



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:12 AM UTC

PDB ID : 1VQ9 / pdb_00001vq9
Title : The structure of CCA-PHE-CAP-BIO and the antibiotic sparsomycin bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

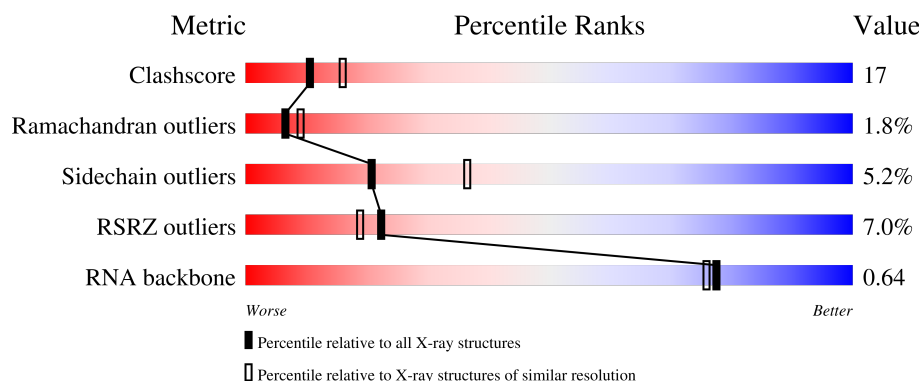
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

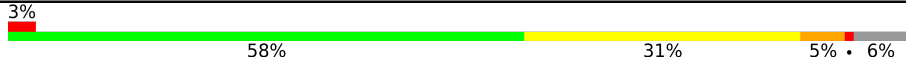
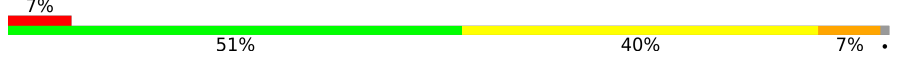
The reported resolution of this entry is 2.40 Å.

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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	
2	9	122	
3	4	5	
4	A	240	
5	B	338	

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Mol	Chain	Length	Quality of chain
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	

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Mol	Chain	Length	Quality of chain
31	3	92	
32	I	162	

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
33	MG	0	8047	-	-	-	X
35	NA	0	9172	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98979 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
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*AP*(PHE)*(ACA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	5	Total	C	N	O	P	0	0	0
			74	40	12	20	2			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501
M	194	ALA	GLY	conflict	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 17 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	95	Total	C	N	O			
			735	450	141	144	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	119	Total	C	N	O			
			950	568	180	202	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	154	Total	C	N	O	S			
			1196	737	209	244	6	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	86	Total	Mg	0	0
			86	86		
33	9	1	Total	Mg	0	0
			1	1		
33	4	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	62	Total	Na	0	0
			62	62		
35	9	2	Total	Na	0	0
			2	2		
35	B	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	D	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	J	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	R	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0
35	T	1	Total 1	Na 1	0	0
35	3	1	Total 1	Na 1	0	0

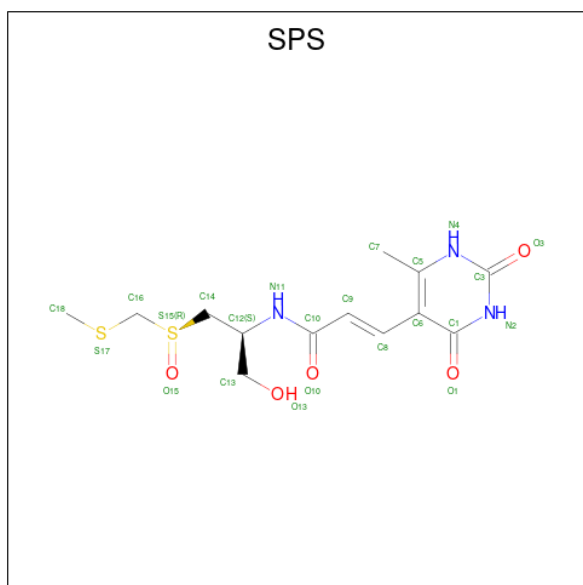
- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	9	Total 9	Cl 9	0	0
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	J	3	Total 3	Cl 3	0	0
36	K	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0

- Molecule 37 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	97	Total 97	Sr 97	0	0
37	9	3	Total 3	Sr 3	0	0
37	A	4	Total 4	Sr 4	0	0
37	B	2	Total 2	Sr 2	0	0
37	F	1	Total 1	Sr 1	0	0
37	H	1	Total 1	Sr 1	0	0
37	L	1	Total 1	Sr 1	0	0
37	R	1	Total 1	Sr 1	0	0
37	S	1	Total 1	Sr 1	0	0
37	1	2	Total 2	Sr 2	0	0
37	3	1	Total 1	Sr 1	0	0

- Molecule 38 is SPARSOMYCIN (CCD ID: SPS) (formula: C₁₃H₁₉N₃O₅S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	4	1	Total	C	N	O	S	0	0
			23	13	3	5	2		

- Molecule 39 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total	Cd	0	0
			1	1		
39	U	1	Total	Cd	0	0
			1	1		
39	Z	1	Total	Cd	0	0
			1	1		
39	1	1	Total	Cd	0	0
			1	1		
39	3	1	Total	Cd	0	0
			1	1		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5630	Total	O	0	0
			5630	5630		
40	9	130	Total	O	0	0
			130	130		
40	4	1	Total	O	0	0
			1	1		
40	A	132	Total	O	0	0
			132	132		
40	B	137	Total	O	0	0
			137	137		
40	C	175	Total	O	0	0
			175	175		
40	D	43	Total	O	0	0
			43	43		
40	E	42	Total	O	0	0
			42	42		
40	F	25	Total	O	0	0
			25	25		
40	G	16	Total	O	0	0
			16	16		
40	H	77	Total	O	0	0
			77	77		
40	J	52	Total	O	0	0
			52	52		

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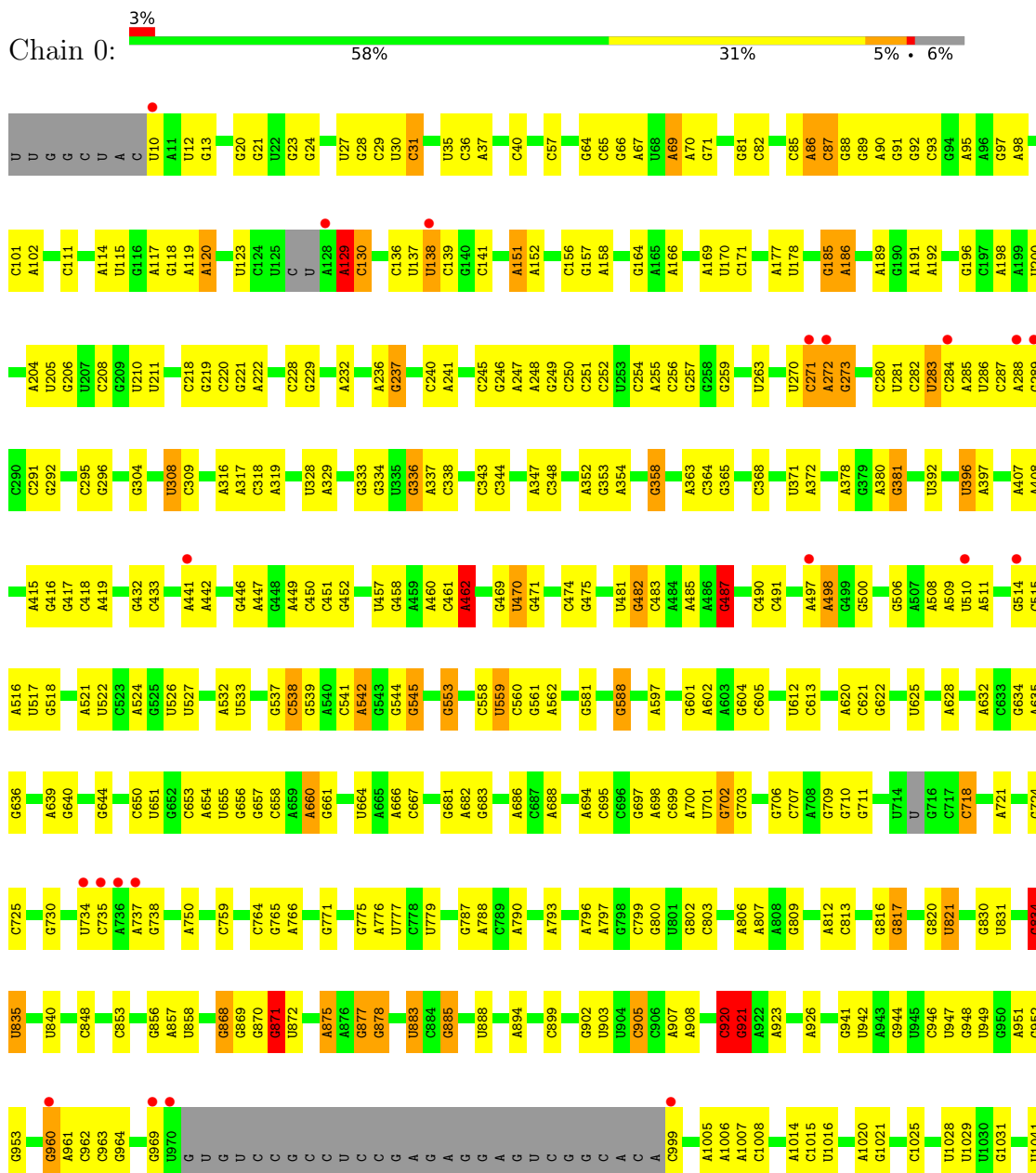
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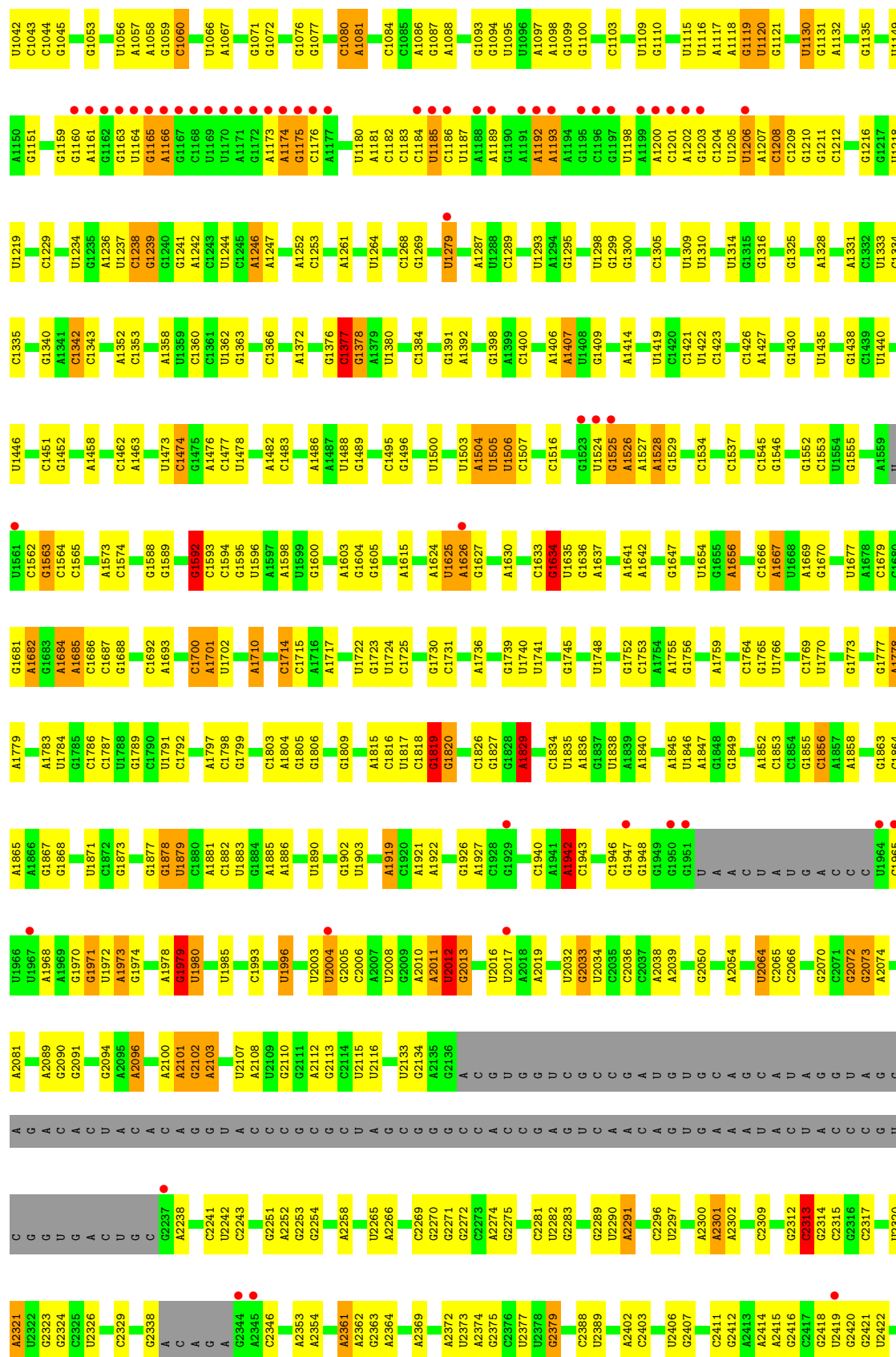
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40	L	93	Total 93	O 93	0	0
40	M	133	Total 133	O 133	0	0
40	N	66	Total 66	O 66	0	0
40	O	42	Total 42	O 42	0	0
40	P	68	Total 68	O 68	0	0
40	Q	53	Total 53	O 53	0	0
40	R	93	Total 93	O 93	0	0
40	S	35	Total 35	O 35	0	0
40	T	40	Total 40	O 40	0	0
40	U	28	Total 28	O 28	0	0
40	V	13	Total 13	O 13	0	0
40	W	70	Total 70	O 70	0	0
40	X	23	Total 23	O 23	0	0
40	Y	93	Total 93	O 93	0	0
40	Z	30	Total 30	O 30	0	0
40	1	60	Total 60	O 60	0	0
40	2	46	Total 46	O 46	0	0
40	3	70	Total 70	O 70	0	0
40	I	9	Total 9	O 9	0	0

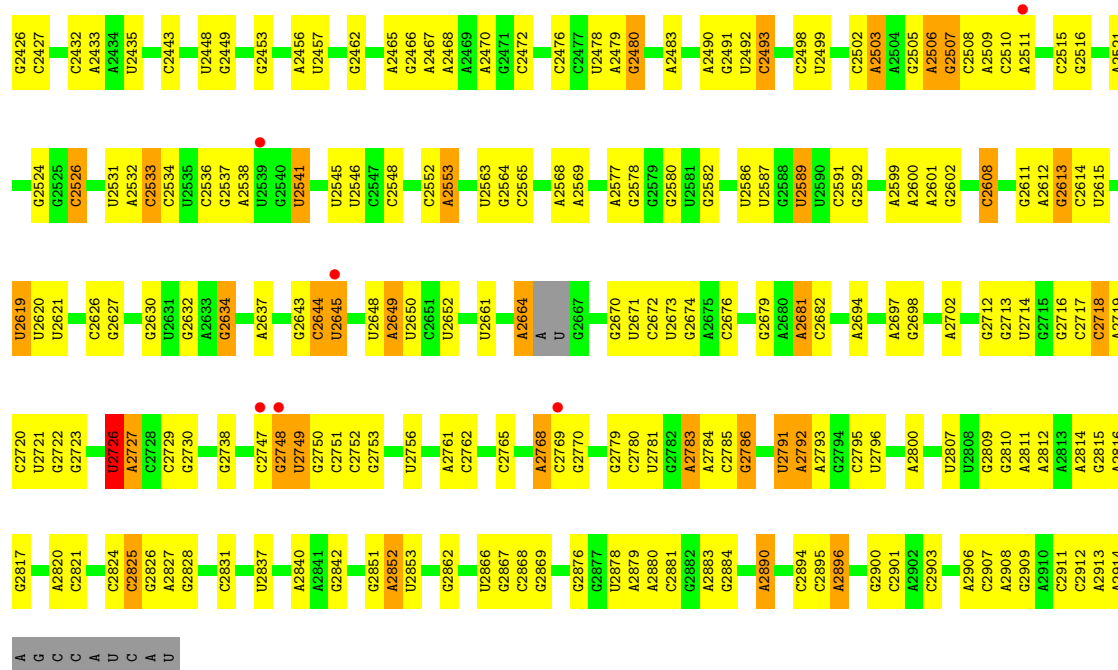
3 Residue-property plots

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



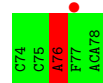
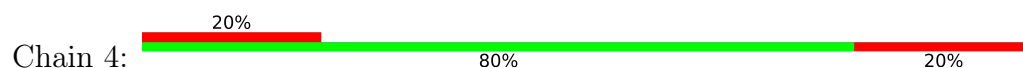




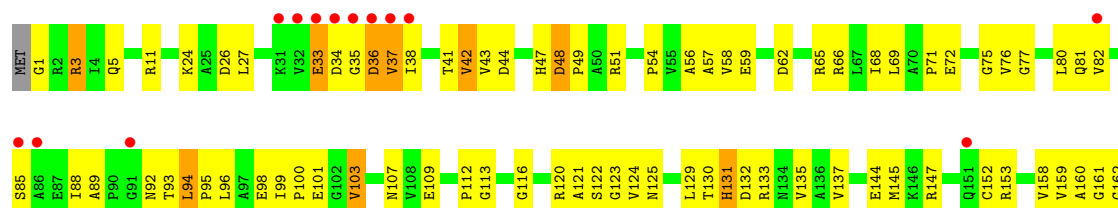
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 5'-R(*CP*CP*AP*(PHE)*(ACA))-3'

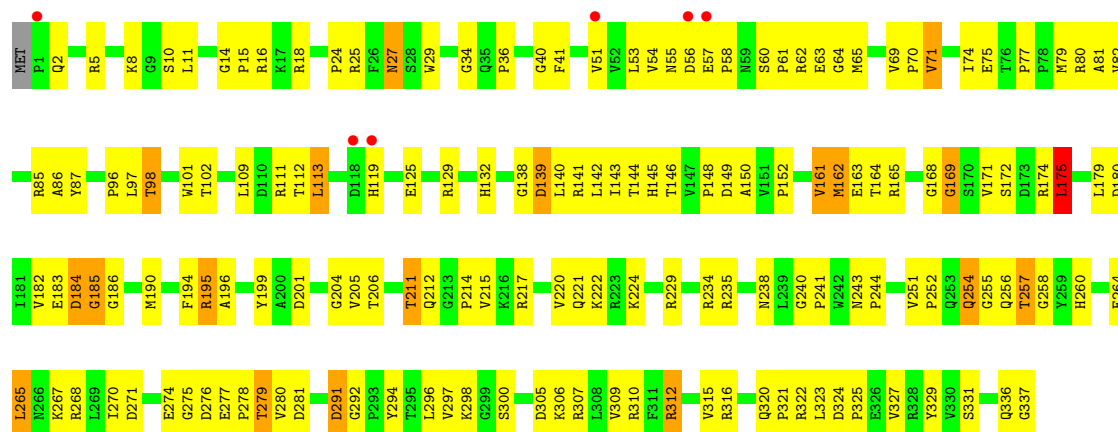


• Molecule 4: 50S ribosomal protein L2P

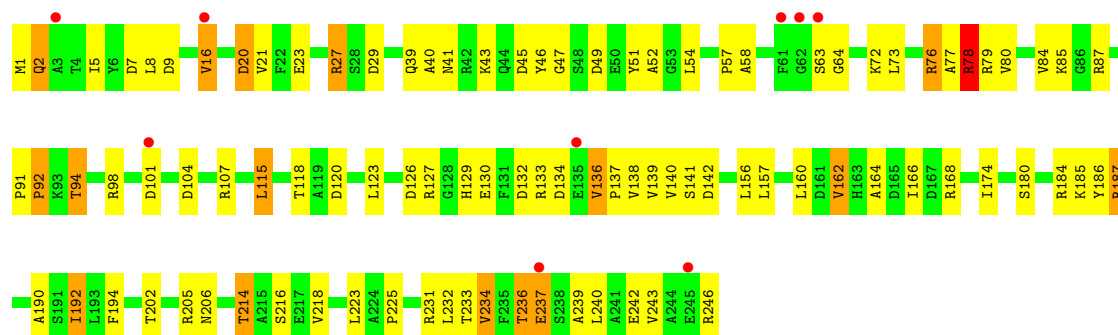




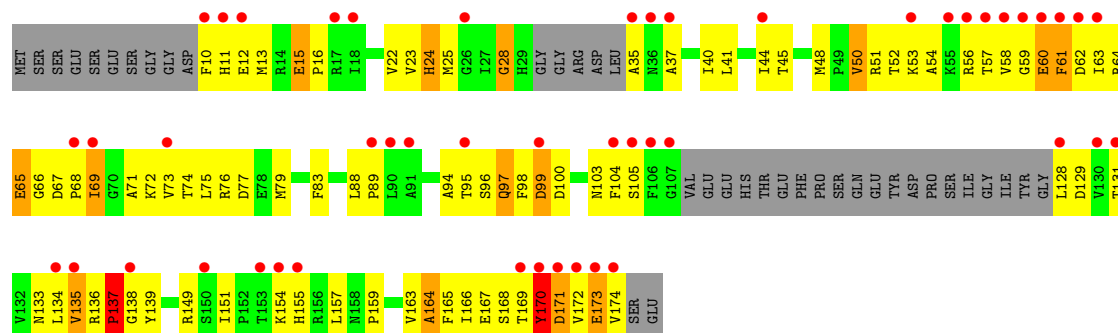
• Molecule 5: 50S ribosomal protein L3P



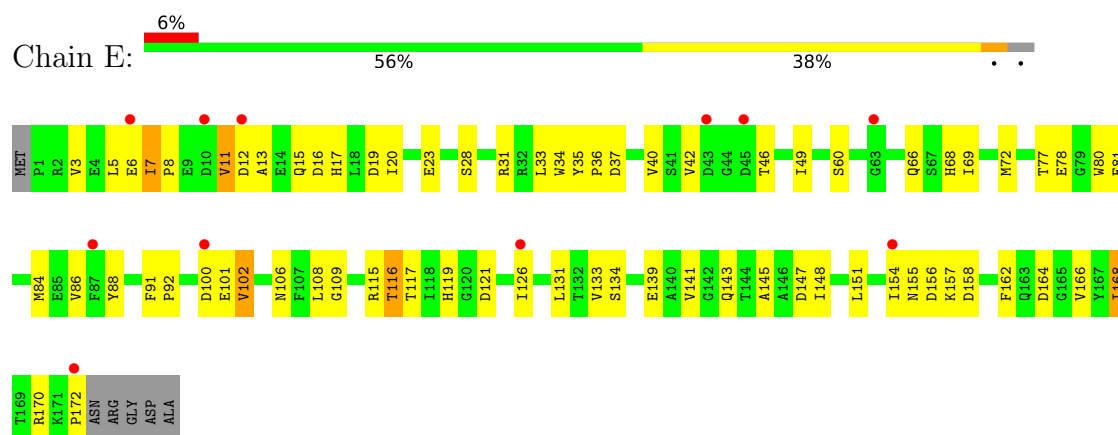
• Molecule 6: 50S ribosomal protein L4E



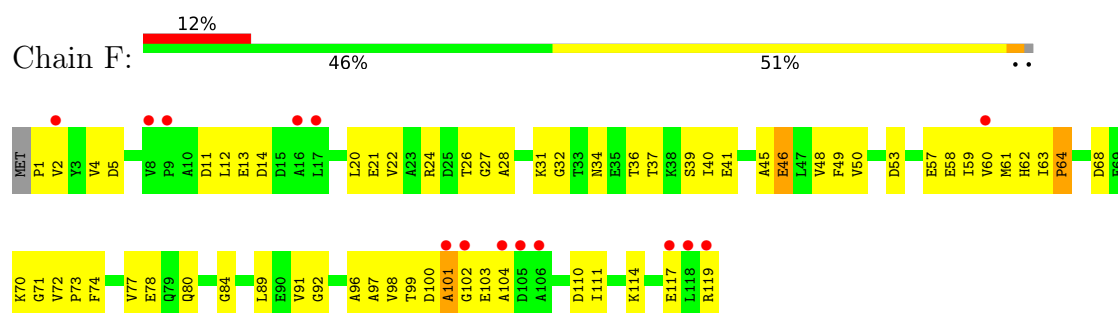
• Molecule 7: 50S ribosomal protein L5P



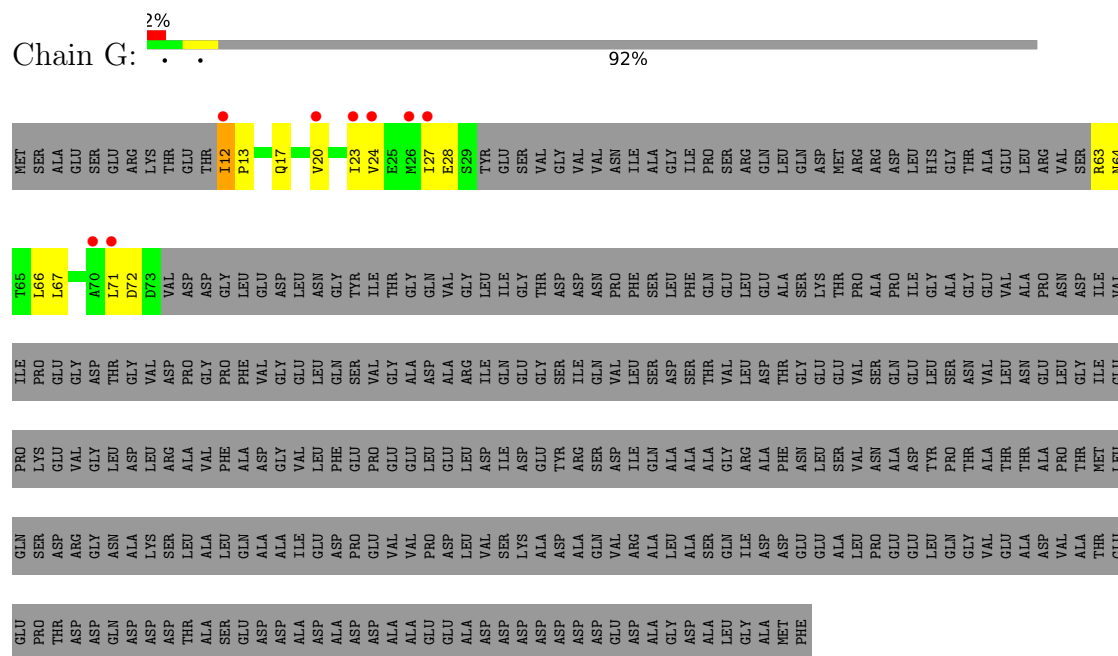
• Molecule 8: 50S ribosomal protein L6P



- Molecule 9: 50S ribosomal protein L7AE

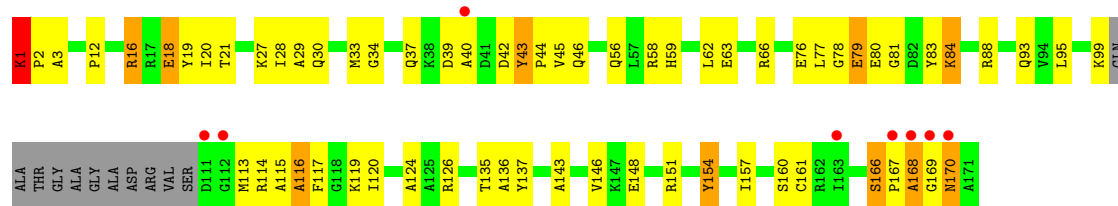


- Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

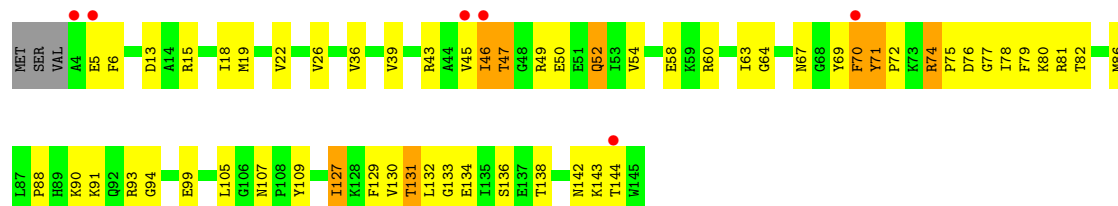


- Molecule 11: 50S RIBOSOMAL PROTEIN L10E

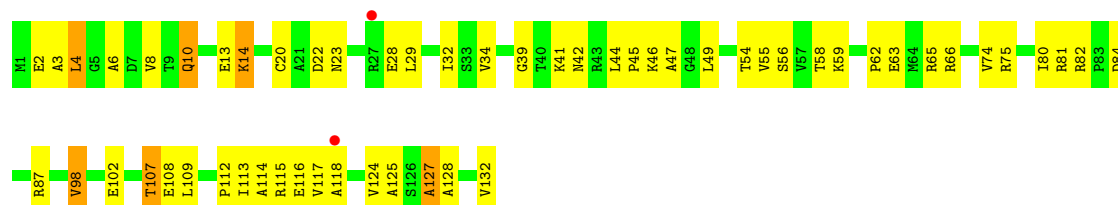




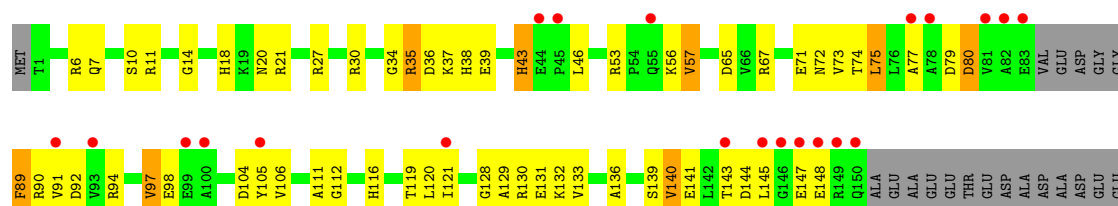
• Molecule 12: 50S ribosomal protein L13P



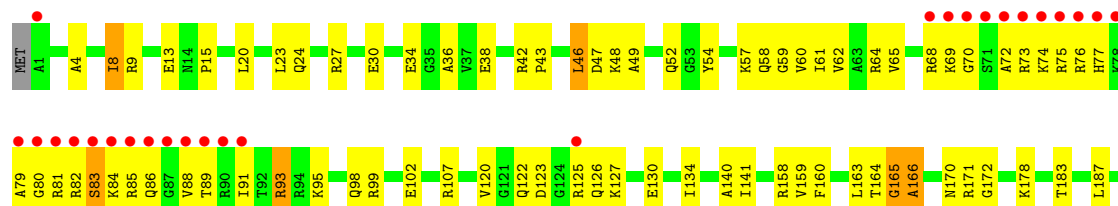
• Molecule 13: 50S ribosomal protein L14P



• Molecule 14: 50S ribosomal protein L15P

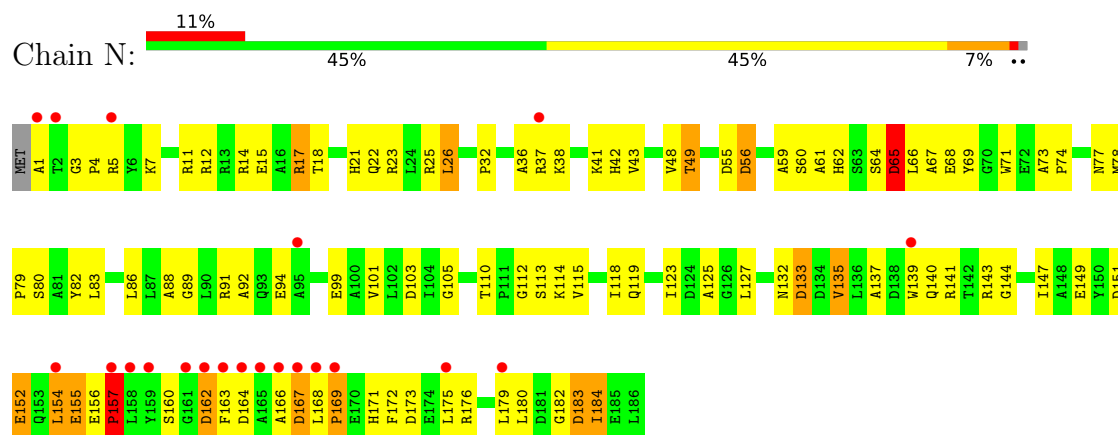


• Molecule 15: 50S Ribosomal Protein L15E

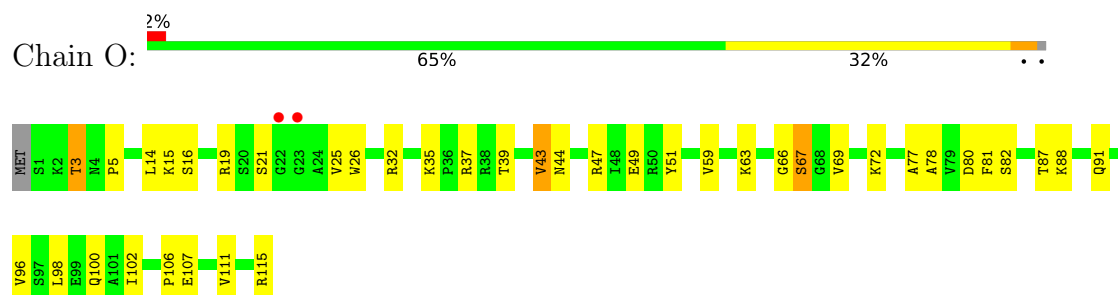


K193
A194

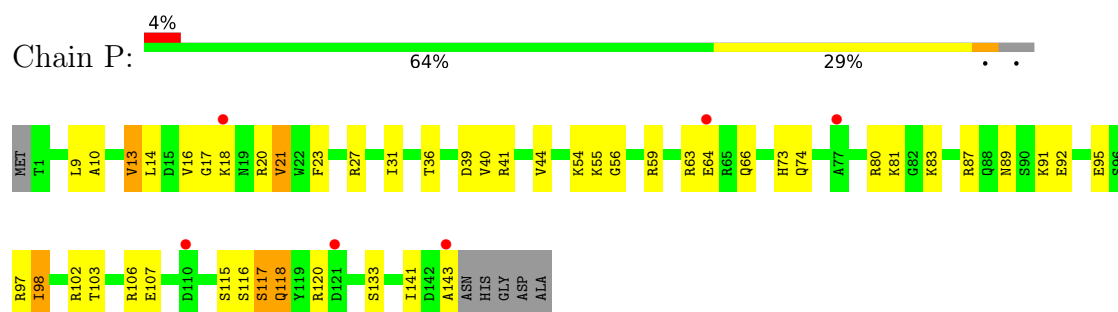
- Molecule 16: 50S ribosomal protein L18P



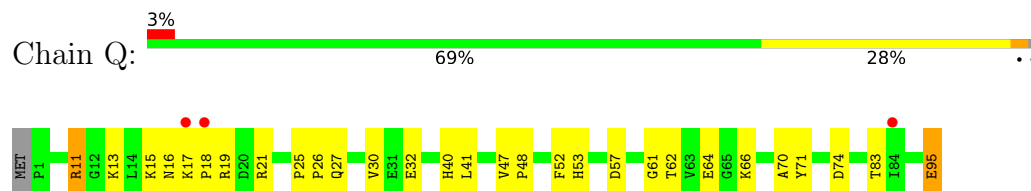
- Molecule 17: 50S ribosomal protein L18e



- Molecule 18: 50S ribosomal protein L19E

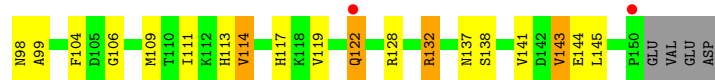


- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P

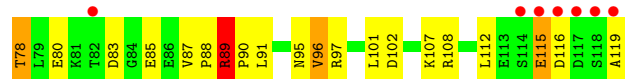
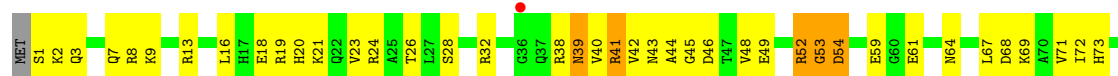




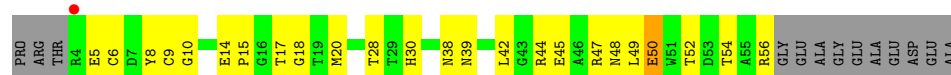
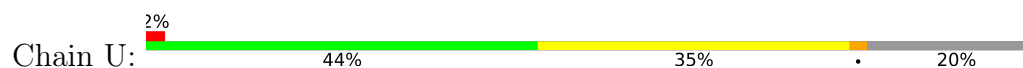
• Molecule 21: 50S ribosomal protein L23P



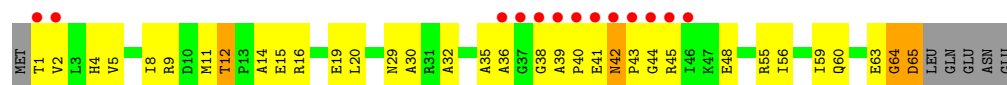
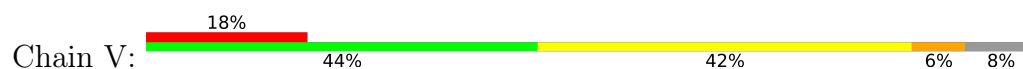
• Molecule 22: 50S ribosomal protein L24P



