



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:58 PM UTC

PDB ID : 1VQ8 / pdb_00001vq8
Title : The structure of CCDA-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 : 2.20 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:

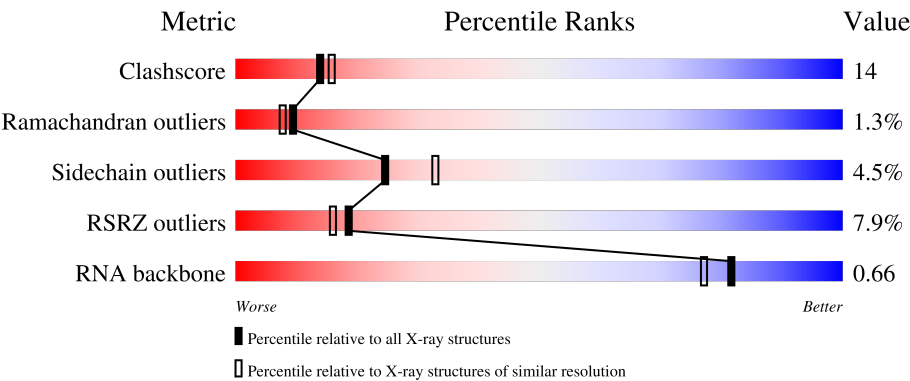
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)
RNA backbone	3983	1052 (2.50-1.90)

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	3% 65% 24% 6%
2	9	122	5% 53% 36% 9%
3	4	5	20% 80% 20%
4	A	240	8% 55% 36% 8%
5	B	338	4% 55% 39% 6%

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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	194	
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
35	NA	0	9169	-	-	-	X
37	SR	0	9500	-	-	-	X
37	SR	B	9521	-	-	-	X
39	CD	O	9205	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 99035 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*(DA)*(PHE)*(ACA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	5	Total	C	N	O	P	0	0	0
			73	40	12	19	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

- 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

- 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

- 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

- 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

- 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

- 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	88	Total	Mg	0	0
			88	88		
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	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	65	Total	Na	0	0
			65	65		
35	9	1	Total	Na	0	0
			1	1		
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		
35	J	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total 10	Cl 10	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	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).

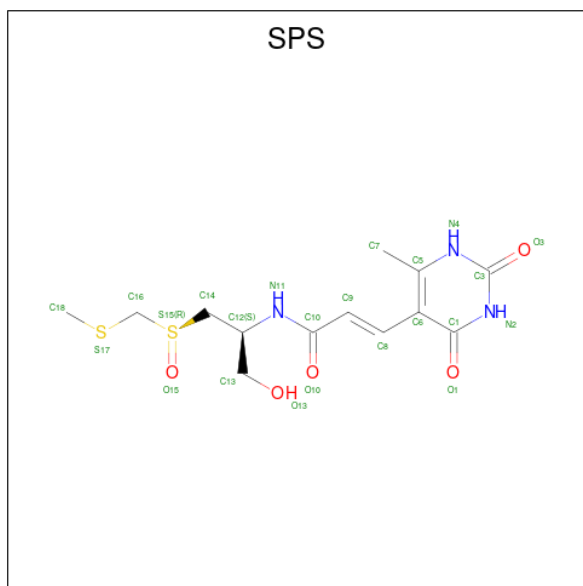
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total 98	Sr 98	0	0
37	9	3	Total 3	Sr 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	3	Total 3	Sr 3	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: $C_{13}H_{19}N_3O_5S_2$).



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

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

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

- Molecule 40 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	0	5743	Total O 5743 5743	0	0
40	9	136	Total O 136 136	0	0
40	4	2	Total O 2 2	0	0
40	A	120	Total O 120 120	0	0
40	B	135	Total O 135 135	0	0
40	C	172	Total O 172 172	0	0
40	D	48	Total O 48 48	0	0
40	E	42	Total O 42 42	0	0
40	F	27	Total O 27 27	0	0
40	G	16	Total O 16 16	0	0
40	H	71	Total O 71 71	0	0
40	J	51	Total O 51 51	0	0
40	K	58	Total O 58 58	0	0
40	L	87	Total O 87 87	0	0
40	M	127	Total O 127 127	0	0

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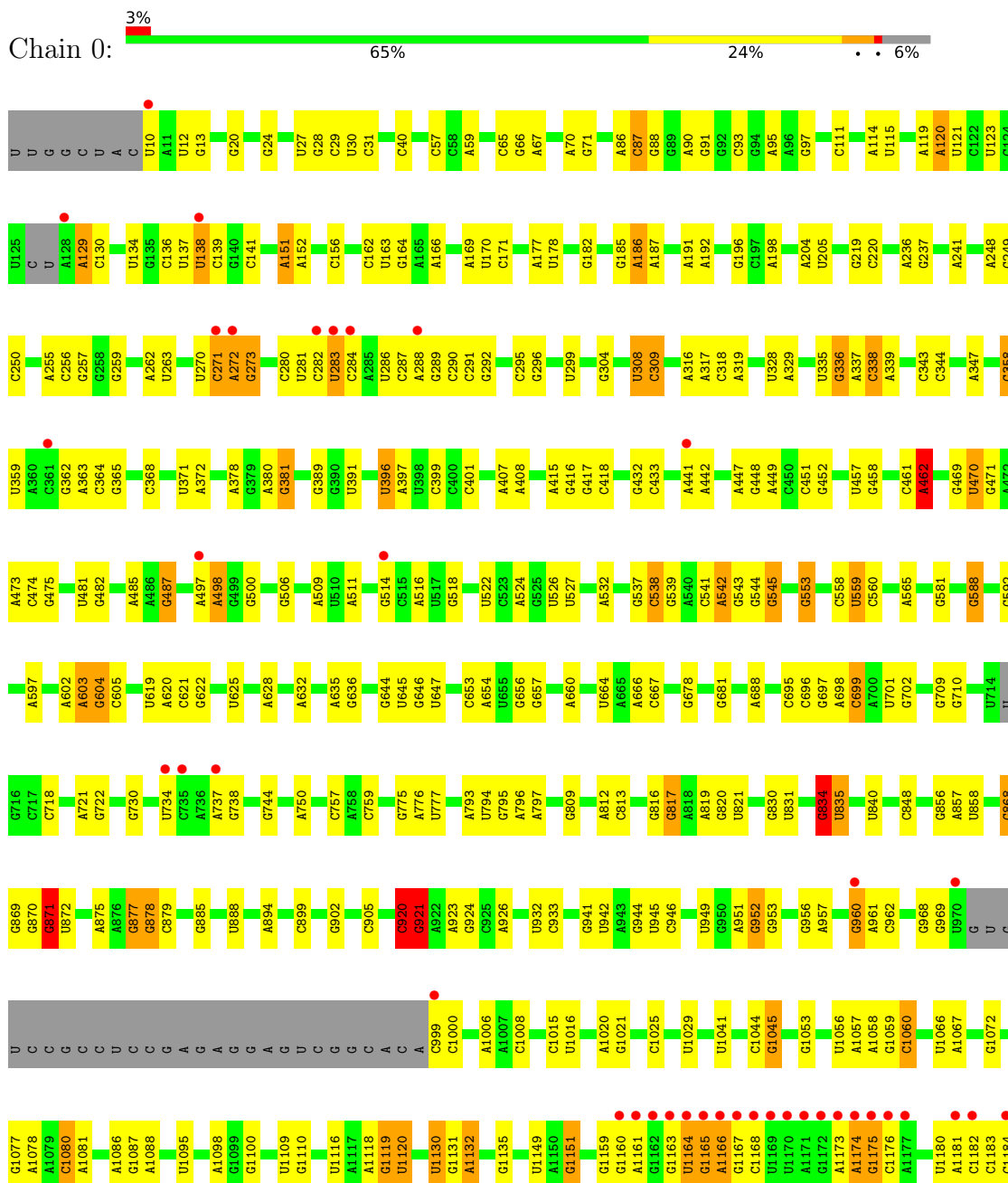
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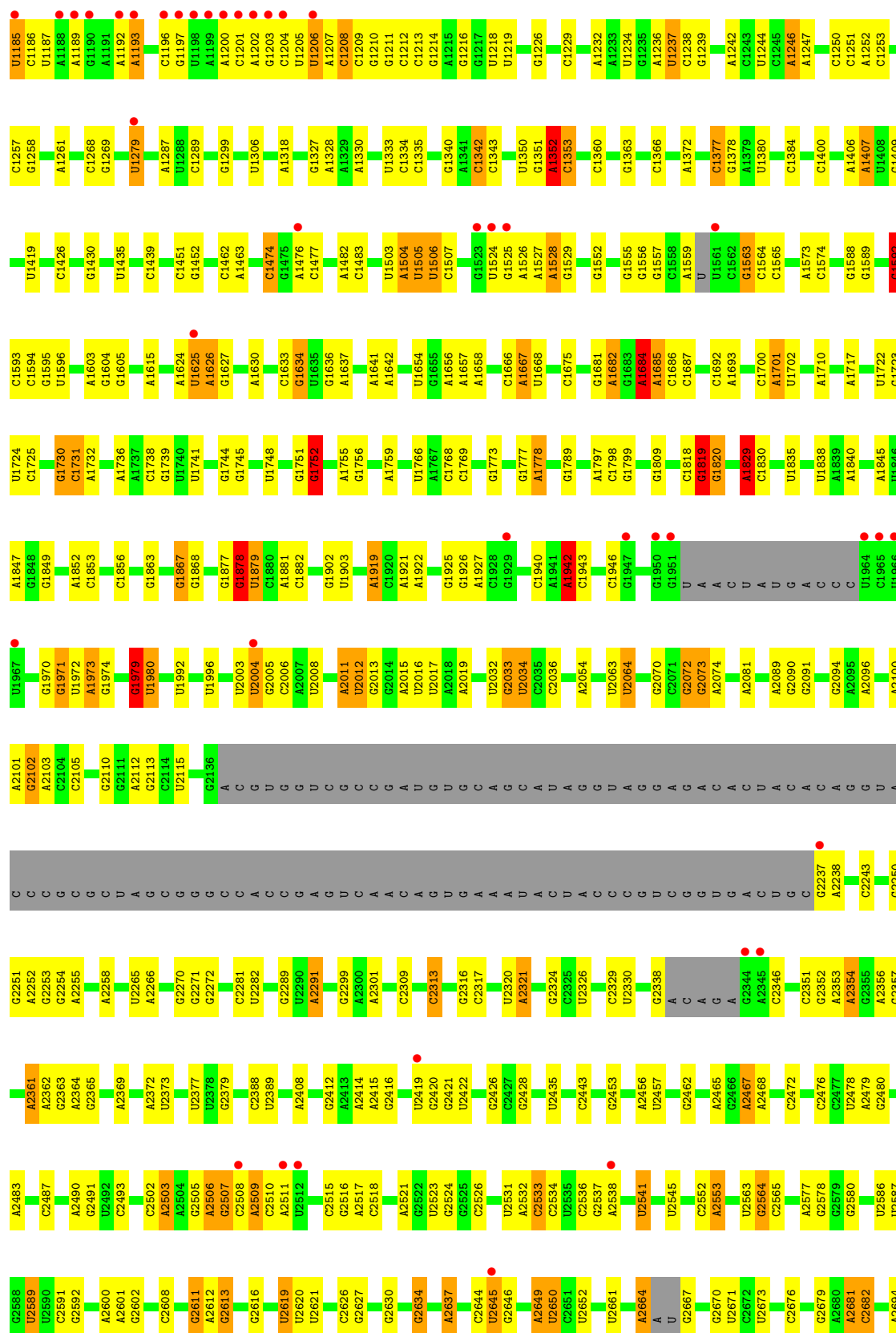
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	N	59	Total	O	0	0
			59	59		
40	O	41	Total	O	0	0
			41	41		
40	P	64	Total	O	0	0
			64	64		
40	Q	58	Total	O	0	0
			58	58		
40	R	85	Total	O	0	0
			85	85		
40	S	30	Total	O	0	0
			30	30		
40	T	36	Total	O	0	0
			36	36		
40	U	28	Total	O	0	0
			28	28		
40	V	15	Total	O	0	0
			15	15		
40	W	68	Total	O	0	0
			68	68		
40	X	23	Total	O	0	0
			23	23		
40	Y	95	Total	O	0	0
			95	95		
40	Z	35	Total	O	0	0
			35	35		
40	1	50	Total	O	0	0
			50	50		
40	2	35	Total	O	0	0
			35	35		
40	3	76	Total	O	0	0
			76	76		
40	I	10	Total	O	0	0
			10	10		

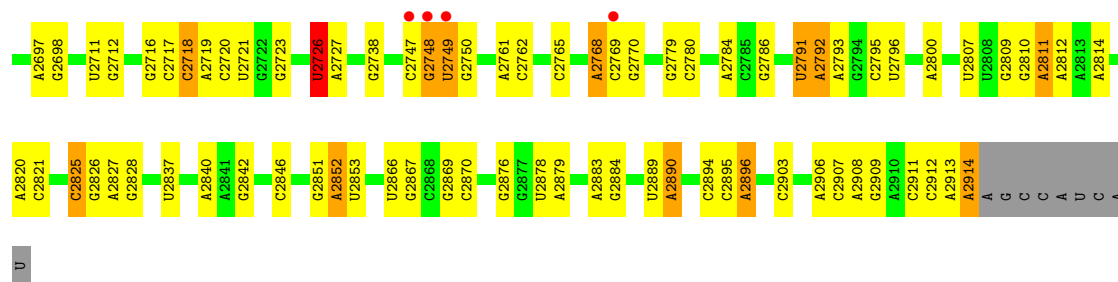
3 Residue-property plots [i](#)

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

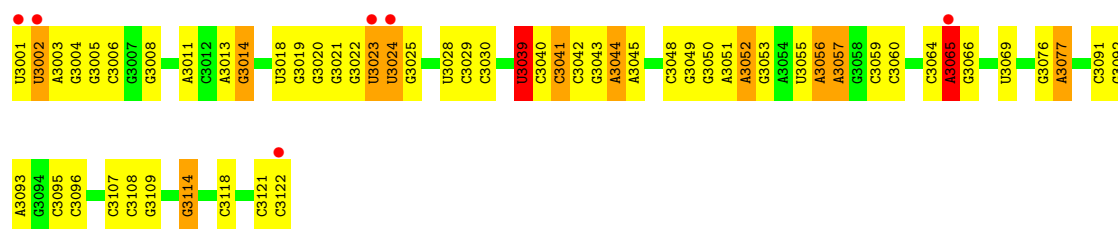
- Molecule 1: 23S ribosomal rna



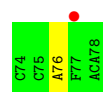




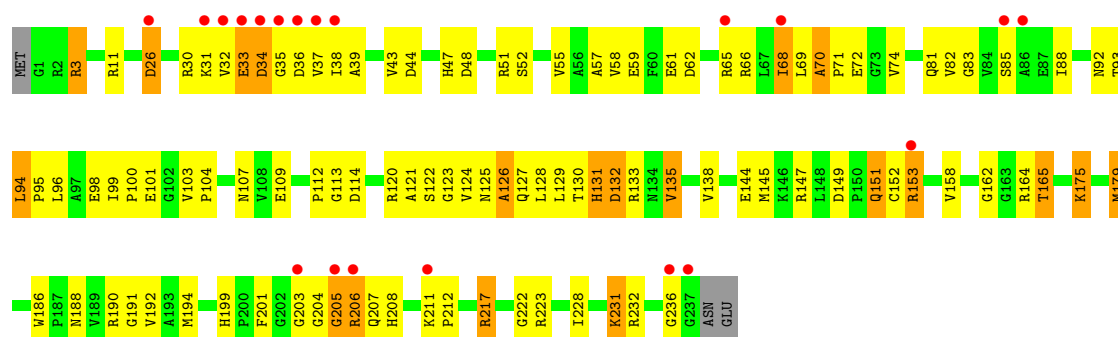
• Molecule 2: 5S ribosomal RNA



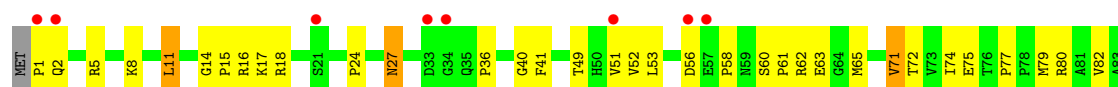
• Molecule 3: 5'-R(*CP*CP*(DA)*(PHE)*(ACA))-3'

