
1	A	1504	A	C1'-O4'-C4'	-6.58	104.64	109.90
2	B	3103	A	C5'-C4'-O4'	6.35	116.72	109.10
1	A	1592	G	N9-C1'-C2'	6.15	121.99	114.00
1	A	1165	G	OP1-P-OP2	6.00	128.60	119.60
1	A	2099	G	C4'-C3'-O3'	-5.89	97.02	109.40
1	A	2313	C	C5'-C4'-O4'	5.85	116.12	109.10
1	A	2097	G	P-O3'-C3'	5.76	126.61	119.70
1	A	2467	A	C1'-O4'-C4'	-5.70	105.34	109.90
10	J	74	ASN	N-CA-C	-5.51	96.11	111.00
1	A	1971	G	N9-C1'-C2'	5.48	121.13	114.00
1	A	2098	C	OP1-P-OP2	5.45	127.78	119.60
1	A	2313	C	C5'-C4'-C3'	5.35	124.56	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2316	G	C5'-C4'-C3'	-5.33	107.47	116.00
2	B	3004	G	O5'-P-OP1	-5.31	100.92	105.70
1	A	1120	U	C5'-C4'-C3'	-5.29	107.54	116.00
1	A	407	A	O4'-C4'-C3'	-5.29	98.71	104.00
1	A	2726	U	N1-C1'-C2'	5.25	120.83	114.00
1	A	1559	A	C2'-C3'-O3'	5.23	122.07	113.70
1	A	1738	C	C5'-C4'-C3'	5.19	124.30	116.00
1	A	2607	U	N1-C1'-C2'	5.18	120.73	114.00
1	A	871	G	C5'-C4'-O4'	-5.17	102.90	109.10
1	A	1942	A	C1'-O4'-C4'	-5.17	105.77	109.90
1	A	2012	U	N1-C1'-C2'	5.16	120.71	114.00
1	A	2291	A	N9-C1'-C2'	5.14	120.68	114.00
1	A	1819	G	C5'-C4'-C3'	5.12	124.19	116.00
1	A	777	U	O4'-C1'-N1	5.07	112.25	108.20
20	T	27	ALA	N-CA-C	-5.06	97.34	111.00
1	A	2526	C	N1-C1'-C2'	5.04	120.56	114.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

All (93) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1017	U	Sidechain
1	A	1056	U	Sidechain
1	A	1078	A	Sidechain
1	A	115	U	Sidechain
1	A	118	G	Sidechain
1	A	1206	U	Sidechain
1	A	1266	U	Sidechain
1	A	1340	G	Sidechain
1	A	1342	C	Sidechain
1	A	1355	A	Sidechain
1	A	1376	G	Sidechain
1	A	1377	C	Sidechain
1	A	1417	G	Sidechain
1	A	1430	G	Sidechain
1	A	1447	U	Sidechain
1	A	1599	U	Sidechain

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Mol	Chain	Res	Type	Group
1	A	169	A	Sidechain
1	A	174	A	Sidechain
1	A	1758	U	Sidechain
1	A	181	G	Sidechain
1	A	182	G	Sidechain
1	A	1828	G	Sidechain
1	A	1829	A	Sidechain
1	A	1845	A	Sidechain
1	A	1867	G	Sidechain
1	A	1877	G	Sidechain
1	A	1878	G	Sidechain
1	A	191	A	Sidechain
1	A	1933	G	Sidechain
1	A	1970	G	Sidechain
1	A	1972	U	Sidechain
1	A	1993	C	Sidechain
1	A	202	U	Sidechain
1	A	2034	U	Sidechain
1	A	2101	A	Sidechain
1	A	2114	C	Sidechain
1	A	2133	U	Sidechain
1	A	214	U	Sidechain
1	A	22	U	Sidechain
1	A	221	G	Sidechain
1	A	2290	U	Sidechain
1	A	2301	A	Sidechain
1	A	2308	U	Sidechain
1	A	2316	G	Sidechain
1	A	237	G	Sidechain
1	A	24	G	Sidechain
1	A	2412	G	Sidechain
1	A	2480	G	Sidechain
1	A	2493	C	Sidechain
1	A	2503	A	Sidechain
1	A	2506	A	Sidechain
1	A	2523	U	Sidechain
1	A	2526	C	Sidechain
1	A	2544	G	Sidechain
1	A	2552	C	Sidechain
1	A	2557	U	Sidechain
1	A	2564	G	Sidechain
1	A	2596	A	Sidechain

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Mol	Chain	Res	Type	Group
1	A	2615	U	Sidechain
1	A	2618	G	Sidechain
1	A	2628	U	Sidechain
1	A	2630	G	Sidechain
1	A	2664	A	Sidechain
1	A	2759	C	Sidechain
1	A	2793	A	Sidechain
1	A	2842	G	Sidechain
1	A	2853	U	Sidechain
1	A	324	G	Sidechain
1	A	332	G	Sidechain
1	A	333	G	Sidechain
1	A	396	U	Sidechain
1	A	402	U	Sidechain
1	A	425	U	Sidechain
1	A	436	A	Sidechain
1	A	44	G	Sidechain
1	A	482	G	Sidechain
1	A	518	G	Sidechain
1	A	532	A	Sidechain
1	A	640	G	Sidechain
1	A	678	G	Sidechain
1	A	690	G	Sidechain
1	A	792	G	Sidechain
1	A	817	G	Sidechain
1	A	818	A	Sidechain
1	A	826	U	Sidechain
1	A	835	U	Sidechain
1	A	864	U	Sidechain
1	A	881	C	Sidechain
1	A	888	U	Sidechain
1	A	952	G	Sidechain
2	B	3008	G	Sidechain
2	B	3039	U	Sidechain
2	B	3065	A	Sidechain