• Molecule 23: 50S ribosomal protein L24E



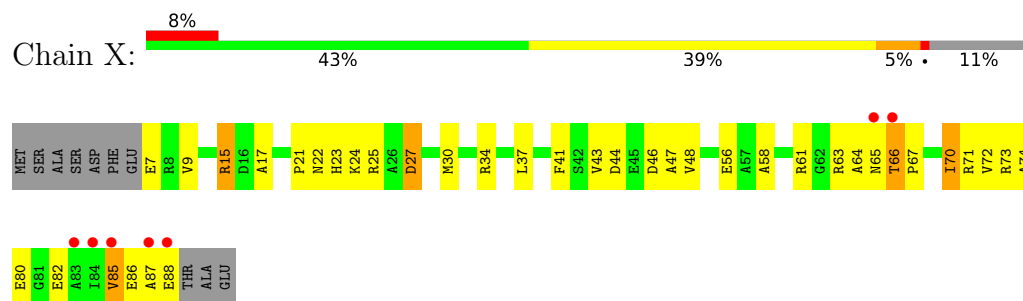
• Molecule 24: 50S ribosomal protein L29P



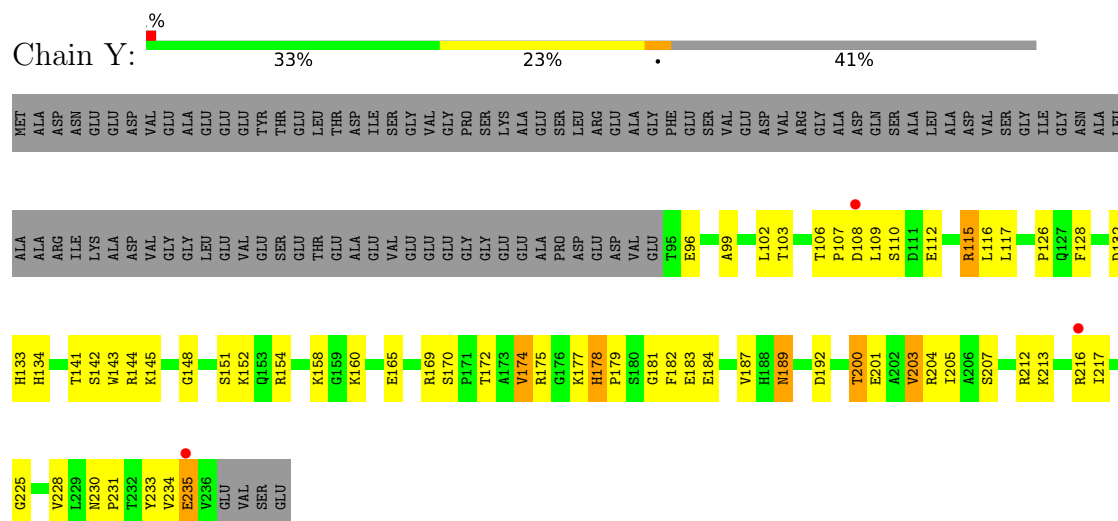
• Molecule 25: 50S ribosomal protein L30P



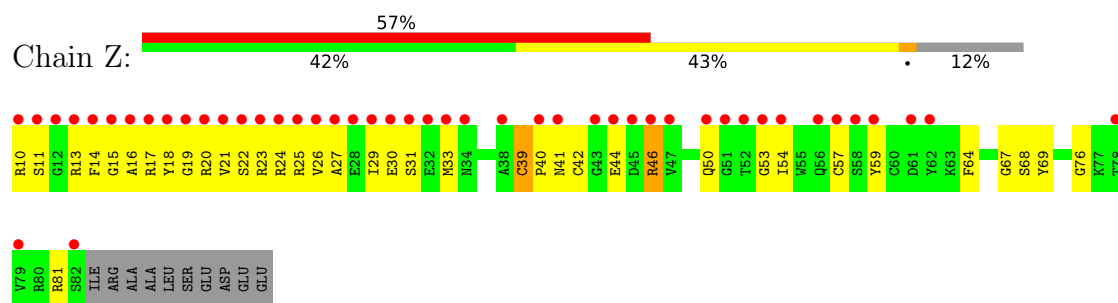
- Molecule 26: 50S ribosomal protein L31e



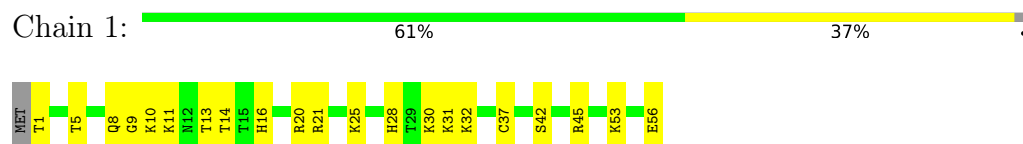
- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: 50S ribosomal protein L37Ae

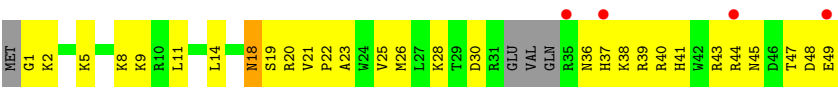


- Molecule 29: 50S ribosomal protein L37e

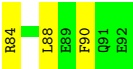
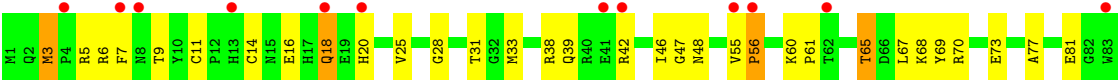


- Molecule 30: 50S ribosomal protein L39e

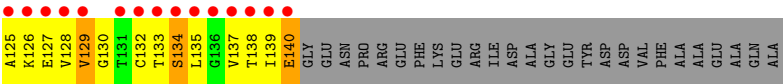
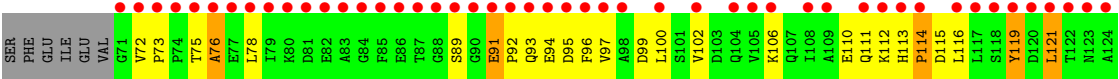
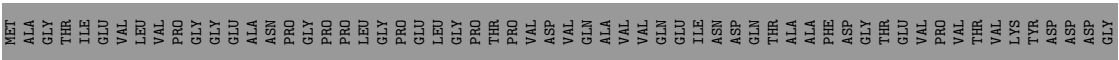
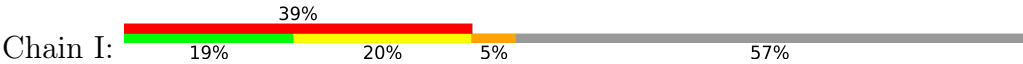




● Molecule 31: 50S ribosomal protein L44E



● Molecule 32: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.82Å 298.60Å 574.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.40) 89.6 (50.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.255 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	98979	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SPS, 1MA, NA, PSU, UR3, K, OMG, CD, OMU, MG, ACA, SR, CL

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	0	0.40	0/65959	0.64	29/102870 (0.0%)
2	9	0.40	0/2905	0.64	2/4528 (0.0%)
3	4	0.42	0/76	0.92	1/112 (0.9%)
4	A	0.43	0/1786	0.97	6/2408 (0.2%)
5	B	0.44	0/2690	0.99	8/3652 (0.2%)
6	C	0.46	0/1884	1.00	8/2551 (0.3%)
7	D	0.38	0/1111	0.96	7/1498 (0.5%)
8	E	0.42	0/1382	0.93	5/1880 (0.3%)
9	F	0.41	0/901	0.90	1/1224 (0.1%)
10	G	0.39	0/241	0.82	0/324
11	H	0.41	0/1287	0.99	7/1725 (0.4%)
12	J	0.42	0/1136	1.01	6/1530 (0.4%)
13	K	0.46	0/1001	0.99	5/1347 (0.4%)
14	L	0.40	0/1130	0.98	5/1509 (0.3%)
15	M	0.44	0/1584	0.90	4/2119 (0.2%)
16	N	0.37	0/1474	1.02	7/1999 (0.4%)
17	O	0.42	0/874	0.95	4/1181 (0.3%)
18	P	0.41	0/1147	0.92	1/1528 (0.1%)
19	Q	0.42	0/749	1.02	1/1005 (0.1%)
20	R	0.44	0/1172	0.99	5/1578 (0.3%)
21	S	0.39	0/648	0.92	1/875 (0.1%)
22	T	0.39	0/958	0.96	9/1289 (0.7%)
23	U	0.40	0/417	0.88	1/562 (0.2%)
24	V	0.37	0/502	0.96	4/675 (0.6%)
25	W	0.46	0/1219	1.00	6/1655 (0.4%)
26	X	0.44	0/664	0.98	4/895 (0.4%)
27	Y	0.45	0/1146	1.03	8/1536 (0.5%)
28	Z	0.38	0/589	0.95	3/787 (0.4%)
29	1	0.48	0/438	0.99	1/578 (0.2%)
30	2	0.45	0/401	0.86	0/529
31	3	0.38	0/771	0.81	1/1024 (0.1%)
32	I	0.38	0/526	0.94	4/716 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.41	0/98768	0.74	154/147689 (0.1%)

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	0	1	44
2	9	0	1
All	All	1	45

There are no bond length outliers.