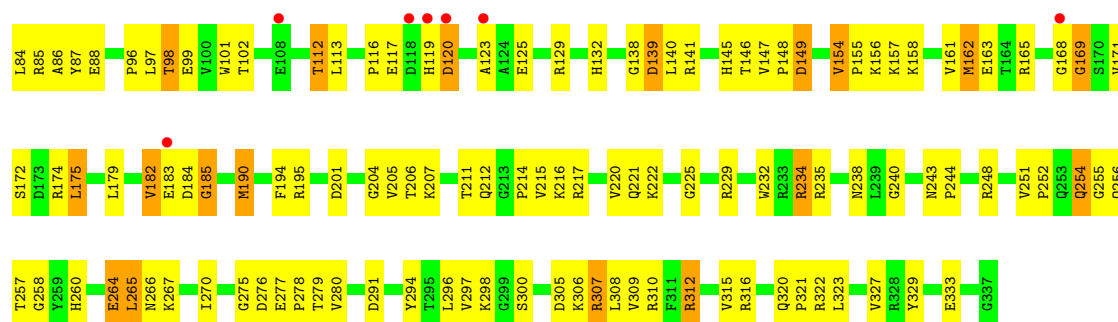


• Molecule 4: 50S ribosomal protein L2P

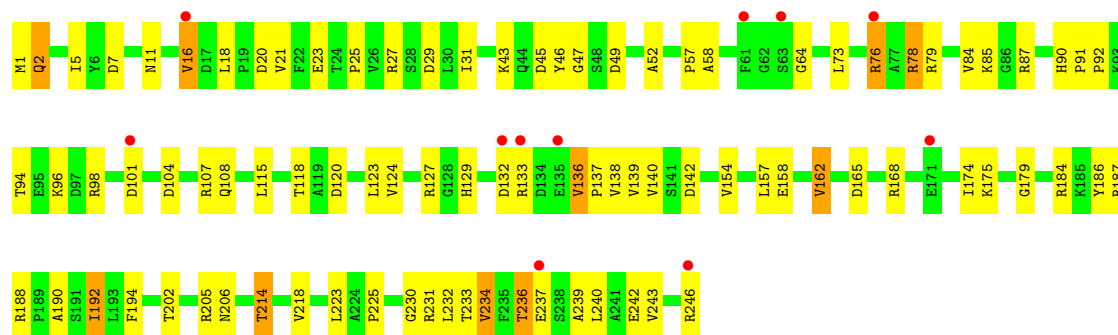


• Molecule 5: 50S ribosomal protein L3P

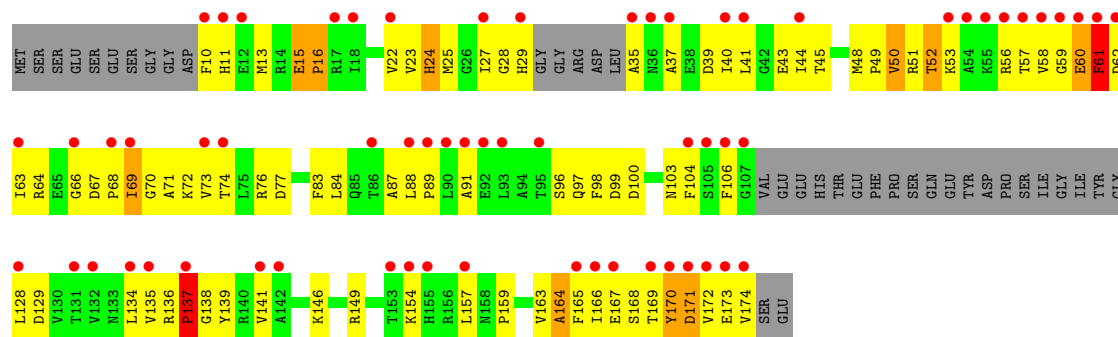




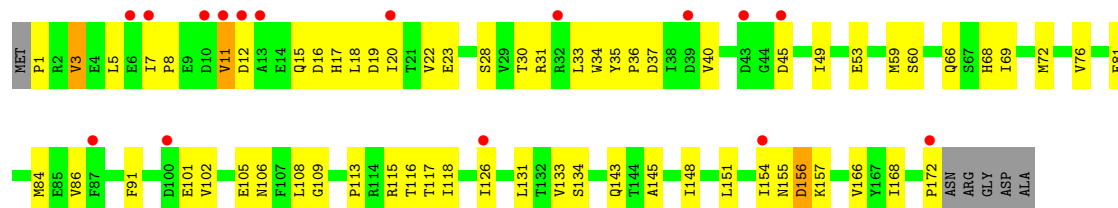
• Molecule 6: 50S ribosomal protein L4E



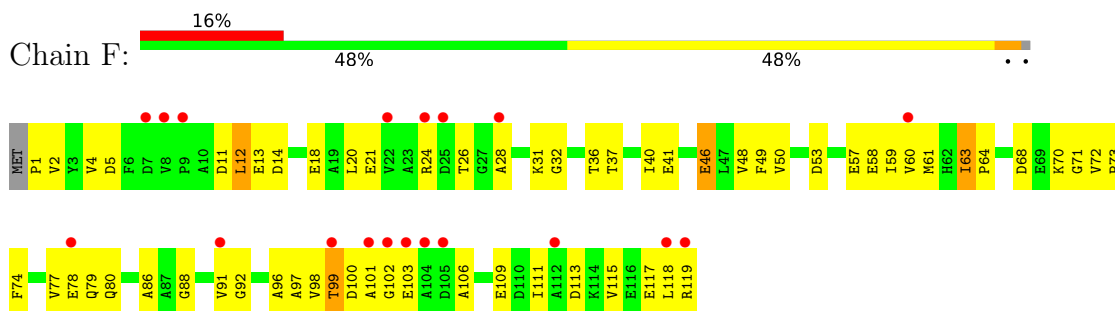
• Molecule 7: 50S ribosomal protein L5P



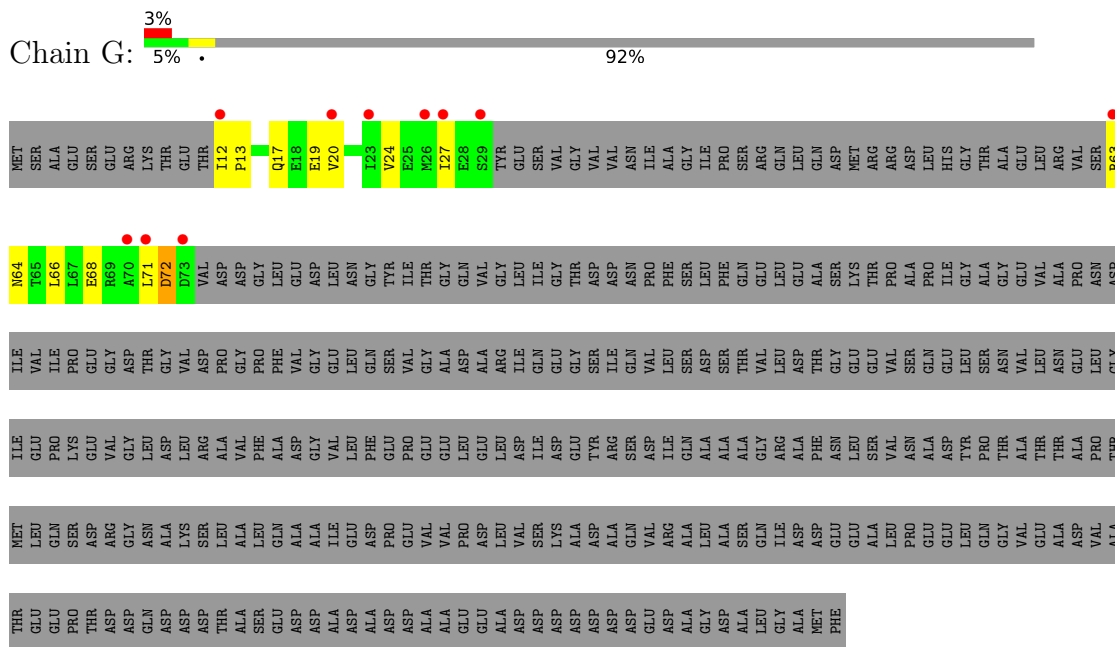
• Molecule 8: 50S ribosomal protein L6P



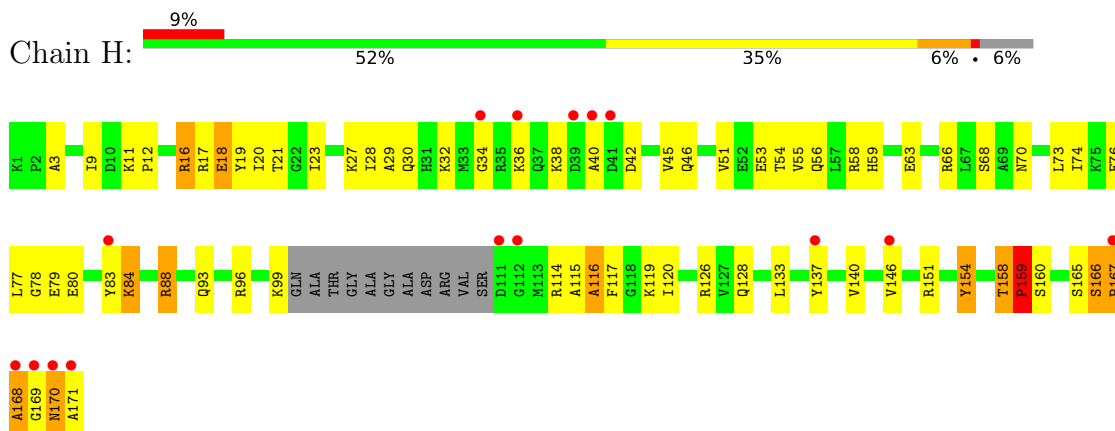
- Molecule 9: 50S ribosomal protein L7AE



- Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

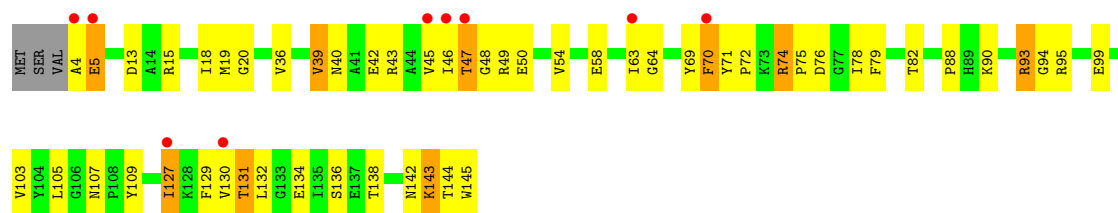


- Molecule 11: 50S RIBOSOMAL PROTEIN L10E



- Molecule 12: 50S ribosomal protein L13P

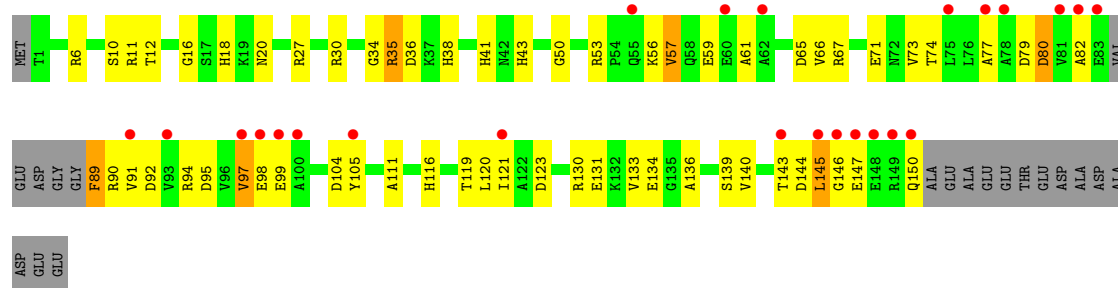




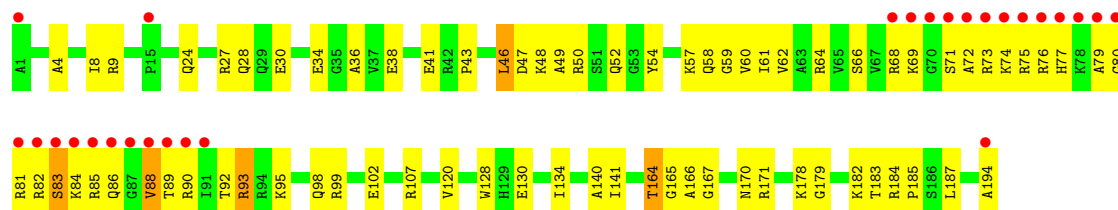
- Molecule 13: 50S ribosomal protein L14P



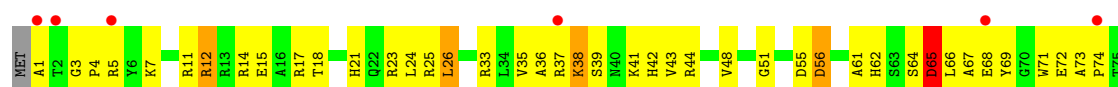
- Molecule 14: 50S ribosomal protein L15P

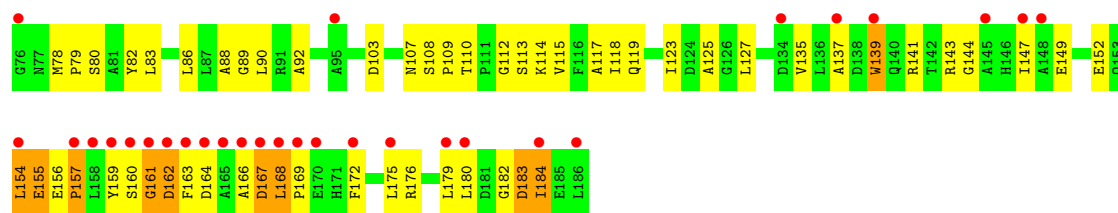


- Molecule 15: 50S Ribosomal Protein L15E

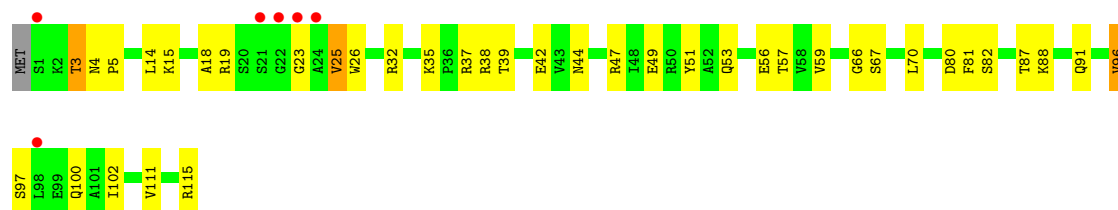


- Molecule 16: 50S ribosomal protein L18P

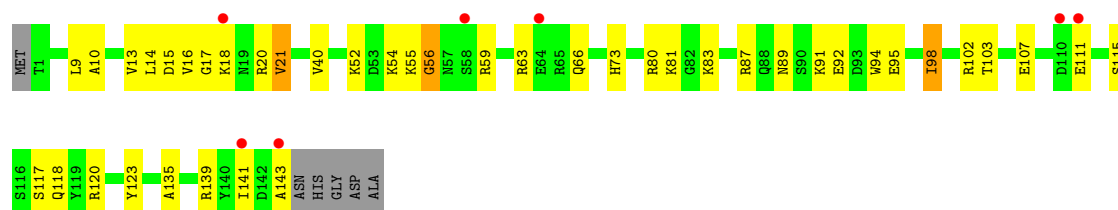




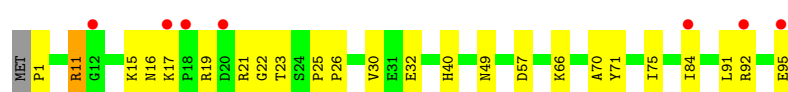
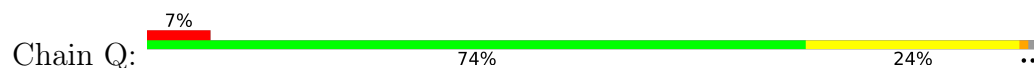
• Molecule 17: 50S ribosomal protein L18e



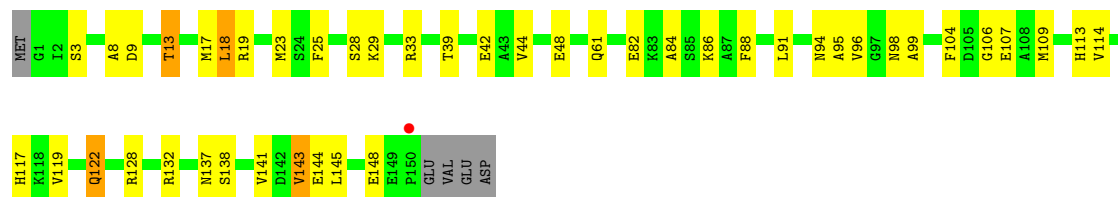
• Molecule 18: 50S ribosomal protein L19E



• Molecule 19: 50S ribosomal protein L21e



• Molecule 20: 50S ribosomal protein L22P



• Molecule 21: 50S ribosomal protein L23P

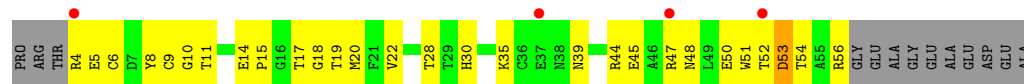




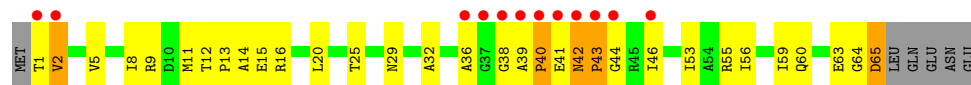
• Molecule 22: 50S ribosomal protein L24P



• Molecule 23: 50S ribosomal protein L24E



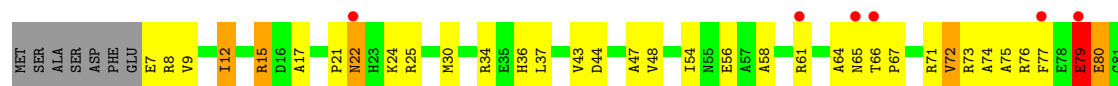
• Molecule 24: 50S ribosomal protein L29P



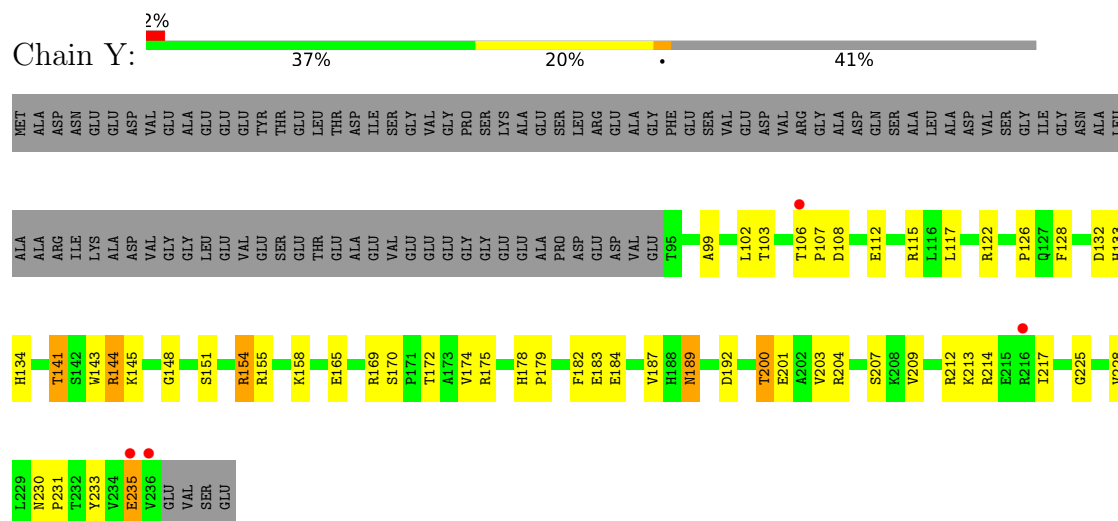
• Molecule 25: 50S ribosomal protein L30P



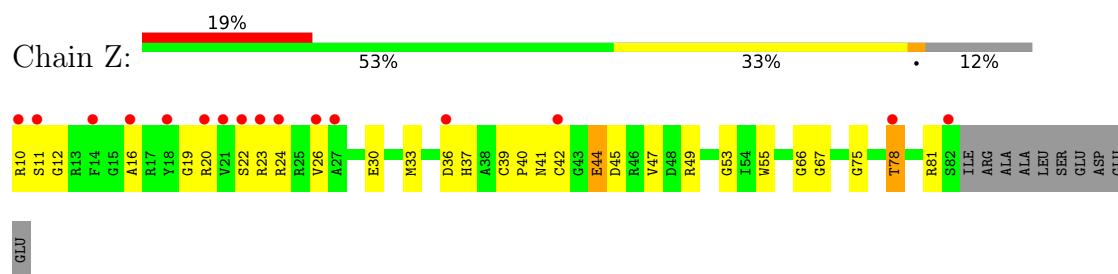
• Molecule 26: 50S ribosomal protein L31e



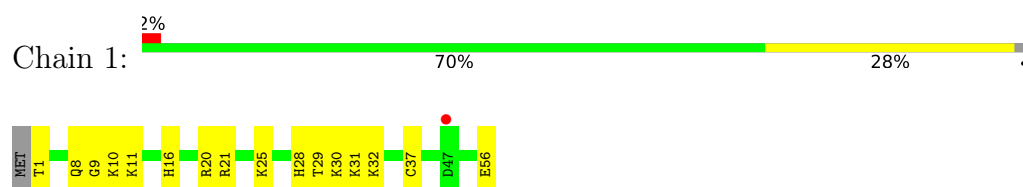
- Molecule 27: 50S ribosomal protein L32E



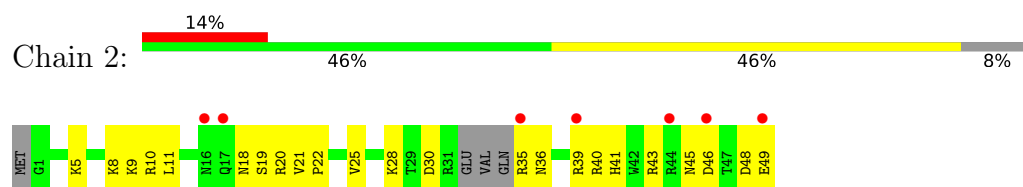
- Molecule 28: 50S ribosomal protein L37Ae



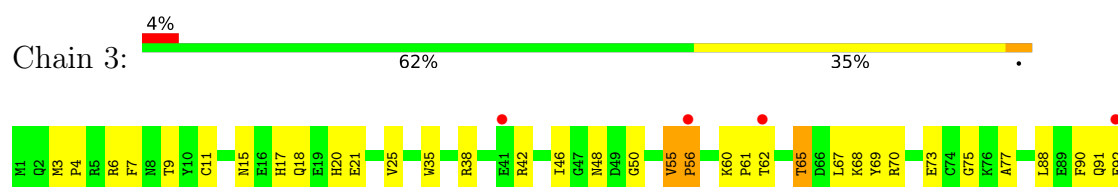
- Molecule 29: 50S ribosomal protein L37e