5.2 Too-close contacts (i)

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	29806	952	0
2	B	2600	0	1326	73	0
3	C	1754	0	1763	128	0
4	D	2624	0	2533	176	0
5	E	1858	0	1816	125	0
6	F	1094	0	1085	127	0
7	G	1357	0	1266	70	0
8	H	885	0	854	64	0
9	I	240	0	231	15	0
10	J	1215	0	1215	152	0
11	K	1119	0	1098	68	0
12	L	993	0	1027	50	0
13	M	1114	0	1072	61	0
14	N	1605	0	1676	160	0
15	O	1444	0	1401	117	0
16	P	864	0	873	32	0
17	Q	1133	0	1127	46	0
18	R	734	0	728	18	0
19	S	1149	0	1122	55	0
20	T	641	0	605	20	0
21	U	949	0	923	55	0
22	V	410	0	365	30	0
23	W	499	0	511	30	0
24	X	1195	0	1137	96	0
25	Y	654	0	653	49	0
26	Z	1130	0	1133	62	0
27	1	563	0	598	59	0
28	2	430	0	426	24	0
29	3	393	0	406	25	0
30	4	755	0	728	35	0
31	1	1	0	0	0	0
31	4	1	0	0	0	0
31	A	109	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	D	1	0	0	0	0
31	L	1	0	0	0	0
31	U	1	0	0	0	0
31	Z	1	0	0	0	0
32	A	2	0	0	0	0
33	A	71	0	0	0	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	E	1	0	0	0	0
33	J	2	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	4	1	0	0	0	0
34	A	9	0	0	0	0
34	C	1	0	0	0	0
34	D	1	0	0	1	0
34	K	3	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	1	0
34	O	1	0	0	0	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Z	1	0	0	0	0
35	A	20	0	11	0	0
36	1	1	0	0	1	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	37	0	0	9	0
37	2	54	0	0	2	0
37	3	43	0	0	4	0
37	4	68	0	0	11	0
37	A	5906	0	0	192	0
37	B	143	0	0	14	0
37	C	123	0	0	19	0
37	D	147	0	0	32	0
37	E	167	0	0	38	0
37	F	50	0	0	19	0
37	G	45	0	0	8	0
37	H	29	0	0	7	0
37	I	21	0	0	1	0
37	J	76	0	0	24	0
37	K	54	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	L	61	0	0	8	0
37	M	78	0	0	16	0
37	N	125	0	0	19	0
37	O	69	0	0	13	0
37	P	45	0	0	7	0
37	Q	73	0	0	6	0
37	R	53	0	0	3	0
37	S	85	0	0	7	0
37	T	35	0	0	4	0
37	U	40	0	0	7	0
37	V	28	0	0	6	0
37	W	17	0	0	2	0
37	X	69	0	0	17	0
37	Y	28	0	0	6	0
37	Z	98	0	0	18	0
All	All	98536	0	59515	2717	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 (2717) 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)
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.57	1.18
5:E:236:THR:HG22	5:E:239:ALA:H	1.03	1.15
1:A:156:C:H5"	14:N:171:ARG:HD3	1.29	1.15
27:1:38:LYS:HE2	27:1:45:LYS:HE2	1.33	1.07
1:A:1160:G:H5'	1:A:1161:A:H5'	1.32	1.06
1:A:1242:A:H5'	11:K:82:THR:HG23	1.34	1.06
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.38	1.06
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.37	1.05
1:A:1134:G:H4'	10:J:151:MET:HE1	1.35	1.04
10:J:45:GLN:HB3	10:J:163:PRO:HD2	1.34	1.04
23:W:12:THR:HG22	23:W:15:GLU:HG3	1.38	1.04
1:A:1751:G:H2'	1:A:1752:G:H5"	1.38	1.03
14:N:164:THR:HG22	14:N:167:GLY:H	1.24	1.02
4:D:140:LEU:HA	37:D:8581:HOH:O	1.60	1.02
6:F:134:LEU:HD11	6:F:166:ILE:HD11	1.40	1.02
12:L:10:GLN:H	12:L:10:GLN:NE2	1.55	1.02
10:J:86:ARG:HH11	10:J:133:ILE:CG1	1.72	1.02
5:E:5:ILE:HD11	5:E:16:VAL:HG23	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:29:LEU:HB3	12:L:55:VAL:HG11	1.43	1.01
27:1:10:ARG:HA	37:1:8415:HOH:O	1.61	1.00
12:L:10:GLN:HE21	12:L:10:GLN:N	1.59	1.00
17:Q:115:SER:H	17:Q:118:GLN:HE21	1.04	1.00
10:J:162:SER:HB2	10:J:163:PRO:HD3	1.41	0.99
2:B:3006:C:H5"	15:O:37:ARG:NH1	1.77	0.99
10:J:26:LYS:HD2	10:J:28:ILE:HD12	1.42	0.99
1:A:1474:C:H6	1:A:1474:C:H5'	1.28	0.98
12:L:81:ARG:HB2	12:L:87:ARG:HH11	1.29	0.97
27:1:38:LYS:HG2	27:1:45:LYS:HG2	1.45	0.97
24:X:88:THR:HG22	24:X:89:ASP:H	1.28	0.97
1:A:21:G:H5'	19:S:2:ILE:HA	1.46	0.97
4:D:62:ARG:HA	4:D:65:MET:HE3	1.46	0.97
2:B:3076:G:H3'	2:B:3077:A:H5"	1.47	0.96
2:B:3023:U:H4'	2:B:3024:U:OP2	1.63	0.95
10:J:86:ARG:HH11	10:J:133:ILE:HG13	0.79	0.95
4:D:264:GLU:HG2	4:D:267:LYS:HE2	1.48	0.95
1:A:962:C:H1'	15:O:5:ARG:NH1	1.82	0.94
15:O:83:LEU:HD13	15:O:175:LEU:HD23	1.50	0.94
14:N:102:GLU:OE1	14:N:164:THR:HG21	1.68	0.94
10:J:150:LYS:HE2	37:J:8382:HOH:O	1.67	0.94
1:A:542:A:H5'	1:A:542:A:H8	1.31	0.94
5:E:78:ARG:HG3	5:E:78:ARG:HH11	1.30	0.93
15:O:47:LEU:HD11	15:O:127:LEU:HD21	1.50	0.93
29:3:41:HIS:H	29:3:45:ASN:HD22	1.17	0.93
2:B:3056:A:H2'	2:B:3057:A:H5"	1.52	0.92
6:F:154:LYS:H	6:F:154:LYS:HD2	1.34	0.92
19:S:99:ALA:HB1	19:S:109:MET:HE1	1.49	0.92
1:A:856:G:H2'	37:A:5400:HOH:O	1.68	0.92
14:N:35:PRO:HG2	14:N:38:VAL:HG23	1.51	0.91
10:J:165:GLY:HA3	37:J:8396:HOH:O	1.68	0.91
12:L:39:GLY:HA2	37:L:4183:HOH:O	1.69	0.91
6:F:25:MET:HE2	6:F:41:LEU:HG	1.53	0.91
1:A:470:U:O2'	28:2:16:HIS:HD2	1.54	0.91
10:J:59:ASN:H	10:J:59:ASN:HD22	1.18	0.91
16:P:42:GLU:HB2	37:P:2176:HOH:O	1.71	0.90
4:D:238:ASN:HD22	4:D:240:GLY:H	1.20	0.90
26:Z:200:THR:HG22	26:Z:201:GLU:HG3	1.54	0.89
1:A:545:G:H5'	1:A:545:G:H8	1.34	0.89
1:A:1835:U:H5	1:A:1840:A:N7	1.69	0.89
20:T:57:THR:HG22	20:T:59:ASP:H	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:ALA:HA	37:D:8581:HOH:O	1.72	0.89
2:B:3006:C:H5"	15:O:37:ARG:HH12	1.37	0.89
37:A:4831:HOH:O	14:N:14:ARG:HG2	1.71	0.88
14:N:52:LEU:HD11	37:N:8613:HOH:O	1.72	0.88
1:A:871:G:H5'	1:A:871:G:C8	2.08	0.88
5:E:236:THR:HG22	5:E:239:ALA:N	1.88	0.88
12:L:81:ARG:HD3	12:L:87:ARG:NH1	1.87	0.88
17:Q:115:SER:OG	17:Q:118:GLN:HG3	1.73	0.87
1:A:645:U:OP2	13:M:4:LYS:HE2	1.73	0.87
12:L:14:LYS:HB2	12:L:45:PRO:HG2	1.56	0.87
7:G:97:VAL:HG12	37:G:4191:HOH:O	1.73	0.87
10:J:4:ALA:HB3	37:J:8365:HOH:O	1.75	0.87
15:O:49:THR:HG22	15:O:56:ASP:HB2	1.57	0.87
15:O:144:GLY:O	15:O:147:ILE:HG22	1.74	0.87
4:D:201:ASP:HB2	4:D:312:ARG:HD2	1.58	0.86
1:A:960:G:H4'	37:A:7402:HOH:O	1.75	0.86
10:J:55:GLN:HE21	10:J:124:ARG:HE	1.22	0.86
5:E:2:GLN:HB3	37:E:8336:HOH:O	1.74	0.86
10:J:139:ASP:N	10:J:140:PRO:HD3	1.89	0.86
14:N:35:PRO:CG	14:N:38:VAL:HG23	2.05	0.86
4:D:321:PRO:HA	37:D:8658:HOH:O	1.75	0.86
10:J:162:SER:HB2	10:J:163:PRO:CD	2.05	0.86
1:A:541:C:H2'	1:A:542:A:H5"	1.58	0.85
1:A:2716:G:H5"	4:D:206:THR:HG21	1.58	0.85
1:A:346:U:H4'	37:A:6815:HOH:O	1.76	0.85
37:A:3699:HOH:O	14:N:157:LEU:HD11	1.74	0.85
10:J:59:ASN:HD22	10:J:59:ASN:N	1.71	0.85
1:A:2717:C:H2'	1:A:2718:C:H5"	1.58	0.85
27:1:46:LYS:HD3	27:1:59:HIS:HB2	1.58	0.85
10:J:27:LYS:H	10:J:58:HIS:HD2	1.20	0.85
3:C:211:LYS:HB3	3:C:212:PRO:HD2	1.56	0.84
24:X:6:GLN:HB2	24:X:26:ILE:HD12	1.56	0.84
30:4:70:ARG:HG2	30:4:77:ALA:HB2	1.58	0.84
23:W:42:ASN:HB3	37:W:7247:HOH:O	1.78	0.84
1:A:1184:C:H1'	37:A:7439:HOH:O	1.77	0.84
6:F:25:MET:HE1	6:F:37:ALA:HB1	1.57	0.84
12:L:74:VAL:HG13	12:L:113:ILE:HG23	1.59	0.84
1:A:1165:G:H4'	1:A:1174:A:O2'	1.77	0.84
37:A:6742:HOH:O	15:O:4:PRO:HD2	1.76	0.84
8:H:91:VAL:HG12	8:H:92:GLY:H	1.42	0.84
8:H:96:ALA:HA	37:H:3111:HOH:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:133:VAL:HA	37:M:8570:HOH:O	1.76	0.84
1:A:2506:A:HO2'	1:A:2507:G:H8	0.89	0.83
10:J:29:ALA:HB3	10:J:65:ARG:HH12	1.43	0.83
37:A:6845:HOH:O	14:N:178:LYS:HB2	1.76	0.83
4:D:212:GLN:HB2	4:D:257:THR:HG21	1.58	0.83
6:F:105:SER:HB2	6:F:131:THR:HG23	1.60	0.83
10:J:2:PRO:HB2	37:J:8365:HOH:O	1.77	0.83
24:X:88:THR:HB	37:X:6679:HOH:O	1.78	0.83
1:A:2717:C:C2'	1:A:2718:C:H5"	2.09	0.83
15:O:87:LEU:HD12	15:O:186:LEU:HD21	1.59	0.83
24:X:88:THR:HG22	24:X:89:ASP:N	1.93	0.83
1:A:711:G:H1'	37:A:7067:HOH:O	1.79	0.83
5:E:115:LEU:HD13	5:E:223:LEU:HD21	1.61	0.82
7:G:15:GLN:HG3	7:G:20:ILE:HG12	1.58	0.82
37:A:4919:HOH:O	2:B:3103:A:H4'	1.78	0.82
5:E:127:ARG:NH2	5:E:225:PRO:HG2	1.94	0.82
1:A:1701:A:H4'	1:A:1702:U:H5"	1.60	0.82
13:M:79:ASP:HB3	37:M:8555:HOH:O	1.80	0.82
15:O:23:ARG:HD3	37:O:8549:HOH:O	1.80	0.82
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.61	0.82
1:A:381:G:H5"	37:A:4287:HOH:O	1.78	0.81
1:A:1116:U:O2'	1:A:1118:A:H2	1.63	0.81
8:H:91:VAL:HG12	8:H:92:GLY:N	1.95	0.81
1:A:1474:C:H5'	1:A:1474:C:C6	2.14	0.81
12:L:81:ARG:HB2	12:L:87:ARG:NH1	1.93	0.81
1:A:560:C:H42	1:A:597:A:H61	1.24	0.81
1:A:1116:U:H3	1:A:1246:A:H62	1.25	0.81
19:S:8:ALA:HB1	19:S:13:THR:HG21	1.60	0.81
3:C:35:GLY:O	3:C:36:ASP:HB3	1.79	0.81
6:F:20:LYS:HA	6:F:75:LEU:O	1.81	0.81
27:1:58:GLY:HA3	37:1:8437:HOH:O	1.80	0.81
1:A:1166:A:H1'	1:A:1192:A:C2	2.15	0.81
14:N:87:MET:HE2	37:N:8592:HOH:O	1.79	0.81
1:A:288:A:H61	1:A:364:C:H42	1.29	0.80
1:A:1372:A:H3'	37:A:7160:HOH:O	1.81	0.80
26:Z:212:ARG:HD2	37:Z:8603:HOH:O	1.81	0.80
1:A:2812:A:H2	1:A:2814:A:H62	1.27	0.80
27:1:38:LYS:HE2	27:1:45:LYS:CE	2.11	0.80
27:1:61:GLY:HA3	37:1:8425:HOH:O	1.81	0.80
1:A:1667:A:H5'	1:A:1667:A:H8	1.46	0.80
14:N:87:MET:HB3	30:4:46:ILE:HD13	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:5:ILE:HD11	5:E:16:VAL:CG2	2.11	0.80
1:A:506:G:H22	1:A:509:A:C5'	1.94	0.80
17:Q:115:SER:H	17:Q:118:GLN:NE2	1.80	0.80
23:W:1:THR:HG23	23:W:2:VAL:H	1.46	0.80
1:A:1160:G:C5'	1:A:1161:A:H5'	2.12	0.80
3:C:100:PRO:HG2	3:C:103:VAL:HG21	1.62	0.80
13:M:68:GLU:HA	37:M:8540:HOH:O	1.81	0.79
1:A:1116:U:HO2'	1:A:1118:A:H2	0.81	0.79
1:A:1751:G:C2'	1:A:1752:G:H5"	2.12	0.79
14:N:172:GLY:O	14:N:183:VAL:HG11	1.82	0.79
10:J:140:PRO:HB3	37:J:8380:HOH:O	1.82	0.79
24:X:137:GLN:HE21	24:X:141:HIS:HE1	1.28	0.79
1:A:559:U:H6	1:A:559:U:H5'	1.48	0.79
37:A:5768:HOH:O	14:N:170:CYS:SG	2.40	0.79
3:C:88:ILE:HD13	3:C:100:PRO:HD3	1.65	0.79
1:A:870:G:H2'	1:A:871:G:H5"	1.62	0.79
10:J:47:GLU:HB3	10:J:133:ILE:CD1	2.12	0.79
4:D:41:PHE:HB3	4:D:190:MET:HE1	1.63	0.79
1:A:1973:A:H5'	1:A:1973:A:H8	1.48	0.78
7:G:81:GLU:HG2	7:G:134:SER:HB3	1.64	0.78
5:E:132:ASP:HB3	37:E:8363:HOH:O	1.84	0.78
23:W:12:THR:HG22	23:W:15:GLU:CG	2.13	0.78
6:F:27:ILE:HG22	6:F:28:GLY:H	1.48	0.78
14:N:106:ASN:HD22	14:N:114:VAL:HG23	1.47	0.78
15:O:113:SER:HB2	37:O:8561:HOH:O	1.82	0.78
25:Y:78:GLU:HG2	25:Y:79:GLU:H	1.48	0.78
5:E:78:ARG:HG3	5:E:78:ARG:NH1	1.98	0.78
1:A:962:C:H1'	15:O:5:ARG:HH12	1.48	0.78
15:O:7:LYS:HE3	18:R:21:ARG:O	1.84	0.78
2:B:3023:U:H3'	37:B:8479:HOH:O	1.83	0.78
1:A:31:C:H2'	37:A:7666:HOH:O	1.84	0.78
4:D:7:ARG:HG2	4:D:7:ARG:HH11	1.49	0.78
13:M:53:ARG:NH2	13:M:57:VAL:HG12	1.97	0.78
21:U:9:LYS:HE3	21:U:13:ARG:NH1	1.99	0.77
27:1:49:ARG:HD2	37:1:8428:HOH:O	1.82	0.77
25:Y:71:ARG:HB3	25:Y:88:GLU:OE1	1.84	0.77
1:A:1209:C:H4'	37:A:5249:HOH:O	1.84	0.77
1:A:2506:A:O2'	1:A:2507:G:H8	1.66	0.77
27:1:40:PRO:HD3	27:1:47:LEU:HD11	1.66	0.77
37:A:4433:HOH:O	14:N:146:GLN:HG2	1.83	0.77
1:A:871:G:C5'	1:A:871:G:H8	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:ARG:HG3	4:D:256:GLN:HG3	1.65	0.77
4:D:223:ARG:HG3	4:D:232:TRP:O	1.84	0.77
1:A:1625:U:H4'	37:A:4636:HOH:O	1.84	0.77
1:A:2468:A:H61	30:4:48:ASN:HD21	1.30	0.76
5:E:214:THR:HG21	37:E:8401:HOH:O	1.84	0.76
12:L:74:VAL:HG11	12:L:113:ILE:HG12	1.66	0.76
11:K:107:ASN:ND2	11:K:109:TYR:H	1.82	0.76
1:A:183:A:H5'	14:N:157:LEU:HD12	1.67	0.76
1:A:1205:U:H2'	1:A:1206:U:H5'	1.66	0.76
1:A:2426:G:H1'	37:A:6067:HOH:O	1.83	0.76
24:X:4:LEU:HD22	24:X:52:VAL:HG21	1.67	0.76
1:A:1603:A:H5'	1:A:1605:G:O4'	1.85	0.76
3:C:36:ASP:OD2	3:C:85:ASP:HB2	1.84	0.76
26:Z:186:ARG:HG2	26:Z:186:ARG:HH11	1.49	0.76
1:A:1701:A:H5'	37:A:6257:HOH:O	1.86	0.76
2:B:3025:G:H3'	2:B:3026:C:C5'	2.16	0.76
30:4:60:LYS:HG3	30:4:61:PRO:HD2	1.68	0.76
10:J:47:GLU:HB3	10:J:133:ILE:HD13	1.66	0.76
30:4:70:ARG:HD3	37:4:8539:HOH:O	1.84	0.76
1:A:871:G:H5'	1:A:871:G:H8	1.47	0.76
10:J:142:VAL:HG13	37:J:8380:HOH:O	1.85	0.76
14:N:104:ARG:O	14:N:108:LYS:HE2	1.86	0.76
37:A:6269:HOH:O	6:F:99:ASP:HA	1.85	0.76
17:Q:59:ARG:NH2	17:Q:66:GLN:HE22	1.83	0.76
37:A:7557:HOH:O	27:1:31:ILE:HG13	1.85	0.75
2:B:3014:G:H5'	2:B:3014:G:H8	1.51	0.75
2:B:3025:G:H3'	2:B:3026:C:H5'	1.67	0.75
1:A:289:G:H22	1:A:363:A:H2	1.35	0.75
1:A:541:C:C2'	1:A:542:A:H5"	2.16	0.75
3:C:55:VAL:HG22	3:C:68:ILE:O	1.86	0.75
11:K:76:ASP:HA	37:K:5907:HOH:O	1.86	0.75
19:S:99:ALA:HB1	19:S:109:MET:CE	2.17	0.75
1:A:2710:U:H1'	37:A:7599:HOH:O	1.86	0.75
5:E:104:ASP:HA	5:E:107:ARG:HH12	1.50	0.75
24:X:13:MET:HE3	24:X:17:ILE:HG22	1.69	0.75
1:A:1244:U:OP1	11:K:18:ILE:HD13	1.86	0.75
6:F:64:ARG:HG2	6:F:67:ASP:HB3	1.68	0.75
24:X:21:LEU:HD13	24:X:26:ILE:HD11	1.69	0.75
7:G:166:VAL:HG12	37:G:3134:HOH:O	1.86	0.75
10:J:26:LYS:HG2	10:J:28:ILE:H	1.51	0.74
1:A:21:G:C5'	19:S:2:ILE:HA	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2890:A:H1'	22:V:56:ARG:NH2	2.02	0.74
13:M:148:GLU:HA	37:M:8569:HOH:O	1.86	0.74
15:O:48:VAL:CG1	15:O:55:ASP:HB3	2.16	0.74
30:4:62:THR:HB	37:4:8549:HOH:O	1.87	0.74
1:A:2586:U:H3	1:A:2592:G:H22	1.32	0.74
14:N:152:ARG:HG3	37:N:8557:HOH:O	1.87	0.74
1:A:396:U:H1'	37:A:7606:HOH:O	1.87	0.74
5:E:115:LEU:HD21	5:E:243:VAL:HG13	1.70	0.74
1:A:1130:U:H5'	37:A:7650:HOH:O	1.86	0.74
3:C:199:HIS:HD2	3:C:201:PHE:H	1.36	0.74
5:E:140:VAL:HB	37:E:8448:HOH:O	1.87	0.74
15:O:164:ASP:CG	15:O:167:ASP:HA	2.08	0.74
24:X:21:LEU:HD21	24:X:48:VAL:HG11	1.69	0.74
1:A:871:G:C8	1:A:871:G:C5'	2.71	0.74
1:A:1164:U:H3	1:A:1192:A:H2	1.33	0.74
1:A:2637:A:H5'	37:A:9262:HOH:O	1.88	0.74
2:B:3024:U:O2'	2:B:3025:G:H4'	1.87	0.74
24:X:88:THR:HG23	24:X:110:GLN:NE2	2.03	0.74
5:E:1:MET:HG2	5:E:2:GLN:H	1.53	0.74
13:M:67:ARG:O	13:M:71:GLU:HG3	1.87	0.73
1:A:2533:C:H6	1:A:2533:C:H5'	1.53	0.73
2:B:3006:C:OP1	15:O:37:ARG:NH1	2.22	0.73
7:G:20:ILE:HD11	7:G:40:VAL:HG11	1.71	0.73
19:S:39:THR:HB	19:S:42:GLU:HG3	1.70	0.73
20:T:57:THR:HG22	20:T:59:ASP:N	2.01	0.73
29:3:41:HIS:N	29:3:45:ASN:HD22	1.86	0.73
1:A:545:G:H5'	1:A:545:G:C8	2.20	0.73
3:C:69:LEU:HD21	3:C:120:ARG:HB3	1.68	0.73
12:L:62:PRO:HG3	12:L:65:ARG:HH21	1.53	0.73
1:A:284:C:H4'	1:A:285:A:O5'	1.86	0.73
5:E:142:ASP:OD1	5:E:237:GLU:HB3	1.89	0.73
5:E:242:GLU:HG3	37:E:8382:HOH:O	1.87	0.73
11:K:74:ARG:HB3	11:K:74:ARG:HH11	1.52	0.73
1:A:1160:G:H5'	1:A:1161:A:C5'	2.16	0.73
5:E:236:THR:HG21	37:E:8374:HOH:O	1.88	0.73
24:X:68:THR:HG23	24:X:69:ARG:HG2	1.70	0.73
24:X:72:PRO:HG2	24:X:77:ALA:HB3	1.70	0.73
1:A:536:A:H3'	37:A:5016:HOH:O	1.89	0.73
1:A:1118:A:C8	1:A:1118:A:H3'	2.23	0.73
10:J:55:GLN:NE2	10:J:124:ARG:HE	1.86	0.73
10:J:150:LYS:HB2	10:J:157:ILE:HD12	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:U:HO2'	1:A:1189:A:H2	1.35	0.72
1:A:2812:A:N7	37:A:7491:HOH:O	2.22	0.72
2:B:3023:U:H6	2:B:3023:U:H5"	1.52	0.72
1:A:877:G:H5'	1:A:878:G:OP1	1.89	0.72
1:A:1666:C:O2'	1:A:1667:A:H5"	1.90	0.72
12:L:34:VAL:HG22	12:L:47:ALA:HB2	1.71	0.72
14:N:164:THR:HG22	14:N:167:GLY:N	2.01	0.72
27:1:37:HIS:HB2	27:1:47:LEU:HB2	1.71	0.72
1:A:1450:C:H4'	1:A:1451:C:OP2	1.89	0.72
1:A:470:U:O2'	28:2:16:HIS:CD2	2.41	0.72
4:D:62:ARG:CA	4:D:65:MET:HE3	2.19	0.72
1:A:450:C:OP1	5:E:184:ARG:NH2	2.21	0.72
9:I:12:ILE:N	9:I:13:PRO:HD3	2.05	0.72
1:A:299:U:H5'	37:A:7308:HOH:O	1.88	0.72
1:A:1080:C:H4'	1:A:1081:A:OP1	1.89	0.72
4:D:62:ARG:HA	4:D:65:MET:CE	2.18	0.72
3:C:153:ARG:HB2	3:C:153:ARG:HH11	1.53	0.72
10:J:33:MET:HB2	10:J:83:PHE:HB3	1.72	0.72
14:N:139:PRO:O	14:N:140:ALA:HB3	1.90	0.72
22:V:14:GLU:O	22:V:17:THR:HB	1.89	0.72
1:A:272:A:H3'	37:A:7504:HOH:O	1.89	0.71
1:A:282:C:H1'	1:A:368:C:N4	2.04	0.71
4:D:190:MET:HE2	4:D:194:PHE:CD1	2.25	0.71
14:N:34:GLU:HB3	14:N:35:PRO:HD2	1.71	0.71
19:S:106:GLY:HA2	19:S:109:MET:HE3	1.72	0.71
24:X:122:ARG:HG2	24:X:122:ARG:HH11	1.54	0.71
2:B:3056:A:C2'	2:B:3057:A:H5"	2.20	0.71
1:A:506:G:H22	1:A:509:A:H5'	1.53	0.71
13:M:53:ARG:HH22	13:M:57:VAL:HG12	1.54	0.71
3:C:131:HIS:O	3:C:132:ASP:HB2	1.90	0.71
1:A:1351:G:OP1	5:E:96:LYS:NZ	2.23	0.71
2:B:3029:C:H2'	2:B:3030:C:H5'	1.72	0.71
20:T:43:GLU:HB3	37:T:8344:HOH:O	1.89	0.71
8:H:63:ILE:HB	8:H:64:PRO:HD3	1.72	0.71
1:A:182:G:H5'	37:A:5123:HOH:O	1.91	0.71
11:K:107:ASN:HD21	11:K:109:TYR:HB2	1.56	0.71
5:E:180:SER:HB2	37:E:8442:HOH:O	1.91	0.71
23:W:39:ALA:N	23:W:40:PRO:HD2	2.06	0.71
37:A:9678:HOH:O	4:D:254:GLN:HG3	1.90	0.71
26:Z:216:ARG:HD3	37:Z:8571:HOH:O	1.90	0.71
1:A:2780:C:H1'	7:G:143:GLN:HE21	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:39:THR:HG22	19:S:42:GLU:H	1.56	0.71
21:U:61:GLU:HG3	37:U:3851:HOH:O	1.90	0.71
26:Z:155:ARG:NH1	37:Z:8558:HOH:O	2.24	0.71
1:A:259:G:H21	14:N:58:GLN:NE2	1.89	0.70
1:A:1003:U:HO2'	10:J:90:PHE:HE1	1.37	0.70
5:E:139:VAL:HG13	37:E:8445:HOH:O	1.91	0.70
1:A:1666:C:H2'	1:A:1667:A:H5'	1.73	0.70
1:A:2054:A:N3	19:S:128:ARG:NH2	2.39	0.70
1:A:2346:C:O2'	6:F:52:THR:HG21	1.92	0.70
10:J:130:HIS:CD2	10:J:133:ILE:HD11	2.26	0.70
1:A:2768:A:H2'	1:A:2769:C:O4'	1.90	0.70
3:C:199:HIS:CD2	3:C:201:PHE:H	2.09	0.70
10:J:46:VAL:HG12	10:J:146:TRP:HZ3	1.56	0.70
6:F:69:ILE:HG22	6:F:69:ILE:O	1.91	0.70
11:K:103:VAL:HG12	37:K:5907:HOH:O	1.92	0.70
3:C:170:VAL:HG22	27:1:22:ILE:HG23	1.73	0.70
10:J:26:LYS:HD2	10:J:28:ILE:CD1	2.20	0.70
13:M:143:THR:HG22	13:M:144:ASP:N	2.05	0.70
1:A:1120:U:C6	1:A:1120:U:H5"	2.27	0.70
1:A:1191:A:H3'	1:A:1192:A:H5"	1.73	0.70
10:J:14:TYR:H	10:J:91:HIS:CE1	2.08	0.70
29:3:41:HIS:H	29:3:45:ASN:ND2	1.90	0.70
1:A:2291:A:C8	1:A:2309:C:H5'	2.26	0.70
4:D:36:PRO:HA	4:D:168:GLY:HA3	1.74	0.70
25:Y:76:ARG:HH11	25:Y:76:ARG:HG3	1.56	0.70
1:A:1835:U:C5	1:A:1840:A:N7	2.57	0.70
4:D:258:GLY:H	4:D:260:HIS:CE1	2.09	0.70
10:J:139:ASP:H	10:J:140:PRO:HD3	1.56	0.70
15:O:164:ASP:OD2	15:O:167:ASP:HA	1.91	0.70
1:A:417:G:P	37:A:7390:HOH:O	2.49	0.70
6:F:146:LYS:NZ	15:O:107:ASN:HD21	1.90	0.70
10:J:69:ASN:O	10:J:72:VAL:HG12	1.92	0.70
16:P:47:ARG:HH11	16:P:47:ARG:HG3	1.57	0.70
1:A:1118:A:H3'	1:A:1118:A:H8	1.56	0.70
1:A:1684:A:H1'	29:3:43:ARG:HH22	1.55	0.69
7:G:101:GLU:HB2	7:G:116:THR:O	1.92	0.69
12:L:81:ARG:HD3	12:L:87:ARG:HH12	1.56	0.69
1:A:603:A:H5"	1:A:604:G:OP1	1.91	0.69
26:Z:187:VAL:HG23	26:Z:192:ASP:CB	2.22	0.69
1:A:111:C:O2'	28:2:20:ARG:HG2	1.92	0.69
6:F:19:GLU:O	6:F:20:LYS:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:88:LEU:HB2	6:F:89:PRO:HD3	1.75	0.69
10:J:41:THR:HA	37:J:8394:HOH:O	1.91	0.69
30:4:73:GLU:HB3	37:4:8559:HOH:O	1.92	0.69
37:A:3759:HOH:O	14:N:189:VAL:HG21	1.92	0.69
37:A:4357:HOH:O	14:N:84:LYS:HE2	1.92	0.69
10:J:137:ASN:O	10:J:139:ASP:N	2.25	0.69
1:A:236:A:H4'	1:A:237:G:H5'	1.75	0.69
1:A:2420:G:O2'	1:A:2421:G:H5'	1.92	0.69
37:A:4160:HOH:O	26:Z:186:ARG:HD2	1.91	0.69
5:E:115:LEU:O	5:E:118:THR:HB	1.91	0.69
21:U:9:LYS:HB2	37:U:7242:HOH:O	1.91	0.69
25:Y:66:THR:HG23	25:Y:67:PRO:HD2	1.75	0.69
1:A:214:U:H5'	37:A:6115:HOH:O	1.91	0.69
10:J:162:SER:CB	10:J:163:PRO:HD3	2.21	0.69
14:N:60:ILE:C	14:N:61:ILE:HD12	2.13	0.69
21:U:32:ARG:NH1	21:U:38:ARG:HH12	1.91	0.69
23:W:49:LEU:O	23:W:53:ILE:HG13	1.92	0.69
1:A:281:U:H2'	1:A:282:C:O4'	1.92	0.69
1:A:1170:U:O2'	1:A:1172:G:N7	2.24	0.69
3:C:191:GLY:HA2	3:C:194:MET:CE	2.23	0.69
29:3:39:ARG:HG2	37:3:3143:HOH:O	1.91	0.69
6:F:54:ALA:HB2	6:F:69:ILE:HD12	1.74	0.69
1:A:1634:G:H3'	37:A:3868:HOH:O	1.93	0.68
1:A:2908:A:H2'	1:A:2909:G:O4'	1.93	0.68
3:C:37:VAL:HG22	37:C:8596:HOH:O	1.93	0.68
10:J:28:ILE:HA	10:J:62:GLU:OE1	1.94	0.68
12:L:62:PRO:HG3	12:L:65:ARG:NH2	2.08	0.68
1:A:1119:G:H22	1:A:1246:A:H2	1.35	0.68
14:N:186:SER:O	14:N:189:VAL:HG12	1.93	0.68
8:H:50:VAL:HG13	8:H:60:VAL:HG11	1.74	0.68
30:4:25:VAL:HG22	30:4:68:LYS:HG3	1.75	0.68
1:A:544:G:H2'	1:A:545:G:H5"	1.73	0.68
19:S:18:LEU:HD12	19:S:143:VAL:HG11	1.75	0.68
4:D:156:LYS:HE3	37:D:8631:HOH:O	1.93	0.68
14:N:164:THR:HG23	14:N:165:SER:N	2.08	0.68
19:S:18:LEU:HB2	19:S:143:VAL:HG12	1.74	0.68
19:S:33:ARG:NH1	37:S:8543:HOH:O	2.24	0.68
4:D:71:VAL:HG11	4:D:296:LEU:HB3	1.75	0.68
4:D:162:MET:HE3	4:D:308:LEU:HD21	1.76	0.68
8:H:50:VAL:HG21	8:H:63:ILE:HG21	1.75	0.68
8:H:99:THR:HA	37:H:3461:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:166:ASN:N	10:J:166:ASN:HD22	1.91	0.68
14:N:139:PRO:O	14:N:140:ALA:CB	2.42	0.68
14:N:138:HIS:ND1	14:N:139:PRO:O	2.19	0.68
1:A:542:A:H5'	1:A:542:A:C8	2.21	0.67
1:A:2779:G:H21	7:G:143:GLN:NE2	1.92	0.67
37:A:4511:HOH:O	10:J:151:MET:HE2	1.94	0.67
24:X:88:THR:HG23	24:X:110:GLN:HE21	1.58	0.67
4:D:7:ARG:NH1	4:D:11:LEU:HD22	2.10	0.67
10:J:59:ASN:H	10:J:59:ASN:ND2	1.89	0.67
26:Z:189:ASN:HA	26:Z:217:ILE:HD11	1.74	0.67
1:A:1328:A:OP1	26:Z:169:ARG:HD2	1.94	0.67
1:A:1679:C:H5'	37:A:9309:HOH:O	1.94	0.67
4:D:51:VAL:CG2	4:D:327:VAL:HG13	2.24	0.67
10:J:3:GLY:HA2	10:J:57:ARG:HH12	1.57	0.67
12:L:10:GLN:H	12:L:10:GLN:HE21	0.77	0.67
21:U:9:LYS:HE3	21:U:13:ARG:HH11	1.59	0.67
1:A:20:G:H21	19:S:117:HIS:HD2	1.43	0.67
24:X:65:VAL:HA	24:X:68:THR:HG22	1.76	0.67
30:4:65:THR:HG23	30:4:67:LEU:HG	1.75	0.67
7:G:11:VAL:HG12	7:G:12:ASP:N	2.08	0.67
10:J:56:ILE:HG22	10:J:61:LEU:HD22	1.75	0.67
19:S:39:THR:HG23	19:S:107:GLU:O	1.95	0.67
1:A:2756:U:H3	1:A:2896:A:H2	1.40	0.67
5:E:236:THR:H	5:E:239:ALA:HB3	1.60	0.67
8:H:39:SER:HB3	8:H:45:ALA:HB2	1.76	0.67
12:L:22:ASP:HB2	37:L:5264:HOH:O	1.94	0.67
15:O:183:ASP:OD2	15:O:186:LEU:HD12	1.93	0.67
28:2:28:HIS:CE1	28:2:31:LYS:HE2	2.30	0.67
2:B:3006:C:C5'	15:O:37:ARG:NH1	2.56	0.67
14:N:114:VAL:HG21	14:N:159:THR:HG21	1.74	0.67
1:A:541:C:H2'	1:A:542:A:C5'	2.24	0.67
27:1:62:TYR:CE2	27:1:64:ILE:HG23	2.30	0.67
1:A:1119:G:N2	1:A:1246:A:C2	2.60	0.67
1:A:1234:U:N3	4:D:244:PRO:HB3	2.10	0.67
14:N:35:PRO:O	37:N:8537:HOH:O	2.12	0.67
20:T:51:GLN:HE21	20:T:53:ASN:HD21	1.42	0.67
23:W:12:THR:CG2	23:W:15:GLU:HG3	2.22	0.67
28:2:21:ARG:HD2	28:2:37:CYS:SG	2.35	0.67
1:A:1058:A:H2'	1:A:1060:C:H5"	1.76	0.66
1:A:1173:A:H2'	37:A:4315:HOH:O	1.94	0.66
6:F:57:THR:HG23	6:F:63:ILE:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:93:ARG:HB3	11:K:93:ARG:HH11	1.58	0.66
1:A:657:G:OP1	5:E:27:ARG:NH2	2.24	0.66
6:F:97:GLN:HG2	6:F:97:GLN:O	1.95	0.66
10:J:46:VAL:O	10:J:146:TRP:HH2	1.79	0.66
15:O:12:ARG:HD3	15:O:18:THR:OG1	1.95	0.66
1:A:282:C:O2'	1:A:283:U:H5'	1.95	0.66
1:A:1594:C:OP2	17:Q:120:ARG:HD2	1.96	0.66
1:A:1771:U:H4'	27:1:20:LEU:HD21	1.77	0.66
37:A:3959:HOH:O	21:U:82:THR:HA	1.96	0.66
4:D:74:ILE:HD13	4:D:309:VAL:HG21	1.78	0.66
4:D:141:ARG:HD2	4:D:163:GLU:OE2	1.96	0.66
11:K:99:GLU:HA	37:K:7377:HOH:O	1.96	0.66
13:M:133:VAL:HB	37:M:8554:HOH:O	1.94	0.66
1:A:1441:G:O2'	1:A:1442:A:H5'	1.95	0.66
4:D:30:PRO:HB2	4:D:39:GLN:NE2	2.11	0.66
4:D:36:PRO:HA	4:D:168:GLY:CA	2.26	0.66
4:D:204:GLY:HA3	37:D:8654:HOH:O	1.96	0.66
7:G:23:GLU:HG2	7:G:28:SER:HB3	1.78	0.66
8:H:53:ASP:OD1	8:H:80:GLN:HB2	1.96	0.66
12:L:82:ARG:NH2	12:L:115:ARG:HG2	2.10	0.66
25:Y:72:VAL:HG22	25:Y:85:VAL:HG12	1.76	0.66
1:A:2840:A:OP1	4:D:211:THR:HG23	1.95	0.66
25:Y:9:VAL:HG13	25:Y:88:GLU:OE2	1.96	0.66
1:A:2578:G:H5'	1:A:2578:G:H8	1.60	0.65
10:J:136:VAL:HG22	10:J:137:ASN:O	1.96	0.65
1:A:338:C:H5"	37:E:8417:HOH:O	1.95	0.65
1:A:1329:A:H2	37:A:4652:HOH:O	1.78	0.65
2:B:3014:G:H5'	2:B:3014:G:C8	2.30	0.65
6:F:41:LEU:HA	6:F:44:ILE:HG22	1.78	0.65
6:F:174:VAL:HG13	37:F:6555:HOH:O	1.94	0.65
1:A:1130:U:H2'	1:A:1131:G:O4'	1.96	0.65
3:C:192:VAL:HB	37:C:8593:HOH:O	1.97	0.65
1:A:396:U:O2'	1:A:418:C:H4'	1.96	0.65
1:A:1377:C:H6	1:A:1377:C:H5'	1.62	0.65
1:A:2064:U:H4'	1:A:2653:A:OP1	1.96	0.65
3:C:53:ALA:HB3	37:C:8606:HOH:O	1.96	0.65
3:C:190:ARG:NH2	3:C:207:GLN:OE1	2.28	0.65
6:F:37:ALA:O	6:F:40:ILE:HG12	1.97	0.65
10:J:44:ALA:HA	10:J:163:PRO:O	1.96	0.65
14:N:87:MET:HB3	30:4:46:ILE:HG21	1.76	0.65
26:Z:187:VAL:HG23	26:Z:192:ASP:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:A:H2'	1:A:286:U:O4'	1.97	0.65
3:C:33:GLU:O	3:C:34:ASP:HB2	1.96	0.65
1:A:1185:U:H2'	1:A:1186:C:C6	2.31	0.65
1:A:2414:A:H2'	1:A:2415:A:C8	2.31	0.65
37:B:8522:HOH:O	15:O:107:ASN:HB3	1.97	0.65
11:K:19:MET:HE3	11:K:132:LEU:HD11	1.79	0.65
17:Q:13:VAL:HG21	17:Q:41:ARG:HG2	1.78	0.65
21:U:53:GLY:HA3	37:U:6384:HOH:O	1.96	0.65
37:A:4491:HOH:O	14:N:94:LYS:HE3	1.97	0.65
7:G:132:THR:HB	37:G:2227:HOH:O	1.95	0.65
1:A:1209:C:H2'	1:A:1210:G:H8	1.60	0.65
1:A:2548:C:OP2	4:D:5:ARG:NH2	2.30	0.65
37:A:7377:HOH:O	21:U:2:LYS:HE2	1.96	0.65
3:C:88:ILE:HG22	3:C:88:ILE:O	1.95	0.65
14:N:87:MET:HB2	14:N:91:ILE:HD11	1.79	0.65
1:A:338:C:H4'	5:E:174:ILE:CD1	2.26	0.65
37:A:6470:HOH:O	26:Z:141:THR:HG23	1.96	0.65
5:E:219:ASN:O	5:E:222:ASP:OD1	2.15	0.65
6:F:64:ARG:CG	6:F:67:ASP:HB3	2.26	0.65
10:J:71:TYR:C	10:J:73:GLN:H	2.00	0.65
14:N:80:GLY:O	14:N:81:ARG:HD3	1.97	0.65
22:V:14:GLU:OE1	22:V:15:PRO:HD2	1.97	0.65
1:A:1819:G:H2'	1:A:1820:G:H4'	1.78	0.65
1:A:2241:C:O2'	1:A:2242:U:H5'	1.97	0.65
13:M:53:ARG:NH2	13:M:57:VAL:CG1	2.60	0.65
4:D:307:ARG:HH11	4:D:307:ARG:HB2	1.61	0.64
5:E:12:THR:HB	37:E:8438:HOH:O	1.96	0.64
15:O:159:TYR:HB3	15:O:162:ASP:HB2	1.79	0.64
1:A:506:G:H22	1:A:509:A:H5"	1.62	0.64
3:C:170:VAL:HG13	27:1:22:ILE:HG21	1.80	0.64
11:K:45:VAL:HG23	11:K:130:VAL:O	1.96	0.64
26:Z:220:GLU:HG2	37:Z:8550:HOH:O	1.97	0.64
1:A:1120:U:H5"	1:A:1120:U:H6	1.60	0.64
12:L:29:LEU:HB3	12:L:55:VAL:CG1	2.24	0.64
15:O:47:LEU:HD13	15:O:97:VAL:HG11	1.79	0.64
24:X:6:GLN:HB2	24:X:26:ILE:CD1	2.28	0.64
6:F:23:VAL:HG23	6:F:23:VAL:O	1.98	0.64
10:J:132:PHE:O	10:J:133:ILE:HD13	1.97	0.64
11:K:131:THR:HG22	11:K:134:GLU:H	1.62	0.64
16:P:14:LEU:HD23	16:P:102:ILE:HD11	1.78	0.64
1:A:57:C:H5"	37:A:6729:HOH:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2004:U:H4'	37:A:5275:HOH:O	1.97	0.64
1:A:2505:G:O2'	1:A:2506:A:H5'	1.98	0.64
2:B:3092:G:H2'	2:B:3093:A:C8	2.32	0.64
5:E:104:ASP:HA	5:E:107:ARG:NH1	2.12	0.64
17:Q:105:LEU:HD21	17:Q:137:LEU:HD21	1.80	0.64
24:X:4:LEU:HD22	24:X:52:VAL:CG2	2.27	0.64
1:A:1741:U:H5'	1:A:1742:A:OP1	1.97	0.64
37:A:7427:HOH:O	4:D:211:THR:HG21	1.97	0.64
5:E:246:ARG:HB3	5:E:246:ARG:NH1	2.12	0.64
6:F:135:VAL:HG21	6:F:139:TYR:CD1	2.33	0.64
17:Q:10:ALA:HA	17:Q:13:VAL:HG12	1.80	0.64
26:Z:185:VAL:HG12	37:Z:8572:HOH:O	1.97	0.64
3:C:105:VAL:HG11	3:C:154:ALA:HB1	1.80	0.64
3:C:191:GLY:HA2	3:C:194:MET:HE3	1.79	0.64
24:X:88:THR:CG2	24:X:89:ASP:H	2.05	0.64
1:A:1641:A:H2'	1:A:1642:A:H5'	1.79	0.64
6:F:99:ASP:HB2	6:F:103:ASN:HB2	1.80	0.64
16:P:38:ARG:NH1	37:P:7674:HOH:O	2.29	0.64
1:A:31:C:H4'	37:U:7242:HOH:O	1.98	0.64
1:A:1406:A:N1	37:A:6009:HOH:O	2.30	0.64
1:A:2878:U:H2'	1:A:2879:A:O4'	1.98	0.64
6:F:38:GLU:HB3	6:F:49:PRO:HG2	1.80	0.64
10:J:27:LYS:N	10:J:58:HIS:HD2	1.94	0.64
10:J:136:VAL:HG23	37:J:8345:HOH:O	1.98	0.64
1:A:2415:A:C2	15:O:25:ARG:HB3	2.33	0.64
6:F:54:ALA:CB	6:F:69:ILE:HD12	2.27	0.64
6:F:105:SER:CB	6:F:131:THR:HG23	2.28	0.64
24:X:137:GLN:HE21	24:X:141:HIS:CE1	2.15	0.64
3:C:105:VAL:CG1	3:C:154:ALA:HB1	2.28	0.63
6:F:135:VAL:HG22	6:F:136:ARG:H	1.62	0.63
7:G:3:VAL:HG22	7:G:49:ILE:HB	1.80	0.63
10:J:144:GLU:OE1	10:J:144:GLU:HA	1.98	0.63
14:N:106:ASN:ND2	34:N:8518:CL:CL	2.68	0.63
1:A:2419:U:H5"	1:A:2420:G:H5'	1.79	0.63
16:P:87:THR:O	16:P:91:GLN:HG3	1.99	0.63
24:X:21:LEU:HD21	24:X:48:VAL:CG1	2.28	0.63
6:F:25:MET:CE	6:F:37:ALA:HB1	2.27	0.63
6:F:136:ARG:HD2	6:F:155:HIS:O	1.97	0.63
7:G:7:ILE:HD11	7:G:11:VAL:C	2.19	0.63
10:J:3:GLY:HA2	10:J:57:ARG:NH1	2.13	0.63
10:J:85:ILE:HB	10:J:132:PHE:CE2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:9:LYS:CE	21:U:13:ARG:NH1	2.61	0.63
1:A:1187:U:O2'	1:A:1189:A:H2	1.81	0.63
8:H:50:VAL:CG1	8:H:60:VAL:HG11	2.29	0.63
1:A:119:A:H2'	1:A:120:A:H5"	1.80	0.63
1:A:200:U:H2'	37:A:3424:HOH:O	1.99	0.63
7:G:31:ARG:NH1	37:G:5919:HOH:O	2.32	0.63
1:A:558:C:C2'	1:A:559:U:H5"	2.29	0.63
1:A:2081:A:H4'	11:K:69:TYR:CE1	2.34	0.63
6:F:95:THR:O	6:F:97:GLN:N	2.28	0.63
8:H:2:VAL:HG22	8:H:57:GLU:OE1	1.98	0.63
14:N:87:MET:CB	30:4:46:ILE:HD13	2.29	0.63
14:N:87:MET:CG	30:4:46:ILE:HG21	2.28	0.63
21:U:69:LYS:O	21:U:71:VAL:HG23	1.99	0.63
28:2:8:GLN:HE22	28:2:11:LYS:NZ	1.97	0.63
1:A:1119:G:H8	11:K:52:GLN:HE22	1.45	0.63
1:A:1162:G:H2'	37:A:6558:HOH:O	1.99	0.63
22:V:9:CYS:HA	22:V:52:THR:HG23	1.81	0.63
24:X:13:MET:CE	24:X:17:ILE:HG22	2.28	0.63
23:W:44:GLY:O	23:W:48:GLU:HG2	1.99	0.63
37:A:3818:HOH:O	10:J:11:LYS:HE2	1.98	0.63
2:B:3023:U:H5"	2:B:3023:U:C6	2.34	0.63
3:C:96:LEU:HD22	3:C:128:LEU:HD13	1.79	0.63
15:O:71:TRP:CE3	15:O:175:LEU:HD22	2.34	0.63
1:A:1205:U:H2'	1:A:1206:U:C5'	2.28	0.62
8:H:58:GLU:OE1	14:N:27:ARG:NH2	2.27	0.62
10:J:53:PRO:HG3	10:J:127:GLY:H	1.64	0.62
29:3:22:PRO:HG2	29:3:25:VAL:HG23	1.81	0.62
1:A:516:A:OP2	37:A:5619:HOH:O	2.16	0.62
1:A:2827:A:H2'	1:A:2828:G:O4'	1.98	0.62
26:Z:112:GLU:CD	26:Z:115:ARG:NH1	2.53	0.62
1:A:182:G:O3'	14:N:157:LEU:HD13	1.99	0.62
1:A:1701:A:H4'	1:A:1702:U:C5'	2.29	0.62
24:X:21:LEU:HD22	24:X:26:ILE:CD1	2.30	0.62
1:A:2270:G:H4'	3:C:223:ARG:HH12	1.64	0.62
3:C:210:GLY:HA3	37:C:8587:HOH:O	1.97	0.62
4:D:145:HIS:HD2	4:D:146:THR:O	1.80	0.62
1:A:1333:U:H2'	1:A:1334:C:C6	2.34	0.62
1:A:1505:U:H6	1:A:1505:U:H5'	1.63	0.62
1:A:2073:G:OP2	1:A:2490:A:H5'	1.99	0.62
1:A:2456:A:H5'	37:A:5669:HOH:O	1.99	0.62
10:J:150:LYS:NZ	37:J:8378:HOH:O	2.27	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:178:HIS:CG	26:Z:179:PRO:HD2	2.35	0.62
6:F:93:LEU:HG	37:F:3862:HOH:O	2.00	0.62
16:P:32:ARG:O	16:P:32:ARG:HD3	1.99	0.62
6:F:99:ASP:CB	6:F:103:ASN:H	2.13	0.62
10:J:65:ARG:HB3	37:J:8384:HOH:O	1.99	0.62
5:E:77:ALA:O	5:E:78:ARG:HG3	2.00	0.62
20:T:81:ILE:HG12	37:T:8336:HOH:O	1.98	0.62
24:X:13:MET:HE1	24:X:18:GLN:HA	1.81	0.62
1:A:681:G:H5'	1:A:681:G:N3	2.15	0.61
1:A:902:G:N7	13:M:18:HIS:HD2	1.98	0.61
1:A:2630:G:O6	3:C:206:ARG:NH2	2.33	0.61
26:Z:165:GLU:HB3	37:Z:8595:HOH:O	1.98	0.61
37:A:9206:HOH:O	3:C:11:ARG:HD3	2.00	0.61
4:D:82:VAL:O	4:D:82:VAL:HG12	1.99	0.61
10:J:49:VAL:O	10:J:157:ILE:HG23	2.00	0.61
15:O:11:ARG:HG3	15:O:14:ARG:NH1	2.15	0.61
15:O:154:LEU:O	15:O:155:GLU:HB3	2.00	0.61
26:Z:235:GLU:H	26:Z:235:GLU:CD	2.02	0.61
1:A:121:U:OP2	29:3:10:ARG:NH2	2.29	0.61
1:A:2768:A:H5"	37:A:4392:HOH:O	2.01	0.61
3:C:153:ARG:HH11	3:C:153:ARG:CB	2.12	0.61
10:J:27:LYS:H	10:J:58:HIS:CD2	2.11	0.61
17:Q:143:ALA:HA	37:Q:170:HOH:O	1.99	0.61
19:S:25:PHE:CE2	19:S:29:LYS:HE2	2.35	0.61
23:W:58:THR:O	23:W:62:GLU:HG3	2.00	0.61
1:A:407:A:H2'	1:A:408:A:C8	2.35	0.61
1:A:2638:G:H5'	37:A:4897:HOH:O	2.00	0.61
3:C:223:ARG:HG3	37:C:8602:HOH:O	2.00	0.61
7:G:7:ILE:HD11	7:G:11:VAL:O	1.99	0.61
9:I:23:ILE:O	9:I:27:ILE:HG13	2.00	0.61
27:1:29:VAL:O	27:1:33:HIS:HB2	2.00	0.61
1:A:2346:C:O5'	1:A:2346:C:H6	1.83	0.61
2:B:3042:C:H2'	37:B:8503:HOH:O	1.99	0.61
6:F:36:ASN:HA	37:F:7500:HOH:O	2.01	0.61
9:I:23:ILE:HD13	9:I:67:LEU:HD23	1.81	0.61
17:Q:71:LYS:HG3	17:Q:71:LYS:O	1.99	0.61
1:A:2718:C:H6	1:A:2718:C:H5'	1.66	0.61
9:I:12:ILE:N	9:I:13:PRO:CD	2.64	0.61
14:N:61:ILE:HD12	14:N:61:ILE:N	2.16	0.61
12:L:32:ILE:HD11	12:L:56:SER:HB3	1.83	0.61
1:A:1730:G:H5'	1:A:1731:C:C5	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2769:C:H2'	1:A:2770:G:O4'	2.00	0.61
6:F:23:VAL:HG22	6:F:73:VAL:HB	1.83	0.61
25:Y:18:ARG:NH1	37:Y:4132:HOH:O	2.29	0.61
1:A:926:A:O2'	13:M:41:HIS:HD2	1.83	0.61
1:A:1189:A:H1'	1:A:1209:C:O4'	2.01	0.61
24:X:81:ASP:OD1	24:X:92:ASP:HB2	2.00	0.61
1:A:282:C:H1'	1:A:368:C:H42	1.66	0.61
1:A:1118:A:H8	1:A:1119:G:H5"	1.65	0.61
2:B:3041:C:O4'	6:F:50:VAL:HG23	2.01	0.61
15:O:48:VAL:HG11	15:O:55:ASP:HB3	1.82	0.61