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	14.42	131.13	109.50
16	N	163	PHE	N-CA-C	-11.59	99.27	113.41
1	0	1979	G	C2'-C3'-O3'	10.25	124.88	109.50
1	0	1563	G	C4'-C3'-O3'	8.40	121.99	109.40
7	D	173	GLU	N-CA-C	8.14	115.46	108.78
14	L	57	VAL	N-CA-C	-7.69	105.35	112.43
2	9	3039	U	N1-C1'-C2'	7.43	123.15	112.00
7	D	170	TYR	N-CA-C	7.39	121.83	111.92
12	J	71	TYR	CA-C-N	7.27	127.03	119.76
12	J	71	TYR	C-N-CA	7.27	127.03	119.76
6	C	78	ARG	N-CA-C	7.25	118.17	108.38
20	R	141	VAL	N-CA-C	7.24	118.24	108.11
5	B	222	LYS	N-CA-C	-7.19	99.28	110.42
1	0	883	U	N1-C1'-C2'	7.10	122.64	112.00
5	B	143	ILE	N-CA-C	-7.05	100.49	109.30
21	S	27	ALA	N-CA-C	-6.98	97.86	108.96
1	0	1592	G	N9-C1'-C2'	6.90	122.34	112.00
1	0	1942	A	C5'-C4'-C3'	6.87	126.30	116.00
1	0	1819	G	C5'-C4'-C3'	6.80	126.21	116.00
27	Y	183	GLU	N-CA-C	-6.75	98.23	109.24
5	B	323	LEU	N-CA-C	6.74	119.00	110.24
19	Q	17	LYS	N-CA-C	-6.69	101.22	109.65
25	W	35	VAL	N-CA-C	6.64	115.51	107.61
16	N	135	VAL	N-CA-C	-6.62	106.84	113.20
8	E	11	VAL	N-CA-C	6.59	119.41	109.20
1	0	1120	U	C5'-C4'-C3'	-6.55	106.18	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	K	124	VAL	N-CA-C	-6.53	104.39	110.53
14	L	145	LEU	N-CA-C	-6.49	104.13	111.07
17	O	82	SER	N-CA-C	-6.45	102.48	110.41
20	R	3	SER	N-CA-C	-6.43	99.56	109.52
1	0	1504	A	N9-C1'-C2'	6.42	121.63	112.00
32	I	91	GLU	CA-C-N	6.38	126.29	119.85
32	I	91	GLU	C-N-CA	6.38	126.29	119.85
25	W	25	ASN	N-CA-C	6.36	120.62	112.86
26	X	79	GLU	N-CA-C	6.34	119.00	111.33
7	D	100	ASP	N-CA-C	-6.33	105.60	113.38
18	P	118	GLN	N-CA-C	-6.28	103.72	112.45
11	H	43	TYR	CA-C-N	6.24	125.65	118.85
11	H	43	TYR	C-N-CA	6.24	125.65	118.85
25	W	113	SER	CA-C-N	6.21	125.91	119.82
25	W	113	SER	C-N-CA	6.21	125.91	119.82
1	0	834	G	C2'-C3'-O3'	-6.17	104.44	113.70
6	C	205	ARG	N-CA-C	6.17	119.65	111.75
20	R	137	ASN	N-CA-C	6.17	119.60	110.46
1	0	871	G	C5'-C4'-O4'	-6.16	100.56	109.80
24	V	64	GLY	N-CA-C	-6.15	106.67	115.64
7	D	15	GLU	CA-C-N	6.13	127.51	119.84
7	D	15	GLU	C-N-CA	6.13	127.51	119.84
28	Z	39	CYS	CA-C-N	6.13	126.31	119.32
28	Z	39	CYS	C-N-CA	6.13	126.31	119.32
4	A	103	VAL	N-CA-C	6.12	114.70	107.73
1	0	921	G	N9-C1'-C2'	6.11	121.17	112.00
1	0	1634	G	N9-C1'-C2'	6.08	121.12	112.00
1	0	2726	U	N1-C1'-C2'	6.04	121.06	112.00
13	K	54	THR	N-CA-C	-6.04	100.72	110.32
22	T	52	ARG	N-CA-C	6.01	123.61	110.80
8	E	17	HIS	CB-CA-C	-5.98	109.69	116.63
16	N	42	HIS	N-CA-C	5.98	118.30	109.69
23	U	50	GLU	N-CA-C	5.97	118.55	111.33
3	4	76	A	C2'-C3'-O3'	5.95	118.42	109.50
7	D	173	GLU	CB-CA-C	-5.94	108.51	117.07
16	N	133	ASP	N-CA-C	5.93	118.23	111.11
27	Y	143	TRP	N-CA-C	5.93	119.05	110.28
13	K	14	LYS	N-CA-C	-5.92	101.28	110.10
1	0	1615	A	C5'-C4'-C3'	5.84	124.77	116.00
5	B	175	LEU	N-CA-C	-5.84	104.92	111.28
28	Z	24	ARG	N-CA-C	-5.84	106.20	113.55
26	X	77	PHE	N-CA-C	5.83	115.54	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	R	122	GLN	N-CA-C	-5.82	100.35	109.25
22	T	16	LEU	N-CA-C	5.80	118.10	111.02
1	0	2313	C	C5'-C4'-C3'	5.80	124.70	116.00
17	O	43	VAL	N-CA-C	5.79	116.93	108.53
4	A	228	ILE	N-CA-C	5.79	116.48	108.84
26	X	22	ASN	N-CA-C	5.76	119.12	111.75
11	H	1	LYS	CA-C-N	5.76	125.69	119.76
11	H	1	LYS	C-N-CA	5.76	125.69	119.76
1	0	920	C	C2'-C3'-O3'	-5.71	105.14	113.70
4	A	99	ILE	N-CA-C	5.68	113.51	108.63
25	W	68	THR	N-CA-C	5.66	118.38	111.82
12	J	81	ARG	N-CA-C	-5.65	105.20	111.36
24	V	42	ASN	CA-C-N	5.63	126.88	119.84
24	V	42	ASN	C-N-CA	5.63	126.88	119.84
22	T	89	ARG	CA-C-N	5.62	125.63	119.90
22	T	89	ARG	C-N-CA	5.62	125.63	119.90
31	3	81	GLU	N-CA-C	-5.62	103.07	110.43
12	J	67	ASN	N-CA-C	-5.60	105.17	111.28
26	X	17	ALA	N-CA-C	-5.57	105.36	111.82
11	H	160	SER	N-CA-C	-5.54	101.52	110.32
11	H	116	ALA	N-CA-C	5.50	119.72	112.89
4	A	48	ASP	CA-C-N	5.50	125.59	119.32
4	A	48	ASP	C-N-CA	5.50	125.59	119.32
22	T	54	ASP	N-CA-C	-5.49	106.54	113.18
6	C	41	ASN	N-CA-C	5.47	119.43	112.87
20	R	18	LEU	N-CA-C	-5.44	101.30	109.95
27	Y	230	ASN	CA-C-N	5.43	125.63	120.31
27	Y	230	ASN	C-N-CA	5.43	125.63	120.31
8	E	168	ILE	N-CA-C	-5.42	101.61	108.93
24	V	30	ALA	N-CA-C	-5.37	105.34	111.14
17	O	69	VAL	N-CA-C	5.33	115.63	108.17
14	L	97	VAL	N-CA-C	5.33	115.96	109.30
15	M	165	GLY	N-CA-C	-5.31	105.97	112.77
13	K	46	LYS	N-CA-C	5.30	118.38	109.95
32	I	134	SER	N-CA-C	-5.30	106.12	112.59
15	M	13	GLU	N-CA-C	-5.29	106.33	112.89
1	0	2291	A	N9-C1'-C2'	5.27	119.91	112.00
16	N	3	GLY	CA-C-N	5.27	124.90	119.05
16	N	3	GLY	C-N-CA	5.27	124.90	119.05
1	0	1504	A	C1'-O4'-C4'	-5.26	104.64	109.90
13	K	8	VAL	N-CA-C	5.26	116.05	108.48
1	0	2301	A	N9-C1'-C2'	5.25	119.88	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Y	178	HIS	N-CA-C	-5.24	102.41	110.01
27	Y	178	HIS	CA-C-N	-5.24	114.42	119.87
27	Y	178	HIS	C-N-CA	-5.24	114.42	119.87
29	1	31	LYS	N-CA-C	-5.23	107.07	113.50
5	B	111	ARG	N-CA-C	-5.23	106.95	113.38
8	E	37	ASP	N-CA-C	5.23	118.93	112.24
17	O	66	GLY	N-CA-C	5.22	125.56	113.18
1	0	1261	A	N9-C1'-C2'	5.21	119.82	112.00
1	0	2012	U	N1-C1'-C2'	5.18	119.77	112.00
25	W	143	THR	N-CA-C	-5.18	105.76	111.71
1	0	206	G	C5'-C4'-C3'	-5.17	108.24	116.00
6	C	80	VAL	CA-C-N	5.17	125.22	119.32
6	C	80	VAL	C-N-CA	5.17	125.22	119.32
6	C	192	ILE	N-CA-C	5.17	116.68	109.55
15	M	8	ILE	N-CA-C	-5.16	105.68	110.53
12	J	91	LYS	N-CA-C	-5.16	102.88	110.52
14	L	7	GLN	N-CA-C	5.16	117.80	111.82
2	9	3039	U	C4'-C3'-O3'	-5.15	105.27	113.00
22	T	101	LEU	N-CA-C	5.15	118.15	110.52
1	0	2615	U	N1-C1'-C2'	5.15	119.72	112.00
15	M	166	ALA	N-CA-C	-5.13	105.86	111.82
27	Y	110	SER	N-CA-C	-5.12	103.77	110.53
7	D	173	GLU	CA-C-O	5.12	120.91	117.94
5	B	265	LEU	N-CA-C	5.10	117.26	110.53
1	0	129	A	C2'-C3'-O3'	5.10	121.34	113.70
4	A	188	ASN	N-CA-C	5.08	116.98	107.99
22	T	3	GLN	CA-C-N	5.07	125.11	119.32
22	T	3	GLN	C-N-CA	5.07	125.11	119.32
32	I	121	LEU	N-CA-C	-5.07	106.35	112.54
5	B	224	LYS	N-CA-C	5.06	118.00	109.95
1	0	718	C	C5'-C4'-C3'	-5.05	108.42	116.00
5	B	161	VAL	N-CA-C	5.05	115.25	108.17
8	E	121	ASP	N-CA-C	-5.05	106.96	112.72
6	C	92	PRO	N-CA-C	-5.05	103.19	111.21
12	J	22	VAL	N-CA-C	-5.04	105.41	110.30
11	H	37	GLN	N-CA-C	-5.04	106.64	112.89
22	T	78	THR	N-CA-C	5.04	116.33	109.18
1	0	1700	C	C2'-C3'-O3'	-5.03	106.16	113.70
9	F	62	HIS	N-CA-C	5.03	117.65	111.82
14	L	20	ASN	N-CA-C	5.01	117.71	111.24
16	N	169	PRO	N-CA-C	-5.01	102.14	112.47
1	0	1452	G	C5'-C4'-C3'	-5.01	108.48	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	462	A	N9-C1'-C2'	5.01	119.52	112.00
6	C	20	ASP	N-CA-C	5.00	117.39	111.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1080	C	Sidechain
1	0	1340	G	Sidechain
1	0	1376	G	Sidechain
1	0	1377	C	Sidechain
1	0	1430	G	Sidechain
1	0	1458	A	Sidechain
1	0	1592	G	Sidechain
1	0	1647	G	Sidechain
1	0	1714	C	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1863	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1993	C	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2664	A	Sidechain
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	460	A	Sidechain
1	0	462	A	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	483	C	Sidechain
1	0	487	G	Sidechain
1	0	518	G	Sidechain
1	0	771	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
2	9	3065	A	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29809	913	0
2	9	2600	0	1326	54	0
3	4	74	0	42	1	0
4	A	1753	0	1765	136	0
5	B	2625	0	2531	159	0
6	C	1859	0	1816	119	0
7	D	1094	0	1085	99	0
8	E	1357	0	1266	71	0
9	F	890	0	843	64	0
10	G	240	0	231	14	0
11	H	1266	0	1268	67	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	61	0
14	L	1118	0	1076	67	0
15	M	1560	0	1567	92	0
16	N	1445	0	1401	101	0
17	O	865	0	873	46	0
18	P	1136	0	1123	45	0
19	Q	735	0	729	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	R	1149	0	1122	53	0
21	S	641	0	605	24	0
22	T	950	0	923	74	0
23	U	410	0	364	24	0
24	V	499	0	511	43	0
25	W	1196	0	1137	106	0
26	X	654	0	653	35	0
27	Y	1130	0	1133	68	0
28	Z	578	0	542	43	0
29	1	431	0	426	27	0
30	2	396	0	413	29	0
31	3	755	0	728	44	0
32	I	519	0	500	43	0
33	0	86	0	0	0	0
33	4	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	62	0	0	0	0
35	3	1	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	9	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	97	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	4	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	4	23	0	19	2	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5630	0	0	126	0
40	1	60	0	0	3	0
40	2	46	0	0	1	0
40	3	70	0	0	6	0
40	4	1	0	0	0	0
40	9	130	0	0	5	0
40	A	132	0	0	13	0
40	B	137	0	0	22	0
40	C	175	0	0	20	0
40	D	43	0	0	8	0
40	E	42	0	0	2	0
40	F	25	0	0	4	0
40	G	16	0	0	2	0
40	H	77	0	0	4	0
40	I	9	0	0	0	0
40	J	52	0	0	1	0
40	K	61	0	0	6	1
40	L	93	0	0	11	0
40	M	133	0	0	8	0
40	N	66	0	0	5	0
40	O	42	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	P	68	0	0	3	0
40	Q	53	0	0	2	0
40	R	93	0	0	5	0
40	S	35	0	0	2	0
40	T	40	0	0	4	0
40	U	28	0	0	2	0
40	V	13	0	0	1	0
40	W	70	0	0	4	0
40	X	23	0	0	3	0
40	Y	93	0	0	9	0
40	Z	30	0	0	5	0
All	All	98979	0	59956	2539	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (2539) 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)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.29	1.15
1:O:1160:G:H5'	1:O:1161:A:H5'	1.27	1.13
15:M:68:ARG:HH21	15:M:73:ARG:HD3	1.12	1.13
6:C:236:THR:HG22	6:C:239:ALA:H	1.06	1.12
9:F:91:VAL:HG12	9:F:92:GLY:H	1.12	1.11
28:Z:46:ARG:HD3	28:Z:59:TYR:HB2	1.37	1.04
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.38	1.04
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.18	1.04
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.40	1.03
21:S:57:THR:HG22	21:S:59:ASP:H	1.23	1.03
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.23	1.02
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.42	1.01
13:K:107:THR:HG22	13:K:108:GLU:HG3	1.43	0.99
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.77	0.99
1:O:156:C:H5''	15:M:171:ARG:HD3	1.44	0.99
13:K:10:GLN:HE21	13:K:10:GLN:N	1.61	0.98
15:M:164:THR:HG22	15:M:166:ALA:H	1.27	0.98
25:W:149:LEU:HG	25:W:153:MET:HE2	1.43	0.98
1:O:1242:A:H5'	12:J:82:THR:HG23	1.47	0.97
13:K:10:GLN:H	13:K:10:GLN:NE2	1.63	0.96
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.29	0.95
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.29	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:C8	1:0:871:G:H5'	2.01	0.95
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.46	0.94
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.46	0.94
4:A:192:VAL:CG1	4:A:207:GLN:HB3	1.97	0.94
1:0:969:G:H1	1:0:999:C:H42	1.13	0.94
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.30	0.94
1:0:656:G:H5'	17:O:3:THR:HG22	1.49	0.93
2:9:3076:G:H3'	2:9:3077:A:H5''	1.50	0.93
2:9:3056:A:H2'	2:9:3057:A:H5''	1.49	0.93
29:1:25:LYS:HD2	30:2:49:GLU:H	1.33	0.93
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.51	0.93
1:0:542:A:H5'	1:0:542:A:H8	1.34	0.93
4:A:33:GLU:H	4:A:33:GLU:CD	1.76	0.93
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.48	0.92
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.03	0.92
16:N:113:SER:HB2	40:N:9358:HOH:O	1.70	0.91
18:P:115:SER:H	18:P:118:GLN:HE21	1.12	0.91
16:N:17:ARG:HB3	16:N:17:ARG:HH11	1.35	0.91
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.49	0.91
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.11	0.91
16:N:11:ARG:HG3	16:N:14:ARG:HH12	1.36	0.91
28:Z:39:CYS:SG	28:Z:57:CYS:HB2	2.11	0.91
1:0:2586:U:H3	1:0:2592:G:H22	1.14	0.90
5:B:86:ALA:HA	40:B:9573:HOH:O	1.70	0.90
1:0:21:G:H5'	20:R:2:ILE:HA	1.51	0.90
7:D:25:MET:HE2	7:D:41:LEU:HG	1.52	0.90
12:J:131:THR:HG22	12:J:134:GLU:H	1.34	0.90
16:N:144:GLY:O	16:N:147:ILE:HG22	1.71	0.89
1:0:1973:A:H5'	1:0:1973:A:H8	1.37	0.89
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.53	0.89
7:D:172:VAL:HG12	7:D:173:GLU:H	1.36	0.89
1:0:1593:C:OP1	18:P:117:SER:HB3	1.73	0.89
6:C:236:THR:HG22	6:C:239:ALA:N	1.87	0.88
5:B:238:ASN:HD22	5:B:240:GLY:H	1.16	0.88
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.88	0.88
1:0:870:G:H2'	1:0:871:G:H5''	1.56	0.88
1:0:2717:C:C2'	1:0:2718:C:H5''	2.04	0.88
1:0:1603:A:H5'	1:0:1605:G:O4'	1.74	0.87
4:A:179:MET:HA	4:A:179:MET:HE3	1.55	0.87
1:0:1835:U:H5	1:0:1840:A:N7	1.73	0.87
1:0:2717:C:H2'	1:0:2718:C:H5''	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.09	0.87
5:B:162:MET:HE3	5:B:310:ARG:HD3	1.57	0.86
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.55	0.86
18:P:115:SER:OG	18:P:118:GLN:HG3	1.75	0.86
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.54	0.86
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.57	0.86
27:Y:174:VAL:HG13	27:Y:177:LYS:HD2	1.57	0.86
1:0:1474:C:H6	1:0:1474:C:H5'	1.39	0.86
1:0:2506:A:HO2'	1:0:2507:G:H8	0.86	0.86
15:M:68:ARG:O	15:M:68:ARG:HD3	1.76	0.85
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.39	0.85
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.58	0.85
15:M:68:ARG:NH2	15:M:73:ARG:HD3	1.89	0.85
9:F:46:GLU:OE1	9:F:100:ASP:HA	1.76	0.85
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.57	0.85
1:0:1160:G:C5'	1:0:1161:A:H5'	2.06	0.85
1:0:871:G:H5'	1:0:871:G:H8	1.38	0.85
5:B:179:LEU:O	5:B:183:GLU:HG2	1.77	0.85
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.60	0.84
1:0:545:G:H5'	1:0:545:G:H8	1.42	0.84
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.57	0.84
1:0:541:C:C2'	1:0:542:A:H5''	2.07	0.84
1:0:1701:A:H4'	1:0:1702:U:H5''	1.59	0.84
1:0:2524:G:H21	1:0:2526:C:H5	1.25	0.84
1:0:288:A:H61	1:0:364:C:H42	1.26	0.83
1:0:289:G:H22	1:0:363:A:H2	1.25	0.83
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.26	0.83
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.60	0.83
4:A:192:VAL:HG22	40:A:9669:HOH:O	1.78	0.83
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.61	0.83
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.59	0.83
1:0:2716:G:H5''	5:B:206:THR:HG21	1.61	0.83
1:0:2840:A:OP1	5:B:211:THR:HG23	1.77	0.83
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.44	0.83
9:F:58:GLU:HA	9:F:61:MET:HE2	1.58	0.82
6:C:236:THR:CG2	6:C:239:ALA:H	1.91	0.82
1:0:2506:A:O2'	1:0:2507:G:H8	1.63	0.82
4:A:194:MET:HE3	4:A:199:HIS:HB2	1.62	0.82
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.62	0.82
18:P:9:LEU:O	18:P:13:VAL:HG12	1.78	0.82
25:W:13:MET:HE2	25:W:18:GLN:HA	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1838:U:O2'	1:0:2644:C:H5'	1.80	0.82
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.60	0.82
6:C:5:ILE:HD11	6:C:16:VAL:HG22	1.60	0.81
24:V:1:THR:HG23	24:V:2:VAL:H	1.44	0.81
1:0:1116:U:O2'	1:0:1118:A:H2	1.63	0.81
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.62	0.81
1:0:1116:U:HO2'	1:0:1118:A:H2	0.81	0.81
27:Y:235:GLU:CD	27:Y:235:GLU:H	1.83	0.81
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.62	0.81
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.63	0.81
9:F:91:VAL:HG12	9:F:92:GLY:N	1.92	0.80
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.46	0.80
7:D:57:THR:HG23	7:D:63:ILE:HA	1.64	0.80
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.61	0.80
1:0:541:C:H2'	1:0:542:A:H5''	1.64	0.80
22:T:115:GLU:HG3	22:T:116:ASP:H	1.44	0.80
25:W:88:THR:HB	40:W:6679:HOH:O	1.80	0.80
40:0:5723:HOH:O	13:K:39:GLY:HA2	1.82	0.80
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.46	0.80
4:A:153:ARG:HB2	4:A:153:ARG:HH11	1.45	0.80
1:0:2812:A:H2	1:0:2814:A:H62	1.24	0.80
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.16	0.80
25:W:125:HIS:HD2	25:W:127:GLY:H	1.25	0.80
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.62	0.79
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.81	0.79
22:T:115:GLU:HG3	22:T:116:ASP:N	1.97	0.79
1:0:553:G:P	27:Y:204:ARG:HH22	2.06	0.79
1:0:1641:A:H2'	1:0:1642:A:H5'	1.64	0.79
20:R:39:THR:HB	20:R:42:GLU:HG3	1.64	0.79
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.46	0.79
21:S:57:THR:HG22	21:S:59:ASP:N	1.95	0.79
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.65	0.79
1:0:111:C:O2'	29:1:20:ARG:HG2	1.84	0.78
1:0:1377:C:H5'	1:0:1377:C:H6	1.47	0.78
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.65	0.78
1:0:871:G:H8	1:0:871:G:C5'	1.96	0.78
14:L:73:VAL:HG23	14:L:74:THR:H	1.48	0.78
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.13	0.78
1:0:1184:C:H4'	32:I:126:LYS:HB3	1.63	0.78
1:0:2005:G:H3'	1:0:2005:G:OP2	1.84	0.78
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1372:A:H3'	40:0:7554:HOH:O	1.84	0.78
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.65	0.78
15:M:79:ALA:HB3	15:M:81:ARG:NH1	1.99	0.78
18:P:91:LYS:O	18:P:95:GLU:HG3	1.84	0.78
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.66	0.77
1:0:1160:G:H5'	1:0:1161:A:C5'	2.10	0.77
29:1:25:LYS:HD2	30:2:49:GLU:N	1.98	0.77
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.66	0.77
1:0:1166:A:H61	1:0:1180:U:H3	1.33	0.77
5:B:162:MET:CE	5:B:310:ARG:HD3	2.14	0.77
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.66	0.77
16:N:37:ARG:HG3	36:N:9307:CL:CL	2.22	0.77
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.67	0.77
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.49	0.77
1:0:1165:G:H1'	1:0:1174:A:H1'	1.64	0.77
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.00	0.77
12:J:74:ARG:NH1	12:J:76:ASP:HB2	1.99	0.77
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.66	0.77
32:I:102:VAL:O	32:I:106:LYS:HG3	1.85	0.77
13:K:81:ARG:HD3	13:K:87:ARG:NH1	1.99	0.76
14:L:80:ASP:HB2	14:L:90:ARG:O	1.83	0.76
20:R:23:MET:HE3	20:R:28:SER:OG	1.84	0.76
4:A:199:HIS:HD2	4:A:201:PHE:H	1.33	0.76
16:N:37:ARG:NH2	16:N:105:GLY:HA3	1.99	0.76
25:W:13:MET:HE1	25:W:21:LEU:HD12	1.67	0.76
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.15	0.76
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.68	0.76
32:I:99:ASP:OD1	32:I:138:THR:HB	1.85	0.76
1:0:506:G:H22	1:0:509:A:C5'	1.98	0.76
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.46	0.76
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.68	0.76
1:0:560:C:H42	1:0:597:A:H61	1.33	0.76
1:0:962:C:H1'	16:N:5:ARG:NH1	2.00	0.76
17:O:32:ARG:NE	17:O:35:LYS:HD2	1.98	0.76
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.68	0.76
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.68	0.75
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.68	0.75
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.11	0.75
16:N:17:ARG:HB3	16:N:17:ARG:NH1	2.00	0.75
15:M:164:THR:HG22	15:M:166:ALA:N	2.00	0.75
4:A:167:LYS:HD2	28:Z:29:ILE:HG21	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:99:ALA:HB1	20:R:109:MET:CE	2.16	0.75
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.67	0.75
1:0:871:G:C8	1:0:871:G:C5'	2.70	0.75
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.67	0.75
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.86	0.75
1:0:1206:U:H5'	1:0:1206:U:H6	1.51	0.75
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.00	0.75
1:0:1118:A:H8	1:0:1118:A:H3'	1.52	0.74
6:C:242:GLU:HB2	40:C:9187:HOH:O	1.85	0.74
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.87	0.74
1:0:123:U:H5'	40:0:7067:HOH:O	1.86	0.74
1:0:506:G:H22	1:0:509:A:H5''	1.51	0.74
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.69	0.74
25:W:122:ARG:HG2	25:W:152:ALA:O	1.86	0.74
27:Y:117:LEU:HD13	27:Y:174:VAL:HG11	1.69	0.74
30:2:18:ASN:HD21	30:2:40:ARG:H	1.34	0.74
1:0:21:G:C5'	20:R:2:ILE:HA	2.17	0.74
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.03	0.74
5:B:321:PRO:HA	40:B:9648:HOH:O	1.87	0.74
6:C:140:VAL:HB	40:C:9257:HOH:O	1.85	0.74
28:Z:19:GLY:O	28:Z:23:ARG:HG2	1.87	0.74
1:0:1700:C:H5''	1:0:1701:A:OP2	1.88	0.73
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.70	0.73
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.88	0.73
1:0:1175:G:H1'	1:0:1193:A:H2'	1.69	0.73
16:N:132:ASN:O	16:N:135:VAL:HG12	1.88	0.73
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.53	0.73
1:0:93:C:H5''	24:V:1:THR:HB	1.69	0.73
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.87	0.73
1:0:381:G:H5''	40:0:4852:HOH:O	1.89	0.73
40:0:5949:HOH:O	10:G:12:ILE:HA	1.89	0.73
15:M:69:LYS:O	15:M:73:ARG:NH2	2.22	0.73
1:0:2346:C:O2'	7:D:52:THR:HG21	1.88	0.73
1:0:1118:A:H3'	1:0:1118:A:C8	2.23	0.72
28:Z:44:GLU:CG	28:Z:46:ARG:HD2	2.18	0.72
8:E:68:HIS:O	8:E:72:MET:HG3	1.90	0.72
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.86	0.72
1:0:481:U:H5''	40:0:6128:HOH:O	1.87	0.72
1:0:2534:C:H1'	40:0:4052:HOH:O	1.89	0.72
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.71	0.72
1:0:1666:C:H2'	1:0:1667:A:H5'	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1919:A:H4'	40:0:5370:HOH:O	1.89	0.72
25:W:80:ASP:O	25:W:84:VAL:HG23	1.89	0.72
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.20	0.72
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.70	0.72
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.89	0.72
32:I:132:CYS:C	32:I:134:SER:H	1.97	0.72
1:0:656:G:OP2	17:O:37:ARG:HD2	1.90	0.72
1:0:2468:A:H61	31:3:48:ASN:HD21	1.36	0.72
5:B:140:LEU:HA	40:B:9573:HOH:O	1.90	0.72
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.04	0.72
7:D:154:LYS:H	7:D:154:LYS:HD2	1.53	0.72
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.37	0.72
28:Z:13:ARG:HD3	40:Z:9214:HOH:O	1.90	0.72
2:9:3029:C:H2'	2:9:3030:C:H5'	1.70	0.72
16:N:154:LEU:HG	16:N:155:GLU:H	1.53	0.72
1:0:450:C:OP1	6:C:184:ARG:NH2	2.22	0.71
1:0:969:G:H1	1:0:999:C:N4	1.86	0.71
1:0:1667:A:H5'	1:0:1667:A:H8	1.53	0.71
4:A:82:VAL:HG13	4:A:93:THR:HB	1.71	0.71
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.55	0.71
1:0:2578:G:H5'	1:0:2578:G:H8	1.55	0.71
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.19	0.71
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.73	0.71
2:9:3014:G:H5'	2:9:3014:G:H8	1.53	0.71
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.71	0.71
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.72	0.71
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.21	0.71
1:0:541:C:H2'	1:0:542:A:C5'	2.21	0.71
1:0:544:G:H2'	1:0:545:G:H5''	1.72	0.71
1:0:1474:C:H5'	1:0:1474:C:C6	2.23	0.71
40:0:7112:HOH:O	27:Y:165:GLU:HB3	1.90	0.71
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.19	0.71
21:S:73:ASP:OD1	21:S:76:GLU:HG3	1.90	0.71
17:O:32:ARG:O	17:O:32:ARG:HD3	1.89	0.71
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.91	0.71
40:0:9959:HOH:O	29:1:1:THR:HA	1.90	0.71
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.73	0.71
25:W:52:VAL:HG22	25:W:53:ALA:H	1.55	0.71
1:0:1687:C:O2	29:1:9:GLY:HA2	1.90	0.71
1:0:1748:U:H4'	40:0:7857:HOH:O	1.90	0.71
8:E:15:GLN:HG2	8:E:19:ASP:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:10:GLN:HE21	13:K:10:GLN:H	0.80	0.71
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.90	0.71
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.02	0.71
26:X:30:MET:HE1	26:X:58:ALA:CB	2.21	0.71
1:O:2851:G:C2'	1:O:2852:A:H5'	2.21	0.70
1:O:281:U:H2'	1:O:282:C:O4'	1.91	0.70
4:A:199:HIS:CD2	4:A:201:PHE:H	2.08	0.70
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.72	0.70
4:A:153:ARG:HB2	4:A:153:ARG:NH1	2.07	0.70
11:H:58:ARG:HH11	11:H:58:ARG:HG3	1.55	0.70
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.73	0.70
11:H:27:LYS:N	11:H:59:HIS:HD2	1.90	0.70
26:X:71:ARG:HD3	40:X:2171:HOH:O	1.91	0.70
1:O:656:G:C5'	17:O:3:THR:HG22	2.20	0.70
1:O:1118:A:H8	1:O:1119:G:H5''	1.56	0.70
1:O:1184:C:H1'	40:O:7803:HOH:O	1.91	0.70
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.72	0.70
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.55	0.70
26:X:25:ARG:HD3	26:X:64:ALA:O	1.92	0.70
1:O:656:G:H5'	17:O:3:THR:CG2	2.21	0.70
6:C:2:GLN:HB3	40:C:9190:HOH:O	1.90	0.70
6:C:139:VAL:HG13	40:C:9254:HOH:O	1.91	0.70
18:P:115:SER:N	18:P:118:GLN:HE21	1.88	0.70
18:P:115:SER:H	18:P:118:GLN:NE2	1.89	0.70
4:A:121:ALA:O	4:A:124:VAL:HG22	1.91	0.69
5:B:238:ASN:HD22	5:B:240:GLY:N	1.89	0.69
31:3:38:ARG:HB3	31:3:42:ARG:NH1	2.04	0.69
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.40	0.69
1:O:474:C:O3'	6:C:73:LEU:HD21	1.91	0.69
1:O:542:A:H5'	1:O:542:A:C8	2.22	0.69
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.75	0.69
1:O:681:G:N3	1:O:681:G:H5'	2.07	0.69
4:A:211:LYS:CG	4:A:212:PRO:HD2	2.23	0.69
22:T:41:ARG:HG2	22:T:41:ARG:NH1	2.00	0.69
1:O:902:G:N7	14:L:18:HIS:HD2	1.91	0.69
9:F:21:GLU:O	9:F:24:ARG:HG3	1.92	0.69
7:D:172:VAL:HG12	7:D:173:GLU:N	2.07	0.69
1:O:1182:C:H1'	1:O:1192:A:H8	1.58	0.69
1:O:1183:C:N4	1:O:1184:C:H41	1.90	0.69
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.75	0.69
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.90	0.69
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.20	0.69
5:B:268:ARG:HH21	5:B:325:PRO:HG3	1.58	0.69
22:T:20:HIS:HB3	22:T:41:ARG:HD2	1.74	0.69
1:O:280:C:H2'	1:O:281:U:O4'	1.92	0.69
25:W:122:ARG:HG2	25:W:122:ARG:HH11	1.57	0.68
1:O:2073:G:H5''	40:O:4373:HOH:O	1.93	0.68
2:9:3056:A:C2'	2:9:3057:A:H5''	2.21	0.68
28:Z:29:ILE:O	28:Z:33:MET:HB2	1.93	0.68
1:O:2748:G:H5'	40:O:7878:HOH:O	1.92	0.68
4:A:51:ARG:HB2	40:A:9641:HOH:O	1.92	0.68
9:F:96:ALA:HA	40:F:3111:HOH:O	1.94	0.68
12:J:75:PRO:HD3	12:J:136:SER:OG	1.92	0.68
25:W:13:MET:HE2	25:W:18:GLN:CA	2.23	0.68
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.16	0.68
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.74	0.68
1:O:447:A:P	22:T:1:SER:HB2	2.34	0.68
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.23	0.68
1:O:2003:U:H4'	1:O:2004:U:C5	2.29	0.68
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.75	0.68
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.08	0.68
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.74	0.68
11:H:169:GLY:C	11:H:170:ASN:HD22	2.00	0.68
13:K:32:ILE:HD11	13:K:56:SER:HB2	1.75	0.68
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.57	0.68
4:A:130:THR:HB	4:A:137:VAL:HB	1.75	0.68
1:O:657:G:OP1	6:C:27:ARG:NH2	2.26	0.68
11:H:30:GLN:H	11:H:66:ARG:NH1	1.92	0.68
27:Y:117:LEU:HD13	27:Y:174:VAL:CG1	2.25	0.68
27:Y:212:ARG:HD2	40:Y:9398:HOH:O	1.93	0.68
24:V:8:ILE:HA	24:V:11:MET:HE3	1.75	0.67
1:O:588:G:O6	25:W:154:ARG:NH1	2.28	0.67
1:O:2491:G:H1'	40:O:7261:HOH:O	1.92	0.67
6:C:132:ASP:HB3	40:C:9171:HOH:O	1.93	0.67
9:F:13:GLU:OE2	9:F:78:GLU:HG2	1.94	0.67
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.28	0.67
13:K:63:GLU:HB2	40:K:6344:HOH:O	1.93	0.67
32:I:125:ALA:O	32:I:129:VAL:HG23	1.93	0.67
1:O:2807:U:P	5:B:27:ASN:HD21	2.18	0.67
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.74	0.67
1:O:797:A:H5'	28:Z:10:ARG:N	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:80:GLY:O	15:M:81:ARG:HD2	1.95	0.67
1:O:1206:U:H2'	1:O:1207:A:O4'	1.93	0.67
5:B:195:ARG:NH1	5:B:324:ASP:OD1	2.28	0.67
12:J:107:ASN:C	12:J:107:ASN:HD22	2.03	0.67
2:9:3040:C:N4	7:D:53:LYS:HE3	2.10	0.67
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.05	0.67
1:O:282:C:O2'	1:O:283:U:H5'	1.93	0.67
1:O:796:A:HO2'	28:Z:10:ARG:N	1.92	0.67
4:A:194:MET:HE3	4:A:199:HIS:CB	2.25	0.67
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.77	0.67
1:O:2676:C:H4'	12:J:70:PHE:CD1	2.29	0.66
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.77	0.66
23:U:47:ARG:HG3	40:U:4381:HOH:O	1.95	0.66
1:O:316:A:N3	1:O:336:G:O2'	2.26	0.66
1:O:2533:C:H5'	1:O:2533:C:H6	1.59	0.66
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.77	0.66
14:L:143:THR:HG22	14:L:144:ASP:N	2.10	0.66
1:O:1377:C:H5'	1:O:1377:C:C6	2.30	0.66
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.75	0.66
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.14	0.66
16:N:37:ARG:CZ	16:N:105:GLY:HA3	2.25	0.66
17:O:32:ARG:HH21	17:O:35:LYS:HZ2	1.40	0.66
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.25	0.66
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.78	0.66
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.20	0.66
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.25	0.66
1:O:95:A:H5''	1:O:97:G:O4'	1.96	0.66
1:O:558:C:H2'	1:O:559:U:H5'	1.77	0.66
1:O:2896:A:N3	1:O:2896:A:H2'	2.11	0.66
4:A:194:MET:CE	4:A:199:HIS:HB2	2.24	0.66
6:C:98:ARG:HG2	6:C:98:ARG:HH11	1.60	0.66
9:F:37:THR:O	9:F:41:GLU:HG3	1.95	0.66
1:O:2054:A:N3	20:R:128:ARG:NH2	2.44	0.66
11:H:27:LYS:H	11:H:59:HIS:HD2	1.44	0.66
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.78	0.66
14:L:35:ARG:C	14:L:35:ARG:HD3	2.21	0.66
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.10	0.66
5:B:275:GLY:O	5:B:291:ASP:HA	1.96	0.66
1:O:870:G:C2'	1:O:871:G:H5''	2.25	0.65
16:N:62:HIS:HB3	16:N:65:ASP:OD1	1.96	0.65
23:U:14:GLU:O	23:U:17:THR:HB	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.79	0.65
31:3:31:THR:HB	31:3:33:MET:HE3	1.77	0.65
1:0:559:U:H5'	1:0:559:U:H6	1.60	0.65
1:0:2816:A:H2'	40:0:8334:HOH:O	1.96	0.65
4:A:135:VAL:HG21	4:A:147:ARG:NH1	2.11	0.65
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.65	0.65
20:R:9:ASP:O	20:R:13:THR:HB	1.96	0.65
24:V:39:ALA:N	24:V:40:PRO:HD2	2.11	0.65
1:0:1476:A:O2'	1:0:1477:C:H5'	1.97	0.65
1:0:1701:A:H4'	1:0:1702:U:C5'	2.27	0.65
1:0:2505:G:O2'	1:0:2506:A:H5'	1.97	0.65
40:9:4707:HOH:O	16:N:147:ILE:HD12	1.95	0.65
4:A:81:GLN:H	4:A:92:ASN:ND2	1.95	0.65
14:L:67:ARG:O	14:L:71:GLU:HG3	1.96	0.65
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.61	0.65
28:Z:44:GLU:HG2	28:Z:46:ARG:HD2	1.79	0.65
1:0:220:C:H1'	40:0:6231:HOH:O	1.94	0.65
1:0:316:A:H5'	22:T:54:ASP:OD2	1.97	0.65
1:0:1183:C:H2'	40:0:6686:HOH:O	1.97	0.65
8:E:6:GLU:HA	8:E:46:THR:HG22	1.79	0.65
16:N:164:ASP:CG	16:N:167:ASP:HA	2.21	0.65
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.26	0.65
25:W:130:HIS:O	25:W:136:GLY:HA3	1.97	0.65
1:0:1528:A:H2'	1:0:1529:G:O4'	1.97	0.65
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.61	0.65
1:0:1973:A:H5'	1:0:1973:A:C8	2.25	0.65
4:A:33:GLU:CD	4:A:33:GLU:N	2.51	0.65
25:W:5:VAL:HG11	25:W:153:MET:HE1	1.77	0.65
1:0:2426:G:H1'	40:0:6540:HOH:O	1.96	0.65
5:B:254:GLN:HG3	40:B:9533:HOH:O	1.97	0.65
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.78	0.65
1:0:1201:C:H2'	1:0:1202:A:H5'	1.79	0.64
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.26	0.64
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.13	0.64
1:0:1119:G:N2	1:0:1246:A:C2	2.56	0.64
1:0:1159:G:H21	1:0:1189:A:H8	1.46	0.64
1:0:1451:C:H5'	1:0:1505:U:C5	2.31	0.64
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.27	0.64
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.79	0.64
1:0:1205:U:H2'	1:0:1206:U:H5''	1.78	0.64
1:0:1299:G:O6	14:L:6:ARG:HD3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:60:VAL:C	15:M:61:ILE:HD12	2.21	0.64
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.78	0.64
1:0:470:U:O2'	29:1:16:HIS:HD2	1.80	0.64
1:0:1165:G:H4'	1:0:1174:A:O2'	1.97	0.64
25:W:48:VAL:O	25:W:48:VAL:HG12	1.97	0.64
1:0:1166:A:H1'	1:0:1192:A:C2	2.33	0.64
7:D:75:LEU:HD22	7:D:79:MET:HB3	1.80	0.64
1:0:282:C:H1'	1:0:368:C:N4	2.12	0.64
1:0:545:G:H5'	1:0:545:G:C8	2.30	0.64
1:0:962:C:H1'	16:N:5:ARG:HH12	1.62	0.64
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.44	0.64
16:N:119:GLN:O	16:N:123:ILE:HG13	1.97	0.64
25:W:88:THR:HG22	25:W:89:ASP:N	2.12	0.64
1:0:1116:U:H3	1:0:1246:A:H62	1.46	0.64
5:B:75:GLU:C	5:B:77:PRO:HD3	2.23	0.64
6:C:162:VAL:HG13	6:C:192:ILE:HD11	1.79	0.64
6:C:236:THR:HA	40:C:9257:HOH:O	1.96	0.64
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.78	0.64
1:0:544:G:C2'	1:0:545:G:H5''	2.27	0.64
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.78	0.64
20:R:99:ALA:HB1	20:R:109:MET:HE3	1.78	0.64
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.61	0.64
1:0:263:U:O4'	9:F:59:ILE:HD13	1.98	0.64
1:0:2908:A:H2'	1:0:2909:G:O4'	1.97	0.64
16:N:164:ASP:OD1	16:N:167:ASP:HA	1.98	0.64
6:C:236:THR:HG21	40:C:9180:HOH:O	1.98	0.63
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.13	0.63
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.80	0.63
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.28	0.63
30:2:18:ASN:ND2	30:2:40:ARG:H	1.96	0.63
1:0:1426:C:H2'	40:0:3189:HOH:O	1.97	0.63
1:0:1882:C:OP1	4:A:192:VAL:HG23	1.99	0.63
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.94	0.63
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.80	0.63
4:A:167:LYS:HB2	28:Z:29:ILE:HD13	1.80	0.63
6:C:77:ALA:O	6:C:78:ARG:HG3	1.97	0.63
32:I:92:PRO:C	32:I:94:GLU:H	2.07	0.63
1:0:1946:C:H2'	1:0:1971:G:C8	2.33	0.63
4:A:161:GLY:O	28:Z:68:SER:HB2	1.97	0.63
5:B:254:GLN:HG2	5:B:255:GLY:N	2.13	0.63
24:V:12:THR:HG23	24:V:14:ALA:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:107:ARG:HG3	15:M:107:ARG:NH1	2.13	0.63
24:V:38:GLY:C	24:V:40:PRO:HD2	2.24	0.63
31:3:3:MET:O	31:3:90:PHE:HA	1.98	0.63
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.99	0.63
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.14	0.63
25:W:5:VAL:O	25:W:52:VAL:HG23	1.98	0.63
1:0:949:U:H4'	19:Q:95:GLU:HA	1.81	0.63
1:0:1835:U:C5	1:0:1840:A:N7	2.63	0.63
1:0:1972:U:H2'	1:0:1973:A:H5''	1.81	0.63
5:B:51:VAL:HG23	5:B:329:TYR:O	1.99	0.63
5:B:62:ARG:HA	5:B:65:MET:HE2	1.81	0.63
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.64	0.63
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.81	0.63
17:O:32:ARG:HH21	17:O:35:LYS:NZ	1.96	0.63
24:V:39:ALA:C	24:V:41:GLU:H	2.06	0.63
1:0:119:A:H2'	1:0:120:A:H5''	1.81	0.63
1:0:635:A:H2'	1:0:636:G:H5''	1.81	0.63
7:D:25:MET:SD	7:D:40:ILE:HD11	2.38	0.63
7:D:51:ARG:HH11	7:D:68:PRO:HB3	1.64	0.63
8:E:126:ILE:HB	8:E:131:LEU:HD23	1.80	0.63
15:M:83:SER:HB3	40:M:9378:HOH:O	1.99	0.63
26:X:71:ARG:HB3	26:X:88:GLU:OE1	1.99	0.63
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.99	0.62
11:H:166:SER:CB	11:H:167:PRO:CD	2.76	0.62
27:Y:189:ASN:C	27:Y:189:ASN:HD22	2.07	0.62
1:0:2073:G:OP2	1:0:2490:A:H5'	1.99	0.62
1:0:2644:C:O2'	1:0:2645:U:H5'	1.99	0.62
5:B:162:MET:HE3	5:B:310:ARG:CD	2.29	0.62
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.34	0.62
15:M:164:THR:HG22	15:M:165:GLY:N	2.13	0.62
28:Z:44:GLU:HG3	28:Z:46:ARG:HD2	1.80	0.62
1:0:2415:A:H2'	1:0:2416:G:H5'	1.80	0.62
9:F:46:GLU:O	9:F:73:PRO:HD2	1.99	0.62
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.13	0.62
25:W:41:TYR:HA	25:W:44:MET:HE3	1.80	0.62
32:I:112:LYS:C	32:I:114:PRO:HD2	2.24	0.62
1:0:1201:C:H5''	40:0:6676:HOH:O	1.97	0.62
1:0:2820:A:OP1	5:B:98:THR:HG22	1.99	0.62
4:A:48:ASP:HB3	40:A:9641:HOH:O	1.99	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.64	0.62
1:0:625:U:H5''	1:0:1044:C:N4	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:797:A:C4'	28:Z:10:ARG:N	2.63	0.62
1:0:2827:A:H2'	1:0:2828:G:O4'	2.00	0.62
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.81	0.62
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.80	0.62
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.29	0.62
25:W:13:MET:HE1	25:W:21:LEU:CD1	2.29	0.62
25:W:119:HIS:HD2	25:W:120:PRO:O	1.81	0.62
1:0:2670:G:O2'	1:0:2671:U:H5'	1.99	0.62
1:0:2718:C:H6	1:0:2718:C:H5'	1.64	0.62
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.15	0.62
21:S:37:VAL:O	21:S:41:VAL:HG23	1.99	0.62
1:0:156:C:H5''	15:M:171:ARG:CD	2.26	0.62
1:0:2291:A:C8	1:0:2309:C:H5'	2.34	0.62
4:A:179:MET:HG2	4:A:186:TRP:CB	2.30	0.62
27:Y:177:LYS:HD3	27:Y:181:GLY:O	1.99	0.62
1:0:2421:G:H1'	40:0:4250:HOH:O	1.98	0.62
40:0:3751:HOH:O	15:M:9:ARG:HG3	1.99	0.62
6:C:107:ARG:NE	40:C:9263:HOH:O	2.29	0.62
11:H:154:TYR:HB2	40:H:9563:HOH:O	2.00	0.62
12:J:107:ASN:ND2	12:J:109:TYR:H	1.97	0.62
25:W:84:VAL:HG12	40:W:6679:HOH:O	1.99	0.62
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.29	0.62
1:0:2064:U:H5'	1:0:2652:U:H4'	1.81	0.62
14:L:10:SER:O	14:L:11:ARG:HB3	1.99	0.62
16:N:110:THR:HB	16:N:113:SER:OG	2.00	0.62
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.15	0.62
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.30	0.62
1:0:2508:C:H2'	40:0:7154:HOH:O	2.00	0.61
4:A:36:ASP:HB3	4:A:85:SER:HB2	1.83	0.61
4:A:206:ARG:H	4:A:206:ARG:HD3	1.65	0.61
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.11	0.61
1:0:558:C:H2'	1:0:559:U:C5'	2.30	0.61
15:M:48:LYS:O	15:M:52:GLN:HG3	1.99	0.61
16:N:17:ARG:HH11	16:N:17:ARG:CB	2.10	0.61
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.98	0.61
6:C:79:ARG:O	6:C:87:ARG:HG2	2.01	0.61
9:F:2:VAL:HG22	9:F:57:GLU:OE1	2.01	0.61
9:F:13:GLU:OE1	9:F:77:VAL:HG13	1.99	0.61
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.34	0.61
25:W:52:VAL:HG22	25:W:53:ALA:N	2.15	0.61
15:M:164:THR:CG2	15:M:165:GLY:N	2.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:447:A:OP2	22:T:1:SER:HB2	2.00	0.61
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.36	0.61
1:0:2894:C:O2'	1:0:2895:C:H5'	1.99	0.61
4:A:164:ARG:HA	28:Z:69:TYR:CE1	2.36	0.61
4:A:203:GLY:HA2	40:A:9581:HOH:O	2.01	0.61
4:A:232:ARG:NH2	4:A:236:GLY:O	2.31	0.61
7:D:170:TYR:O	7:D:171:ASP:HB3	1.99	0.61
10:G:12:ILE:N	10:G:13:PRO:HD3	2.15	0.61
10:G:63:ARG:HB2	10:G:66:LEU:HG	1.82	0.61
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.99	0.61
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.00	0.61
15:M:70:GLY:HA3	15:M:73:ARG:HH22	1.66	0.61
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.30	0.61
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.83	0.61
22:T:49:GLU:HB3	22:T:59:GLU:CG	2.31	0.61
7:D:25:MET:HE2	7:D:41:LEU:CG	2.28	0.61
31:3:55:VAL:HG22	40:3:9444:HOH:O	2.00	0.61
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.19	0.60
11:H:170:ASN:HD22	11:H:170:ASN:N	1.99	0.60
22:T:48:VAL:HG13	22:T:97:ARG:O	2.01	0.60
1:0:343:C:O2'	1:0:344:C:H5'	2.00	0.60
1:0:1773:G:C8	28:Z:16:ALA:HA	2.36	0.60
1:0:2420:G:O2'	1:0:2421:G:H5'	2.00	0.60
2:9:3014:G:H5'	2:9:3014:G:C8	2.36	0.60
5:B:56:ASP:OD1	5:B:322:ARG:HB3	2.02	0.60
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.82	0.60
11:H:157:ILE:HD11	11:H:161:CYS:SG	2.41	0.60
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.82	0.60
32:I:113:HIS:N	32:I:114:PRO:HD2	2.15	0.60
1:0:1189:A:O2'	1:0:1208:C:H2'	2.00	0.60
4:A:75:GLY:HA2	28:Z:64:PHE:HA	1.83	0.60
21:S:33:SER:O	21:S:37:VAL:HG23	2.01	0.60
25:W:4:LEU:CD2	25:W:54:PHE:HB3	2.28	0.60
1:0:371:U:H2'	1:0:372:A:H8	1.66	0.60
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.00	0.60
1:0:2524:G:N2	1:0:2526:C:H5	1.97	0.60
5:B:125:GLU:O	5:B:129:ARG:HG3	2.00	0.60
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.83	0.60
14:L:133:VAL:HA	40:L:9477:HOH:O	2.00	0.60
27:Y:117:LEU:CD1	27:Y:174:VAL:HG11	2.32	0.60
1:0:1666:C:O2'	1:0:1667:A:H5''	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:138:GLY:O	5:B:139:ASP:O	2.20	0.60
5:B:305:ASP:O	5:B:306:LYS:HB2	2.00	0.60
24:V:1:THR:HG23	24:V:2:VAL:N	2.16	0.60
1:O:396:U:O2'	1:O:418:C:H4'	2.01	0.60
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.83	0.60
18:P:14:LEU:O	18:P:16:VAL:HG23	2.01	0.60
1:O:289:G:N2	1:O:363:A:H2	1.96	0.60
8:E:69:ILE:HA	8:E:72:MET:HE3	1.83	0.60
14:L:136:ALA:HB3	40:L:9477:HOH:O	2.02	0.60
18:P:97:ARG:HD2	40:P:163:HOH:O	2.02	0.60
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.84	0.60
9:F:58:GLU:HG3	9:F:61:MET:HE2	1.82	0.60
12:J:45:VAL:HG23	12:J:130:VAL:O	2.01	0.60
32:I:134:SER:O	32:I:135:LEU:HD23	2.00	0.60
23:U:5:GLU:HG2	23:U:10:GLY:O	2.02	0.60
1:O:899:C:H5'	40:O:3768:HOH:O	2.00	0.60
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.67	0.60
27:Y:144:ARG:NE	40:Y:9410:HOH:O	2.34	0.60
1:O:2003:U:H4'	1:O:2004:U:H5	1.67	0.59
1:O:2541:U:H5'	1:O:2541:U:H6	1.65	0.59
25:W:108:ARG:HH21	25:W:114:PRO:HG2	1.66	0.59
31:3:70:ARG:HB3	40:3:9506:HOH:O	2.02	0.59
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.84	0.59
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.17	0.59
11:H:116:ALA:O	11:H:117:PHE:C	2.46	0.59
13:K:82:ARG:NH2	13:K:115:ARG:HG2	2.17	0.59
14:L:148:GLU:HB2	40:L:9496:HOH:O	2.00	0.59
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.84	0.59
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.82	0.59
1:O:1681:G:H5''	1:O:1682:A:H5'	1.83	0.59
4:A:179:MET:HG2	4:A:186:TRP:HB2	1.83	0.59
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.37	0.59
16:N:80:SER:HB2	40:N:9339:HOH:O	2.01	0.59
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.82	0.59
32:I:99:ASP:O	32:I:100:LEU:HD23	2.02	0.59
1:O:1060:C:H6	1:O:1060:C:H5'	1.68	0.59
1:O:1118:A:C8	1:O:1119:G:H5''	2.37	0.59
1:O:1333:U:H2'	1:O:1334:C:C6	2.38	0.59
4:A:41:THR:HG23	4:A:77:GLY:O	2.03	0.59
7:D:41:LEU:HA	7:D:44:ILE:CG2	2.31	0.59
16:N:49:THR:HG22	16:N:56:ASP:CB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:78:ALA:C	17:O:98:LEU:HD13	2.28	0.59
4:A:65:ARG:C	4:A:66:ARG:HG3	2.28	0.59
5:B:217:ARG:HG3	5:B:257:THR:CG2	2.32	0.59
22:T:48:VAL:CG1	22:T:96:VAL:HG22	2.32	0.59
23:U:52:THR:HG22	23:U:54:THR:N	2.17	0.59
1:O:2101:A:H2'	6:C:63:SER:OG	2.01	0.59
11:H:76:GLU:C	11:H:77:LEU:HD23	2.28	0.59
15:M:68:ARG:HH21	15:M:73:ARG:CD	2.02	0.59
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.03	0.59
1:O:1595:G:O2'	1:O:1596:U:H5'	2.02	0.59
40:9:5071:HOH:O	16:N:23:ARG:HD3	2.01	0.59
5:B:175:LEU:O	5:B:175:LEU:HD23	2.03	0.59
11:H:63:GLU:HA	40:H:9551:HOH:O	2.02	0.59
11:H:79:GLU:C	11:H:80:GLU:HG3	2.26	0.59
25:W:142:ASP:HB3	25:W:145:GLY:H	1.68	0.59
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.38	0.59
8:E:84:MET:HE2	8:E:133:VAL:CG2	2.32	0.59
19:Q:25:PRO:HB2	40:Q:4350:HOH:O	2.03	0.59
20:R:82:GLU:O	20:R:86:LYS:HG3	2.03	0.59
1:O:1878:G:H1'	40:O:6567:HOH:O	2.02	0.58
1:O:2032:U:H2'	1:O:2033:G:C5'	2.33	0.58
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.32	0.58
17:O:14:LEU:HG	17:O:102:ILE:HD11	1.84	0.58
21:S:77:VAL:O	21:S:80:ARG:HG2	2.03	0.58
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.43	0.58
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.67	0.58
2:9:3039:U:H3'	2:9:3040:C:H5''	1.85	0.58
6:C:1:MET:HG2	6:C:2:GLN:H	1.67	0.58
13:K:75:ARG:HD3	13:K:112:PRO:O	2.02	0.58
1:O:558:C:O2'	1:O:559:U:H5''	2.02	0.58
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.03	0.58
1:O:1555:G:H4'	1:O:1630:A:H2	1.69	0.58
4:A:122:SER:O	4:A:124:VAL:HG13	2.02	0.58