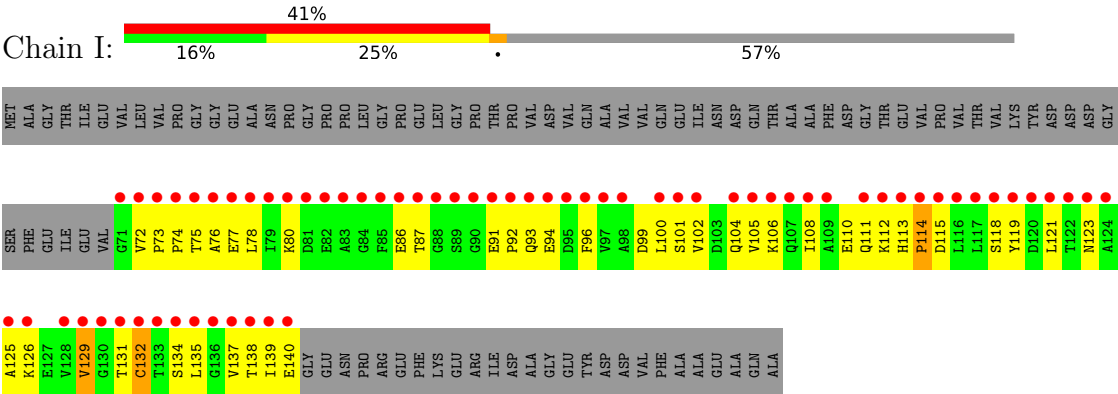
- Molecule 30: 50S ribosomal protein L39e



- 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	211.52Å 298.48Å 574.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.1 (50.00-2.20) 90.0 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.247 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.3	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	0.95	EDS
Total number of atoms	99035	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% 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: PSU, UR3, SPS, NA, SR, 1MA, ACA, K, OMG, CL, MG, CD, OMU

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	0.39	0/65959	0.63	35/102870 (0.0%)
2	9	0.39	0/2905	0.62	3/4528 (0.1%)
3	4	0.42	0/75	0.65	0/110
4	A	0.42	0/1786	0.99	7/2408 (0.3%)
5	B	0.41	0/2690	1.01	14/3652 (0.4%)
6	C	0.44	0/1884	0.99	10/2551 (0.4%)
7	D	0.35	0/1111	0.91	5/1498 (0.3%)
8	E	0.38	0/1382	0.86	3/1880 (0.2%)
9	F	0.39	0/901	0.88	2/1224 (0.2%)
10	G	0.35	0/241	0.77	0/324
11	H	0.37	0/1287	0.95	6/1725 (0.3%)
12	J	0.39	0/1136	0.92	2/1530 (0.1%)
13	K	0.41	0/1001	0.96	1/1347 (0.1%)
14	L	0.39	0/1130	0.99	4/1509 (0.3%)
15	M	0.40	0/1584	0.90	3/2119 (0.1%)
16	N	0.35	0/1474	0.97	8/1999 (0.4%)
17	O	0.40	0/874	0.94	4/1181 (0.3%)
18	P	0.39	0/1147	0.90	1/1528 (0.1%)
19	Q	0.41	0/749	1.03	2/1005 (0.2%)
20	R	0.41	0/1172	0.95	5/1578 (0.3%)
21	S	0.36	0/648	0.88	2/875 (0.2%)
22	T	0.36	0/958	0.94	7/1289 (0.5%)
23	U	0.40	0/417	0.88	2/562 (0.4%)
24	V	0.34	0/502	0.91	2/675 (0.3%)
25	W	0.44	0/1219	0.94	3/1655 (0.2%)
26	X	0.42	0/664	0.94	4/895 (0.4%)
27	Y	0.43	0/1146	0.99	4/1536 (0.3%)
28	Z	0.38	0/589	0.94	1/787 (0.1%)
29	1	0.45	0/438	0.92	0/578
30	2	0.44	0/401	0.85	0/529
31	3	0.39	0/771	0.87	2/1024 (0.2%)
32	I	0.36	0/526	0.89	2/716 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	0/98767	0.73	144/147687 (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	51
2	9	0	2
All	All	1	53

There are no bond length outliers.

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	14.47	131.21	109.50
19	Q	17	LYS	N-CA-C	-10.26	96.81	109.83
16	N	163	PHE	N-CA-C	-9.35	100.65	112.90
1	0	1563	G	C4'-C3'-O3'	8.50	122.15	109.40
1	0	1352	A	C2'-C3'-O3'	8.37	122.06	109.50
4	A	222	GLY	N-CA-C	-7.78	105.22	114.48
8	E	11	VAL	N-CA-C	7.73	120.63	108.89
1	0	1942	A	C5'-C4'-C3'	7.71	127.56	116.00
5	B	157	LYS	N-CA-C	-7.53	105.00	114.56
26	X	12	ILE	N-CA-C	7.52	115.36	107.76
5	B	222	LYS	N-CA-C	-7.50	99.43	110.52
1	0	1979	G	C2'-C3'-O3'	7.43	124.85	113.70
1	0	1819	G	C5'-C4'-C3'	7.39	127.09	116.00
2	9	3039	U	N1-C1'-C2'	7.26	122.89	112.00
27	Y	143	TRP	N-CA-C	7.07	120.63	110.10
1	0	1592	G	N9-C1'-C2'	7.03	122.54	112.00
21	S	27	ALA	N-CA-C	-7.00	97.85	109.46
27	Y	183	GLU	N-CA-C	-6.97	98.33	109.76
6	C	78	ARG	N-CA-C	6.83	118.17	108.74
1	0	871	G	C5'-C4'-O4'	-6.77	99.64	109.80
5	B	120	ASP	CA-C-N	6.77	126.47	119.56
5	B	120	ASP	C-N-CA	6.77	126.47	119.56
6	C	188	ARG	N-CA-C	6.75	114.29	108.22
1	0	920	C	C2'-C3'-O3'	-6.70	103.64	113.70
20	R	141	VAL	N-CA-C	6.67	117.45	108.11
5	B	266	ASN	N-CA-C	6.57	120.43	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	89	THR	N-CA-C	6.55	119.75	111.69
7	D	170	TYR	N-CA-C	6.51	120.64	111.52
15	M	8	ILE	N-CA-C	-6.49	104.43	110.53
16	N	42	HIS	N-CA-C	6.49	118.39	109.18
27	Y	230	ASN	CA-C-N	6.48	126.66	120.31
27	Y	230	ASN	C-N-CA	6.48	126.66	120.31
6	C	192	ILE	N-CA-C	6.45	117.97	109.21
16	N	51	GLY	CA-C-N	6.42	125.92	119.24
16	N	51	GLY	C-N-CA	6.42	125.92	119.24
11	H	160	SER	N-CA-C	-6.38	101.94	110.55
14	L	57	VAL	N-CA-C	-6.32	105.20	111.77
17	O	82	SER	N-CA-C	-6.32	102.38	110.53
6	C	205	ARG	N-CA-C	6.32	119.83	111.75
31	3	55	VAL	CA-C-N	6.22	127.61	119.84
31	3	55	VAL	C-N-CA	6.22	127.61	119.84
7	D	15	GLU	CA-C-N	6.21	127.61	119.84
7	D	15	GLU	C-N-CA	6.21	127.61	119.84
1	0	2291	A	N9-C1'-C2'	6.21	121.32	112.00
20	R	137	ASN	N-CA-C	6.21	120.04	110.42
1	0	1684	A	C2'-C3'-O3'	6.20	118.80	109.50
22	T	89	ARG	CA-C-N	6.16	126.18	119.90
22	T	89	ARG	C-N-CA	6.16	126.18	119.90
11	H	116	ALA	N-CA-C	6.13	120.49	112.89
4	A	228	ILE	N-CA-C	6.04	117.08	108.93
1	0	2726	U	N1-C1'-C2'	5.99	120.98	112.00
14	L	97	VAL	N-CA-C	5.98	116.77	109.30
26	X	22	ASN	N-CA-C	5.97	118.56	111.33
32	I	91	GLU	CA-C-N	5.95	125.86	119.85
32	I	91	GLU	C-N-CA	5.95	125.86	119.85
18	P	56	GLY	N-CA-C	-5.93	101.08	111.46
5	B	323	LEU	N-CA-C	5.92	118.40	110.35
1	0	1504	A	N9-C1'-C2'	5.87	120.81	112.00
4	A	135	VAL	N-CA-C	5.85	116.29	108.27
14	L	145	LEU	N-CA-C	-5.83	104.84	111.07
17	O	66	GLY	N-CA-C	5.82	125.06	115.34
1	0	921	G	N9-C1'-C2'	5.82	120.73	112.00
4	A	70	ALA	N-CA-C	5.78	117.10	109.93
23	U	50	GLU	N-CA-C	5.78	118.33	111.33
1	0	1878	G	O4'-C1'-C2'	-5.75	101.85	107.60
4	A	188	ASN	N-CA-C	5.73	117.86	108.52
1	0	1615	A	C5'-C4'-C3'	5.71	124.56	116.00
1	0	1819	G	C4'-C3'-C2'	-5.71	96.89	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	20	ASN	N-CA-C	5.70	118.59	111.24
20	R	122	GLN	N-CA-C	-5.69	99.91	108.96
25	W	35	VAL	N-CA-C	5.68	114.37	107.61
5	B	49	THR	N-CA-C	-5.67	100.73	108.38
20	R	3	SER	N-CA-C	-5.66	100.74	109.52
1	0	129	A	C2'-C3'-O3'	5.66	122.19	113.70
7	D	77	ASP	CB-CA-C	-5.66	110.06	116.63
1	0	1261	A	N9-C1'-C2'	5.64	120.46	112.00
1	0	1559	A	C2'-C3'-O3'	5.61	122.11	113.70
8	E	156	ASP	N-CA-C	5.59	117.38	111.28
6	C	179	GLY	N-CA-C	-5.58	106.04	112.73
4	A	231	LYS	N-CA-C	-5.58	105.97	112.89
22	T	47	THR	N-CA-C	-5.58	101.08	109.95
26	X	17	ALA	N-CA-C	-5.58	105.74	112.54
22	T	52	ARG	N-CA-C	5.56	122.65	110.80
9	F	63	ILE	CB-CA-C	-5.54	108.44	113.70
1	0	2301	A	N9-C1'-C2'	5.53	120.30	112.00
1	0	834	G	C2'-C3'-O3'	-5.53	105.41	113.70
9	F	79	GLN	N-CA-C	5.53	118.41	109.40
1	0	1452	G	C5'-C4'-C3'	-5.52	107.71	116.00
4	A	126	ALA	N-CA-C	-5.51	102.36	110.52
11	H	159	PRO	N-CA-C	5.50	118.92	111.22
5	B	117	GLU	N-CA-C	-5.50	106.62	113.55
7	D	100	ASP	N-CA-C	-5.49	106.62	113.38
5	B	147	VAL	CA-C-N	5.45	125.53	119.32
5	B	147	VAL	C-N-CA	5.45	125.53	119.32
5	B	161	VAL	N-CA-C	5.45	115.80	108.17
1	0	2467	A	O4'-C4'-C3'	-5.44	100.66	106.10
19	Q	49	ASN	N-CA-C	5.44	118.48	110.59
12	J	47	THR	N-CA-C	5.43	117.88	110.55
5	B	154	VAL	CA-C-N	5.42	125.07	119.05
5	B	154	VAL	C-N-CA	5.42	125.07	119.05
11	H	16	ARG	N-CA-C	5.42	117.31	108.63
20	R	18	LEU	N-CA-C	-5.42	101.34	109.95
11	H	158	THR	N-CA-C	5.37	121.67	109.81
22	T	16	LEU	N-CA-C	5.35	116.79	111.07
16	N	117	ALA	N-CA-C	-5.34	105.54	111.36
6	C	90	HIS	CA-C-N	5.33	125.87	120.38
6	C	90	HIS	C-N-CA	5.33	125.87	120.38
6	C	186	TYR	N-CA-C	5.32	118.66	110.42
26	X	79	GLU	N-CA-C	5.31	117.07	111.28
22	T	3	GLN	CA-C-N	5.31	125.37	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	3	GLN	C-N-CA	5.31	125.37	119.32
16	N	3	GLY	CA-C-N	5.30	124.75	119.24
16	N	3	GLY	C-N-CA	5.30	124.75	119.24
28	Z	24	ARG	N-CA-C	-5.29	105.59	111.36
16	N	168	LEU	N-CA-C	5.29	121.51	109.81
24	V	42	ASN	CA-C-N	5.29	126.45	119.84
24	V	42	ASN	C-N-CA	5.29	126.45	119.84
12	J	36	VAL	N-CA-C	5.29	116.20	108.53
8	E	37	ASP	N-CA-C	5.29	119.01	112.24
1	0	462	A	N9-C1'-C2'	5.27	119.90	112.00
11	H	88	ARG	N-CA-C	5.27	119.57	113.20
17	O	4	ASN	CA-C-N	5.26	124.89	119.05
17	O	4	ASN	C-N-CA	5.26	124.89	119.05
21	S	59	ASP	N-CA-C	-5.26	106.09	112.88
25	W	113	SER	CA-C-N	5.25	124.97	119.82
25	W	113	SER	C-N-CA	5.25	124.97	119.82
1	0	2313	C	C5'-C4'-C3'	5.23	123.84	116.00
5	B	175	LEU	N-CA-C	-5.22	105.58	111.28
1	0	1752	G	C5'-C4'-C3'	5.22	123.03	115.20
13	K	8	VAL	N-CA-C	5.20	115.39	108.11
6	C	18	LEU	N-CA-C	-5.16	101.78	109.42
1	0	1979	G	N9-C1'-C2'	5.09	119.64	112.00
1	0	1120	U	C5'-C4'-C3'	-5.09	108.37	116.00
2	9	3039	U	C4'-C3'-O3'	-5.08	105.38	113.00
1	0	2673	U	N1-C1'-C2'	5.08	119.61	112.00
6	C	175	LYS	N-CA-C	5.08	117.25	110.35
1	0	718	C	C5'-C4'-C3'	-5.06	108.41	116.00
15	M	4	ALA	N-CA-C	-5.04	105.97	111.82
1	0	1330	A	C2'-C3'-O3'	-5.03	106.15	113.70
1	0	389	G	C5'-C4'-C3'	-5.02	108.46	116.00
1	0	1504	A	C1'-O4'-C4'	-5.02	104.88	109.90
1	0	1504	A	O4'-C4'-C3'	-5.02	98.98	104.00
23	U	53	ASP	N-CA-C	-5.02	105.70	111.07
2	9	3065	A	N9-C1'-C2'	5.01	119.52	112.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1080	C	Sidechain
1	0	1132	A	Sidechain
1	0	1327	G	Sidechain
1	0	1340	G	Sidechain
1	0	1430	G	Sidechain
1	0	1592	G	Sidechain
1	0	1744	G	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	182	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	2036	C	Sidechain
1	0	2115	U	Sidechain
1	0	2316	G	Sidechain
1	0	24	G	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	2564	G	Sidechain
1	0	2616	G	Sidechain
1	0	2630	G	Sidechain
1	0	2664	A	Sidechain
1	0	270	U	Sidechain
1	0	2793	A	Sidechain
1	0	2811	A	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	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