24:X:122:ARG:CZ	37:X:5817:HOH:O	2.47	0.61
1:A:553:G:P	26:Z:204:ARG:HH22	2.24	0.60
1:A:558:C:O2'	1:A:559:U:H5"	2.01	0.60
1:A:1268:C:O2'	1:A:1269:G:H5'	2.01	0.60
5:E:246:ARG:NH2	37:E:8420:HOH:O	2.34	0.60
10:J:35:ASN:ND2	10:J:80:ASN:HA	2.16	0.60
13:M:136:ALA:HB3	37:M:8570:HOH:O	1.99	0.60
22:V:37:GLU:HB3	37:V:408:HOH:O	2.01	0.60
24:X:122:ARG:NH2	37:X:4276:HOH:O	2.23	0.60
2:B:3039:U:H1'	2:B:3044:A:H61	1.64	0.60
37:B:8465:HOH:O	15:O:147:ILE:HD12	2.01	0.60
10:J:45:GLN:HE21	10:J:135:TRP:HE1	1.49	0.60
25:Y:15:ARG:HB3	25:Y:15:ARG:HH11	1.66	0.60
37:A:3658:HOH:O	14:N:79:LYS:HD3	2.00	0.60
15:O:170:GLU:O	15:O:174:GLU:HG3	2.01	0.60
1:A:1187:U:H2'	37:A:6866:HOH:O	2.01	0.60
37:A:5501:HOH:O	14:N:58:GLN:HG3	2.00	0.60
4:D:305:ASP:O	4:D:306:LYS:HB2	2.01	0.60
5:E:246:ARG:NE	37:E:8420:HOH:O	2.33	0.60
14:N:74:ARG:HH11	14:N:74:ARG:HG3	1.66	0.60
14:N:87:MET:CB	30:4:46:ILE:HG21	2.30	0.60
24:X:122:ARG:NE	37:X:5817:HOH:O	2.33	0.60
28:2:28:HIS:CD2	28:2:31:LYS:HG3	2.36	0.60
37:A:7658:HOH:O	14:N:154:ARG:HB2	2.01	0.60
6:F:35:ALA:N	37:F:5576:HOH:O	2.34	0.60
6:F:93:LEU:HB3	6:F:97:GLN:OE1	2.02	0.60
11:K:45:VAL:HG21	11:K:129:PHE:CD1	2.37	0.60
19:S:9:ASP:O	19:S:13:THR:HB	2.01	0.60
27:1:56:MET:HE2	27:1:63:LYS:HG3	1.84	0.60
1:A:2310:G:OP2	10:J:114:PRO:HD2	2.01	0.60
2:B:3001:U:O3'	2:B:3003:A:H5"	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2301:A:H5"	1:A:2302:A:H5'	1.84	0.60
1:A:2363:G:O3'	18:R:11:ARG:NH1	2.35	0.60
1:A:2821:C:H4'	4:D:116:PRO:HB3	1.83	0.60
13:M:143:THR:HG22	13:M:145:LEU:H	1.66	0.60
15:O:49:THR:CG2	15:O:56:ASP:HB2	2.30	0.60
15:O:169:PRO:O	15:O:172:PHE:HB3	2.02	0.60
24:X:21:LEU:HD22	24:X:26:ILE:HD11	1.84	0.60
1:A:344:C:H2'	1:A:345:G:O4'	2.01	0.60
37:A:9074:HOH:O	4:D:214:PRO:HD2	2.00	0.60
37:E:8357:HOH:O	16:P:3:THR:HG21	2.01	0.60
8:H:46:GLU:O	8:H:73:PRO:HD2	2.01	0.60
11:K:107:ASN:C	11:K:107:ASN:HD22	2.05	0.60
15:O:61:ALA:HB3	15:O:88:ALA:HB2	1.83	0.60
21:U:47:THR:HB	21:U:100:ASP:HB3	1.83	0.60
24:X:80:ASP:O	24:X:84:VAL:HG23	2.01	0.60
26:Z:187:VAL:HG12	26:Z:205:ILE:HA	1.83	0.60
29:3:22:PRO:HG2	29:3:25:VAL:CG2	2.31	0.60
1:A:138:U:H5"	1:A:139:C:OP2	2.02	0.60
1:A:182:G:H4'	14:N:157:LEU:HD13	1.84	0.60
1:A:1667:A:H5'	1:A:1667:A:C8	2.34	0.60
12:L:34:VAL:CG2	12:L:47:ALA:HB2	2.31	0.60
23:W:64:GLY:O	23:W:65:ASP:HB2	2.01	0.60
24:X:106:THR:OG1	24:X:109:GLU:HG3	2.02	0.60
26:Z:200:THR:HG22	26:Z:201:GLU:CG	2.31	0.60
1:A:1119:G:H2'	11:K:52:GLN:NE2	2.17	0.60
5:E:162:VAL:HG12	5:E:192:ILE:HD11	1.84	0.60
14:N:169:ARG:HD2	37:N:8589:HOH:O	2.01	0.60
17:Q:59:ARG:HH22	17:Q:66:GLN:HE22	1.50	0.60
1:A:558:C:H2'	1:A:559:U:C5'	2.32	0.59
3:C:88:ILE:HD13	3:C:100:PRO:CD	2.31	0.59
14:N:183:VAL:HG12	14:N:184:ARG:N	2.16	0.59
1:A:1440:U:OP2	37:A:4436:HOH:O	2.16	0.59
5:E:236:THR:HA	37:E:8448:HOH:O	2.02	0.59
10:J:75:SER:O	10:J:79:ALA:HB2	2.02	0.59
19:S:111:ILE:HG23	19:S:145:LEU:HD11	1.83	0.59
24:X:4:LEU:HD23	24:X:54:PHE:HB3	1.83	0.59
26:Z:115:ARG:NE	37:Z:8556:HOH:O	2.35	0.59
1:A:485:A:N3	1:A:487:G:H5"	2.17	0.59
1:A:2672:C:H1'	37:D:8635:HOH:O	2.02	0.59
6:F:44:ILE:HG12	6:F:83:PHE:HE1	1.66	0.59
10:J:139:ASP:N	10:J:140:PRO:CD	2.64	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:47:LEU:CD1	15:O:97:VAL:HG11	2.31	0.59
1:A:567:U:H5"	37:X:5817:HOH:O	2.02	0.59
1:A:2587:U:H2'	1:A:2589:U:H5"	1.85	0.59
1:A:2635:A:O2'	1:A:2636:C:H5'	2.03	0.59
4:D:179:LEU:O	4:D:183:GLU:HG2	2.03	0.59
22:V:52:THR:HG22	22:V:54:THR:N	2.17	0.59
1:A:1242:A:C5'	11:K:82:THR:HG23	2.23	0.59
1:A:1299:G:O6	13:M:6:ARG:HD3	2.02	0.59
13:M:145:LEU:O	13:M:148:GLU:HG3	2.01	0.59
14:N:30:GLU:O	14:N:34:GLU:HG3	2.03	0.59
1:A:1189:A:H1'	1:A:1209:C:C1'	2.32	0.59
1:A:1393:A:H2'	1:A:1394:C:C6	2.38	0.59
1:A:2064:U:H5'	1:A:2652:U:O3'	2.03	0.59
37:A:9382:HOH:O	14:N:94:LYS:HE2	2.02	0.59
24:X:125:HIS:CD2	24:X:127:GLY:H	2.21	0.59
1:A:870:G:C2'	1:A:871:G:H5"	2.30	0.59
1:A:2748:G:H2'	37:A:7516:HOH:O	2.02	0.59
1:A:538:C:OP2	26:Z:134:HIS:HE1	1.86	0.59
1:A:544:G:C2'	1:A:545:G:H5"	2.32	0.59
2:B:3013:A:O2'	2:B:3014:G:H5"	2.03	0.59
3:C:125:ASN:HB3	3:C:158:VAL:HG12	1.84	0.59
10:J:83:PHE:HZ	10:J:146:TRP:HE1	1.47	0.59
25:Y:43:VAL:HG12	25:Y:44:ASP:N	2.17	0.59
1:A:21:G:H5"	19:S:1:GLY:O	2.03	0.59
7:G:172:PRO:HB3	37:G:6931:HOH:O	2.03	0.59
15:O:151:ASP:O	15:O:154:LEU:HB2	2.03	0.59
27:1:30:GLU:HA	27:1:33:HIS:HB3	1.85	0.59
2:B:3049:G:H5"	37:B:8465:HOH:O	2.03	0.58
5:E:107:ARG:NH1	5:E:107:ARG:HB3	2.18	0.58
7:G:68:HIS:O	7:G:72:MET:HG3	2.03	0.58
14:N:38:VAL:C	14:N:63:VAL:HG13	2.23	0.58
15:O:24:LEU:O	15:O:28:LYS:HG2	2.02	0.58
21:U:41:ARG:HG2	21:U:41:ARG:HH11	1.67	0.58
23:W:39:ALA:C	23:W:41:GLU:H	2.06	0.58
1:A:2690:U:O2'	7:G:111:LYS:HE3	2.04	0.58
2:B:3048:C:H4'	15:O:141:ARG:HH21	1.67	0.58
4:D:185:GLY:HA2	37:D:8634:HOH:O	2.01	0.58
10:J:166:ASN:N	10:J:166:ASN:ND2	2.51	0.58
12:L:55:VAL:HG12	12:L:56:SER:N	2.18	0.58
12:L:115:ARG:HG3	12:L:116:GLU:N	2.18	0.58
27:1:28:ASP:O	27:1:31:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:G:O3'	14:N:157:LEU:CD1	2.51	0.58
1:A:1701:A:H5"	1:A:1702:U:H3'	1.85	0.58
1:A:2326:U:H4'	1:A:2412:G:H4'	1.85	0.58
5:E:107:ARG:NE	37:E:8453:HOH:O	2.25	0.58
6:F:44:ILE:HG23	6:F:45:THR:HG23	1.85	0.58
8:H:110:GLU:HG2	37:H:6926:HOH:O	2.03	0.58
11:K:19:MET:CE	11:K:132:LEU:HD11	2.34	0.58
11:K:75:PRO:HG2	11:K:105:LEU:HD21	1.85	0.58
14:N:52:LEU:HD13	14:N:116:ASN:HB3	1.85	0.58
24:X:4:LEU:O	24:X:32:CYS:HA	2.03	0.58
1:A:2851:G:O2'	1:A:2852:A:H5'	2.03	0.58
4:D:329:TYR:CE2	22:V:15:PRO:HG2	2.38	0.58
1:A:513:A:N3	37:A:3637:HOH:O	2.32	0.58
1:A:738:G:H3'	37:A:7019:HOH:O	2.03	0.58
37:B:8465:HOH:O	15:O:147:ILE:HB	2.03	0.58
4:D:162:MET:CE	4:D:308:LEU:HD21	2.33	0.58
5:E:1:MET:HG2	5:E:2:GLN:N	2.17	0.58
10:J:84:ARG:NH2	10:J:135:TRP:HH2	2.01	0.58
19:S:61:GLN:NE2	37:S:8540:HOH:O	2.35	0.58
25:Y:37:LEU:CD1	25:Y:85:VAL:HG21	2.25	0.58
3:C:36:ASP:O	3:C:38:ILE:N	2.37	0.58
3:C:101:GLU:OE2	3:C:131:HIS:HB2	2.04	0.58
4:D:41:PHE:HA	4:D:79:MET:HE2	1.84	0.58
4:D:264:GLU:HG2	4:D:267:LYS:CE	2.28	0.58
19:S:39:THR:HB	19:S:42:GLU:CG	2.32	0.58
1:A:272:A:H5'	1:A:273:G:OP2	2.03	0.58
3:C:95:PRO:HG2	3:C:98:GLU:HG2	1.86	0.58
3:C:211:LYS:HD3	37:C:8611:HOH:O	2.04	0.58
6:F:86:THR:O	6:F:90:LEU:HG	2.04	0.58
6:F:166:ILE:HD12	37:F:6326:HOH:O	2.03	0.58
4:D:221:GLN:HE22	12:L:42:ASN:HD22	1.51	0.58
7:G:23:GLU:HG2	7:G:28:SER:CB	2.34	0.58
2:B:3003:A:N6	2:B:3022:G:H1'	2.19	0.58
11:K:74:ARG:HH11	11:K:74:ARG:CB	2.16	0.58
15:O:86:LEU:HD12	15:O:125:ALA:HB2	1.86	0.58
28:2:25:LYS:HG2	28:2:25:LYS:O	2.04	0.58
1:A:1197:G:N2	37:A:6207:HOH:O	2.36	0.58
4:D:175:LEU:HD23	4:D:175:LEU:C	2.23	0.58
4:D:195:ARG:HD2	4:D:324:ASP:OD1	2.04	0.58
9:I:64:ASN:HD22	9:I:64:ASN:N	2.01	0.58
15:O:184:ILE:HG22	15:O:185:GLU:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:84:VAL:HG12	37:X:6679:HOH:O	2.03	0.58
1:A:204:A:C2'	1:A:205:U:H5'	2.33	0.57
1:A:558:C:H5'	37:A:5228:HOH:O	2.04	0.57
1:A:2320:U:H4'	1:A:2321:A:O4'	2.04	0.57
1:A:2604:A:H5'	37:A:5766:HOH:O	2.04	0.57
10:J:127:GLY:O	10:J:128:ALA:HB3	2.04	0.57
11:K:107:ASN:HD22	11:K:109:TYR:H	1.51	0.57
15:O:38:LYS:HD2	15:O:114:LYS:HE3	1.85	0.57
19:S:18:LEU:HD12	19:S:143:VAL:CG1	2.34	0.57
24:X:22:GLU:HG2	24:X:27:HIS:CD2	2.39	0.57
25:Y:41:PHE:O	25:Y:43:VAL:HG23	2.03	0.57
1:A:1787:C:OP1	17:Q:68:LYS:HE2	2.04	0.57
2:B:3044:A:O4'	6:F:76:ARG:NE	2.37	0.57
4:D:125:GLU:O	4:D:129:ARG:HG3	2.03	0.57
4:D:140:LEU:HD23	37:D:8581:HOH:O	2.04	0.57
5:E:129:HIS:CE1	5:E:231:ARG:HA	2.40	0.57
8:H:91:VAL:CG1	8:H:92:GLY:H	2.13	0.57
24:X:149:LEU:HG	24:X:153:MET:HE2	1.86	0.57
1:A:204:A:H2'	1:A:205:U:H5'	1.85	0.57
1:A:1299:G:N2	37:A:4652:HOH:O	2.36	0.57
1:A:1362:U:H5'	37:A:3248:HOH:O	2.04	0.57
1:A:1766:U:O2	1:A:1778:A:H5'	2.04	0.57
1:A:2547:C:OP2	4:D:5:ARG:NH1	2.38	0.57
2:B:3023:U:H3'	2:B:3024:U:H5"	1.86	0.57
3:C:192:VAL:CG1	3:C:207:GLN:HB3	2.33	0.57
15:O:89:GLY:O	15:O:92:ALA:HB3	2.04	0.57
15:O:157:PRO:HA	37:O:8527:HOH:O	2.04	0.57
1:A:960:G:H2'	1:A:960:G:N3	2.20	0.57
1:A:1528:A:H2'	1:A:1529:G:O4'	2.04	0.57
2:B:3039:U:H1'	2:B:3044:A:N6	2.18	0.57
3:C:94:LEU:N	3:C:94:LEU:HD23	2.20	0.57
3:C:175:LYS:HE2	37:C:8577:HOH:O	2.03	0.57
4:D:66:GLU:OE1	4:D:328:ARG:HD2	2.04	0.57
4:D:119:HIS:O	4:D:121:PRO:HD3	2.04	0.57
8:H:37:THR:O	8:H:41:GLU:HG3	2.04	0.57
8:H:58:GLU:HA	8:H:61:MET:HE2	1.86	0.57
19:S:18:LEU:HB2	19:S:143:VAL:CG1	2.34	0.57
26:Z:144:ARG:NE	37:Z:8614:HOH:O	2.36	0.57
26:Z:163:THR:HG23	37:Z:8528:HOH:O	2.05	0.57
1:A:263:U:O4'	8:H:59:ILE:HD13	2.05	0.57
11:K:80:LYS:HE2	11:K:98:PHE:CZ	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:45:PRO:HB2	37:L:7169:HOH:O	2.03	0.57
14:N:37:VAL:CG1	14:N:63:VAL:HG11	2.35	0.57
25:Y:78:GLU:CG	25:Y:79:GLU:H	2.17	0.57
26:Z:112:GLU:OE2	26:Z:115:ARG:NH1	2.36	0.57
1:A:289:G:N2	1:A:363:A:H2	1.99	0.57
1:A:1181:A:H2'	1:A:1182:C:O4'	2.04	0.57
1:A:2717:C:O2'	1:A:2718:C:H5"	2.04	0.57
10:J:48:LEU:HG	10:J:157:ILE:HG21	1.87	0.57
1:A:280:C:H2'	1:A:281:U:O4'	2.05	0.57
1:A:951:A:C2'	1:A:952:G:H5'	2.34	0.57
1:A:1753:C:O2	4:D:229:ARG:NH2	2.38	0.57
1:A:1996:U:O2'	1:A:1997:A:H5'	2.05	0.57
1:A:2768:A:O2'	1:A:2769:C:H5'	2.05	0.57
2:B:3002:U:OP2	2:B:3002:U:H4'	2.04	0.57
4:D:314:ALA:HB3	4:D:317:PRO:HG3	1.87	0.57
1:A:1168:C:H2'	1:A:1169:U:O4'	2.05	0.57
1:A:2679:G:H2'	1:A:2681:A:OP2	2.05	0.57
1:A:2795:C:O2'	1:A:2796:U:H5'	2.03	0.57
4:D:74:ILE:HG13	37:D:8606:HOH:O	2.04	0.57
7:G:84:MET:HE1	7:G:148:ILE:HD12	1.86	0.57
9:I:12:ILE:HG22	9:I:12:ILE:O	2.04	0.57
1:A:1172:G:H1'	37:A:4942:HOH:O	2.03	0.57
1:A:2300:A:H4'	1:A:2301:A:O5'	2.05	0.57
3:C:36:ASP:HA	3:C:83:GLY:HA3	1.87	0.57
5:E:107:ARG:NH2	37:E:8453:HOH:O	2.35	0.57
5:E:127:ARG:HG2	5:E:127:ARG:HH11	1.69	0.57
5:E:233:THR:HG22	5:E:234:VAL:N	2.19	0.57
7:G:31:ARG:HH12	7:G:68:HIS:CD2	2.23	0.57
13:M:143:THR:CG2	13:M:144:ASP:N	2.67	0.57
14:N:12:TRP:CE2	14:N:20:ILE:HD11	2.40	0.57
1:A:1333:U:H2'	1:A:1334:C:H6	1.69	0.56
11:K:130:VAL:HG12	11:K:131:THR:N	2.20	0.56
14:N:63:VAL:HG21	14:N:109:PHE:CE1	2.40	0.56
24:X:21:LEU:HB3	24:X:26:ILE:HG12	1.87	0.56
25:Y:30:MET:CE	25:Y:58:ALA:HB3	2.35	0.56
1:A:1159:G:H21	1:A:1189:A:H8	1.52	0.56
1:A:2533:C:H5'	1:A:2533:C:C6	2.38	0.56
1:A:2676:C:H4'	11:K:70:PHE:CE1	2.40	0.56
37:A:4804:HOH:O	11:K:47:THR:HB	2.05	0.56
2:B:3020:G:O2'	2:B:3021:G:H5'	2.05	0.56
4:D:238:ASN:HD22	4:D:240:GLY:N	1.95	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:49:ILE:HD11	7:G:69:ILE:HD12	1.85	0.56
14:N:37:VAL:HG21	14:N:108:LYS:CG	2.35	0.56
14:N:61:ILE:HG13	37:N:8621:HOH:O	2.06	0.56
14:N:113:ARG:NH2	14:N:156:ARG:HG2	2.20	0.56
16:P:14:LEU:CD2	16:P:102:ILE:HD11	2.34	0.56
19:S:119:VAL:O	19:S:119:VAL:HG12	2.04	0.56
22:V:52:THR:HG22	22:V:54:THR:H	1.70	0.56
25:Y:30:MET:HE1	25:Y:58:ALA:HB3	1.87	0.56
1:A:371:U:H2'	1:A:372:A:H8	1.70	0.56
1:A:1053:G:OP1	10:J:12:PRO:HG3	2.05	0.56
1:A:1878:G:H1'	37:A:6096:HOH:O	2.04	0.56
2:B:3030:C:OP1	6:F:137:PRO:O	2.23	0.56
8:H:21:GLU:O	8:H:24:ARG:HG3	2.05	0.56
17:Q:16:VAL:HG12	17:Q:17:GLY:N	2.20	0.56
19:S:104:PHE:HB2	19:S:109:MET:HE1	1.87	0.56
20:T:33:SER:OG	20:T:36:GLU:HG3	2.04	0.56
24:X:38:THR:HG22	37:X:3580:HOH:O	2.06	0.56
3:C:81:GLN:HB2	3:C:92:ASN:ND2	2.20	0.56
4:D:51:VAL:HG23	4:D:329:TYR:O	2.06	0.56
11:K:131:THR:HG22	11:K:133:GLY:N	2.20	0.56
11:K:133:GLY:O	11:K:137:GLU:HG3	2.05	0.56
12:L:74:VAL:CG1	12:L:113:ILE:HG12	2.33	0.56
23:W:55:ARG:O	23:W:59:ILE:HG12	2.04	0.56
1:A:1086:A:N6	24:X:11:VAL:HG11	2.21	0.56
1:A:1134:G:H4'	10:J:151:MET:CE	2.24	0.56
2:B:3076:G:C3'	2:B:3077:A:H5"	2.30	0.56
3:C:105:VAL:HG12	3:C:106:CYS:N	2.21	0.56
4:D:279:THR:OG1	4:D:290:VAL:HB	2.06	0.56
6:F:95:THR:C	6:F:97:GLN:H	2.09	0.56
8:H:107:VAL:O	8:H:111:ILE:HG13	2.04	0.56
19:S:44:VAL:O	19:S:48:GLU:HG3	2.05	0.56
24:X:129:LYS:HG2	37:X:1990:HOH:O	2.06	0.56
27:1:30:GLU:HA	27:1:33:HIS:CB	2.36	0.56
30:4:55:VAL:HB	30:4:56:PRO:HD2	1.87	0.56
1:A:317:A:H5"	21:U:52:ARG:HD2	1.86	0.56
1:A:644:G:H1'	37:A:6378:HOH:O	2.06	0.56
1:A:1213:C:O2'	1:A:1214:G:H5'	2.06	0.56
1:A:2094:G:H4'	4:D:245:SER:HB3	1.88	0.56
4:D:55:ASN:HB3	4:D:63:GLU:HA	1.87	0.56
8:H:50:VAL:CG2	8:H:63:ILE:HG21	2.34	0.56
10:J:45:GLN:HG3	10:J:135:TRP:NE1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:115:SER:N	17:Q:118:GLN:HE21	1.88	0.56
1:A:447:A:OP1	21:U:2:LYS:HG2	2.06	0.56
1:A:2434:A:O3'	30:4:28:GLY:HA3	2.06	0.56
2:B:3006:C:C5'	15:O:37:ARG:HH12	2.15	0.56
8:H:91:VAL:CG1	8:H:92:GLY:N	2.66	0.56
27:1:38:LYS:CE	27:1:45:LYS:HE2	2.22	0.56
1:A:899:C:H5'	37:A:3184:HOH:O	2.05	0.56
1:A:1086:A:C6	24:X:11:VAL:HG11	2.40	0.56
1:A:1314:U:H2'	37:A:5849:HOH:O	2.06	0.56
1:A:1667:A:H2'	1:A:1668:U:C6	2.40	0.56
1:A:1778:A:H2'	1:A:1779:A:H5'	1.88	0.56
6:F:23:VAL:HG21	6:F:45:THR:HG21	1.87	0.56
11:K:39:VAL:HG12	11:K:40:ASN:ND2	2.20	0.56
12:L:75:ARG:CZ	37:L:4172:HOH:O	2.52	0.56
26:Z:187:VAL:CG2	26:Z:192:ASP:HB2	2.35	0.56
1:A:644:G:N3	1:A:644:G:H5'	2.21	0.56
1:A:2862:G:H4'	4:D:336:GLN:O	2.05	0.56
13:M:90:ARG:NH2	13:M:121:ILE:HD11	2.20	0.56
15:O:78:MET:HB2	15:O:79:PRO:HD3	1.88	0.56
15:O:90:LEU:HB2	15:O:186:LEU:HD22	1.87	0.56
25:Y:74:ALA:CB	25:Y:85:VAL:HG22	2.36	0.56
1:A:1014:A:H2'	1:A:1015:C:H5'	1.88	0.56
1:A:1654:U:H2'	3:C:47:HIS:HD2	1.70	0.56
4:D:7:ARG:HG2	4:D:7:ARG:NH1	2.20	0.56
4:D:195:ARG:HG2	4:D:323:LEU:HD22	1.87	0.56
7:G:69:ILE:HA	7:G:72:MET:CE	2.36	0.56
13:M:77:ALA:HB3	37:M:8527:HOH:O	2.05	0.56
22:V:17:THR:HG22	22:V:18:GLY:N	2.21	0.56
24:X:139:GLY:O	24:X:141:HIS:HD2	1.89	0.56
6:F:94:ALA:HB3	6:F:174:VAL:HA	1.89	0.55
15:O:86:LEU:O	15:O:90:LEU:HG	2.06	0.55
27:1:53:GLY:HA2	27:1:67:GLY:O	2.05	0.55
1:A:797:A:C4'	27:1:10:ARG:N	2.69	0.55
1:A:1182:C:H1'	1:A:1192:A:H8	1.71	0.55
1:A:1741:U:O2'	1:A:2723:G:H4'	2.06	0.55
1:A:2638:G:H1'	37:A:7737:HOH:O	2.07	0.55
3:C:8:ARG:HG2	37:C:8550:HOH:O	2.06	0.55
3:C:94:LEU:HG	3:C:99:ILE:HD11	1.89	0.55
13:M:104:ASP:O	13:M:105:TYR:HB3	2.05	0.55
18:R:64:GLU:HG3	18:R:74:ASP:OD2	2.07	0.55
24:X:5:VAL:HG22	24:X:32:CYS:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:A:O2'	1:A:672:G:H2'	2.06	0.55
1:A:1559:A:H1'	37:A:5840:HOH:O	2.06	0.55
1:A:2837:U:H1'	4:D:307:ARG:HH12	1.71	0.55
6:F:55:LYS:HA	37:F:6752:HOH:O	2.06	0.55
7:G:15:GLN:HG2	7:G:19:ASP:O	2.06	0.55
1:A:431:G:P	14:N:48:ARG:HH12	2.28	0.55
1:A:1003:U:O2'	10:J:90:PHE:HE1	1.88	0.55
1:A:2503:A:OP1	10:J:147:ARG:NH2	2.36	0.55
2:B:3025:G:C3'	2:B:3026:C:H5'	2.33	0.55
3:C:200:PRO:HG2	3:C:225:VAL:HG21	1.89	0.55
4:D:154:VAL:HG12	4:D:156:LYS:HG2	1.87	0.55
5:E:88:SER:O	5:E:91:PRO:HD3	2.05	0.55
10:J:31:PHE:HE2	10:J:87:LYS:O	1.89	0.55
23:W:39:ALA:N	23:W:40:PRO:CD	2.69	0.55
26:Z:144:ARG:CZ	37:Z:8614:HOH:O	2.54	0.55
27:1:19:GLY:O	27:1:23:ARG:HG2	2.07	0.55
3:C:186:TRP:CG	3:C:187:PRO:HA	2.41	0.55
19:S:29:LYS:HB3	37:S:8532:HOH:O	2.06	0.55
19:S:119:VAL:HG21	19:S:142:ASP:CG	2.26	0.55
24:X:110:GLN:NE2	24:X:110:GLN:HA	2.21	0.55
1:A:65:C:O2'	1:A:66:G:H5'	2.06	0.55
1:A:1119:G:H8	11:K:52:GLN:NE2	2.03	0.55
1:A:2403:C:H3'	37:A:5181:HOH:O	2.07	0.55
7:G:6:GLU:HA	7:G:46:THR:HG22	1.89	0.55
10:J:58:HIS:HA	10:J:61:LEU:HD23	1.89	0.55
14:N:61:ILE:HA	37:N:8621:HOH:O	2.07	0.55
14:N:162:GLY:HA2	37:N:8519:HOH:O	2.06	0.55
25:Y:43:VAL:CG1	25:Y:47:ALA:HB3	2.37	0.55
25:Y:75:ALA:O	25:Y:83:ALA:HA	2.06	0.55
27:1:38:LYS:HG3	37:1:8429:HOH:O	2.06	0.55
1:A:1441:G:H1'	37:A:7743:HOH:O	2.06	0.55
1:A:1743:G:N7	37:A:9247:HOH:O	2.33	0.55
1:A:2467:A:H2'	37:A:5429:HOH:O	2.07	0.55
2:B:3078:G:N2	2:B:3103:A:OP2	2.37	0.55
5:E:16:VAL:HG12	5:E:17:ASP:N	2.21	0.55
6:F:10:PHE:CG	6:F:11:HIS:N	2.74	0.55
6:F:25:MET:CE	6:F:41:LEU:HG	2.31	0.55
7:G:31:ARG:NH1	7:G:68:HIS:CG	2.75	0.55
19:S:18:LEU:HG	19:S:91:LEU:HD13	1.89	0.55
22:V:44:ARG:HB3	37:V:3805:HOH:O	2.06	0.55
1:A:1615:A:H5'	37:A:4153:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2890:A:H1'	22:V:56:ARG:HH21	1.72	0.55
3:C:192:VAL:HG12	3:C:207:GLN:HB3	1.88	0.55
6:F:64:ARG:CD	6:F:67:ASP:HB3	2.37	0.55
24:X:31:HIS:HB3	37:X:5420:HOH:O	2.06	0.55
25:Y:78:GLU:HG2	25:Y:79:GLU:N	2.20	0.55
1:A:1940:C:H4'	37:A:7319:HOH:O	2.06	0.55
3:C:109:GLU:HG2	3:C:116:GLY:N	2.22	0.55
2:B:3055:U:H4'	2:B:3056:A:C8	2.41	0.55
3:C:66:ARG:HB2	3:C:66:ARG:HH11	1.71	0.55
5:E:237:GLU:HB2	37:E:8426:HOH:O	2.06	0.55
6:F:135:VAL:HG22	6:F:136:ARG:N	2.21	0.55
6:F:163:VAL:HA	37:F:6326:HOH:O	2.07	0.55
11:K:75:PRO:HG2	11:K:105:LEU:CD2	2.36	0.55
23:W:4:HIS:HB3	37:W:6622:HOH:O	2.06	0.55
23:W:39:ALA:O	23:W:41:GLU:N	2.40	0.55
26:Z:187:VAL:HG23	26:Z:192:ASP:HB3	1.87	0.55
1:A:69:A:H5'	1:A:69:A:C8	2.42	0.54
1:A:394:G:H1	14:N:181:GLU:CD	2.11	0.54
2:B:3025:G:N2	37:B:8510:HOH:O	2.39	0.54
6:F:154:LYS:H	6:F:154:LYS:CD	2.09	0.54
7:G:11:VAL:HG13	7:G:23:GLU:O	2.07	0.54
7:G:20:ILE:CD1	7:G:40:VAL:HG11	2.35	0.54
21:U:111:ARG:HB3	21:U:119:ALA:HB2	1.90	0.54
5:E:61:PHE:HB3	37:E:8441:HOH:O	2.07	0.54
6:F:23:VAL:HG12	6:F:130:VAL:HG22	1.89	0.54
6:F:57:THR:HG23	6:F:63:ILE:CB	2.37	0.54
10:J:139:ASP:HA	37:J:8370:HOH:O	2.07	0.54
15:O:77:ASN:OD1	15:O:80:SER:HB2	2.07	0.54
15:O:155:GLU:O	15:O:156:GLU:HG3	2.08	0.54
25:Y:25:ARG:HD2	37:Y:3861:HOH:O	2.06	0.54
25:Y:71:ARG:HD3	37:Y:2171:HOH:O	2.07	0.54
1:A:1477:C:H5'	1:A:1868:G:C5'	2.37	0.54
5:E:235:PHE:HE2	5:E:243:VAL:HG21	1.73	0.54
6:F:50:VAL:O	6:F:71:ALA:HA	2.07	0.54
13:M:57:VAL:HG12	13:M:57:VAL:O	2.07	0.54
14:N:74:ARG:HG3	14:N:74:ARG:NH1	2.22	0.54
15:O:73:ALA:N	37:O:8567:HOH:O	2.41	0.54
17:Q:103:THR:O	17:Q:107:GLU:HG3	2.07	0.54
18:R:66:LYS:HB2	18:R:70:ALA:O	2.07	0.54
1:A:281:U:O2'	1:A:282:C:H5'	2.08	0.54
5:E:46:TYR:CE2	5:E:98:ARG:NH1	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:75:SER:C	10:J:79:ALA:HB2	2.28	0.54
10:J:163:PRO:HG2	37:J:8340:HOH:O	2.07	0.54
27:1:38:LYS:CG	27:1:45:LYS:HG2	2.30	0.54
1:A:926:A:O2'	13:M:41:HIS:CD2	2.61	0.54
1:A:1209:C:H2'	1:A:1210:G:C8	2.41	0.54
1:A:2649:A:H5'	1:A:2649:A:H8	1.73	0.54
1:A:2769:C:C2'	1:A:2770:G:H5'	2.38	0.54
37:A:9878:HOH:O	11:K:46:ILE:HA	2.08	0.54
37:C:8613:HOH:O	27:1:75:ALA:HB3	2.06	0.54
5:E:76:ARG:HG2	5:E:78:ARG:HH12	1.72	0.54
5:E:214:THR:HG23	37:E:8433:HOH:O	2.08	0.54
8:H:101:ALA:HA	37:H:5413:HOH:O	2.08	0.54
20:T:56:ASN:O	29:3:8:LYS:HE2	2.08	0.54
1:A:542:A:H2'	1:A:543:G:O4'	2.07	0.54
3:C:132:ASP:OD1	3:C:133:ARG:N	2.40	0.54
25:Y:27:ASP:OD2	25:Y:27:ASP:N	2.40	0.54
26:Z:189:ASN:HD22	26:Z:189:ASN:C	2.10	0.54
27:1:11:THR:OG1	27:1:23:ARG:HB2	2.08	0.54
3:C:109:GLU:HG2	3:C:116:GLY:H	1.73	0.54
4:D:108:GLU:HB3	4:D:111:ARG:HD2	1.90	0.54
10:J:53:PRO:HA	10:J:125:VAL:O	2.08	0.54
15:O:34:LEU:HA	15:O:47:LEU:HD23	1.90	0.54
17:Q:38:GLU:HA	17:Q:41:ARG:NH1	2.23	0.54
17:Q:105:LEU:CD2	17:Q:137:LEU:HD21	2.37	0.54
19:S:106:GLY:HA2	19:S:109:MET:CE	2.37	0.54
26:Z:126:PRO:HG2	26:Z:128:PHE:CE1	2.43	0.54
1:A:56:G:H5"	23:W:50:ARG:NH1	2.23	0.54
1:A:2896:A:H5"	37:A:6074:HOH:O	2.07	0.54
3:C:76:VAL:HG23	27:1:63:LYS:HB3	1.89	0.54
3:C:121:ALA:O	3:C:124:VAL:HG22	2.08	0.54
7:G:34:TRP:O	11:K:127:ILE:HD11	2.07	0.54
10:J:150:LYS:CE	37:J:8378:HOH:O	2.56	0.54
11:K:74:ARG:O	11:K:78:ILE:HG12	2.07	0.54
13:M:12:THR:HG21	13:M:16:GLY:O	2.08	0.54
16:P:41:ALA:HA	37:P:5104:HOH:O	2.07	0.54
19:S:17:MET:HE1	19:S:19:ARG:NH2	2.22	0.54
1:A:1942:A:O2'	1:A:1943:C:H5'	2.08	0.54
1:A:2265:U:H2'	1:A:2266:A:C8	2.43	0.54
4:D:275:GLY:O	4:D:291:ASP:HA	2.08	0.54
1:A:1139:U:H2'	1:A:1140:C:C6	2.43	0.54
1:A:2783:A:H3'	37:A:5201:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:93:THR:HG23	3:C:154:ALA:O	2.08	0.54
5:E:47:GLY:HA2	5:E:92:PRO:HB2	1.89	0.54
6:F:41:LEU:HA	6:F:44:ILE:CG2	2.37	0.54
7:G:100:ASP:HB2	37:G:2789:HOH:O	2.06	0.54
10:J:75:SER:HB3	10:J:79:ALA:HB1	1.89	0.54
20:T:81:ILE:HG23	37:T:8336:HOH:O	2.08	0.54
24:X:54:PHE:CZ	24:X:140:LYS:HB2	2.42	0.54
1:A:155:C:OP2	14:N:188:ARG:HD3	2.07	0.53
1:A:941:G:O2'	1:A:942:U:H5'	2.07	0.53
1:A:2326:U:H4'	1:A:2412:G:C4'	2.38	0.53
1:A:2815:G:OP2	11:K:99:GLU:HG2	2.08	0.53
6:F:170:TYR:O	6:F:171:ASP:HB3	2.07	0.53
10:J:46:VAL:HG12	10:J:146:TRP:CZ3	2.42	0.53
10:J:117:LYS:HB2	37:J:8341:HOH:O	2.07	0.53
15:O:139:TRP:HA	15:O:139:TRP:CE3	2.42	0.53
21:U:49:GLU:OE2	21:U:97:ARG:HD2	2.07	0.53
24:X:125:HIS:HD2	24:X:127:GLY:H	1.55	0.53
25:Y:21:PRO:HG2	25:Y:24:LYS:HD3	1.89	0.53
1:A:35:U:H5'	5:E:47:GLY:O	2.08	0.53
1:A:128:A:O2'	1:A:129:A:H5'	2.08	0.53
1:A:821:U:H2'	1:A:822:C:H6	1.72	0.53
10:J:5:MET:HG3	37:J:8365:HOH:O	2.08	0.53
14:N:114:VAL:HB	14:N:159:THR:HG23	1.88	0.53
15:O:71:TRP:HE3	15:O:175:LEU:HD22	1.73	0.53
26:Z:106:THR:HG23	26:Z:107:PRO:HD2	1.90	0.53
26:Z:107:PRO:HB3	26:Z:182:PHE:CE2	2.44	0.53
1:A:183:A:C5'	14:N:157:LEU:HD12	2.37	0.53
1:A:820:G:O2'	1:A:856:G:H4'	2.08	0.53
1:A:1834:C:H2'	1:A:1840:A:N6	2.24	0.53
10:J:150:LYS:HE2	37:J:8378:HOH:O	2.07	0.53
24:X:122:ARG:HH21	24:X:154:ARG:HD2	1.73	0.53
27:1:11:THR:CG2	27:1:23:ARG:HB2	2.38	0.53
1:A:625:U:H5"	1:A:1044:C:N4	2.23	0.53
1:A:1398:G:H2'	1:A:1399:A:C8	2.44	0.53
1:A:1973:A:H5'	1:A:1973:A:C8	2.36	0.53
37:A:3732:HOH:O	21:U:9:LYS:CD	2.55	0.53
4:D:198:GLU:HB3	37:D:8596:HOH:O	2.08	0.53
5:E:76:ARG:HG2	5:E:78:ARG:NH1	2.22	0.53
10:J:59:ASN:N	10:J:59:ASN:ND2	2.44	0.53
13:M:72:ASN:HB2	37:M:8578:HOH:O	2.09	0.53
25:Y:31:ILE:O	25:Y:35:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:122:ARG:NH2	37:Z:8535:HOH:O	2.40	0.53
1:A:136:C:H2'	1:A:137:U:O4'	2.08	0.53
6:F:19:GLU:HG3	37:F:6165:HOH:O	2.08	0.53
13:M:73:VAL:HG23	13:M:74:THR:H	1.72	0.53
1:A:656:G:OP2	16:P:37:ARG:HD2	2.09	0.53
1:A:1060:C:H6	1:A:1060:C:H5'	1.74	0.53
1:A:1700:C:OP2	37:A:6009:HOH:O	2.19	0.53
1:A:2506:A:O2'	1:A:2507:G:O5'	2.26	0.53
3:C:88:ILE:CD1	3:C:100:PRO:HD3	2.37	0.53
12:L:99:ASP:OD1	12:L:101:ASN:N	2.41	0.53
13:M:143:THR:HG22	13:M:144:ASP:H	1.74	0.53
15:O:110:THR:HB	15:O:113:SER:OG	2.09	0.53
16:P:96:VAL:HA	37:P:4258:HOH:O	2.09	0.53
29:3:18:ASN:HD21	29:3:40:ARG:H	1.56	0.53
1:A:21:G:H4'	19:S:2:ILE:HG22	1.90	0.53
1:A:558:C:H2'	1:A:559:U:H5'	1.91	0.53
1:A:1189:A:H3'	37:A:7659:HOH:O	2.08	0.53
1:A:2721:U:H4'	12:L:87:ARG:HG3	1.91	0.53
2:B:3023:U:C3'	2:B:3024:U:H5"	2.39	0.53
4:D:63:GLU:O	4:D:63:GLU:HG3	2.08	0.53
10:J:84:ARG:CZ	10:J:135:TRP:HH2	2.21	0.53
14:N:45:ARG:CZ	14:N:48:ARG:HG3	2.39	0.53
27:1:39:CYS:HA	27:1:47:LEU:HD11	1.91	0.53
29:3:35:ARG:HB2	37:3:2691:HOH:O	2.07	0.53
1:A:1189:A:H1'	1:A:1209:C:H1'	1.91	0.53
1:A:2270:G:H4'	3:C:223:ARG:NH1	2.24	0.53
3:C:200:PRO:HD3	37:C:8520:HOH:O	2.08	0.53
5:E:162:VAL:HG13	5:E:232:LEU:HD21	1.91	0.53
5:E:185:LYS:HD3	5:E:186:TYR:CE1	2.44	0.53
5:E:246:ARG:HB3	5:E:246:ARG:HH11	1.72	0.53
6:F:99:ASP:HB3	6:F:103:ASN:H	1.74	0.53
7:G:81:GLU:HG2	7:G:134:SER:CB	2.35	0.53
8:H:47:LEU:HB2	8:H:108:LEU:HD11	1.91	0.53
22:V:52:THR:CG2	22:V:54:THR:HB	2.39	0.53
24:X:149:LEU:HG	24:X:153:MET:CE	2.39	0.53
1:A:401:C:C5'	37:A:5768:HOH:O	2.56	0.53
1:A:1132:A:N6	1:A:1229:C:H2'	2.24	0.53
1:A:1384:C:H5'	25:Y:30:MET:HG2	1.91	0.53
1:A:2329:C:O2'	1:A:2330:U:H5'	2.08	0.53
4:D:144:THR:HG22	4:D:145:HIS:N	2.23	0.53
4:D:307:ARG:HH11	4:D:307:ARG:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:38:GLU:OE2	6:F:51:ARG:CZ	2.57	0.53
6:F:57:THR:HG23	6:F:63:ILE:CG2	2.38	0.53
15:O:154:LEU:HG	15:O:155:GLU:H	1.73	0.53
25:Y:76:ARG:O	25:Y:77:PHE:HB3	2.08	0.53
1:A:1972:U:H2'	1:A:1973:A:C5'	2.39	0.53
5:E:236:THR:CG2	5:E:239:ALA:H	1.96	0.53
6:F:58:VAL:HG12	6:F:59:GLY:N	2.24	0.53
19:S:39:THR:CB	19:S:42:GLU:HG3	2.39	0.53
24:X:3:ALA:O	24:X:54:PHE:HA	2.09	0.53
24:X:26:ILE:HG13	24:X:26:ILE:O	2.08	0.53
24:X:108:ARG:HE	24:X:114:PRO:HG3	1.73	0.53
25:Y:12:ILE:HD12	25:Y:36:HIS:ND1	2.24	0.53
1:A:639:A:H2'	1:A:640:G:C8	2.44	0.52
37:A:4052:HOH:O	8:H:31:LYS:HE3	2.07	0.52
3:C:199:HIS:HD2	3:C:201:PHE:HB2	1.74	0.52
4:D:7:ARG:NH1	4:D:11:LEU:CD2	2.72	0.52
8:H:99:THR:O	8:H:100:ASP:HB2	2.08	0.52
12:L:109:LEU:HD13	12:L:113:ILE:HD11	1.90	0.52
1:A:283:U:H5"	1:A:284:C:P	2.49	0.52
1:A:920:C:H5"	1:A:921:G:O5'	2.10	0.52
1:A:1123:A:C6	1:A:1238:C:H5'	2.44	0.52
1:A:2502:C:C2'	1:A:2503:A:H5'	2.38	0.52
4:D:1:PRO:O	4:D:2:GLN:HB2	2.09	0.52
5:E:76:ARG:HD2	37:E:8429:HOH:O	2.08	0.52
5:E:79:ARG:O	5:E:87:ARG:HG2	2.09	0.52
9:I:63:ARG:N	37:I:2569:HOH:O	2.43	0.52
10:J:147:ARG:HA	10:J:150:LYS:HZ2	1.75	0.52
18:R:40:HIS:CE1	18:R:94:GLN:HA	2.45	0.52
4:D:27:ASN:HD22	4:D:27:ASN:H	1.57	0.52
5:E:84:VAL:O	5:E:85:LYS:HB2	2.10	0.52
8:H:48:VAL:CG2	8:H:74:PHE:HB3	2.39	0.52
8:H:117:GLU:C	8:H:119:ARG:H	2.12	0.52
15:O:43:VAL:HG11	15:O:81:ALA:HA	1.91	0.52
15:O:152:GLU:C	15:O:154:LEU:H	2.11	0.52
18:R:25:PRO:HB2	37:R:4350:HOH:O	2.08	0.52
26:Z:117:LEU:HD12	26:Z:174:VAL:HG11	1.92	0.52
1:A:256:C:H2'	1:A:257:G:O4'	2.09	0.52
1:A:380:A:H5"	14:N:48:ARG:NH2	2.24	0.52
1:A:581:G:H5'	37:A:7661:HOH:O	2.09	0.52
1:A:1733:A:H4'	4:D:212:GLN:HA	1.90	0.52
1:A:2421:G:H3'	1:A:2422:U:H5"	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:14:GLY:HA3	37:D:8609:HOH:O	2.09	0.52
6:F:62:ASP:HA	37:F:4233:HOH:O	2.09	0.52
1:A:593:A:N7	37:A:4367:HOH:O	2.41	0.52
1:A:816:G:C6	1:A:817:G:N1	2.77	0.52
1:A:1015:C:H2'	1:A:1016:U:H6	1.75	0.52
1:A:1523:G:H2'	1:A:1524:U:C6	2.45	0.52
1:A:2361:A:H5'	1:A:2361:A:H8	1.74	0.52
1:A:2385:G:H2'	1:A:2386:U:C6	2.44	0.52
1:A:2508:C:H2'	37:A:6724:HOH:O	2.08	0.52
1:A:2781:U:C2'	1:A:2782:G:H5'	2.39	0.52
4:D:248:ARG:NH2	37:D:8526:HOH:O	2.42	0.52
5:E:246:ARG:CZ	37:E:8420:HOH:O	2.58	0.52
11:K:39:VAL:HG13	11:K:106:GLY:O	2.09	0.52
14:N:48:ARG:NH2	37:N:8564:HOH:O	2.43	0.52
17:Q:18:LYS:O	17:Q:21:VAL:HG22	2.08	0.52
1:A:447:A:O2'	1:A:448:G:H5'	2.10	0.52
1:A:1167:G:O2'	1:A:1168:C:H5'	2.09	0.52
1:A:1972:U:H2'	1:A:1973:A:H5"	1.90	0.52
4:D:149:ASP:HB2	37:D:8582:HOH:O	2.10	0.52
13:M:72:ASN:O	13:M:76:LEU:HG	2.09	0.52
26:Z:107:PRO:HB3	26:Z:182:PHE:CD2	2.45	0.52
1:A:1205:U:C2'	1:A:1206:U:C5'	2.87	0.52
1:A:2004:U:O2	1:A:2004:U:H2'	2.08	0.52
1:A:2720:C:O2	12:L:87:ARG:NH2	2.42	0.52
7:G:11:VAL:CG1	7:G:12:ASP:N	2.72	0.52
10:J:55:GLN:HE22	10:J:91:HIS:CD2	2.27	0.52
14:N:98:GLN:O	14:N:102:GLU:HG3	2.09	0.52
26:Z:186:ARG:HG2	26:Z:186:ARG:NH1	2.15	0.52
1:A:401:C:H5'	37:A:5768:HOH:O	2.09	0.52
1:A:2866:U:H4'	1:A:2867:G:H5'	1.91	0.52
2:B:3055:U:H4'	2:B:3056:A:H8	1.72	0.52
6:F:65:GLU:HG3	37:F:6752:HOH:O	2.08	0.52
1:A:1119:G:N2	1:A:1246:A:H2	2.05	0.52
1:A:1669:A:H2'	1:A:1670:G:C8	2.45	0.52
1:A:2010:A:H2'	37:A:5933:HOH:O	2.10	0.52
1:A:2064:U:H5'	1:A:2652:U:H4'	1.91	0.52
37:A:4696:HOH:O	15:O:21:HIS:HD2	1.93	0.52
3:C:51:ARG:NH1	3:C:120:ARG:O	2.43	0.52
3:C:51:ARG:NH2	3:C:69:LEU:HD13	2.24	0.52
3:C:191:GLY:HA2	3:C:194:MET:HE2	1.90	0.52
8:H:46:GLU:OE1	8:H:100:ASP:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:64:SER:C	15:O:66:LEU:H	2.14	0.52
25:Y:70:ILE:O	25:Y:70:ILE:HG23	2.09	0.52
1:A:703:G:O2'	1:A:704:C:H5'	2.10	0.52
1:A:834:G:H4'	1:A:835:U:OP2	2.10	0.52
5:E:127:ARG:HG2	5:E:127:ARG:NH1	2.25	0.52
10:J:71:TYR:C	10:J:73:GLN:N	2.61	0.52
15:O:182:GLY:O	15:O:183:ASP:O	2.28	0.52
19:S:132:ARG:CZ	37:S:8584:HOH:O	2.58	0.52
20:T:57:THR:CG2	20:T:58:MET:N	2.73	0.52
21:U:71:VAL:HG11	21:U:90:PRO:CB	2.26	0.52
29:3:22:PRO:HB2	29:3:24:TRP:CD1	2.45	0.52
1:A:669:G:O2'	1:A:670:G:H5'	2.10	0.51
5:E:234:VAL:HG22	5:E:234:VAL:O	2.10	0.51
7:G:69:ILE:HA	7:G:72:MET:HE2	1.92	0.51
10:J:47:GLU:HG2	10:J:133:ILE:HD12	1.91	0.51
10:J:109:ASP:HB2	37:J:8347:HOH:O	2.10	0.51
14:N:55:LYS:O	14:N:60:ILE:HD12	2.10	0.51
15:O:23:ARG:NH1	37:O:8549:HOH:O	2.43	0.51
24:X:143:THR:N	37:X:3520:HOH:O	2.43	0.51
26:Z:133:HIS:HD2	37:Z:8584:HOH:O	1.91	0.51
1:A:184:G:H5"	14:N:153:THR:HG22	1.92	0.51
1:A:1008:C:H5"	10:J:16:ARG:HH12	1.75	0.51
1:A:2896:A:OP1	25:Y:15:ARG:NH1	2.44	0.51
3:C:199:HIS:CD2	3:C:201:PHE:HB2	2.45	0.51
4:D:307:ARG:HH11	4:D:307:ARG:CG	2.22	0.51
5:E:118:THR:O	5:E:136:VAL:HG13	2.10	0.51
8:H:58:GLU:HB3	14:N:8:ILE:HG23	1.92	0.51
13:M:73:VAL:HG23	13:M:74:THR:N	2.25	0.51
14:N:37:VAL:HG21	14:N:108:LYS:HG3	1.92	0.51
24:X:139:GLY:O	24:X:141:HIS:CD2	2.63	0.51
1:A:558:C:H2'	1:A:559:U:H5"	1.92	0.51
1:A:941:G:C5	1:A:942:U:C4	2.98	0.51
1:A:962:C:C1'	15:O:5:ARG:NH1	2.66	0.51
1:A:2266:A:OP2	14:N:90:ARG:NH2	2.44	0.51
2:B:3029:C:C2'	2:B:3030:C:H5'	2.40	0.51
3:C:130:THR:HG22	3:C:131:HIS:O	2.10	0.51
6:F:11:HIS:C	6:F:13:MET:H	2.13	0.51
13:M:149:ARG:O	13:M:150:GLN:HB2	2.10	0.51
14:N:37:VAL:HG13	14:N:63:VAL:HG11	1.92	0.51
14:N:134:ILE:HG23	14:N:141:ILE:HD13	1.93	0.51
19:S:132:ARG:HG2	19:S:133:ALA:N	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:38:ARG:HH11	21:U:38:ARG:HG3	1.75	0.51
30:4:17:HIS:O	30:4:18:GLN:HG3	2.10	0.51
1:A:314:G:N2	1:A:316:A:H3'	2.25	0.51
1:A:1118:A:C8	1:A:1119:G:H5"	2.46	0.51
1:A:2589:U:H2'	1:A:2590:U:C6	2.45	0.51
1:A:2777:G:O2'	1:A:2778:A:H5'	2.09	0.51
1:A:2812:A:H1'	37:A:5764:HOH:O	2.10	0.51
2:B:3049:G:H2'	2:B:3050:G:O4'	2.10	0.51
4:D:138:GLY:O	4:D:139:ASP:O	2.27	0.51
17:Q:14:LEU:HD13	17:Q:51:ALA:HB2	1.92	0.51
17:Q:91:LYS:O	17:Q:95:GLU:HG3	2.09	0.51
21:U:24:ARG:HH21	21:U:39:ASN:HD22	1.58	0.51
25:Y:76:ARG:HG3	25:Y:76:ARG:NH1	2.24	0.51
1:A:514:G:H8	1:A:514:G:O5'	1.92	0.51
1:A:1118:A:H62	1:A:1244:U:H3	1.58	0.51
1:A:1189:A:O2'	1:A:1208:C:H2'	2.10	0.51
1:A:2361:A:H2'	1:A:2362:A:C8	2.45	0.51
1:A:2910:A:H5"	37:A:4101:HOH:O	2.10	0.51
6:F:99:ASP:HB2	6:F:103:ASN:H	1.76	0.51
14:N:57:LYS:HE2	14:N:140:ALA:O	2.10	0.51
14:N:169:ARG:NH2	37:N:8548:HOH:O	2.27	0.51
15:O:159:TYR:HE2	15:O:163:PHE:HE2	1.59	0.51
1:A:333:G:O2'	1:A:334:G:H5'	2.11	0.51
1:A:1236:A:H2'	1:A:1237:U:O4'	2.11	0.51
1:A:1377:C:H5'	1:A:1377:C:C6	2.43	0.51
1:A:2488:A:H2	37:A:7250:HOH:O	1.93	0.51
5:E:168:ARG:NH2	5:E:190:ALA:O	2.44	0.51
6:F:27:ILE:HG22	6:F:28:GLY:N	2.19	0.51
15:O:11:ARG:O	15:O:15:GLU:HG3	2.11	0.51
19:S:25:PHE:CE2	19:S:29:LYS:CE	2.93	0.51
1:A:2649:A:H5'	1:A:2649:A:C8	2.46	0.51
1:A:2782:G:O6	1:A:2790:C:H5"	2.10	0.51
2:B:3025:G:H2'	37:B:8461:HOH:O	2.09	0.51
3:C:232:ARG:NH2	3:C:236:GLY:O	2.29	0.51
5:E:27:ARG:HG3	5:E:29:ASP:OD1	2.11	0.51
10:J:157:ILE:CG2	10:J:158:ASN:N	2.74	0.51
13:M:104:ASP:HB3	37:M:8560:HOH:O	2.10	0.51
17:Q:98:ILE:HD12	17:Q:102:ARG:NE	2.26	0.51
20:T:32:ALA:HA	20:T:36:GLU:OE1	2.11	0.51
21:U:73:HIS:CD2	21:U:88:PRO:HG3	2.46	0.51
26:Z:172:THR:HG22	26:Z:173:ALA:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:G:H5'	1:A:88:G:H8	1.76	0.51
1:A:157:G:H4'	14:N:95:LYS:HE3	1.93	0.51
1:A:500:G:H21	19:S:98:ASN:HD21	1.58	0.51
1:A:638:C:H2'	1:A:639:A:C8	2.45	0.51
1:A:797:A:H4'	27:1:10:ARG:N	2.25	0.51
1:A:2070:G:H5"	37:A:3756:HOH:O	2.11	0.51
1:A:2435:U:H1'	37:A:5403:HOH:O	2.10	0.51
4:D:56:ASP:OD1	4:D:322:ARG:HB3	2.10	0.51
8:H:19:ALA:O	8:H:22:VAL:HG22	2.11	0.51
1:A:1420:C:C2	1:A:1445:G:N2	2.79	0.51