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.18	0.58
21:S:57:THR:CG2	21:S:59:ASP:HB2	2.33	0.58
22:T:89:ARG:HG3	22:T:89:ARG:O	2.03	0.58
1:O:2563:U:H2'	1:O:2565:C:O5'	2.03	0.58
1:O:2643:G:H5''	40:O:4473:HOH:O	2.03	0.58
7:D:50:VAL:O	7:D:71:ALA:HA	2.03	0.58
18:P:55:LYS:HG2	18:P:56:GLY:N	2.17	0.58
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.58
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.87	0.58
1:0:1666:C:H2'	1:0:1667:A:C5'	2.33	0.58
1:0:2749:U:H5'	40:0:8329:HOH:O	2.03	0.58
4:A:36:ASP:C	4:A:38:ILE:H	2.12	0.58
5:B:140:LEU:HD23	40:B:9573:HOH:O	2.03	0.58
5:B:214:PRO:HD2	40:B:9524:HOH:O	2.02	0.58
7:D:167:GLU:C	7:D:169:THR:H	2.10	0.58
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.52	0.58
18:P:89:ASN:HB3	18:P:92:GLU:HB2	1.84	0.58
24:V:5:VAL:HG23	40:V:2271:HOH:O	2.03	0.58
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.37	0.58
1:0:87:C:H2'	30:2:28:LYS:O	2.03	0.58
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.31	0.58
12:J:26:VAL:HG13	12:J:36:VAL:HG11	1.85	0.58
14:L:143:THR:HG22	14:L:144:ASP:H	1.69	0.58
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.51	0.58
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.67	0.58
6:C:233:THR:HG22	6:C:234:VAL:H	1.69	0.58
9:F:34:ASN:HA	15:M:4:ALA:HB2	1.86	0.58
1:0:1384:C:H5'	26:X:30:MET:HG2	1.84	0.58
8:E:11:VAL:HG12	8:E:12:ASP:N	2.18	0.58
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.86	0.58
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.39	0.58
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.50	0.58
30:2:41:HIS:H	30:2:45:ASN:HD22	1.50	0.58
1:0:151:A:H2'	1:0:152:A:O4'	2.04	0.58
1:0:200:U:H2'	40:0:4002:HOH:O	2.04	0.58
1:0:877:G:H5'	1:0:878:G:OP1	2.03	0.58
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.04	0.58
1:0:1714:C:O2'	1:0:1715:C:H5'	2.03	0.58
1:0:1819:G:H2'	1:0:1820:G:H4'	1.85	0.58
1:0:2769:C:C2'	1:0:2770:G:H5'	2.34	0.58
40:0:6006:HOH:O	5:B:298:LYS:HG2	2.03	0.58
40:0:6143:HOH:O	28:Z:17:ARG:HD3	2.04	0.58
4:A:94:LEU:HD23	4:A:94:LEU:N	2.19	0.58
8:E:116:THR:CG2	8:E:151:LEU:HD22	2.30	0.58
1:0:120:A:H5'	29:1:20:ARG:HH21	1.69	0.58
1:0:380:A:OP2	15:M:9:ARG:HD2	2.03	0.58
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.19	0.58
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.04	0.58
22:T:71:VAL:HG13	22:T:91:LEU:O	2.03	0.58
23:U:52:THR:CG2	23:U:54:THR:HB	2.34	0.58
26:X:43:VAL:HG12	26:X:44:ASP:N	2.19	0.58
31:3:70:ARG:NH1	31:3:77:ALA:HB2	2.18	0.58
1:0:236:A:H8	1:0:236:A:OP1	1.87	0.57
1:0:263:U:O2	15:M:42:ARG:HD2	2.04	0.57
9:F:48:VAL:HG23	9:F:74:PHE:HB3	1.86	0.57
16:N:169:PRO:O	16:N:172:PHE:HB3	2.03	0.57
1:0:920:C:H4'	1:0:921:G:C2	2.39	0.57
40:0:4766:HOH:O	30:2:38:LYS:HE3	2.04	0.57
4:A:43:VAL:HG21	4:A:59:GLU:HG3	1.86	0.57
1:0:775:G:OP1	29:1:16:HIS:HE1	1.87	0.57
1:0:1205:U:H2'	1:0:1206:U:C5'	2.35	0.57
1:0:1209:C:H2'	1:0:1210:G:H8	1.69	0.57
5:B:102:THR:HG23	5:B:182:VAL:HG12	1.85	0.57
11:H:56:GLN:NE2	11:H:93:GLN:HG2	2.19	0.57
22:T:38:ARG:NH1	40:T:6217:HOH:O	2.37	0.57
1:0:1778:A:H2'	1:0:1779:A:H5'	1.86	0.57
1:0:2103:A:H5'	40:0:4975:HOH:O	2.04	0.57
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.86	0.57
1:0:2851:G:O2'	1:0:2852:A:H5'	2.04	0.57
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.35	0.57
1:0:2320:U:H4'	1:0:2321:A:O4'	2.04	0.57
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.86	0.57
20:R:44:VAL:O	20:R:48:GLU:HG3	2.03	0.57
22:T:28:SER:O	22:T:32:ARG:HG3	2.03	0.57
22:T:71:VAL:HG12	22:T:72:ILE:N	2.19	0.57
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.86	0.57
1:0:12:U:H2'	1:0:13:G:H5'	1.86	0.57
4:A:165:THR:HG22	40:A:9656:HOH:O	2.04	0.57
8:E:23:GLU:HG2	8:E:28:SER:CB	2.35	0.57
9:F:57:GLU:HB2	15:M:23:LEU:HD11	1.85	0.57
17:O:15:LYS:HD3	17:O:19:ARG:NH2	2.20	0.57
22:T:26:THR:HA	22:T:39:ASN:HB3	1.86	0.57
31:3:25:VAL:HG13	31:3:68:LYS:HE3	1.87	0.57
1:0:204:A:H2'	1:0:205:U:H5'	1.86	0.57
1:0:2851:G:H2'	1:0:2852:A:H5'	1.86	0.57
4:A:109:GLU:HG2	4:A:116:GLY:N	2.20	0.57
5:B:41:PHE:HB3	5:B:190:MET:HE1	1.87	0.57
11:H:166:SER:HB3	11:H:167:PRO:CD	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:16:VAL:HG12	18:P:17:GLY:N	2.19	0.57
22:T:48:VAL:HG11	22:T:96:VAL:HG13	1.87	0.57
26:X:78:GLU:HG2	26:X:79:GLU:OE2	2.05	0.57
40:O:7894:HOH:O	31:3:60:LYS:HG3	2.04	0.57
7:D:51:ARG:NH1	7:D:68:PRO:HB3	2.19	0.57
12:J:74:ARG:HH11	12:J:74:ARG:CB	2.17	0.57
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.45	0.57
31:3:65:THR:HG22	31:3:67:LEU:HG	1.86	0.57
1:O:1165:G:O3'	1:O:1174:A:H4'	2.04	0.57
1:O:1187:U:O2'	1:O:1189:A:H2	1.88	0.57
7:D:138:GLY:N	40:D:7597:HOH:O	2.38	0.57
8:E:84:MET:HE1	8:E:148:ILE:CD1	2.34	0.57
15:M:77:HIS:HD2	15:M:79:ALA:O	1.88	0.57
16:N:49:THR:HG22	16:N:56:ASP:HB3	1.87	0.57
1:O:946:C:H2'	1:O:947:U:C6	2.38	0.57
2:9:3011:A:P	19:Q:19:ARG:HH21	2.28	0.57
11:H:45:VAL:HA	11:H:167:PRO:O	2.05	0.57
15:M:58:GLN:HG3	40:M:9410:HOH:O	2.05	0.57
1:O:816:G:OP1	18:P:91:LYS:HE2	2.04	0.56
1:O:2081:A:H4'	12:J:69:TYR:CE1	2.40	0.56
5:B:58:PRO:HA	5:B:63:GLU:CD	2.31	0.56
6:C:1:MET:HG2	6:C:2:GLN:N	2.20	0.56
16:N:162:ASP:HA	40:N:9333:HOH:O	2.03	0.56
17:O:59:VAL:HG23	17:O:111:VAL:CG2	2.35	0.56
21:S:52:VAL:C	21:S:53:ASN:HD22	2.12	0.56
1:O:709:G:O2'	17:O:25:VAL:HG12	2.05	0.56
1:O:2415:A:N3	16:N:26:LEU:HD13	2.20	0.56
1:O:2878:U:H2'	1:O:2879:A:O4'	2.05	0.56
4:A:88:ILE:O	4:A:88:ILE:HG22	2.03	0.56
5:B:85:ARG:NH1	40:B:9628:HOH:O	2.38	0.56
5:B:199:TYR:CE2	5:B:268:ARG:HB2	2.40	0.56
7:D:37:ALA:O	7:D:40:ILE:HG12	2.06	0.56
12:J:74:ARG:O	12:J:78:ILE:HG12	2.05	0.56
25:W:38:THR:HG22	25:W:39:ASP:N	2.19	0.56
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.87	0.56
1:O:1066:U:H2'	1:O:1067:A:C8	2.41	0.56
1:O:1116:U:O2'	1:O:1118:A:C2	2.45	0.56
1:O:1641:A:C2'	1:O:1642:A:H5'	2.34	0.56
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.40	0.56
10:G:24:VAL:O	10:G:28:GLU:HB2	2.04	0.56
24:V:42:ASN:O	24:V:44:GLY:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:364:C:H2'	1:0:365:G:O4'	2.05	0.56
1:0:506:G:H22	1:0:509:A:H5'	1.71	0.56
1:0:2432:C:O2'	1:0:2433:A:H5'	2.06	0.56
1:0:2812:A:N7	40:0:7853:HOH:O	2.33	0.56
2:9:3029:C:O3'	7:D:138:GLY:HA2	2.06	0.56
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.36	0.56
1:0:737:A:H2'	1:0:738:G:O4'	2.06	0.56
1:0:853:C:H3'	40:0:5080:HOH:O	2.04	0.56
1:0:2531:U:O2'	1:0:2532:A:H5'	2.05	0.56
7:D:57:THR:HA	40:D:5146:HOH:O	2.05	0.56
7:D:173:GLU:HG3	7:D:174:VAL:N	2.21	0.56
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.27	0.56
32:I:132:CYS:C	32:I:134:SER:N	2.63	0.56
1:0:338:C:H4'	6:C:174:ILE:CD1	2.36	0.56
1:0:432:G:O2'	1:0:433:C:H5'	2.06	0.56
1:0:1766:U:O2	1:0:1778:A:H5'	2.06	0.56
2:9:3013:A:O2'	2:9:3014:G:H5''	2.05	0.56
2:9:3042:C:H5'	2:9:3043:G:OP2	2.06	0.56
4:A:69:LEU:HB3	40:A:9612:HOH:O	2.05	0.56
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.88	0.56
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.36	0.56
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.88	0.56
13:K:115:ARG:HG3	13:K:116:GLU:N	2.21	0.56
22:T:48:VAL:O	22:T:59:GLU:HA	2.06	0.56
1:0:241:A:C2	1:0:378:A:H4'	2.41	0.56
1:0:482:G:H4'	1:0:508:A:N1	2.21	0.56
1:0:500:G:H21	20:R:98:ASN:HD21	1.53	0.56
1:0:558:C:C2'	1:0:559:U:H5''	2.36	0.56
1:0:1603:A:H5''	1:0:1604:G:H3'	1.87	0.56
1:0:2072:G:C6	1:0:2533:C:H1'	2.41	0.56
1:0:2480:G:H3'	40:0:4723:HOH:O	2.06	0.56
1:0:2502:C:C2'	1:0:2503:A:H5'	2.35	0.56
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.35	0.56
6:C:233:THR:HG22	6:C:234:VAL:N	2.20	0.56
27:Y:200:THR:CG2	27:Y:201:GLU:HG3	2.35	0.56
30:2:20:ARG:HG3	30:2:21:VAL:N	2.21	0.56
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.86	0.56
30:2:48:ASP:O	30:2:49:GLU:HB2	2.06	0.56
1:0:1241:G:N3	12:J:86:MET:HE2	2.20	0.55
1:0:2645:U:C6	1:0:2645:U:OP2	2.59	0.55
4:A:179:MET:HA	4:A:179:MET:CE	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:64:ASN:HD22	10:G:64:ASN:N	2.02	0.55
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.06	0.55
4:A:129:LEU:CD1	4:A:145:MET:HE1	2.36	0.55
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.41	0.55
1:0:272:A:H5'	1:0:273:G:OP2	2.06	0.55
1:0:288:A:H2'	1:0:289:G:C8	2.40	0.55
1:0:797:A:H4'	28:Z:10:ARG:N	2.21	0.55
1:0:2649:A:H5'	1:0:2649:A:C8	2.41	0.55
1:0:2649:A:H5'	1:0:2649:A:H8	1.71	0.55
4:A:43:VAL:O	4:A:44:ASP:HB2	2.07	0.55
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.26	0.55
1:0:271:C:H41	1:0:378:A:H2	1.54	0.55
13:K:23:ASN:HD21	13:K:107:THR:HB	1.71	0.55
32:I:106:LYS:O	32:I:110:GLU:HG3	2.06	0.55
1:0:1972:U:C2'	1:0:1973:A:H5''	2.36	0.55
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.89	0.55
6:C:184:ARG:HB3	40:C:9172:HOH:O	2.07	0.55
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.37	0.55
27:Y:106:THR:HG22	27:Y:107:PRO:O	2.07	0.55
32:I:128:VAL:C	32:I:130:GLY:H	2.15	0.55
1:0:2419:U:H5''	1:0:2420:G:H5'	1.89	0.55
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.71	0.55
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.71	0.55
1:0:138:U:H5''	1:0:139:C:OP2	2.06	0.55
1:0:2515:C:H2'	1:0:2516:G:O4'	2.06	0.55
12:J:131:THR:HG22	12:J:134:GLU:N	2.15	0.55
21:S:53:ASN:HD22	21:S:53:ASN:N	2.05	0.55
1:0:21:G:H5''	20:R:1:GLY:O	2.07	0.55
1:0:1736:A:H1'	40:0:7921:HOH:O	2.06	0.55
4:A:167:LYS:CB	28:Z:29:ILE:HD13	2.36	0.55
9:F:31:LYS:HE3	40:F:2623:HOH:O	2.06	0.55
1:0:291:C:H2'	1:0:292:G:O4'	2.06	0.55
1:0:952:G:N3	1:0:2302:A:H2'	2.22	0.55
1:0:1189:A:H1'	1:0:1209:C:H1'	1.89	0.55
9:F:11:ASP:O	9:F:14:ASP:HB2	2.07	0.55
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.37	0.55
1:0:20:G:H21	20:R:117:HIS:HD2	1.53	0.55
1:0:1724:U:H5''	40:0:4281:HOH:O	2.06	0.55
1:0:1886:A:H4'	40:Z:9206:HOH:O	2.07	0.55
2:9:3002:U:OP2	2:9:3003:A:H5'	2.07	0.55
2:9:3051:A:H5'	16:N:160:SER:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.36	0.55
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.36	0.55
1:O:485:A:N3	1:O:487:G:H5''	2.21	0.54
1:O:2421:G:H2'	40:O:4620:HOH:O	2.06	0.54
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.37	0.54
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.42	0.54
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.37	0.54
23:U:17:THR:HG22	23:U:18:GLY:N	2.21	0.54
25:W:13:MET:CE	25:W:18:GLN:HA	2.36	0.54
32:I:129:VAL:O	32:I:129:VAL:HG12	2.07	0.54
1:O:1786:C:OP1	18:P:74:GLN:HG2	2.06	0.54
1:O:2102:G:H5''	1:O:2538:A:C2	2.42	0.54
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.88	0.54
1:O:475:G:OP1	6:C:73:LEU:HD22	2.07	0.54
1:O:1086:A:C6	25:W:11:VAL:HG11	2.42	0.54
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.89	0.54
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.37	0.54
12:J:107:ASN:HD22	12:J:109:TYR:H	1.53	0.54
1:O:709:G:O2'	17:O:25:VAL:CG1	2.55	0.54
1:O:1926:G:H2'	1:O:1927:A:C8	2.42	0.54
1:O:2032:U:C2'	1:O:2033:G:H5''	2.38	0.54
1:O:2748:G:H2'	40:O:7878:HOH:O	2.06	0.54
5:B:40:GLY:HA3	40:B:9639:HOH:O	2.08	0.54
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.37	0.54
26:X:72:VAL:CG2	26:X:85:VAL:HG12	2.33	0.54
30:2:20:ARG:HG3	30:2:21:VAL:H	1.72	0.54
1:O:834:G:H4'	1:O:835:U:OP2	2.07	0.54
1:O:951:A:C2'	1:O:952:G:H5'	2.38	0.54
1:O:1132:A:N6	1:O:1229:C:H2'	2.23	0.54
5:B:97:LEU:O	5:B:98:THR:HG23	2.07	0.54
6:C:76:ARG:HH11	6:C:76:ARG:CG	2.21	0.54
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.42	0.54
1:O:497:A:H2'	1:O:498:A:C5'	2.38	0.54
4:A:36:ASP:O	4:A:38:ILE:N	2.38	0.54
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.38	0.54
5:B:297:VAL:HB	40:B:9599:HOH:O	2.08	0.54
16:N:154:LEU:CG	16:N:155:GLU:H	2.19	0.54
22:T:41:ARG:HH11	22:T:41:ARG:CG	2.07	0.54
1:O:415:A:O2'	1:O:416:G:H5'	2.08	0.54
1:O:1626:A:H2'	1:O:1627:G:O4'	2.08	0.54
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.90	0.54
4:A:153:ARG:HH11	4:A:153:ARG:CB	2.17	0.54
6:C:214:THR:HG22	6:C:216:SER:H	1.72	0.54
32:I:113:HIS:N	32:I:114:PRO:CD	2.70	0.54
1:O:69:A:H5'	1:O:69:A:C8	2.42	0.54
1:O:1119:G:N2	1:O:1246:A:N1	2.56	0.54
1:O:1829:A:H61	28:Z:18:TYR:H	1.56	0.54
1:O:1838:U:H1'	1:O:2644:C:O4'	2.08	0.54
1:O:2326:U:H4'	1:O:2412:G:C4'	2.38	0.54
1:O:2717:C:O2'	1:O:2718:C:H5''	2.06	0.54
40:O:5195:HOH:O	21:S:23:LYS:HE2	2.07	0.54
7:D:25:MET:CE	7:D:37:ALA:HB1	2.37	0.54
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.56	0.54
24:V:20:LEU:HD22	24:V:60:GLN:NE2	2.18	0.54
1:O:1525:G:H5'	1:O:1526:A:OP2	2.08	0.54
1:O:2717:C:H2'	1:O:2718:C:C5'	2.35	0.54
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.43	0.54
17:O:39:THR:O	17:O:115:ARG:NH2	2.41	0.54
1:O:2862:G:H4'	5:B:336:GLN:O	2.07	0.54
2:9:3076:G:C3'	2:9:3077:A:H5''	2.31	0.54
7:D:59:GLY:O	7:D:61:PHE:N	2.39	0.54
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.43	0.54
15:M:89:THR:O	15:M:89:THR:HG22	2.08	0.54
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.89	0.54
31:3:38:ARG:CB	31:3:42:ARG:HH12	2.11	0.54
1:O:1667:A:H5'	1:O:1667:A:C8	2.40	0.53
9:F:40:ILE:HD11	9:F:48:VAL:HG11	1.89	0.53
1:O:441:A:H1'	1:O:442:A:N7	2.23	0.53
1:O:1181:A:N1	1:O:1192:A:O2'	2.40	0.53
1:O:1834:C:H2'	1:O:1840:A:N6	2.23	0.53
11:H:21:THR:O	11:H:120:ILE:HD12	2.07	0.53
1:O:1086:A:OP1	25:W:9:GLY:N	2.40	0.53
1:O:1654:U:H2'	4:A:47:HIS:HD2	1.72	0.53
1:O:1677:U:OP2	30:2:8:LYS:NZ	2.41	0.53
1:O:1943:C:H4'	4:A:211:LYS:O	2.09	0.53
2:9:3092:G:H2'	2:9:3093:A:C8	2.44	0.53
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.24	0.53
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.73	0.53
17:O:88:LYS:HD3	40:O:7061:HOH:O	2.08	0.53
19:Q:62:THR:O	19:Q:64:GLU:HG2	2.08	0.53
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2795:C:O2'	1:0:2796:U:H5'	2.09	0.53
2:9:3020:G:O2'	2:9:3021:G:H5'	2.08	0.53
2:9:3052:A:H2'	2:9:3053:G:O4'	2.08	0.53
5:B:185:GLY:HA2	40:B:9627:HOH:O	2.08	0.53
2:9:3029:C:C2'	2:9:3030:C:H5'	2.38	0.53
5:B:10:SER:O	5:B:16:ARG:NH1	2.40	0.53
5:B:139:ASP:HB2	5:B:165:ARG:HE	1.73	0.53
5:B:321:PRO:HG3	40:B:9594:HOH:O	2.08	0.53
6:C:27:ARG:HD2	17:O:5:PRO:HD2	1.89	0.53
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.91	0.53
12:J:131:THR:HB	12:J:134:GLU:OE1	2.09	0.53
20:R:104:PHE:CB	20:R:109:MET:HE2	2.38	0.53
28:Z:11:SER:O	28:Z:14:PHE:HB2	2.08	0.53
1:0:2502:C:H2'	1:0:2503:A:H5'	1.91	0.53
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.91	0.53
13:K:49:LEU:CD1	13:K:80:ILE:HD13	2.37	0.53
25:W:139:GLY:O	25:W:141:HIS:HD2	1.90	0.53
28:Z:50:GLN:HB2	28:Z:54:ILE:HG22	1.91	0.53
29:1:10:LYS:HG3	40:1:9489:HOH:O	2.07	0.53
1:0:622:G:P	27:Y:148:GLY:HA3	2.48	0.53
1:0:706:G:N2	1:0:707:C:N4	2.57	0.53
1:0:1202:A:H2'	1:0:1203:G:O4'	2.09	0.53
1:0:1205:U:C2'	1:0:1206:U:H5''	2.37	0.53
1:0:1295:G:H5''	14:L:14:GLY:O	2.09	0.53
6:C:218:VAL:HG12	40:C:9232:HOH:O	2.08	0.53
20:R:114:VAL:HA	20:R:144:GLU:O	2.08	0.53
22:T:48:VAL:HG12	22:T:49:GLU:N	2.24	0.53
25:W:88:THR:HG22	25:W:89:ASP:H	1.72	0.53
1:0:816:G:C6	1:0:817:G:N1	2.77	0.53
14:L:36:ASP:HB2	40:L:9434:HOH:O	2.08	0.53
22:T:41:ARG:NH1	22:T:42:VAL:O	2.42	0.53
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.41	0.53
29:1:25:LYS:O	29:1:25:LYS:HG2	2.09	0.53
1:0:185:G:O3'	1:0:186:A:H4'	2.09	0.53
1:0:553:G:P	27:Y:204:ARG:NH2	2.81	0.53
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.44	0.53
1:0:1845:A:OP2	4:A:190:ARG:NH1	2.42	0.53
1:0:2414:A:H2'	1:0:2415:A:C8	2.44	0.53
2:9:3014:G:H2'	2:9:3015:C:H5'	1.91	0.53
4:A:217:ARG:HH11	4:A:217:ARG:CG	2.21	0.53
8:E:7:ILE:HD11	8:E:11:VAL:C	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:104:ASP:HB2	40:L:9464:HOH:O	2.09	0.53
22:T:48:VAL:HG13	22:T:97:ARG:C	2.33	0.53
25:W:4:LEU:HD23	25:W:54:PHE:CB	2.35	0.53
4:A:96:LEU:O	4:A:131:HIS:HE1	1.92	0.53
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.91	0.53
6:C:180:SER:HB2	40:C:9252:HOH:O	2.08	0.53
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.90	0.53
7:D:172:VAL:CG1	7:D:173:GLU:H	2.14	0.53
9:F:27:GLY:HA3	9:F:101:ALA:O	2.09	0.53
17:O:87:THR:O	17:O:91:GLN:HG3	2.09	0.53
25:W:78:ASP:HB2	40:W:6694:HOH:O	2.09	0.53
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.09	0.52
1:0:2720:C:O2	13:K:87:ARG:NH2	2.42	0.52
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.90	0.52
24:V:12:THR:HB	24:V:15:GLU:OE2	2.09	0.52
1:0:204:A:C2'	1:0:205:U:H5'	2.38	0.52
1:0:949:U:C4'	19:Q:95:GLU:HA	2.39	0.52
1:0:2533:C:H5'	1:0:2533:C:C6	2.43	0.52
1:0:2896:A:H5''	40:X:5399:HOH:O	2.08	0.52
4:A:35:GLY:O	4:A:36:ASP:CB	2.56	0.52
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.74	0.52
5:B:145:HIS:HD2	5:B:146:THR:O	1.91	0.52
6:C:118:THR:O	6:C:136:VAL:HG13	2.09	0.52
6:C:236:THR:H	6:C:239:ALA:HB3	1.73	0.52
11:H:39:ASP:HB2	11:H:42:ASP:OD2	2.08	0.52
14:L:144:ASP:HA	14:L:147:GLU:OE1	2.10	0.52
18:P:141:ILE:C	18:P:143:ALA:H	2.16	0.52
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.44	0.52
1:0:1482:A:O2'	1:0:1483:C:H5'	2.09	0.52
1:0:2324:G:N2	1:0:2377:U:H1'	2.24	0.52
12:J:130:VAL:HG12	12:J:131:THR:H	1.74	0.52
15:M:158:ARG:HB2	15:M:163:LEU:HB2	1.89	0.52
1:0:1118:A:C8	1:0:1118:A:C3'	2.87	0.52
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.09	0.52
2:9:3044:A:O4'	7:D:76:ARG:NE	2.42	0.52
11:H:16:ARG:HH21	11:H:18:GLU:CD	2.17	0.52
12:J:76:ASP:HA	40:J:5907:HOH:O	2.09	0.52
15:M:83:SER:HB2	31:3:47:GLY:CA	2.39	0.52
1:0:2296:C:H2'	1:0:2297:U:H6	1.73	0.52
1:0:2883:A:H2'	1:0:2884:G:O4'	2.10	0.52
2:9:3023:U:O2'	2:9:3024:U:H4'	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.91	0.52
22:T:48:VAL:HG12	22:T:96:VAL:HG22	1.92	0.52
1:0:40:C:H4'	40:0:7388:HOH:O	2.08	0.52
1:0:338:C:H5''	40:C:9229:HOH:O	2.10	0.52
1:0:1189:A:H1'	1:0:1209:C:C1'	2.40	0.52
40:0:7894:HOH:O	31:3:61:PRO:HG2	2.09	0.52
13:K:118:ALA:CA	13:K:125:ALA:HB2	2.35	0.52
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.21	0.52
1:0:2786:G:H2'	40:0:7552:HOH:O	2.10	0.52
1:0:2812:A:C2	1:0:2814:A:N6	2.69	0.52
2:9:3107:C:H5	40:9:3167:HOH:O	1.92	0.52
5:B:53:LEU:HD21	5:B:270:ILE:HD12	1.92	0.52
15:M:68:ARG:HE	15:M:73:ARG:NE	2.08	0.52
15:M:70:GLY:HA3	15:M:73:ARG:NH2	2.25	0.52
16:N:154:LEU:O	16:N:155:GLU:CB	2.58	0.52
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.92	0.52
25:W:65:VAL:HA	25:W:68:THR:HG22	1.91	0.52
1:0:558:C:C2'	1:0:559:U:C5'	2.88	0.52
1:0:1333:U:H2'	1:0:1334:C:H6	1.74	0.52
1:0:1943:C:O4'	4:A:212:PRO:HA	2.08	0.52
1:0:944:G:C8	25:W:23:MET:HE1	2.45	0.52
1:0:1476:A:O2'	1:0:1868:G:H5'	2.10	0.52
1:0:2840:A:OP1	5:B:211:THR:CG2	2.54	0.52
2:9:3008:G:H4'	19:Q:27:GLN:NE2	2.25	0.52
2:9:3041:C:H4'	7:D:48:MET:HB3	1.92	0.52
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.92	0.52
7:D:128:LEU:HB2	40:D:6007:HOH:O	2.08	0.52
9:F:84:GLY:O	9:F:89:LEU:HB2	2.10	0.52
14:L:35:ARG:HH12	14:L:43:HIS:CD2	2.28	0.52
15:M:57:LYS:HE2	15:M:140:ALA:O	2.10	0.52
1:0:516:A:H5'	40:0:6128:HOH:O	2.10	0.52
6:C:194:PHE:HA	6:C:234:VAL:HG13	1.92	0.52
8:E:133:VAL:HG12	8:E:141:VAL:HG13	1.92	0.52
13:K:14:LYS:HG3	13:K:32:ILE:O	2.09	0.52
1:0:92:G:H4'	24:V:44:GLY:HA3	1.92	0.51
1:0:706:G:N2	1:0:707:C:H41	2.08	0.51
1:0:2825:C:H4'	1:0:2826:G:O5'	2.10	0.51
40:0:7793:HOH:O	5:B:211:THR:HG21	2.08	0.51
14:L:11:ARG:NH2	14:L:18:HIS:CG	2.78	0.51
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.10	0.51
27:Y:115:ARG:HB3	27:Y:115:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:144:ARG:NH1	40:Y:9374:HOH:O	2.38	0.51
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.10	0.51
1:O:475:G:OP1	6:C:73:LEU:CD2	2.58	0.51
1:O:1057:A:H1'	1:O:2492:U:O2'	2.10	0.51
1:O:2578:G:H5'	1:O:2578:G:C8	2.42	0.51
4:A:129:LEU:HD13	4:A:145:MET:HE1	1.92	0.51
6:C:133:ARG:HG2	6:C:134:ASP:N	2.25	0.51
15:M:81:ARG:HG2	15:M:85:ARG:O	2.09	0.51
18:P:40:VAL:O	18:P:44:VAL:HG23	2.10	0.51
22:T:48:VAL:HG11	22:T:96:VAL:CG1	2.38	0.51
25:W:105:THR:HA	25:W:109:GLU:OE1	2.10	0.51
1:O:447:A:OP1	22:T:2:LYS:HG2	2.11	0.51
1:O:1878:G:O2'	1:O:1879:U:C6	2.61	0.51
6:C:156:LEU:O	6:C:160:LEU:HG	2.11	0.51
18:P:89:ASN:HB3	18:P:92:GLU:CB	2.40	0.51
23:U:17:THR:CG2	23:U:18:GLY:N	2.73	0.51
31:3:70:ARG:NH1	31:3:77:ALA:CB	2.73	0.51
1:O:236:A:H4'	1:O:237:G:H5'	1.92	0.51
1:O:451:C:O2'	1:O:452:G:H5'	2.09	0.51
1:O:1186:C:H5''	32:I:119:TYR:CE1	2.45	0.51
1:O:1342:C:C2'	1:O:1343:C:H5'	2.40	0.51
4:A:223:ARG:NH1	40:A:9549:HOH:O	2.41	0.51
15:M:120:VAL:HG11	15:M:130:GLU:HG3	1.91	0.51
26:X:41:PHE:O	26:X:43:VAL:HG23	2.11	0.51
27:Y:174:VAL:CG1	27:Y:177:LYS:HD2	2.35	0.51
1:O:1679:C:H5'	40:O:9927:HOH:O	2.11	0.51
6:C:21:VAL:C	6:C:23:GLU:H	2.19	0.51
6:C:84:VAL:HG12	6:C:85:LYS:HG2	1.93	0.51
8:E:131:LEU:HD12	8:E:166:VAL:HG11	1.92	0.51
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.92	0.51
11:H:78:GLY:C	11:H:80:GLU:H	2.18	0.51
11:H:148:GLU:OE1	11:H:148:GLU:HA	2.10	0.51
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.24	0.51
12:J:130:VAL:HG12	12:J:131:THR:N	2.26	0.51
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.93	0.51
27:Y:151:SER:HB3	27:Y:154:ARG:CB	2.38	0.51
1:O:157:G:H4'	15:M:95:LYS:HE2	1.92	0.51
1:O:164:G:H4'	14:L:30:ARG:HD3	1.93	0.51
1:O:304:G:H1'	1:O:347:A:N6	2.25	0.51
1:O:1745:G:H22	1:O:2033:G:H5'	1.76	0.51
1:O:2779:G:H21	8:E:143:GLN:NE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:O:5465:HOH:O	6:C:202:THR:HB	2.10	0.51
40:9:1361:HOH:O	16:N:41:LYS:HE3	2.10	0.51
8:E:81:GLU:O	8:E:172:PRO:HD3	2.11	0.51
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.17	0.51
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.93	0.51
20:R:104:PHE:HB2	20:R:109:MET:HE2	1.91	0.51
1:O:21:G:H4'	20:R:2:ILE:HG22	1.92	0.51
1:O:1098:A:O3'	25:W:129:LYS:HE2	2.10	0.51
1:O:2769:C:H2'	1:O:2770:G:H5'	1.92	0.51
40:O:7883:HOH:O	15:M:91:ILE:HG23	2.11	0.51
7:D:51:ARG:HD3	40:D:7636:HOH:O	2.11	0.51
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.34	0.51
12:J:50:GLU:O	12:J:54:VAL:HG23	2.10	0.51
27:Y:170:SER:OG	27:Y:175:ARG:HG3	2.10	0.51
1:O:117:A:H2'	1:O:118:G:O4'	2.11	0.51
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.76	0.51
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.46	0.51
26:X:15:ARG:HB3	26:X:15:ARG:NH1	2.25	0.51
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.46	0.51
29:1:13:THR:HG22	29:1:14:THR:N	2.26	0.51
31:3:56:PRO:HA	40:3:9483:HOH:O	2.11	0.51
31:3:65:THR:CG2	31:3:88:LEU:HD22	2.41	0.51
1:O:317:A:H5''	22:T:52:ARG:HD2	1.93	0.51
1:O:776:A:OP1	29:1:28:HIS:HE1	1.94	0.51
1:O:2676:C:H4'	12:J:70:PHE:CE1	2.45	0.51
40:O:3716:HOH:O	31:3:46:ILE:HG12	2.11	0.51
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.93	0.51
11:H:143:ALA:O	11:H:146:VAL:HG12	2.11	0.51
20:R:4:TYR:CE1	20:R:15:LYS:HD3	2.46	0.51
29:1:45:ARG:NH2	40:1:9484:HOH:O	2.28	0.51
1:O:249:G:O2'	1:O:250:C:H5'	2.11	0.51
1:O:949:U:O2'	19:Q:40:HIS:HE1	1.94	0.51
1:O:1118:A:H62	1:O:1244:U:H3	1.59	0.51
1:O:1234:U:N3	5:B:244:PRO:HB3	2.26	0.51
1:O:2011:A:H5'	1:O:2013:G:H1'	1.93	0.51
1:O:2032:U:H2'	1:O:2033:G:H5''	1.91	0.51
7:D:159:PRO:O	7:D:163:VAL:HG23	2.11	0.51
11:H:170:ASN:N	11:H:170:ASN:ND2	2.59	0.51
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.41	0.51
14:L:75:LEU:N	14:L:75:LEU:HD23	2.26	0.51
24:V:12:THR:HG23	24:V:14:ALA:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:4:LEU:CD2	25:W:52:VAL:HG21	2.36	0.51
30:2:36:ASN:HB3	30:2:39:ARG:HG3	1.93	0.51
1:0:407:A:H2'	1:0:408:A:C8	2.46	0.50
1:0:721:A:H4'	17:O:51:TYR:CD1	2.46	0.50
1:0:2070:G:H2'	1:0:2072:G:OP1	2.10	0.50
1:0:2432:C:H2'	1:0:2433:A:H8	1.76	0.50
2:9:3049:G:O2'	2:9:3050:G:H5'	2.12	0.50
5:B:171:VAL:HG23	5:B:172:SER:N	2.26	0.50
7:D:25:MET:HE1	7:D:40:ILE:HD11	1.93	0.50
9:F:70:LYS:C	9:F:72:VAL:H	2.19	0.50
16:N:167:ASP:C	16:N:168:LEU:HG	2.36	0.50
24:V:64:GLY:O	24:V:65:ASP:HB2	2.09	0.50
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.40	0.50
1:0:812:A:H1'	40:0:4503:HOH:O	2.12	0.50
1:0:1803:C:H2'	1:0:1804:A:C8	2.47	0.50
1:0:2054:A:C2	20:R:128:ARG:NH2	2.79	0.50
5:B:51:VAL:HG22	5:B:53:LEU:CD1	2.41	0.50
5:B:150:ALA:O	5:B:152:PRO:HD3	2.11	0.50
6:C:234:VAL:HG13	6:C:234:VAL:O	2.11	0.50
16:N:36:ALA:HB1	16:N:118:ILE:HD12	1.92	0.50
25:W:13:MET:CE	25:W:17:ILE:HG22	2.32	0.50
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.41	0.50
1:0:1180:U:H1'	40:0:3801:HOH:O	2.12	0.50
1:0:1203:G:O2'	1:0:1204:C:H5'	2.11	0.50
1:0:1268:C:O2'	1:0:1269:G:H5'	2.11	0.50
1:0:1902:G:H2'	1:0:1903:U:O4'	2.11	0.50
1:0:2895:C:H4'	40:X:4132:HOH:O	2.11	0.50
5:B:140:LEU:HD13	5:B:175:LEU:HA	1.91	0.50
12:J:6:PHE:HB3	12:J:109:TYR:OH	2.11	0.50
15:M:83:SER:HB2	31:3:47:GLY:HA3	1.93	0.50
19:Q:64:GLU:HG3	19:Q:74:ASP:CG	2.36	0.50
1:0:1500:U:P	18:P:41:ARG:HH22	2.34	0.50
1:0:2612:A:H4'	40:0:4231:HOH:O	2.10	0.50
1:0:2661:U:H3	1:0:2812:A:H62	1.59	0.50
1:0:2769:C:H2'	1:0:2770:G:C5'	2.41	0.50
1:0:2769:C:O2'	1:0:2770:G:H5'	2.12	0.50
5:B:62:ARG:HA	5:B:65:MET:CE	2.40	0.50
6:C:236:THR:O	6:C:237:GLU:C	2.54	0.50
14:L:143:THR:O	14:L:147:GLU:HG3	2.11	0.50
16:N:115:VAL:HG22	40:N:9358:HOH:O	2.11	0.50
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:497:A:H2'	1:0:498:A:H5'	1.94	0.50
1:0:1972:U:H2'	1:0:1973:A:C5'	2.41	0.50
1:0:2089:A:O2'	1:0:2090:G:H5'	2.11	0.50
4:A:210:GLY:N	40:A:9621:HOH:O	2.44	0.50
7:D:99:ASP:HB2	7:D:103:ASN:HB2	1.93	0.50
7:D:103:ASN:ND2	7:D:133:ASN:HD22	2.09	0.50
15:M:76:ARG:HA	40:M:9329:HOH:O	2.11	0.50
27:Y:145:LYS:HE2	40:Y:9404:HOH:O	2.11	0.50
1:0:1298:U:H2'	1:0:1299:G:C8	2.45	0.50
1:0:1942:A:H3'	40:0:7693:HOH:O	2.12	0.50
5:B:294:TYR:CD1	5:B:294:TYR:C	2.89	0.50
6:C:236:THR:HG22	6:C:239:ALA:CB	2.42	0.50
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.93	0.50
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.93	0.50
12:J:19:MET:HE2	12:J:79:PHE:HA	1.92	0.50
14:L:77:ALA:C	14:L:79:ASP:H	2.19	0.50
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.47	0.50
1:0:1198:U:H2'	1:0:1200:A:OP2	2.11	0.50
1:0:1666:C:C2'	1:0:1667:A:C5'	2.90	0.50
9:F:99:THR:O	9:F:100:ASP:HB2	2.10	0.50
25:W:122:ARG:NH2	40:W:5817:HOH:O	2.40	0.50
26:X:34:ARG:NH1	26:X:48:VAL:O	2.45	0.50
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.94	0.50
6:C:57:PRO:HG2	6:C:73:LEU:HD13	1.94	0.50
11:H:30:GLN:H	11:H:66:ARG:HH11	1.60	0.50
11:H:83:TYR:CD1	11:H:83:TYR:C	2.90	0.50
25:W:128:VAL:O	25:W:138:LEU:HD11	2.12	0.50
1:0:812:A:H2'	1:0:813:C:C6	2.46	0.50
4:A:36:ASP:CB	4:A:85:SER:HB2	2.41	0.50
5:B:132:HIS:NE2	5:B:171:VAL:HG23	2.27	0.50
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.41	0.50
22:T:23:VAL:HG23	22:T:41:ARG:HG3	1.93	0.50
26:X:7:GLU:HA	26:X:74:ALA:O	2.12	0.50
27:Y:189:ASN:CA	27:Y:217:ILE:HD11	2.38	0.50
1:0:475:G:C5'	6:C:73:LEU:HD23	2.43	0.49
1:0:797:A:C5'	28:Z:10:ARG:N	2.73	0.49
1:0:834:G:H3'	1:0:835:U:H4'	1.94	0.49
1:0:1853:C:OP1	4:A:231:LYS:HG3	2.12	0.49
1:0:2472:C:O2'	1:0:2634:G:H4'	2.12	0.49
1:0:2748:G:H4'	1:0:2749:U:C5'	2.41	0.49
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:255:A:H2'	1:0:256:C:C6	2.47	0.49
1:0:799:C:O2'	1:0:800:G:H5'	2.12	0.49
1:0:1180:U:O2'	32:I:92:PRO:HD2	2.13	0.49
1:0:1486:A:C5	30:2:2:LYS:HG3	2.46	0.49
2:9:3049:G:C2'	2:9:3050:G:H5'	2.42	0.49
5:B:41:PHE:CG	5:B:79:MET:HE2	2.47	0.49
8:E:20:ILE:HD12	8:E:33:LEU:CD1	2.41	0.49
8:E:154:ILE:HD11	8:E:157:LYS:HE2	1.94	0.49
1:0:248:A:H5'	1:0:249:G:OP2	2.13	0.49
1:0:905:C:OP1	27:Y:144:ARG:NH1	2.45	0.49
1:0:1845:A:O2'	1:0:1846:U:H5'	2.12	0.49
1:0:1878:G:O2'	1:0:1879:U:OP2	2.29	0.49
1:0:1881:A:OP1	4:A:199:HIS:HE1	1.95	0.49
1:0:2050:G:H5''	20:R:80:TYR:O	2.13	0.49
1:0:2072:G:H3'	1:0:2073:G:C5'	2.42	0.49
1:0:2265:U:H2'	1:0:2266:A:C8	2.47	0.49
5:B:276:ASP:O	5:B:279:THR:HG22	2.12	0.49
7:D:10:PHE:CG	7:D:11:HIS:N	2.81	0.49
26:X:61:ARG:HB2	26:X:65:ASN:HB2	1.94	0.49
32:I:138:THR:HG22	32:I:139:ILE:N	2.27	0.49
1:0:1826:C:O2'	1:0:1827:G:H5'	2.12	0.49
1:0:2326:U:H4'	1:0:2412:G:H4'	1.95	0.49
5:B:144:THR:HG21	40:B:9618:HOH:O	2.12	0.49
9:F:5:ASP:O	9:F:119:ARG:NH1	2.45	0.49
12:J:131:THR:HG23	12:J:133:GLY:H	1.78	0.49
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.94	0.49
17:O:14:LEU:CG	17:O:102:ILE:HD11	2.42	0.49
31:3:69:TYR:O	31:3:77:ALA:HA	2.13	0.49
1:0:259:G:H21	15:M:58:GLN:NE2	2.10	0.49
1:0:816:G:H5'	1:0:1598:A:H4'	1.94	0.49
1:0:1077:G:H2'	1:0:1080:C:H42	1.76	0.49
1:0:1940:C:H4'	40:0:7693:HOH:O	2.11	0.49
1:0:2016:U:H2'	1:0:2017:U:O4'	2.13	0.49
5:B:54:VAL:O	5:B:55:ASN:C	2.55	0.49
5:B:101:TRP:HB2	5:B:119:HIS:CD2	2.47	0.49
5:B:254:GLN:HG2	5:B:255:GLY:H	1.77	0.49
5:B:277:GLU:N	5:B:278:PRO:HD2	2.27	0.49
7:D:96:SER:C	7:D:98:PHE:H	2.20	0.49
14:L:27:ARG:HH21	14:L:30:ARG:HG2	1.77	0.49
14:L:74:THR:OG1	14:L:75:LEU:HD23	2.13	0.49
23:U:47:ARG:HG2	23:U:54:THR:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:42:CYS:SG	28:Z:44:GLU:HB2	2.53	0.49
1:0:218:C:P	31:3:39:GLN:HE21	2.34	0.49
1:0:1264:U:P	25:W:117:ARG:HH22	2.35	0.49
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.27	0.49
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	2.13	0.49
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.12	0.49
28:Z:15:GLY:HA3	40:Z:9229:HOH:O	2.12	0.49
1:0:380:A:H2'	40:M:9440:HOH:O	2.12	0.49
1:0:1474:C:H6	1:0:1474:C:C5'	2.18	0.49
1:0:2036:C:O4'	13:K:44:LEU:HG	2.13	0.49
1:0:2101:A:H5'	6:C:63:SER:HB3	1.95	0.49
1:0:2112:A:H2'	1:0:2113:G:C8	2.48	0.49
1:0:2372:A:H2'	1:0:2373:U:C6	2.48	0.49
1:0:2374:A:H2'	1:0:2375:G:C8	2.48	0.49
2:9:3052:A:O2'	2:9:3053:G:H5'	2.12	0.49
5:B:77:PRO:HG3	40:B:9571:HOH:O	2.12	0.49
7:D:25:MET:CE	7:D:40:ILE:HD11	2.43	0.49
7:D:62:ASP:HA	40:D:4233:HOH:O	2.12	0.49
8:E:166:VAL:HG12	40:E:3134:HOH:O	2.13	0.49
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.43	0.49
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.77	0.49
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.76	0.49
18:P:103:THR:O	18:P:107:GLU:HG3	2.13	0.49
1:0:120:A:H2'	1:0:120:A:N3	2.28	0.49
1:0:317:A:OP1	22:T:52:ARG:O	2.31	0.49
1:0:653:C:H2'	1:0:654:A:C8	2.47	0.49
1:0:1688:G:O2'	29:1:5:THR:HG23	2.13	0.49
11:H:88:ARG:NH1	11:H:135:THR:OG1	2.45	0.49
21:S:57:THR:HG22	21:S:59:ASP:HB2	1.95	0.49
22:T:78:THR:HB	22:T:87:VAL:O	2.13	0.49
1:0:946:C:H2'	1:0:947:U:H6	1.78	0.49
1:0:1314:U:H2'	40:0:6340:HOH:O	2.13	0.49
1:0:1476:A:H1'	1:0:1867:G:O2'	2.12	0.49
1:0:2133:U:H4'	1:0:2134:G:H5'	1.93	0.49
1:0:2281:C:C2'	1:0:2282:U:H5'	2.42	0.49
1:0:2415:A:C2'	1:0:2416:G:H5'	2.43	0.49
1:0:2912:C:H2'	1:0:2913:A:O4'	2.12	0.49
4:A:81:GLN:H	4:A:92:ASN:CG	2.20	0.49
5:B:102:THR:HG21	5:B:182:VAL:O	2.13	0.49
7:D:23:VAL:HG23	7:D:23:VAL:O	2.12	0.49
8:E:84:MET:HB2	8:E:131:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:119:HIS:HE1	8:E:147:ASP:OD2	1.95	0.49
14:L:119:THR:HG23	14:L:139:SER:OG	2.12	0.49
16:N:67:ALA:HA	16:N:71:TRP:HB3	1.94	0.49
22:T:48:VAL:HG11	22:T:96:VAL:HG22	1.95	0.49
25:W:149:LEU:CG	25:W:153:MET:HE2	2.31	0.49
31:3:7:PHE:CE1	31:3:9:THR:HB	2.48	0.49
1:0:1204:C:H2'	1:0:1205:U:O4'	2.12	0.49
1:0:2824:C:O3'	1:0:2825:C:H6	1.96	0.49
2:9:3114:G:O6	16:N:11:ARG:HD3	2.12	0.49
5:B:214:PRO:C	5:B:220:VAL:HG22	2.38	0.49
6:C:20:ASP:O	6:C:23:GLU:HB2	2.12	0.49
6:C:45:ASP:OD2	6:C:98:ARG:HD2	2.13	0.49
9:F:57:GLU:O	9:F:61:MET:HG3	2.13	0.49
9:F:110:ASP:O	9:F:114:LYS:HG3	2.12	0.49
20:R:132:ARG:NH2	40:R:9500:HOH:O	2.46	0.49
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.13	0.49
25:W:38:THR:O	25:W:42:ARG:HB2	2.12	0.49
1:0:371:U:H2'	1:0:372:A:C8	2.46	0.48
1:0:1166:A:H1'	1:0:1192:A:N3	2.27	0.48
1:0:1878:G:O2'	1:0:1879:U:P	2.71	0.48
2:9:3092:G:H2'	2:9:3093:A:H8	1.78	0.48
5:B:254:GLN:NE2	40:B:9585:HOH:O	2.46	0.48
13:K:2:GLU:O	13:K:3:ALA:C	2.56	0.48
14:L:129:ALA:O	14:L:133:VAL:HG23	2.13	0.48
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.94	0.48
17:O:25:VAL:HG23	17:O:26:TRP:H	1.78	0.48
1:0:1174:A:C6	1:0:1201:C:H4'	2.48	0.48
1:0:1218:U:H2'	1:0:1219:U:C6	2.49	0.48
1:0:2748:G:H4'	1:0:2749:U:H5'	1.94	0.48
2:9:3064:C:C2'	2:9:3065:A:H5'	2.42	0.48
5:B:51:VAL:HG23	5:B:327:VAL:HG13	1.94	0.48
5:B:96:PRO:HG3	40:B:9628:HOH:O	2.13	0.48
6:C:237:GLU:HB2	40:C:9238:HOH:O	2.13	0.48
11:H:167:PRO:O	11:H:168:ALA:HB2	2.12	0.48
15:M:107:ARG:NH1	40:M:9380:HOH:O	2.46	0.48
1:0:1149:U:H5''	1:0:1151:G:O4'	2.13	0.48
1:0:1741:U:H3'	40:0:3343:HOH:O	2.12	0.48
40:0:7400:HOH:O	15:M:68:ARG:HB2	2.13	0.48
2:9:3008:G:O6	16:N:11:ARG:NH1	2.44	0.48
2:9:3108:C:O2'	2:9:3109:G:H5'	2.12	0.48
27:Y:144:ARG:CZ	40:Y:9410:HOH:O	2.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:319:A:H4'	1:0:338:C:C5	2.48	0.48
1:0:951:A:O2'	1:0:952:G:H5'	2.13	0.48
1:0:1185:U:H5'	40:0:7803:HOH:O	2.13	0.48
1:0:1242:A:C5'	12:J:82:THR:HG23	2.31	0.48
1:0:1600:G:OP2	1:0:1600:G:H8	1.96	0.48
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.39	0.48
1:0:2809:G:H2'	1:0:2810:G:O4'	2.13	0.48
4:A:69:LEU:O	4:A:71:PRO:HD3	2.13	0.48
10:G:20:VAL:O	10:G:24:VAL:HG23	2.13	0.48
11:H:95:LEU:HD11	11:H:124:ALA:HB2	1.95	0.48
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.78	0.48
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.43	0.48
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.67	0.48
27:Y:144:ARG:NH2	40:Y:9410:HOH:O	2.47	0.48
1:0:1187:U:H2'	1:0:1189:A:OP2	2.12	0.48
1:0:1741:U:O2'	1:0:2723:G:H4'	2.14	0.48
5:B:305:ASP:O	5:B:306:LYS:CB	2.60	0.48
9:F:60:VAL:O	9:F:60:VAL:HG12	2.14	0.48
15:M:48:LYS:HE3	15:M:52:GLN:NE2	2.28	0.48
21:S:57:THR:HG21	21:S:59:ASP:HB2	1.96	0.48
22:T:69:LYS:O	22:T:71:VAL:HG23	2.14	0.48
1:0:368:C:H1'	40:0:5722:HOH:O	2.12	0.48
1:0:1422:U:H2'	1:0:1423:C:C6	2.49	0.48
5:B:81:ALA:O	5:B:186:GLY:HA3	2.13	0.48
7:D:134:LEU:CD1	7:D:166:ILE:HD11	2.40	0.48
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.96	0.48
14:L:34:GLY:HA3	14:L:38:HIS:CE1	2.49	0.48
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.12	0.48
18:P:55:LYS:CG	18:P:56:GLY:N	2.76	0.48
23:U:47:ARG:HG2	23:U:54:THR:HG21	1.95	0.48
24:V:55:ARG:O	24:V:59:ILE:HG12	2.14	0.48
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.96	0.48
25:W:64:THR:O	25:W:68:THR:HG22	2.13	0.48
27:Y:108:ASP:OD1	27:Y:108:ASP:N	2.40	0.48
1:0:894:A:C2	6:C:87:ARG:NH2	2.81	0.48
1:0:1058:A:H2'	1:0:1060:C:H5''	1.95	0.48
1:0:1947:G:H2'	1:0:1948:G:C8	2.47	0.48
1:0:1947:G:H2'	1:0:1948:G:H8	1.78	0.48
1:0:2289:G:O2'	1:0:2290:U:H5'	2.14	0.48
2:9:3051:A:H5'	16:N:160:SER:CB	2.43	0.48
2:9:3064:C:H2'	2:9:3065:A:H5'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:12:GLU:O	7:D:15:GLU:HG2	2.13	0.48
7:D:60:GLU:HG3	7:D:60:GLU:O	2.14	0.48
7:D:103:ASN:HD21	7:D:133:ASN:HD22	1.59	0.48
18:P:36:THR:O	18:P:39:ASP:HB2	2.13	0.48
20:R:84:ALA:O	20:R:88:PHE:HD1	1.97	0.48
22:T:48:VAL:HG11	22:T:96:VAL:CG2	2.44	0.48
25:W:5:VAL:O	25:W:52:VAL:CG2	2.62	0.48
31:3:6:ARG:HA	31:3:20:HIS:O	2.13	0.48
1:0:524:A:H5''	20:R:29:LYS:HD3	1.96	0.48
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.12	0.48
1:0:1435:U:H5'	40:0:3189:HOH:O	2.13	0.48
1:0:2591:C:H2'	1:0:2592:G:O4'	2.14	0.48
1:0:2676:C:H4'	12:J:70:PHE:HD1	1.74	0.48
5:B:24:PRO:HG3	5:B:204:GLY:HA2	1.95	0.48
5:B:81:ALA:HB1	5:B:142:LEU:HD13	1.94	0.48
6:C:49:ASP:HB3	6:C:52:ALA:HB2	1.94	0.48
6:C:120:ASP:C	6:C:120:ASP:OD1	2.56	0.48
9:F:102:GLY:O	9:F:103:GLU:HB2	2.13	0.48
14:L:53:ARG:NH2	14:L:57:VAL:CG1	2.77	0.48
27:Y:178:HIS:CD2	27:Y:179:PRO:HD2	2.49	0.48
31:3:67:LEU:HD21	31:3:88:LEU:CD2	2.43	0.48
1:0:247:A:H2'	40:0:4470:HOH:O	2.13	0.48
1:0:2411:C:H4'	40:0:5466:HOH:O	2.12	0.48
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.95	0.48
5:B:14:GLY:HA2	5:B:15:PRO:C	2.39	0.48
5:B:16:ARG:NH1	40:B:9610:HOH:O	2.46	0.48
7:D:10:PHE:CD1	7:D:11:HIS:N	2.82	0.48
15:M:68:ARG:O	15:M:68:ARG:CD	2.56	0.48
1:0:329:A:OP2	6:C:206:ASN:HB2	2.14	0.48
1:0:1189:A:H3'	40:0:8033:HOH:O	2.13	0.48
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.45	0.48
1:0:2868:C:H2'	1:0:2869:G:O4'	2.14	0.48
38:4:9701:SPS:O1	38:4:9701:SPS:H91	2.14	0.48
8:E:81:GLU:HG2	8:E:134:SER:CB	2.42	0.48
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.96	0.48
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.49	0.48
15:M:102:GLU:CD	15:M:164:THR:HG21	2.38	0.48
24:V:12:THR:HG22	24:V:15:GLU:H	1.78	0.48
1:0:328:U:O2	6:C:202:THR:HG21	2.15	0.47
1:0:802:G:H2'	1:0:803:C:C6	2.49	0.47
1:0:1787:C:H4'	1:0:2883:A:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2498:C:O2'	1:0:2499:U:H5'	2.13	0.47
4:A:204:GLY:O	4:A:205:GLY:C	2.57	0.47
5:B:80:ARG:HB2	5:B:145:HIS:CE1	2.49	0.47
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.22	0.47
25:W:4:LEU:O	25:W:32:CYS:HA	2.13	0.47
26:X:61:ARG:HH11	26:X:61:ARG:HG3	1.79	0.47
1:0:285:A:H2'	1:0:286:U:O4'	2.14	0.47
1:0:462:A:H2'	40:0:5402:HOH:O	2.14	0.47
1:0:907:A:H4'	1:0:1328:A:C2	2.49	0.47
1:0:2506:A:O2'	1:0:2507:G:P	2.72	0.47
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.49	0.47
13:K:74:VAL:HG11	13:K:113:ILE:CG1	2.37	0.47
24:V:44:GLY:O	24:V:48:GLU:HG2	2.13	0.47
25:W:48:VAL:CG1	25:W:48:VAL:O	2.62	0.47
28:Z:59:TYR:HA	40:Z:9233:HOH:O	2.14	0.47
1:0:960:G:N3	1:0:960:G:H2'	2.29	0.47
6:C:218:VAL:N	40:C:9232:HOH:O	2.47	0.47
7:D:40:ILE:HG13	7:D:41:LEU:N	2.29	0.47
12:J:45:VAL:HG22	12:J:46:ILE:N	2.29	0.47
14:L:6:ARG:NH2	40:L:9445:HOH:O	2.47	0.47
14:L:72:ASN:HB2	40:L:9486:HOH:O	2.14	0.47
14:L:73:VAL:HG23	14:L:74:THR:N	2.22	0.47
22:T:19:ARG:HD3	22:T:67:LEU:O	2.14	0.47
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.45	0.47
1:0:655:U:O2'	17:O:3:THR:HB	2.13	0.47
1:0:2090:G:H2'	1:0:2091:G:C8	2.48	0.47
1:0:2824:C:H5''	1:0:2825:C:H5'	1.97	0.47
2:9:3014:G:C2'	2:9:3015:C:H5'	2.45	0.47
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.15	0.47
4:A:112:PRO:HD3	4:A:152:CYS:SG	2.55	0.47
4:A:123:GLY:HA2	4:A:159:VAL:O	2.14	0.47
6:C:54:LEU:HD23	6:C:79:ARG:HG3	1.96	0.47
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.47	0.47
25:W:13:MET:HE2	25:W:18:GLN:N	2.29	0.47
1:0:57:C:H42	1:0:89:G:H1	1.61	0.47
1:0:137:U:H2'	1:0:139:C:C5	2.49	0.47
1:0:1120:U:H5'	1:0:1121:G:OP2	2.14	0.47
1:0:2032:U:H2'	1:0:2033:G:H5'	1.95	0.47
1:0:2906:A:H5'	1:0:2907:C:O4'	2.15	0.47
7:D:164:ALA:O	7:D:165:PHE:C	2.57	0.47
12:J:19:MET:CE	12:J:132:LEU:HD11	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:112:GLY:HA2	16:N:137:ALA:N	2.29	0.47
17:O:77:ALA:HA	17:O:96:VAL:O	2.15	0.47
24:V:4:HIS:O	24:V:8:ILE:HG13	2.13	0.47
1:O:541:C:O2'	1:O:542:A:H5''	2.14	0.47
1:O:883:U:H2'	1:O:883:U:O2	2.14	0.47
1:O:1015:C:H2'	1:O:1016:U:H6	1.79	0.47
1:O:1309:U:O2'	1:O:1310:U:H5'	2.15	0.47
1:O:1477:C:H5'	1:O:1868:G:C5'	2.43	0.47
1:O:2784:A:H1'	8:E:60:SER:OG	2.15	0.47
1:O:2866:U:H4'	1:O:2867:G:H5'	1.95	0.47
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.48	0.47
4:A:207:GLN:O	4:A:208:HIS:HB3	2.14	0.47
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.12	0.47
5:B:215:VAL:HA	5:B:220:VAL:HG22	1.97	0.47
6:C:123:LEU:O	6:C:126:ASP:N	2.47	0.47
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.80	0.47
13:K:125:ALA:O	13:K:127:ALA:N	2.44	0.47
20:R:68:HIS:CD2	20:R:76:ASP:HB2	2.49	0.47
22:T:41:ARG:NH1	22:T:41:ARG:CG	2.71	0.47
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.50	0.47
1:O:65:C:O2'	1:O:66:G:H5'	2.15	0.47
1:O:256:C:H2'	1:O:257:G:O4'	2.14	0.47
1:O:517:U:H1'	40:O:7913:HOH:O	2.14	0.47
1:O:1020:A:H2'	1:O:1021:G:C8	2.49	0.47
1:O:1119:G:H2'	12:J:52:GLN:HE22	1.74	0.47
1:O:1163:G:H5'	32:I:115:ASP:O	2.15	0.47
1:O:1174:A:C5	1:O:1201:C:H4'	2.50	0.47
1:O:2019:A:H5'	40:O:5068:HOH:O	2.15	0.47
1:O:2580:G:N3	1:O:2600:A:H2	2.13	0.47
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.80	0.47
6:C:76:ARG:CG	6:C:76:ARG:NH1	2.78	0.47
6:C:84:VAL:O	6:C:85:LYS:HB2	2.15	0.47
7:D:64:ARG:HB3	7:D:67:ASP:OD2	2.15	0.47
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.38	0.47
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.96	0.47
12:J:64:GLY:HA3	36:J:9321:CL:CL	2.51	0.47
13:K:49:LEU:HD12	13:K:80:ILE:HG21	1.95	0.47
14:L:57:VAL:HG12	14:L:57:VAL:O	2.15	0.47
16:N:182:GLY:O	16:N:183:ASP:C	2.57	0.47
17:O:21:SER:OG	17:O:106:PRO:HB2	2.14	0.47
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:64:GLU:HG2	40:P:168:HOH:O	2.15	0.47
24:V:39:ALA:C	24:V:41:GLU:N	2.73	0.47
25:W:38:THR:HG22	25:W:40:ALA:H	1.79	0.47
27:Y:216:ARG:HD2	40:Y:9367:HOH:O	2.14	0.47
30:2:14:LEU:HD13	30:2:47:THR:CG2	2.45	0.47
1:0:559:U:H5'	1:0:559:U:C6	2.45	0.47
1:0:2253:G:O2'	1:0:2254:G:H5'	2.15	0.47
1:0:2312:G:H2'	1:0:2313:C:H5'	1.96	0.47
1:0:2619:UR3:H2'	1:0:2620:U:C6	2.49	0.47
40:0:7136:HOH:O	19:Q:13:LYS:HE2	2.14	0.47
4:A:43:VAL:O	4:A:43:VAL:HG12	2.14	0.47
5:B:87:TYR:O	5:B:138:GLY:N	2.33	0.47
6:C:168:ARG:NH2	6:C:190:ALA:O	2.47	0.47
8:E:102:VAL:HG11	8:E:148:ILE:HD11	1.96	0.47
15:M:98:GLN:O	15:M:102:GLU:HG3	2.15	0.47
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.79	0.47
1:0:333:G:O2'	1:0:334:G:H5'	2.15	0.47
1:0:407:A:H8	40:0:4990:HOH:O	1.96	0.47
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.79	0.47
1:0:2032:U:O2'	1:0:2033:G:H5''	2.14	0.47
1:0:2478:U:O2'	1:0:2479:A:H5'	2.15	0.47
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.97	0.47
9:F:11:ASP:HA	9:F:14:ASP:OD2	2.14	0.47
12:J:54:VAL:O	12:J:58:GLU:HG3	2.15	0.47
1:0:1753:C:O2	5:B:229:ARG:NH2	2.48	0.47
1:0:2269:C:H2'	1:0:2270:G:O4'	2.15	0.47
1:0:2679:G:H2'	1:0:2681:A:OP2	2.14	0.47
4:A:81:GLN:N	4:A:92:ASN:ND2	2.62	0.47
5:B:264:GLU:HG2	5:B:267:LYS:CE	2.45	0.47
5:B:274:GLU:HA	5:B:292:GLY:O	2.14	0.47
5:B:307:ARG:HG3	5:B:307:ARG:NH1	2.21	0.47
6:C:45:ASP:OD2	6:C:98:ARG:CD	2.63	0.47
8:E:11:VAL:CG1	8:E:12:ASP:N	2.78	0.47
8:E:101:GLU:HB3	8:E:117:THR:HA	1.97	0.47
9:F:1:PRO:H3	9:F:4:VAL:HG23	1.79	0.47
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.45	0.47
4:A:109:GLU:HG2	4:A:116:GLY:H	1.80	0.46
6:C:140:VAL:HG12	6:C:141:SER:N	2.29	0.46
7:D:95:THR:OG1	7:D:174:VAL:HG22	2.15	0.46
7:D:151:ILE:HG23	7:D:155:HIS:HB3	1.97	0.46
8:E:80:TRP:O	8:E:134:SER:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:12:ILE:HD12	40:G:692:HOH:O	2.16	0.46
15:M:82:ARG:O	15:M:83:SER:C	2.57	0.46
18:P:27:ARG:O	18:P:31:ILE:HG13	2.15	0.46
23:U:45:GLU:HB2	23:U:48:ASN:HD22	1.78	0.46
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.96	0.46
1:0:35:U:O2'	1:0:36:C:H5'	2.16	0.46
1:0:40:C:O5'	1:0:40:C:H6	1.99	0.46
1:0:793:A:H5''	18:P:83:LYS:HG2	1.97	0.46
1:0:817:G:OP2	18:P:91:LYS:HE3	2.16	0.46
1:0:848:C:H5'	40:0:7630:HOH:O	2.16	0.46
1:0:1965:C:O5'	1:0:1965:C:H6	1.98	0.46
40:0:3801:HOH:O	32:I:92:PRO:HD3	2.14	0.46