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Mol	Chain	Res	Type	Group
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
1	0	952	G	Sidechain
2	9	3039	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	29811	706	0
2	9	2600	0	1326	60	0
3	4	73	0	42	2	0
4	A	1753	0	1766	117	0
5	B	2625	0	2532	142	0
6	C	1859	0	1816	88	0
7	D	1094	0	1085	91	0
8	E	1357	0	1266	60	0
9	F	890	0	843	61	0
10	G	240	0	231	12	0
11	H	1266	0	1268	68	0
12	J	1120	0	1098	64	0
13	K	992	0	1031	59	0
14	L	1118	0	1076	66	0
15	M	1560	0	1567	76	0
16	N	1445	0	1401	99	0
17	O	865	0	873	41	0
18	P	1136	0	1123	40	0
19	Q	735	0	729	19	0
20	R	1149	0	1122	42	0
21	S	641	0	605	21	0
22	T	950	0	923	59	0
23	U	410	0	364	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	V	499	0	511	42	0
25	W	1196	0	1137	84	0
26	X	654	0	653	39	0
27	Y	1130	0	1133	57	0
28	Z	578	0	539	23	0
29	1	431	0	426	21	0
30	2	396	0	413	26	0
31	3	755	0	728	33	0
32	I	519	0	500	49	0
33	0	88	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	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	65	0	0	0	0
35	9	1	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
36	0	10	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	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	A	3	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	4	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	5743	0	0	113	0
40	1	50	0	0	1	0
40	2	35	0	0	3	0
40	3	76	0	0	5	0
40	4	2	0	0	1	0
40	9	136	0	0	4	0
40	A	120	0	0	11	0
40	B	135	0	0	24	0
40	C	172	0	0	14	0
40	D	48	0	0	5	0
40	E	42	0	0	1	0
40	F	27	0	0	4	0
40	G	16	0	0	1	0
40	H	71	0	0	6	0
40	I	10	0	0	0	0
40	J	51	0	0	4	0
40	K	58	0	0	6	0
40	L	87	0	0	10	0
40	M	127	0	0	6	0
40	N	59	0	0	8	0
40	O	41	0	0	6	0
40	P	64	0	0	1	0
40	Q	58	0	0	2	0
40	R	85	0	0	3	0
40	S	30	0	0	1	0
40	T	36	0	0	5	0
40	U	28	0	0	2	0
40	V	15	0	0	1	0
40	W	68	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	X	23	0	0	4	0
40	Y	95	0	0	9	0
40	Z	35	0	0	2	0
All	All	99035	0	59957	2176	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (2176) 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)
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.28	1.10
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.31	1.10
6:C:236:THR:HG22	6:C:239:ALA:H	1.10	1.09
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.28	1.08
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.36	1.06
25:W:6:GLN:HB2	25:W:26:ILE:HD11	1.37	1.06
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.39	1.04
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.39	1.02
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.40	1.02
1:O:156:C:H5''	15:M:171:ARG:HD3	1.44	1.00
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.41	1.00
2:9:3076:G:H3'	2:9:3077:A:H5''	1.42	0.99
1:O:289:G:H22	1:O:363:A:H2	1.04	0.98
25:W:149:LEU:HG	25:W:153:MET:HE2	1.44	0.97
1:O:1160:G:H5'	1:O:1161:A:H5'	1.47	0.97
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.47	0.97
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.11	0.95
5:B:86:ALA:HA	40:B:9578:HOH:O	1.66	0.95
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.49	0.95
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.47	0.94
5:B:238:ASN:HD22	5:B:240:GLY:H	1.10	0.94
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.31	0.94
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.49	0.93
9:F:91:VAL:HG12	9:F:92:GLY:H	1.34	0.93
18:P:115:SER:H	18:P:118:GLN:HE21	1.11	0.93
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.82	0.93
13:K:10:GLN:NE2	13:K:10:GLN:H	1.64	0.93
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.10	0.93
1:O:1242:A:H5'	12:J:82:THR:HG23	1.50	0.93
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.09	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1701:A:H4'	1:O:1702:U:H5''	1.50	0.92
5:B:140:LEU:HA	40:B:9578:HOH:O	1.71	0.91
1:O:656:G:H5'	17:O:3:THR:HG22	1.53	0.90
1:O:1166:A:H61	1:O:1180:U:H3	1.18	0.90
13:K:10:GLN:HE21	13:K:10:GLN:N	1.69	0.89
16:N:113:SER:HB2	40:N:9354:HOH:O	1.73	0.89
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.54	0.89
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.02	0.89
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.52	0.89
4:A:153:ARG:HB2	4:A:153:ARG:HH11	1.38	0.88
1:O:871:G:C8	1:O:871:G:H5'	2.09	0.88
1:O:1372:A:H3'	40:O:7650:HOH:O	1.73	0.88
9:F:46:GLU:OE1	9:F:100:ASP:HA	1.71	0.88
1:O:2840:A:OP1	5:B:211:THR:HG23	1.73	0.88
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.38	0.88
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.55	0.88
1:O:542:A:H5'	1:O:542:A:H8	1.39	0.87
1:O:1474:C:H6	1:O:1474:C:H5'	1.39	0.87
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.56	0.87
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.56	0.87
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.89	0.87
4:A:179:MET:HA	4:A:179:MET:HE3	1.56	0.87
29:1:25:LYS:HD2	30:2:49:GLU:H	1.40	0.87
13:K:10:GLN:H	13:K:10:GLN:HE21	0.87	0.86
13:K:107:THR:HG22	13:K:108:GLU:HG3	1.54	0.86
13:K:39:GLY:HA2	40:K:4183:HOH:O	1.74	0.86
1:O:2812:A:H2	1:O:2814:A:H62	1.17	0.86
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.39	0.86
1:O:288:A:H61	1:O:364:C:H42	1.19	0.86
2:9:3056:A:H2'	2:9:3057:A:H5''	1.56	0.86
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.57	0.86
1:O:1973:A:H5'	1:O:1973:A:H8	1.41	0.86
12:J:93:ARG:HB3	12:J:93:ARG:HH11	1.37	0.85
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.59	0.85
1:O:541:C:H2'	1:O:542:A:H5''	1.59	0.85
1:O:1206:U:H5'	1:O:1206:U:H6	1.40	0.85
1:O:2586:U:H3	1:O:2592:G:H22	1.26	0.84
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.59	0.84
6:C:236:THR:HG22	6:C:239:ALA:N	1.92	0.84
1:O:2506:A:O2'	1:O:2507:G:H8	1.61	0.83
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:162:MET:HE1	5:B:308:LEU:HD21	1.58	0.83
1:0:2748:G:H5'	40:0:7982:HOH:O	1.77	0.83
1:0:1835:U:H5	1:0:1840:A:N7	1.77	0.83
1:0:2506:A:HO2'	1:0:2507:G:H8	0.85	0.83
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.60	0.83
1:0:1603:A:H5'	1:0:1605:G:O4'	1.77	0.83
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.59	0.83
4:A:192:VAL:HB	40:A:9579:HOH:O	1.78	0.82
1:0:2534:C:H1'	40:0:4078:HOH:O	1.80	0.82
6:C:236:THR:CG2	6:C:239:ALA:H	1.91	0.82
27:Y:235:GLU:CD	27:Y:235:GLU:H	1.85	0.82
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.94	0.82
7:D:25:MET:HE2	7:D:41:LEU:HG	1.59	0.81
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.80	0.81
16:N:144:GLY:O	16:N:147:ILE:HG22	1.80	0.81
1:0:1041:U:H5'	40:L:9495:HOH:O	1.80	0.81
1:0:2054:A:N3	20:R:128:ARG:NH2	2.29	0.81
7:D:136:ARG:HH12	7:D:157:LEU:HA	1.43	0.81
25:W:88:THR:HB	40:W:6679:HOH:O	1.79	0.81
1:0:1116:U:O2'	1:0:1118:A:H2	1.64	0.81
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.63	0.81
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.44	0.81
40:0:5382:HOH:O	12:J:47:THR:HB	1.81	0.80
6:C:1:MET:HG2	6:C:2:GLN:H	1.45	0.80
1:0:2717:C:C2'	1:0:2718:C:H5''	2.12	0.80
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.63	0.80
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.62	0.80
1:0:541:C:C2'	1:0:542:A:H5''	2.12	0.80
1:0:545:G:H5'	1:0:545:G:H8	1.45	0.80
15:M:80:GLY:O	15:M:81:ARG:HD2	1.81	0.79
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.48	0.79
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.82	0.79
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.11	0.79
18:P:115:SER:H	18:P:118:GLN:NE2	1.80	0.79
1:0:111:C:O2'	29:1:20:ARG:HG2	1.82	0.79
2:9:3029:C:H2'	2:9:3030:C:H5'	1.65	0.79
6:C:139:VAL:HG13	40:C:9249:HOH:O	1.82	0.79
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.46	0.79
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.00	0.79
4:A:192:VAL:HG22	40:A:9617:HOH:O	1.80	0.79
1:0:2003:U:H4'	1:0:2004:U:H5	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.62	0.78
1:O:1878:G:H1'	40:O:6629:HOH:O	1.82	0.78
5:B:162:MET:CE	5:B:310:ARG:HD3	2.12	0.78
1:O:870:G:H2'	1:O:871:G:H5''	1.65	0.78
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.13	0.78
1:O:93:C:H5''	24:V:1:THR:HB	1.65	0.78
11:H:27:LYS:H	11:H:59:HIS:HD2	1.32	0.77
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.66	0.77
23:U:20:MET:HE2	23:U:30:HIS:NE2	1.99	0.77
7:D:172:VAL:HG12	7:D:173:GLU:H	1.49	0.77
25:W:125:HIS:HD2	25:W:127:GLY:H	1.32	0.77
1:O:2541:U:H4'	40:O:5938:HOH:O	1.83	0.77
1:O:797:A:H5'	28:Z:10:ARG:N	1.99	0.77
1:O:871:G:C8	1:O:871:G:C5'	2.68	0.77
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.15	0.77
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.85	0.77
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.67	0.77
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.67	0.76
1:O:871:G:C5'	1:O:871:G:H8	1.96	0.76
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.67	0.76
27:Y:154:ARG:HH12	27:Y:155:ARG:HG2	1.49	0.76
11:H:21:THR:O	11:H:120:ILE:HD12	1.85	0.76
4:A:35:GLY:O	4:A:36:ASP:HB3	1.84	0.76
32:I:99:ASP:OD1	32:I:138:THR:HB	1.84	0.76
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.20	0.76
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.68	0.76
27:Y:151:SER:O	27:Y:155:ARG:HG3	1.86	0.76
1:O:1377:C:H5'	1:O:1377:C:H6	1.50	0.76
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.67	0.76
1:O:289:G:N2	1:O:363:A:H2	1.83	0.76
4:A:194:MET:HE3	4:A:199:HIS:HB2	1.68	0.76
18:P:115:SER:OG	18:P:118:GLN:HG3	1.85	0.76
1:O:2851:G:C2'	1:O:2852:A:H5'	2.15	0.76
6:C:5:ILE:HD11	6:C:16:VAL:HG22	1.68	0.76
1:O:481:U:H5''	40:O:6177:HOH:O	1.85	0.75
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.68	0.75
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.50	0.75
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.67	0.75
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.01	0.75
18:P:91:LYS:O	18:P:95:GLU:HG3	1.86	0.75
15:M:99:ARG:NH2	15:M:170:ASN:HD22	1.83	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.02	0.74
40:9:4707:HOH:O	16:N:147:ILE:HD12	1.87	0.74
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.17	0.74
16:N:11:ARG:HG3	16:N:14:ARG:HH12	1.51	0.74
9:F:58:GLU:CD	15:M:27:ARG:HH22	1.94	0.74
24:V:12:THR:HG22	24:V:15:GLU:CG	2.13	0.74
1:0:1667:A:H8	1:0:1667:A:H5'	1.52	0.74
4:A:153:ARG:HB2	4:A:153:ARG:NH1	2.01	0.74
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.15	0.74
1:0:506:G:H22	1:0:509:A:C5'	2.01	0.74
1:0:1751:G:H2'	1:0:1752:G:H5''	1.69	0.74
1:0:2717:C:H2'	1:0:2718:C:H5''	1.69	0.74
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.03	0.74
31:3:6:ARG:NH1	31:3:21:GLU:HG3	2.02	0.74
6:C:2:GLN:HB3	40:C:9189:HOH:O	1.86	0.74
7:D:154:LYS:H	7:D:154:LYS:HD2	1.52	0.74
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.13	0.74
1:0:1160:G:C5'	1:0:1161:A:H5'	2.18	0.74
9:F:91:VAL:HG12	9:F:92:GLY:N	2.01	0.74
9:F:96:ALA:HA	40:F:3111:HOH:O	1.88	0.74
1:0:1119:G:N2	1:0:1246:A:C2	2.55	0.73
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.03	0.73
26:X:54:ILE:HD11	26:X:85:VAL:HG12	1.69	0.73
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.68	0.73
1:0:280:C:H2'	1:0:281:U:O4'	1.89	0.73
1:0:544:G:H2'	1:0:545:G:H5''	1.70	0.73
1:0:1118:A:H62	1:0:1244:U:H3	1.36	0.73
40:0:9966:HOH:O	29:1:1:THR:HA	1.88	0.73
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.69	0.73
1:0:871:G:H5'	1:0:871:G:H8	1.52	0.73
1:0:1205:U:H2'	1:0:1206:U:H5''	1.71	0.73
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.70	0.73
24:V:39:ALA:C	24:V:41:GLU:H	1.97	0.72
4:A:51:ARG:HB2	40:A:9592:HOH:O	1.89	0.72
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.71	0.72
1:0:1206:U:H2'	1:0:1207:A:O4'	1.89	0.72
4:A:199:HIS:HD2	4:A:201:PHE:H	1.38	0.72
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.54	0.72
14:L:73:VAL:HG23	14:L:74:THR:H	1.55	0.72
1:0:1116:U:HO2'	1:0:1118:A:H2	0.80	0.72
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:48:ASP:HB3	40:A:9592:HOH:O	1.90	0.72
10:G:12:ILE:N	10:G:13:PRO:HD3	2.04	0.72
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.04	0.72
32:I:74:PRO:HG2	32:I:77:GLU:OE1	1.89	0.72
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.55	0.72
1:O:1175:G:H1'	1:O:1193:A:H2'	1.70	0.71
1:O:2644:C:H2'	40:O:7574:HOH:O	1.90	0.71
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.55	0.71
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.72	0.71
30:2:41:HIS:H	30:2:45:ASN:HD22	1.37	0.71
16:N:164:ASP:CG	16:N:167:ASP:HA	2.15	0.71
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.72	0.71
1:O:902:G:N7	14:L:18:HIS:HD2	1.88	0.71
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.72	0.71
1:O:2346:C:O2'	7:D:52:THR:HG21	1.89	0.71
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.26	0.71
25:W:5:VAL:HG11	25:W:153:MET:HE1	1.71	0.71
1:O:2716:G:H5''	5:B:206:THR:HG21	1.73	0.71
40:O:7900:HOH:O	5:B:211:THR:HG21	1.91	0.71
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.55	0.71
1:O:474:C:O3'	6:C:73:LEU:HD21	1.91	0.71
1:O:1244:U:OP1	12:J:18:ILE:HD13	1.91	0.71
5:B:16:ARG:NH1	40:B:9610:HOH:O	2.23	0.71
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.71	0.71
11:H:154:TYR:HB2	40:H:9557:HOH:O	1.91	0.71
16:N:80:SER:HB2	40:N:9332:HOH:O	1.91	0.71
26:X:30:MET:HE1	26:X:58:ALA:CB	2.20	0.71
25:W:13:MET:CE	25:W:17:ILE:HG22	2.20	0.70
1:O:1700:C:H5''	1:O:1701:A:OP2	1.91	0.70
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.87	0.70
1:O:541:C:H2'	1:O:542:A:C5'	2.22	0.70
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.74	0.70
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.89	0.70
1:O:559:U:H6	1:O:559:U:H5'	1.55	0.70
1:O:1189:A:H3'	40:O:8198:HOH:O	1.91	0.70
2:9:3014:G:H5'	2:9:3014:G:H8	1.56	0.70
1:O:1118:A:H8	1:O:1118:A:H3'	1.56	0.70
1:O:1166:A:H1'	1:O:1192:A:C2	2.27	0.70
4:A:82:VAL:HG13	4:A:93:THR:HB	1.74	0.70
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.74	0.70
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:125:HIS:CD2	25:W:127:GLY:H	2.10	0.70
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.15	0.70
1:0:1118:A:H3'	1:0:1118:A:C8	2.27	0.69
1:0:1183:C:N4	1:0:1184:C:H41	1.89	0.69
25:W:52:VAL:HG22	25:W:53:ALA:H	1.56	0.69
1:0:1666:C:H2'	1:0:1667:A:H5'	1.73	0.69
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.23	0.69
1:0:381:G:H5''	40:M:9371:HOH:O	1.91	0.69
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.74	0.69
1:0:2468:A:H61	31:3:48:ASN:HD21	1.40	0.69
1:0:1116:U:H3	1:0:1246:A:H62	1.40	0.69
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.27	0.69
5:B:112:THR:HG23	5:B:158:LYS:NZ	2.07	0.69
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.25	0.69
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.74	0.69
15:M:164:THR:HG22	15:M:166:ALA:H	1.57	0.69
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.75	0.69
6:C:1:MET:HG2	6:C:2:GLN:N	2.08	0.69
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.74	0.69
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.53	0.69
22:T:115:GLU:HG3	22:T:116:ASP:N	2.08	0.69
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.87	0.69
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.23	0.68
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.23	0.68