1:A:1743:G:H1'	37:A:4861:HOH:O	2.10	0.51
1:A:1972:U:C2'	1:A:1973:A:H5"	2.41	0.51
1:A:2570:G:H5"	37:A:4881:HOH:O	2.11	0.51
2:B:3020:G:H3'	37:B:8435:HOH:O	2.10	0.51
3:C:57:ALA:HA	3:C:67:LEU:HD23	1.93	0.51
4:D:280:VAL:CG1	4:D:334:SER:HA	2.40	0.51
6:F:22:VAL:HG22	6:F:74:THR:HG22	1.93	0.51
8:H:113:ASP:O	8:H:117:GLU:HG3	2.11	0.51
14:N:114:VAL:HG21	14:N:159:THR:CG2	2.40	0.51
1:A:42:C:H1'	37:A:4645:HOH:O	2.09	0.51
1:A:709:G:O2'	16:P:25:VAL:HG12	2.10	0.51
1:A:1164:U:C4'	1:A:1165:G:OP1	2.54	0.51
1:A:1266:U:H4'	26:Z:115:ARG:HH21	1.75	0.51
1:A:1500:U:P	17:Q:41:ARG:HH22	2.34	0.51
1:A:1909:A:N1	1:A:2128:G:H1'	2.25	0.51
1:A:1919:A:H4'	37:A:4818:HOH:O	2.11	0.51
5:E:200:PRO:HB3	5:E:212:VAL:HG23	1.93	0.51
7:G:15:GLN:NE2	7:G:40:VAL:O	2.43	0.51
16:P:39:THR:O	16:P:115:ARG:NH2	2.44	0.51
20:T:51:GLN:NE2	20:T:53:ASN:HD21	2.07	0.51
29:3:48:ASP:O	29:3:49:GLU:HB2	2.11	0.51
1:A:1003:U:O2	10:J:90:PHE:CZ	2.64	0.50
1:A:1595:G:O2'	1:A:1596:U:H5'	2.11	0.50
4:D:240:GLY:HA3	37:D:8656:HOH:O	2.10	0.50
10:J:39:GLY:O	10:J:41:THR:N	2.44	0.50
14:N:185:PRO:HG2	14:N:189:VAL:HG11	1.93	0.50
26:Z:112:GLU:CD	26:Z:115:ARG:HH12	2.13	0.50
30:4:74:CYS:N	37:4:8559:HOH:O	2.43	0.50
1:A:88:G:N7	29:3:28:LYS:HD2	2.26	0.50
1:A:775:G:OP1	28:2:16:HIS:HE1	1.94	0.50
1:A:1180:U:H2'	1:A:1181:A:O4'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:6969:HOH:O	18:R:9:GLY:HA2	2.12	0.50
3:C:192:VAL:HG13	37:C:8555:HOH:O	2.10	0.50
8:H:16:ALA:HA	8:H:111:ILE:HD13	1.93	0.50
13:M:143:THR:CG2	13:M:144:ASP:H	2.24	0.50
19:S:128:ARG:HB2	19:S:132:ARG:O	2.10	0.50
27:1:11:THR:HG23	27:1:11:THR:O	2.10	0.50
27:1:57:CYS:SG	27:1:59:HIS:HB3	2.50	0.50
1:A:661:G:C5	1:A:686:A:C2	2.98	0.50
1:A:1603:A:H5"	1:A:1605:G:H5'	1.93	0.50
1:A:1827:G:H2'	1:A:1828:G:C8	2.46	0.50
2:B:3041:C:C6	6:F:50:VAL:HG21	2.46	0.50
3:C:1:GLY:HA2	3:C:197:VAL:HG23	1.94	0.50
4:D:267:LYS:HD3	37:D:8528:HOH:O	2.11	0.50
4:D:320:GLN:HG3	4:D:321:PRO:HD2	1.93	0.50
6:F:11:HIS:O	6:F:12:GLU:HB3	2.11	0.50
6:F:140:ARG:O	6:F:144:ARG:HG2	2.10	0.50
7:G:31:ARG:CZ	37:G:5919:HOH:O	2.60	0.50
8:H:58:GLU:CD	14:N:27:ARG:HH22	2.15	0.50
8:H:99:THR:O	8:H:99:THR:HG23	2.10	0.50
8:H:101:ALA:HB2	8:H:108:LEU:HD22	1.93	0.50
10:J:141:ASN:HA	37:J:8366:HOH:O	2.11	0.50
14:N:115:LEU:HD13	14:N:116:ASN:HB2	1.93	0.50
19:S:17:MET:CE	19:S:19:ARG:NH2	2.74	0.50
24:X:38:THR:HB	37:X:5390:HOH:O	2.10	0.50
24:X:154:ARG:C	37:X:4276:HOH:O	2.49	0.50
1:A:1506:U:H6	1:A:1506:U:H5'	1.76	0.50
7:G:22:VAL:O	7:G:28:SER:HA	2.12	0.50
13:M:120:LEU:HD12	13:M:133:VAL:HG21	1.94	0.50
14:N:55:LYS:HB2	14:N:60:ILE:CD1	2.42	0.50
20:T:6:LYS:HB2	20:T:27:ALA:O	2.10	0.50
22:V:46:ALA:HB1	22:V:52:THR:HG21	1.93	0.50
27:1:58:GLY:CA	37:1:8437:HOH:O	2.50	0.50
1:A:1056:U:H2'	1:A:1057:A:O4'	2.11	0.50
1:A:2251:G:H2'	1:A:2252:A:C8	2.47	0.50
1:A:2526:C:O2'	1:A:2527:U:H5'	2.11	0.50
1:A:2781:U:H1'	7:G:139:GLU:OE2	2.10	0.50
37:A:3732:HOH:O	21:U:9:LYS:HD2	2.11	0.50
6:F:41:LEU:CA	6:F:44:ILE:HG22	2.41	0.50
14:N:47:ASP:CG	14:N:48:ARG:N	2.65	0.50
23:W:56:ILE:O	23:W:60:GLN:HG3	2.10	0.50
1:A:328:U:O4'	5:E:202:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:U:H4'	18:R:95:GLU:HA	1.93	0.50
1:A:2756:U:N3	1:A:2896:A:H2	2.09	0.50
1:A:2781:U:H2'	1:A:2782:G:H5'	1.93	0.50
2:B:3064:C:H2'	2:B:3065:A:H5'	1.94	0.50
4:D:301:VAL:HG13	4:D:302:PRO:HD2	1.94	0.50
10:J:129:ASN:HD22	10:J:129:ASN:N	2.09	0.50
13:M:89:PHE:N	37:M:8568:HOH:O	2.44	0.50
15:O:154:LEU:O	15:O:155:GLU:CB	2.60	0.50
22:V:52:THR:HG22	22:V:54:THR:HB	1.93	0.50
27:1:31:ILE:HG23	27:1:32:LYS:N	2.27	0.50
1:A:660:A:H4'	1:A:661:G:O5'	2.12	0.50
1:A:1028:U:H1'	37:A:3624:HOH:O	2.12	0.50
1:A:1592:G:O2'	1:A:1593:C:O5'	2.29	0.50
1:A:2507:G:H2'	1:A:2510:C:H42	1.77	0.50
3:C:125:ASN:CB	3:C:158:VAL:HG12	2.42	0.50
4:D:258:GLY:N	4:D:260:HIS:CE1	2.79	0.50
5:E:35:VAL:HG21	5:E:227:GLY:HA2	1.92	0.50
12:L:28:GLU:HB3	12:L:59:LYS:HB2	1.94	0.50
14:N:155:HIS:CE1	14:N:158:ARG:HE	2.29	0.50
14:N:184:ARG:HG3	14:N:185:PRO:HA	1.93	0.50
1:A:1176:C:H1'	37:A:3903:HOH:O	2.12	0.50
1:A:1423:C:O2'	1:A:1424:A:H5'	2.12	0.50
1:A:2104:C:O2	1:A:2485:A:N1	2.44	0.50
1:A:2256:G:H2'	1:A:2257:G:H5'	1.94	0.50
4:D:139:ASP:HB2	4:D:165:ARG:HE	1.77	0.50
6:F:19:GLU:O	6:F:133:ASN:HB3	2.12	0.50
10:J:118:PRO:HD2	37:J:8341:HOH:O	2.11	0.50
22:V:35:LYS:HB2	37:V:774:HOH:O	2.12	0.50
24:X:122:ARG:NH2	24:X:154:ARG:HD2	2.27	0.50
1:A:664:U:O4	1:A:681:G:H5"	2.11	0.50
1:A:1151:G:OP1	9:I:63:ARG:NH1	2.44	0.50
1:A:2717:C:H2'	1:A:2718:C:C5'	2.38	0.50
37:A:9639:HOH:O	34:D:8519:CL:CL	2.57	0.50
2:B:3054:A:O2'	2:B:3055:U:H5'	2.12	0.50
8:H:101:ALA:HB2	8:H:108:LEU:CD2	2.41	0.50
10:J:157:ILE:HG22	10:J:158:ASN:N	2.27	0.50
25:Y:9:VAL:HG13	25:Y:88:GLU:CD	2.31	0.50
1:A:377:C:H5	37:A:3292:HOH:O	1.95	0.49
1:A:1118:A:C8	1:A:1118:A:C3'	2.85	0.49
1:A:1527:A:H1'	1:A:1528:A:C8	2.47	0.49
8:H:46:GLU:N	37:H:3461:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:56:ILE:HG22	10:J:61:LEU:CD2	2.40	0.49
14:N:38:VAL:O	14:N:63:VAL:HG13	2.11	0.49
14:N:107:ARG:NH1	37:N:8578:HOH:O	2.38	0.49
15:O:62:HIS:HB3	15:O:65:ASP:OD1	2.11	0.49
16:P:26:TRP:HB2	37:P:3062:HOH:O	2.11	0.49
19:S:34:GLU:HG2	19:S:46:TYR:OH	2.13	0.49
24:X:90:TYR:N	24:X:90:TYR:CD1	2.79	0.49
26:Z:189:ASN:ND2	26:Z:192:ASP:H	2.10	0.49
1:A:1462:C:H2'	1:A:1463:A:C8	2.47	0.49
1:A:1864:C:OP1	14:N:75:THR:HG23	2.12	0.49
1:A:2473:U:O3'	1:A:2474:A:H3'	2.11	0.49
1:A:2815:G:N7	11:K:80:LYS:NZ	2.60	0.49
6:F:27:ILE:HD11	6:F:37:ALA:CB	2.42	0.49
8:H:48:VAL:HG23	8:H:74:PHE:CB	2.42	0.49
16:P:47:ARG:HG3	16:P:47:ARG:NH1	2.25	0.49
28:2:10:LYS:HG3	37:2:2979:HOH:O	2.12	0.49
28:2:28:HIS:CD2	28:2:30:LYS:HB2	2.46	0.49
30:4:3:MET:O	30:4:90:PHE:HA	2.12	0.49
1:A:2072:G:C6	1:A:2533:C:H1'	2.47	0.49
1:A:2314:G:C2'	1:A:2315:C:H5'	2.42	0.49
1:A:2385:G:H2'	1:A:2386:U:H6	1.77	0.49
1:A:2613:G:O2'	1:A:2614:C:H5'	2.12	0.49
4:D:7:ARG:CD	4:D:9:GLY:O	2.59	0.49
4:D:103:ASP:HB2	37:D:8593:HOH:O	2.12	0.49
6:F:86:THR:C	6:F:89:PRO:HD2	2.32	0.49
7:G:107:PHE:CE2	7:G:108:LEU:HD13	2.47	0.49
9:I:20:VAL:O	9:I:24:VAL:HG23	2.13	0.49
14:N:81:ARG:HG3	14:N:85:ARG:HB2	1.93	0.49
1:A:156:C:H5"	14:N:171:ARG:CD	2.21	0.49
1:A:1166:A:H1'	1:A:1192:A:N1	2.26	0.49
37:A:9107:HOH:O	5:E:103:ASN:HB3	2.12	0.49
3:C:128:LEU:HG	37:C:8574:HOH:O	2.11	0.49
6:F:99:ASP:CB	6:F:103:ASN:HB2	2.42	0.49
10:J:110:GLY:N	37:J:8395:HOH:O	2.45	0.49
20:T:23:LYS:HE2	37:T:8331:HOH:O	2.12	0.49
25:Y:71:ARG:CD	37:Y:2171:HOH:O	2.60	0.49
1:A:512:G:O3'	1:A:513:A:H8	1.96	0.49
37:A:3728:HOH:O	14:N:108:LYS:HD2	2.13	0.49
3:C:211:LYS:HB3	3:C:212:PRO:CD	2.32	0.49
4:D:248:ARG:O	4:D:251:VAL:CG1	2.61	0.49
5:E:153:VAL:O	5:E:157:LEU:HG	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:30:MET:HE1	25:Y:55:ASN:HA	1.94	0.49
26:Z:109:LEU:HA	37:Z:8573:HOH:O	2.13	0.49
1:A:56:G:H5"	23:W:50:ARG:HH12	1.76	0.49
1:A:289:G:O2'	1:A:290:C:H5'	2.13	0.49
1:A:338:C:H4'	5:E:174:ILE:HD12	1.93	0.49
1:A:790:A:H2'	1:A:791:A:O4'	2.12	0.49
1:A:1098:A:H2'	1:A:1099:G:O4'	2.13	0.49
1:A:1477:C:H5'	1:A:1868:G:H5'	1.94	0.49
22:V:9:CYS:CA	22:V:52:THR:HG23	2.42	0.49
24:X:65:VAL:HA	24:X:68:THR:CG2	2.42	0.49
1:A:1289:C:O2'	1:A:1290:G:H5'	2.13	0.49
1:A:1477:C:O2'	1:A:1478:U:H5'	2.11	0.49
1:A:1636:G:O2'	1:A:1637:A:H5'	2.11	0.49
1:A:1657:A:H2'	1:A:1658:A:C8	2.47	0.49
1:A:1804:A:H2'	1:A:1805:G:C8	2.46	0.49
1:A:2256:G:H2'	1:A:2257:G:C5'	2.43	0.49
4:D:16:ARG:NE	37:D:8554:HOH:O	2.26	0.49
10:J:35:ASN:HD21	10:J:80:ASN:HA	1.78	0.49
10:J:47:GLU:CB	10:J:133:ILE:CD1	2.88	0.49
15:O:143:ARG:HA	15:O:172:PHE:CD2	2.48	0.49
15:O:154:LEU:HG	15:O:155:GLU:N	2.27	0.49
24:X:38:THR:HG22	24:X:39:ASP:N	2.27	0.49
24:X:122:ARG:HH22	24:X:154:ARG:C	2.16	0.49
28:2:8:GLN:HE22	28:2:11:LYS:HZ2	1.60	0.49
30:4:91:GLN:O	30:4:92:GLU:HB2	2.12	0.49
1:A:175:G:H2'	14:N:192:ALA:HB3	1.93	0.49
1:A:1165:G:OP1	1:A:1165:G:H3'	2.13	0.49
6:F:99:ASP:O	6:F:159:PRO:HG3	2.12	0.49
6:F:103:ASN:ND2	6:F:134:LEU:H	2.09	0.49
7:G:132:THR:O	7:G:132:THR:HG23	2.13	0.49
13:M:61:ALA:HA	37:M:8560:HOH:O	2.12	0.49
24:X:38:THR:O	24:X:42:ARG:HB2	2.13	0.49
1:A:1654:U:H2'	3:C:47:HIS:CD2	2.48	0.49
1:A:2472:C:O2'	1:A:2634:G:H4'	2.13	0.49
1:A:2488:A:H61	1:A:2534:C:H42	1.60	0.49
7:G:37:ASP:OD1	11:K:125:SER:HB3	2.13	0.49
10:J:14:TYR:N	10:J:91:HIS:CE1	2.77	0.49
1:A:484:A:N1	1:A:506:G:H4'	2.27	0.49
4:D:55:ASN:HB3	4:D:64:GLY:H	1.78	0.49
4:D:314:ALA:CB	4:D:317:PRO:HG3	2.43	0.49
6:F:94:ALA:HB3	6:F:174:VAL:CA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:75:ARG:HG2	12:L:90:PHE:CD2	2.48	0.49
14:N:64:ARG:HD2	37:N:8586:HOH:O	2.11	0.49
30:4:56:PRO:N	37:4:8548:HOH:O	2.46	0.49
1:A:2676:C:H4'	11:K:70:PHE:HE1	1.77	0.48
2:B:3023:U:H6	2:B:3023:U:C5'	2.23	0.48
2:B:3031:C:H1'	37:B:8393:HOH:O	2.13	0.48
3:C:165:THR:HG22	37:C:8618:HOH:O	2.13	0.48
4:D:177:HIS:O	4:D:181:ILE:HG13	2.12	0.48
10:J:56:ILE:HG21	10:J:61:LEU:HD13	1.95	0.48
14:N:108:LYS:HE3	37:N:8611:HOH:O	2.11	0.48
15:O:184:ILE:HG22	15:O:185:GLU:N	2.28	0.48
1:A:2271:G:H2'	1:A:2271:G:N3	2.28	0.48
4:D:127:GLN:HG3	37:D:8642:HOH:O	2.13	0.48
4:D:280:VAL:HG13	4:D:333:GLU:O	2.14	0.48
10:J:35:ASN:ND2	10:J:79:ALA:O	2.46	0.48
11:K:45:VAL:HG22	11:K:46:ILE:N	2.27	0.48
15:O:58:LEU:HD12	15:O:58:LEU:N	2.28	0.48
18:R:30:VAL:O	18:R:30:VAL:HG12	2.13	0.48
21:U:38:ARG:HG3	21:U:38:ARG:NH1	2.27	0.48
27:1:26:VAL:O	27:1:30:GLU:HG3	2.13	0.48
1:A:371:U:H2'	1:A:372:A:C8	2.47	0.48
1:A:794:U:H3	1:A:819:A:H61	1.60	0.48
1:A:1269:G:H2'	1:A:1270:U:C6	2.48	0.48
1:A:1666:C:C2'	1:A:1667:A:C5'	2.91	0.48
1:A:1717:A:H5"	17:Q:54:LYS:HB2	1.95	0.48
1:A:2001:G:O2'	1:A:2002:C:H5'	2.13	0.48
1:A:2114:C:OP1	3:C:1:GLY:HA2	2.13	0.48
4:D:14:GLY:HA2	4:D:15:PRO:C	2.33	0.48
6:F:94:ALA:O	6:F:95:THR:O	2.31	0.48
16:P:44:ASN:HA	16:P:65:LEU:O	2.12	0.48
24:X:90:TYR:CE2	24:X:99:ALA:HB2	2.49	0.48
1:A:188:C:H5"	14:N:163:LEU:HD21	1.95	0.48
1:A:245:C:H2'	1:A:246:G:H5'	1.95	0.48
1:A:278:A:H2'	1:A:279:C:O4'	2.13	0.48
1:A:380:A:OP2	14:N:9:ARG:HD2	2.14	0.48
1:A:474:C:O3'	5:E:73:LEU:HD21	2.13	0.48
1:A:547:A:H3'	37:A:4914:HOH:O	2.13	0.48
1:A:1249:U:H2'	1:A:1250:C:C6	2.48	0.48
37:A:3732:HOH:O	21:U:9:LYS:HD3	2.13	0.48
4:D:16:ARG:NH2	37:D:8554:HOH:O	2.35	0.48
5:E:76:ARG:HD3	37:E:8367:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:101:THR:HG22	37:F:7400:HOH:O	2.14	0.48
10:J:47:GLU:CB	10:J:133:ILE:HD13	2.38	0.48
17:Q:10:ALA:HA	17:Q:13:VAL:CG1	2.43	0.48
24:X:42:ARG:O	24:X:45:VAL:HG22	2.13	0.48
30:4:57:GLY:HA2	37:4:8525:HOH:O	2.13	0.48
1:A:128:A:H3'	1:A:128:A:C8	2.48	0.48
1:A:283:U:H5"	1:A:284:C:OP2	2.14	0.48
1:A:558:C:C2'	1:A:559:U:C5'	2.91	0.48
1:A:588:G:O6	24:X:154:ARG:NH1	2.47	0.48
1:A:797:A:O4'	27:1:10:ARG:N	2.46	0.48
1:A:949:U:O2'	18:R:40:HIS:HE1	1.97	0.48
1:A:1205:U:C2'	1:A:1206:U:H5"	2.43	0.48
1:A:1306:U:OP1	5:E:184:ARG:HD2	2.13	0.48
1:A:2694:A:H4'	7:G:91:PHE:CE1	2.48	0.48
3:C:107:ASN:OD1	3:C:120:ARG:HD2	2.14	0.48
4:D:42:ALA:HB1	4:D:308:LEU:HD11	1.94	0.48
6:F:167:GLU:OE2	6:F:173:GLU:HG2	2.13	0.48
16:P:63:LYS:HG3	16:P:80:ASP:O	2.14	0.48
28:2:2:GLY:O	28:2:6:PRO:HG2	2.14	0.48
1:A:629:A:H2'	1:A:630:A:O4'	2.14	0.48
1:A:2361:A:H5"	37:A:9002:HOH:O	2.12	0.48
3:C:34:ASP:OD1	3:C:35:GLY:N	2.44	0.48
5:E:95:GLU:HG3	37:E:8470:HOH:O	2.14	0.48
6:F:51:ARG:HD3	37:F:7636:HOH:O	2.13	0.48
7:G:9:GLU:HG3	7:G:10:ASP:N	2.27	0.48
10:J:84:ARG:CZ	10:J:135:TRP:CH2	2.97	0.48
12:L:125:ALA:C	12:L:127:ALA:H	2.16	0.48
15:O:171:HIS:CE1	37:O:8567:HOH:O	2.66	0.48
19:S:39:THR:CG2	19:S:42:GLU:HG3	2.44	0.48
20:T:8:PRO:HD2	23:W:32:ALA:HA	1.96	0.48
23:W:64:GLY:O	23:W:65:ASP:CB	2.62	0.48
1:A:2724:U:H2'	1:A:2725:G:O4'	2.13	0.48
1:A:2768:A:H3'	37:A:4392:HOH:O	2.13	0.48
1:A:2769:C:O2'	1:A:2770:G:H5'	2.13	0.48
37:A:9969:HOH:O	13:M:22:ARG:HG2	2.12	0.48
5:E:129:HIS:HE1	5:E:231:ARG:HA	1.79	0.48
7:G:93:MET:HE1	7:G:165:GLY:N	2.29	0.48
15:O:138:ASP:O	15:O:140:GLN:N	2.45	0.48
24:X:34:LEU:CD1	24:X:100:LEU:HD13	2.44	0.48
28:2:1:THR:HA	37:2:435:HOH:O	2.13	0.48
1:A:39:G:N2	1:A:444:C:C2	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:C:H6	1:A:168:C:O5'	1.97	0.48
1:A:1304:U:H2'	1:A:1305:C:C6	2.49	0.48
1:A:2832:C:H5	37:A:7185:HOH:O	1.96	0.48
13:M:97:VAL:HG12	13:M:98:GLU:O	2.14	0.48
14:N:67:ILE:HD11	14:N:104:ARG:HD2	1.95	0.48
15:O:163:PHE:HE1	15:O:171:HIS:HD1	1.61	0.48
1:A:1123:A:C2	1:A:1129:C:H4'	2.49	0.48
1:A:1168:C:H5	37:A:7471:HOH:O	1.96	0.48
1:A:2501:G:H1'	37:A:4511:HOH:O	2.13	0.48
5:E:19:PRO:HG2	5:E:22:PHE:CD1	2.49	0.48
11:K:70:PHE:CD2	11:K:70:PHE:O	2.67	0.48
14:N:69:LYS:HG2	14:N:127:LYS:HG3	1.96	0.48
16:P:112:ARG:HA	37:P:1484:HOH:O	2.13	0.48
19:S:132:ARG:NH2	37:S:8584:HOH:O	2.46	0.48
1:A:714:U:H3'	37:A:6913:HOH:O	2.14	0.48
1:A:1007:A:H2'	10:J:19:TYR:CZ	2.49	0.48
1:A:1268:C:H2'	1:A:1269:G:H8	1.79	0.48
1:A:1515:A:H2'	1:A:1516:C:C6	2.49	0.48
1:A:1594:C:C5	17:Q:120:ARG:NH1	2.82	0.48
4:D:217:ARG:HG3	4:D:257:THR:HG22	1.94	0.48
6:F:58:VAL:CG1	6:F:59:GLY:N	2.75	0.48
10:J:97:LYS:HD3	10:J:117:LYS:HE2	1.96	0.48
19:S:39:THR:HB	19:S:42:GLU:CD	2.34	0.48
19:S:111:ILE:HG23	19:S:145:LEU:CD1	2.44	0.48
1:A:710:G:OP1	16:P:24:ALA:HB3	2.14	0.47
1:A:1450:C:C4'	1:A:1451:C:OP2	2.60	0.47
1:A:1861:C:H4'	3:C:6:GLY:O	2.13	0.47
1:A:2793:A:H5'	37:A:4524:HOH:O	2.14	0.47
3:C:8:ARG:NH1	37:C:8550:HOH:O	2.42	0.47
4:D:79:MET:HE1	37:D:8626:HOH:O	2.14	0.47
5:E:57:PRO:O	5:E:58:ALA:C	2.52	0.47
6:F:10:PHE:CD1	6:F:11:HIS:N	2.82	0.47
8:H:22:VAL:HG21	8:H:104:ALA:HB2	1.96	0.47
10:J:46:VAL:O	10:J:146:TRP:CH2	2.63	0.47
10:J:86:ARG:HD3	10:J:130:HIS:HD2	1.79	0.47
13:M:101:ASP:C	13:M:103:ALA:H	2.17	0.47
14:N:87:MET:H	14:N:87:MET:HG3	1.20	0.47
16:P:21:SER:OG	16:P:106:PRO:HB2	2.14	0.47
16:P:25:VAL:HG23	16:P:26:TRP:N	2.29	0.47
20:T:29:ASP:OD1	20:T:31:ARG:HG3	2.14	0.47
24:X:141:HIS:HB2	24:X:146:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:43:VAL:CG1	25:Y:44:ASP:N	2.76	0.47
26:Z:112:GLU:OE1	26:Z:115:ARG:NH1	2.46	0.47
1:A:249:G:O2'	1:A:250:C:H5'	2.14	0.47
1:A:383:A:H4'	37:A:5297:HOH:O	2.14	0.47
1:A:482:G:H4'	1:A:508:A:N1	2.29	0.47
1:A:951:A:O2'	1:A:952:G:H5'	2.14	0.47
1:A:958:G:H2'	1:A:959:C:C6	2.48	0.47
1:A:1593:C:OP1	17:Q:117:SER:HB3	2.14	0.47
1:A:1666:C:C2'	1:A:1667:A:H5'	2.41	0.47
2:B:3035:C:H5"	37:B:8455:HOH:O	2.14	0.47
3:C:123:GLY:HA3	3:C:162:GLY:HA2	1.96	0.47
5:E:236:THR:O	5:E:237:GLU:C	2.52	0.47
7:G:80:TRP:O	7:G:134:SER:HA	2.13	0.47
13:M:128:GLY:O	13:M:132:LYS:HG3	2.14	0.47
14:N:67:ILE:CD1	14:N:104:ARG:HD2	2.43	0.47
24:X:122:ARG:NH2	37:X:5817:HOH:O	2.48	0.47
1:A:2020:C:N4	1:A:2021:C:N4	2.62	0.47
1:A:2428:G:N7	30:4:60:LYS:NZ	2.60	0.47
1:A:2831:C:H2'	1:A:2832:C:H5'	1.96	0.47
37:A:4198:HOH:O	29:3:38:LYS:HE3	2.14	0.47
37:A:4535:HOH:O	5:E:50:GLU:HG2	2.14	0.47
8:H:107:VAL:HG23	37:H:6617:HOH:O	2.14	0.47
14:N:122:GLU:HB2	14:N:126:HIS:O	2.14	0.47
19:S:114:VAL:O	19:S:114:VAL:HG13	2.13	0.47
1:A:407:A:H5'	37:A:5999:HOH:O	2.14	0.47
1:A:816:G:H5'	1:A:1598:A:H4'	1.95	0.47
1:A:1414:A:N6	1:A:1415:G:C2	2.82	0.47
1:A:1470:A:OP1	14:N:93:ARG:NH1	2.44	0.47
3:C:164:ARG:HB2	27:1:68:CYS:SG	2.53	0.47
4:D:43:GLY:O	4:D:308:LEU:HD12	2.14	0.47
6:F:146:LYS:NZ	15:O:107:ASN:ND2	2.60	0.47
7:G:32:ARG:O	7:G:33:LEU:HD23	2.14	0.47
10:J:31:PHE:HA	10:J:85:ILE:CG2	2.45	0.47
17:Q:80:ARG:HG2	17:Q:87:ARG:CZ	2.44	0.47
1:A:120:A:H2'	1:A:120:A:N3	2.28	0.47
1:A:602:A:O2'	1:A:605:C:H4'	2.15	0.47
1:A:1525:G:H5'	1:A:1526:A:OP2	2.15	0.47
4:D:7:ARG:NH1	4:D:7:ARG:CG	2.77	0.47
8:H:21:GLU:HA	8:H:24:ARG:HE	1.79	0.47
8:H:100:ASP:HB3	37:H:5691:HOH:O	2.15	0.47
10:J:26:LYS:HG2	10:J:28:ILE:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:66:ARG:HG2	12:L:66:ARG:HH11	1.80	0.47
15:O:139:TRP:HA	15:O:139:TRP:HE3	1.80	0.47
17:Q:38:GLU:HA	17:Q:41:ARG:HH11	1.80	0.47
18:R:32:GLU:HA	18:R:71:TYR:OH	2.15	0.47
19:S:14:ALA:HB3	19:S:147:LEU:HB2	1.96	0.47
24:X:64:THR:O	24:X:68:THR:HG22	2.14	0.47
25:Y:9:VAL:HG13	25:Y:88:GLU:OE1	2.14	0.47
25:Y:25:ARG:HG2	37:Y:5356:HOH:O	2.14	0.47
1:A:170:U:OP1	14:N:83:SER:OG	2.31	0.47
1:A:538:C:H5"	1:A:539:G:C8	2.49	0.47
1:A:1183:C:N4	37:A:4368:HOH:O	2.44	0.47
1:A:2825:C:H4'	1:A:2826:G:O5'	2.14	0.47
1:A:2830:U:H3'	37:A:5197:HOH:O	2.14	0.47
1:A:2896:A:H2'	1:A:2896:A:N3	2.29	0.47
37:A:4160:HOH:O	26:Z:186:ARG:CD	2.58	0.47
37:A:5688:HOH:O	12:L:87:ARG:CZ	2.62	0.47
4:D:254:GLN:HG2	4:D:255:GLY:N	2.29	0.47
11:K:93:ARG:HB3	11:K:93:ARG:NH1	2.27	0.47
14:N:78:ASN:C	14:N:79:LYS:HG2	2.35	0.47
24:X:38:THR:HG22	24:X:39:ASP:H	1.80	0.47
1:A:349:U:O2'	1:A:350:C:H5'	2.15	0.47
1:A:449:A:N7	5:E:43:LYS:HG2	2.30	0.47
1:A:559:U:H5'	1:A:559:U:C6	2.38	0.47
1:A:657:G:H2'	1:A:658:C:C6	2.50	0.47
1:A:858:U:H2'	1:A:859:C:H6	1.79	0.47
1:A:960:G:N3	1:A:960:G:C2'	2.77	0.47
1:A:970:U:H2'	37:A:6301:HOH:O	2.14	0.47
1:A:1415:G:H5'	28:2:12:ASN:O	2.14	0.47
1:A:2353:A:H4'	1:A:2354:A:O5'	2.14	0.47
1:A:2421:G:H3'	1:A:2422:U:C5'	2.45	0.47
37:A:4035:HOH:O	4:D:27:ASN:HB2	2.15	0.47
2:B:3049:G:O2'	2:B:3050:G:H5'	2.15	0.47
4:D:84:LEU:O	4:D:84:LEU:HD13	2.13	0.47
4:D:162:MET:HG3	4:D:310:ARG:NH1	2.28	0.47
5:E:133:ARG:HD2	37:E:8408:HOH:O	2.15	0.47
6:F:23:VAL:HG21	6:F:45:THR:CG2	2.44	0.47
11:K:59:LYS:O	11:K:63:ILE:HG13	2.13	0.47
15:O:82:TYR:OH	15:O:176:ARG:NH1	2.48	0.47
19:S:113:HIS:O	19:S:145:LEU:HD12	2.15	0.47
1:A:929:A:H8	1:A:929:A:O5'	1.98	0.47
1:A:1517:U:C2	1:A:1670:G:N2	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1656:A:H2'	1:A:1657:A:O4'	2.15	0.47
1:A:1819:G:H2'	1:A:1820:G:C4'	2.45	0.47
6:F:65:GLU:HA	37:F:6752:HOH:O	2.14	0.47
1:A:654:A:OP2	16:P:38:ARG:HD3	2.14	0.47
1:A:1267:C:O2'	1:A:1268:C:H5'	2.15	0.47
1:A:2456:A:H2'	1:A:2457:U:C6	2.50	0.47
3:C:18:ALA:O	3:C:20:SER:N	2.43	0.47
3:C:94:LEU:HG	3:C:99:ILE:CD1	2.44	0.47
6:F:67:ASP:O	6:F:69:ILE:HG13	2.15	0.47
1:A:907:A:H2'	1:A:908:A:H8	1.79	0.47
1:A:1192:A:O2'	1:A:1193:A:OP1	2.29	0.47
1:A:1299:G:H5'	37:A:4043:HOH:O	2.14	0.47
4:D:162:MET:CE	4:D:310:ARG:HD3	2.45	0.47
4:D:207:LYS:HG2	4:D:304:PRO:HB3	1.95	0.47
5:E:140:VAL:HG12	5:E:141:SER:N	2.29	0.47
37:L:7438:HOH:O	22:V:20:MET:HE1	2.15	0.47
15:O:167:ASP:O	15:O:168:LEU:HD23	2.15	0.47
24:X:26:ILE:O	24:X:26:ILE:CG1	2.62	0.47
26:Z:144:ARG:NH1	37:Z:8578:HOH:O	2.37	0.47
28:2:28:HIS:O	28:2:32:LYS:N	2.48	0.47
1:A:401:C:P	37:A:5768:HOH:O	2.73	0.46
1:A:832:U:H2'	1:A:833:G:C8	2.50	0.46
1:A:1191:A:N1	1:A:1206:U:O4	2.48	0.46
1:A:1535:G:H2'	1:A:1536:C:C6	2.50	0.46
1:A:2429:A:H2'	1:A:2430:A:C8	2.50	0.46
4:D:305:ASP:O	4:D:306:LYS:CB	2.62	0.46
5:E:104:ASP:O	5:E:108:GLN:HG3	2.15	0.46
5:E:165:ASP:O	5:E:168:ARG:HB3	2.15	0.46
21:U:9:LYS:HD2	37:U:7242:HOH:O	2.16	0.46
30:4:18:GLN:OE1	30:4:73:GLU:HB3	2.15	0.46
1:A:407:A:H2'	1:A:408:A:H8	1.80	0.46
1:A:639:A:H2'	1:A:640:G:H8	1.79	0.46
1:A:795:G:N3	1:A:817:G:C2	2.83	0.46
1:A:1850:U:H2'	1:A:1851:G:C8	2.49	0.46
1:A:2433:A:H2'	1:A:2434:A:C8	2.49	0.46
1:A:2780:C:H1'	7:G:143:GLN:NE2	2.26	0.46
2:B:3042:C:O2	6:F:76:ARG:NH1	2.48	0.46
4:D:2:GLN:HA	37:D:8621:HOH:O	2.14	0.46
6:F:55:LYS:O	6:F:56:ARG:HB2	2.14	0.46
6:F:92:GLU:O	6:F:93:LEU:O	2.32	0.46
7:G:84:MET:HB2	7:G:131:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:28:GLU:OE2	12:L:58:THR:HG21	2.15	0.46
21:U:49:GLU:HB3	21:U:59:GLU:CG	2.45	0.46
1:A:12:U:H2'	1:A:13:G:H5'	1.97	0.46
1:A:1114:A:H2'	1:A:1115:U:H6	1.80	0.46
1:A:1135:G:H5'	37:A:5903:HOH:O	2.14	0.46
1:A:1503:U:H2'	1:A:1504:A:O4'	2.15	0.46
1:A:1878:G:O2'	1:A:1879:U:OP2	2.33	0.46
1:A:2314:G:H2'	1:A:2315:C:H5'	1.98	0.46
1:A:2730:G:O2'	1:A:2731:G:H5'	2.15	0.46
37:A:6105:HOH:O	29:3:20:ARG:HB3	2.16	0.46
8:H:79:GLN:HG3	8:H:82:ASP:OD2	2.14	0.46
14:N:182:LYS:HB2	14:N:194:ALA:HB2	1.98	0.46
15:O:61:ALA:CB	15:O:88:ALA:HB2	2.46	0.46
15:O:180:LEU:O	15:O:181:ASP:HB3	2.15	0.46
15:O:182:GLY:N	37:O:8571:HOH:O	2.46	0.46
17:Q:103:THR:HA	17:Q:106:ARG:NH1	2.31	0.46
27:1:51:GLY:HA3	37:1:8416:HOH:O	2.15	0.46
27:1:56:MET:HA	27:1:62:TYR:O	2.14	0.46
1:A:138:U:OP2	1:A:139:C:H5	1.99	0.46
1:A:424:C:H2'	1:A:425:U:C6	2.50	0.46
1:A:1166:A:H61	1:A:1180:U:H3	1.63	0.46
1:A:1593:C:OP1	17:Q:117:SER:CB	2.63	0.46
10:J:45:GLN:NE2	10:J:135:TRP:HE1	2.14	0.46
13:M:90:ARG:NH1	13:M:119:THR:HG21	2.30	0.46
1:A:1116:U:H3	1:A:1246:A:N6	2.04	0.46
1:A:1734:C:OP1	4:D:234:ARG:HD3	2.15	0.46
1:A:2834:G:OP1	25:Y:39:LYS:HE2	2.15	0.46
5:E:164:ALA:O	5:E:167:ASP:HB2	2.15	0.46
6:F:23:VAL:O	6:F:23:VAL:CG2	2.62	0.46
8:H:60:VAL:HG13	8:H:63:ILE:HG13	1.98	0.46
10:J:130:HIS:CG	10:J:133:ILE:HD11	2.50	0.46
12:L:58:THR:HG22	12:L:59:LYS:HG3	1.98	0.46
12:L:81:ARG:CD	12:L:87:ARG:NH1	2.71	0.46
13:M:143:THR:HG21	37:M:8535:HOH:O	2.14	0.46
15:O:132:ASN:O	15:O:135:VAL:HG12	2.15	0.46
21:U:37:GLN:OE1	21:U:118:SER:HA	2.14	0.46
1:A:1943:C:O4'	3:C:212:PRO:HA	2.15	0.46
1:A:2911:C:H2'	1:A:2912:C:C6	2.51	0.46
4:D:75:GLU:C	4:D:77:PRO:HD3	2.36	0.46
4:D:146:THR:O	4:D:159:PRO:HB3	2.14	0.46
4:D:248:ARG:HG2	37:D:8577:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:180:SER:N	37:E:8375:HOH:O	2.46	0.46
10:J:114:PRO:O	10:J:115:PHE:C	2.53	0.46
10:J:163:PRO:O	10:J:164:ALA:HB2	2.16	0.46
13:M:6:ARG:NH2	37:M:8545:HOH:O	2.48	0.46
14:N:172:GLY:C	14:N:183:VAL:HG11	2.34	0.46
20:T:51:GLN:HE21	20:T:53:ASN:ND2	2.12	0.46
30:4:73:GLU:HB2	37:4:8526:HOH:O	2.16	0.46
1:A:37:A:H2'	1:A:38:G:C8	2.50	0.46
1:A:154:C:P	14:N:188:ARG:HH12	2.39	0.46
1:A:283:U:H5	1:A:284:C:N4	2.13	0.46
1:A:559:U:H2'	1:A:560:C:O4'	2.16	0.46
1:A:646:G:H2'	1:A:647:U:C6	2.51	0.46
1:A:1183:C:N3	37:A:6020:HOH:O	2.48	0.46
1:A:2769:C:H2'	1:A:2770:G:C5'	2.45	0.46
37:A:7430:HOH:O	5:E:188:ARG:HD2	2.15	0.46
4:D:41:PHE:CZ	4:D:79:MET:HG3	2.50	0.46
7:G:86:VAL:CG1	7:G:129:GLU:HA	2.45	0.46
17:Q:101:GLN:HG3	37:Q:165:HOH:O	2.16	0.46
24:X:119:HIS:HD2	24:X:120:PRO:O	1.98	0.46
1:A:1015:C:H2'	1:A:1016:U:C6	2.51	0.46
1:A:2010:A:C2'	37:A:5933:HOH:O	2.64	0.46
1:A:2607:U:C4	4:D:242:TRP:CZ2	3.03	0.46
1:A:2748:G:H5'	37:A:7516:HOH:O	2.16	0.46
1:A:2766:A:O2'	1:A:2767:C:H5'	2.16	0.46
37:A:4940:HOH:O	10:J:57:ARG:HG3	2.15	0.46
5:E:223:LEU:HD12	5:E:223:LEU:HA	1.72	0.46
7:G:34:TRP:HA	37:G:4572:HOH:O	2.14	0.46
7:G:108:LEU:HD11	7:G:164:ASP:HB2	1.98	0.46
11:K:39:VAL:CG1	11:K:107:ASN:HB2	2.46	0.46
1:A:1413:A:H2'	1:A:1414:A:O4'	2.16	0.46
1:A:2719:A:C2	4:D:70:PRO:HG3	2.51	0.46
4:D:51:VAL:HG21	4:D:327:VAL:HG13	1.98	0.46
15:O:127:LEU:HD12	15:O:127:LEU:HA	1.75	0.46
22:V:17:THR:CG2	22:V:18:GLY:N	2.79	0.46
22:V:33:SER:O	22:V:37:GLU:HG3	2.15	0.46
24:X:11:VAL:O	24:X:12:ASN:HB2	2.15	0.46
25:Y:15:ARG:HB3	25:Y:15:ARG:NH1	2.30	0.46
1:A:894:A:C2	5:E:87:ARG:NH2	2.84	0.46
1:A:1418:U:OP1	29:3:42:TRP:HB3	2.16	0.46
1:A:1562:C:O2	1:A:1562:C:H2'	2.15	0.46
1:A:1850:U:H2'	1:A:1851:G:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2256:G:C2'	1:A:2257:G:H5'	2.46	0.46
1:A:2642:G:H2'	1:A:2643:G:O4'	2.15	0.46
2:B:3069:U:OP1	15:O:4:PRO:HG3	2.15	0.46
5:E:162:VAL:HG12	5:E:162:VAL:O	2.16	0.46
11:K:39:VAL:HG11	11:K:107:ASN:HB2	1.98	0.46
11:K:142:ASN:O	11:K:144:THR:N	2.49	0.46
14:N:137:ASP:HA	14:N:142:LYS:HE3	1.97	0.46
21:U:9:LYS:NZ	21:U:13:ARG:NH1	2.64	0.46
1:A:92:G:H4'	23:W:44:GLY:HA3	1.98	0.45
1:A:1562:C:H42	1:A:2738:G:H1	1.62	0.45
1:A:1842:A:C4	1:A:1979:G:C6	3.04	0.45
37:A:5381:HOH:O	3:C:164:ARG:NE	2.48	0.45
37:A:9313:HOH:O	24:X:9:GLY:HA3	2.16	0.45
2:B:3064:C:C2'	2:B:3065:A:H5'	2.46	0.45
4:D:82:VAL:O	4:D:82:VAL:CG1	2.61	0.45
7:G:31:ARG:HH12	7:G:68:HIS:CE1	2.34	0.45
8:H:26:THR:HB	8:H:102:GLY:HA3	1.97	0.45
12:L:74:VAL:HG12	12:L:75:ARG:HG3	1.97	0.45
14:N:68:ARG:O	14:N:68:ARG:HD3	2.16	0.45
14:N:79:LYS:HD2	37:N:8558:HOH:O	2.15	0.45
17:Q:16:VAL:CG1	17:Q:17:GLY:N	2.79	0.45
19:S:39:THR:O	19:S:40:ALA:C	2.54	0.45
1:A:393:G:C6	1:A:394:G:C6	3.05	0.45
1:A:2064:U:H2'	1:A:2065:C:H6	1.81	0.45
1:A:2670:G:O2'	1:A:2671:U:H5'	2.16	0.45
3:C:105:VAL:HG11	3:C:154:ALA:CB	2.44	0.45
3:C:170:VAL:HG13	27:1:22:ILE:CG2	2.45	0.45
8:H:28:ALA:HB3	8:H:99:THR:O	2.15	0.45
10:J:71:TYR:O	10:J:73:GLN:N	2.49	0.45
11:K:74:ARG:NH1	11:K:76:ASP:HB2	2.31	0.45
17:Q:120:ARG:NH2	17:Q:123:TYR:CD2	2.84	0.45
19:S:84:ALA:O	19:S:88:PHE:HD1	1.99	0.45
24:X:41:TYR:O	24:X:45:VAL:HG13	2.16	0.45
25:Y:20:GLU:CD	25:Y:21:PRO:HD2	2.36	0.45
27:1:60:CYS:HG	36:1:8403:CD:CD	1.48	0.45
30:4:15:ASN:ND2	37:4:8546:HOH:O	2.49	0.45
30:4:40:ARG:HD2	37:4:8547:HOH:O	2.15	0.45
1:A:303:C:H2'	1:A:304:G:O4'	2.17	0.45
1:A:1010:C:H4'	15:O:4:PRO:HB2	1.99	0.45
1:A:2698:G:H2'	1:A:2699:A:C8	2.51	0.45
4:D:221:GLN:HE22	12:L:42:ASN:ND2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:16:VAL:HG12	5:E:17:ASP:H	1.80	0.45
7:G:5:LEU:HD21	7:G:66:GLN:HG3	1.99	0.45
7:G:77:THR:OG1	7:G:78:GLU:N	2.47	0.45
16:P:26:TRP:HA	16:P:26:TRP:CE3	2.51	0.45
21:U:48:VAL:HG13	21:U:49:GLU:N	2.31	0.45
25:Y:51:ASP:OD2	25:Y:52:PRO:HD2	2.17	0.45
1:A:244:C:O5'	1:A:244:C:H6	1.98	0.45
1:A:329:A:OP2	5:E:206:ASN:HB2	2.17	0.45
1:A:398:U:H2'	1:A:399:C:C6	2.52	0.45
1:A:1116:U:O2'	1:A:1118:A:C2	2.50	0.45
1:A:2274:A:H1'	14:N:86:MET:SD	2.57	0.45
1:A:2515:C:C2'	1:A:2516:G:H5'	2.46	0.45
1:A:2515:C:H2'	1:A:2516:G:O4'	2.15	0.45
2:B:3056:A:C3'	2:B:3057:A:H5"	2.46	0.45
4:D:60:SER:C	4:D:62:ARG:H	2.19	0.45
10:J:150:LYS:HA	10:J:153:VAL:HG22	1.99	0.45
12:L:34:VAL:HB	37:L:7169:HOH:O	2.14	0.45
29:3:36:ASN:HB3	29:3:39:ARG:NE	2.32	0.45
1:A:485:A:O2'	1:A:487:G:H5'	2.16	0.45
1:A:657:G:H2'	1:A:658:C:H6	1.80	0.45
1:A:1391:G:H2'	1:A:1392:A:H5'	1.98	0.45
1:A:1544:U:O2'	1:A:1545:C:H5'	2.16	0.45
1:A:2506:A:H1'	37:A:6029:HOH:O	2.17	0.45
4:D:127:GLN:HA	37:D:8597:HOH:O	2.17	0.45
6:F:84:LEU:C	6:F:86:THR:H	2.20	0.45
7:G:31:ARG:HH12	7:G:68:HIS:CG	2.33	0.45
7:G:152:THR:HG21	7:G:165:GLY:HA2	1.97	0.45
10:J:48:LEU:HD13	10:J:146:TRP:HB3	1.98	0.45
14:N:122:GLU:OE2	14:N:127:LYS:HE2	2.16	0.45
15:O:91:ARG:HG3	15:O:186:LEU:HD23	1.98	0.45
16:P:25:VAL:HG23	16:P:26:TRP:H	1.82	0.45
29:3:19:SER:O	29:3:36:ASN:ND2	2.50	0.45
30:4:11:CYS:HB2	30:4:20:HIS:CE1	2.52	0.45
1:A:584:U:H3'	37:A:6070:HOH:O	2.16	0.45
1:A:818:A:O2'	27:1:13:ARG:HD3	2.16	0.45
1:A:945:U:H2'	1:A:946:C:C6	2.52	0.45
1:A:1667:A:H2'	1:A:1668:U:H6	1.81	0.45
1:A:2005:G:H3'	1:A:2005:G:OP2	2.17	0.45
1:A:2559:C:H4'	37:A:7230:HOH:O	2.15	0.45
3:C:179:MET:HG2	3:C:186:TRP:CG	2.52	0.45
4:D:53:LEU:HD21	4:D:270:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:49:ASP:HB3	5:E:52:ALA:HB2	1.97	0.45
6:F:76:ARG:O	6:F:77:ASP:HB2	2.17	0.45
8:H:22:VAL:CG2	8:H:104:ALA:HB2	2.46	0.45
11:K:42:GLU:O	11:K:131:THR:HG23	2.16	0.45
14:N:74:ARG:HD3	14:N:91:ILE:HD12	1.99	0.45
14:N:104:ARG:O	14:N:108:LYS:HG2	2.16	0.45
18:R:25:PRO:HA	18:R:26:PRO:HD3	1.81	0.45
24:X:122:ARG:HH11	24:X:122:ARG:CG	2.26	0.45
24:X:151:GLU:O	24:X:154:ARG:HB3	2.16	0.45
1:A:420:U:H2'	1:A:421:C:C6	2.51	0.45
1:A:716:G:C2'	1:A:717:C:O5'	2.65	0.45
1:A:920:C:H5'	1:A:921:G:C4	2.52	0.45
1:A:1826:C:O2'	1:A:1827:G:H5'	2.16	0.45
2:B:3031:C:H2'	2:B:3032:G:O4'	2.17	0.45
3:C:26:ASP:OD1	3:C:28:GLU:HG3	2.17	0.45
3:C:97:ALA:HB2	3:C:150:PRO:HB2	1.98	0.45
3:C:211:LYS:NZ	37:C:8620:HOH:O	2.45	0.45
17:Q:16:VAL:CG1	17:Q:20:ARG:HB2	2.47	0.45
21:U:41:ARG:NH1	21:U:42:VAL:O	2.49	0.45
23:W:51:LYS:O	23:W:55:ARG:HG3	2.16	0.45
1:A:716:G:H2'	1:A:717:C:O5'	2.17	0.45
1:A:778:C:C4	1:A:779:U:C4	3.05	0.45
1:A:1334:C:H2'	1:A:1335:C:H6	1.82	0.45
1:A:1730:G:H5'	1:A:1731:C:C6	2.52	0.45
2:B:3028:U:H2'	2:B:3029:C:C6	2.52	0.45
3:C:128:LEU:HD21	3:C:131:HIS:HE1	1.81	0.45
4:D:274:GLU:HA	4:D:292:GLY:O	2.17	0.45
6:F:63:ILE:C	37:F:5728:HOH:O	2.55	0.45
9:I:63:ARG:O	9:I:67:LEU:HG	2.17	0.45
13:M:130:ARG:O	13:M:134:GLU:HG3	2.16	0.45
22:V:6:CYS:C	22:V:8:TYR:H	2.19	0.45
26:Z:187:VAL:HB	37:Z:8572:HOH:O	2.16	0.45
27:1:22:ILE:O	27:1:26:VAL:HG23	2.17	0.45
27:1:42:CYS:SG	27:1:44:PHE:HB2	2.56	0.45
30:4:87:ARG:NH1	37:4:8523:HOH:O	2.49	0.45
1:A:120:A:H5'	28:2:20:ARG:HH21	1.82	0.45
1:A:424:C:H2'	1:A:425:U:H6	1.82	0.45
1:A:2072:G:H3'	1:A:2073:G:C5'	2.47	0.45
37:A:6215:HOH:O	3:C:22:ARG:HG2	2.17	0.45
2:B:3008:G:O6	15:O:11:ARG:NH1	2.49	0.45
2:B:3039:U:H3'	2:B:3040:C:H5"	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:VAL:O	3:C:43:VAL:HG12	2.16	0.45
15:O:87:LEU:CD1	15:O:186:LEU:HD21	2.40	0.45
18:R:75:ILE:CD1	18:R:84:ILE:HD11	2.47	0.45
19:S:69:LYS:HE2	19:S:78:GLY:O	2.17	0.45
19:S:82:GLU:HG3	19:S:83:LYS:N	2.31	0.45
21:U:27:LEU:HD23	21:U:98:VAL:HB	1.99	0.45
26:Z:126:PRO:HG2	26:Z:128:PHE:CZ	2.51	0.45
1:A:319:A:H4'	1:A:338:C:C5	2.51	0.45
1:A:451:C:O2'	1:A:452:G:H5'	2.17	0.45
1:A:876:A:N3	1:A:876:A:H2'	2.32	0.45
1:A:1114:A:H2'	1:A:1115:U:C6	2.52	0.45
1:A:1175:G:H1'	1:A:1193:A:H2'	1.99	0.45
1:A:1815:A:HO2'	1:A:2750:G:HO2'	1.61	0.45
1:A:1883:U:O2'	1:A:1884:G:H5'	2.17	0.45
4:D:312:ARG:HD3	4:D:315:VAL:HG13	1.98	0.45
6:F:59:GLY:O	6:F:61:PHE:N	2.38	0.45
10:J:81:TYR:CD1	10:J:81:TYR:C	2.89	0.45
11:K:63:ILE:HG22	11:K:64:GLY:N	2.31	0.45
15:O:43:VAL:O	15:O:43:VAL:HG12	2.17	0.45
17:Q:94:TRP:CZ2	17:Q:98:ILE:HG13	2.52	0.45
24:X:122:ARG:HG2	24:X:152:ALA:O	2.16	0.45
24:X:126:ASP:HB3	24:X:135:GLY:O	2.17	0.45
1:A:113:A:OP2	1:A:114:A:H2'	2.17	0.44
1:A:603:A:H4'	1:A:604:G:O5'	2.16	0.44
1:A:825:U:H5"	1:A:826:U:OP1	2.18	0.44
1:A:1787:C:H4'	1:A:2883:A:O4'	2.17	0.44
1:A:2502:C:H4'	10:J:151:MET:HG2	1.99	0.44
1:A:2851:G:C2'	1:A:2852:A:H5'	2.47	0.44
2:B:3036:C:C5	2:B:3037:C:C5	3.05	0.44
3:C:35:GLY:O	3:C:36:ASP:CB	2.57	0.44
4:D:41:PHE:CD1	4:D:79:MET:HE2	2.52	0.44
4:D:310:ARG:NH2	37:D:8557:HOH:O	2.49	0.44
7:G:126:ILE:HB	7:G:131:LEU:CD2	2.47	0.44
8:H:79:GLN:HB2	8:H:82:ASP:OD2	2.16	0.44
22:V:11:THR:HG22	22:V:53:ASP:OD2	2.17	0.44
1:A:134:U:C2	1:A:145:A:C2	3.06	0.44
1:A:612:U:H2'	1:A:613:C:C6	2.53	0.44
1:A:858:U:H2'	1:A:859:C:C6	2.52	0.44
1:A:1902:G:H2'	1:A:1903:U:O4'	2.17	0.44
1:A:1926:G:H2'	1:A:1927:A:C8	2.53	0.44
1:A:2578:G:H5'	1:A:2578:G:C8	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2821:C:H4'	4:D:116:PRO:CB	2.44	0.44
1:A:2846:C:H4'	37:A:5046:HOH:O	2.16	0.44
2:B:3051:A:H5'	15:O:160:SER:HB3	2.00	0.44
3:C:100:PRO:HG2	3:C:103:VAL:CG2	2.40	0.44
4:D:41:PHE:CE1	4:D:79:MET:HG3	2.52	0.44
4:D:69:VAL:HA	4:D:70:PRO:HD3	1.84	0.44
5:E:145:GLU:HG3	37:E:8374:HOH:O	2.18	0.44
10:J:13:ALA:HA	10:J:91:HIS:CE1	2.53	0.44
15:O:15:GLU:HB2	15:O:17:ARG:HG3	1.98	0.44
26:Z:187:VAL:CG1	26:Z:205:ILE:HA	2.47	0.44
1:A:162:C:H2'	1:A:163:U:H5'	1.99	0.44
1:A:251:C:H5'	14:N:140:ALA:HA	1.98	0.44
1:A:952:G:OP1	18:R:42:LYS:HE2	2.17	0.44
1:A:2718:C:H5'	1:A:2718:C:C6	2.49	0.44
3:C:33:GLU:H	3:C:33:GLU:CD	2.21	0.44
3:C:173:GLY:O	3:C:176:HIS:HB3	2.17	0.44
4:D:2:GLN:HB2	37:D:8637:HOH:O	2.17	0.44
14:N:25:TRP:HE3	14:N:26:HIS:HD2	1.64	0.44