5:B:241:PRO:HD2	40:B:9646:HOH:O	2.15	0.46
8:E:100:ASP:HB2	40:E:2789:HOH:O	2.16	0.46
13:K:114:ALA:HA	13:K:132:VAL:O	2.15	0.46
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.15	0.46
20:R:39:THR:HB	20:R:42:GLU:CG	2.40	0.46
20:R:122:GLN:HB3	20:R:138:SER:HB2	1.96	0.46
24:V:64:GLY:O	24:V:65:ASP:CB	2.62	0.46
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.44	0.46
1:0:660:A:H4'	1:0:661:G:O5'	2.15	0.46
1:0:1183:C:H5	1:0:1192:A:OP1	1.97	0.46
1:0:1406:A:H4'	1:0:1407:A:H5''	1.95	0.46
4:A:109:GLU:CD	4:A:153:ARG:NH1	2.73	0.46
5:B:243:ASN:HA	5:B:244:PRO:C	2.39	0.46
6:C:98:ARG:HG2	6:C:98:ARG:NH1	2.29	0.46
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.98	0.46
9:F:20:LEU:HB2	9:F:49:PHE:CZ	2.50	0.46
10:G:12:ILE:N	10:G:13:PRO:CD	2.78	0.46
16:N:140:GLN:HA	16:N:143:ARG:HD3	1.97	0.46
16:N:156:GLU:O	16:N:157:PRO:C	2.59	0.46
22:T:32:ARG:HH12	22:T:38:ARG:HH12	1.62	0.46
22:T:83:ASP:OD1	22:T:85:GLU:HB3	2.15	0.46
23:U:9:CYS:HA	23:U:52:THR:HG23	1.96	0.46
24:V:32:ALA:O	24:V:35:ALA:HB3	2.16	0.46
25:W:73:LEU:HD12	25:W:73:LEU:HA	1.82	0.46
1:0:87:C:C2	30:2:30:ASP:OD2	2.68	0.46
1:0:171:C:OP2	15:M:84:LYS:HG3	2.16	0.46
1:0:710:G:O2'	1:0:711:G:H5'	2.15	0.46
1:0:1044:C:H5''	40:0:9647:HOH:O	2.14	0.46
1:0:1236:A:C8	12:J:63:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1363:G:OP1	6:C:76:ARG:NH2	2.47	0.46
1:O:1636:G:O2'	1:O:1637:A:H5'	2.15	0.46
1:O:2613:G:O2'	1:O:2614:C:H5'	2.15	0.46
8:E:106:ASN:ND2	8:E:109:GLY:HA2	2.31	0.46
10:G:64:ASN:N	10:G:64:ASN:ND2	2.63	0.46
15:M:99:ARG:HH21	15:M:170:ASN:ND2	2.10	0.46
15:M:172:GLY:HA2	40:M:9321:HOH:O	2.15	0.46
16:N:89:GLY:O	16:N:92:ALA:HB3	2.15	0.46
25:W:88:THR:CG2	25:W:89:ASP:N	2.78	0.46
1:O:81:G:N3	1:O:98:A:C2	2.84	0.46
1:O:392:U:H5''	15:M:193:LYS:HB3	1.96	0.46
1:O:500:G:O2'	20:R:94:ASN:ND2	2.49	0.46
1:O:1562:C:N4	40:O:6331:HOH:O	2.47	0.46
1:O:2453:G:H5''	40:L:9440:HOH:O	2.15	0.46
40:O:3152:HOH:O	25:W:119:HIS:HE1	1.99	0.46
4:A:206:ARG:HD3	4:A:206:ARG:N	2.30	0.46
5:B:183:GLU:O	5:B:184:ASP:C	2.59	0.46
26:X:86:GLU:HG3	26:X:87:ALA:O	2.16	0.46
32:I:139:ILE:HG22	32:I:140:GLU:N	2.29	0.46
1:O:129:A:H4'	1:O:130:C:OP1	2.16	0.46
1:O:1067:A:H5'	40:O:4882:HOH:O	2.15	0.46
1:O:1071:G:H4'	27:Y:154:ARG:NH2	2.31	0.46
1:O:1103:C:O2	12:J:86:MET:HG2	2.16	0.46
1:O:1462:C:H2'	1:O:1463:A:C8	2.51	0.46
1:O:1759:A:N3	1:O:1818:C:H2'	2.31	0.46
1:O:2748:G:OP1	1:O:2749:U:H5''	2.16	0.46
4:A:72:GLU:CD	28:Z:76:GLY:HA3	2.40	0.46
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.96	0.46
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.15	0.46
11:H:154:TYR:CD1	11:H:154:TYR:C	2.93	0.46
15:M:30:GLU:O	15:M:34:GLU:HG3	2.15	0.46
20:R:61:GLN:CD	40:R:9451:HOH:O	2.58	0.46
31:3:11:CYS:HB2	31:3:20:HIS:HE1	1.77	0.46
1:O:136:C:H2'	1:O:137:U:O4'	2.15	0.46
1:O:2432:C:H2'	1:O:2433:A:C8	2.50	0.46
1:O:2443:C:H1'	14:L:56:LYS:HE3	1.98	0.46
1:O:2831:C:O3'	20:R:71:LYS:HE2	2.15	0.46
5:B:337:GLY:N	40:B:9542:HOH:O	2.49	0.46
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.98	0.46
9:F:91:VAL:CG1	9:F:92:GLY:H	1.97	0.46
12:J:88:PRO:O	12:J:94:GLY:HA3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:62:PRO:HA	13:K:65:ARG:HH21	1.80	0.46
20:R:119:VAL:O	20:R:119:VAL:CG1	2.63	0.46
21:S:81:ILE:HG22	24:V:29:ASN:OD1	2.15	0.46
22:T:43:ASN:C	22:T:45:GLY:H	2.24	0.46
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.15	0.46
32:I:132:CYS:O	32:I:134:SER:N	2.49	0.46
1:0:189:A:OP1	15:M:171:ARG:NH2	2.48	0.46
1:0:289:G:N1	1:0:363:A:C2	2.73	0.46
1:0:601:G:O2'	1:0:602:A:H5'	2.16	0.46
1:0:870:G:OP2	4:A:3:ARG:HD3	2.15	0.46
1:0:1159:G:H1	1:0:1208:C:H42	1.64	0.46
1:0:1200:A:H3'	40:0:6230:HOH:O	2.15	0.46
1:0:1849:G:H1'	1:0:2011:A:N1	2.31	0.46
1:0:2300:A:H4'	1:0:2301:A:O5'	2.16	0.46
1:0:2448:U:O2'	1:0:2449:G:H5'	2.16	0.46
4:A:217:ARG:CG	4:A:217:ARG:NH1	2.78	0.46
6:C:57:PRO:O	6:C:58:ALA:C	2.58	0.46
20:R:29:LYS:NZ	40:R:9451:HOH:O	2.39	0.46
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.97	0.46
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.51	0.46
1:0:10:U:O4	1:0:532:A:OP2	2.33	0.46
1:0:328:U:O4'	6:C:202:THR:HG22	2.15	0.46
1:0:820:G:C5	4:A:171:LYS:HB2	2.50	0.46
1:0:1056:U:H2'	1:0:1057:A:O4'	2.15	0.46
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.15	0.46
1:0:1634:G:H2'	1:0:1635:U:C6	2.51	0.46
1:0:1755:A:H2'	1:0:1756:G:O4'	2.16	0.46
1:0:1829:A:C8	1:0:1885:A:C8	3.04	0.46
1:0:2064:U:H5'	1:0:2652:U:O3'	2.16	0.46
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.16	0.46
1:0:2866:U:C4	23:U:50:GLU:HB3	2.51	0.46
40:0:9643:HOH:O	14:L:30:ARG:HD2	2.14	0.46
5:B:139:ASP:CB	5:B:165:ARG:HE	2.29	0.46
16:N:36:ALA:O	16:N:37:ARG:HD2	2.15	0.46
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.51	0.46
20:R:47:LEU:O	20:R:51:ILE:HG13	2.15	0.46
24:V:1:THR:CG2	24:V:2:VAL:H	2.13	0.46
1:0:1130:U:H2'	1:0:1131:G:O4'	2.15	0.46
1:0:1504:A:H5'	40:0:4945:HOH:O	2.15	0.46
1:0:1789:G:O6	18:P:73:HIS:HE1	1.99	0.46
4:A:94:LEU:HD12	4:A:98:GLU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:41:PHE:HB3	5:B:190:MET:CE	2.46	0.46
7:D:35:ALA:C	7:D:37:ALA:H	2.23	0.46
11:H:79:GLU:O	11:H:80:GLU:HG3	2.16	0.46
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.97	0.46
27:Y:203:VAL:HG12	27:Y:228:VAL:HG22	1.97	0.46
30:2:5:LYS:O	30:2:9:LYS:HG3	2.15	0.46
31:3:55:VAL:HG23	40:3:9457:HOH:O	2.15	0.46
31:3:73:GLU:HB2	40:3:9462:HOH:O	2.15	0.46
1:0:292:G:H2'	1:0:358:G:N2	2.32	0.45
1:0:1182:C:C1'	1:0:1192:A:H8	2.28	0.45
1:0:1299:G:N7	14:L:6:ARG:NH1	2.64	0.45
2:9:3042:C:O2	7:D:76:ARG:NH1	2.49	0.45
4:A:93:THR:C	4:A:94:LEU:HD23	2.40	0.45
5:B:53:LEU:CD1	5:B:327:VAL:HG22	2.45	0.45
7:D:136:ARG:HB3	7:D:137:PRO:HD2	1.97	0.45
7:D:170:TYR:O	7:D:171:ASP:CB	2.64	0.45
13:K:4:LEU:CD2	13:K:116:GLU:HB3	2.44	0.45
15:M:64:ARG:HD2	40:M:9388:HOH:O	2.16	0.45
15:M:125:ARG:HE	15:M:126:GLN:HE21	1.64	0.45
1:0:875:A:C2	4:A:194:MET:SD	3.09	0.45
1:0:920:C:H4'	1:0:921:G:N2	2.31	0.45
1:0:920:C:H5''	1:0:921:G:O5'	2.16	0.45
1:0:1042:U:O2'	1:0:1043:C:H5'	2.16	0.45
1:0:1819:G:H2'	1:0:1820:G:C5'	2.46	0.45
1:0:2769:C:H2'	1:0:2770:G:O4'	2.16	0.45
7:D:154:LYS:H	7:D:154:LYS:CD	2.27	0.45
11:H:18:GLU:HG3	11:H:19:TYR:CE1	2.51	0.45
14:L:35:ARG:NH1	14:L:43:HIS:CD2	2.83	0.45
15:M:49:ALA:C	15:M:54:TYR:HB3	2.41	0.45
16:N:59:ALA:O	16:N:60:SER:HB3	2.16	0.45
25:W:38:THR:CG2	25:W:39:ASP:N	2.78	0.45
30:2:14:LEU:HD13	30:2:47:THR:HG21	1.98	0.45
31:3:20:HIS:HA	31:3:70:ARG:O	2.16	0.45
1:0:97:G:N1	22:T:107:LYS:HD2	2.31	0.45
1:0:1438:G:N7	1:0:1684:A:O2'	2.46	0.45
4:A:81:GLN:CB	4:A:92:ASN:ND2	2.79	0.45
6:C:7:ASP:O	6:C:9:ASP:N	2.49	0.45
6:C:51:TYR:CE2	29:1:53:LYS:HB3	2.51	0.45
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.97	0.45
16:N:183:ASP:O	16:N:184:ILE:C	2.58	0.45
17:O:49:GLU:OE1	17:O:72:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:561:G:O2'	1:0:562:A:H5'	2.16	0.45
1:0:1427:A:H61	1:0:1440:U:H1'	1.81	0.45
1:0:1574:C:O5'	1:0:1574:C:H6	1.99	0.45
1:0:2283:G:C6	11:H:113:MET:HB3	2.52	0.45
1:0:2672:C:O2'	1:0:2673:U:H5'	2.17	0.45
1:0:2852:A:H5''	40:0:5736:HOH:O	2.16	0.45
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.17	0.45
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.76	0.45
14:L:97:VAL:HG12	14:L:98:GLU:O	2.16	0.45
15:M:59:GLY:C	15:M:141:ILE:HD11	2.40	0.45
22:T:73:HIS:HD2	22:T:88:PRO:HG3	1.81	0.45
26:X:70:ILE:HG23	26:X:70:ILE:O	2.17	0.45
28:Z:14:PHE:HE1	28:Z:26:VAL:HG21	1.81	0.45
31:3:5:ARG:HG3	31:3:6:ARG:HG3	1.99	0.45
1:0:352:A:H2'	1:0:353:G:C8	2.51	0.45
1:0:541:C:H2'	1:0:542:A:H5'	1.99	0.45
1:0:1400:C:H4'	26:X:56:GLU:HG2	1.98	0.45
1:0:1701:A:H5''	1:0:1702:U:H3'	1.98	0.45
1:0:2716:G:H5''	5:B:206:THR:CG2	2.41	0.45
1:0:2716:G:C5'	5:B:206:THR:HG21	2.42	0.45
2:9:3029:C:H2'	2:9:3030:C:C5'	2.43	0.45
6:C:46:TYR:HE2	6:C:98:ARG:HH12	1.55	0.45
12:J:13:ASP:OD1	12:J:15:ARG:HB3	2.17	0.45
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.46	0.45
15:M:123:ASP:OD1	15:M:123:ASP:C	2.59	0.45
17:O:32:ARG:HB2	40:O:4656:HOH:O	2.16	0.45
18:P:59:ARG:HH22	18:P:66:GLN:NE2	2.04	0.45
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.79	0.45
25:W:29:VAL:O	25:W:30:ASN:HB2	2.16	0.45
1:0:1342:C:O2'	1:0:1343:C:H5'	2.17	0.45
8:E:145:ALA:HB1	8:E:168:ILE:HD11	1.98	0.45
8:E:154:ILE:CD1	8:E:157:LYS:HE2	2.47	0.45
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.98	0.45
23:U:52:THR:HG22	23:U:54:THR:HB	1.98	0.45
30:2:41:HIS:HB3	30:2:44:ARG:HB2	1.98	0.45
1:0:666:A:H2'	1:0:667:C:O4'	2.17	0.45
1:0:2435:U:H1'	40:0:5923:HOH:O	2.17	0.45
1:0:2880:A:H2'	1:0:2881:C:H5'	1.99	0.45
40:0:3526:HOH:O	6:C:78:ARG:HD3	2.16	0.45
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.44	0.45
4:A:113:GLY:HA2	4:A:153:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:C:9175:HOH:O	22:T:2:LYS:HE2	2.16	0.45
7:D:105:SER:HB2	7:D:131:THR:HG23	1.98	0.45
16:N:166:ALA:O	16:N:167:ASP:O	2.35	0.45
17:O:81:PHE:N	17:O:81:PHE:CD1	2.85	0.45
20:R:92:LEU:HD23	20:R:145:LEU:HD21	1.97	0.45
1:0:37:A:C2	1:0:446:G:C2	3.05	0.45
1:0:1495:C:H2'	1:0:1496:G:C8	2.52	0.45
1:0:1871:U:O4'	1:0:1873:G:C8	2.70	0.45
1:0:2608:C:H3'	40:0:8217:HOH:O	2.16	0.45
1:0:2672:C:P	5:B:25:ARG:NH1	2.90	0.45
40:0:3136:HOH:O	18:P:81:LYS:HG2	2.17	0.45
4:A:35:GLY:O	4:A:36:ASP:HB2	2.15	0.45
4:A:217:ARG:HH11	4:A:217:ARG:HG3	1.82	0.45
5:B:146:THR:C	5:B:148:PRO:HD3	2.41	0.45
7:D:170:TYR:CD1	7:D:170:TYR:N	2.85	0.45
11:H:56:GLN:NE2	11:H:126:ARG:HE	2.14	0.45
14:L:104:ASP:O	14:L:105:TYR:HB3	2.17	0.45
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.99	0.45
1:0:541:C:C2'	1:0:542:A:C5'	2.83	0.45
1:0:764:C:H2'	1:0:765:G:O4'	2.17	0.45
1:0:907:A:H2'	1:0:908:A:C8	2.52	0.45
1:0:1421:C:O2'	1:0:1422:U:H5'	2.17	0.45
1:0:2785:C:H4'	1:0:2786:G:OP2	2.17	0.45
40:0:6724:HOH:O	27:Y:158:LYS:HD3	2.16	0.45
4:A:54:PRO:HG2	4:A:160:ALA:HB3	1.99	0.45
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.99	0.45
16:N:67:ALA:C	16:N:69:TYR:H	2.24	0.45
16:N:168:LEU:HA	16:N:169:PRO:HD3	1.84	0.45
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.81	0.45
26:X:23:HIS:O	26:X:63:ARG:HD3	2.16	0.45
26:X:27:ASP:OD2	26:X:27:ASP:N	2.49	0.45
29:1:28:HIS:HD2	29:1:30:LYS:H	1.64	0.45
1:0:432:G:H2'	1:0:433:C:H6	1.82	0.45
1:0:806:A:H2'	1:0:807:A:O4'	2.17	0.45
1:0:1014:A:H2'	1:0:1015:C:H5'	1.98	0.45
1:0:1086:A:N6	25:W:11:VAL:HG11	2.32	0.45
1:0:1119:G:H8	12:J:52:GLN:HE22	1.65	0.45
1:0:2323:G:H5'	40:0:7402:HOH:O	2.17	0.45
40:0:5790:HOH:O	25:W:119:HIS:CG	2.70	0.45
40:9:466:HOH:O	19:Q:25:PRO:HB3	2.17	0.45
4:A:192:VAL:HB	40:A:9627:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.47	0.45
5:B:205:VAL:O	5:B:307:ARG:NE	2.49	0.45
9:F:26:THR:HG21	9:F:102:GLY:C	2.41	0.45
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.54	0.45
16:N:175:LEU:O	16:N:179:LEU:HG	2.17	0.45
32:I:75:THR:O	32:I:76:ALA:C	2.60	0.45
1:O:661:G:C5	1:O:686:A:C2	3.05	0.44
1:O:734:U:H1'	1:O:737:A:N6	2.32	0.44
1:O:877:G:C2	1:O:885:G:O4'	2.70	0.44
1:O:960:G:N3	1:O:960:G:C2'	2.80	0.44
1:O:1007:A:H2'	11:H:19:TYR:CZ	2.52	0.44
1:O:1185:U:H2'	1:O:1186:C:C6	2.51	0.44
1:O:1218:U:H2'	1:O:1219:U:H6	1.80	0.44
1:O:1819:G:H2'	1:O:1820:G:C4'	2.47	0.44
1:O:1942:A:H2'	1:O:1943:C:H6	1.81	0.44
40:O:5790:HOH:O	25:W:122:ARG:NH2	2.51	0.44
4:A:81:GLN:HG3	4:A:92:ASN:HD21	1.83	0.44
5:B:41:PHE:HA	5:B:79:MET:HE1	1.98	0.44
5:B:195:ARG:O	5:B:196:ALA:C	2.59	0.44
9:F:101:ALA:HA	40:F:5413:HOH:O	2.17	0.44
14:L:128:GLY:O	14:L:132:LYS:HG3	2.16	0.44
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.48	0.44
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.47	0.44
23:U:49:LEU:HG	40:U:3805:HOH:O	2.16	0.44
31:3:14:CYS:HB3	31:3:16:GLU:HG2	2.00	0.44
32:I:113:HIS:CE1	32:I:121:LEU:HD22	2.48	0.44
1:O:750:A:O3'	6:C:101:ASP:HB2	2.17	0.44
1:O:1093:G:H2'	1:O:1094:G:O4'	2.18	0.44
40:O:5905:HOH:O	4:A:164:ARG:CZ	2.65	0.44
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.82	0.44
13:K:74:VAL:O	13:K:74:VAL:HG12	2.15	0.44
16:N:64:SER:C	16:N:66:LEU:H	2.25	0.44
16:N:154:LEU:O	16:N:155:GLU:HB2	2.16	0.44
23:U:52:THR:HG21	23:U:54:THR:HB	1.99	0.44
25:W:131:PRO:O	25:W:136:GLY:N	2.46	0.44
27:Y:152:LYS:HB3	27:Y:160:LYS:HG3	2.00	0.44
1:O:1180:U:H2'	1:O:1181:A:C8	2.52	0.44
1:O:1331:A:OP2	27:Y:142:SER:OG	2.28	0.44
1:O:1419:U:H2'	1:O:1685:A:C2	2.52	0.44
40:O:5254:HOH:O	16:N:21:HIS:HD2	2.00	0.44
4:A:217:ARG:HG2	4:A:229:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.98	0.44
5:B:175:LEU:C	5:B:175:LEU:CD2	2.91	0.44
6:C:72:LYS:HE3	40:C:9107:HOH:O	2.17	0.44
7:D:22:VAL:HA	7:D:73:VAL:O	2.17	0.44
8:E:34:TRP:O	12:J:127:ILE:HD11	2.16	0.44
11:H:46:GLN:HG3	11:H:137:TYR:CD2	2.52	0.44
11:H:114:ARG:O	11:H:115:ALA:C	2.60	0.44
16:N:11:ARG:O	16:N:15:GLU:HG3	2.17	0.44
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.32	0.44
29:1:28:HIS:O	29:1:32:LYS:N	2.44	0.44
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.82	0.44
1:0:963:C:H2'	1:0:964:G:C8	2.53	0.44
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.17	0.44
4:A:36:ASP:HB2	4:A:85:SER:H	1.81	0.44
5:B:58:PRO:HA	5:B:63:GLU:OE2	2.16	0.44
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.47	0.44
8:E:13:ALA:O	8:E:42:VAL:HG11	2.18	0.44
9:F:28:ALA:CB	9:F:99:THR:HG23	2.47	0.44
15:M:74:LYS:HG2	15:M:75:ARG:N	2.32	0.44
21:S:51:GLN:NE2	21:S:53:ASN:HD21	2.16	0.44
25:W:92:ASP:N	25:W:92:ASP:OD1	2.51	0.44
1:0:251:C:H2'	1:0:252:C:H6	1.82	0.44
1:0:308:U:H5'	22:T:97:ARG:NH2	2.33	0.44
1:0:1098:A:H2'	1:0:1099:G:O4'	2.17	0.44
1:0:2470:A:H5''	40:0:3808:HOH:O	2.16	0.44
4:A:163:GLY:HA2	4:A:166:ASP:OD2	2.17	0.44
5:B:109:LEU:HD11	5:B:113:LEU:HD11	1.99	0.44
5:B:138:GLY:O	5:B:139:ASP:C	2.59	0.44
6:C:54:LEU:O	29:1:53:LYS:HE3	2.17	0.44
7:D:76:ARG:O	7:D:77:ASP:HB2	2.18	0.44
11:H:29:ALA:C	11:H:30:GLN:HG3	2.43	0.44
14:L:143:THR:CG2	14:L:144:ASP:N	2.79	0.44
15:M:61:ILE:HD12	15:M:61:ILE:N	2.32	0.44
16:N:103:ASP:C	16:N:103:ASP:OD1	2.60	0.44
17:O:25:VAL:HG23	17:O:26:TRP:N	2.33	0.44
20:R:144:GLU:HB3	40:R:9460:HOH:O	2.17	0.44
29:1:10:LYS:N	40:1:9489:HOH:O	2.48	0.44
1:0:245:C:H2'	1:0:246:G:H5'	2.00	0.44
1:0:625:U:H5''	1:0:1044:C:H41	1.81	0.44
1:0:694:A:H2'	1:0:695:C:H5'	1.99	0.44
1:0:1298:U:H2'	1:0:1299:G:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2241:C:O2'	1:0:2242:U:H5'	2.18	0.44
2:9:3059:C:H2'	2:9:3060:C:C6	2.53	0.44
5:B:277:GLU:N	5:B:278:PRO:CD	2.81	0.44
5:B:320:GLN:HE21	5:B:321:PRO:CD	2.31	0.44
6:C:138:VAL:O	6:C:234:VAL:HA	2.17	0.44
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.53	0.44
11:H:1:LYS:HA	11:H:2:PRO:HD3	1.84	0.44
14:L:89:PHE:CD1	14:L:89:PHE:N	2.86	0.44
15:M:125:ARG:HE	15:M:126:GLN:NE2	2.16	0.44
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.47	0.44
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.99	0.44
17:O:26:TRP:N	40:O:3062:HOH:O	2.51	0.44
17:O:44:ASN:OD1	17:O:67:SER:HB2	2.17	0.44
22:T:18:GLU:O	22:T:21:LYS:HG2	2.17	0.44
25:W:65:VAL:CG1	25:W:116:LEU:HD13	2.47	0.44
31:3:65:THR:HG23	31:3:88:LEU:HD22	1.99	0.44
1:0:392:U:C5'	15:M:193:LYS:HB3	2.48	0.44
1:0:1025:C:H5'	25:W:23:MET:O	2.17	0.44
1:0:1180:U:H2'	1:0:1181:A:O4'	2.18	0.44
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.47	0.44
1:0:1486:A:C4	30:2:2:LYS:HG3	2.53	0.44
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.17	0.44
1:0:1942:A:H2'	1:0:1943:C:C6	2.53	0.44
1:0:2100:A:H4'	6:C:64:GLY:O	2.18	0.44
4:A:36:ASP:O	4:A:36:ASP:CG	2.59	0.44
4:A:48:ASP:HA	4:A:49:PRO:HD3	1.84	0.44
5:B:60:SER:HA	5:B:61:PRO:HD3	1.86	0.44
5:B:102:THR:HB	40:B:9627:HOH:O	2.17	0.44
6:C:130:GLU:O	6:C:164:ALA:HB3	2.18	0.44
7:D:35:ALA:C	7:D:37:ALA:N	2.74	0.44
9:F:58:GLU:HB3	15:M:8:ILE:HG23	1.99	0.44
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.99	0.44
13:K:98:VAL:HG11	13:K:102:GLU:HA	2.00	0.44
15:M:46:LEU:HG	40:M:9422:HOH:O	2.18	0.44
15:M:73:ARG:HD2	15:M:73:ARG:N	2.33	0.44
22:T:71:VAL:CG1	22:T:72:ILE:N	2.80	0.44
22:T:80:GLU:HG2	40:T:2885:HOH:O	2.17	0.44
24:V:39:ALA:O	24:V:41:GLU:N	2.44	0.44
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.18	0.44
27:Y:96:GLU:O	27:Y:235:GLU:HA	2.18	0.44
27:Y:109:LEU:HA	40:Y:9369:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:634:G:O2'	1:0:1358:A:OP1	2.34	0.44
1:0:820:G:H5'	1:0:821:U:H5'	1.98	0.44
1:0:1883:U:H5'	1:0:2012:U:OP2	2.17	0.44
4:A:43:VAL:HG21	4:A:59:GLU:CG	2.47	0.44
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.44
5:B:168:GLY:O	5:B:169:GLY:O	2.36	0.44
5:B:221:GLN:HE22	13:K:42:ASN:ND2	2.14	0.44
7:D:75:LEU:HD13	7:D:79:MET:O	2.18	0.44
9:F:117:GLU:C	9:F:119:ARG:H	2.25	0.44
11:H:66:ARG:HD3	40:H:9551:HOH:O	2.18	0.44
30:2:19:SER:HB3	40:2:4479:HOH:O	2.18	0.44
1:0:36:C:C2	1:0:447:A:C2	3.06	0.44
1:0:177:A:H2'	1:0:178:U:O4'	2.18	0.44
1:0:1739:G:O2'	1:0:1740:U:H5'	2.18	0.44
1:0:2505:G:C2'	1:0:2506:A:H5'	2.48	0.44
1:0:2911:C:O2'	1:0:2912:C:H5'	2.18	0.44
40:0:7267:HOH:O	15:M:178:LYS:HB2	2.18	0.44
2:9:3031:C:H2'	2:9:3032:G:O4'	2.18	0.44
2:9:3091:C:H2'	2:9:3092:G:O4'	2.17	0.44
5:B:260:HIS:HE1	40:B:9581:HOH:O	2.00	0.44
8:E:101:GLU:OE2	8:E:115:ARG:HD3	2.18	0.44
8:E:116:THR:HG22	8:E:151:LEU:CD2	2.38	0.44
13:K:22:ASP:C	13:K:22:ASP:OD1	2.61	0.44
17:O:63:LYS:HA	17:O:80:ASP:O	2.18	0.44
23:U:20:MET:HG3	23:U:30:HIS:CD2	2.53	0.44
26:X:43:VAL:HG12	26:X:47:ALA:HB3	2.00	0.44
31:3:67:LEU:HD21	31:3:88:LEU:HD23	2.00	0.44
1:0:254:C:O2	1:0:254:C:H2'	2.17	0.43
2:9:3095:C:O2'	2:9:3096:C:H5'	2.18	0.43
4:A:41:THR:O	4:A:43:VAL:HG23	2.18	0.43
4:A:171:LYS:NZ	40:A:9557:HOH:O	2.51	0.43
5:B:55:ASN:HB3	5:B:64:GLY:H	1.83	0.43
7:D:68:PRO:C	7:D:69:ILE:HG13	2.43	0.43
8:E:84:MET:HE2	8:E:133:VAL:HG23	1.99	0.43
13:K:87:ARG:NH1	40:K:4066:HOH:O	2.51	0.43
14:L:35:ARG:HH11	14:L:35:ARG:CB	2.15	0.43
15:M:120:VAL:CG1	15:M:130:GLU:HG3	2.47	0.43
15:M:159:VAL:HG13	15:M:160:PHE:N	2.33	0.43
16:N:67:ALA:C	16:N:69:TYR:N	2.76	0.43
16:N:137:ALA:HB1	16:N:141:ARG:HD3	2.00	0.43
21:S:57:THR:CG2	21:S:58:MET:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.43	0.43
1:0:1015:C:H2'	1:0:1016:U:C6	2.53	0.43
1:0:1362:U:H2'	1:0:1363:G:C8	2.53	0.43
1:0:1503:U:H2'	1:0:1504:A:O4'	2.19	0.43
1:0:1516:C:H42	1:0:1670:G:H1	1.65	0.43
1:0:2673:U:C4	1:0:2674:G:C6	3.06	0.43
1:0:2768:A:O2'	1:0:2769:C:H5'	2.17	0.43
4:A:206:ARG:H	4:A:206:ARG:CD	2.29	0.43
5:B:113:LEU:HD21	5:B:161:VAL:HG21	2.00	0.43
14:L:21:ARG:N	40:L:9428:HOH:O	2.50	0.43
16:N:11:ARG:HA	16:N:14:ARG:CZ	2.48	0.43
16:N:77:ASN:O	16:N:80:SER:HB3	2.18	0.43
1:0:101:C:H2'	1:0:102:A:C8	2.53	0.43
1:0:288:A:H2'	1:0:289:G:H8	1.83	0.43
1:0:407:A:O2'	1:0:408:A:H5'	2.18	0.43
1:0:766:A:H5'	40:0:5178:HOH:O	2.18	0.43
1:0:790:A:H1'	1:0:1710:A:O2'	2.18	0.43
1:0:1166:A:N6	1:0:1180:U:H3	2.08	0.43
1:0:1391:G:H2'	1:0:1392:A:H5'	2.01	0.43
1:0:1527:A:H1'	1:0:1528:A:C8	2.54	0.43
1:0:2453:G:H5'	40:0:5219:HOH:O	2.18	0.43
4:A:42:VAL:O	4:A:76:VAL:HG13	2.17	0.43
9:F:68:ASP:C	9:F:70:LYS:H	2.26	0.43
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.80	0.43
14:L:53:ARG:HH22	14:L:57:VAL:HG12	1.79	0.43
16:N:61:ALA:HA	16:N:91:ARG:NH1	2.34	0.43
22:T:1:SER:O	22:T:7:GLN:NE2	2.51	0.43
1:0:289:G:H1	1:0:363:A:H2	1.56	0.43
1:0:347:A:H2'	1:0:348:C:O4'	2.19	0.43
1:0:449:A:N7	6:C:43:LYS:HG2	2.33	0.43
1:0:926:A:H5'	14:L:39:GLU:OE2	2.18	0.43
1:0:1025:C:OP1	25:W:108:ARG:NH1	2.52	0.43
1:0:1669:A:H2'	1:0:1670:G:C8	2.54	0.43
1:0:2406:U:O2'	1:0:2407:G:H5'	2.19	0.43
1:0:2726:U:O2	1:0:2749:U:O5'	2.37	0.43
5:B:258:GLY:O	5:B:260:HIS:CD2	2.71	0.43
6:C:7:ASP:C	6:C:9:ASP:H	2.26	0.43
6:C:157:LEU:CD1	6:C:166:ILE:HD11	2.48	0.43
8:E:77:THR:OG1	8:E:78:GLU:N	2.49	0.43
8:E:88:TYR:CE1	8:E:92:PRO:HA	2.53	0.43
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:107:ASN:C	12:J:107:ASN:ND2	2.71	0.43
13:K:66:ARG:HD3	40:K:2777:HOH:O	2.18	0.43
21:S:56:ASN:O	30:2:8:LYS:NZ	2.46	0.43
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.52	0.43
24:V:64:GLY:O	24:V:65:ASP:OD1	2.36	0.43
32:I:119:TYR:N	32:I:119:TYR:CD1	2.85	0.43
1:0:941:G:C5	1:0:942:U:C4	3.07	0.43
1:0:1211:G:H2'	1:0:1212:C:C6	2.53	0.43
1:0:1335:C:OP2	27:Y:207:SER:HB3	2.18	0.43
1:0:1377:C:H6	1:0:1377:C:C5'	2.25	0.43
1:0:1414:A:P	30:2:1:GLY:HA2	2.58	0.43
1:0:2644:C:H6	40:0:7480:HOH:O	2.02	0.43
1:0:2712:G:H5'	40:0:5723:HOH:O	2.19	0.43
1:0:2900:G:H2'	1:0:2901:C:O4'	2.17	0.43
40:0:5197:HOH:O	5:B:300:SER:HB3	2.18	0.43
40:0:6140:HOH:O	22:T:68:ASP:HB2	2.18	0.43
4:A:95:PRO:HA	4:A:153:ARG:HA	2.01	0.43
6:C:40:ALA:O	6:C:43:LYS:HB2	2.18	0.43
9:F:91:VAL:CG1	9:F:92:GLY:N	2.65	0.43
12:J:142:ASN:O	12:J:144:THR:N	2.52	0.43
16:N:82:TYR:OH	16:N:176:ARG:NH1	2.52	0.43
21:S:43:GLU:HB3	40:S:9501:HOH:O	2.18	0.43
25:W:60:GLU:O	25:W:63:GLU:HB2	2.18	0.43
25:W:139:GLY:O	25:W:141:HIS:CD2	2.69	0.43
26:X:15:ARG:HH11	26:X:15:ARG:CB	2.32	0.43
28:Z:57:CYS:C	28:Z:59:TYR:N	2.75	0.43
1:0:85:C:H3'	1:0:86:A:H2'	2.01	0.43
1:0:1625:U:H4'	40:0:5193:HOH:O	2.18	0.43
1:0:1717:A:H5''	18:P:54:LYS:HB2	2.01	0.43
1:0:2765:C:H4'	40:0:6006:HOH:O	2.18	0.43
2:9:3007:G:H4'	16:N:55:ASP:OD2	2.19	0.43
7:D:60:GLU:O	7:D:61:PHE:C	2.60	0.43
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.33	0.43
15:M:47:ASP:CG	15:M:48:LYS:N	2.76	0.43
27:Y:189:ASN:C	27:Y:189:ASN:ND2	2.76	0.43
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.33	0.43
1:0:271:C:N4	1:0:378:A:H2	2.17	0.43
1:0:353:G:O2'	1:0:354:A:H5'	2.18	0.43
1:0:1135:G:H5'	40:0:6389:HOH:O	2.18	0.43
1:0:1427:A:H61	1:0:1440:U:C1'	2.32	0.43
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2338:G:OP1	7:D:97:GLN:HG2	2.18	0.43
1:O:2506:A:O2'	1:O:2507:G:C8	2.48	0.43
1:O:2634:G:OP2	4:A:204:GLY:N	2.48	0.43
1:O:2713:G:O2'	1:O:2714:U:H5'	2.19	0.43
40:O:4941:HOH:O	4:A:11:ARG:CZ	2.65	0.43
5:B:41:PHE:HA	5:B:79:MET:CE	2.49	0.43
6:C:57:PRO:HG2	6:C:73:LEU:CD1	2.49	0.43
6:C:162:VAL:HG13	6:C:192:ILE:CD1	2.48	0.43
7:D:12:GLU:HA	7:D:15:GLU:OE1	2.19	0.43
7:D:151:ILE:CG2	7:D:155:HIS:HB3	2.49	0.43
9:F:32:GLY:N	40:F:3111:HOH:O	2.51	0.43
10:G:12:ILE:HG22	10:G:17:GLN:HE21	1.83	0.43
16:N:32:PRO:HD2	16:N:99:GLU:O	2.19	0.43
17:O:49:GLU:O	17:O:72:LYS:HE3	2.19	0.43
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.84	0.43
1:O:208:C:C2	1:O:232:A:C2	3.07	0.43
1:O:1014:A:H5''	2:9:3101:G:O2'	2.19	0.43
1:O:1209:C:H2'	1:O:1210:G:C8	2.53	0.43
1:O:1279:U:O2	1:O:1279:U:H2'	2.18	0.43
1:O:1926:G:H2'	1:O:1927:A:H8	1.82	0.43
1:O:2361:A:H2'	1:O:2362:A:C8	2.53	0.43
1:O:2524:G:N2	1:O:2526:C:H41	2.17	0.43
1:O:2545:U:OP2	5:B:2:GLN:NE2	2.52	0.43
1:O:2577:A:H5'	40:O:8161:HOH:O	2.19	0.43
2:9:3001:U:O3'	2:9:3003:A:H5''	2.19	0.43
4:A:37:VAL:HG22	40:A:9631:HOH:O	2.19	0.43
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.46	0.43
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.84	0.43
5:B:278:PRO:HD3	5:B:294:TYR:CE2	2.54	0.43
8:E:162:PHE:N	8:E:162:PHE:CD1	2.86	0.43
11:H:77:LEU:HD12	11:H:83:TYR:HD2	1.83	0.43
13:K:6:ALA:HB1	13:K:81:ARG:O	2.19	0.43
18:P:115:SER:O	18:P:116:SER:C	2.60	0.43
21:S:81:ILE:HG23	40:S:9492:HOH:O	2.18	0.43
22:T:53:GLY:HA3	40:T:6384:HOH:O	2.18	0.43
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.19	0.43
1:O:82:C:OP1	22:T:67:LEU:HB2	2.19	0.43
1:O:170:U:H2'	1:O:171:C:H5'	2.01	0.43
1:O:1310:U:OP2	6:C:168:ARG:NH1	2.51	0.43
1:O:1446:U:H2'	21:S:55:GLN:NE2	2.34	0.43
1:O:1985:U:C2	1:O:1996:U:O4'	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:133:ARG:HG2	6:C:134:ASP:H	1.83	0.43
13:K:10:GLN:N	13:K:10:GLN:NE2	2.42	0.43
13:K:13:GLU:OE1	13:K:44:LEU:HD12	2.19	0.43
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.49	0.43
18:P:63:ARG:NH2	40:P:194:HOH:O	2.49	0.43
24:V:56:ILE:O	24:V:60:GLN:HG3	2.19	0.43
28:Z:33:MET:HG3	28:Z:69:TYR:O	2.18	0.43
1:0:1211:G:O2'	1:0:1212:C:H5'	2.19	0.43
1:0:1238:C:H5'	1:0:1239:G:OP2	2.18	0.43
1:0:1473:U:C1'	29:1:42:SER:HB3	2.49	0.43
1:0:2011:A:H5'	1:0:2013:G:C1'	2.48	0.43
1:0:2415:A:C2	16:N:25:ARG:HB3	2.54	0.43
1:0:2722:G:H4'	40:K:5029:HOH:O	2.18	0.43
1:0:2780:C:C1'	8:E:143:GLN:HE21	2.28	0.43
1:0:2783:A:H3'	40:0:5734:HOH:O	2.19	0.43
2:9:3059:C:H6	2:9:3059:C:O5'	2.01	0.43
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.54	0.43
16:N:26:LEU:HD12	16:N:101:VAL:CG1	2.48	0.43
16:N:151:ASP:OD1	16:N:166:ALA:HA	2.19	0.43
24:V:42:ASN:C	24:V:44:GLY:H	2.27	0.43
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.33	0.43
31:3:55:VAL:HB	31:3:56:PRO:HD2	2.00	0.43
1:0:2402:A:O2'	1:0:2403:C:H5'	2.19	0.42
1:0:2506:A:O2'	1:0:2507:G:O5'	2.37	0.42
6:C:187:ARG:NH2	40:C:9173:HOH:O	2.52	0.42
11:H:18:GLU:H	11:H:18:GLU:HG2	1.58	0.42
14:L:121:ILE:HG12	14:L:141:GLU:HB2	2.01	0.42
16:N:149:GLU:HA	16:N:152:GLU:HB2	2.01	0.42
20:R:39:THR:O	20:R:40:ALA:C	2.61	0.42
22:T:64:ASN:HB3	22:T:73:HIS:HB2	2.00	0.42
25:W:88:THR:C	25:W:90:TYR:H	2.26	0.42
30:2:48:ASP:O	30:2:49:GLU:CB	2.67	0.42
1:0:1081:A:H5''	40:0:3720:HOH:O	2.18	0.42
1:0:1815:A:H4'	1:0:2751:C:O4'	2.18	0.42
1:0:2251:G:H2'	1:0:2252:A:C8	2.54	0.42
1:0:2274:A:O2'	1:0:2275:G:H5'	2.19	0.42
1:0:2353:A:O2'	16:N:7:LYS:HB3	2.18	0.42
1:0:2456:A:H2'	1:0:2457:U:C6	2.54	0.42
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.83	0.42
4:A:1:GLY:HA2	4:A:197:VAL:HG23	2.01	0.42
5:B:41:PHE:CD1	5:B:79:MET:CE	3.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:214:PRO:HB2	5:B:220:VAL:HG21	2.00	0.42
8:E:81:GLU:HA	8:E:133:VAL:O	2.19	0.42
8:E:102:VAL:HG11	8:E:148:ILE:CD1	2.48	0.42
9:F:99:THR:O	9:F:99:THR:HG23	2.19	0.42
11:H:33:MET:HE1	11:H:66:ARG:HG3	2.02	0.42
1:0:553:G:OP2	27:Y:204:ARG:NH2	2.51	0.42
1:0:1537:C:H1'	40:0:7007:HOH:O	2.18	0.42
1:0:1855:G:H4'	1:0:1856:C:O5'	2.19	0.42
1:0:2296:C:H2'	1:0:2297:U:C6	2.53	0.42
1:0:2817:G:P	40:0:8334:HOH:O	2.77	0.42
4:A:89:ALA:HB3	40:A:9662:HOH:O	2.18	0.42
5:B:29:TRP:CZ3	5:B:164:THR:HG23	2.55	0.42
7:D:128:LEU:C	7:D:128:LEU:HD23	2.44	0.42
8:E:15:GLN:NE2	8:E:40:VAL:O	2.51	0.42
11:H:27:LYS:H	11:H:59:HIS:CD2	2.31	0.42
11:H:46:GLN:HG3	11:H:137:TYR:CE2	2.54	0.42
14:L:94:ARG:HG2	14:L:106:VAL:HG21	2.00	0.42
15:M:77:HIS:CE1	15:M:86:GLN:HG2	2.53	0.42
20:R:39:THR:HG22	20:R:41:GLY:N	2.34	0.42
25:W:125:HIS:HB2	25:W:137:GLN:OE1	2.19	0.42
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.48	0.42
1:0:64:G:H2'	1:0:65:C:O4'	2.20	0.42
1:0:639:A:C6	1:0:640:G:C6	3.08	0.42
1:0:1305:C:H5'	40:0:3410:HOH:O	2.18	0.42
1:0:1666:C:C2'	1:0:1667:A:H5''	2.49	0.42
1:0:2346:C:H6	1:0:2346:C:O5'	2.02	0.42
1:0:2727:A:C6	1:0:2756:U:C2	3.07	0.42
1:0:2729:C:O2'	1:0:2730:G:H5'	2.20	0.42
1:0:2837:U:H2'	40:0:7233:HOH:O	2.20	0.42
7:D:66:GLY:O	7:D:67:ASP:HB3	2.17	0.42
7:D:173:GLU:HG3	7:D:174:VAL:H	1.83	0.42
8:E:170:ARG:HE	8:E:170:ARG:HB2	1.60	0.42
14:L:35:ARG:NE	14:L:46:LEU:HD21	2.34	0.42
16:N:179:LEU:HD23	16:N:184:ILE:HD12	2.01	0.42
19:Q:61:GLY:HA2	40:Q:6286:HOH:O	2.19	0.42
22:T:73:HIS:CD2	22:T:88:PRO:CG	3.03	0.42
25:W:122:ARG:NH1	25:W:152:ALA:O	2.52	0.42
26:X:74:ALA:CB	26:X:85:VAL:HG13	2.46	0.42
1:0:240:C:OP2	1:0:270:U:H5	2.02	0.42
1:0:664:U:O4	1:0:681:G:H5''	2.19	0.42
1:0:1184:C:O2'	1:0:1185:U:OP2	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1241:G:C2	12:J:86:MET:HE2	2.54	0.42
1:0:1545:C:H2'	1:0:1546:G:O4'	2.20	0.42
1:0:1890:U:H4'	1:0:2010:A:C6	2.55	0.42
1:0:2112:A:H2'	1:0:2113:G:H8	1.84	0.42
1:0:2816:A:H5''	1:0:2817:G:H5'	2.02	0.42
4:A:27:LEU:HD13	4:A:69:LEU:HA	2.00	0.42
4:A:36:ASP:C	4:A:38:ILE:N	2.77	0.42
5:B:139:ASP:HB2	5:B:165:ARG:NE	2.35	0.42
6:C:123:LEU:HA	6:C:123:LEU:HD23	1.84	0.42
12:J:78:ILE:HG21	12:J:132:LEU:HD21	2.01	0.42
12:J:132:LEU:HD23	12:J:132:LEU:HA	1.88	0.42
14:L:144:ASP:O	14:L:147:GLU:HB2	2.20	0.42
22:T:102:ASP:OD1	22:T:102:ASP:C	2.62	0.42
31:3:70:ARG:HH11	31:3:77:ALA:HB2	1.82	0.42
1:0:612:U:H2'	1:0:613:C:C6	2.55	0.42
1:0:779:U:H5'	1:0:1836:A:C2	2.55	0.42
1:0:1805:G:O2'	1:0:1806:G:H5'	2.20	0.42
1:0:2388:C:H5'	19:Q:83:THR:O	2.20	0.42
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.52	0.42
1:0:2697:A:H2'	1:0:2698:G:O4'	2.19	0.42
4:A:56:ALA:O	4:A:68:ILE:HG22	2.19	0.42
4:A:58:VAL:HG21	4:A:80:LEU:HD12	2.02	0.42
4:A:203:GLY:CA	40:A:9581:HOH:O	2.63	0.42
5:B:71:VAL:HG11	5:B:296:LEU:HD22	2.01	0.42
7:D:94:ALA:HA	7:D:174:VAL:O	2.19	0.42
16:N:66:LEU:HG	16:N:175:LEU:HD21	2.01	0.42
16:N:171:HIS:CE1	40:N:9364:HOH:O	2.71	0.42
25:W:125:HIS:CD2	25:W:127:GLY:H	2.17	0.42
1:0:23:G:C6	1:0:24:G:N1	2.88	0.42
1:0:490:C:O2'	1:0:491:C:H5'	2.20	0.42
1:0:1076:G:C2	1:0:1084:C:C2	3.08	0.42
1:0:1477:C:H2'	1:0:1478:U:O4'	2.20	0.42
1:0:1864:C:H2'	1:0:1865:A:O4'	2.19	0.42
40:0:4008:HOH:O	4:A:5:GLN:HB2	2.18	0.42
4:A:3:ARG:H	4:A:3:ARG:HG2	1.55	0.42
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.68	0.42
12:J:77:GLY:O	12:J:78:ILE:C	2.62	0.42
24:V:19:GLU:OE1	24:V:19:GLU:HA	2.19	0.42
25:W:65:VAL:HA	25:W:68:THR:CG2	2.49	0.42
1:0:130:C:H5'	40:0:5715:HOH:O	2.19	0.42
1:0:255:A:H2'	1:0:256:C:H6	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:682:A:H2'	1:0:683:G:O4'	2.18	0.42
1:0:1588:G:C6	1:0:1589:G:N1	2.88	0.42
1:0:1816:C:H2'	1:0:1817:U:O4'	2.20	0.42
1:0:1829:A:H61	28:Z:18:TYR:N	2.18	0.42
1:0:2094:G:O6	1:0:2649:A:H2	2.03	0.42
1:0:2568:A:H5''	1:0:2702:A:O2'	2.19	0.42
1:0:2718:C:H5'	1:0:2718:C:C6	2.50	0.42
1:0:2748:G:H8	40:0:7878:HOH:O	2.03	0.42
40:0:5358:HOH:O	12:J:47:THR:HB	2.19	0.42
40:0:7512:HOH:O	29:1:1:THR:HB	2.19	0.42
3:4:76:A:H8	38:4:9701:SPS:H81	1.84	0.42
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.48	0.42
9:F:20:LEU:HD12	9:F:20:LEU:O	2.20	0.42
9:F:21:GLU:HG2	9:F:24:ARG:HH21	1.84	0.42
14:L:89:PHE:N	40:L:9474:HOH:O	2.52	0.42
19:Q:47:VAL:HA	19:Q:48:PRO:HD3	1.83	0.42
25:W:5:VAL:C	25:W:52:VAL:HG23	2.45	0.42
32:I:92:PRO:C	32:I:94:GLU:N	2.74	0.42
1:0:29:C:C2'	1:0:30:U:H5'	2.49	0.42
1:0:196:G:H1'	1:0:198:A:N7	2.35	0.42
1:0:506:G:N2	1:0:509:A:H5''	2.27	0.42
1:0:553:G:O4'	1:0:1325:G:H5'	2.20	0.42
1:0:2379:G:N3	1:0:2418:G:H2'	2.34	0.42
1:0:2507:G:H2'	1:0:2510:C:H42	1.85	0.42
1:0:2582:G:O3'	13:K:41:LYS:HA	2.20	0.42
5:B:175:LEU:HD23	5:B:175:LEU:C	2.44	0.42
11:H:34:GLY:HA3	11:H:84:LYS:HA	2.02	0.42
15:M:36:ALA:O	15:M:65:VAL:HA	2.19	0.42
16:N:86:LEU:HD21	16:N:180:LEU:HD12	2.02	0.42
17:O:14:LEU:HD23	17:O:102:ILE:HD11	2.00	0.42
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.26	0.42
28:Z:29:ILE:HA	40:Z:9225:HOH:O	2.19	0.42
28:Z:39:CYS:HA	28:Z:40:PRO:HD3	1.89	0.42
1:0:31:C:OP2	22:T:8:ARG:NH1	2.52	0.42
1:0:396:U:C2	31:3:38:ARG:NH1	2.87	0.42
1:0:697:G:H4'	1:0:730:G:O3'	2.19	0.42
1:0:963:C:O2	1:0:1005:A:N1	2.53	0.42
1:0:1293:U:H5'	27:Y:154:ARG:HH21	1.85	0.42
1:0:1979:G:O2'	1:0:1980:U:OP1	2.36	0.42
1:0:2107:U:O2'	1:0:2108:A:H5'	2.20	0.42
1:0:2363:G:O3'	19:Q:11:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2748:G:C5'	40:0:7878:HOH:O	2.61	0.42
12:J:19:MET:HE3	12:J:132:LEU:CD1	2.49	0.42
14:L:130:ARG:O	14:L:133:VAL:N	2.53	0.42
22:T:61:GLU:HG3	40:T:3851:HOH:O	2.19	0.42
23:U:52:THR:HG22	23:U:54:THR:H	1.84	0.42
27:Y:107:PRO:HD3	27:Y:182:PHE:CE1	2.55	0.42
27:Y:133:HIS:HD2	40:Y:9381:HOH:O	2.01	0.42
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.52	0.42
1:0:93:C:H5''	24:V:1:THR:CB	2.42	0.41
1:0:228:C:H2'	1:0:229:G:H5'	2.02	0.41
1:0:526:U:H2'	1:0:527:U:C6	2.55	0.41
1:0:1380:U:O4	1:0:2748:G:O2'	2.24	0.41
1:0:1845:A:O3'	4:A:187:PRO:HB2	2.20	0.41
5:B:309:VAL:HG12	40:B:9644:HOH:O	2.20	0.41
6:C:107:ARG:HB3	6:C:107:ARG:HH11	1.84	0.41
8:E:7:ILE:HG13	8:E:8:PRO:HD2	2.01	0.41
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.55	0.41
17:O:98:LEU:O	17:O:102:ILE:HG13	2.20	0.41
18:P:18:LYS:O	18:P:21:VAL:HG13	2.20	0.41
1:0:650:C:O2'	1:0:651:U:H5'	2.20	0.41
1:0:907:A:H2'	1:0:908:A:H8	1.85	0.41
1:0:1097:A:H5''	25:W:125:HIS:CE1	2.55	0.41
1:0:1552:G:C6	1:0:1553:C:C4	3.08	0.41
1:0:2038:A:O2'	1:0:2039:A:H5'	2.19	0.41
1:0:2115:U:H2'	1:0:2116:U:C6	2.54	0.41
5:B:145:HIS:CD2	5:B:146:THR:O	2.73	0.41
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.55	0.41
7:D:28:GLY:CA	7:D:69:ILE:HG23	2.42	0.41
7:D:58:VAL:CB	7:D:62:ASP:HB3	2.47	0.41
13:K:115:ARG:HG3	13:K:116:GLU:H	1.85	0.41
18:P:103:THR:HA	18:P:106:ARG:NH2	2.35	0.41
25:W:122:ARG:HG2	25:W:122:ARG:NH1	2.31	0.41
27:Y:213:LYS:HB2	27:Y:213:LYS:HE3	1.87	0.41
1:0:282:C:O2'	1:0:283:U:C5'	2.67	0.41
1:0:1398:G:H5'	18:P:23:PHE:O	2.19	0.41
1:0:1565:C:O4'	1:0:2738:G:H1'	2.20	0.41
1:0:2032:U:C2'	1:0:2033:G:C5'	2.95	0.41
1:0:2820:A:H2'	1:0:2821:C:C6	2.54	0.41
1:0:2908:A:C2'	1:0:2909:G:H5'	2.50	0.41
2:9:3005:G:OP1	16:N:17:ARG:NH2	2.53	0.41
4:A:33:GLU:O	4:A:34:ASP:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:34:ASN:O	9:F:37:THR:HB	2.20	0.41
11:H:28:ILE:HG23	40:H:9551:HOH:O	2.19	0.41
11:H:154:TYR:C	11:H:154:TYR:HD1	2.28	0.41
17:O:59:VAL:CG2	17:O:111:VAL:CG2	2.98	0.41
17:O:106:PRO:HG2	17:O:107:GLU:OE2	2.20	0.41
25:W:122:ARG:NH2	25:W:154:ARG:HG2	2.35	0.41
30:2:11:LEU:HD23	30:2:11:LEU:HA	1.88	0.41
1:0:221:G:H2'	1:0:222:A:C8	2.55	0.41
1:0:787:G:O2'	1:0:788:A:H5'	2.20	0.41
1:0:1028:U:H5'	1:0:1031:G:O4'	2.20	0.41
1:0:1175:G:H2'	1:0:1176:C:O4'	2.20	0.41
1:0:1878:G:O2'	1:0:1879:U:H6	2.01	0.41
1:0:2435:U:OP1	31:3:28:GLY:HA3	2.21	0.41
1:0:2568:A:H2'	1:0:2569:A:O4'	2.21	0.41
40:0:3398:HOH:O	5:B:252:PRO:HD3	2.20	0.41
2:9:3001:U:H5'	2:9:3121:C:O2	2.20	0.41
4:A:132:ASP:OD1	4:A:133:ARG:N	2.38	0.41
6:C:104:ASP:OD1	6:C:107:ARG:NH1	2.52	0.41
11:H:59:HIS:HA	11:H:62:LEU:HD23	2.02	0.41
14:L:34:GLY:C	14:L:36:ASP:H	2.28	0.41
14:L:130:ARG:O	14:L:131:GLU:C	2.64	0.41
17:O:37:ARG:HG3	40:O:3002:HOH:O	2.20	0.41
20:R:15:LYS:HE3	40:R:9492:HOH:O	2.20	0.41
28:Z:25:ARG:HB3	28:Z:29:ILE:CD1	2.51	0.41
32:I:75:THR:HA	32:I:112:LYS:HZ3	1.85	0.41
1:0:27:U:H2'	1:0:28:G:O4'	2.20	0.41
1:0:295:C:H2'	1:0:296:G:O4'	2.21	0.41
1:0:522:U:O2'	1:0:1366:C:H5'	2.21	0.41
1:0:1406:A:H4'	1:0:1407:A:C5'	2.51	0.41
1:0:1488:U:H4'	1:0:1489:G:OP1	2.20	0.41
1:0:1507:C:H4'	40:0:4154:HOH:O	2.20	0.41
1:0:1783:A:O2'	1:0:1784:U:H5'	2.20	0.41
1:0:1856:C:H5'	1:0:1858:A:O4'	2.21	0.41
1:0:2091:G:O3'	5:B:235:ARG:HD3	2.19	0.41
1:0:2096:A:N3	1:0:2096:A:H3'	2.35	0.41
40:0:7171:HOH:O	16:N:4:PRO:HD2	2.20	0.41
2:9:3018:U:H2'	2:9:3019:G:H8	1.86	0.41
5:B:294:TYR:HE2	40:B:9641:HOH:O	2.02	0.41
6:C:115:LEU:HA	6:C:115:LEU:HD12	1.77	0.41
7:D:65:GLU:HA	40:D:6752:HOH:O	2.20	0.41
7:D:71:ALA:HB2	40:D:7636:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:99:ASP:CB	7:D:103:ASN:H	2.33	0.41
30:2:19:SER:O	30:2:36:ASN:ND2	2.53	0.41
1:0:90:A:H2'	1:0:91:G:O4'	2.21	0.41
1:0:157:G:C6	1:0:158:A:N7	2.89	0.41
1:0:702:G:O2'	1:0:703:G:H5'	2.21	0.41
1:0:1634:G:H2'	1:0:1635:U:H6	1.85	0.41
1:0:1921:A:O2'	1:0:1922:A:H5'	2.21	0.41
1:0:2553:A:H2'	1:0:2553:A:N3	2.35	0.41
6:C:246:ARG:NH1	40:C:9177:HOH:O	2.49	0.41
9:F:26:THR:CG2	9:F:102:GLY:HA3	2.51	0.41
9:F:60:VAL:O	9:F:60:VAL:CG1	2.69	0.41
25:W:88:THR:CG2	25:W:89:ASP:H	2.33	0.41
31:3:73:GLU:HG2	40:3:9493:HOH:O	2.19	0.41
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.35	0.41
1:0:441:A:C2	1:0:442:A:N6	2.89	0.41
1:0:521:A:H2'	1:0:522:U:H5'	2.02	0.41
1:0:830:G:O2'	1:0:831:U:H5'	2.21	0.41
1:0:1041:U:H2'	1:0:1042:U:H5'	2.02	0.41
1:0:1182:C:H1'	1:0:1192:A:C8	2.47	0.41
1:0:1202:A:C2'	1:0:1203:G:H5'	2.51	0.41
1:0:2815:G:N7	12:J:80:LYS:NZ	2.68	0.41
40:0:4062:HOH:O	18:P:133:SER:HA	2.20	0.41
40:0:7765:HOH:O	22:T:9:LYS:HB2	2.19	0.41
4:A:65:ARG:HG2	4:A:65:ARG:HH11	1.85	0.41
6:C:78:ARG:NH1	6:C:78:ARG:CG	2.79	0.41
11:H:78:GLY:C	11:H:80:GLU:N	2.77	0.41
13:K:80:ILE:HG23	40:K:7064:HOH:O	2.20	0.41
15:M:122:GLN:HB2	15:M:126:GLN:O	2.20	0.41
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.20	0.41
21:S:33:SER:OG	21:S:36:GLU:HG3	2.20	0.41
24:V:1:THR:O	24:V:2:VAL:C	2.64	0.41
27:Y:187:VAL:CG1	27:Y:205:ILE:HA	2.51	0.41
1:0:363:A:H1'	40:0:5783:HOH:O	2.21	0.41
1:0:1252:A:H2'	1:0:1253:C:O4'	2.21	0.41
1:0:1463:A:O5'	1:0:1463:A:H8	2.03	0.41
1:0:2314:G:C2'	1:0:2315:C:H5'	2.51	0.41
1:0:2532:A:H2	40:0:7900:HOH:O	2.03	0.41
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.55	0.41
6:C:98:ARG:HH11	6:C:98:ARG:CG	2.29	0.41
7:D:166:ILE:HB	40:D:6326:HOH:O	2.20	0.41
10:G:63:ARG:N	40:G:2569:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:19:MET:HE1	12:J:132:LEU:HD21	2.02	0.41
15:M:43:PRO:HG3	15:M:62:VAL:HG21	2.02	0.41
16:N:22:GLN:O	16:N:26:LEU:HD22	2.21	0.41
22:T:18:GLU:O	22:T:21:LYS:HE2	2.20	0.41
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.21	0.41
28:Z:27:ALA:O	28:Z:31:SER:HB2	2.20	0.41
1:O:481:U:H4'	1:O:515:C:H2'	2.03	0.41
1:O:560:C:C2	1:O:561:G:C8	3.09	0.41
1:O:700:A:C2	14:L:71:GLU:HG2	2.56	0.41
1:O:724:G:O2'	1:O:725:C:H5'	2.21	0.41
1:O:1119:G:H22	1:O:1246:A:H2	1.48	0.41
1:O:1314:U:H5''	1:O:1316:G:O4'	2.20	0.41
1:O:1406:A:H5'	1:O:1407:A:C8	2.56	0.41
1:O:1477:C:O2'	1:O:1478:U:H5'	2.21	0.41
1:O:1506:U:H5'	1:O:1506:U:H6	1.86	0.41
1:O:1764:C:H2'	1:O:1765:G:O4'	2.21	0.41
1:O:2065:C:O2'	1:O:2066:C:H5'	2.21	0.41
1:O:2089:A:C2'	1:O:2090:G:H5'	2.51	0.41
1:O:2362:A:H2'	1:O:2363:G:C8	2.56	0.41
1:O:2364:A:H5''	19:Q:15:LYS:HD3	2.03	0.41
1:O:2546:U:H4'	40:O:6621:HOH:O	2.20	0.41
1:O:2582:G:H4'	40:K:4440:HOH:O	2.20	0.41
1:O:2626:C:H2'	1:O:2627:G:C8	2.56	0.41
1:O:2752:C:O2'	1:O:2753:G:H5'	2.20	0.41
1:O:2908:A:H2'	1:O:2909:G:C4'	2.51	0.41
5:B:190:MET:CE	5:B:194:PHE:CD1	2.91	0.41
5:B:331:SER:OG	23:U:14:GLU:OE2	2.26	0.41
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.50	0.41
8:E:31:ARG:HH11	8:E:68:HIS:HB3	1.85	0.41
8:E:108:LEU:CD1	8:E:164:ASP:HB2	2.51	0.41
11:H:29:ALA:CB	11:H:66:ARG:HH12	2.28	0.41
13:K:113:ILE:HD12	13:K:128:ALA:HB2	2.02	0.41
13:K:114:ALA:HB3	13:K:117:VAL:HG23	2.02	0.41
14:L:67:ARG:HB2	14:L:112:GLY:HA3	2.03	0.41
14:L:92:ASP:HA	14:L:121:ILE:HB	2.03	0.41
18:P:16:VAL:HG12	18:P:17:GLY:H	1.83	0.41
20:R:4:TYR:CE1	20:R:17:MET:HE2	2.56	0.41
22:T:43:ASN:HD22	22:T:108:ARG:NH2	2.19	0.41
23:U:38:ASN:O	23:U:42:LEU:HG	2.21	0.41
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.55	0.41
32:I:114:PRO:HG2	32:I:115:ASP:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:128:VAL:C	32:I:130:GLY:N	2.77	0.41
1:0:657:G:H2'	1:0:658:C:O4'	2.21	0.41
1:0:903:U:O4	14:L:18:HIS:HB2	2.21	0.41
1:0:1119:G:H8	12:J:52:GLN:NE2	2.18	0.41
1:0:1534:C:O2'	1:0:1656:A:OP1	2.34	0.41
1:0:2493:C:O2	1:0:2493:C:H2'	2.20	0.41
15:M:164:THR:CG2	15:M:165:GLY:H	2.33	0.41
20:R:96:VAL:O	20:R:99:ALA:HB3	2.19	0.41
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.79	0.41
29:1:56:GLU:OXT	29:1:56:GLU:HG2	2.20	0.41
32:I:72:VAL:HG11	32:I:111:GLN:O	2.21	0.41
1:0:286:U:H2'	1:0:287:C:C6	2.56	0.40
1:0:419:A:H1'	1:0:1921:A:C2	2.56	0.40
1:0:1095:U:O2	25:W:120:PRO:HG2	2.20	0.40
1:0:1791:U:O2'	1:0:1792:C:H5'	2.21	0.40
6:C:107:ARG:HH11	6:C:107:ARG:CB	2.33	0.40
6:C:157:LEU:HD22	6:C:162:VAL:CG1	2.51	0.40
7:D:103:ASN:OD1	7:D:133:ASN:ND2	2.54	0.40
13:K:62:PRO:HA	13:K:65:ARG:HE	1.86	0.40
14:L:140:VAL:HB	40:L:9454:HOH:O	2.20	0.40
15:M:163:LEU:N	15:M:163:LEU:HD23	2.36	0.40
20:R:98:ASN:N	20:R:98:ASN:HD22	2.18	0.40
25:W:146:ILE:HD13	25:W:146:ILE:HA	1.85	0.40
30:2:23:ALA:O	30:2:26:MET:HG2	2.21	0.40
1:0:95:A:O5'	1:0:97:G:H5'	2.21	0.40
1:0:790:A:H8	40:0:6549:HOH:O	2.04	0.40
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.55	0.40
1:0:1173:A:H4'	1:0:1174:A:C8	2.56	0.40
1:0:1377:C:O2'	1:0:1378:G:H5''	2.22	0.40
1:0:1592:G:O2'	1:0:1593:C:O4'	2.25	0.40
1:0:2389:U:H4'	19:Q:53:HIS:CD2	2.56	0.40
2:9:3056:A:C3'	2:9:3057:A:H5''	2.51	0.40
15:M:34:GLU:HB3	15:M:38:GLU:HG3	2.02	0.40
16:N:91:ARG:O	16:N:94:GLU:HB2	2.22	0.40
16:N:114:LYS:O	16:N:118:ILE:HG13	2.21	0.40
16:N:133:ASP:C	16:N:135:VAL:H	2.29	0.40
17:O:47:ARG:NH1	40:O:4564:HOH:O	2.54	0.40
21:S:5:ILE:HD11	21:S:41:VAL:HG22	2.04	0.40
22:T:21:LYS:HA	22:T:24:ARG:HG3	2.03	0.40
23:U:6:CYS:C	23:U:8:TYR:H	2.28	0.40
32:I:92:PRO:HB2	32:I:134:SER:C	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:119:A:H2'	1:0:120:A:C5'	2.50	0.40
1:0:210:U:H2'	1:0:211:U:C6	2.56	0.40
1:0:533:U:C5	1:0:2812:A:C2	3.09	0.40
1:0:711:G:C2	1:0:718:C:C2	3.09	0.40
1:0:947:U:O2'	1:0:948:G:H5'	2.21	0.40
1:0:1115:U:O2'	1:0:1116:U:H5'	2.21	0.40
1:0:1299:G:H5'	40:0:4616:HOH:O	2.20	0.40
1:0:2791:U:H1'	1:0:2792:A:H5''	2.03	0.40
5:B:205:VAL:HB	5:B:307:ARG:HD3	2.03	0.40
5:B:280:VAL:HG12	5:B:281:ASP:N	2.36	0.40
6:C:94:THR:HB	40:C:9162:HOH:O	2.20	0.40
6:C:118:THR:HG23	40:C:9106:HOH:O	2.21	0.40
9:F:22:VAL:HG23	9:F:104:ALA:HB2	2.02	0.40
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.54	0.40
28:Z:39:CYS:O	28:Z:42:CYS:O	2.39	0.40
29:1:53:LYS:HD3	29:1:53:LYS:HA	1.92	0.40
32:I:132:CYS:O	32:I:135:LEU:N	2.53	0.40
1:0:1071:G:H4'	27:Y:154:ARG:HH22	1.86	0.40
1:0:1165:G:H21	1:0:1173:A:C5'	2.34	0.40
1:0:1342:C:H2'	1:0:1343:C:H5'	2.04	0.40
1:0:1573:A:N7	1:0:1574:C:C2	2.90	0.40
1:0:1592:G:H2'	1:0:1593:C:C6	2.56	0.40
1:0:1624:A:H4'	1:0:1625:U:H5'	2.02	0.40
1:0:1803:C:H2'	1:0:1804:A:H8	1.86	0.40
1:0:1852:A:H5''	4:A:232:ARG:O	2.22	0.40
1:0:2466:G:OP2	14:L:37:LYS:HE2	2.22	0.40
2:9:3088:G:OP1	25:W:130:HIS:NE2	2.39	0.40
7:D:13:MET:HA	7:D:137:PRO:HG2	2.02	0.40
8:E:158:ASP:C	8:E:158:ASP:OD1	2.65	0.40
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.50	0.40
22:T:40:VAL:HG22	22:T:41:ARG:N	2.35	0.40
24:V:12:THR:H	24:V:15:GLU:CD	2.30	0.40
1:0:475:G:H5'	6:C:73:LEU:HD23	2.04	0.40
1:0:820:G:O2'	1:0:856:G:H4'	2.21	0.40
1:0:951:A:H2'	1:0:952:G:H5'	2.03	0.40
1:0:1117:A:C2	1:0:1244:U:C2	3.09	0.40
1:0:1603:A:H5'	1:0:1605:G:C4'	2.51	0.40
1:0:1769:C:O2'	1:0:1770:U:H5'	2.22	0.40
1:0:1797:A:H2'	1:0:1799:G:O5'	2.21	0.40
1:0:2346:C:O3'	7:D:52:THR:CG2	2.70	0.40
1:0:2565:C:H4'	40:0:5357:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2896:A:N3	1:0:2896:A:C2'	2.81	0.40
4:A:81:GLN:CG	4:A:92:ASN:HD21	2.34	0.40
5:B:57:GLU:OE1	5:B:60:SER:HB2	2.21	0.40
5:B:270:ILE:O	5:B:271:ASP:HB2	2.22	0.40
6:C:39:GLN:O	6:C:43:LYS:HD3	2.22	0.40
7:D:149:ARG:HH12	16:N:15:GLU:HA	1.86	0.40
13:K:66:ARG:HH11	13:K:66:ARG:HG2	1.86	0.40
15:M:77:HIS:HB2	15:M:81:ARG:HD3	2.03	0.40
15:M:82:ARG:O	15:M:84:LYS:N	2.55	0.40
16:N:74:PRO:HB2	16:N:77:ASN:ND2	2.37	0.40
19:Q:41:LEU:HB3	19:Q:52:PHE:CZ	2.56	0.40
20:R:99:ALA:HB1	20:R:109:MET:HE1	2.02	0.40
25:W:146:ILE:HG22	25:W:147:ASP:N	2.36	0.40
27:Y:102:LEU:HD11	27:Y:225:GLY:HA2	2.04	0.40
27:Y:112:GLU:O	27:Y:116:LEU:HG	2.21	0.40
32:I:91:GLU:HB2	32:I:95:ASP:OD2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:K:6344:HOH:O	40:K:6344:HOH:O[3_655]	2.05	0.15