1:0:1165:G:H1'	1:0:1174:A:H1'	1.74	0.68
40:0:5995:HOH:O	10:G:12:ILE:HA	1.91	0.68
4:A:153:ARG:HH11	4:A:153:ARG:CB	2.06	0.68
5:B:264:GLU:HG2	5:B:267:LYS:CE	2.20	0.68
22:T:26:THR:HA	22:T:39:ASN:HB3	1.76	0.68
24:V:1:THR:HG23	24:V:2:VAL:H	1.57	0.68
1:0:560:C:H42	1:0:597:A:H61	1.41	0.68
5:B:51:VAL:HG23	5:B:329:TYR:O	1.94	0.68
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.58	0.68
1:0:2807:U:P	5:B:27:ASN:HD21	2.16	0.68
15:M:164:THR:HG22	15:M:166:ALA:N	2.08	0.68
23:U:17:THR:HG22	23:U:18:GLY:N	2.08	0.68
1:0:506:G:H22	1:0:509:A:H5''	1.57	0.68
7:D:39:ASP:O	7:D:43:GLU:HG3	1.94	0.68
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.08	0.68
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.16	0.68
1:0:316:A:H5'	22:T:54:ASP:OD2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1168:C:H5''	32:I:87:THR:HG23	1.74	0.68
8:E:15:GLN:HG2	8:E:19:ASP:O	1.94	0.68
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.24	0.68
20:R:23:MET:HE3	20:R:28:SER:OG	1.92	0.68
5:B:125:GLU:O	5:B:129:ARG:HG3	1.94	0.68
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.09	0.68
16:N:154:LEU:HG	16:N:155:GLU:H	1.59	0.67
24:V:43:PRO:O	24:V:46:ILE:HG22	1.94	0.67
1:O:328:U:O4'	6:C:202:THR:HG22	1.93	0.67
4:A:191:GLY:HA2	4:A:194:MET:CE	2.18	0.67
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.24	0.67
16:N:110:THR:HB	16:N:113:SER:OG	1.93	0.67
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.93	0.67
1:O:87:C:H2'	30:2:28:LYS:O	1.94	0.67
1:O:2005:G:H3'	1:O:2005:G:OP2	1.95	0.67
6:C:132:ASP:HB3	40:C:9166:HOH:O	1.94	0.67
1:O:1730:G:H5'	1:O:1731:C:C5	2.29	0.67
4:A:33:GLU:H	4:A:33:GLU:CD	2.03	0.67
1:O:796:A:HO2'	28:Z:10:ARG:N	1.93	0.67
1:O:1973:A:H5'	1:O:1973:A:C8	2.28	0.67
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.40	0.67
18:P:103:THR:O	18:P:107:GLU:HG3	1.93	0.67
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.25	0.67
1:O:2003:U:H4'	1:O:2004:U:C5	2.29	0.67
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.59	0.67
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.74	0.67
1:O:2578:G:H5'	1:O:2578:G:H8	1.58	0.67
5:B:62:ARG:HA	5:B:65:MET:HE2	1.75	0.67
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.75	0.67
11:H:27:LYS:N	11:H:59:HIS:HD2	1.91	0.67
23:U:52:THR:HG22	23:U:54:THR:N	2.10	0.67
1:O:962:C:H1'	16:N:5:ARG:NH1	2.10	0.67
1:O:282:C:O2'	1:O:283:U:H5'	1.95	0.66
26:X:71:ARG:HB3	26:X:88:GLU:OE1	1.95	0.66
1:O:1165:G:H4'	1:O:1174:A:O2'	1.95	0.66
15:M:107:ARG:HG3	15:M:107:ARG:NH1	2.08	0.66
1:O:1159:G:H21	1:O:1189:A:H8	1.42	0.66
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.25	0.66
1:O:1201:C:H2'	1:O:1202:A:H5'	1.76	0.66
1:O:2718:C:H6	1:O:2718:C:H5'	1.60	0.66
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.78	0.66
5:B:179:LEU:O	5:B:183:GLU:HG2	1.94	0.66
1:0:447:A:P	22:T:1:SER:HB2	2.35	0.66
1:0:524:A:H5''	20:R:29:LYS:HD3	1.77	0.66
1:0:1701:A:H4'	1:0:1702:U:C5'	2.23	0.66
17:O:14:LEU:HG	17:O:102:ILE:HD11	1.76	0.66
25:W:21:LEU:O	25:W:26:ILE:HG23	1.95	0.66
1:0:681:G:N3	1:0:681:G:H5'	2.11	0.66
1:0:1299:G:O6	14:L:6:ARG:HD3	1.96	0.66
1:0:1838:U:O2'	1:0:2644:C:H5'	1.96	0.66
13:K:49:LEU:HD12	13:K:80:ILE:HG21	1.77	0.66
22:T:71:VAL:HG12	22:T:72:ILE:N	2.11	0.66
1:0:2505:G:O2'	1:0:2506:A:H5'	1.96	0.66
5:B:254:GLN:HG2	5:B:255:GLY:N	2.10	0.66
14:L:133:VAL:HA	40:L:9475:HOH:O	1.96	0.65
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.77	0.65
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.10	0.65
25:W:88:THR:HG22	25:W:89:ASP:N	2.11	0.65
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.96	0.65
9:F:14:ASP:O	9:F:18:GLU:HG3	1.96	0.65
14:L:143:THR:HG22	14:L:144:ASP:N	2.10	0.65
4:A:33:GLU:CD	4:A:33:GLU:N	2.55	0.65
4:A:194:MET:HE3	4:A:199:HIS:CB	2.26	0.65
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.42	0.65
16:N:33:ARG:NH1	16:N:103:ASP:OD2	2.28	0.65
1:0:291:C:H2'	1:0:292:G:O4'	1.95	0.65
27:Y:144:ARG:CZ	40:Y:9411:HOH:O	2.44	0.65
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.77	0.65
40:O:6989:HOH:O	27:Y:141:THR:HG23	1.97	0.65
4:A:211:LYS:CG	4:A:212:PRO:HD2	2.27	0.65
17:O:32:ARG:O	17:O:32:ARG:HD3	1.97	0.65
25:W:108:ARG:HH21	25:W:114:PRO:HG2	1.61	0.65
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.10	0.65
1:0:2480:G:H3'	40:O:4750:HOH:O	1.96	0.65
1:0:2769:C:H2'	1:0:2770:G:O4'	1.97	0.65
25:W:41:TYR:HA	25:W:44:MET:HE3	1.78	0.65
1:0:1919:A:H4'	40:O:5395:HOH:O	1.97	0.64
4:A:199:HIS:CD2	4:A:201:PHE:H	2.15	0.64
1:0:470:U:O2'	29:1:16:HIS:HD2	1.79	0.64
1:0:544:G:C2'	1:0:545:G:H5''	2.26	0.64
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:75:PRO:HD3	12:J:136:SER:OG	1.96	0.64
25:W:80:ASP:O	25:W:84:VAL:HG23	1.97	0.64
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.28	0.64
1:O:2270:G:H4'	4:A:223:ARG:HH12	1.61	0.64
5:B:238:ASN:ND2	5:B:240:GLY:H	1.90	0.64
5:B:297:VAL:HB	40:B:9599:HOH:O	1.97	0.64
7:D:138:GLY:N	40:D:7597:HOH:O	2.31	0.64
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.63	0.64
26:X:72:VAL:HG13	26:X:85:VAL:HG13	1.79	0.64
1:O:1183:C:H2'	40:O:6750:HOH:O	1.98	0.64
24:V:39:ALA:N	24:V:40:PRO:HD2	2.12	0.64
25:W:13:MET:HE2	25:W:18:GLN:HA	1.79	0.64
1:O:281:U:H2'	1:O:282:C:O4'	1.97	0.64
1:O:949:U:H4'	19:Q:95:GLU:HA	1.80	0.64
2:9:3056:A:C2'	2:9:3057:A:H5''	2.26	0.64
4:A:203:GLY:HA2	40:A:9536:HOH:O	1.97	0.64
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.37	0.64
1:O:1184:C:H1'	40:O:7910:HOH:O	1.98	0.64
1:O:2507:G:H2'	1:O:2510:C:H42	1.61	0.64
25:W:130:HIS:O	25:W:136:GLY:HA3	1.98	0.64
1:O:1666:C:O2'	1:O:1667:A:H5''	1.97	0.64
11:H:166:SER:CB	11:H:167:PRO:CD	2.75	0.64
17:O:57:THR:O	17:O:111:VAL:HG23	1.97	0.64
30:2:20:ARG:HD2	30:2:39:ARG:NH2	2.12	0.64
32:I:92:PRO:C	32:I:94:GLU:H	2.06	0.64
5:B:307:ARG:HG3	5:B:307:ARG:NH1	2.05	0.64
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.79	0.64
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.13	0.64
25:W:149:LEU:CG	25:W:153:MET:HE2	2.26	0.64
30:2:20:ARG:HD2	30:2:39:ARG:HH21	1.62	0.64
1:O:1160:G:H5'	1:O:1161:A:C5'	2.23	0.63
32:I:125:ALA:O	32:I:129:VAL:HG23	1.96	0.63
1:O:123:U:H5'	40:O:7139:HOH:O	1.99	0.63
1:O:2851:G:H2'	1:O:2852:A:H5'	1.79	0.63
5:B:238:ASN:HD22	5:B:240:GLY:N	1.90	0.63
12:J:131:THR:HG22	12:J:134:GLU:H	1.63	0.63
13:K:115:ARG:HG3	13:K:116:GLU:N	2.13	0.63
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.98	0.63
27:Y:165:GLU:HB3	40:Y:9393:HOH:O	1.97	0.63
28:Z:53:GLY:HA2	28:Z:67:GLY:O	1.99	0.63
25:W:48:VAL:O	25:W:48:VAL:HG12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.80	0.63
1:0:1184:C:H4'	32:I:126:LYS:HB3	1.80	0.63
1:0:1377:C:H5'	1:0:1377:C:C6	2.33	0.63
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.33	0.63
1:0:558:C:H2'	1:0:559:U:H5'	1.80	0.63
2:9:3004:G:H21	16:N:44:ARG:NH1	1.97	0.63
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.67	0.63
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.79	0.63
15:M:99:ARG:HH21	15:M:170:ASN:ND2	1.89	0.63
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.33	0.63
24:V:55:ARG:O	24:V:59:ILE:HG12	1.99	0.63
4:A:33:GLU:O	4:A:34:ASP:HB2	1.98	0.63
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.81	0.63
1:0:380:A:OP2	15:M:9:ARG:HD2	1.99	0.63
1:0:1116:U:O2'	1:0:1118:A:C2	2.45	0.63
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.29	0.63
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.81	0.63
2:9:3013:A:O2'	2:9:3014:G:H5''	1.99	0.63
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.34	0.63
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.81	0.62
15:M:24:GLN:O	15:M:28:GLN:HG3	1.99	0.62
23:U:45:GLU:HB2	23:U:48:ASN:HD22	1.64	0.62
1:0:1053:G:OP1	11:H:12:PRO:HG3	1.98	0.62
1:0:1333:U:H2'	1:0:1334:C:C6	2.35	0.62
1:0:1426:C:H2'	40:0:3201:HOH:O	1.97	0.62
1:0:1552:G:N2	1:0:1634:G:H1'	2.13	0.62
11:H:166:SER:HB3	11:H:167:PRO:CD	2.29	0.62
14:L:104:ASP:HB2	40:L:9465:HOH:O	1.99	0.62
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.64	0.62
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.79	0.62
1:0:343:C:O2'	1:0:344:C:H5'	1.99	0.62
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.80	0.62
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.35	0.62
7:D:172:VAL:HG12	7:D:173:GLU:N	2.14	0.62
11:H:58:ARG:HH11	11:H:58:ARG:HG3	1.63	0.62
12:J:107:ASN:C	12:J:107:ASN:HD22	2.07	0.62
18:P:9:LEU:O	18:P:13:VAL:HG12	1.98	0.62
25:W:88:THR:HG22	25:W:89:ASP:H	1.64	0.62
27:Y:189:ASN:C	27:Y:189:ASN:HD22	2.07	0.62
1:0:282:C:H1'	1:0:368:C:N4	2.14	0.62
1:0:960:G:H4'	40:0:7877:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2878:U:H2'	1:0:2879:A:O4'	1.99	0.62
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.00	0.62
4:A:131:HIS:O	4:A:132:ASP:HB2	2.00	0.62
1:0:120:A:H5'	29:1:20:ARG:HH21	1.64	0.62
1:0:656:G:H5'	17:O:3:THR:CG2	2.28	0.62
1:0:1118:A:H8	1:0:1119:G:H5''	1.65	0.62
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.30	0.62
15:M:69:LYS:O	15:M:73:ARG:NH2	2.32	0.62
1:0:797:A:C4'	28:Z:10:ARG:N	2.63	0.62
1:0:2073:G:OP2	1:0:2490:A:H5'	1.98	0.62
1:0:2649:A:H5'	1:0:2649:A:H8	1.64	0.62
5:B:88:GLU:HB3	5:B:97:LEU:HD12	1.82	0.62
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.18	0.62
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.98	0.62
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.29	0.62
1:0:338:C:H4'	6:C:174:ILE:CD1	2.30	0.62
1:0:877:G:H5'	1:0:878:G:OP1	2.00	0.62
1:0:1474:C:H5'	1:0:1474:C:C6	2.28	0.62
1:0:2768:A:H2'	1:0:2769:C:C6	2.35	0.62
18:P:115:SER:N	18:P:118:GLN:HE21	1.92	0.62
1:0:960:G:H3'	1:0:960:G:N3	2.15	0.61
1:0:2533:C:H5'	1:0:2533:C:H6	1.65	0.61
1:0:2769:C:C2'	1:0:2770:G:H5'	2.30	0.61
5:B:58:PRO:HA	5:B:63:GLU:OE2	1.99	0.61
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.65	0.61
25:W:84:VAL:HG12	40:W:6679:HOH:O	1.99	0.61
1:0:545:G:H5'	1:0:545:G:C8	2.31	0.61
11:H:63:GLU:HA	40:H:9545:HOH:O	2.00	0.61
13:K:75:ARG:HD3	13:K:112:PRO:O	2.00	0.61
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.15	0.61
22:T:38:ARG:NH1	40:T:6217:HOH:O	2.33	0.61
1:0:1926:G:H2'	1:0:1927:A:C8	2.35	0.61
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.81	0.61
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.30	0.61
25:W:137:GLN:NE2	25:W:141:HIS:HE1	1.91	0.61
1:0:164:G:H4'	14:L:30:ARG:HD3	1.83	0.61
1:0:542:A:H5'	1:0:542:A:C8	2.28	0.61
1:0:625:U:H5''	1:0:1044:C:N4	2.15	0.61
1:0:1119:G:H22	1:0:1246:A:H2	1.43	0.61
1:0:1882:C:OP1	4:A:192:VAL:HG23	2.01	0.61
5:B:41:PHE:HB3	5:B:190:MET:HE1	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:316:A:N3	1:0:336:G:O2'	2.32	0.61
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.81	0.61
8:E:68:HIS:O	8:E:72:MET:HG3	1.99	0.61
17:O:32:ARG:HB2	40:O:4656:HOH:O	2.01	0.61
5:B:72:THR:HB	40:B:9599:HOH:O	1.99	0.61
7:D:149:ARG:HH12	16:N:15:GLU:HA	1.65	0.61
20:R:44:VAL:O	20:R:48:GLU:HG3	1.99	0.61
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.81	0.61
1:0:1189:A:O2'	1:0:1208:C:H2'	2.00	0.61
1:0:1205:U:C2'	1:0:1206:U:H5''	2.30	0.61
7:D:25:MET:SD	7:D:40:ILE:HD11	2.40	0.61
40:O:6053:HOH:O	5:B:298:LYS:HG2	2.00	0.61
8:E:101:GLU:HB2	8:E:116:THR:O	2.00	0.61
20:R:9:ASP:O	20:R:13:THR:HB	2.00	0.61
1:0:1058:A:H2'	1:0:1060:C:H5''	1.82	0.61
5:B:154:VAL:HG12	5:B:156:LYS:HG2	1.83	0.61
7:D:51:ARG:HH11	7:D:68:PRO:HB3	1.65	0.61
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.30	0.61
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.83	0.61
1:0:2649:A:H5'	1:0:2649:A:C8	2.36	0.61
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.81	0.61
9:F:37:THR:O	9:F:41:GLU:HG3	2.01	0.61
11:H:76:GLU:C	11:H:77:LEU:HD23	2.26	0.61
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.82	0.61
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.31	0.60
1:0:656:G:C5'	17:O:3:THR:HG22	2.29	0.60
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.82	0.60
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.82	0.60
1:0:553:G:P	27:Y:204:ARG:HH22	2.24	0.60
1:0:2426:G:H1'	40:O:6602:HOH:O	1.99	0.60
9:F:1:PRO:H3	9:F:4:VAL:HG23	1.66	0.60
12:J:76:ASP:HA	40:J:5907:HOH:O	2.00	0.60
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.02	0.60
1:0:1946:C:H2'	1:0:1971:G:C8	2.36	0.60
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.17	0.60
4:A:194:MET:CE	4:A:199:HIS:HB2	2.32	0.60
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.83	0.60
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.01	0.60
2:9:3020:G:O2'	2:9:3021:G:H5'	2.01	0.60
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.82	0.60
12:J:74:ARG:O	12:J:78:ILE:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:143:THR:HG22	14:L:144:ASP:H	1.67	0.60
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.02	0.60
21:S:57:THR:HG22	21:S:58:MET:N	2.15	0.60
11:H:30:GLN:H	11:H:66:ARG:NH1	1.99	0.60
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.01	0.60
25:W:139:GLY:O	25:W:141:HIS:HD2	1.85	0.60
29:1:10:LYS:HG3	40:1:9489:HOH:O	2.00	0.60
1:0:1159:G:H1	1:0:1208:C:H42	1.50	0.60
4:A:88:ILE:O	4:A:88:ILE:HG22	2.02	0.60
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.84	0.60
5:B:275:GLY:O	5:B:291:ASP:HA	2.01	0.60
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.31	0.60
32:I:112:LYS:C	32:I:114:PRO:HD2	2.27	0.60
1:0:635:A:H2'	1:0:636:G:H5''	1.83	0.60
1:0:1451:C:H5'	1:0:1505:U:C5	2.37	0.60
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.83	0.60
23:U:14:GLU:O	23:U:17:THR:HB	2.02	0.60
23:U:17:THR:CG2	23:U:18:GLY:N	2.64	0.60
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.16	0.60
26:X:72:VAL:HG13	26:X:85:VAL:CG1	2.32	0.60
1:0:1205:U:H2'	1:0:1206:U:C5'	2.32	0.60
2:9:3040:C:N4	7:D:53:LYS:HE3	2.17	0.60
9:F:99:THR:O	9:F:100:ASP:HB2	2.01	0.60
27:Y:144:ARG:HH11	27:Y:144:ARG:HG3	1.67	0.60
1:0:396:U:O2'	1:0:418:C:H4'	2.02	0.59
1:0:2064:U:H5'	1:0:2652:U:H4'	1.83	0.59
1:0:2524:G:H21	1:0:2526:C:H41	1.48	0.59
1:0:2896:A:N3	1:0:2896:A:H2'	2.17	0.59
4:A:179:MET:HG2	4:A:186:TRP:CB	2.32	0.59
1:0:1119:G:OP2	12:J:49:ARG:HD3	2.02	0.59
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.02	0.59
8:E:84:MET:HE1	8:E:148:ILE:CD1	2.31	0.59
1:0:2820:A:OP1	5:B:98:THR:HG22	2.03	0.59
1:0:2851:G:O2'	1:0:2852:A:H5'	2.01	0.59
9:F:2:VAL:HG22	9:F:57:GLU:OE1	2.03	0.59
27:Y:212:ARG:HD2	40:Y:9401:HOH:O	2.01	0.59
25:W:13:MET:HE2	25:W:18:GLN:CA	2.33	0.59
1:0:1182:C:H1'	1:0:1192:A:H8	1.68	0.59
1:0:2443:C:H5'	14:L:57:VAL:HG21	1.83	0.59
40:0:7995:HOH:O	31:3:60:LYS:HG3	2.02	0.59
5:B:85:ARG:NH1	40:B:9626:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:170:TYR:O	7:D:171:ASP:HB3	2.02	0.59
14:L:67:ARG:O	14:L:71:GLU:HG3	2.03	0.59
1:0:1766:U:O2	1:0:1778:A:H5'	2.03	0.59
1:0:2726:U:O2'	26:X:22:ASN:ND2	2.35	0.59
2:9:3029:C:C2'	2:9:3030:C:H5'	2.33	0.59
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.83	0.59
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.85	0.59
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.67	0.59
17:O:39:THR:O	17:O:115:ARG:NH2	2.33	0.59
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.17	0.59
1:0:391:U:OP2	15:M:84:LYS:NZ	2.35	0.59
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.84	0.59
5:B:145:HIS:HD2	5:B:146:THR:O	1.86	0.59
14:L:36:ASP:HB2	40:L:9437:HOH:O	2.02	0.59