15:O:33:ARG:NH1	15:O:103:ASP:OD2	2.46	0.44
15:O:73:ALA:HB1	15:O:74:PRO:CD	2.47	0.44
19:S:33:ARG:NH2	37:S:8532:HOH:O	2.42	0.44
21:U:71:VAL:HG12	21:U:72:ILE:N	2.32	0.44
24:X:6:GLN:HA	24:X:52:VAL:HG23	1.99	0.44
1:A:613:C:H2'	1:A:614:U:H6	1.83	0.44
1:A:736:A:H2'	1:A:737:A:O4'	2.17	0.44
1:A:795:G:H1'	1:A:817:G:N2	2.32	0.44
1:A:821:U:H5"	37:A:3033:HOH:O	2.16	0.44
1:A:862:U:H2'	1:A:863:G:H8	1.82	0.44
1:A:1311:G:C2	1:A:1312:G:C8	3.06	0.44
1:A:1805:G:H2'	1:A:1806:G:H8	1.82	0.44
1:A:2088:C:H1'	1:A:2841:A:N1	2.32	0.44
1:A:2397:G:C5	1:A:2465:A:C6	3.06	0.44
3:C:30:ARG:HE	3:C:30:ARG:HB3	1.68	0.44
4:D:329:TYR:HE2	22:V:15:PRO:HG2	1.79	0.44
5:E:5:ILE:CD1	5:E:16:VAL:HG23	2.30	0.44
6:F:59:GLY:C	6:F:61:PHE:H	2.16	0.44
9:I:64:ASN:N	9:I:64:ASN:ND2	2.65	0.44
14:N:99:ARG:CD	14:N:167:GLY:HA2	2.47	0.44
15:O:32:PRO:HD2	15:O:99:GLU:O	2.18	0.44
16:P:26:TRP:HA	16:P:26:TRP:HE3	1.81	0.44
16:P:98:LEU:HD12	16:P:98:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:42:GLU:HG2	20:T:49:VAL:HG23	1.98	0.44
21:U:48:VAL:HG22	21:U:97:ARG:O	2.18	0.44
1:A:553:G:O2'	26:Z:179:PRO:HG3	2.18	0.44
1:A:1759:A:N3	1:A:1818:C:H2'	2.33	0.44
1:A:2502:C:C4'	10:J:151:MET:HG2	2.48	0.44
3:C:105:VAL:CG1	3:C:106:CYS:N	2.80	0.44
5:E:115:LEU:HD12	5:E:115:LEU:HA	1.88	0.44
5:E:133:ARG:NH2	37:E:8422:HOH:O	2.51	0.44
6:F:84:LEU:HA	6:F:87:ALA:HB3	2.00	0.44
6:F:149:ARG:NH1	37:F:3066:HOH:O	2.35	0.44
6:F:166:ILE:O	6:F:169:THR:N	2.51	0.44
10:J:62:GLU:HA	37:J:8384:HOH:O	2.17	0.44
13:M:121:ILE:HG12	13:M:141:GLU:HB2	1.99	0.44
21:U:50:VAL:HG12	21:U:56:ALA:HA	1.99	0.44
24:X:14:HIS:HA	37:X:2978:HOH:O	2.18	0.44
24:X:21:LEU:HB3	24:X:26:ILE:CG1	2.47	0.44
26:Z:185:VAL:HA	37:Z:8564:HOH:O	2.17	0.44
30:4:48:ASN:ND2	30:4:50:GLY:H	2.16	0.44
30:4:65:THR:HB	30:4:83:TRP:H	1.82	0.44
1:A:240:C:H4'	14:N:146:GLN:NE2	2.33	0.44
1:A:582:C:O2'	1:A:583:G:H5'	2.18	0.44
1:A:1679:C:O2'	1:A:1685:A:N1	2.48	0.44
1:A:1768:C:H2'	1:A:1769:C:O4'	2.17	0.44
1:A:2044:G:OP1	25:Y:23:HIS:HE1	2.00	0.44
1:A:2443:C:H3'	37:A:3453:HOH:O	2.16	0.44
37:A:4377:HOH:O	3:C:11:ARG:CZ	2.66	0.44
4:D:36:PRO:CA	4:D:168:GLY:HA3	2.46	0.44
4:D:54:VAL:HB	37:D:8613:HOH:O	2.16	0.44
5:E:5:ILE:HD13	37:E:8426:HOH:O	2.17	0.44
5:E:98:ARG:NH1	37:E:8356:HOH:O	2.47	0.44
5:E:200:PRO:HB3	5:E:212:VAL:CG2	2.48	0.44
6:F:95:THR:CG2	6:F:174:VAL:HG22	2.48	0.44
6:F:128:LEU:HD23	6:F:128:LEU:C	2.37	0.44
10:J:149:ALA:C	10:J:151:MET:H	2.21	0.44
10:J:151:MET:HA	10:J:151:MET:HE3	2.00	0.44
14:N:123:ASP:C	14:N:123:ASP:OD1	2.56	0.44
30:4:69:TYR:HB2	30:4:78:HIS:CE1	2.53	0.44
1:A:514:G:OP1	1:A:514:G:H2'	2.18	0.44
1:A:1613:C:H2'	1:A:1614:G:O4'	2.18	0.44
1:A:1789:G:O6	17:Q:73:HIS:HE1	2.01	0.44
5:E:214:THR:HB	37:E:8326:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:111:ILE:O	8:H:115:VAL:HG23	2.16	0.44
14:N:61:ILE:N	14:N:61:ILE:CD1	2.81	0.44
21:U:88:PRO:HB3	37:U:6320:HOH:O	2.17	0.44
22:V:9:CYS:HA	22:V:52:THR:CG2	2.47	0.44
23:W:20:LEU:HD22	23:W:60:GLN:HE22	1.82	0.44
26:Z:189:ASN:HD22	26:Z:192:ASP:H	1.66	0.44
27:1:10:ARG:HG3	27:1:11:THR:N	2.33	0.44
27:1:30:GLU:HB3	27:1:34:LYS:HE3	2.00	0.44
29:3:30:ASP:O	29:3:31:GLU:HB2	2.16	0.44
1:A:101:C:H2'	1:A:102:A:H8	1.83	0.44
1:A:777:U:O2'	28:2:11:LYS:HG2	2.18	0.44
1:A:797:A:H5'	27:1:10:ARG:HG2	2.00	0.44
1:A:1044:C:H5"	37:A:9022:HOH:O	2.18	0.44
1:A:1688:G:C6	1:A:1692:C:C6	3.05	0.44
1:A:1829:A:H5"	37:A:3065:HOH:O	2.18	0.44
1:A:2656:G:C2'	1:A:2657:G:H5'	2.47	0.44
3:C:153:ARG:HB2	3:C:153:ARG:NH1	2.28	0.44
5:E:1:MET:HG2	5:E:2:GLN:NE2	2.33	0.44
8:H:47:LEU:HD22	8:H:108:LEU:CD1	2.48	0.44
12:L:30:LYS:O	12:L:55:VAL:HG13	2.18	0.44
14:N:5:TYR:HE2	14:N:46:LEU:HD13	1.83	0.44
14:N:52:LEU:HD21	37:N:8613:HOH:O	2.18	0.44
18:R:75:ILE:HD13	18:R:84:ILE:HD11	1.99	0.44
22:V:47:ARG:HG3	37:V:4381:HOH:O	2.17	0.44
24:X:146:ILE:HG22	24:X:147:ASP:N	2.33	0.44
1:A:820:G:C5	3:C:171:LYS:HB2	2.53	0.44
1:A:1857:A:N6	1:A:2247:C:H1'	2.33	0.44
1:A:2281:C:C2'	1:A:2282:U:H5'	2.47	0.44
1:A:2324:G:H4'	1:A:2418:G:O2'	2.18	0.44
3:C:211:LYS:HB2	37:C:8619:HOH:O	2.17	0.44
5:E:187:ARG:NH2	37:E:8365:HOH:O	2.42	0.44
7:G:137:ASP:OD1	7:G:139:GLU:HB2	2.18	0.44
14:N:99:ARG:HD2	14:N:167:GLY:HA2	2.00	0.44
17:Q:63:ARG:NH2	37:Q:198:HOH:O	2.39	0.44
29:3:40:ARG:HG2	29:3:40:ARG:HH11	1.82	0.44
1:A:553:G:O4'	1:A:1325:G:H5'	2.18	0.43
1:A:1730:G:C5'	1:A:1731:C:C6	3.01	0.43
1:A:2807:U:P	4:D:27:ASN:HD21	2.41	0.43
4:D:132:HIS:HB2	4:D:137:LEU:HD22	1.99	0.43
4:D:320:GLN:HG3	4:D:321:PRO:CD	2.47	0.43
10:J:147:ARG:HA	10:J:150:LYS:NZ	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:22:VAL:O	11:K:26:VAL:HG23	2.17	0.43
12:L:41:LYS:O	12:L:42:ASN:HB2	2.18	0.43
21:U:80:GLU:OE2	21:U:84:GLY:HA2	2.18	0.43
1:A:426:G:H2'	1:A:427:C:O4'	2.18	0.43
1:A:1447:U:H3'	1:A:1506:U:O2	2.18	0.43
4:D:125:GLU:OE2	4:D:129:ARG:NH1	2.51	0.43
5:E:51:TYR:CE2	28:2:53:LYS:HB3	2.53	0.43
5:E:150:THR:HA	5:E:203:ALA:O	2.18	0.43
15:O:44:ARG:HG3	15:O:45:ALA:N	2.33	0.43
21:U:41:ARG:O	21:U:43:ASN:ND2	2.51	0.43
22:V:31:PHE:CG	22:V:37:GLU:HG2	2.53	0.43
22:V:39:ASN:ND2	22:V:44:ARG:HH11	2.16	0.43
1:A:308:U:H5'	21:U:97:ARG:NH2	2.33	0.43
1:A:316:A:H5'	21:U:54:ASP:OD2	2.18	0.43
1:A:319:A:H4'	1:A:338:C:C4	2.53	0.43
1:A:902:G:N7	13:M:18:HIS:CD2	2.83	0.43
2:B:3003:A:H2'	37:B:8422:HOH:O	2.17	0.43
3:C:43:VAL:O	3:C:43:VAL:CG1	2.66	0.43
4:D:85:ARG:NH1	37:D:8635:HOH:O	2.51	0.43
7:G:119:HIS:HE1	7:G:147:ASP:OD2	2.01	0.43
7:G:126:ILE:HB	7:G:131:LEU:HD23	2.00	0.43
10:J:139:ASP:HB2	37:J:8348:HOH:O	2.17	0.43
21:U:14:ALA:HA	21:U:15:PRO:HD3	1.89	0.43
26:Z:234:VAL:HG12	26:Z:235:GLU:N	2.33	0.43
1:A:1313:A:H5'	26:Z:208:LYS:O	2.18	0.43
1:A:1887:U:OP1	27:1:21:LYS:HE3	2.18	0.43
1:A:2073:G:C6	1:A:2607:U:C2	3.06	0.43
3:C:215:ILE:HG13	3:C:216:SER:N	2.34	0.43
4:D:168:GLY:O	4:D:169:GLY:O	2.37	0.43
5:E:107:ARG:CZ	37:E:8453:HOH:O	2.63	0.43
5:E:218:VAL:HG12	37:E:8420:HOH:O	2.18	0.43
6:F:81:GLU:O	6:F:85:GLN:HG3	2.19	0.43
14:N:43:PRO:HG3	14:N:62:VAL:HG21	2.01	0.43
15:O:100:ALA:O	15:O:129:ILE:HG23	2.18	0.43
27:1:25:ARG:O	27:1:29:VAL:HG23	2.19	0.43
29:3:40:ARG:HA	29:3:45:ASN:ND2	2.32	0.43
1:A:324:G:O2'	1:A:325:U:H5'	2.19	0.43
1:A:820:G:C6	3:C:171:LYS:HB2	2.54	0.43
1:A:1495:C:H1'	1:A:1573:A:H1'	2.01	0.43
1:A:1523:G:C6	1:A:1524:U:O4	2.71	0.43
1:A:1846:U:O2'	3:C:172:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1874:U:H2'	3:C:120:ARG:HG3	2.00	0.43
1:A:1946:C:H2'	1:A:1971:G:C8	2.53	0.43
1:A:2498:C:O2'	1:A:2499:U:H5'	2.18	0.43
1:A:2502:C:H2'	1:A:2503:A:H5'	1.99	0.43
1:A:2904:U:H4'	25:Y:8:ARG:NH1	2.33	0.43
2:B:3026:C:P	37:B:8441:HOH:O	2.76	0.43
6:F:44:ILE:HG12	6:F:83:PHE:CE1	2.51	0.43
8:H:58:GLU:HG3	8:H:61:MET:HE1	1.99	0.43
37:L:1387:HOH:O	22:V:20:MET:HE3	2.17	0.43
13:M:130:ARG:HA	37:M:8554:HOH:O	2.18	0.43
14:N:66:ALA:O	14:N:67:ILE:HD13	2.19	0.43
15:O:37:ARG:NE	37:O:8535:HOH:O	2.50	0.43
15:O:161:GLY:O	15:O:162:ASP:C	2.56	0.43
24:X:125:HIS:HE1	37:X:3071:HOH:O	2.01	0.43
1:A:771:G:OP2	14:N:79:LYS:HE3	2.17	0.43
1:A:1438:G:HO2'	1:A:1684:A:H2	1.67	0.43
1:A:1543:G:N1	1:A:1641:A:OP2	2.42	0.43
1:A:1555:G:H4'	1:A:1630:A:H2	1.84	0.43
1:A:2595:U:H2'	1:A:2596:A:C8	2.53	0.43
1:A:2780:C:H2'	1:A:2781:U:C6	2.54	0.43
2:B:3092:G:C6	2:B:3093:A:C6	3.07	0.43
4:D:88:GLU:O	4:D:88:GLU:HG3	2.18	0.43
5:E:25:PRO:HG2	37:E:8324:HOH:O	2.18	0.43
9:I:66:LEU:O	9:I:69:ARG:HB3	2.19	0.43
11:K:6:PHE:O	11:K:8:ALA:N	2.52	0.43
12:L:49:LEU:HD21	12:L:74:VAL:O	2.18	0.43
14:N:78:ASN:O	14:N:79:LYS:HG2	2.19	0.43
15:O:116:PHE:N	37:O:8561:HOH:O	2.28	0.43
15:O:163:PHE:O	15:O:164:ASP:O	2.36	0.43
19:S:119:VAL:O	19:S:119:VAL:CG1	2.66	0.43
24:X:1:MET:HB2	24:X:103:GLU:HG2	2.01	0.43
1:A:10:U:H5'	37:A:6012:HOH:O	2.18	0.43
1:A:168:C:O2'	1:A:169:A:H5'	2.19	0.43
1:A:695:C:H2'	1:A:696:C:C6	2.53	0.43
1:A:737:A:H2'	1:A:738:G:O4'	2.18	0.43
1:A:1845:A:OP2	3:C:190:ARG:NH1	2.50	0.43
1:A:2729:C:O2'	1:A:2730:G:H5'	2.19	0.43
1:A:2781:U:H2'	1:A:2782:G:C5'	2.48	0.43
2:B:3025:G:H5"	2:B:3026:C:C6	2.53	0.43
4:D:82:VAL:HG12	4:D:101:TRP:CE3	2.54	0.43
5:E:139:VAL:CG1	37:E:8445:HOH:O	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:35:TYR:HA	11:K:127:ILE:HD12	2.01	0.43
8:H:28:ALA:CB	8:H:99:THR:HG23	2.48	0.43
13:M:34:GLY:C	13:M:36:ASP:H	2.22	0.43
19:S:96:VAL:HG13	19:S:106:GLY:HA3	2.01	0.43
21:U:55:PHE:CD2	21:U:77:VAL:HG13	2.53	0.43
23:W:7:GLU:O	23:W:11:MET:HG3	2.18	0.43
1:A:80:A:H5"	21:U:41:ARG:CZ	2.48	0.43
1:A:151:A:H2'	1:A:152:A:O4'	2.18	0.43
1:A:290:C:O2'	1:A:291:C:H5'	2.18	0.43
1:A:675:U:H2'	1:A:676:C:H5'	2.01	0.43
1:A:2274:A:H4'	14:N:77:PHE:HE1	1.84	0.43
2:B:3024:U:O2	2:B:3024:U:O4'	2.37	0.43
4:D:310:ARG:HD2	37:D:8649:HOH:O	2.19	0.43
5:E:7:ASP:OD1	5:E:11:ASN:O	2.36	0.43
5:E:27:ARG:HG2	5:E:30:LEU:HG	2.01	0.43
5:E:33:LYS:HD2	37:E:8455:HOH:O	2.19	0.43
8:H:34:ASN:O	8:H:38:LYS:HG3	2.19	0.43
10:J:154:THR:HB	10:J:155:PRO:HD3	2.01	0.43
10:J:162:SER:CB	10:J:163:PRO:CD	2.84	0.43
15:O:73:ALA:HB2	15:O:163:PHE:CZ	2.54	0.43
24:X:76:ASP:O	24:X:77:ALA:C	2.57	0.43
25:Y:74:ALA:HB1	25:Y:85:VAL:HG22	2.01	0.43
1:A:226:A:H1'	1:A:393:G:C5	2.54	0.43
1:A:1058:A:H2'	1:A:1060:C:C5'	2.46	0.43
1:A:1211:G:O2'	1:A:1212:C:H5'	2.18	0.43
1:A:1681:G:H5"	1:A:1682:A:H5'	2.00	0.43
1:A:1878:G:C1'	37:A:6096:HOH:O	2.66	0.43
1:A:2269:C:C2'	1:A:2270:G:H5'	2.48	0.43
1:A:2388:C:O2'	1:A:2389:U:H5'	2.18	0.43
1:A:2667:G:H1'	1:A:2914:A:N3	2.33	0.43
1:A:2769:C:H2'	1:A:2770:G:H5'	2.01	0.43
1:A:2791:U:H1'	1:A:2792:A:H5"	2.00	0.43
37:A:6656:HOH:O	21:U:38:ARG:NH1	2.50	0.43
4:D:162:MET:HG3	4:D:310:ARG:CZ	2.49	0.43
6:F:23:VAL:CG2	6:F:73:VAL:HB	2.47	0.43
6:F:95:THR:HG21	6:F:174:VAL:HG22	2.01	0.43
7:G:20:ILE:O	7:G:30:THR:HA	2.18	0.43
10:J:14:TYR:N	10:J:91:HIS:HE1	2.17	0.43
13:M:73:VAL:HG21	13:M:116:HIS:CD2	2.54	0.43
15:O:47:LEU:HD12	15:O:92:ALA:HB1	2.00	0.43
28:2:25:LYS:HE2	37:3:7213:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:53:LYS:HD3	28:2:53:LYS:HA	1.84	0.43
1:A:1160:G:HO2'	1:A:1190:G:H8	1.67	0.43
1:A:1422:U:H2'	1:A:1423:C:C6	2.54	0.43
1:A:2715:G:N2	4:D:264:GLU:OE1	2.52	0.43
37:A:6520:HOH:O	27:1:22:ILE:HG13	2.18	0.43
4:D:154:VAL:HA	4:D:155:PRO:HD3	1.86	0.43
4:D:238:ASN:ND2	4:D:240:GLY:H	2.01	0.43
10:J:165:GLY:C	10:J:166:ASN:HD22	2.21	0.43
13:M:125:PHE:CZ	13:M:140:VAL:HG13	2.54	0.43
21:U:26:THR:HA	21:U:39:ASN:HB3	2.00	0.43
1:A:187:A:H3'	1:A:188:C:H6	1.84	0.42
1:A:553:G:OP2	26:Z:204:ARG:NH2	2.51	0.42
1:A:1383:U:H2'	1:A:1384:C:C6	2.54	0.42
1:A:1706:G:C6	1:A:1707:G:C6	3.06	0.42
3:C:211:LYS:CB	37:C:8619:HOH:O	2.66	0.42
6:F:146:LYS:HZ3	15:O:107:ASN:HD21	1.64	0.42
7:G:107:PHE:CZ	7:G:152:THR:HB	2.54	0.42
8:H:110:GLU:O	8:H:114:LYS:HG3	2.18	0.42
10:J:65:ARG:CZ	37:J:8384:HOH:O	2.67	0.42
10:J:83:PHE:HE1	10:J:146:TRP:CZ2	2.37	0.42
10:J:113:ALA:N	10:J:114:PRO:HD3	2.33	0.42
13:M:148:GLU:HG2	37:M:8548:HOH:O	2.18	0.42
14:N:72:SER:HB2	14:N:93:ARG:HG2	2.01	0.42
14:N:99:ARG:NH1	37:N:8559:HOH:O	2.47	0.42
14:N:182:LYS:HD2	14:N:193:LYS:HB2	2.01	0.42
26:Z:184:GLU:OE1	26:Z:204:ARG:NH1	2.52	0.42
1:A:806:A:H2'	1:A:807:A:O4'	2.19	0.42
1:A:877:G:C5'	1:A:878:G:OP1	2.64	0.42
1:A:955:A:C2	1:A:1013:A:C4	3.07	0.42
1:A:1051:C:H2'	1:A:1052:G:O4'	2.19	0.42
1:A:1192:A:H3'	1:A:1193:A:H5'	2.00	0.42
1:A:1850:U:O4'	1:A:1941:A:C2	2.72	0.42
1:A:2356:A:H2'	1:A:2357:G:O4'	2.19	0.42
1:A:2481:G:H3'	1:A:2482:G:H5"	2.01	0.42
1:A:2757:A:H2'	1:A:2758:G:O4'	2.19	0.42
6:F:173:GLU:O	6:F:174:VAL:C	2.57	0.42
11:K:130:VAL:CG1	11:K:131:THR:N	2.81	0.42
13:M:55:GLN:HA	13:M:58:GLN:NE2	2.34	0.42
13:M:73:VAL:HG11	13:M:118:LEU:HD21	2.00	0.42
14:N:173:LEU:HD23	14:N:183:VAL:HG12	2.01	0.42
15:O:164:ASP:C	15:O:164:ASP:OD1	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:44:ARG:CB	37:V:3805:HOH:O	2.64	0.42
1:A:154:C:H2'	1:A:155:C:H6	1.84	0.42
1:A:331:A:C6	1:A:332:G:C4	3.07	0.42
1:A:907:A:H2'	1:A:908:A:C8	2.52	0.42
1:A:2004:U:H1'	37:A:3176:HOH:O	2.19	0.42
1:A:2274:A:C4'	14:N:77:PHE:HE1	2.32	0.42
1:A:2668:G:H2'	1:A:2669:U:C6	2.54	0.42
4:D:217:ARG:HG3	4:D:257:THR:CG2	2.50	0.42
14:N:32:ARG:NH2	37:N:8596:HOH:O	2.52	0.42
14:N:164:THR:CG2	14:N:165:SER:N	2.71	0.42
15:O:80:SER:HB2	37:O:8537:HOH:O	2.20	0.42
15:O:90:LEU:CB	15:O:186:LEU:HD22	2.49	0.42
15:O:93:GLN:HG2	37:O:8559:HOH:O	2.17	0.42
24:X:146:ILE:HD13	24:X:146:ILE:HA	1.90	0.42
1:A:628:A:C8	1:A:2071:C:N4	2.88	0.42
1:A:875:A:C2	3:C:194:MET:SD	3.13	0.42
1:A:1483:C:O2'	1:A:1484:G:H5'	2.20	0.42
1:A:1819:G:H2'	1:A:1820:G:C5'	2.50	0.42
1:A:2093:G:H5"	37:A:9461:HOH:O	2.18	0.42
1:A:2898:G:H4'	4:D:288:GLY:HA2	2.01	0.42
37:A:7644:HOH:O	26:Z:172:THR:HB	2.19	0.42
10:J:26:LYS:HD2	10:J:28:ILE:CG1	2.49	0.42
14:N:35:PRO:HD2	14:N:38:VAL:HG21	2.02	0.42
21:U:18:GLU:O	21:U:21:LYS:HG2	2.19	0.42
21:U:48:VAL:HG22	21:U:97:ARG:C	2.39	0.42
27:1:30:GLU:O	27:1:33:HIS:HB3	2.19	0.42
27:1:41:VAL:HG12	27:1:42:CYS:N	2.34	0.42
28:2:28:HIS:HD2	28:2:30:LYS:H	1.67	0.42
1:A:23:G:H1'	1:A:520:A:N6	2.35	0.42
1:A:255:A:H2'	1:A:256:C:C6	2.54	0.42
1:A:871:G:H5"	1:A:871:G:H8	1.78	0.42
1:A:1419:U:H2'	1:A:1685:A:C2	2.54	0.42
1:A:2392:C:H4'	37:R:2875:HOH:O	2.19	0.42
1:A:2723:G:H1'	37:A:4809:HOH:O	2.19	0.42
1:A:2734:G:O2'	1:A:2735:U:H5'	2.19	0.42
1:A:2912:C:H2'	1:A:2913:A:O4'	2.20	0.42
37:A:9954:HOH:O	24:X:10:GLU:HG2	2.19	0.42
4:D:24:PRO:HG2	4:D:204:GLY:HA2	2.01	0.42
8:H:110:GLU:HA	8:H:113:ASP:OD2	2.19	0.42
9:I:27:ILE:HD12	9:I:70:ALA:HB1	2.01	0.42
13:M:54:PRO:HG2	13:M:57:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:52:ARG:HB2	21:U:95:ASN:HB3	2.02	0.42
25:Y:78:GLU:CG	25:Y:79:GLU:N	2.80	0.42
1:A:1470:A:OP1	14:N:93:ARG:HD2	2.19	0.42
1:A:1883:U:H5'	1:A:2012:U:OP2	2.20	0.42
1:A:2621:U:H5	37:A:9965:HOH:O	2.03	0.42
1:A:2691:A:H8	1:A:2691:A:OP1	2.02	0.42
1:A:2694:A:H4'	7:G:91:PHE:HE1	1.85	0.42
3:C:36:ASP:HB2	3:C:84:VAL:N	2.35	0.42
3:C:69:LEU:CD2	3:C:120:ARG:HB3	2.44	0.42
3:C:194:MET:CE	3:C:199:HIS:HB2	2.50	0.42
4:D:147:VAL:O	4:D:147:VAL:HG12	2.19	0.42
5:E:39:GLN:O	5:E:43:LYS:HD3	2.19	0.42
6:F:35:ALA:C	6:F:37:ALA:N	2.73	0.42
6:F:146:LYS:HZ1	15:O:107:ASN:HD21	1.62	0.42
7:G:119:HIS:CE1	7:G:147:ASP:OD2	2.72	0.42
8:H:12:LEU:HD23	8:H:12:LEU:O	2.20	0.42
10:J:113:ALA:N	10:J:114:PRO:CD	2.82	0.42
13:M:146:GLY:C	13:M:148:GLU:H	2.23	0.42
1:A:24:G:N2	1:A:518:G:H1'	2.34	0.42
1:A:338:C:H4'	5:E:174:ILE:HD11	2.01	0.42
1:A:941:G:C6	1:A:942:U:C4	3.07	0.42
1:A:1067:A:H5'	37:X:2978:HOH:O	2.20	0.42
1:A:1702:U:H5"	37:A:7189:HOH:O	2.20	0.42
10:J:43:PRO:HD2	10:J:137:ASN:HA	2.02	0.42
14:N:174:ARG:HG3	37:N:8521:HOH:O	2.18	0.42
20:T:38:ALA:O	20:T:42:GLU:HG3	2.19	0.42
24:X:5:VAL:O	24:X:52:VAL:HG22	2.19	0.42
26:Z:106:THR:CG2	26:Z:107:PRO:HD2	2.50	0.42
26:Z:216:ARG:CD	37:Z:8571:HOH:O	2.59	0.42
1:A:152:A:O2'	1:A:153:C:H5'	2.19	0.42
1:A:291:C:H2'	1:A:292:G:O4'	2.20	0.42
1:A:1191:A:C3'	1:A:1192:A:H5"	2.47	0.42
1:A:1342:C:O2'	1:A:1343:C:H5'	2.19	0.42
1:A:1440:U:P	37:A:4436:HOH:O	2.77	0.42
1:A:1762:C:H2'	1:A:1763:C:H6	1.85	0.42
1:A:2092:G:H5"	1:A:2613:G:OP1	2.20	0.42
1:A:2443:C:O3'	13:M:56:LYS:HE3	2.20	0.42
1:A:2511:A:H1'	37:A:4768:HOH:O	2.19	0.42
1:A:2547:C:H2'	1:A:2548:C:H6	1.84	0.42
1:A:2781:U:O2'	1:A:2782:G:H5'	2.19	0.42
4:D:279:THR:CG2	4:D:280:VAL:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:77:GLY:O	11:K:78:ILE:C	2.58	0.42
12:L:106:GLY:HA3	37:L:5264:HOH:O	2.19	0.42
14:N:37:VAL:HG21	14:N:108:LYS:HG2	2.01	0.42
21:U:32:ARG:NH1	21:U:38:ARG:NH1	2.63	0.42
23:W:1:THR:HG23	23:W:2:VAL:N	2.25	0.42
25:Y:15:ARG:HH11	25:Y:15:ARG:CB	2.31	0.42
1:A:101:C:H2'	1:A:102:A:C8	2.55	0.42
1:A:111:C:H2'	1:A:112:G:O4'	2.20	0.42
1:A:137:U:OP1	1:A:259:G:O2'	2.38	0.42
1:A:1238:C:H4'	37:A:5994:HOH:O	2.20	0.42
1:A:1592:G:HO2'	1:A:1593:C:C4'	2.33	0.42
1:A:2121:G:O2'	1:A:2122:C:H5'	2.20	0.42
2:B:3057:A:O2'	6:F:152:PRO:HD2	2.20	0.42
10:J:117:LYS:O	10:J:119:VAL:HG13	2.20	0.42
15:O:37:ARG:NH2	37:O:8535:HOH:O	2.52	0.42
15:O:163:PHE:HA	37:O:8520:HOH:O	2.19	0.42
21:U:43:ASN:C	21:U:45:GLY:H	2.23	0.42
24:X:65:VAL:CA	24:X:68:THR:HG22	2.49	0.42
27:1:32:LYS:HZ2	27:1:70:GLN:NE2	2.18	0.42
1:A:245:C:C2'	1:A:246:G:H5'	2.50	0.42
1:A:764:C:H2'	1:A:765:G:O4'	2.20	0.42
1:A:1079:A:H4'	1:A:2078:U:H5'	2.02	0.42
1:A:1119:G:C8	11:K:52:GLN:NE2	2.86	0.42
1:A:1505:U:H5'	1:A:1505:U:C6	2.50	0.42
1:A:1641:A:C2'	1:A:1642:A:H5'	2.47	0.42
1:A:2362:A:H2'	1:A:2363:G:C8	2.55	0.42
1:A:2544:G:H2'	1:A:2545:U:O4'	2.20	0.42
1:A:2591:C:H2'	1:A:2592:G:O4'	2.20	0.42
1:A:2894:C:O2'	1:A:2895:C:H5'	2.19	0.42
1:A:2909:G:O2'	1:A:2910:A:H5'	2.20	0.42
4:D:24:PRO:CG	4:D:204:GLY:HA2	2.50	0.42
4:D:76:THR:N	4:D:77:PRO:HD3	2.35	0.42
4:D:168:GLY:N	4:D:174:ARG:HD3	2.34	0.42
9:I:71:LEU:C	9:I:73:ASP:H	2.23	0.42
14:N:95:LYS:HG2	14:N:99:ARG:HB3	2.01	0.42
27:1:11:THR:HG21	27:1:23:ARG:HB2	2.01	0.42
1:A:20:G:H1'	19:S:5:SER:HB3	2.01	0.41
1:A:946:C:H2'	1:A:947:U:C6	2.55	0.41
1:A:951:A:H2'	1:A:952:G:H5'	2.01	0.41
1:A:1312:G:O2'	26:Z:208:LYS:HB3	2.19	0.41
1:A:1434:A:H2'	1:A:1436:C:C5	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2276:U:H2'	1:A:2277:U:C6	2.55	0.41
1:A:2755:G:H1'	37:A:4651:HOH:O	2.21	0.41
2:B:3074:G:C6	2:B:3075:G:N7	2.87	0.41
3:C:39:ALA:HB3	3:C:61:GLU:OE2	2.20	0.41
3:C:192:VAL:CG1	3:C:192:VAL:O	2.67	0.41
10:J:30:GLN:H	10:J:65:ARG:NH1	2.18	0.41
10:J:57:ARG:HG3	10:J:57:ARG:HH11	1.85	0.41
11:K:107:ASN:ND2	11:K:107:ASN:C	2.69	0.41
11:K:131:THR:HB	11:K:134:GLU:HG3	2.01	0.41
12:L:34:VAL:HG21	12:L:46:LYS:O	2.20	0.41
15:O:67:ALA:HA	15:O:71:TRP:HB3	2.02	0.41
1:A:113:A:H2'	1:A:115:U:O4	2.20	0.41
1:A:213:G:N2	1:A:225:G:H2'	2.35	0.41
1:A:419:A:H1'	1:A:1921:A:C2	2.56	0.41
1:A:590:A:H2'	1:A:591:A:H5'	2.02	0.41
1:A:667:C:H2'	1:A:668:C:H6	1.84	0.41
1:A:843:A:C2	1:A:846:A:C8	3.08	0.41
1:A:1706:G:C5	1:A:1707:G:C6	3.09	0.41
1:A:1756:G:H1'	37:A:6237:HOH:O	2.19	0.41
1:A:2423:C:H2'	1:A:2424:U:C6	2.55	0.41
1:A:2775:A:C6	1:A:2776:A:C6	3.08	0.41
1:A:2833:C:C2	1:A:2848:G:N2	2.88	0.41
3:C:70:ALA:HA	3:C:71:PRO:HD3	1.81	0.41
6:F:99:ASP:HB2	6:F:103:ASN:CB	2.49	0.41
8:H:20:LEU:O	8:H:23:ALA:HB3	2.21	0.41
11:K:51:GLU:O	11:K:55:GLU:HG3	2.20	0.41
13:M:65:ASP:CG	13:M:111:ALA:HB3	2.41	0.41
13:M:72:ASN:OD1	13:M:75:LEU:HD12	2.20	0.41
14:N:138:HIS:C	14:N:139:PRO:O	2.52	0.41
15:O:66:LEU:HD12	15:O:66:LEU:HA	1.94	0.41
28:2:17:THR:N	28:2:27:TYR:O	2.45	0.41
29:3:18:ASN:ND2	29:3:40:ARG:H	2.19	0.41
1:A:74:A:H2'	1:A:75:U:C6	2.56	0.41
1:A:336:G:OP1	37:A:3700:HOH:O	2.21	0.41
1:A:391:U:OP2	14:N:84:LYS:NZ	2.50	0.41
1:A:1375:A:C2'	1:A:1376:G:H5'	2.51	0.41
1:A:2377:U:O5'	1:A:2377:U:H6	2.03	0.41
1:A:2456:A:H2'	1:A:2457:U:H6	1.84	0.41
1:A:2541:U:H5'	1:A:2611:G:O6	2.20	0.41
3:C:36:ASP:O	3:C:37:VAL:C	2.59	0.41
3:C:135:VAL:N	37:C:8595:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:MET:HG2	3:C:186:TRP:CB	2.50	0.41
4:D:215:VAL:HA	4:D:220:VAL:HG22	2.02	0.41
4:D:243:ASN:HA	4:D:244:PRO:C	2.40	0.41
5:E:13:ASP:OD1	5:E:13:ASP:O	2.38	0.41
6:F:49:PRO:HG3	37:F:5828:HOH:O	2.19	0.41
6:F:60:GLU:C	6:F:62:ASP:N	2.73	0.41
14:N:134:ILE:CG2	14:N:141:ILE:HD13	2.50	0.41
19:S:29:LYS:HD3	37:S:8532:HOH:O	2.20	0.41
21:U:41:ARG:HG2	21:U:41:ARG:NH1	2.34	0.41
23:W:42:ASN:O	23:W:44:GLY:N	2.53	0.41
24:X:154:ARG:HB3	24:X:154:ARG:HE	1.60	0.41
25:Y:43:VAL:HG12	25:Y:47:ALA:HB3	2.01	0.41
27:1:38:LYS:HD3	37:1:8423:HOH:O	2.19	0.41
1:A:128:A:C8	1:A:128:A:C3'	3.02	0.41
1:A:282:C:H2'	1:A:283:U:O4'	2.19	0.41
1:A:952:G:N3	1:A:2302:A:H2'	2.35	0.41
1:A:1504:A:O2'	1:A:1506:U:OP2	2.32	0.41
1:A:1516:C:H2'	1:A:1517:U:C6	2.55	0.41
1:A:2134:G:C6	1:A:2258:A:C8	3.09	0.41
1:A:2494:G:H4'	10:J:5:MET:SD	2.60	0.41
1:A:2646:G:C2	1:A:2647:C:C6	3.09	0.41
1:A:2890:A:C1'	22:V:56:ARG:NH2	2.80	0.41
4:D:139:ASP:HB3	37:D:8550:HOH:O	2.19	0.41
7:G:112:ALA:HA	7:G:113:PRO:HD3	1.92	0.41
8:H:117:GLU:C	8:H:119:ARG:N	2.72	0.41
21:U:71:VAL:CG1	21:U:72:ILE:N	2.83	0.41
24:X:4:LEU:HD23	24:X:4:LEU:HA	1.88	0.41
1:A:506:G:N2	1:A:509:A:H5"	2.34	0.41
1:A:1730:G:H5'	1:A:1731:C:H5	1.81	0.41
3:C:135:VAL:HG21	3:C:147:ARG:NH1	2.35	0.41
4:D:71:VAL:CG1	4:D:296:LEU:HB3	2.47	0.41
4:D:102:THR:HG21	4:D:182:VAL:O	2.20	0.41
4:D:277:GLU:N	4:D:278:PRO:HD2	2.35	0.41
6:F:93:LEU:CB	6:F:97:GLN:OE1	2.67	0.41
6:F:128:LEU:N	37:F:6007:HOH:O	2.53	0.41
9:I:67:LEU:O	9:I:71:LEU:HG	2.20	0.41
13:M:62:ALA:HB2	13:M:103:ALA:CB	2.50	0.41
15:O:67:ALA:C	15:O:69:TYR:N	2.74	0.41
17:Q:13:VAL:CG2	17:Q:41:ARG:HG2	2.50	0.41
17:Q:28:GLN:NE2	37:Q:160:HOH:O	2.54	0.41
24:X:137:GLN:HG3	24:X:137:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:187:VAL:O	26:Z:187:VAL:HG13	2.21	0.41
1:A:128:A:HO2'	1:A:129:A:H5'	1.85	0.41
1:A:776:A:OP1	28:2:28:HIS:HE1	2.03	0.41
1:A:814:G:H8	37:A:7181:HOH:O	2.03	0.41
1:A:907:A:H4'	1:A:1328:A:C2	2.56	0.41
1:A:920:C:H4'	1:A:921:G:C2	2.55	0.41
1:A:1524:U:O2'	1:A:1525:G:P	2.78	0.41
1:A:2607:U:H4'	37:A:9422:HOH:O	2.20	0.41
37:A:3148:HOH:O	14:N:87:MET:HE3	2.19	0.41
37:A:7430:HOH:O	5:E:188:ARG:CD	2.67	0.41
3:C:36:ASP:CB	3:C:85:ASP:H	2.33	0.41
3:C:103:VAL:HA	3:C:104:PRO:HD3	1.93	0.41
3:C:125:ASN:ND2	37:C:8535:HOH:O	2.49	0.41
5:E:236:THR:C	37:E:8445:HOH:O	2.59	0.41
1:A:37:A:H2'	1:A:38:G:H8	1.85	0.41
1:A:295:C:H2'	1:A:296:G:O4'	2.20	0.41
1:A:1474:C:H6	1:A:1474:C:C5'	2.15	0.41
1:A:1584:C:O2'	1:A:1585:C:H5'	2.20	0.41
1:A:1666:C:O2'	1:A:1667:A:C5'	2.65	0.41
1:A:2420:G:H4'	37:A:4066:HOH:O	2.20	0.41
1:A:2820:A:H2'	1:A:2821:C:C6	2.56	0.41
1:A:2826:G:C6	1:A:2913:A:N6	2.89	0.41
37:A:5688:HOH:O	12:L:87:ARG:NE	2.53	0.41
6:F:24:HIS:HB2	6:F:72:LYS:CB	2.51	0.41
10:J:86:ARG:H	10:J:86:ARG:HG2	1.54	0.41
11:K:19:MET:HE2	11:K:79:PHE:HA	2.03	0.41
11:K:26:VAL:HG13	11:K:36:VAL:HG11	2.02	0.41
11:K:47:THR:HG22	11:K:48:GLY:N	2.36	0.41
15:O:38:LYS:HE2	15:O:107:ASN:ND2	2.36	0.41
25:Y:74:ALA:HB2	25:Y:85:VAL:HG13	2.01	0.41
1:A:69:A:H5'	1:A:69:A:H8	1.81	0.41
1:A:195:C:H2'	1:A:196:G:H5'	2.03	0.41
1:A:466:A:H2'	1:A:467:G:O4'	2.20	0.41
1:A:921:G:H4'	1:A:924:G:N1	2.35	0.41
1:A:932:U:H2'	1:A:933:C:C6	2.56	0.41
1:A:2505:G:H8	37:A:5612:HOH:O	2.03	0.41
1:A:2654:C:H5'	37:D:8663:HOH:O	2.21	0.41
4:D:268:ARG:NE	37:D:8608:HOH:O	2.54	0.41
7:G:69:ILE:HA	7:G:72:MET:HE3	2.01	0.41
10:J:47:GLU:CG	10:J:133:ILE:HD12	2.51	0.41
14:N:134:ILE:O	14:N:136:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:25:ARG:HA	15:O:28:LYS:HG3	2.03	0.41
16:P:96:VAL:HG13	16:P:100:GLN:HB2	2.02	0.41
16:P:98:LEU:O	16:P:102:ILE:HG13	2.19	0.41
16:P:115:ARG:NH1	37:P:6194:HOH:O	2.53	0.41
17:Q:10:ALA:CA	17:Q:13:VAL:HG12	2.48	0.41
17:Q:115:SER:HG	17:Q:118:GLN:HG3	1.77	0.41
30:4:69:TYR:CZ	30:4:80:ARG:HD2	2.56	0.41
1:A:545:G:H2'	1:A:546:C:O4'	2.21	0.41
1:A:702:G:O2'	1:A:703:G:H5'	2.21	0.41
1:A:821:U:O2'	1:A:822:C:H5'	2.21	0.41
1:A:869:G:OP1	14:N:79:LYS:HE2	2.20	0.41
1:A:876:A:N3	1:A:876:A:C2'	2.84	0.41
1:A:1218:U:H2'	1:A:1219:U:C6	2.56	0.41
1:A:1269:G:H2'	1:A:1270:U:H6	1.84	0.41
1:A:1298:U:H2'	1:A:1299:G:C8	2.55	0.41
1:A:1457:U:O2'	1:A:1458:A:H5'	2.20	0.41
1:A:1739:G:O2'	1:A:1740:U:H5'	2.21	0.41
1:A:1754:A:H2'	1:A:1755:A:O4'	2.21	0.41
1:A:2283:G:C5	10:J:111:MET:HB3	2.56	0.41
1:A:2478:U:O2'	1:A:2479:A:H5'	2.20	0.41
1:A:2481:G:C3'	1:A:2482:G:H5"	2.50	0.41
1:A:2819:C:H2'	1:A:2820:A:C8	2.56	0.41
1:A:2831:C:H2'	1:A:2832:C:C5'	2.50	0.41
1:A:2900:G:H2'	1:A:2901:C:O4'	2.21	0.41
37:A:6996:HOH:O	3:C:211:LYS:HG2	2.21	0.41
2:B:3047:A:C2	2:B:3048:C:C2	3.08	0.41
2:B:3057:A:N6	37:B:8443:HOH:O	2.51	0.41
4:D:4:SER:O	4:D:5:ARG:HB2	2.21	0.41
5:E:33:LYS:HE2	37:E:8360:HOH:O	2.20	0.41
5:E:166:ILE:CD1	5:E:207:LEU:HD13	2.51	0.41
6:F:35:ALA:HB1	37:F:3279:HOH:O	2.21	0.41
6:F:95:THR:C	6:F:97:GLN:N	2.71	0.41
7:G:31:ARG:NH1	7:G:68:HIS:CD2	2.89	0.41
7:G:133:VAL:HG12	7:G:141:VAL:HG13	2.03	0.41
8:H:39:SER:CB	8:H:45:ALA:HB2	2.47	0.41
14:N:42:ARG:HA	14:N:43:PRO:HD3	1.90	0.41
18:R:28:ARG:HG2	37:R:4350:HOH:O	2.21	0.41
21:U:43:ASN:HD22	21:U:108:ARG:NH2	2.19	0.41
22:V:47:ARG:CG	37:V:4381:HOH:O	2.69	0.41
23:W:57:LYS:HA	23:W:60:GLN:HE21	1.86	0.41
1:A:492:C:O2'	1:A:493:U:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:A:C2	13:M:71:GLU:HG2	2.56	0.41
1:A:1076:G:C2	1:A:1084:C:C2	3.09	0.41
1:A:1494:A:C4	1:A:1495:C:C5	3.09	0.41
1:A:1735:C:O2'	1:A:1736:A:H5'	2.20	0.41
1:A:1820:G:C6	1:A:2030:A:C2	3.09	0.41
1:A:2297:U:H1'	37:A:5144:HOH:O	2.20	0.41
2:B:3052:A:H2'	2:B:3053:G:O4'	2.21	0.41
4:D:26:PHE:CE1	4:D:310:ARG:HB3	2.56	0.41
4:D:217:ARG:HE	4:D:257:THR:HG22	1.86	0.41
7:G:36:PRO:HD3	11:K:127:ILE:HD12	2.02	0.41
7:G:81:GLU:HA	7:G:133:VAL:O	2.20	0.41
11:K:39:VAL:HG12	11:K:40:ASN:CG	2.42	0.41
11:K:107:ASN:HD22	11:K:108:PRO:N	2.19	0.41
12:L:118:ALA:C	12:L:120:ARG:H	2.24	0.41
14:N:157:LEU:HB3	14:N:160:PHE:HD1	1.85	0.41
16:P:73:ASP:HA	16:P:92:VAL:O	2.21	0.41
17:Q:121:ASP:HB2	37:Q:201:HOH:O	2.20	0.41
18:R:16:ASN:HD22	18:R:16:ASN:HA	1.61	0.41
20:T:10:VAL:HG11	23:W:36:ALA:HA	2.03	0.41
20:T:57:THR:C	20:T:59:ASP:H	2.24	0.41
23:W:42:ASN:N	23:W:43:PRO:HD3	2.36	0.41
24:X:40:ALA:HB3	37:X:5390:HOH:O	2.21	0.41
29:3:35:ARG:N	37:3:2691:HOH:O	2.53	0.41
1:A:656:G:H5'	16:P:3:THR:CG2	2.51	0.40
1:A:1132:A:H2'	1:A:1133:A:C8	2.56	0.40
1:A:1375:A:O2'	1:A:1376:G:H5'	2.21	0.40
1:A:1771:U:O2'	1:A:1773:G:N7	2.52	0.40
1:A:2591:C:OP2	4:D:1:PRO:HD3	2.21	0.40
2:B:3040:C:N4	6:F:51:ARG:HB2	2.35	0.40
5:E:166:ILE:HD11	5:E:207:LEU:HD13	2.03	0.40
12:L:55:VAL:CG1	12:L:56:SER:N	2.84	0.40
13:M:148:GLU:HB2	37:M:8586:HOH:O	2.20	0.40
15:O:120:GLU:HG3	15:O:136:LEU:HD13	2.03	0.40
21:U:1:SER:N	37:U:5837:HOH:O	2.54	0.40
1:A:130:C:H2'	37:A:3143:HOH:O	2.21	0.40
1:A:587:A:H5"	37:A:7260:HOH:O	2.20	0.40
1:A:1250:C:O2'	1:A:1251:C:H5'	2.21	0.40
1:A:1462:C:H2'	1:A:1463:A:H8	1.84	0.40
1:A:1485:A:H4'	37:A:3269:HOH:O	2.21	0.40
1:A:1909:A:H2'	1:A:1910:A:C8	2.56	0.40
1:A:2251:G:H4'	37:A:7380:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:A:4804:HOH:O	11:K:47:THR:CB	2.65	0.40
37:A:9519:HOH:O	17:Q:81:LYS:HG2	2.21	0.40
4:D:315:VAL:HG23	4:D:316:ARG:HG2	2.04	0.40
5:E:220:THR:O	5:E:220:THR:HG22	2.21	0.40
6:F:59:GLY:C	6:F:61:PHE:N	2.75	0.40
6:F:91:ALA:HB1	37:F:5198:HOH:O	2.21	0.40
8:H:57:GLU:O	8:H:61:MET:HG3	2.21	0.40
14:N:84:LYS:O	14:N:87:MET:HG2	2.22	0.40
18:R:40:HIS:HD2	18:R:60:THR:OG1	2.05	0.40
26:Z:144:ARG:NH2	37:Z:8614:HOH:O	2.53	0.40
27:1:46:LYS:NZ	37:1:8440:HOH:O	2.54	0.40
30:4:11:CYS:SG	30:4:14:CYS:HB2	2.61	0.40
1:A:581:G:O2'	1:A:582:C:H5'	2.22	0.40
1:A:1029:U:O2'	1:A:1273:C:OP1	2.35	0.40
1:A:1352:A:N1	5:E:48:SER:HB3	2.36	0.40
1:A:1497:G:H4'	1:A:1627:G:O2'	2.21	0.40
1:A:1545:C:H2'	1:A:1546:G:O4'	2.21	0.40
1:A:2684:A:H2'	1:A:2685:C:C6	2.56	0.40
1:A:2714:U:H4'	4:D:10:SER:HB2	2.03	0.40
1:A:2906:A:H5'	1:A:2907:C:O4'	2.20	0.40
4:D:7:ARG:HD3	4:D:9:GLY:O	2.21	0.40
4:D:148:PRO:HD2	37:D:8582:HOH:O	2.21	0.40
6:F:57:THR:HG23	6:F:63:ILE:HA	2.04	0.40
11:K:39:VAL:CG1	11:K:40:ASN:N	2.85	0.40
11:K:54:VAL:HG11	11:K:138:THR:HG21	2.03	0.40
14:N:65:VAL:HG21	14:N:105:ALA:HB2	2.03	0.40
23:W:39:ALA:C	23:W:41:GLU:N	2.74	0.40
24:X:67:ALA:HB2	24:X:93:ILE:HD13	2.02	0.40
25:Y:8:ARG:NH1	37:Y:2479:HOH:O	2.48	0.40
26:Z:187:VAL:HB	26:Z:203:VAL:HG22	2.01	0.40
1:A:61:G:OP1	29:3:17:GLN:HG2	2.22	0.40
1:A:263:U:C2	8:H:59:ILE:CD1	3.04	0.40
1:A:396:U:H5'	30:4:42:ARG:NH1	2.36	0.40
1:A:539:G:H2'	1:A:540:A:C8	2.56	0.40
1:A:832:U:H2'	1:A:833:G:H8	1.86	0.40
1:A:1003:U:O2	10:J:90:PHE:HZ	2.03	0.40
1:A:1181:A:C2	1:A:1192:A:C8	3.10	0.40
1:A:1425:G:O2'	1:A:1426:C:H5'	2.21	0.40
1:A:1588:G:C6	1:A:1589:G:N1	2.90	0.40
1:A:2083:A:N6	11:K:90:LYS:HE2	2.36	0.40
1:A:2408:A:H2	37:4:8514:HOH:O	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2563:U:H2'	1:A:2565:C:O5'	2.21	0.40
4:D:102:THR:HG23	4:D:182:VAL:HG12	2.02	0.40
4:D:129:ARG:NH2	4:D:176:ASP:OD1	2.51	0.40
4:D:132:HIS:CE1	4:D:171:VAL:HG21	2.56	0.40
5:E:191:SER:OG	5:E:192:ILE:N	2.54	0.40
6:F:49:PRO:HA	6:F:73:VAL:HG22	2.04	0.40
8:H:34:ASN:HA	14:N:4:ALA:HB2	2.03	0.40
8:H:38:LYS:NZ	14:N:3:SER:HA	2.36	0.40
10:J:72:VAL:HG11	10:J:81:TYR:CZ	2.57	0.40
10:J:143:GLU:N	37:J:8380:HOH:O	2.55	0.40
12:L:78:LYS:HA	12:L:79:PRO:HD3	1.90	0.40
14:N:77:PHE:HD2	37:N:8526:HOH:O	2.03	0.40
15:O:129:ILE:HA	15:O:130:PRO:HD3	1.97	0.40
16:P:59:VAL:HG23	16:P:111:VAL:HG23	2.03	0.40
17:Q:7:LYS:HD2	17:Q:21:VAL:CG2	2.51	0.40
24:X:21:LEU:CD2	24:X:48:VAL:HG11	2.46	0.40
1:A:308:U:C4	1:A:342:C:H1'	2.55	0.40
1:A:1450:C:O2'	1:A:1494:A:H5'	2.21	0.40
1:A:1614:G:H2'	37:A:4595:HOH:O	2.21	0.40
1:A:2090:G:H2'	1:A:2091:G:C8	2.56	0.40
1:A:2119:C:H2'	1:A:2120:U:O4'	2.21	0.40
1:A:2266:A:H2'	1:A:2267:G:C8	2.57	0.40
1:A:2366:C:H6	1:A:2366:C:O5'	2.05	0.40
1:A:2518:C:H2'	1:A:2519:C:O4'	2.20	0.40
37:A:9307:HOH:O	27:1:16:PRO:HG3	2.21	0.40
3:C:99:ILE:O	3:C:131:HIS:CE1	2.74	0.40
3:C:105:VAL:HG13	3:C:155:THR:O	2.21	0.40
3:C:220:PRO:HD2	3:C:223:ARG:HD3	2.03	0.40
13:M:34:GLY:O	13:M:36:ASP:N	2.54	0.40
14:N:38:VAL:O	14:N:38:VAL:HG12	2.19	0.40
17:Q:134:VAL:O	17:Q:137:LEU:HB3	2.22	0.40
17:Q:143:ALA:HB2	37:Q:196:HOH:O	2.21	0.40
21:U:28:SER:O	21:U:32:ARG:HG3	2.21	0.40
25:Y:25:ARG:HD3	25:Y:64:ALA:O	2.22	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
3	C	235/239 (98%)	210 (89%)	20 (8%)	5 (2%)	7 33
4	D	335/337 (99%)	304 (91%)	24 (7%)	7 (2%)	7 33
5	E	244/246 (99%)	219 (90%)	24 (10%)	1 (0%)	34 72
6	F	134/176 (76%)	96 (72%)	29 (22%)	9 (7%)	1 6
7	G	170/177 (96%)	162 (95%)	8 (5%)	0	100 100
8	H	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	9 39
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100 100
10	J	152/167 (91%)	135 (89%)	12 (8%)	5 (3%)	4 21
11	K	140/145 (97%)	129 (92%)	8 (6%)	3 (2%)	7 33
12	L	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	10 42
13	M	141/164 (86%)	122 (86%)	16 (11%)	3 (2%)	7 33
14	N	192/194 (99%)	170 (88%)	20 (10%)	2 (1%)	15 53
15	O	184/186 (99%)	167 (91%)	10 (5%)	7 (4%)	3 18
16	P	113/115 (98%)	108 (96%)	5 (4%)	0	100 100
17	Q	141/148 (95%)	137 (97%)	4 (3%)	0	100 100
18	R	93/95 (98%)	87 (94%)	6 (6%)	0	100 100
19	S	148/154 (96%)	138 (93%)	9 (6%)	1 (1%)	22 60
20	T	79/84 (94%)	75 (95%)	4 (5%)	0	100 100
21	U	117/119 (98%)	110 (94%)	6 (5%)	1 (1%)	17 55
22	V	51/66 (77%)	46 (90%)	5 (10%)	0	100 100
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4 22
24	X	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	12 45
25	Y	80/91 (88%)	70 (88%)	9 (11%)	1 (1%)	12 45
26	Z	140/240 (58%)	136 (97%)	4 (3%)	0	100 100
27	1	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	5 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	85 (94%)	3 (3%)	2 (2%)	6	31
All	All	3633/4235 (86%)	3317 (91%)	259 (7%)	57 (2%)	9	40