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	208 (88%)	20 (8%)	7 (3%)	3	3
5	B	335/338 (99%)	296 (88%)	32 (10%)	7 (2%)	5	7
6	C	244/246 (99%)	221 (91%)	22 (9%)	1 (0%)	30	43
7	D	134/177 (76%)	104 (78%)	19 (14%)	11 (8%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	E	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
9	F	117/120 (98%)	102 (87%)	12 (10%)	3 (3%)	4	4
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	136 (87%)	15 (10%)	5 (3%)	3	3
12	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	9	13
13	K	130/132 (98%)	118 (91%)	11 (8%)	1 (1%)	16	25
14	L	141/165 (86%)	115 (82%)	25 (18%)	1 (1%)	18	28
15	M	192/195 (98%)	179 (93%)	11 (6%)	2 (1%)	12	20
16	N	184/187 (98%)	158 (86%)	17 (9%)	9 (5%)	1	1
17	O	113/116 (97%)	105 (93%)	8 (7%)	0	100	100
18	P	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
19	Q	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	11	18
20	R	148/155 (96%)	137 (93%)	10 (7%)	1 (1%)	18	28
21	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
22	T	117/120 (98%)	110 (94%)	4 (3%)	3 (3%)	4	4
23	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
24	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	7	11
25	W	152/154 (99%)	145 (95%)	7 (5%)	0	100	100
26	X	80/92 (87%)	71 (89%)	8 (10%)	1 (1%)	9	14
27	Y	140/241 (58%)	135 (96%)	5 (4%)	0	100	100
28	Z	71/83 (86%)	58 (82%)	9 (13%)	4 (6%)	1	1
29	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
30	2	42/50 (84%)	39 (93%)	2 (5%)	1 (2%)	4	5
31	3	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
32	I	68/162 (42%)	52 (76%)	12 (18%)	4 (6%)	1	0
All	All	3705/4431 (84%)	3338 (90%)	302 (8%)	65 (2%)	6	9