1:0:2644:C:O2'	1:0:2645:U:H5'	2.03	0.59
9:F:58:GLU:HG3	9:F:61:MET:HE2	1.83	0.59
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.64	0.59
1:0:2291:A:C8	1:0:2309:C:H5'	2.38	0.59
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.03	0.59
1:0:2765:C:H4'	40:0:6053:HOH:O	2.02	0.59
1:0:2827:A:H2'	1:0:2828:G:O4'	2.03	0.59
1:0:516:A:H5'	40:0:6177:HOH:O	2.03	0.59
1:0:2072:G:H4'	40:0:4372:HOH:O	2.02	0.58
40:0:9737:HOH:O	15:M:82:ARG:HD2	2.01	0.58
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.85	0.58
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.59	0.58
29:1:56:GLU:HG2	29:1:56:GLU:OXT	2.03	0.58
1:0:1201:C:H5''	40:0:6739:HOH:O	2.03	0.58
1:0:2419:U:H5''	1:0:2420:G:H5'	1.84	0.58
11:H:169:GLY:C	11:H:170:ASN:HD22	2.11	0.58
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.65	0.58
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.68	0.58
32:I:102:VAL:O	32:I:106:LYS:HG3	2.03	0.58
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.36	0.58
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.85	0.58
16:N:162:ASP:HA	40:N:9327:HOH:O	2.02	0.58
1:0:138:U:H5''	1:0:139:C:OP2	2.03	0.58
1:0:2524:G:H21	1:0:2526:C:H5	1.49	0.58
7:D:49:PRO:HB3	7:D:73:VAL:HG22	1.84	0.58
11:H:79:GLU:C	11:H:80:GLU:HG3	2.28	0.58
16:N:143:ARG:HH21	16:N:169:PRO:HB2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.67	0.58
1:O:2420:G:O2'	1:O:2421:G:H5'	2.04	0.58
5:B:305:ASP:O	5:B:306:LYS:HB2	2.04	0.58
12:J:107:ASN:ND2	12:J:109:TYR:H	2.01	0.58
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.67	0.58
1:O:263:U:O4'	9:F:59:ILE:HD13	2.03	0.58
2:9:3039:U:H1'	2:9:3044:A:H61	1.68	0.58
16:N:69:TYR:HE2	16:N:184:ILE:HG13	1.68	0.58
20:R:17:MET:HE1	20:R:19:ARG:NH2	2.19	0.58
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.18	0.58
2:9:3051:A:H5'	16:N:160:SER:CB	2.34	0.58
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.58
31:3:65:THR:HG22	31:3:67:LEU:HG	1.85	0.58
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.03	0.58
4:A:121:ALA:O	4:A:124:VAL:HG22	2.03	0.58
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.19	0.58
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.85	0.58
13:K:4:LEU:CD2	13:K:116:GLU:HB3	2.32	0.58
14:L:57:VAL:HG12	14:L:57:VAL:O	2.04	0.58
31:3:70:ARG:HB3	40:3:9510:HOH:O	2.04	0.58
32:I:113:HIS:N	32:I:114:PRO:HD2	2.18	0.58
1:O:797:A:C5'	28:Z:10:ARG:N	2.67	0.58
1:O:1168:C:H5''	32:I:87:THR:CG2	2.34	0.58
1:O:1384:C:H5'	26:X:30:MET:HG2	1.85	0.58
1:O:1687:C:O2	29:1:9:GLY:HA2	2.04	0.58
5:B:190:MET:HA	5:B:190:MET:HE3	1.86	0.58
9:F:58:GLU:HA	9:F:61:MET:HG3	1.85	0.58
12:J:19:MET:CE	12:J:132:LEU:HD11	2.31	0.58
1:O:441:A:H1'	1:O:442:A:N7	2.19	0.58
1:O:657:G:OP1	6:C:27:ARG:NH2	2.29	0.58
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.16	0.58
1:O:1730:G:H5''	1:O:1731:C:H6	1.69	0.57
15:M:60:VAL:C	15:M:61:ILE:HD12	2.28	0.57
1:O:121:U:OP2	30:2:10:ARG:NH2	2.33	0.57
1:O:2795:C:O2'	1:O:2796:U:H5'	2.04	0.57
1:O:2908:A:H2'	1:O:2909:G:O4'	2.02	0.57
25:W:13:MET:HE3	25:W:17:ILE:CG2	2.34	0.57
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.85	0.57
1:O:506:G:H22	1:O:509:A:H5'	1.69	0.57
1:O:1943:C:H4'	4:A:211:LYS:O	2.05	0.57
1:O:2237:G:H1'	1:O:2238:A:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2769:C:O2'	1:O:2770:G:H5'	2.04	0.57
2:9:3018:U:H2'	2:9:3019:G:H8	1.70	0.57
5:B:62:ARG:HA	5:B:65:MET:CE	2.34	0.57
5:B:175:LEU:O	5:B:175:LEU:HD23	2.05	0.57
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.33	0.57
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.34	0.57
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.87	0.57
2:9:3014:G:H5'	2:9:3014:G:C8	2.39	0.57
6:C:79:ARG:O	6:C:87:ARG:HG2	2.04	0.57
9:F:13:GLU:OE1	9:F:77:VAL:HG13	2.05	0.57
16:N:23:ARG:HG2	16:N:23:ARG:HH11	1.69	0.57
23:U:47:ARG:HG3	40:U:4381:HOH:O	2.03	0.57
5:B:102:THR:HG21	5:B:182:VAL:O	2.04	0.57
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.40	0.57
25:W:26:ILE:HB	40:W:5420:HOH:O	2.03	0.57
26:X:43:VAL:HG12	26:X:44:ASP:N	2.19	0.57
32:I:139:ILE:HG22	32:I:140:GLU:N	2.20	0.57
1:O:20:G:H21	20:R:117:HIS:HD2	1.52	0.57
1:O:1634:G:H3'	40:O:4466:HOH:O	2.04	0.57
1:O:2694:A:H4'	8:E:91:PHE:HE1	1.69	0.57
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.86	0.57
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.68	0.57
6:C:129:HIS:HD2	6:C:165:ASP:OD2	1.88	0.57
1:O:2676:C:H4'	12:J:70:PHE:CD1	2.39	0.57
5:B:96:PRO:HG3	40:B:9626:HOH:O	2.02	0.57
10:G:64:ASN:HD22	10:G:64:ASN:N	2.01	0.57
1:O:1180:U:O2'	32:I:92:PRO:HD2	2.05	0.57
1:O:1189:A:H1'	1:O:1209:C:O4'	2.04	0.57
5:B:17:LYS:O	5:B:260:HIS:HD2	1.86	0.57
6:C:140:VAL:HB	40:C:9252:HOH:O	2.04	0.57
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.03	0.57
22:T:41:ARG:HG2	22:T:41:ARG:NH1	2.19	0.57
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.35	0.57
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.40	0.57
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.87	0.57
20:R:39:THR:HG22	20:R:107:GLU:O	2.05	0.57
21:S:77:VAL:O	21:S:80:ARG:HG2	2.05	0.57
27:Y:154:ARG:HB3	27:Y:154:ARG:HH11	1.69	0.57
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.69	0.57
40:O:4931:HOH:O	15:M:83:SER:HB3	2.04	0.57
11:H:170:ASN:HD22	11:H:170:ASN:N	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.05	0.57
1:0:256:C:H2'	1:0:257:G:O4'	2.05	0.56
2:9:3041:C:O4'	7:D:50:VAL:HG13	2.05	0.56
6:C:242:GLU:HB2	40:C:9186:HOH:O	2.05	0.56
1:0:2779:G:H21	8:E:143:GLN:NE2	2.03	0.56
7:D:59:GLY:O	7:D:61:PHE:N	2.38	0.56
25:W:5:VAL:O	25:W:52:VAL:HG23	2.04	0.56
31:3:3:MET:O	31:3:90:PHE:HA	2.05	0.56
32:I:74:PRO:C	32:I:112:LYS:HZ1	2.13	0.56
1:0:500:G:H21	20:R:98:ASN:HD21	1.51	0.56
1:0:1730:G:C5'	1:0:1731:C:C6	2.87	0.56
1:0:2524:G:N2	1:0:2526:C:H41	2.03	0.56
1:0:2717:C:O2'	1:0:2718:C:H5''	2.05	0.56
1:0:2912:C:H2'	1:0:2913:A:O4'	2.05	0.56
13:K:125:ALA:C	13:K:127:ALA:H	2.13	0.56
15:M:107:ARG:NH1	40:M:9378:HOH:O	2.38	0.56
16:N:115:VAL:HG22	40:N:9354:HOH:O	2.05	0.56
25:W:4:LEU:O	25:W:32:CYS:HA	2.05	0.56
5:B:267:LYS:HE3	5:B:300:SER:O	2.05	0.56
4:A:113:GLY:HA2	4:A:153:ARG:NH2	2.20	0.56
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.87	0.56
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.86	0.56
23:U:4:ARG:HG2	23:U:4:ARG:HH11	1.71	0.56
1:0:871:G:H5''	1:0:871:G:H8	1.70	0.56
1:0:1681:G:H5''	1:0:1682:A:H5'	1.87	0.56
1:0:2105:C:H5'	40:4:7933:HOH:O	2.05	0.56
2:9:3051:A:H5'	16:N:160:SER:HB3	1.87	0.56
11:H:116:ALA:O	11:H:117:PHE:C	2.49	0.56
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.87	0.56
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.88	0.56
1:0:737:A:H2'	1:0:738:G:O4'	2.05	0.56
4:A:206:ARG:H	4:A:206:ARG:HD3	1.71	0.56
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.88	0.56
12:J:74:ARG:NH1	12:J:105:LEU:HD11	2.21	0.56
13:K:55:VAL:HG12	13:K:56:SER:N	2.20	0.56
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.31	0.56
22:T:48:VAL:HG22	22:T:96:VAL:HG22	1.87	0.56
24:V:64:GLY:O	24:V:65:ASP:HB2	2.03	0.56
12:J:93:ARG:HB3	12:J:93:ARG:NH1	2.17	0.56
14:L:79:ASP:HB2	40:L:9459:HOH:O	2.06	0.56
1:0:1595:G:O2'	1:0:1596:U:H5'	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2563:U:H2'	1:0:2565:C:O5'	2.05	0.56
5:B:40:GLY:HA3	40:B:9637:HOH:O	2.04	0.56
7:D:57:THR:HG23	7:D:63:ILE:HA	1.88	0.56
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.87	0.56
16:N:11:ARG:O	16:N:15:GLU:HG3	2.06	0.56
25:W:52:VAL:HG22	25:W:53:ALA:N	2.20	0.56
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.41	0.56
27:Y:154:ARG:NH1	27:Y:155:ARG:HG2	2.19	0.56
30:2:48:ASP:O	30:2:49:GLU:HB2	2.05	0.56
1:0:1592:G:O2'	1:0:1593:C:O4'	2.24	0.56
29:1:25:LYS:HD2	30:2:49:GLU:N	2.18	0.56
1:0:95:A:H5''	1:0:97:G:O4'	2.06	0.55
1:0:1878:G:O2'	1:0:1879:U:OP2	2.24	0.55
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.86	0.55
4:A:135:VAL:HG21	4:A:147:ARG:NH1	2.20	0.55
8:E:69:ILE:HA	8:E:72:MET:HE3	1.87	0.55
31:3:62:THR:HB	40:3:9487:HOH:O	2.05	0.55
1:0:2320:U:H4'	1:0:2321:A:O4'	2.06	0.55
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.88	0.55
8:E:34:TRP:O	12:J:127:ILE:HD11	2.06	0.55
16:N:149:GLU:O	16:N:152:GLU:HB3	2.05	0.55
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.64	0.55
1:0:2453:G:H5''	40:L:9442:HOH:O	2.04	0.55
40:0:6753:HOH:O	23:U:56:ARG:HB3	2.05	0.55
16:N:154:LEU:O	16:N:155:GLU:HB2	2.06	0.55
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.88	0.55
1:0:248:A:H5'	1:0:249:G:OP2	2.07	0.55
2:9:3041:C:H4'	7:D:48:MET:HB3	1.88	0.55
2:9:3076:G:C3'	2:9:3077:A:H5''	2.27	0.55
6:C:236:THR:HG21	40:C:9178:HOH:O	2.05	0.55
14:L:80:ASP:CB	14:L:90:ARG:HB3	2.36	0.55
16:N:183:ASP:O	16:N:184:ILE:O	2.25	0.55
28:Z:10:ARG:HA	40:Z:9215:HOH:O	2.06	0.55
4:A:179:MET:HA	4:A:179:MET:CE	2.33	0.55
5:B:120:ASP:OD2	5:B:123:ALA:HB2	2.07	0.55
10:G:12:ILE:N	10:G:13:PRO:CD	2.69	0.55
12:J:70:PHE:CG	12:J:70:PHE:O	2.60	0.55
19:Q:25:PRO:HB2	40:Q:4350:HOH:O	2.07	0.55
22:T:40:VAL:HG22	22:T:41:ARG:N	2.22	0.55
24:V:56:ILE:O	24:V:60:GLN:HG3	2.05	0.55
1:0:558:C:O2'	1:0:559:U:H5''	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1200:A:H4'	40:0:7793:HOH:O	2.07	0.55
1:0:1209:C:H2'	1:0:1210:G:H8	1.71	0.55
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.05	0.55
2:9:3041:C:H5'	7:D:48:MET:HE2	1.89	0.55
4:A:36:ASP:C	4:A:38:ILE:H	2.15	0.55
5:B:84:LEU:HB2	5:B:182:VAL:HG21	1.89	0.55
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.72	0.55
18:P:111:GLU:O	18:P:111:GLU:HG2	2.06	0.55
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.06	0.55
25:W:64:THR:O	25:W:68:THR:HG22	2.06	0.55
1:0:870:G:C2'	1:0:871:G:H5''	2.35	0.55
1:0:2072:G:C6	1:0:2533:C:H1'	2.42	0.55
11:H:171:ALA:HA	40:H:9535:HOH:O	2.06	0.55
14:L:136:ALA:HB3	40:L:9475:HOH:O	2.06	0.55
16:N:89:GLY:O	16:N:92:ALA:HB3	2.07	0.55
1:0:272:A:H5'	1:0:273:G:OP2	2.07	0.55
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.07	0.55
1:0:2645:U:C6	1:0:2645:U:OP2	2.59	0.55
5:B:185:GLY:HA2	40:B:9625:HOH:O	2.05	0.55
9:F:58:GLU:HA	9:F:61:MET:HE2	1.89	0.55
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.89	0.55
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.88	0.55
1:0:1236:A:C8	12:J:63:ILE:HD11	2.41	0.55
2:9:3057:A:H8	7:D:141:VAL:HG21	1.72	0.55
6:C:214:THR:HG23	40:C:9237:HOH:O	2.06	0.55
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.07	0.55
24:V:1:THR:HG23	24:V:2:VAL:N	2.22	0.55
30:2:36:ASN:HB3	30:2:39:ARG:HG3	1.89	0.55
1:0:2365:G:H5''	40:Q:6597:HOH:O	2.06	0.55
1:0:2502:C:C2'	1:0:2503:A:H5'	2.36	0.55
40:0:3147:HOH:O	18:P:81:LYS:HG2	2.06	0.55
40:0:9698:HOH:O	5:B:214:PRO:HD2	2.06	0.55
15:M:79:ALA:HB3	15:M:81:ARG:NH1	2.22	0.55
24:V:42:ASN:HB3	40:V:7247:HOH:O	2.06	0.55
1:0:1406:A:H4'	1:0:1407:A:H5''	1.88	0.54
1:0:1528:A:H2'	1:0:1529:G:O4'	2.07	0.54
1:0:2524:G:H21	1:0:2526:C:N4	2.04	0.54
9:F:13:GLU:OE2	9:F:78:GLU:HG2	2.07	0.54
15:M:68:ARG:O	15:M:68:ARG:HD3	2.08	0.54
1:0:485:A:N3	1:0:487:G:H5''	2.22	0.54
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.72	0.54
5:B:97:LEU:O	5:B:98:THR:HG23	2.06	0.54
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.89	0.54
17:O:59:VAL:CG2	17:O:111:VAL:HG21	2.37	0.54
1:O:949:U:C4'	19:Q:95:GLU:HA	2.37	0.54
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.07	0.54
5:B:321:PRO:HA	40:B:9646:HOH:O	2.07	0.54
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.25	0.54
9:F:31:LYS:HE3	40:F:2623:HOH:O	2.06	0.54
21:S:57:THR:CG2	21:S:58:MET:N	2.69	0.54
32:I:134:SER:O	32:I:135:LEU:HD23	2.07	0.54
1:O:1067:A:H5'	40:O:4901:HOH:O	2.06	0.54
4:A:34:ASP:OD1	4:A:35:GLY:N	2.41	0.54
40:K:7438:HOH:O	23:U:20:MET:HE1	2.07	0.54
17:O:59:VAL:HG23	17:O:111:VAL:CG2	2.37	0.54
1:O:2670:G:O2'	1:O:2671:U:H5'	2.07	0.54
1:O:2717:C:OP1	5:B:207:LYS:HG3	2.08	0.54
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.08	0.54
18:P:141:ILE:C	18:P:143:ALA:H	2.14	0.54
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.72	0.54
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.89	0.54
32:I:72:VAL:HG11	32:I:111:GLN:O	2.07	0.54
1:O:2720:C:O2	13:K:87:ARG:NH2	2.41	0.54
1:O:2748:G:OP1	1:O:2749:U:H5''	2.07	0.54
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.42	0.54
18:P:98:ILE:O	18:P:98:ILE:HD13	2.08	0.54
1:O:2866:U:H4'	1:O:2867:G:H5'	1.89	0.54
2:9:3029:C:O3'	7:D:138:GLY:HA2	2.07	0.54
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.54	0.54
1:O:656:G:OP2	17:O:37:ARG:HD2	2.08	0.54
1:O:1667:A:H2'	1:O:1668:U:C6	2.43	0.54
40:O:3309:HOH:O	5:B:254:GLN:HG3	2.08	0.54
5:B:321:PRO:HG3	40:B:9595:HOH:O	2.08	0.54
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.13	0.54
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.43	0.54
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.89	0.54
1:O:12:U:H2'	1:O:13:G:H5'	1.90	0.54
1:O:1853:C:OP1	4:A:231:LYS:HG3	2.08	0.54
2:9:3114:G:O6	16:N:11:ARG:HD3	2.07	0.54
17:O:53:GLN:HE21	17:O:56:GLU:CD	2.15	0.54
1:O:151:A:H2'	1:O:152:A:O4'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:834:G:H4'	1:0:835:U:OP2	2.08	0.54
1:0:1187:U:O2'	1:0:1189:A:H2	1.91	0.54
1:0:2894:C:O2'	1:0:2895:C:H5'	2.07	0.54
1:0:286:U:H2'	1:0:287:C:C6	2.43	0.53
1:0:1641:A:H2'	1:0:1642:A:H5'	1.90	0.53
1:0:1902:G:H2'	1:0:1903:U:O4'	2.08	0.53
14:L:80:ASP:HB2	14:L:90:ARG:O	2.06	0.53
15:M:58:GLN:HG3	40:M:9405:HOH:O	2.07	0.53
1:0:757:C:OP1	14:L:27:ARG:HD2	2.07	0.53
1:0:1335:C:OP2	27:Y:207:SER:HB3	2.08	0.53
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.89	0.53
1:0:156:C:H5''	15:M:171:ARG:CD	2.27	0.53
1:0:1189:A:H1'	1:0:1209:C:C1'	2.38	0.53
4:A:94:LEU:HD23	4:A:94:LEU:N	2.24	0.53
5:B:139:ASP:HB3	40:B:9552:HOH:O	2.08	0.53
6:C:236:THR:HA	40:C:9252:HOH:O	2.07	0.53
9:F:60:VAL:O	9:F:60:VAL:HG12	2.09	0.53
14:L:150:GLN:HB3	40:L:9471:HOH:O	2.08	0.53
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.38	0.53
16:N:167:ASP:C	16:N:168:LEU:HG	2.34	0.53
1:0:558:C:H2'	1:0:559:U:C5'	2.38	0.53
1:0:709:G:O2'	17:O:25:VAL:CG1	2.56	0.53
1:0:1819:G:H2'	1:0:1820:G:H4'	1.89	0.53
6:C:194:PHE:HA	6:C:234:VAL:HG13	1.91	0.53
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.38	0.53
22:T:47:THR:HB	22:T:100:ASP:HB3	1.90	0.53
1:0:40:C:H4'	40:0:7476:HOH:O	2.08	0.53
1:0:2711:U:H1'	40:0:4024:HOH:O	2.08	0.53
4:A:165:THR:HG22	40:A:9604:HOH:O	2.09	0.53
5:B:310:ARG:HD2	40:B:9587:HOH:O	2.08	0.53
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.89	0.53
10:G:20:VAL:O	10:G:24:VAL:HG23	2.08	0.53
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.09	0.53
16:N:169:PRO:O	16:N:172:PHE:HB3	2.09	0.53
23:U:5:GLU:HG2	23:U:10:GLY:O	2.07	0.53
6:C:20:ASP:O	6:C:23:GLU:HB2	2.08	0.53
15:M:77:HIS:HD2	15:M:79:ALA:O	1.91	0.53
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.91	0.53
1:0:793:A:H5''	18:P:83:LYS:HG2	1.91	0.53
1:0:1555:G:H4'	1:0:1630:A:H2	1.73	0.53
18:P:16:VAL:HG12	18:P:17:GLY:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:122:GLN:HB3	20:R:138:SER:HB2	1.89	0.53
1:O:1363:G:OP1	6:C:76:ARG:NH2	2.42	0.53
4:A:164:ARG:CZ	40:A:9572:HOH:O	2.56	0.53
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.90	0.53
15:M:167:GLY:O	15:M:171:ARG:HG3	2.09	0.53
31:3:70:ARG:HH11	31:3:70:ARG:HG2	1.74	0.53