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	20	LYS
6	F	93	LEU
6	F	95	THR
6	F	173	GLU
8	H	101	ALA
10	J	162	SER
13	M	80	ASP
15	O	154	LEU
15	O	164	ASP
15	O	183	ASP
3	C	34	ASP
3	C	37	VAL
3	C	132	ASP
4	D	34	GLY
4	D	169	GLY
5	E	58	ALA
6	F	11	HIS
6	F	137	PRO
6	F	171	ASP
10	J	164	ALA
11	K	5	GLU
11	K	143	LYS
23	W	43	PRO
24	X	49	ASN
24	X	77	ALA
27	1	81	LYS
3	C	119	ALA
10	J	138	PRO
11	K	7	ASP
12	L	119	GLN
13	M	21	ARG
14	N	140	ALA

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Mol	Chain	Res	Type
15	O	162	ASP
15	O	181	ASP
21	U	53	GLY
25	Y	77	PHE
30	4	56	PRO
30	4	57	GLY
4	D	184	ASP
4	D	185	GLY
6	F	61	PHE
8	H	64	PRO
10	J	40	PRO
12	L	126	SER
14	N	165	SER
15	O	167	ASP
4	D	2	GLN
4	D	107	SER
6	F	36	ASN
13	M	35	ARG
10	J	72	VAL
15	O	155	GLU
23	W	40	PRO
27	1	41	VAL
3	C	112	PRO
19	S	81	PRO