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	36	ASP
4	A	37	VAL
5	B	139	ASP

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Mol	Chain	Res	Type
5	B	169	GLY
7	D	164	ALA
9	F	101	ALA
11	H	166	SER
11	H	168	ALA
14	L	80	ASP
16	N	154	LEU
16	N	167	ASP
16	N	184	ILE
28	Z	20	ARG
28	Z	81	ARG
4	A	205	GLY
5	B	34	GLY
5	B	279	THR
5	B	291	ASP
6	C	8	LEU
7	D	16	PRO
7	D	56	ARG
7	D	60	GLU
7	D	65	GLU
7	D	97	GLN
7	D	137	PRO
13	K	127	ALA
16	N	155	GLU
16	N	183	ASP
24	V	43	PRO
32	I	76	ALA
32	I	129	VAL
5	B	184	ASP
7	D	168	SER
7	D	171	ASP
11	H	16	ARG
12	J	5	GLU
15	M	83	SER
26	X	70	ILE
32	I	133	THR
4	A	24	LYS
5	B	185	GLY
9	F	64	PRO
11	H	79	GLU
12	J	143	LYS
16	N	157	PRO

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Mol	Chain	Res	Type
16	N	162	ASP
22	T	46	ASP
22	T	53	GLY
28	Z	41	ASN
16	N	65	ASP
16	N	68	GLU
22	T	44	ALA
30	2	37	HIS
32	I	114	PRO
4	A	208	HIS
4	A	42	VAL
7	D	69	ILE
11	H	81	GLY
7	D	28	GLY
15	M	88	VAL
28	Z	21	VAL
9	F	71	GLY
4	A	204	GLY
19	Q	18	PRO
20	R	114	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	167 (93%)	12 (7%)	15	26
5	B	282/283 (100%)	265 (94%)	17 (6%)	17	31
6	C	193/193 (100%)	175 (91%)	18 (9%)	8	14
7	D	117/148 (79%)	110 (94%)	7 (6%)	17	31
8	E	152/156 (97%)	144 (95%)	8 (5%)	20	36
9	F	93/94 (99%)	92 (99%)	1 (1%)	65	82
10	G	27/283 (10%)	25 (93%)	2 (7%)	13	22
11	H	132/138 (96%)	127 (96%)	5 (4%)	29	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	J	118/121 (98%)	108 (92%)	10 (8%)	10	16
13	K	106/106 (100%)	100 (94%)	6 (6%)	18	33
14	L	113/127 (89%)	108 (96%)	5 (4%)	25	43
15	M	158/159 (99%)	156 (99%)	2 (1%)	61	80
16	N	149/150 (99%)	140 (94%)	9 (6%)	17	31
17	O	93/94 (99%)	89 (96%)	4 (4%)	26	44
18	P	113/117 (97%)	109 (96%)	4 (4%)	32	53
19	Q	79/80 (99%)	75 (95%)	4 (5%)	21	37
20	R	117/122 (96%)	112 (96%)	5 (4%)	26	44
21	S	71/74 (96%)	70 (99%)	1 (1%)	59	79
22	T	105/106 (99%)	100 (95%)	5 (5%)	23	40
23	U	44/52 (85%)	43 (98%)	1 (2%)	44	66
24	V	51/57 (90%)	48 (94%)	3 (6%)	18	31
25	W	130/130 (100%)	124 (95%)	6 (5%)	24	41
26	X	66/74 (89%)	58 (88%)	8 (12%)	5	7
27	Y	120/196 (61%)	110 (92%)	10 (8%)	10	17
28	Z	60/68 (88%)	59 (98%)	1 (2%)	53	74
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	43	65
31	3	79/79 (100%)	75 (95%)	4 (5%)	21	37
32	I	58/130 (45%)	56 (97%)	2 (3%)	32	54
All	All	3093/3612 (86%)	2932 (95%)	161 (5%)	21	36

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	26	ASP
4	A	33	GLU
4	A	62	ASP
4	A	94	LEU
4	A	131	HIS
4	A	144	GLU
4	A	165	THR
4	A	175	LYS

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Mol	Chain	Res	Type
4	A	179	MET
4	A	206	ARG
4	A	217	ARG
5	B	11	LEU
5	B	27	ASN
5	B	71	VAL
5	B	82	VAL
5	B	98	THR
5	B	112	THR
5	B	113	LEU
5	B	149	ASP
5	B	162	MET
5	B	175	LEU
5	B	180	ASP
5	B	195	ARG
5	B	211	THR
5	B	251	VAL
5	B	254	GLN
5	B	257	THR
5	B	312	ARG
6	C	2	GLN
6	C	16	VAL
6	C	27	ARG
6	C	76	ARG
6	C	78	ARG
6	C	91	PRO
6	C	94	THR
6	C	115	LEU
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	223	LEU
6	C	234	VAL
6	C	236	THR
6	C	237	GLU
6	C	240	LEU
6	C	243	VAL
7	D	24	HIS
7	D	50	VAL
7	D	61	PHE
7	D	99	ASP

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Mol	Chain	Res	Type
7	D	135	VAL
7	D	137	PRO
7	D	170	TYR
8	E	3	VAL
8	E	7	ILE
8	E	16	ASP
8	E	86	VAL
8	E	102	VAL
8	E	116	THR
8	E	155	ASN
8	E	156	ASP
9	F	46	GLU
10	G	12	ILE
10	G	72	ASP
11	H	1	LYS
11	H	18	GLU
11	H	84	LYS
11	H	154	TYR
11	H	170	ASN
12	J	39	VAL
12	J	46	ILE
12	J	47	THR
12	J	49	ARG
12	J	52	GLN
12	J	70	PHE
12	J	74	ARG
12	J	93	ARG
12	J	127	ILE
12	J	131	THR
13	K	4	LEU
13	K	10	GLN
13	K	55	VAL
13	K	84	ASP
13	K	98	VAL
13	K	107	THR
14	L	35	ARG
14	L	43	HIS
14	L	75	LEU
14	L	89	PHE
14	L	140	VAL
15	M	46	LEU
15	M	93	ARG

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Mol	Chain	Res	Type
16	N	17	ARG
16	N	26	LEU
16	N	38	LYS
16	N	49	THR
16	N	56	ASP
16	N	65	ASP
16	N	127	LEU
16	N	152	GLU
16	N	157	PRO
17	O	3	THR
17	O	16	SER
17	O	43	VAL
17	O	67	SER
18	P	13	VAL
18	P	21	VAL
18	P	98	ILE
18	P	117	SER
19	Q	11	ARG
19	Q	16	ASN
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	39	THR
20	R	82	GLU
20	R	132	ARG
20	R	143	VAL
21	S	53	ASN
22	T	39	ASN
22	T	41	ARG
22	T	89	ARG
22	T	96	VAL
22	T	115	GLU
23	U	28	THR
24	V	12	THR
24	V	45	ARG
24	V	65	ASP
25	W	4	LEU
25	W	26	ILE
25	W	35	VAL
25	W	122	ARG
25	W	146	ILE
25	W	154	ARG

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Mol	Chain	Res	Type
26	X	15	ARG
26	X	27	ASP
26	X	46	ASP
26	X	66	THR
26	X	79	GLU
26	X	80	GLU
26	X	82	GLU
26	X	85	VAL
27	Y	103	THR
27	Y	115	ARG
27	Y	141	THR
27	Y	172	THR
27	Y	174	VAL
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	231	PRO
27	Y	235	GLU
28	Z	46	ARG
30	2	18	ASN
31	3	3	MET
31	3	18	GLN
31	3	56	PRO
31	3	65	THR
32	I	119	TYR
32	I	140	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	29	HIS
4	A	92	ASN
4	A	134	ASN
4	A	151	GLN
4	A	199	HIS
4	A	218	ASN
5	B	2	GLN
5	B	27	ASN
5	B	55	ASN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN

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Mol	Chain	Res	Type
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	11	ASN
6	C	39	GLN
6	C	129	HIS
7	D	47	GLN
7	D	103	ASN
7	D	133	ASN
8	E	106	ASN
8	E	119	HIS
8	E	143	GLN
9	F	80	GLN
10	G	17	GLN
10	G	64	ASN
11	H	31	HIS
11	H	37	GLN
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	72	HIS
11	H	170	ASN
12	J	25	GLN
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
13	K	119	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	43	HIS
15	M	24	GLN
15	M	58	GLN
15	M	77	HIS
15	M	126	GLN
15	M	143	ASN
15	M	170	ASN
16	N	22	GLN
16	N	93	GLN
16	N	107	ASN
18	P	50	GLN

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Mol	Chain	Res	Type
18	P	66	GLN
18	P	73	HIS
18	P	118	GLN
19	Q	40	HIS
19	Q	67	GLN
20	R	22	GLN
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
20	R	122	GLN
20	R	140	GLN
21	S	53	ASN
21	S	55	GLN
22	T	37	GLN
22	T	39	ASN
22	T	43	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	27	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
27	Y	129	ASN
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	188	HIS
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	2	GLN

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Mol	Chain	Res	Type
31	3	13	HIS
31	3	20	HIS
31	3	30	GLN
31	3	39	GLN
31	3	48	ASN
31	3	78	HIS
32	I	111	GLN
32	I	113	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	256 (9%)	33 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
3	4	2/5 (40%)	1 (50%)	0
All	All	2868/3049 (94%)	275 (9%)	34 (1%)

All (275) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	138	U
1	0	141	C
1	0	151	A
1	0	166	A
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G

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Mol	Chain	Res	Type
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	702	G
1	0	735	C

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Mol	Chain	Res	Type
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A

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Mol	Chain	Res	Type
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1246	A
1	0	1247	A
1	0	1279	U
1	0	1287	A
1	0	1289	C
1	0	1300	G
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1564	C
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1686	C

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Mol	Chain	Res	Type
1	0	1692	C
1	0	1693	A
1	0	1701	A
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1968	A
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G

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Mol	Chain	Res	Type
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2329	C
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2611	G
1	0	2613	G
1	0	2634	G
1	0	2637	A
1	0	2644	C
1	0	2645	U
1	0	2648	U
1	0	2649	A
1	0	2650	U
1	0	2664	A

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Mol	Chain	Res	Type
1	0	2681	A
1	0	2682	C
1	0	2718	C
1	0	2719	A
1	0	2726	U
1	0	2727	A
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2783	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2852	A
1	0	2853	U
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3039	U
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G

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Mol	Chain	Res	Type
2	9	3122	C
3	4	76	A

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	87	C
1	0	129	A
1	0	169	A
1	0	604	G
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1165	G
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1563	G
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1856	C
1	0	1973	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2791	U
1	0	2852	A
2	9	3065	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	0	2587	1	19,22,23	0.22	0	25,31,34	0.43	0
1	1MA	0	628	1,35	21,25,26	0.78	1 (4%)	30,37,40	0.81	2 (6%)
1	UR3	0	2619	1	19,22,23	0.49	0	26,32,35	0.69	1 (3%)
1	OMG	0	2588	1	23,26,27	0.31	0	32,38,41	0.38	0
1	PSU	0	2621	1	18,21,22	1.60	2 (11%)	21,30,33	1.38	3 (14%)
3	ACA	4	78	3	3,3,8	0.54	0	1,2,8	0.67	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	1MA	0	628	1,35	-	2/7/25/26	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	0/9/27/28	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
3	ACA	4	78	3	-	0/0/1/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.18	1.43	1.36
1	0	2621	PSU	C6-C5	3.39	1.39	1.35
1	0	628	1MA	C6-N6	2.54	1.34	1.28

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.47	120.52	118.17
1	0	2621	PSU	C6-N1-C2	-3.31	119.61	122.69
1	0	2621	PSU	O2-C2-N1	2.72	125.59	122.79
1	0	628	1MA	N1-C2-N3	2.69	129.19	126.00
1	0	2619	UR3	C4-N3-C2	2.68	126.74	124.58
1	0	628	1MA	CM1-N1-C6	2.05	123.32	120.15

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8
1	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2619	UR3	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 313 ligands modelled in this entry, 312 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
38	SPS	4	9701	33	20,23,23	1.46	3 (15%)	23,30,30	2.09	6 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	SPS	4	9701	33	-	5/15/18/18	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	9701	SPS	C6-C1	4.40	1.53	1.45
38	4	9701	SPS	C9-C10	-2.99	1.41	1.48
38	4	9701	SPS	O15-S15	-2.03	1.43	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	9701	SPS	C7-C5-N4	4.97	119.19	113.42
38	4	9701	SPS	C7-C5-C6	-3.93	121.38	126.47
38	4	9701	SPS	N4-C3-N2	3.88	121.84	115.74
38	4	9701	SPS	C1-N2-C3	-3.76	121.19	126.37
38	4	9701	SPS	C6-C1-N2	2.43	118.70	114.45
38	4	9701	SPS	O15-S15-C16	2.10	108.97	106.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	4	9701	SPS	N11-C12-C13-O13
38	4	9701	SPS	C14-C12-C13-O13
38	4	9701	SPS	C12-C14-S15-O15
38	4	9701	SPS	C12-C14-S15-C16
38	4	9701	SPS	C5-C6-C8-C9

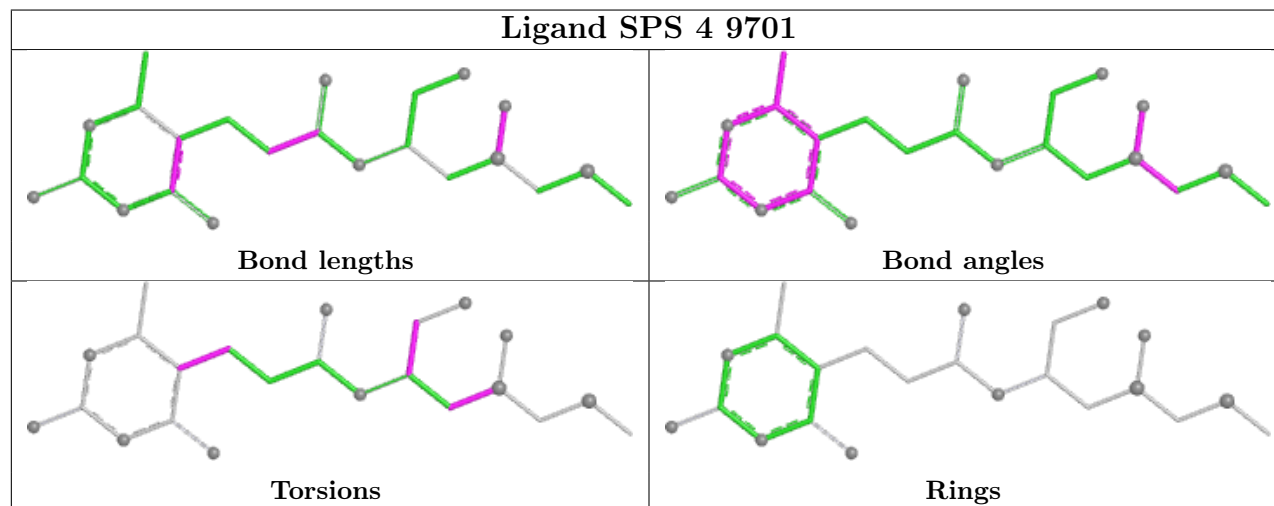
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	4	9701	SPS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	76:A	O3'	77:PHE	C	1.60

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.23	80 (2%) 53 50	19, 43, 80, 130	0
2	9	122/122 (100%)	0.40	5 (4%) 41 37	35, 59, 79, 129	0
3	4	4/5 (80%)	0.45	1 (25%) 2 1	44, 46, 51, 57	0
4	A	237/240 (98%)	0.67	17 (7%) 21 18	28, 51, 79, 92	0
5	B	337/338 (99%)	0.33	6 (1%) 67 63	25, 46, 66, 77	0
6	C	246/246 (100%)	0.34	9 (3%) 45 41	24, 43, 61, 72	0
7	D	140/177 (79%)	1.91	48 (34%) 1 1	53, 76, 103, 111	0
8	E	172/178 (96%)	0.71	11 (6%) 25 22	37, 55, 69, 73	0
9	F	119/120 (99%)	1.07	14 (11%) 9 6	45, 64, 88, 91	0
10	G	29/348 (8%)	1.64	8 (27%) 1 1	60, 77, 82, 85	0
11	H	160/171 (93%)	0.69	8 (5%) 34 30	39, 54, 80, 84	0
12	J	142/145 (97%)	0.39	6 (4%) 40 36	32, 43, 59, 75	0
13	K	132/132 (100%)	0.22	2 (1%) 72 68	30, 42, 59, 67	0
14	L	145/165 (87%)	0.94	21 (14%) 6 4	26, 60, 92, 101	0
15	M	194/195 (99%)	0.77	26 (13%) 7 5	31, 42, 80, 85	0
16	N	186/187 (99%)	1.02	21 (11%) 10 7	43, 58, 93, 98	0
17	O	115/116 (99%)	0.58	2 (1%) 69 65	36, 49, 61, 67	0
18	P	143/149 (95%)	0.61	6 (4%) 40 36	35, 47, 58, 66	0
19	Q	95/96 (98%)	0.48	3 (3%) 50 46	39, 46, 58, 65	0
20	R	150/155 (96%)	-0.05	2 (1%) 75 71	27, 39, 56, 67	0
21	S	81/85 (95%)	0.58	4 (4%) 35 31	39, 52, 69, 84	0
22	T	119/120 (99%)	0.66	8 (6%) 24 20	35, 50, 72, 96	0
23	U	53/66 (80%)	0.46	1 (1%) 66 62	39, 50, 66, 72	0
24	V	65/71 (91%)	1.43	13 (20%) 3 2	47, 65, 94, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.32	5 (3%)	50	46	31, 44, 58, 68	0
26	X	82/92 (89%)	0.61	7 (8%)	16	13	37, 49, 69, 85	0
27	Y	142/241 (58%)	0.25	3 (2%)	63	59	24, 41, 57, 76	0
28	Z	73/83 (87%)	2.97	47 (64%)	0	0	63, 85, 94, 98	0
29	1	56/57 (98%)	-0.19	0	100	100	25, 31, 38, 47	0
30	2	46/50 (92%)	0.87	4 (8%)	16	13	32, 51, 65, 70	0
31	3	92/92 (100%)	1.15	12 (13%)	7	5	48, 65, 72, 81	0
32	I	70/162 (43%)	3.47	63 (90%)	0	0	92, 106, 120, 121	0
All	All	6650/7480 (88%)	0.32	463 (6%)	22	19	19, 47, 85, 130	0

All (463) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	V	1	THR	11.7
32	I	133	THR	9.9
15	M	70	GLY	9.4
28	Z	22	SER	9.2
28	Z	12	GLY	8.3
7	D	10	PHE	7.6
28	Z	21	VAL	7.5
32	I	118	SER	7.5
15	M	74	LYS	7.4
15	M	80	GLY	7.2
28	Z	11	SER	7.1
7	D	63	ILE	7.0
2	9	3001	U	6.7
15	M	89	THR	6.7
16	N	166	ALA	6.6
28	Z	14	PHE	6.3
15	M	72	ALA	6.3
32	I	129	VAL	6.3
4	A	37	VAL	6.0
28	Z	16	ALA	6.0
16	N	154	LEU	5.9
7	D	174	VAL	5.8
28	Z	18	TYR	5.8
30	2	49	GLU	5.8
24	V	40	PRO	5.8
7	D	90	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
22	T	117	ASP	5.7
28	Z	29	ILE	5.7
32	I	90	GLY	5.6
15	M	79	ALA	5.5
28	Z	26	VAL	5.5
7	D	107	GLY	5.5
32	I	121	LEU	5.5
32	I	137	VAL	5.4
32	I	117	LEU	5.4
15	M	78	LYS	5.3
15	M	81	ARG	5.3
32	I	85	PHE	5.2
26	X	88	GLU	5.2
24	V	2	VAL	5.1
4	A	36	ASP	5.0
28	Z	10	ARG	5.0
16	N	168	LEU	5.0
28	Z	27	ALA	5.0
10	G	26	MET	5.0
32	I	79	ILE	5.0
7	D	172	VAL	5.0
32	I	96	PHE	4.9
7	D	57	THR	4.9
15	M	88	VAL	4.9
22	T	118	SER	4.9
32	I	76	ALA	4.8
32	I	139	ILE	4.8
1	0	1173	A	4.8
32	I	116	LEU	4.8
32	I	125	ALA	4.7
2	9	3002	U	4.7
1	0	2748	G	4.7
7	D	55	LYS	4.7
15	M	71	SER	4.7
24	V	39	ALA	4.7
2	9	3024	U	4.6
28	Z	34	ASN	4.6
15	M	86	GLN	4.6
15	M	73	ARG	4.6
1	0	10	U	4.5
28	Z	40	PRO	4.5
32	I	124	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
14	L	82	ALA	4.5
28	Z	17	ARG	4.5
28	Z	13	ARG	4.4
7	D	61	PHE	4.4
16	N	165	ALA	4.4
28	Z	19	GLY	4.3
5	B	1	PRO	4.3
15	M	83	SER	4.3
28	Z	20	ARG	4.3
15	M	76	ARG	4.3
32	I	78	LEU	4.2
32	I	97	VAL	4.2
15	M	82	ARG	4.2
2	9	3023	U	4.2
24	V	43	PRO	4.1
28	Z	33	MET	4.1
15	M	75	ARG	4.1
32	I	138	THR	4.1
1	0	1172	G	4.1
7	D	171	ASP	4.1
32	I	132	CYS	4.1
28	Z	23	ARG	4.0
1	0	1169	U	4.0
32	I	93	GLN	4.0
12	J	70	PHE	4.0
14	L	77	ALA	4.0
9	F	102	GLY	4.0
24	V	37	GLY	4.0
28	Z	15	GLY	4.0
10	G	23	ILE	4.0
15	M	84	LYS	3.9
22	T	119	ALA	3.9
32	I	100	LEU	3.9
11	H	168	ALA	3.9
12	J	4	ALA	3.9
1	0	1165	G	3.8
17	O	22	GLY	3.8
28	Z	54	ILE	3.8
32	I	128	VAL	3.8
26	X	65	ASN	3.8
22	T	116	ASP	3.8
14	L	78	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	0	1175	G	3.8
32	I	135	LEU	3.8
32	I	134	SER	3.8
7	D	11	HIS	3.8
28	Z	31	SER	3.7
32	I	109	ALA	3.7
28	Z	30	GLU	3.7
32	I	77	GLU	3.7
28	Z	24	ARG	3.7
32	I	123	ASN	3.7
21	S	81	ILE	3.7
11	H	111	ASP	3.7
1	0	1161	A	3.7
28	Z	82	SER	3.6
1	0	138	U	3.6
16	N	95	ALA	3.6
27	Y	216	ARG	3.6
15	M	87	GLY	3.6
10	G	12	ILE	3.6
1	0	2345	A	3.6
32	I	105	VAL	3.5
32	I	119	TYR	3.5
7	D	59	GLY	3.5
14	L	83	GLU	3.5
14	L	146	GLY	3.5
32	I	88	GLY	3.5
31	3	41	GLU	3.5
1	0	1164	U	3.5
18	P	143	ALA	3.5
24	V	38	GLY	3.5
4	A	237	GLY	3.5
6	C	63	SER	3.5
7	D	36	ASN	3.4
14	L	81	VAL	3.4
4	A	35	GLY	3.4
31	3	4	PRO	3.4
32	I	108	ILE	3.4
1	0	1192	A	3.4
1	0	514	G	3.4
1	0	1964	U	3.4
7	D	105	SER	3.4
1	0	2237	G	3.4