1:O:538:C:OP2	27:Y:134:HIS:HE1	1.91	0.53
1:O:1476:A:O2'	1:O:1477:C:H5'	2.08	0.53
5:B:58:PRO:HA	5:B:63:GLU:CD	2.34	0.53
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.38	0.53
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.65	0.53
32:I:138:THR:HG22	32:I:139:ILE:H	1.74	0.53
1:O:1118:A:C8	1:O:1119:G:H5''	2.44	0.53
1:O:2812:A:C2	1:O:2814:A:N6	2.65	0.53
5:B:264:GLU:CG	5:B:267:LYS:HE2	2.29	0.53
16:N:36:ALA:C	16:N:37:ARG:HD2	2.34	0.53
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.91	0.52
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.39	0.52
15:M:30:GLU:O	15:M:34:GLU:HG3	2.09	0.52
1:O:1268:C:O2'	27:Y:169:ARG:HB2	2.09	0.52
1:O:1626:A:H2'	1:O:1627:G:O4'	2.08	0.52
1:O:1666:C:H2'	1:O:1667:A:C5'	2.37	0.52
1:O:1730:G:H5'	1:O:1731:C:H5	1.74	0.52
1:O:2541:U:H5'	1:O:2541:U:H6	1.74	0.52
2:9:3049:G:O2'	2:9:3050:G:H5'	2.10	0.52
16:N:64:SER:C	16:N:66:LEU:H	2.17	0.52
22:T:19:ARG:HD3	22:T:67:LEU:O	2.09	0.52
25:W:38:THR:HG22	25:W:39:ASP:N	2.24	0.52
32:I:99:ASP:O	32:I:100:LEU:HD23	2.09	0.52
1:O:288:A:H2'	1:O:289:G:C8	2.43	0.52
1:O:951:A:C2'	1:O:952:G:H5'	2.39	0.52
1:O:1352:A:O2'	1:O:1353:C:OP1	2.24	0.52
6:C:84:VAL:HG12	6:C:85:LYS:HG2	1.92	0.52
17:O:87:THR:O	17:O:91:GLN:HG3	2.08	0.52
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.24	0.52
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.90	0.52
32:I:105:VAL:HG11	32:I:129:VAL:CG2	2.39	0.52
1:O:1166:A:H1'	1:O:1192:A:N3	2.25	0.52
14:L:35:ARG:C	14:L:35:ARG:HD3	2.35	0.52
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.23	0.52
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.93	0.52
1:0:1878:G:O2'	1:0:1879:U:C6	2.60	0.52
2:9:3008:G:O6	16:N:11:ARG:NH1	2.42	0.52
5:B:232:TRP:HD1	5:B:235:ARG:HD2	1.74	0.52
5:B:232:TRP:CD1	5:B:235:ARG:HD2	2.44	0.52
14:L:134:GLU:HG3	40:L:9458:HOH:O	2.10	0.52
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	1.91	0.52
1:0:1878:G:O2'	1:0:1879:U:P	2.68	0.52
1:0:2032:U:H2'	1:0:2033:G:C5'	2.40	0.52
16:N:152:GLU:C	16:N:154:LEU:H	2.16	0.52
1:0:894:A:N1	6:C:87:ARG:NH2	2.57	0.52
6:C:233:THR:HG22	6:C:234:VAL:N	2.25	0.52
15:M:57:LYS:HE2	15:M:140:ALA:O	2.10	0.52
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.56	0.52
1:0:750:A:O3'	6:C:101:ASP:HB2	2.09	0.52
1:0:2626:C:H2'	1:0:2627:G:C8	2.45	0.52
4:A:217:ARG:HH11	4:A:217:ARG:CG	2.23	0.52
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.90	0.52
14:L:73:VAL:HG23	14:L:74:THR:N	2.25	0.52
14:L:92:ASP:HB3	14:L:95:ASP:OD2	2.10	0.52
23:U:20:MET:HE2	23:U:30:HIS:CE1	2.44	0.52
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.92	0.52
1:0:364:C:H2'	1:0:365:G:O4'	2.10	0.52
1:0:848:C:H5'	40:0:7728:HOH:O	2.09	0.52
1:0:2346:C:H6	1:0:2346:C:O5'	1.93	0.52
13:K:98:VAL:HG22	13:K:102:GLU:C	2.35	0.52
14:L:119:THR:HG23	14:L:139:SER:OG	2.10	0.52
16:N:72:GLU:O	16:N:72:GLU:HG2	2.10	0.52
32:I:114:PRO:HG2	32:I:115:ASP:H	1.75	0.52
1:0:1738:C:H1'	40:0:7770:HOH:O	2.10	0.51
1:0:2415:A:N3	16:N:26:LEU:HD13	2.25	0.51
40:0:7093:HOH:O	27:Y:155:ARG:HD2	2.08	0.51
15:M:98:GLN:O	15:M:102:GLU:HG3	2.10	0.51
1:0:962:C:H1'	16:N:5:ARG:HH12	1.75	0.51
1:0:1060:C:H6	1:0:1060:C:H5'	1.76	0.51
1:0:1328:A:OP1	27:Y:169:ARG:HD2	2.10	0.51
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.45	0.51
2:9:3042:C:O2	7:D:76:ARG:NH1	2.43	0.51
4:A:128:LEU:HD21	4:A:131:HIS:HE1	1.75	0.51
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.41	0.51
12:J:19:MET:HE2	12:J:79:PHE:HA	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:92:ASP:HA	14:L:121:ILE:HB	1.92	0.51
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.40	0.51
16:N:154:LEU:O	16:N:155:GLU:CB	2.58	0.51
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.71	0.51
1:O:920:C:H5''	1:O:921:G:O5'	2.10	0.51
1:O:1181:A:N1	1:O:1192:A:O2'	2.40	0.51
1:O:1242:A:C5'	12:J:82:THR:HG23	2.31	0.51
1:O:2064:U:H5'	1:O:2652:U:O3'	2.10	0.51
2:9:3049:G:C2'	2:9:3050:G:H5'	2.41	0.51
5:B:258:GLY:H	5:B:260:HIS:CE1	2.28	0.51
8:E:11:VAL:HG12	8:E:12:ASP:N	2.24	0.51
8:E:154:ILE:HG13	8:E:156:ASP:OD1	2.10	0.51
27:Y:112:GLU:HA	27:Y:112:GLU:OE1	2.10	0.51
28:Z:42:CYS:SG	28:Z:44:GLU:HB2	2.51	0.51
9:F:53:ASP:OD1	9:F:80:GLN:HB2	2.11	0.51
13:K:74:VAL:HG11	13:K:113:ILE:CG1	2.32	0.51
15:M:71:SER:O	15:M:73:ARG:NH1	2.43	0.51
20:R:39:THR:HB	20:R:42:GLU:HG3	1.93	0.51
1:O:2769:C:H2'	1:O:2770:G:C5'	2.40	0.51
6:C:154:VAL:O	6:C:158:GLU:HG3	2.11	0.51
8:E:23:GLU:HG2	8:E:28:SER:CB	2.41	0.51
9:F:28:ALA:CB	9:F:99:THR:HG23	2.41	0.51
11:H:170:ASN:N	11:H:170:ASN:ND2	2.59	0.51
24:V:25:THR:HG22	24:V:29:ASN:HD21	1.75	0.51
32:I:113:HIS:N	32:I:114:PRO:CD	2.73	0.51
1:O:1234:U:N3	5:B:244:PRO:HB3	2.26	0.51
1:O:1594:C:OP2	18:P:120:ARG:HD2	2.10	0.51
1:O:2505:G:C2'	1:O:2506:A:H5'	2.41	0.51
5:B:243:ASN:HA	5:B:244:PRO:C	2.36	0.51
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.93	0.51
7:D:128:LEU:HB2	40:D:6007:HOH:O	2.11	0.51
9:F:48:VAL:HG23	9:F:74:PHE:HB3	1.93	0.51
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.91	0.51
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.10	0.51
1:O:1730:G:C5'	1:O:1731:C:H6	2.23	0.51
1:O:2712:G:H5'	40:K:4183:HOH:O	2.11	0.51
9:F:91:VAL:CG1	9:F:92:GLY:H	2.14	0.51
11:H:56:GLN:NE2	11:H:126:ARG:HE	2.09	0.51
12:J:88:PRO:O	12:J:94:GLY:HA3	2.11	0.51
15:M:64:ARG:HD2	40:M:9384:HOH:O	2.09	0.51
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:299:U:H5'	40:0:7789:HOH:O	2.11	0.51
1:0:475:G:OP1	6:C:73:LEU:CD2	2.58	0.51
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.39	0.51
1:0:1400:C:H4'	26:X:56:GLU:HG2	1.92	0.51
1:0:1701:A:H5''	1:0:1702:U:H3'	1.93	0.51
4:A:129:LEU:CD1	4:A:145:MET:HE1	2.41	0.51
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.76	0.51
5:B:254:GLN:HG2	5:B:255:GLY:H	1.76	0.51
20:R:82:GLU:O	20:R:86:LYS:HG3	2.11	0.51
25:W:5:VAL:O	25:W:52:VAL:CG2	2.59	0.51
25:W:38:THR:O	25:W:42:ARG:HB2	2.10	0.51
1:0:134:U:H6	1:0:134:U:H5''	1.75	0.51
1:0:328:U:O4'	6:C:202:THR:CG2	2.59	0.51
1:0:2456:A:H2'	1:0:2457:U:C6	2.46	0.51
2:9:3002:U:OP2	2:9:3003:A:H5'	2.10	0.51
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.93	0.51
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.92	0.51
14:L:145:LEU:HD23	14:L:145:LEU:O	2.10	0.51
1:0:776:A:OP1	29:1:28:HIS:HE1	1.95	0.50
1:0:1218:U:H2'	1:0:1219:U:C6	2.46	0.50
1:0:2718:C:H5'	1:0:2718:C:C6	2.44	0.50
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.92	0.50
12:J:107:ASN:HD22	12:J:109:TYR:H	1.58	0.50
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.93	0.50
23:U:9:CYS:HA	23:U:52:THR:HG23	1.93	0.50
25:W:139:GLY:O	25:W:141:HIS:CD2	2.63	0.50
1:0:588:G:O6	25:W:154:ARG:NH1	2.45	0.50
1:0:1462:C:H2'	1:0:1463:A:C8	2.47	0.50
1:0:2896:A:H5''	40:X:5399:HOH:O	2.10	0.50
40:9:1361:HOH:O	16:N:41:LYS:HE3	2.10	0.50
17:O:42:GLU:HB2	40:O:2176:HOH:O	2.10	0.50
32:I:101:SER:H	32:I:104:GLN:NE2	2.09	0.50
1:0:870:G:OP2	4:A:3:ARG:HD3	2.12	0.50
1:0:945:U:H2'	1:0:946:C:C6	2.46	0.50
1:0:2661:U:H3	1:0:2812:A:H62	1.60	0.50
2:9:3057:A:C8	7:D:141:VAL:HG21	2.46	0.50
23:U:9:CYS:O	23:U:52:THR:HG23	2.11	0.50
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.92	0.50
1:0:241:A:C2	1:0:378:A:H4'	2.47	0.50
1:0:407:A:H2'	1:0:408:A:C8	2.47	0.50
1:0:2414:A:H2'	1:0:2415:A:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2487:C:H1'	40:O:5938:HOH:O	2.10	0.50
4:A:192:VAL:HG11	4:A:207:GLN:HB3	1.93	0.50
14:L:104:ASP:O	14:L:105:TYR:HB3	2.11	0.50
14:L:143:THR:O	14:L:147:GLU:HG3	2.10	0.50
1:O:447:A:OP2	22:T:1:SER:HB2	2.11	0.50
1:O:2726:U:O2	1:O:2749:U:O5'	2.30	0.50
4:A:36:ASP:O	4:A:36:ASP:CG	2.54	0.50
5:B:307:ARG:HB3	40:B:9642:HOH:O	2.11	0.50
6:C:236:THR:HG22	6:C:239:ALA:CB	2.41	0.50
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.93	0.50
15:M:164:THR:CG2	15:M:165:GLY:N	2.74	0.50
20:R:119:VAL:HG12	20:R:119:VAL:O	2.11	0.50
22:T:71:VAL:CG1	22:T:72:ILE:N	2.74	0.50
32:I:138:THR:HG22	32:I:139:ILE:N	2.26	0.50
1:O:1350:U:H2'	1:O:1351:G:O4'	2.11	0.50
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.11	0.50
5:B:16:ARG:NH2	40:B:9557:HOH:O	2.39	0.50
5:B:162:MET:CE	5:B:308:LEU:HD21	2.36	0.50
15:M:41:GLU:HG3	40:M:9344:HOH:O	2.12	0.50
15:M:48:LYS:O	15:M:52:GLN:HG3	2.12	0.50
1:O:119:A:H2'	1:O:120:A:H5''	1.93	0.50
1:O:2265:U:H2'	1:O:2266:A:C8	2.47	0.50
1:O:2507:G:H2'	1:O:2510:C:N4	2.27	0.50
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.41	0.50
12:J:47:THR:HG22	12:J:48:GLY:N	2.26	0.50
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.93	0.50
13:K:132:VAL:HG11	23:U:22:VAL:HG22	1.93	0.50
21:S:33:SER:O	21:S:37:VAL:HG23	2.10	0.50
31:3:35:TRP:HB2	40:3:9493:HOH:O	2.12	0.50
1:O:292:G:H2'	1:O:358:G:N2	2.27	0.50
1:O:1477:C:H5'	1:O:1868:G:C5'	2.41	0.50
1:O:2524:G:N2	1:O:2526:C:H5	2.10	0.50
40:O:3164:HOH:O	25:W:119:HIS:HE1	1.95	0.50
7:D:136:ARG:HB3	7:D:137:PRO:HD2	1.93	0.50
11:H:158:THR:HB	11:H:159:PRO:HD3	1.94	0.50
12:J:13:ASP:OD1	12:J:15:ARG:HB3	2.12	0.50
16:N:36:ALA:O	16:N:37:ARG:HD2	2.12	0.50
1:O:65:C:O2'	1:O:66:G:H5'	2.12	0.50
6:C:104:ASP:O	6:C:108:GLN:HG3	2.12	0.50
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.39	0.50
10:G:12:ILE:HD12	40:G:692:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:6:CYS:C	23:U:8:TYR:H	2.19	0.50
40:O:5157:HOH:O	4:A:206:ARG:HD3	2.11	0.49
2:9:3023:U:O2'	2:9:3024:U:H4'	2.12	0.49
8:E:7:ILE:HG22	8:E:45:ASP:O	2.11	0.49
8:E:166:VAL:HG12	40:E:3134:HOH:O	2.12	0.49
17:O:97:SER:OG	17:O:100:GLN:HG3	2.12	0.49
20:R:84:ALA:O	20:R:88:PHE:HD1	1.95	0.49
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.45	0.49
27:Y:115:ARG:NE	40:Y:9356:HOH:O	2.45	0.49
1:O:1279:U:O2	1:O:1279:U:H2'	2.12	0.49
1:O:2072:G:H3'	1:O:2073:G:C5'	2.42	0.49
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.38	0.49
6:C:236:THR:O	6:C:237:GLU:C	2.54	0.49
7:D:25:MET:CE	7:D:40:ILE:HD11	2.42	0.49
9:F:68:ASP:C	9:F:70:LYS:H	2.20	0.49
16:N:114:LYS:O	16:N:118:ILE:HG13	2.12	0.49
24:V:38:GLY:C	24:V:40:PRO:HD2	2.36	0.49
24:V:39:ALA:O	24:V:41:GLU:N	2.44	0.49
1:O:944:G:H21	25:W:44:MET:CE	2.26	0.49
1:O:2911:C:O2'	1:O:2912:C:H5'	2.12	0.49
7:D:25:MET:HE1	7:D:40:ILE:HD11	1.94	0.49
7:D:60:GLU:O	7:D:61:PHE:C	2.55	0.49
11:H:27:LYS:H	11:H:59:HIS:CD2	2.20	0.49
14:L:145:LEU:HD23	14:L:145:LEU:C	2.37	0.49
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.77	0.49
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.42	0.49
1:O:2889:U:H4'	1:O:2890:A:H5'	1.95	0.49
4:A:232:ARG:NH2	4:A:236:GLY:O	2.37	0.49
5:B:112:THR:HG23	5:B:158:LYS:HZ2	1.76	0.49
6:C:236:THR:H	6:C:239:ALA:HB3	1.77	0.49
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.27	0.49
12:J:4:ALA:O	12:J:5:GLU:HB2	2.11	0.49
1:O:926:A:O2'	14:L:41:HIS:HD2	1.96	0.49
1:O:1200:A:H3'	40:O:6281:HOH:O	2.11	0.49
1:O:2502:C:H2'	1:O:2503:A:H5'	1.95	0.49
6:C:118:THR:O	6:C:136:VAL:HG13	2.11	0.49
11:H:45:VAL:HA	11:H:167:PRO:O	2.12	0.49
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.94	0.49
29:1:25:LYS:O	29:1:25:LYS:HG2	2.12	0.49
1:O:309:C:OP1	22:T:97:ARG:NH2	2.39	0.49
1:O:678:G:OP2	6:C:107:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1592:G:H2'	1:0:1593:C:C6	2.48	0.49
1:0:2100:A:H4'	6:C:64:GLY:O	2.12	0.49
1:0:2346:C:H4'	7:D:52:THR:CG2	2.42	0.49
4:A:217:ARG:HH11	4:A:217:ARG:HG3	1.76	0.49
5:B:320:GLN:HE21	5:B:321:PRO:HD2	1.77	0.49
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.43	0.49
11:H:29:ALA:C	11:H:30:GLN:HG3	2.38	0.49
12:J:142:ASN:O	12:J:144:THR:N	2.46	0.49
14:L:144:ASP:HA	14:L:147:GLU:OE1	2.11	0.49
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.95	0.49
1:0:820:G:O2'	1:0:856:G:H4'	2.13	0.49
1:0:1118:A:C8	1:0:1118:A:C3'	2.90	0.49
2:9:3052:A:O2'	2:9:3053:G:H5'	2.13	0.49
6:C:27:ARG:O	6:C:31:ILE:HG13	2.13	0.49
7:D:25:MET:CE	7:D:37:ALA:HB1	2.42	0.49
8:E:81:GLU:HG2	8:E:134:SER:CB	2.42	0.49
9:F:117:GLU:C	9:F:119:ARG:H	2.21	0.49
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.08	0.49
12:J:45:VAL:HG22	12:J:46:ILE:N	2.27	0.49
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.26	0.49
25:W:13:MET:HE2	25:W:18:GLN:N	2.28	0.49
27:Y:145:LYS:HE2	40:Y:9405:HOH:O	2.11	0.49
1:0:1666:C:C2'	1:0:1667:A:C5'	2.91	0.49
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.94	0.49
1:0:542:A:H2'	1:0:543:G:O4'	2.12	0.49
7:D:50:VAL:O	7:D:71:ALA:HA	2.13	0.49
7:D:167:GLU:C	7:D:169:THR:H	2.20	0.49
9:F:111:ILE:O	9:F:115:VAL:HG23	2.13	0.49
16:N:82:TYR:OH	16:N:176:ARG:NH1	2.46	0.49
20:R:132:ARG:NH2	40:R:9494:HOH:O	2.46	0.49
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.93	0.49
1:0:775:G:OP1	29:1:16:HIS:HE1	1.96	0.49
1:0:797:A:H4'	28:Z:10:ARG:N	2.28	0.49
1:0:1506:U:H6	1:0:1506:U:H5'	1.78	0.49
1:0:2090:G:H2'	1:0:2091:G:C8	2.47	0.49
1:0:2846:C:H4'	40:0:5619:HOH:O	2.11	0.49
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.95	0.49
30:2:35:ARG:HB2	40:2:2691:HOH:O	2.11	0.49
40:0:4331:HOH:O	22:T:9:LYS:HD3	2.13	0.48
5:B:14:GLY:HA2	5:B:15:PRO:C	2.37	0.48
6:C:246:ARG:NH1	40:C:9174:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.94	0.48
22:T:71:VAL:HG13	22:T:91:LEU:O	2.13	0.48
22:T:89:ARG:O	22:T:89:ARG:HG3	2.13	0.48
24:V:64:GLY:O	24:V:65:ASP:CB	2.60	0.48
1:O:920:C:H4'	1:O:921:G:C2	2.49	0.48
1:O:999:C:H2'	1:O:1000:C:O4'	2.12	0.48
1:O:1119:G:N2	1:O:1246:A:N1	2.61	0.48
17:O:14:LEU:CG	17:O:102:ILE:HD11	2.43	0.48
1:O:475:G:OP1	6:C:73:LEU:HD22	2.12	0.48
1:O:2408:A:H4'	31:3:15:ASN:O	2.13	0.48
4:A:52:SER:HB2	4:A:164:ARG:HH11	1.78	0.48
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.27	0.48
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.49	0.48
28:Z:36:ASP:HB3	28:Z:45:ASP:O	2.13	0.48
1:O:319:A:H4'	1:O:338:C:C5	2.48	0.48
1:O:1183:C:H5	1:O:1192:A:OP1	1.96	0.48
1:O:1527:A:H1'	1:O:1528:A:C8	2.48	0.48
1:O:2102:G:H5''	1:O:2538:A:C2	2.48	0.48
1:O:2508:C:H2'	40:O:7232:HOH:O	2.12	0.48
26:X:34:ARG:NH1	26:X:48:VAL:O	2.46	0.48
6:C:157:LEU:HD22	6:C:162:VAL:CG1	2.43	0.48
7:D:25:MET:HE2	7:D:41:LEU:CG	2.36	0.48
16:N:36:ALA:HB1	16:N:118:ILE:HD12	1.96	0.48
18:P:115:SER:HG	18:P:118:GLN:HG3	1.77	0.48
22:T:38:ARG:NH1	22:T:38:ARG:HG3	2.29	0.48
1:O:1921:A:O2'	1:O:1922:A:H5'	2.14	0.48
1:O:2472:C:O2'	1:O:2634:G:H4'	2.13	0.48
1:O:2509:A:H2'	1:O:2510:C:O4'	2.13	0.48
11:H:34:GLY:HA3	11:H:84:LYS:HA	1.95	0.48
16:N:69:TYR:CE2	16:N:184:ILE:HG13	2.49	0.48
16:N:73:ALA:N	40:N:9360:HOH:O	2.45	0.48
17:O:80:ASP:OD1	17:O:81:PHE:N	2.45	0.48
1:O:666:A:H2'	1:O:667:C:O4'	2.14	0.48
1:O:2032:U:H2'	1:O:2033:G:H5'	1.94	0.48
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.95	0.48
5:B:56:ASP:HB3	5:B:322:ARG:HE	1.79	0.48
12:J:131:THR:HB	12:J:134:GLU:OE1	2.14	0.48
13:K:27:ARG:HD2	40:K:4747:HOH:O	2.14	0.48
14:L:10:SER:O	14:L:11:ARG:HB3	2.14	0.48
15:M:24:GLN:NE2	15:M:24:GLN:HA	2.28	0.48
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:7:GLU:HA	26:X:74:ALA:O	2.14	0.48
1:0:969:G:H1	1:0:999:C:H42	1.62	0.48
1:0:1724:U:H5''	40:0:4309:HOH:O	2.12	0.48
1:0:2883:A:H2'	1:0:2884:G:O4'	2.14	0.48
9:F:60:VAL:O	9:F:60:VAL:CG1	2.61	0.48
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.78	0.48
14:L:97:VAL:HG12	14:L:98:GLU:O	2.13	0.48
14:L:123:ASP:O	14:L:146:GLY:HA2	2.13	0.48
15:M:184:ARG:HG3	15:M:185:PRO:HA	1.96	0.48
18:P:98:ILE:HD12	18:P:102:ARG:CZ	2.43	0.48
25:W:65:VAL:CG1	25:W:116:LEU:HD13	2.42	0.48