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	
3	C	179/181 (99%)	165 (92%)	14 (8%)	12	42
4	D	282/282 (100%)	266 (94%)	16 (6%)	20	56
5	E	193/193 (100%)	178 (92%)	15 (8%)	12	42
6	F	117/147 (80%)	108 (92%)	9 (8%)	13	42
7	G	152/155 (98%)	148 (97%)	4 (3%)	46	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	92/92 (100%)	92 (100%)	0	100	100
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	112 (92%)	10 (8%)	11	39
11	K	118/121 (98%)	109 (92%)	9 (8%)	13	43
12	L	106/106 (100%)	103 (97%)	3 (3%)	43	77
13	M	112/126 (89%)	108 (96%)	4 (4%)	35	70
14	N	166/166 (100%)	157 (95%)	9 (5%)	22	57
15	O	149/149 (100%)	143 (96%)	6 (4%)	31	68
16	P	93/93 (100%)	91 (98%)	2 (2%)	52	81
17	Q	113/116 (97%)	110 (97%)	3 (3%)	44	77
18	R	79/79 (100%)	75 (95%)	4 (5%)	24	60
19	S	117/121 (97%)	113 (97%)	4 (3%)	37	72
20	T	71/73 (97%)	71 (100%)	0	100	100
21	U	105/105 (100%)	102 (97%)	3 (3%)	42	76
22	V	44/52 (85%)	44 (100%)	0	100	100
23	W	51/56 (91%)	50 (98%)	1 (2%)	55	83
24	X	130/130 (100%)	122 (94%)	8 (6%)	18	52
25	Y	66/73 (90%)	62 (94%)	4 (6%)	18	53
26	Z	120/195 (62%)	110 (92%)	10 (8%)	11	39
27	1	56/56 (100%)	53 (95%)	3 (5%)	22	57
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	49	79
30	4	79/79 (100%)	77 (98%)	2 (2%)	47	79
All	All	3027/3441 (88%)	2883 (95%)	144 (5%)	25	62

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3	ARG
3	C	33	GLU
3	C	36	ASP
3	C	55	VAL
3	C	68	ILE
3	C	69	LEU

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Mol	Chain	Res	Type
3	C	78	ASP
3	C	94	LEU
3	C	120	ARG
3	C	131	HIS
3	C	153	ARG
3	C	179	MET
3	C	187	PRO
3	C	217	ARG
4	D	7	ARG
4	D	11	LEU
4	D	27	ASN
4	D	33	ASP
4	D	63	GLU
4	D	97	LEU
4	D	98	THR
4	D	103	ASP
4	D	162	MET
4	D	234	ARG
4	D	251	VAL
4	D	254	GLN
4	D	256	GLN
4	D	264	GLU
4	D	307	ARG
4	D	312	ARG
5	E	2	GLN
5	E	27	ARG
5	E	67	GLN
5	E	76	ARG
5	E	78	ARG
5	E	94	THR
5	E	115	LEU
5	E	136	VAL
5	E	187	ARG
5	E	214	THR
5	E	222	ASP
5	E	223	LEU
5	E	234	VAL
5	E	236	THR
5	E	240	LEU
6	F	24	HIS
6	F	61	PHE
6	F	99	ASP

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Mol	Chain	Res	Type
6	F	100	ASP
6	F	131	THR
6	F	133	ASN
6	F	136	ARG
6	F	137	PRO
6	F	149	ARG
7	G	7	ILE
7	G	54	ASP
7	G	102	VAL
7	G	164	ASP
10	J	59	ASN
10	J	61	LEU
10	J	72	VAL
10	J	73	GLN
10	J	82	LYS
10	J	85	ILE
10	J	86	ARG
10	J	142	VAL
10	J	150	LYS
10	J	166	ASN
11	K	46	ILE
11	K	52	GLN
11	K	74	ARG
11	K	79	PHE
11	K	107	ASN
11	K	112	ASP
11	K	120	SER
11	K	125	SER
11	K	127	ILE
12	L	7	ASP
12	L	10	GLN
12	L	98	VAL
13	M	30	ARG
13	M	35	ARG
13	M	80	ASP
13	M	117	GLU
14	N	38	VAL
14	N	46	LEU
14	N	48	ARG
14	N	68	ARG
14	N	81	ARG
14	N	87	MET

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Mol	Chain	Res	Type
14	N	93	ARG
14	N	99	ARG
14	N	164	THR
15	O	26	LEU
15	O	43	VAL
15	O	127	LEU
15	O	128	ASP
15	O	152	GLU
15	O	163	PHE
16	P	3	THR
16	P	28	ASP
17	Q	52	LYS
17	Q	91	LYS
17	Q	98	ILE
18	R	11	ARG
18	R	16	ASN
18	R	57	ASP
18	R	95	GLU
19	S	13	THR
19	S	39	THR
19	S	82	GLU
19	S	132	ARG
21	U	39	ASN
21	U	48	VAL
21	U	73	HIS
23	W	43	PRO
24	X	4	LEU
24	X	35	VAL
24	X	52	VAL
24	X	73	LEU
24	X	122	ARG
24	X	142	ASP
24	X	146	ILE
24	X	154	ARG
25	Y	15	ARG
25	Y	27	ASP
25	Y	49	ARG
25	Y	72	VAL
26	Z	141	THR
26	Z	154	ARG
26	Z	163	THR
26	Z	172	THR

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Mol	Chain	Res	Type
26	Z	186	ARG
26	Z	189	ASN
26	Z	200	THR
26	Z	203	VAL
26	Z	231	PRO
26	Z	235	GLU
27	1	11	THR
27	1	44	PHE
27	1	64	ILE
29	3	18	ASN
30	4	56	PRO
30	4	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	47	HIS
3	C	92	ASN
3	C	127	GLN
3	C	199	HIS
4	D	27	ASN
4	D	145	HIS
4	D	238	ASN
4	D	256	GLN
4	D	260	HIS
4	D	332	ASN
5	E	2	GLN
5	E	39	GLN
5	E	129	HIS
5	E	163	HIS
6	F	103	ASN
7	G	106	ASN
7	G	119	HIS
7	G	143	GLN
9	I	17	GLN
9	I	64	ASN
10	J	8	ASN
10	J	35	ASN
10	J	55	GLN
10	J	58	HIS
10	J	59	ASN
10	J	69	ASN

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Mol	Chain	Res	Type
10	J	74	ASN
10	J	91	HIS
10	J	129	ASN
10	J	130	HIS
10	J	166	ASN
11	K	52	GLN
11	K	107	ASN
11	K	126	ASN
12	L	10	GLN
12	L	42	ASN
13	M	18	HIS
13	M	41	HIS
13	M	42	ASN
13	M	58	GLN
13	M	116	HIS
14	N	26	HIS
14	N	58	GLN
14	N	89	ASN
14	N	176	GLN
15	O	107	ASN
15	O	153	GLN
16	P	53	GLN
17	Q	50	GLN
17	Q	66	GLN
17	Q	73	HIS
17	Q	118	GLN
18	R	16	ASN
18	R	40	HIS
19	S	61	GLN
19	S	94	ASN
19	S	98	ASN
19	S	113	HIS
19	S	117	HIS
20	T	53	ASN
21	U	39	ASN
21	U	43	ASN
21	U	73	HIS
22	V	39	ASN
22	V	48	ASN
23	W	60	GLN
24	X	27	HIS
24	X	87	HIS

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Mol	Chain	Res	Type
24	X	110	GLN
24	X	119	HIS
24	X	125	HIS
24	X	141	HIS
25	Y	23	HIS
26	Z	133	HIS
26	Z	134	HIS
26	Z	149	GLN
26	Z	189	ASN
27	1	33	HIS
27	1	70	GLN
28	2	8	GLN
28	2	16	HIS
28	2	28	HIS
29	3	16	ASN
29	3	18	ASN
29	3	41	HIS
29	3	45	ASN
30	4	15	ASN
30	4	30	GLN
30	4	48	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	239 (8%)	38 (1%)
2	B	121/122 (99%)	18 (14%)	6 (4%)
All	All	2868/3044 (94%)	257 (8%)	44 (1%)

All (257) 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

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Mol	Chain	Res	Type
1	A	114	A
1	A	115	U
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	186	A
1	A	191	A
1	A	192	A
1	A	200	U
1	A	219	G
1	A	237	G
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

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Mol	Chain	Res	Type
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	717	C
1	A	759	C
1	A	777	U
1	A	809	G
1	A	821	U
1	A	835	U
1	A	840	U
1	A	857	A
1	A	858	U
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	884	C
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

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Mol	Chain	Res	Type
1	A	1081	A
1	A	1088	A
1	A	1109	U
1	A	1110	G
1	A	1119	G
1	A	1130	U
1	A	1137	G
1	A	1162	G
1	A	1164	U
1	A	1165	G
1	A	1166	A
1	A	1171	A
1	A	1174	A
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	1234	U
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	1409	G
1	A	1451	C
1	A	1474	C
1	A	1485	A
1	A	1505	U
1	A	1506	U
1	A	1524	U
1	A	1525	G
1	A	1526	A
1	A	1564	C

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Mol	Chain	Res	Type
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
1	A	1723	G
1	A	1725	C
1	A	1731	C
1	A	1752	G
1	A	1778	A
1	A	1779	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	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

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Mol	Chain	Res	Type
1	A	2072	G
1	A	2073	G
1	A	2074	A
1	A	2096	A
1	A	2097	G
1	A	2101	A
1	A	2102	G
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
1	A	2346	C
1	A	2354	A
1	A	2361	A
1	A	2369	A
1	A	2422	U
1	A	2462	G
1	A	2467	A
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	2638	G
1	A	2649	A
1	A	2664	A
1	A	2681	A
1	A	2682	C

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Mol	Chain	Res	Type
1	A	2718	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	2840	A
1	A	2850	C
1	A	2876	G
1	A	2890	A
1	A	2896	A
1	A	2914	A
2	B	3002	U
2	B	3003	A
2	B	3014	G
2	B	3022	G
2	B	3023	U
2	B	3024	U
2	B	3025	G
2	B	3026	C
2	B	3040	C
2	B	3041	C
2	B	3043	G
2	B	3044	A
2	B	3052	A
2	B	3057	A
2	B	3066	G
2	B	3077	A
2	B	3114	G
2	B	3122	C

All (44) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type

Mol	Chain	Res	Type
1	A	10	U
1	A	69	A
1	A	129	A
1	A	284	C
1	A	338	C
1	A	545	G
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	898	G
1	A	1080	C
1	A	1164	U
1	A	1237	U
1	A	1246	A
1	A	1352	A
1	A	1377	C
1	A	1450	C
1	A	1563	G
1	A	1692	C
1	A	1856	C
1	A	1942	A
1	A	1979	G
1	A	2011	A
1	A	2313	C
1	A	2361	A
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	3003	A
2	B	3023	U
2	B	3024	U

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Mol	Chain	Res	Type
2	B	3043	G
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 232 ligands modelled in this entry, 231 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
35	CLM	A	9001	-	19,20,20	1.41	1 (5%)	23,27,27	1.16	3 (13%)

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
35	CLM	A	9001	-	-	2/20/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A	9001	CLM	C5-C3	-4.46	1.47	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	A	9001	CLM	O4-C4-C3	2.43	116.97	111.09
35	A	9001	CLM	C11-C10-C9	-2.31	116.87	120.08
35	A	9001	CLM	C8-C9-N9	-2.10	117.80	119.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

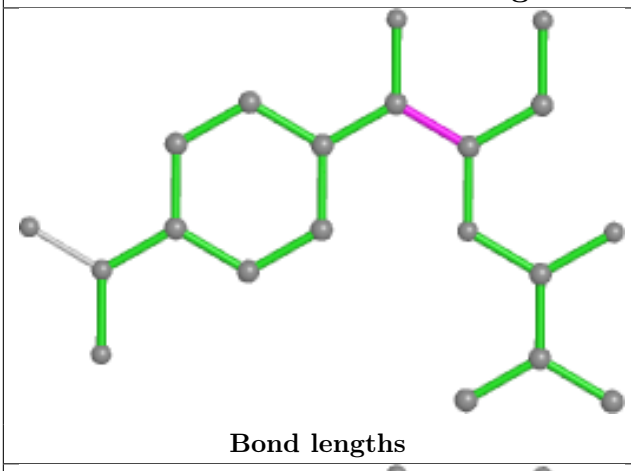
Mol	Chain	Res	Type	Atoms
35	A	9001	CLM	CL2-C1-C2-O2
35	A	9001	CLM	CL2-C1-C2-N2

There are no ring outliers.