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Mol	Chain	Res	Type	RSRZ
32	I	89	SER	3.4
14	L	149	ARG	3.4
24	V	41	GLU	3.4
14	L	150	GLN	3.4
7	D	135	VAL	3.4
7	D	89	PRO	3.4
4	A	203	GLY	3.4
17	O	23	GLY	3.4
32	I	83	ALA	3.4
14	L	148	GLU	3.4
10	G	71	LEU	3.3
32	I	102	VAL	3.3
15	M	77	HIS	3.3
4	A	32	VAL	3.3
11	H	40	ALA	3.3
28	Z	58	SER	3.3
28	Z	45	ASP	3.3
1	0	2645	U	3.3
1	0	1951	G	3.3
1	0	271	C	3.3
32	I	94	GLU	3.3
1	0	1171	A	3.2
16	N	37	ARG	3.2
32	I	92	PRO	3.2
32	I	114	PRO	3.2
31	3	62	THR	3.2
8	E	154	ILE	3.2
1	0	735	C	3.2
32	I	87	THR	3.2
1	0	1162	G	3.2
8	E	45	ASP	3.2
7	D	35	ALA	3.2
7	D	170	TYR	3.2
4	A	38	ILE	3.2
9	F	101	ALA	3.1
14	L	99	GLU	3.1
25	W	86	GLU	3.1
1	0	1199	A	3.1
1	0	1184	C	3.1
7	D	44	ILE	3.1
7	D	12	GLU	3.1
8	E	12	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
7	D	26	GLY	3.1
1	0	288	A	3.1
32	I	74	PRO	3.1
28	Z	25	ARG	3.1
27	Y	235	GLU	3.0
31	3	20	HIS	3.0
8	E	10	ASP	3.0
32	I	95	ASP	3.0
11	H	112	GLY	3.0
8	E	6	GLU	3.0
16	N	163	PHE	3.0
7	D	154	LYS	3.0
32	I	98	ALA	3.0
1	0	1176	C	3.0
10	G	27	ILE	3.0
28	Z	79	VAL	3.0
32	I	75	THR	3.0
28	Z	59	TYR	3.0
8	E	100	ASP	3.0
4	A	33	GLU	2.9
5	B	57	GLU	2.9
32	I	72	VAL	2.9
32	I	126	LYS	2.9
1	0	2747	C	2.9
1	0	1170	U	2.9
15	M	85	ARG	2.9
14	L	145	LEU	2.9
1	0	284	C	2.9
7	D	56	ARG	2.9
18	P	18	LYS	2.9
7	D	138	GLY	2.9
11	H	169	GLY	2.9
24	V	42	ASN	2.8
32	I	122	THR	2.8
9	F	105	ASP	2.8
32	I	81	ASP	2.8
1	0	1168	C	2.8
7	D	106	PHE	2.8
1	0	272	A	2.8
32	I	82	GLU	2.8
32	I	111	GLN	2.8
6	C	16	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
28	Z	46	ARG	2.8
1	0	1193	A	2.8
32	I	113	HIS	2.8
7	D	18	ILE	2.7
7	D	69	ILE	2.7
16	N	169	PRO	2.7
22	T	114	SER	2.7
31	3	55	VAL	2.7
1	0	960	G	2.7
16	N	162	ASP	2.7
3	4	77	PHE	2.7
7	D	131	THR	2.7
1	0	1950	G	2.7
7	D	58	VAL	2.7
9	F	119	ARG	2.7
15	M	90	ARG	2.7
32	I	127	GLU	2.7
1	0	1524	U	2.7
1	0	441	A	2.7
15	M	68	ARG	2.7
16	N	158	LEU	2.7
24	V	44	GLY	2.6
30	2	35	ARG	2.6
1	0	2769	C	2.6
14	L	91	VAL	2.6
16	N	159	TYR	2.6
1	0	970	U	2.6
1	0	2004	U	2.6
16	N	167	ASP	2.6
9	F	2	VAL	2.6
1	0	1166	A	2.6
1	0	1200	A	2.6
1	0	1202	A	2.6
32	I	131	THR	2.6
1	0	1523	G	2.6
14	L	105	TYR	2.6
28	Z	62	TYR	2.6
32	I	136	GLY	2.6
26	X	85	VAL	2.6
21	S	78	ALA	2.6
1	0	1177	A	2.6
31	3	7	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	0	2419	U	2.5
7	D	134	LEU	2.5
9	F	8	VAL	2.5
21	S	21	GLN	2.5
28	Z	41	ASN	2.5
7	D	37	ALA	2.5
28	Z	38	ALA	2.5
1	0	128	A	2.5
8	E	63	GLY	2.5
16	N	161	GLY	2.5
19	Q	18	PRO	2.5
24	V	46	ILE	2.5
12	J	5	GLU	2.5
8	E	87	PHE	2.5
7	D	155	HIS	2.5
9	F	106	ALA	2.5
32	I	73	PRO	2.5
32	I	84	GLY	2.5
5	B	56	ASP	2.5
16	N	164	ASP	2.5
15	M	91	ILE	2.5
1	0	734	U	2.5
1	0	1163	G	2.5
4	A	31	LYS	2.5
1	0	999	C	2.5
7	D	91	ALA	2.5
16	N	1	ALA	2.5
1	0	1160	G	2.5
28	Z	57	CYS	2.4
28	Z	51	GLY	2.4
1	0	737	A	2.4
1	0	1174	A	2.4
28	Z	50	GLN	2.4
28	Z	56	GLN	2.4
30	2	44	ARG	2.4
28	Z	47	VAL	2.4
13	K	118	ALA	2.4
7	D	95	THR	2.4
16	N	157	PRO	2.4
1	0	1525	G	2.4
32	I	104	GLN	2.4
1	0	2511	A	2.4

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Mol	Chain	Res	Type	RSRZ
1	0	1279	U	2.4
7	D	153	THR	2.4
14	L	44	GLU	2.4
19	Q	84	ILE	2.4
1	0	1203	G	2.4
14	L	147	GLU	2.4
18	P	64	GLU	2.4
1	0	1967	U	2.4
7	D	62	ASP	2.4
7	D	169	THR	2.3
20	R	150	PRO	2.3
2	9	3122	C	2.3
32	I	71	GLY	2.3
32	I	120	ASP	2.3
7	D	104	PHE	2.3
9	F	104	ALA	2.3
25	W	74	GLU	2.3
26	X	87	ALA	2.3
13	K	27	ARG	2.3
5	B	119	HIS	2.3
9	F	118	LEU	2.3
16	N	179	LEU	2.3
1	0	1196	C	2.3
32	I	112	LYS	2.3
11	H	167	PRO	2.3
25	W	77	ALA	2.3
31	3	56	PRO	2.3
1	0	289	G	2.3
23	U	4	ARG	2.3
1	0	736	A	2.3
4	A	85	SER	2.3
7	D	150	SER	2.3
4	A	211	LYS	2.3
15	M	69	LYS	2.3
28	Z	32	GLU	2.3
4	A	151	GLN	2.3
14	L	55	GLN	2.3
1	0	1561	U	2.3
7	D	173	GLU	2.3
32	I	86	GLU	2.3
7	D	130	VAL	2.3
9	F	16	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
28	Z	52	THR	2.2
6	C	62	GLY	2.2
28	Z	43	GLY	2.2
28	Z	53	GLY	2.2
1	0	1189	A	2.2
1	0	1197	G	2.2
1	0	510	U	2.2
6	C	237	GLU	2.2
7	D	17	ARG	2.2
7	D	73	VAL	2.2
14	L	93	VAL	2.2
24	V	45	ARG	2.2
26	X	66	THR	2.2
28	Z	78	THR	2.2
32	I	80	LYS	2.2
9	F	17	LEU	2.2
18	P	121	ASP	2.2
28	Z	61	ASP	2.2
1	0	1188	A	2.2
1	0	1185	U	2.2
1	0	2344	G	2.2
6	C	61	PHE	2.2
10	G	20	VAL	2.2
12	J	45	VAL	2.2
1	0	1186	C	2.2
7	D	53	LYS	2.2
31	3	13	HIS	2.2
31	3	18	GLN	2.2
7	D	128	LEU	2.2
22	T	36	GLY	2.2
26	X	84	ILE	2.2
5	B	118	ASP	2.2
27	Y	108	ASP	2.2
6	C	135	GLU	2.2
4	A	206	ARG	2.2
31	3	83	TRP	2.2
7	D	68	PRO	2.2
1	0	1929	G	2.2
18	P	77	ALA	2.2
19	Q	17	LYS	2.2
26	X	83	ALA	2.2
1	0	1201	C	2.2

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Mol	Chain	Res	Type	RSRZ
12	J	46	ILE	2.2
9	F	117	GLU	2.2
32	I	91	GLU	2.2
31	3	42	ARG	2.2
14	L	45	PRO	2.2
4	A	82	VAL	2.1
11	H	170	ASN	2.1
1	0	969	G	2.1
1	0	1167	G	2.1
14	L	121	ILE	2.1
5	B	51	VAL	2.1
6	C	3	ALA	2.1
10	G	70	ALA	2.1
16	N	175	LEU	2.1
1	0	1195	G	2.1
32	I	140	GLU	2.1
4	A	34	ASP	2.1
9	F	9	PRO	2.1
20	R	122	GLN	2.1
1	0	2017	U	2.1
4	A	86	ALA	2.1
14	L	100	ALA	2.1
31	3	8	ASN	2.1
1	0	497	A	2.1
16	N	2	THR	2.1
22	T	82	THR	2.1
16	N	5	ARG	2.1
7	D	60	GLU	2.1
8	E	43	ASP	2.1
32	I	106	LYS	2.1
1	0	1965	C	2.1
21	S	20	PHE	2.1
15	M	1	ALA	2.1
24	V	36	ALA	2.1
6	C	245	GLU	2.1
28	Z	28	GLU	2.1
1	0	1626	A	2.1
8	E	126	ILE	2.1
6	C	101	ASP	2.1
18	P	110	ASP	2.1
8	E	172	PRO	2.1
10	G	24	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
15	M	125	ARG	2.0
28	Z	44	GLU	2.0
1	0	1206	U	2.0
1	0	2539	U	2.0
11	H	163	ILE	2.0
12	J	144	THR	2.0
14	L	143	THR	2.0
1	0	1191	A	2.0
30	2	37	HIS	2.0
9	F	60	VAL	2.0
1	0	1947	G	2.0
22	T	115	GLU	2.0
4	A	91	GLY	2.0
25	W	26	ILE	2.0
16	N	139	TRP	2.0
7	D	99	ASP	2.0
25	W	76	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ACA	4	78	4/9	0.80	0.29	52,52,52,52	0
1	OMG	0	2588	24/25	0.97	0.07	31,32,34,36	0
1	UR3	0	2619	21/22	0.97	0.07	30,33,37,40	0
1	PSU	0	2621	20/21	0.97	0.07	32,35,39,40	0
1	1MA	0	628	23/24	0.97	0.07	27,30,32,32	0
1	OMU	0	2587	21/22	0.98	0.07	31,34,36,38	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	MG	0	8102	1/1	0.50	0.19	94,94,94,94	0
33	MG	0	8050	1/1	0.67	0.19	91,91,91,91	0
35	NA	S	9112	1/1	0.67	0.17	71,71,71,71	0
33	MG	0	8108	1/1	0.69	0.33	88,88,88,88	0
33	MG	B	8055	1/1	0.69	0.17	85,85,85,85	0
33	MG	0	8047	1/1	0.69	0.43	92,92,92,92	0
35	NA	0	9172	1/1	0.70	0.46	76,76,76,76	0
33	MG	0	8092	1/1	0.73	0.30	68,68,68,68	0
35	NA	0	9122	1/1	0.74	0.29	75,75,75,75	0
35	NA	0	9184	1/1	0.76	0.20	87,87,87,87	0
33	MG	0	8014	1/1	0.77	0.30	74,74,74,74	0
33	MG	0	8045	1/1	0.78	0.24	73,73,73,73	0
35	NA	0	9177	1/1	0.78	0.40	76,76,76,76	0
33	MG	0	8099	1/1	0.78	0.21	77,77,77,77	0
35	NA	0	9124	1/1	0.78	0.30	52,52,52,52	0
37	SR	A	9537	1/1	0.78	0.18	159,159,159,159	0
37	SR	0	9501	1/1	0.79	0.21	193,193,193,193	0
39	CD	O	9205	1/1	0.79	0.37	196,196,196,196	0
33	MG	0	8052	1/1	0.80	0.26	75,75,75,75	0
37	SR	0	9601	1/1	0.80	0.32	196,196,196,196	0
35	NA	0	9168	1/1	0.80	0.47	74,74,74,74	0
37	SR	0	9482	1/1	0.80	0.39	175,175,175,175	0
35	NA	9	9183	1/1	0.82	0.29	84,84,84,84	0
35	NA	0	9164	1/1	0.82	0.30	56,56,56,56	0
33	MG	0	8113	1/1	0.82	0.15	78,78,78,78	0
35	NA	0	9171	1/1	0.82	0.27	67,67,67,67	0
34	K	0	9002	1/1	0.82	0.22	91,91,91,91	0
35	NA	0	9129	1/1	0.82	0.26	74,74,74,74	0
35	NA	0	9163	1/1	0.82	0.19	72,72,72,72	0
35	NA	0	9185	1/1	0.83	0.36	53,53,53,53	0
33	MG	0	8101	1/1	0.83	0.11	68,68,68,68	0
35	NA	0	9140	1/1	0.83	0.29	65,65,65,65	0
33	MG	0	8107	1/1	0.83	0.24	61,61,61,61	0
35	NA	0	9150	1/1	0.84	0.13	44,44,44,44	0
35	NA	0	9132	1/1	0.84	0.25	77,77,77,77	0
35	NA	3	9169	1/1	0.84	0.27	84,84,84,84	0
33	MG	0	8114	1/1	0.84	0.20	74,74,74,74	0
33	MG	0	8022	1/1	0.85	0.29	67,67,67,67	0
37	SR	0	9484	1/1	0.85	0.14	148,148,148,148	0
35	NA	D	9151	1/1	0.85	0.14	60,60,60,60	0
35	NA	0	9179	1/1	0.86	0.31	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	9182	1/1	0.86	0.14	68,68,68,68	0
33	MG	0	8063	1/1	0.86	0.14	74,74,74,74	0
35	NA	0	9170	1/1	0.86	0.46	92,92,92,92	0
35	NA	0	9126	1/1	0.86	0.14	49,49,49,49	0
35	NA	0	9127	1/1	0.86	0.27	75,75,75,75	0
35	NA	0	9166	1/1	0.86	0.36	76,76,76,76	0
33	MG	0	8110	1/1	0.87	0.23	40,40,40,40	0
35	NA	0	9120	1/1	0.87	0.17	59,59,59,59	0
37	SR	0	9490	1/1	0.87	0.14	129,129,129,129	0
35	NA	0	9175	1/1	0.87	0.20	42,42,42,42	0
33	MG	0	8060	1/1	0.87	0.20	88,88,88,88	0
33	MG	0	8083	1/1	0.87	0.14	51,51,51,51	0
33	MG	0	8090	1/1	0.87	0.19	67,67,67,67	0
33	MG	0	8089	1/1	0.88	0.23	54,54,54,54	0
33	MG	0	8094	1/1	0.88	0.14	65,65,65,65	0
37	SR	0	9547	1/1	0.88	0.22	175,175,175,175	0
36	CL	0	9316	1/1	0.88	0.26	74,74,74,74	0
34	K	0	9001	1/1	0.88	0.37	101,101,101,101	0
33	MG	0	8057	1/1	0.88	0.16	64,64,64,64	0
35	NA	0	9174	1/1	0.89	0.27	67,67,67,67	0
35	NA	0	9157	1/1	0.89	0.15	35,35,35,35	0
35	NA	0	9159	1/1	0.89	0.25	56,56,56,56	0
33	MG	0	8046	1/1	0.89	0.09	37,37,37,37	0
33	MG	0	8040	1/1	0.89	0.18	73,73,73,73	0
33	MG	0	8024	1/1	0.89	0.37	87,87,87,87	0
35	NA	0	9102	1/1	0.89	0.40	68,68,68,68	0
35	NA	0	9111	1/1	0.89	0.08	46,46,46,46	0
33	MG	0	8097	1/1	0.89	0.12	65,65,65,65	0
37	SR	B	9521	1/1	0.89	0.52	196,196,196,196	0
33	MG	9	8095	1/1	0.89	0.21	46,46,46,46	0
35	NA	0	9167	1/1	0.90	0.25	59,59,59,59	0
36	CL	3	9304	1/1	0.90	0.12	74,74,74,74	0
37	SR	0	9459	1/1	0.90	0.10	93,93,93,93	0
37	SR	0	9468	1/1	0.90	0.11	113,113,113,113	0
33	MG	0	8103	1/1	0.90	0.14	53,53,53,53	0
35	NA	0	9154	1/1	0.90	0.21	54,54,54,54	0
33	MG	A	8066	1/1	0.90	0.13	57,57,57,57	0
37	SR	0	9500	1/1	0.90	0.37	196,196,196,196	0
35	NA	9	9152	1/1	0.90	0.25	59,59,59,59	0
33	MG	0	8065	1/1	0.90	0.23	92,92,92,92	0
37	SR	0	9590	1/1	0.90	0.13	131,131,131,131	0
35	NA	B	9161	1/1	0.90	0.24	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8088	1/1	0.90	0.07	42,42,42,42	0
33	MG	0	8115	1/1	0.90	0.08	58,58,58,58	0
35	NA	0	9141	1/1	0.90	0.17	64,64,64,64	0
35	NA	J	9146	1/1	0.91	0.09	58,58,58,58	0
33	MG	0	8059	1/1	0.91	0.12	46,46,46,46	0
35	NA	0	9173	1/1	0.91	0.09	57,57,57,57	0
33	MG	0	8076	1/1	0.91	0.10	57,57,57,57	0
36	CL	A	9309	1/1	0.91	0.25	70,70,70,70	0
35	NA	0	9113	1/1	0.91	0.18	67,67,67,67	0
37	SR	0	9425	1/1	0.91	0.15	151,151,151,151	0
37	SR	9	9588	1/1	0.91	0.12	132,132,132,132	0
35	NA	0	9114	1/1	0.91	0.17	56,56,56,56	0
35	NA	0	9178	1/1	0.91	0.22	44,44,44,44	0
35	NA	0	9116	1/1	0.91	0.12	51,51,51,51	0
35	NA	0	9115	1/1	0.92	0.15	42,42,42,42	0
33	MG	0	8042	1/1	0.92	0.06	50,50,50,50	0
33	MG	0	8061	1/1	0.92	0.10	78,78,78,78	0
33	MG	0	8116	1/1	0.92	0.11	69,69,69,69	0
35	NA	0	9155	1/1	0.92	0.13	65,65,65,65	0
35	NA	0	9106	1/1	0.92	0.24	39,39,39,39	0
35	NA	0	9125	1/1	0.92	0.15	93,93,93,93	0
35	NA	0	9107	1/1	0.92	0.16	52,52,52,52	0
33	MG	0	8084	1/1	0.92	0.29	107,107,107,107	0
35	NA	0	9165	1/1	0.92	0.20	37,37,37,37	0
35	NA	0	9181	1/1	0.92	0.16	58,58,58,58	0
33	MG	0	8091	1/1	0.92	0.07	55,55,55,55	0
33	MG	0	8085	1/1	0.92	0.23	69,69,69,69	0
33	MG	T	8073	1/1	0.93	0.12	34,34,34,34	0
33	MG	0	8072	1/1	0.93	0.09	65,65,65,65	0
37	SR	0	9515	1/1	0.93	0.23	109,109,109,109	0
37	SR	0	9529	1/1	0.93	0.10	123,123,123,123	0
37	SR	0	9530	1/1	0.93	0.12	107,107,107,107	0
33	MG	0	8117	1/1	0.93	0.12	40,40,40,40	0
35	NA	0	9101	1/1	0.93	0.07	41,41,41,41	0
33	MG	0	8075	1/1	0.93	0.06	49,49,49,49	0
33	MG	0	8043	1/1	0.93	0.08	56,56,56,56	0
35	NA	R	9186	1/1	0.93	0.16	75,75,75,75	0
35	NA	0	9139	1/1	0.93	0.12	61,61,61,61	0
33	MG	0	8082	1/1	0.93	0.32	80,80,80,80	0
33	MG	0	8098	1/1	0.94	0.08	40,40,40,40	0
33	MG	0	8036	1/1	0.94	0.06	47,47,47,47	0
36	CL	B	9319	1/1	0.94	0.22	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CL	J	9321	1/1	0.94	0.10	65,65,65,65	0
36	CL	L	9310	1/1	0.94	0.14	51,51,51,51	0
37	SR	0	9534	1/1	0.94	0.30	113,113,113,113	0
37	SR	0	9539	1/1	0.94	0.36	173,173,173,173	0
33	MG	0	8093	1/1	0.94	0.06	45,45,45,45	0
37	SR	0	9566	1/1	0.94	0.14	97,97,97,97	0
35	NA	0	9110	1/1	0.94	0.14	39,39,39,39	0
33	MG	0	8041	1/1	0.94	0.09	52,52,52,52	0
37	SR	0	9626	1/1	0.94	0.37	146,146,146,146	0
35	NA	0	9156	1/1	0.94	0.17	57,57,57,57	0
35	NA	0	9135	1/1	0.94	0.16	42,42,42,42	0
35	NA	0	9158	1/1	0.94	0.14	46,46,46,46	0
37	SR	H	9486	1/1	0.94	0.26	121,121,121,121	0
38	SPS	4	9701	23/23	0.94	0.11	39,45,57,60	0
33	MG	0	8051	1/1	0.94	0.09	24,24,24,24	0
39	CD	Z	9203	1/1	0.94	0.15	155,155,155,155	0
33	MG	0	8019	1/1	0.95	0.07	52,52,52,52	0
33	MG	0	8054	1/1	0.95	0.07	61,61,61,61	0
37	SR	0	9532	1/1	0.95	0.11	114,114,114,114	0
35	NA	T	9143	1/1	0.95	0.09	37,37,37,37	0
37	SR	0	9465	1/1	0.95	0.08	105,105,105,105	0
35	NA	0	9128	1/1	0.95	0.13	40,40,40,40	0
35	NA	0	9149	1/1	0.95	0.07	46,46,46,46	0
37	SR	0	9483	1/1	0.95	0.07	77,77,77,77	0
36	CL	0	9317	1/1	0.95	0.10	58,58,58,58	0
35	NA	0	9123	1/1	0.95	0.13	50,50,50,50	0
37	SR	0	9495	1/1	0.95	0.06	90,90,90,90	0
35	NA	C	9104	1/1	0.95	0.09	26,26,26,26	0
33	MG	0	8104	1/1	0.95	0.08	58,58,58,58	0
37	SR	0	9504	1/1	0.95	0.07	92,92,92,92	0
37	SR	0	9505	1/1	0.95	0.20	117,117,117,117	0
37	SR	0	9506	1/1	0.95	0.15	108,108,108,108	0
35	NA	0	9118	1/1	0.95	0.13	43,43,43,43	0
33	MG	0	8058	1/1	0.96	0.12	34,34,34,34	0
36	CL	0	9322	1/1	0.96	0.29	53,53,53,53	0
35	NA	0	9134	1/1	0.96	0.04	38,38,38,38	0
33	MG	4	8118	1/1	0.96	0.09	29,29,29,29	0
33	MG	0	8067	1/1	0.96	0.15	35,35,35,35	0
33	MG	0	8112	1/1	0.96	0.04	44,44,44,44	0
36	CL	M	9318	1/1	0.96	0.07	40,40,40,40	0
36	CL	N	9307	1/1	0.96	0.08	60,60,60,60	0
36	CL	Y	9320	1/1	0.96	0.07	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8031	1/1	0.96	0.05	48,48,48,48	0
33	MG	0	8032	1/1	0.96	0.08	34,34,34,34	0
37	SR	0	9446	1/1	0.96	0.07	93,93,93,93	0
37	SR	0	9452	1/1	0.96	0.09	94,94,94,94	0
37	SR	0	9568	1/1	0.96	0.06	86,86,86,86	0
37	SR	0	9581	1/1	0.96	0.06	105,105,105,105	0
37	SR	0	9585	1/1	0.96	0.06	91,91,91,91	0
33	MG	0	8025	1/1	0.96	0.18	19,19,19,19	0
33	MG	0	8106	1/1	0.96	0.05	39,39,39,39	0
33	MG	0	8037	1/1	0.96	0.05	42,42,42,42	0
37	SR	9	9503	1/1	0.96	0.06	105,105,105,105	0
37	SR	0	9469	1/1	0.96	0.07	88,88,88,88	0
36	CL	0	9303	1/1	0.96	0.09	47,47,47,47	0
36	CL	0	9311	1/1	0.96	0.09	66,66,66,66	0
36	CL	0	9313	1/1	0.96	0.07	51,51,51,51	0
37	SR	0	9489	1/1	0.96	0.07	101,101,101,101	0
36	CL	0	9315	1/1	0.96	0.10	58,58,58,58	0
35	NA	0	9130	1/1	0.96	0.05	41,41,41,41	0
33	MG	Y	8109	1/1	0.97	0.04	39,39,39,39	0
33	MG	0	8013	1/1	0.97	0.20	10,10,10,10	0
37	SR	0	9508	1/1	0.97	0.07	87,87,87,87	0
37	SR	0	9432	1/1	0.97	0.10	65,65,65,65	0
37	SR	0	9517	1/1	0.97	0.06	94,94,94,94	0
37	SR	0	9522	1/1	0.97	0.07	100,100,100,100	0
37	SR	0	9433	1/1	0.97	0.10	74,74,74,74	0
33	MG	0	8096	1/1	0.97	0.06	37,37,37,37	0
33	MG	0	8039	1/1	0.97	0.08	45,45,45,45	0
33	MG	0	8009	1/1	0.97	0.05	31,31,31,31	0
37	SR	0	9461	1/1	0.97	0.07	86,86,86,86	0
37	SR	0	9545	1/1	0.97	0.07	84,84,84,84	0
37	SR	0	9464	1/1	0.97	0.06	80,80,80,80	0
37	SR	0	9560	1/1	0.97	0.07	94,94,94,94	0
35	NA	0	9117	1/1	0.97	0.05	31,31,31,31	0
37	SR	0	9467	1/1	0.97	0.06	73,73,73,73	0
37	SR	0	9570	1/1	0.97	0.09	117,117,117,117	0
35	NA	0	9105	1/1	0.97	0.06	36,36,36,36	0
35	NA	0	9131	1/1	0.97	0.08	51,51,51,51	0
37	SR	0	9475	1/1	0.97	0.06	80,80,80,80	0
37	SR	0	9477	1/1	0.97	0.06	79,79,79,79	0
33	MG	0	8029	1/1	0.97	0.09	22,22,22,22	0
36	CL	J	9301	1/1	0.97	0.12	50,50,50,50	0
33	MG	B	8056	1/1	0.97	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	A	9436	1/1	0.97	0.17	87,87,87,87	0
37	SR	A	9497	1/1	0.97	0.06	99,99,99,99	0
33	MG	0	8080	1/1	0.97	0.12	46,46,46,46	0
35	NA	0	9160	1/1	0.97	0.11	45,45,45,45	0
37	SR	F	9595	1/1	0.97	0.11	92,92,92,92	0
35	NA	0	9162	1/1	0.97	0.08	43,43,43,43	0
37	SR	S	9470	1/1	0.97	0.07	98,98,98,98	0
36	CL	O	9308	1/1	0.97	0.16	56,56,56,56	0
36	CL	R	9306	1/1	0.97	0.06	45,45,45,45	0
35	NA	0	9136	1/1	0.97	0.10	32,32,32,32	0
33	MG	0	8070	1/1	0.98	0.06	26,26,26,26	0
37	SR	0	9454	1/1	0.98	0.04	79,79,79,79	0
37	SR	0	9455	1/1	0.98	0.04	66,66,66,66	0
33	MG	0	8079	1/1	0.98	0.03	29,29,29,29	0
33	MG	0	8026	1/1	0.98	0.08	25,25,25,25	0
35	NA	M	9147	1/1	0.98	0.05	33,33,33,33	0
36	CL	0	9305	1/1	0.98	0.07	58,58,58,58	0
37	SR	0	9466	1/1	0.98	0.06	95,95,95,95	0
37	SR	0	9629	1/1	0.98	0.04	73,73,73,73	0
37	SR	9	9481	1/1	0.98	0.04	86,86,86,86	0
37	SR	0	9509	1/1	0.98	0.05	86,86,86,86	0
37	SR	0	9405	1/1	0.98	0.06	81,81,81,81	0
37	SR	0	9420	1/1	0.98	0.09	74,74,74,74	0
37	SR	A	9437	1/1	0.98	0.05	70,70,70,70	0
35	NA	Q	9148	1/1	0.98	0.05	48,48,48,48	0
35	NA	R	9137	1/1	0.98	0.04	23,23,23,23	0
36	CL	0	9314	1/1	0.98	0.19	52,52,52,52	0
37	SR	0	9478	1/1	0.98	0.05	72,72,72,72	0
37	SR	0	9480	1/1	0.98	0.04	83,83,83,83	0
37	SR	0	9438	1/1	0.98	0.05	66,66,66,66	0
37	SR	0	9441	1/1	0.98	0.04	64,64,64,64	0
33	MG	0	8002	1/1	0.98	0.04	33,33,33,33	0
37	SR	0	9447	1/1	0.98	0.04	62,62,62,62	0
37	SR	0	9473	1/1	0.99	0.06	77,77,77,77	0
37	SR	0	9474	1/1	0.99	0.04	68,68,68,68	0
33	MG	0	8020	1/1	0.99	0.06	37,37,37,37	0
37	SR	0	9407	1/1	0.99	0.09	50,50,50,50	0
37	SR	0	9410	1/1	0.99	0.09	46,46,46,46	0
37	SR	0	9411	1/1	0.99	0.10	49,49,49,49	0
37	SR	0	9412	1/1	0.99	0.05	51,51,51,51	0
37	SR	0	9413	1/1	0.99	0.05	50,50,50,50	0
37	SR	0	9414	1/1	0.99	0.06	56,56,56,56	0

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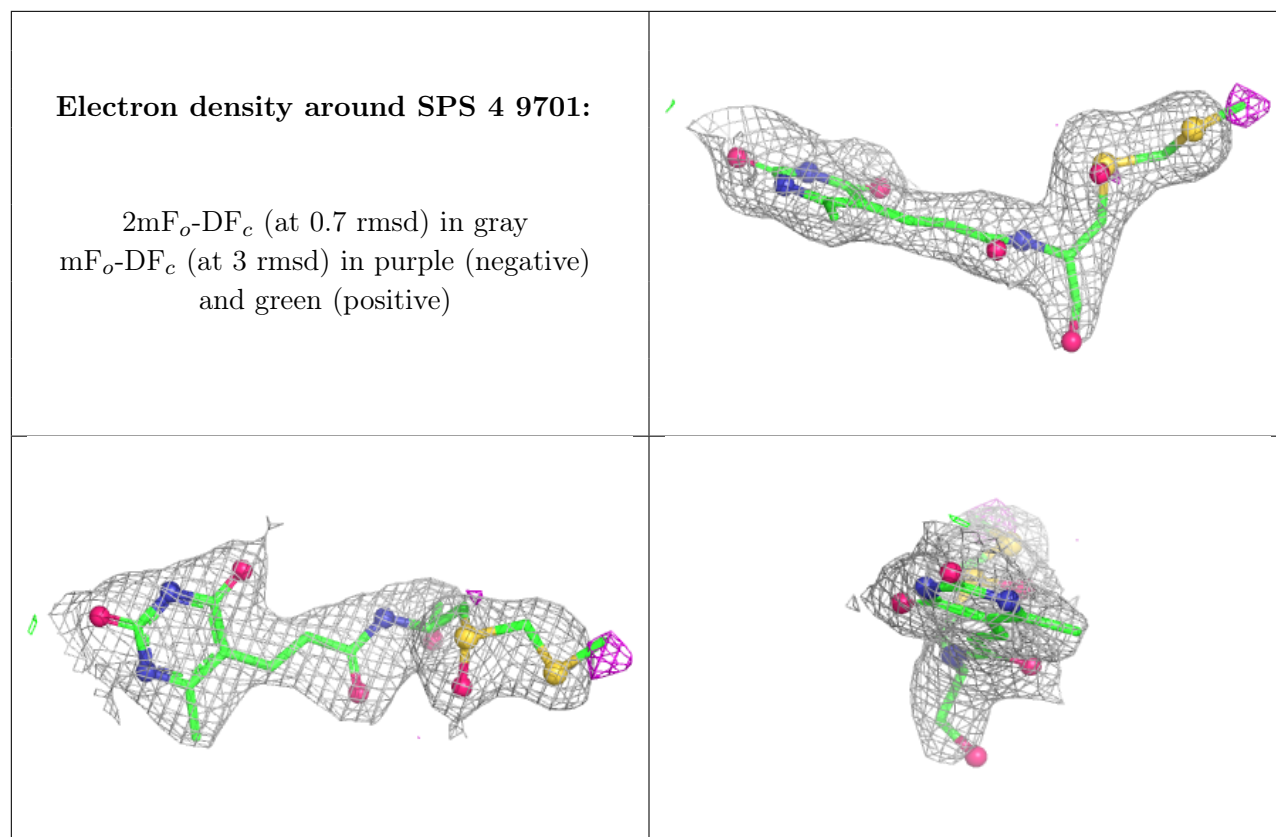
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	9488	1/1	0.99	0.04	80,80,80,80	0
37	SR	0	9416	1/1	0.99	0.04	48,48,48,48	0
37	SR	0	9417	1/1	0.99	0.05	58,58,58,58	0
33	MG	0	8021	1/1	0.99	0.07	49,49,49,49	0
37	SR	0	9498	1/1	0.99	0.03	65,65,65,65	0
37	SR	0	9421	1/1	0.99	0.05	68,68,68,68	0
37	SR	0	9422	1/1	0.99	0.03	57,57,57,57	0
37	SR	0	9423	1/1	0.99	0.03	56,56,56,56	0
33	MG	0	8038	1/1	0.99	0.10	16,16,16,16	0
37	SR	0	9426	1/1	0.99	0.03	72,72,72,72	0
37	SR	0	9427	1/1	0.99	0.06	55,55,55,55	0
37	SR	0	9428	1/1	0.99	0.04	51,51,51,51	0
37	SR	0	9429	1/1	0.99	0.06	67,67,67,67	0
37	SR	0	9431	1/1	0.99	0.05	57,57,57,57	0
33	MG	0	8001	1/1	0.99	0.10	17,17,17,17	0
33	MG	0	8012	1/1	0.99	0.09	26,26,26,26	0
37	SR	0	9434	1/1	0.99	0.07	61,61,61,61	0
37	SR	0	9435	1/1	0.99	0.03	71,71,71,71	0
33	MG	0	8003	1/1	0.99	0.03	24,24,24,24	0
37	SR	0	9440	1/1	0.99	0.03	60,60,60,60	0
35	NA	0	9138	1/1	0.99	0.06	56,56,56,56	0
37	SR	0	9442	1/1	0.99	0.04	63,63,63,63	0
37	SR	0	9443	1/1	0.99	0.03	62,62,62,62	0
37	SR	0	9444	1/1	0.99	0.03	52,52,52,52	0
37	SR	0	9445	1/1	0.99	0.04	62,62,62,62	0
33	MG	K	8069	1/1	0.99	0.07	20,20,20,20	0
33	MG	0	8004	1/1	0.99	0.02	24,24,24,24	0
37	SR	0	9448	1/1	0.99	0.03	64,64,64,64	0
37	SR	0	9449	1/1	0.99	0.03	61,61,61,61	0
37	SR	0	9450	1/1	0.99	0.03	63,63,63,63	0
37	SR	0	9451	1/1	0.99	0.07	57,57,57,57	0
33	MG	0	8027	1/1	0.99	0.14	31,31,31,31	0
37	SR	0	9453	1/1	0.99	0.05	76,76,76,76	0
36	CL	J	9302	1/1	0.99	0.04	54,54,54,54	0
33	MG	0	8044	1/1	0.99	0.03	35,35,35,35	0
37	SR	0	9456	1/1	0.99	0.04	69,69,69,69	0
37	SR	0	9457	1/1	0.99	0.05	50,50,50,50	0
36	CL	K	9312	1/1	0.99	0.04	45,45,45,45	0
33	MG	0	8028	1/1	0.99	0.02	31,31,31,31	0
37	SR	B	9458	1/1	0.99	0.04	66,66,66,66	0
37	SR	0	9462	1/1	0.99	0.05	67,67,67,67	0
33	MG	0	8068	1/1	0.99	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8015	1/1	0.99	0.02	29,29,29,29	0
37	SR	R	9418	1/1	0.99	0.06	58,58,58,58	0
33	MG	0	8030	1/1	0.99	0.03	38,38,38,38	0
37	SR	1	9419	1/1	0.99	0.07	47,47,47,47	0
37	SR	1	9460	1/1	0.99	0.04	52,52,52,52	0
37	SR	3	9439	1/1	0.99	0.06	79,79,79,79	0
33	MG	0	8017	1/1	0.99	0.06	18,18,18,18	0
33	MG	0	8005	1/1	0.99	0.05	31,31,31,31	0
35	NA	0	9108	1/1	0.99	0.03	31,31,31,31	0
39	CD	1	9202	1/1	0.99	0.04	58,58,58,58	0
39	CD	3	9204	1/1	0.99	0.10	70,70,70,70	0
33	MG	0	8008	1/1	1.00	0.09	15,15,15,15	0
37	SR	0	9415	1/1	1.00	0.06	57,57,57,57	0
37	SR	0	9406	1/1	1.00	0.10	45,45,45,45	0
37	SR	0	9430	1/1	1.00	0.05	48,48,48,48	0
37	SR	0	9424	1/1	1.00	0.08	49,49,49,49	0
39	CD	U	9201	1/1	1.00	0.02	61,61,61,61	0
37	SR	L	9409	1/1	1.00	0.05	46,46,46,46	0
33	MG	0	8074	1/1	1.00	0.13	15,15,15,15	0
37	SR	0	9408	1/1	1.00	0.11	48,48,48,48	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.