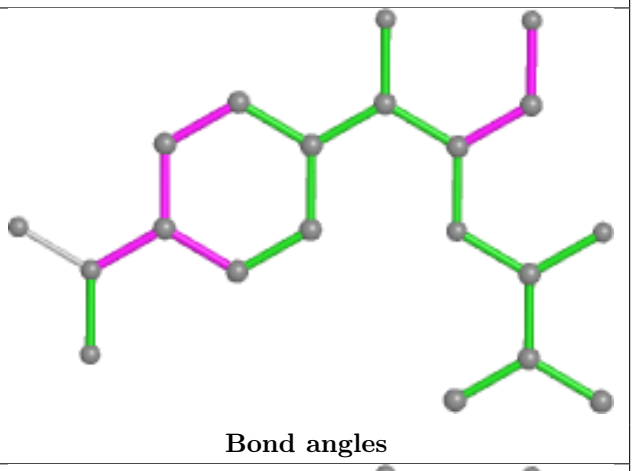
No monomer is involved in short contacts.

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 then 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.

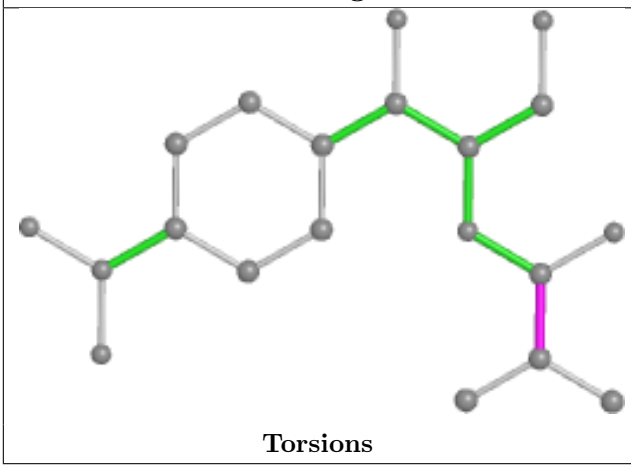
Ligand CLM A 9001



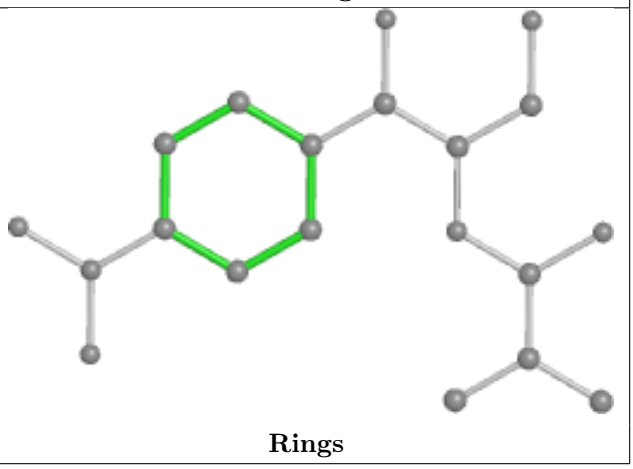
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	2754/2922 (94%)	-0.34	35 (1%) 77 51	14, 38, 82, 130	0
2	B	122/122 (100%)	-0.09	6 (4%) 29 11	31, 55, 80, 139	0
3	C	237/239 (99%)	-0.17	3 (1%) 77 51	21, 42, 74, 95	0
4	D	337/337 (100%)	-0.30	1 (0%) 94 84	20, 49, 73, 84	0
5	E	246/246 (100%)	-0.42	0 100 100	16, 39, 62, 72	0
6	F	140/176 (79%)	1.22	31 (22%) 0 0	46, 89, 107, 111	0
7	G	172/177 (97%)	0.29	3 (1%) 70 41	39, 61, 80, 85	0
8	H	119/119 (100%)	0.07	2 (1%) 70 41	39, 61, 86, 93	0
9	I	29/348 (8%)	1.50	5 (17%) 1 0	65, 82, 89, 92	0
10	J	156/167 (93%)	-0.07	1 (0%) 89 72	31, 51, 77, 81	0
11	K	142/145 (97%)	-0.25	0 100 100	29, 43, 64, 83	0
12	L	132/132 (100%)	-0.45	0 100 100	28, 45, 63, 70	0
13	M	145/164 (88%)	0.14	6 (4%) 37 14	17, 57, 93, 107	0
14	N	194/194 (100%)	-0.46	0 100 100	22, 36, 55, 65	0
15	O	186/186 (100%)	0.06	4 (2%) 62 33	31, 54, 93, 107	0
16	P	115/115 (100%)	-0.29	0 100 100	31, 47, 63, 67	0
17	Q	143/148 (96%)	-0.13	0 100 100	30, 47, 59, 68	0
18	R	95/95 (100%)	-0.40	1 (1%) 80 56	27, 37, 53, 66	0
19	S	150/154 (97%)	-0.32	0 100 100	24, 39, 58, 66	0
20	T	81/84 (96%)	-0.32	0 100 100	37, 51, 70, 72	0
21	U	119/119 (100%)	0.00	3 (2%) 57 29	33, 49, 73, 86	0
22	V	53/66 (80%)	-0.05	0 100 100	33, 49, 65, 73	0
23	W	65/70 (92%)	0.68	4 (6%) 20 7	43, 64, 99, 103	0
24	X	154/154 (100%)	-0.41	0 100 100	28, 41, 58, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Y	82/91 (90%)	0.20	2 (2%) 59 30	36, 51, 74, 93	0
26	Z	142/240 (59%)	-0.28	3 (2%) 63 34	18, 38, 59, 78	0
27	1	73/73 (100%)	-0.31	0 100 100	36, 52, 68, 75	0
28	2	56/56 (100%)	-0.64	0 100 100	18, 27, 32, 41	0
29	3	46/48 (95%)	0.04	1 (2%) 62 33	28, 52, 78, 91	0
30	4	92/92 (100%)	-0.06	0 100 100	26, 47, 61, 73	0
All	All	6577/7279 (90%)	-0.21	111 (1%) 70 41	14, 44, 83, 139	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	W	1	THR	8.4
2	B	3001	U	5.9
2	B	3025	G	5.7
25	Y	88	GLU	4.6
6	F	57	THR	4.6
6	F	63	ILE	4.4
1	A	1172	G	4.3
1	A	1198	U	4.2
1	A	1177	A	4.1
9	I	27	ILE	4.0
6	F	66	GLY	4.0
23	W	40	PRO	3.9
26	Z	235	GLU	3.9
1	A	1173	A	3.9
15	O	162	ASP	3.8
9	I	26	MET	3.7
3	C	35	GLY	3.6
6	F	69	ILE	3.5
6	F	85	GLN	3.5
7	G	45	ASP	3.5
6	F	18	ILE	3.4
6	F	62	ASP	3.4
23	W	38	GLY	3.4
23	W	39	ALA	3.4
1	A	1199	A	3.3
1	A	1203	G	3.3
25	Y	80	GLU	3.3
6	F	67	ASP	3.2
13	M	60	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
6	F	64	ARG	3.2
1	A	1169	U	3.2
3	C	85	ASP	3.2
1	A	735	C	3.1
6	F	56	ARG	3.1
1	A	1202	A	3.1
6	F	92	GLU	3.1
3	C	36	ASP	3.0
1	A	282	C	3.0
2	B	3023	U	3.0
9	I	23	ILE	3.0
1	A	1204	C	3.0
1	A	2237	G	2.9
1	A	2637	A	2.9
6	F	170	TYR	2.9
6	F	25	MET	2.9
6	F	102	GLY	2.9
1	A	970	U	2.9
13	M	80	ASP	2.8
6	F	75	LEU	2.8
4	D	1	PRO	2.8
1	A	1178	G	2.8
15	O	186	LEU	2.8
2	B	3002	U	2.8
6	F	88	LEU	2.7
6	F	90	LEU	2.7
6	F	27	ILE	2.7
1	A	960	G	2.7
1	A	1163	G	2.7
1	A	284	C	2.7
1	A	1162	G	2.6
6	F	171	ASP	2.6
1	A	1168	C	2.5
1	A	1195	G	2.5
18	R	95	GLU	2.5
1	A	1165	G	2.5
7	G	100	ASP	2.5
26	Z	95	THR	2.5
15	O	138	ASP	2.5
1	A	1525	G	2.5
7	G	128	GLY	2.4
6	F	61	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
13	M	104	ASP	2.4
1	A	1171	A	2.4
21	U	119	ALA	2.4
6	F	70	GLY	2.3
6	F	65	GLU	2.3
13	M	100	ALA	2.3
6	F	89	PRO	2.3
2	B	3024	U	2.3
21	U	116	ASP	2.3
1	A	1190	G	2.3
1	A	1279	U	2.3
1	A	999	C	2.2
1	A	10	U	2.2
15	O	152	GLU	2.2
1	A	1197	G	2.2
1	A	1175	G	2.2
1	A	1170	U	2.2
1	A	1205	U	2.2
1	A	1200	A	2.2
6	F	10	PHE	2.1
6	F	86	THR	2.1
10	J	80	ASN	2.1
1	A	1174	A	2.1
6	F	23	VAL	2.1
26	Z	108	ASP	2.1
8	H	26	THR	2.1
2	B	3122	C	2.1
13	M	106	VAL	2.1
9	I	71	LEU	2.1
9	I	72	ASP	2.1
6	F	58	VAL	2.1
29	3	49	GLU	2.1
6	F	134	LEU	2.1
13	M	59	GLU	2.0
8	H	107	VAL	2.0
6	F	45	THR	2.0
21	U	1	SER	2.0
1	A	1181	A	2.0
6	F	41	LEU	2.0
6	F	44	ILE	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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	NA	A	8371	1/1	0.39	0.49	55,55,55,55	0
33	NA	A	8384	1/1	0.39	0.56	59,59,59,59	0
33	NA	A	8357	1/1	0.57	0.17	56,56,56,56	0
31	MG	A	8049	1/1	0.62	0.51	69,69,69,69	0
33	NA	A	8364	1/1	0.62	0.27	33,33,33,33	0
33	NA	A	8307	1/1	0.66	0.25	51,51,51,51	0
33	NA	A	8329	1/1	0.67	0.24	48,48,48,48	0
33	NA	A	8382	1/1	0.69	0.54	74,74,74,74	0
34	CL	K	8502	1/1	0.72	0.23	72,72,72,72	0
31	MG	A	8088	1/1	0.74	0.24	44,44,44,44	0
31	MG	A	8089	1/1	0.75	0.13	68,68,68,68	0
33	NA	J	8322	1/1	0.75	0.37	63,63,63,63	0
33	NA	A	8333	1/1	0.75	0.12	24,24,24,24	0
31	MG	A	8022	1/1	0.77	0.11	26,26,26,26	0
33	NA	A	8376	1/1	0.78	0.46	53,53,53,53	0
33	NA	A	8377	1/1	0.78	0.70	66,66,66,66	0
35	CLM	A	9001	20/20	0.78	0.31	57,61,68,69	0
33	NA	A	8373	1/1	0.79	0.30	49,49,49,49	0
33	NA	A	8359	1/1	0.79	0.38	49,49,49,49	0
31	MG	A	8050	1/1	0.79	0.17	79,79,79,79	0
31	MG	A	8114	1/1	0.79	0.13	52,52,52,52	0
33	NA	B	8383	1/1	0.80	0.25	45,45,45,45	0
31	MG	A	8068	1/1	0.80	0.11	61,61,61,61	0
33	NA	S	8386	1/1	0.81	0.50	83,83,83,83	0
33	NA	T	8312	1/1	0.81	0.16	44,44,44,44	0
33	NA	A	8340	1/1	0.81	0.60	41,41,41,41	0
33	NA	A	8326	1/1	0.81	0.27	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	NA	A	8324	1/1	0.82	0.20	46,46,46,46	0
31	MG	A	8087	1/1	0.82	0.24	71,71,71,71	0
33	NA	A	8368	1/1	0.83	0.27	63,63,63,63	0
33	NA	A	8363	1/1	0.83	0.33	64,64,64,64	0
33	NA	E	8304	1/1	0.83	0.16	30,30,30,30	0
34	CL	4	8504	1/1	0.83	0.23	72,72,72,72	0
33	NA	A	8352	1/1	0.83	0.30	51,51,51,51	0
31	MG	A	8113	1/1	0.84	0.19	35,35,35,35	0
34	CL	Z	8520	1/1	0.84	0.16	39,39,39,39	0
33	NA	A	8310	1/1	0.84	0.29	21,21,21,21	0
31	MG	A	8103	1/1	0.84	0.17	56,56,56,56	0
34	CL	A	8503	1/1	0.85	0.22	49,49,49,49	0
33	NA	A	8369	1/1	0.85	0.26	51,51,51,51	0
31	MG	B	8095	1/1	0.85	0.14	61,61,61,61	0
31	MG	A	8076	1/1	0.85	0.18	71,71,71,71	0
33	NA	A	8342	1/1	0.85	0.24	40,40,40,40	0
33	NA	A	8355	1/1	0.86	0.62	57,57,57,57	0
33	NA	B	8351	1/1	0.86	0.14	49,49,49,49	0
33	NA	A	8306	1/1	0.87	0.34	51,51,51,51	0
31	MG	A	8085	1/1	0.87	0.17	59,59,59,59	0
31	MG	A	8072	1/1	0.87	0.18	56,56,56,56	0
33	NA	A	8316	1/1	0.87	0.28	53,53,53,53	0
31	MG	U	8073	1/1	0.87	0.09	52,52,52,52	0
31	MG	1	8105	1/1	0.88	0.24	28,28,28,28	0
33	NA	A	8372	1/1	0.88	0.31	62,62,62,62	0
31	MG	A	8028	1/1	0.88	0.08	28,28,28,28	0
33	NA	A	8385	1/1	0.88	0.35	45,45,45,45	0
33	NA	A	8315	1/1	0.88	0.22	34,34,34,34	0
31	MG	A	8066	1/1	0.89	0.47	38,38,38,38	0
31	MG	A	8046	1/1	0.89	0.08	45,45,45,45	0
33	NA	K	8346	1/1	0.89	0.14	43,43,43,43	0
33	NA	A	8378	1/1	0.89	0.86	47,47,47,47	0
33	NA	A	8370	1/1	0.89	0.23	55,55,55,55	0
33	NA	A	8362	1/1	0.89	0.28	65,65,65,65	0
33	NA	A	8302	1/1	0.89	0.28	34,34,34,34	0
31	MG	A	8051	1/1	0.89	0.13	61,61,61,61	0
33	NA	A	8375	1/1	0.89	0.24	48,48,48,48	0
33	NA	C	8345	1/1	0.89	0.15	49,49,49,49	0
34	CL	A	8517	1/1	0.90	0.14	51,51,51,51	0
34	CL	D	8519	1/1	0.90	0.30	53,53,53,53	0
33	NA	A	8330	1/1	0.90	0.30	27,27,27,27	0
31	MG	A	8042	1/1	0.90	0.22	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	NA	A	8308	1/1	0.90	0.15	49,49,49,49	0
33	NA	A	8381	1/1	0.90	0.21	45,45,45,45	0
33	NA	S	8337	1/1	0.91	0.11	35,35,35,35	0
31	MG	A	8037	1/1	0.91	0.06	39,39,39,39	0
31	MG	A	8101	1/1	0.91	0.15	55,55,55,55	0
33	NA	A	8327	1/1	0.91	0.17	47,47,47,47	0
31	MG	A	8063	1/1	0.91	0.07	74,74,74,74	0
31	MG	A	8106	1/1	0.91	0.17	51,51,51,51	0
33	NA	A	8332	1/1	0.91	0.24	28,28,28,28	0
31	MG	4	8078	1/1	0.91	0.12	35,35,35,35	0
31	MG	A	8082	1/1	0.91	0.13	66,66,66,66	0
33	NA	A	8319	1/1	0.91	0.11	40,40,40,40	0
32	K	A	8202	1/1	0.92	0.20	56,56,56,56	0
33	NA	A	8335	1/1	0.92	0.25	53,53,53,53	0
33	NA	A	8339	1/1	0.92	0.18	17,17,17,17	0
33	NA	A	8374	1/1	0.92	0.62	56,56,56,56	0
31	MG	A	8045	1/1	0.92	0.11	63,63,63,63	0
31	MG	A	8108	1/1	0.92	0.07	77,77,77,77	0
33	NA	A	8350	1/1	0.92	0.28	44,44,44,44	0
31	MG	A	8102	1/1	0.92	0.18	60,60,60,60	0
31	MG	A	8090	1/1	0.92	0.22	46,46,46,46	0
33	NA	M	8380	1/1	0.92	0.55	57,57,57,57	0
33	NA	A	8341	1/1	0.93	0.15	25,25,25,25	0
31	MG	A	8111	1/1	0.93	0.09	54,54,54,54	0
34	CL	N	8518	1/1	0.93	0.21	41,41,41,41	0
31	MG	A	8081	1/1	0.93	0.07	47,47,47,47	0
34	CL	A	8505	1/1	0.93	0.14	53,53,53,53	0
33	NA	A	8379	1/1	0.93	0.16	51,51,51,51	0
36	CD	V	8401	1/1	0.93	0.08	63,63,63,63	0
31	MG	A	8094	1/1	0.94	0.12	61,61,61,61	0
33	NA	A	8313	1/1	0.94	0.22	66,66,66,66	0
31	MG	A	8100	1/1	0.94	0.12	80,80,80,80	0
31	MG	A	8044	1/1	0.94	0.15	42,42,42,42	0
33	NA	A	8318	1/1	0.94	0.17	53,53,53,53	0
31	MG	Z	8109	1/1	0.94	0.11	33,33,33,33	0
31	MG	A	8024	1/1	0.94	0.10	18,18,18,18	0
31	MG	A	8023	1/1	0.94	0.08	36,36,36,36	0
34	CL	A	8515	1/1	0.94	0.26	67,67,67,67	0
31	MG	A	8075	1/1	0.94	0.08	52,52,52,52	0
34	CL	C	8509	1/1	0.94	0.19	67,67,67,67	0
33	NA	A	8328	1/1	0.94	0.28	30,30,30,30	0
31	MG	A	8057	1/1	0.94	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	CL	K	8521	1/1	0.94	0.16	50,50,50,50	0
33	NA	A	8305	1/1	0.94	0.12	32,32,32,32	0
31	MG	A	8047	1/1	0.94	0.10	65,65,65,65	0
31	MG	A	8112	1/1	0.94	0.17	49,49,49,49	0
33	NA	A	8334	1/1	0.94	0.05	27,27,27,27	0
31	MG	A	8091	1/1	0.94	0.05	37,37,37,37	0
31	MG	A	8062	1/1	0.95	0.10	58,58,58,58	0
33	NA	A	8311	1/1	0.95	0.17	51,51,51,51	0
33	NA	A	8367	1/1	0.95	0.09	42,42,42,42	0
31	MG	D	8055	1/1	0.95	0.07	48,48,48,48	0
31	MG	A	8011	1/1	0.95	0.07	35,35,35,35	0
31	MG	A	8015	1/1	0.95	0.05	41,41,41,41	0
33	NA	A	8317	1/1	0.95	0.12	29,29,29,29	0
31	MG	A	8018	1/1	0.95	0.11	50,50,50,50	0
33	NA	U	8343	1/1	0.95	0.10	34,34,34,34	0
31	MG	A	8053	1/1	0.95	0.12	49,49,49,49	0
33	NA	A	8344	1/1	0.95	0.05	15,15,15,15	0
34	CL	A	8514	1/1	0.95	0.12	47,47,47,47	0
33	NA	A	8349	1/1	0.95	0.22	37,37,37,37	0
31	MG	A	8043	1/1	0.95	0.11	41,41,41,41	0
31	MG	A	8059	1/1	0.95	0.12	37,37,37,37	0
33	NA	A	8353	1/1	0.95	0.12	27,27,27,27	0
33	NA	A	8354	1/1	0.95	0.14	32,32,32,32	0
31	MG	A	8093	1/1	0.95	0.09	40,40,40,40	0
31	MG	A	8061	1/1	0.95	0.09	35,35,35,35	0
34	CL	R	8511	1/1	0.95	0.13	49,49,49,49	0
31	MG	A	8099	1/1	0.95	0.22	48,48,48,48	0
33	NA	A	8360	1/1	0.95	0.41	42,42,42,42	0
33	NA	A	8361	1/1	0.95	0.20	58,58,58,58	0
31	MG	A	8115	1/1	0.95	0.08	44,44,44,44	0
31	MG	A	8033	1/1	0.96	0.05	31,31,31,31	0
33	NA	R	8348	1/1	0.96	0.08	27,27,27,27	0
31	MG	A	8004	1/1	0.96	0.09	33,33,33,33	0
31	MG	A	8092	1/1	0.96	0.13	89,89,89,89	0
31	MG	A	8038	1/1	0.96	0.10	31,31,31,31	0
31	MG	C	8065	1/1	0.96	0.11	50,50,50,50	0
33	NA	A	8356	1/1	0.96	0.22	40,40,40,40	0
31	MG	A	8104	1/1	0.96	0.14	42,42,42,42	0
34	CL	A	8513	1/1	0.96	0.11	52,52,52,52	0
31	MG	A	8064	1/1	0.96	0.17	20,20,20,20	0
33	NA	A	8314	1/1	0.96	0.08	28,28,28,28	0
34	CL	A	8516	1/1	0.96	0.19	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	A	8107	1/1	0.96	0.04	34,34,34,34	0
33	NA	A	8338	1/1	0.96	0.14	43,43,43,43	0
31	MG	A	8096	1/1	0.96	0.06	42,42,42,42	0
31	MG	A	8110	1/1	0.96	0.05	34,34,34,34	0
33	NA	A	8365	1/1	0.96	0.21	33,33,33,33	0
33	NA	A	8366	1/1	0.96	0.15	53,53,53,53	0
34	CL	O	8507	1/1	0.96	0.19	61,61,61,61	0
34	CL	P	8508	1/1	0.96	0.14	71,71,71,71	0
31	MG	A	8097	1/1	0.96	0.09	46,46,46,46	0
33	NA	A	8301	1/1	0.96	0.17	24,24,24,24	0
33	NA	J	8309	1/1	0.96	0.07	24,24,24,24	0
31	MG	A	8041	1/1	0.96	0.20	66,66,66,66	0
33	NA	A	8325	1/1	0.96	0.39	58,58,58,58	0
36	CD	1	8403	1/1	0.96	0.10	56,56,56,56	0
36	CD	4	8404	1/1	0.96	0.07	59,59,59,59	0
31	MG	A	8054	1/1	0.97	0.11	38,38,38,38	0
33	NA	A	8303	1/1	0.97	0.17	41,41,41,41	0
31	MG	A	8005	1/1	0.97	0.10	36,36,36,36	0
31	MG	A	8058	1/1	0.97	0.12	43,43,43,43	0
31	MG	A	8017	1/1	0.97	0.04	22,22,22,22	0
31	MG	A	8009	1/1	0.97	0.06	32,32,32,32	0
31	MG	A	8035	1/1	0.97	0.04	39,39,39,39	0
31	MG	A	8020	1/1	0.97	0.08	36,36,36,36	0
31	MG	A	8048	1/1	0.97	0.06	43,43,43,43	0
31	MG	A	8021	1/1	0.97	0.09	36,36,36,36	0
31	MG	A	8067	1/1	0.97	0.13	49,49,49,49	0
31	MG	A	8117	1/1	0.97	0.09	25,25,25,25	0
34	CL	A	8522	1/1	0.97	0.18	66,66,66,66	0
31	MG	A	8040	1/1	0.97	0.11	54,54,54,54	0
31	MG	A	8070	1/1	0.97	0.09	47,47,47,47	0
34	CL	K	8501	1/1	0.97	0.18	61,61,61,61	0
31	MG	A	8071	1/1	0.97	0.08	72,72,72,72	0
33	NA	A	8321	1/1	0.97	0.23	45,45,45,45	0
34	CL	M	8510	1/1	0.97	0.12	60,60,60,60	0
33	NA	A	8323	1/1	0.97	0.14	37,37,37,37	0
31	MG	L	8069	1/1	0.97	0.08	64,64,64,64	0
31	MG	A	8098	1/1	0.97	0.13	29,29,29,29	0
31	MG	A	8001	1/1	0.97	0.04	22,22,22,22	0
31	MG	A	8052	1/1	0.97	0.18	52,52,52,52	0
31	MG	A	8013	1/1	0.97	0.12	48,48,48,48	0
32	K	A	8201	1/1	0.97	0.14	55,55,55,55	0
36	CD	P	8405	1/1	0.97	0.04	90,90,90,90	0

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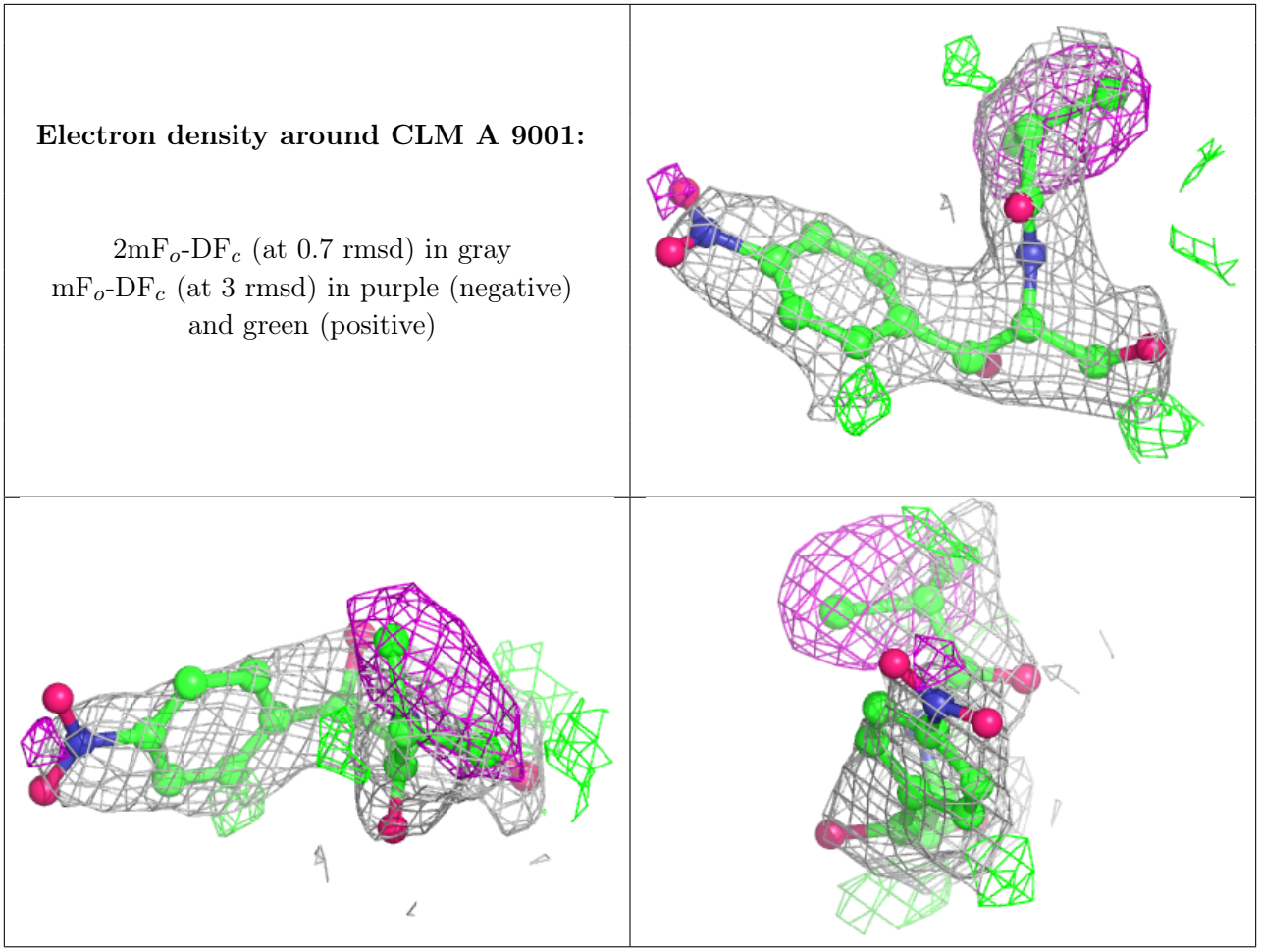
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	MG	A	8077	1/1	0.97	0.09	40,40,40,40	0
31	MG	A	8080	1/1	0.97	0.08	42,42,42,42	0
33	NA	N	8347	1/1	0.97	0.08	17,17,17,17	0
31	MG	A	8074	1/1	0.98	0.06	28,28,28,28	0
31	MG	A	8008	1/1	0.98	0.06	43,43,43,43	0
33	NA	A	8320	1/1	0.98	0.07	20,20,20,20	0
31	MG	A	8036	1/1	0.98	0.03	39,39,39,39	0
31	MG	A	8014	1/1	0.98	0.06	30,30,30,30	0
31	MG	A	8056	1/1	0.98	0.07	44,44,44,44	0
31	MG	A	8006	1/1	0.98	0.04	28,28,28,28	0
31	MG	A	8016	1/1	0.98	0.10	27,27,27,27	0
31	MG	A	8083	1/1	0.98	0.07	42,42,42,42	0
31	MG	A	8010	1/1	0.98	0.05	29,29,29,29	0
31	MG	A	8086	1/1	0.98	0.18	35,35,35,35	0
31	MG	A	8025	1/1	0.98	0.09	47,47,47,47	0
33	NA	A	8331	1/1	0.98	0.14	38,38,38,38	0
31	MG	A	8026	1/1	0.98	0.09	27,27,27,27	0
31	MG	A	8027	1/1	0.98	0.04	30,30,30,30	0
31	MG	A	8007	1/1	0.98	0.07	26,26,26,26	0
31	MG	A	8029	1/1	0.98	0.07	40,40,40,40	0
34	CL	S	8506	1/1	0.98	0.12	43,43,43,43	0
33	NA	A	8336	1/1	0.98	0.04	34,34,34,34	0
31	MG	A	8030	1/1	0.98	0.06	30,30,30,30	0
31	MG	A	8116	1/1	0.98	0.10	60,60,60,60	0
31	MG	A	8031	1/1	0.98	0.03	22,22,22,22	0
31	MG	A	8032	1/1	0.98	0.05	26,26,26,26	0
31	MG	A	8019	1/1	0.98	0.05	27,27,27,27	0
36	CD	2	8402	1/1	0.98	0.07	57,57,57,57	0
31	MG	A	8034	1/1	0.98	0.04	26,26,26,26	0
31	MG	A	8060	1/1	0.99	0.18	36,36,36,36	0
31	MG	A	8039	1/1	0.99	0.05	52,52,52,52	0
31	MG	A	8012	1/1	0.99	0.12	37,37,37,37	0
31	MG	A	8002	1/1	0.99	0.06	38,38,38,38	0
31	MG	A	8084	1/1	0.99	0.10	60,60,60,60	0
31	MG	A	8003	1/1	0.99	0.06	18,18,18,18	0
34	CL	A	8512	1/1	0.99	0.07	41,41,41,41	0
31	MG	A	8079	1/1	0.99	0.09	36,36,36,36	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.

Electron density around CLM A 9001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.