1:0:653:C:H2'	1:0:654:A:C8	2.48	0.48
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.13	0.48
6:C:84:VAL:O	6:C:85:LYS:HB2	2.14	0.48
9:F:46:GLU:O	9:F:73:PRO:HD2	2.14	0.48
15:M:182:LYS:O	15:M:194:ALA:HB2	2.14	0.48
16:N:156:GLU:O	16:N:157:PRO:C	2.57	0.48
21:S:56:ASN:O	30:2:8:LYS:NZ	2.42	0.48
1:0:558:C:C2'	1:0:559:U:H5''	2.44	0.48
1:0:1739:G:H1'	1:0:2726:U:O4	2.13	0.48
1:0:1789:G:O6	18:P:73:HIS:HE1	1.97	0.48
1:0:2769:C:H2'	1:0:2770:G:H5'	1.95	0.48
40:0:5826:HOH:O	25:W:122:ARG:NH2	2.41	0.48
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.95	0.48
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.28	0.48
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.43	0.48
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.96	0.48
24:V:1:THR:CG2	24:V:2:VAL:H	2.20	0.48
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.96	0.48
25:W:142:ASP:HB2	40:W:2729:HOH:O	2.14	0.48
1:0:1044:C:H5''	40:0:9649:HOH:O	2.13	0.47
1:0:1603:A:H5''	1:0:1605:G:H5'	1.96	0.47
1:0:1736:A:H1'	40:0:8086:HOH:O	2.14	0.47
1:0:2852:A:H5''	40:0:5770:HOH:O	2.14	0.47
8:E:69:ILE:HA	8:E:72:MET:CE	2.43	0.47
11:H:83:TYR:CD1	11:H:83:TYR:C	2.92	0.47
14:L:61:ALA:HB2	14:L:105:TYR:CZ	2.49	0.47
15:M:43:PRO:HG3	15:M:62:VAL:HG21	1.95	0.47
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.79	0.47
1:0:2112:A:H2'	1:0:2113:G:C8	2.49	0.47
1:0:2895:C:H4'	40:X:4132:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.79	0.47
5:B:267:LYS:HD2	40:B:9530:HOH:O	2.13	0.47
13:K:14:LYS:HG3	13:K:32:ILE:O	2.13	0.47
20:R:106:GLY:HA2	20:R:109:MET:CE	2.44	0.47
1:0:1730:G:H5''	1:0:1731:C:C6	2.49	0.47
1:0:2749:U:H5'	40:0:8433:HOH:O	2.13	0.47
1:0:2812:A:N7	40:0:7959:HOH:O	2.35	0.47
4:A:149:ASP:OD1	4:A:151:GLN:HB2	2.14	0.47
13:K:55:VAL:CG1	13:K:56:SER:N	2.77	0.47
22:T:81:LYS:HD2	22:T:87:VAL:HG11	1.96	0.47
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.21	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.44	0.47
1:0:2611:G:H5'	1:0:2613:G:C8	2.49	0.47
5:B:51:VAL:HG22	5:B:52:VAL:N	2.29	0.47
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.44	0.47
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.50	0.47
1:0:317:A:OP1	22:T:52:ARG:O	2.33	0.47
1:0:558:C:C2'	1:0:559:U:C5'	2.93	0.47
1:0:944:G:C8	25:W:23:MET:HE1	2.49	0.47
40:0:7351:HOH:O	15:M:178:LYS:HB2	2.14	0.47
5:B:53:LEU:HD21	5:B:270:ILE:HD12	1.97	0.47
5:B:162:MET:HE2	5:B:310:ARG:CD	2.32	0.47
6:C:133:ARG:HH11	6:C:133:ARG:HG3	1.79	0.47
7:D:52:THR:HB	7:D:70:GLY:C	2.39	0.47
12:J:130:VAL:HG12	12:J:131:THR:N	2.30	0.47
17:O:59:VAL:HG21	17:O:111:VAL:HG21	1.94	0.47
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.15	0.47
32:I:106:LYS:O	32:I:110:GLU:HG3	2.14	0.47
1:0:1979:G:O2'	1:0:1980:U:OP1	2.27	0.47
1:0:2545:U:OP2	5:B:2:GLN:NE2	2.47	0.47
1:0:2681:A:H4'	1:0:2682:C:H5'	1.97	0.47
1:0:2717:C:H2'	1:0:2718:C:C5'	2.40	0.47
1:0:2906:A:H5'	1:0:2907:C:O4'	2.15	0.47
2:9:3018:U:H2'	2:9:3019:G:C8	2.50	0.47
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.30	0.47
5:B:41:PHE:CG	5:B:79:MET:HE2	2.50	0.47
6:C:25:PRO:HG2	40:C:9125:HOH:O	2.14	0.47
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.80	0.47
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.96	0.47
16:N:166:ALA:O	16:N:167:ASP:O	2.33	0.47
1:0:29:C:C2'	1:0:30:U:H5'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:185:G:H4'	1:0:186:A:H4'	1.96	0.47
1:0:1185:U:H2'	1:0:1186:C:C6	2.48	0.47
1:0:1406:A:H4'	1:0:1407:A:C5'	2.45	0.47
1:0:1881:A:OP1	4:A:199:HIS:HE1	1.97	0.47
1:0:2421:G:H4'	40:0:5324:HOH:O	2.13	0.47
1:0:2443:C:H1'	14:L:56:LYS:HE3	1.97	0.47
40:0:3822:HOH:O	32:I:92:PRO:HD3	2.13	0.47
2:9:3059:C:H2'	2:9:3060:C:C6	2.50	0.47
5:B:75:GLU:C	5:B:77:PRO:HD3	2.40	0.47
6:C:218:VAL:N	40:C:9225:HOH:O	2.48	0.47
7:D:25:MET:CE	7:D:41:LEU:HG	2.38	0.47
7:D:84:LEU:HA	7:D:87:ALA:HB3	1.97	0.47
7:D:146:LYS:NZ	16:N:107:ASN:HD21	2.13	0.47
8:E:106:ASN:ND2	8:E:109:GLY:HA2	2.30	0.47
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.61	0.47
14:L:80:ASP:HB2	14:L:90:ARG:HB3	1.96	0.47
14:L:98:GLU:O	14:L:99:GLU:HB2	2.15	0.47
16:N:182:GLY:O	16:N:183:ASP:C	2.57	0.47
23:U:52:THR:HG22	23:U:54:THR:H	1.77	0.47
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.78	0.47
26:X:25:ARG:HD2	40:X:5356:HOH:O	2.15	0.47
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.48	0.47
28:Z:10:ARG:C	28:Z:12:GLY:H	2.23	0.47
1:0:710:G:H5'	17:O:25:VAL:HG13	1.97	0.47
1:0:932:U:H2'	1:0:933:C:C6	2.50	0.47
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.14	0.47
1:0:2503:A:P	11:H:151:ARG:HH22	2.38	0.47
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.29	0.47
9:F:118:LEU:O	9:F:119:ARG:HB3	2.15	0.47
14:L:53:ARG:HH22	14:L:57:VAL:HG12	1.80	0.47
32:I:131:THR:O	32:I:135:LEU:HG	2.15	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.49	0.47
6:C:133:ARG:HE	6:C:138:VAL:HG22	1.79	0.47
13:K:101:ASN:O	13:K:102:GLU:HB2	2.15	0.47
26:X:61:ARG:HB2	26:X:65:ASN:HB2	1.97	0.47
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.96	0.47
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.50	0.47
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.96	0.47
31:3:55:VAL:HG22	40:3:9444:HOH:O	2.15	0.47
1:0:475:G:C5'	6:C:73:LEU:HD23	2.45	0.47
1:0:1853:C:O2'	4:A:217:ARG:NH2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3091:C:H2'	2:9:3092:G:O4'	2.15	0.47
12:J:43:ARG:HG2	40:J:5361:HOH:O	2.15	0.47
16:N:37:ARG:NE	40:N:9330:HOH:O	2.47	0.47
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.50	0.47
1:0:1667:A:H5'	1:0:1667:A:C8	2.41	0.46
40:0:5274:HOH:O	16:N:21:HIS:HD2	1.97	0.46
4:A:36:ASP:HB2	4:A:85:SER:H	1.79	0.46
5:B:87:TYR:O	5:B:138:GLY:N	2.34	0.46
8:E:1:PRO:HG2	8:E:59:MET:SD	2.56	0.46
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.46	0.46
16:N:119:GLN:O	16:N:123:ILE:HG13	2.15	0.46
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.80	0.46
18:P:89:ASN:HB3	18:P:92:GLU:HB2	1.96	0.46
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.80	0.46
1:0:447:A:OP1	22:T:2:LYS:HG2	2.15	0.46
1:0:1333:U:H2'	1:0:1334:C:H6	1.80	0.46
40:0:3549:HOH:O	6:C:78:ARG:HD3	2.15	0.46
2:9:3001:U:H5'	2:9:3121:C:O2	2.15	0.46
6:C:120:ASP:C	6:C:120:ASP:OD1	2.57	0.46
9:F:70:LYS:C	9:F:72:VAL:H	2.23	0.46
10:G:64:ASN:N	10:G:64:ASN:ND2	2.63	0.46
11:H:30:GLN:H	11:H:66:ARG:HH11	1.63	0.46
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.97	0.46
25:W:88:THR:CG2	25:W:89:ASP:H	2.28	0.46
26:X:85:VAL:HG12	26:X:86:GLU:N	2.30	0.46
32:I:139:ILE:CG2	32:I:140:GLU:N	2.78	0.46
1:0:57:C:H5'	24:V:46:ILE:HG21	1.98	0.46
2:9:3039:U:H1'	2:9:3044:A:N6	2.30	0.46
7:D:154:LYS:H	7:D:154:LYS:CD	2.24	0.46
16:N:167:ASP:O	16:N:168:LEU:HG	2.15	0.46
25:W:122:ARG:HG3	25:W:152:ALA:O	2.14	0.46
30:2:5:LYS:O	30:2:9:LYS:HG3	2.15	0.46
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.96	0.46
1:0:500:G:O2'	20:R:94:ASN:ND2	2.48	0.46
1:0:1211:G:O2'	1:0:1212:C:H5'	2.16	0.46
4:A:71:PRO:HD2	4:A:74:VAL:HG21	1.98	0.46
5:B:305:ASP:O	5:B:306:LYS:CB	2.63	0.46
15:M:68:ARG:NH2	15:M:73:ARG:HD3	2.31	0.46
16:N:152:GLU:C	16:N:154:LEU:N	2.74	0.46
17:O:88:LYS:HD3	40:O:7061:HOH:O	2.15	0.46
20:R:119:VAL:O	20:R:119:VAL:CG1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:399:C:H5'	15:M:179:GLY:O	2.15	0.46
2:9:3029:C:H2'	2:9:3030:C:C5'	2.42	0.46
3:4:76:DA:H5''	38:4:9701:SPS:C6	2.45	0.46
4:A:58:VAL:HG21	4:A:68:ILE:HD12	1.98	0.46
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.76	0.46
4:A:132:ASP:OD1	4:A:133:ARG:N	2.49	0.46
9:F:21:GLU:O	9:F:24:ARG:HG3	2.15	0.46
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.46	0.46
20:R:33:ARG:NH1	40:R:9454:HOH:O	2.40	0.46
22:T:40:VAL:HG22	22:T:41:ARG:H	1.81	0.46
1:0:462:A:H2'	40:0:5427:HOH:O	2.15	0.46
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.97	0.46
1:0:2019:A:H5'	40:0:5087:HOH:O	2.16	0.46
1:0:2453:G:H4'	14:L:50:GLY:C	2.40	0.46
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.97	0.46
14:L:143:THR:CG2	14:L:144:ASP:N	2.78	0.46
16:N:67:ALA:C	16:N:69:TYR:H	2.23	0.46
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.50	0.46
1:0:622:G:P	27:Y:148:GLY:HA3	2.55	0.46
1:0:1299:G:H5'	40:0:4642:HOH:O	2.15	0.46
4:A:96:LEU:HG	4:A:152:CYS:O	2.16	0.46
5:B:51:VAL:HG23	5:B:327:VAL:HG13	1.97	0.46
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.97	0.46
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.97	0.46
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.41	0.46
13:K:114:ALA:HB3	13:K:117:VAL:HG23	1.96	0.46
15:M:90:ARG:HB2	31:3:46:ILE:HD11	1.98	0.46
23:U:17:THR:CG2	23:U:18:GLY:H	2.27	0.46
25:W:29:VAL:O	25:W:30:ASN:HB2	2.16	0.46
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.15	0.46
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.15	0.46
1:0:57:C:H5'	24:V:46:ILE:CG2	2.46	0.46
1:0:951:A:O2'	1:0:952:G:H5'	2.16	0.46
1:0:2837:U:H2'	40:0:7315:HOH:O	2.14	0.46
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.80	0.46
11:H:18:GLU:HG3	11:H:19:TYR:CE1	2.51	0.46
15:M:95:LYS:HA	15:M:170:ASN:HD21	1.81	0.46
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.27	0.46
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.59	0.46
31:3:69:TYR:O	31:3:77:ALA:HA	2.16	0.46
1:0:204:A:C2'	1:0:205:U:H5'	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:432:G:O2'	1:0:433:C:H5'	2.16	0.46
1:0:451:C:O2'	1:0:452:G:H5'	2.15	0.46
1:0:834:G:H3'	1:0:835:U:H4'	1.98	0.46
1:0:1940:C:H4'	40:0:7797:HOH:O	2.14	0.46
2:9:3006:C:H4'	16:N:35:VAL:HG11	1.98	0.46
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.98	0.46
4:A:126:ALA:HB1	4:A:138:VAL:CG1	2.46	0.46
5:B:140:LEU:HD23	40:B:9578:HOH:O	2.16	0.46
17:O:25:VAL:HG23	40:O:3062:HOH:O	2.16	0.46
19:Q:22:GLY:O	19:Q:23:THR:C	2.58	0.46
22:T:41:ARG:NH1	22:T:42:VAL:O	2.49	0.46
24:V:1:THR:O	24:V:2:VAL:C	2.59	0.46
26:X:25:ARG:NH2	40:X:5740:HOH:O	2.48	0.46
27:Y:144:ARG:NH1	40:Y:9377:HOH:O	2.49	0.46
1:0:1202:A:H2'	1:0:1203:G:O4'	2.16	0.46
2:9:3028:U:H2'	2:9:3029:C:C6	2.51	0.46
38:4:9701:SPS:O1	38:4:9701:SPS:H91	2.16	0.46
5:B:146:THR:C	5:B:148:PRO:HD3	2.41	0.46
11:H:73:LEU:HD21	11:H:146:VAL:HA	1.98	0.46
14:L:144:ASP:O	14:L:147:GLU:HB2	2.16	0.46
15:M:82:ARG:O	15:M:83:SER:C	2.59	0.46
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.80	0.46
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.98	0.46
27:Y:189:ASN:C	27:Y:189:ASN:ND2	2.74	0.46
1:0:664:U:O4	1:0:681:G:H5''	2.16	0.45
1:0:1086:A:C6	25:W:11:VAL:HG11	2.51	0.45
1:0:1167:G:H2'	1:0:1168:C:O4'	2.16	0.45
1:0:1419:U:H2'	1:0:1685:A:C2	2.52	0.45
1:0:1730:G:H5'	1:0:1731:C:C6	2.50	0.45
1:0:2531:U:O2'	1:0:2532:A:H5'	2.16	0.45
1:0:2679:G:H2'	1:0:2681:A:OP2	2.15	0.45
5:B:71:VAL:CG1	5:B:296:LEU:HD22	2.46	0.45
5:B:138:GLY:O	5:B:139:ASP:O	2.34	0.45
7:D:159:PRO:O	7:D:163:VAL:HG23	2.17	0.45
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.97	0.45
8:E:81:GLU:O	8:E:172:PRO:HD3	2.16	0.45
15:M:66:SER:HB3	15:M:128:TRP:NE1	2.31	0.45
18:P:135:ALA:HB1	18:P:139:ARG:NH1	2.31	0.45
20:R:82:GLU:OE1	20:R:86:LYS:HE3	2.16	0.45
23:U:52:THR:CG2	23:U:54:THR:HB	2.46	0.45
1:0:136:C:H2'	1:0:137:U:O4'	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:415:A:O2'	1:0:416:G:H5'	2.17	0.45
1:0:1165:G:O3'	1:0:1174:A:H4'	2.16	0.45
1:0:2825:C:H4'	1:0:2826:G:O5'	2.15	0.45
9:F:26:THR:HG21	9:F:103:GLU:HG3	1.97	0.45
17:O:23:GLY:C	40:O:3062:HOH:O	2.59	0.45
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.31	0.45
26:X:76:ARG:O	26:X:77:PHE:HB3	2.16	0.45
1:0:249:G:O2'	1:0:250:C:H5'	2.17	0.45
1:0:1135:G:H5'	40:0:6446:HOH:O	2.16	0.45
1:0:1829:A:H2'	1:0:1830:C:H5'	1.99	0.45
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.16	0.45
9:F:20:LEU:HB2	9:F:49:PHE:CZ	2.51	0.45
14:L:89:PHE:CD1	14:L:89:PHE:N	2.85	0.45
16:N:33:ARG:NH2	40:N:9350:HOH:O	2.50	0.45
17:O:32:ARG:HH21	17:O:35:LYS:HZ1	1.64	0.45
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.17	0.45
25:W:88:THR:CG2	25:W:89:ASP:N	2.78	0.45
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.47	0.45
1:0:289:G:H5'	40:0:5159:HOH:O	2.17	0.45
1:0:2619:UR3:H2'	1:0:2620:U:C6	2.51	0.45
2:9:3005:G:OP1	16:N:17:ARG:NH2	2.50	0.45
6:C:124:VAL:HA	6:C:230:GLY:O	2.16	0.45
8:E:16:ASP:O	8:E:17:HIS:HB2	2.15	0.45
8:E:101:GLU:HA	8:E:118:ILE:HG13	1.97	0.45
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.99	0.45
15:M:107:ARG:NH1	15:M:107:ARG:CG	2.78	0.45
22:T:12:ARG:NH1	40:T:3035:HOH:O	2.49	0.45
23:U:20:MET:CG	23:U:28:THR:HG23	2.47	0.45
1:0:734:U:H1'	1:0:737:A:N6	2.32	0.45
40:0:9834:HOH:O	4:A:11:ARG:HD3	2.17	0.45
7:D:51:ARG:HD3	40:D:7636:HOH:O	2.16	0.45
9:F:102:GLY:O	9:F:103:GLU:HB2	2.16	0.45
12:J:103:VAL:HG12	40:J:5907:HOH:O	2.16	0.45
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.46	0.45
15:M:164:THR:CG2	15:M:166:ALA:H	2.27	0.45
17:O:59:VAL:CG2	17:O:111:VAL:CG2	2.95	0.45
24:V:25:THR:HG22	24:V:29:ASN:ND2	2.32	0.45
32:I:108:ILE:C	32:I:110:GLU:H	2.24	0.45
1:0:371:U:H2'	1:0:372:A:H8	1.80	0.45
1:0:1130:U:H2'	1:0:1131:G:O4'	2.17	0.45
1:0:1624:A:H4'	1:0:1625:U:H5'	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2697:A:H2'	1:0:2698:G:O4'	2.17	0.45
4:A:129:LEU:HD13	4:A:145:MET:HE1	1.98	0.45
5:B:217:ARG:HG3	5:B:257:THR:CG2	2.47	0.45
6:C:168:ARG:NH2	6:C:190:ALA:O	2.50	0.45
14:L:66:VAL:HG23	14:L:67:ARG:N	2.31	0.45
16:N:86:LEU:O	16:N:90:LEU:HG	2.15	0.45
20:R:25:PHE:CZ	20:R:29:LYS:HE2	2.50	0.45
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.45	0.45
1:0:968:G:O2'	1:0:969:G:H5'	2.17	0.45
1:0:1149:U:H5''	1:0:1151:G:O4'	2.17	0.45
1:0:1745:G:H22	1:0:2033:G:H5'	1.82	0.45
1:0:2289:G:H21	1:0:2291:A:H2	1.62	0.45
1:0:2356:A:H2'	1:0:2357:G:O4'	2.16	0.45
1:0:2506:A:O2'	1:0:2507:G:O5'	2.35	0.45
40:0:5514:HOH:O	11:H:58:ARG:HG3	2.16	0.45
4:A:122:SER:O	4:A:124:VAL:HG13	2.17	0.45
12:J:107:ASN:C	12:J:107:ASN:ND2	2.73	0.45
15:M:81:ARG:HG2	15:M:85:ARG:O	2.16	0.45
16:N:110:THR:HB	16:N:113:SER:HG	1.79	0.45
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.25	0.45
25:W:3:ALA:O	25:W:54:PHE:HA	2.17	0.45
26:X:73:ARG:NH1	26:X:88:GLU:HG2	2.32	0.45
1:0:59:A:H5'	40:0:4886:HOH:O	2.15	0.45
1:0:497:A:H2'	1:0:498:A:C5'	2.47	0.45
1:0:1741:U:H3'	40:0:3369:HOH:O	2.16	0.45
4:A:130:THR:HG22	4:A:131:HIS:O	2.17	0.45
5:B:80:ARG:HB2	5:B:145:HIS:CE1	2.52	0.45
6:C:233:THR:HG22	6:C:234:VAL:H	1.82	0.45
23:U:9:CYS:CA	23:U:52:THR:HG23	2.47	0.45
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.50	0.45
1:0:1180:U:H1'	40:0:3822:HOH:O	2.17	0.45
1:0:1654:U:H2'	4:A:47:HIS:HD2	1.82	0.45
4:A:66:ARG:HH11	4:A:66:ARG:CB	2.29	0.45
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.46	0.45
5:B:254:GLN:NE2	40:B:9588:HOH:O	2.49	0.45
11:H:166:SER:O	11:H:167:PRO:C	2.59	0.45
13:K:119:GLN:O	13:K:119:GLN:HG2	2.17	0.45
30:2:20:ARG:HG3	30:2:21:VAL:N	2.31	0.45
31:3:75:GLY:HA2	40:3:9510:HOH:O	2.16	0.45
1:0:120:A:H2'	1:0:120:A:N3	2.32	0.45
1:0:968:G:H1'	11:H:32:LYS:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2073:G:H5''	40:0:4398:HOH:O	2.16	0.45
1:0:2329:C:O2'	1:0:2330:U:H5'	2.17	0.45
4:A:128:LEU:HD21	4:A:131:HIS:CE1	2.51	0.45
7:D:10:PHE:CD1	7:D:11:HIS:N	2.85	0.45
7:D:96:SER:C	7:D:98:PHE:H	2.24	0.45
7:D:170:TYR:O	7:D:171:ASP:CB	2.65	0.45
9:F:26:THR:HG21	9:F:102:GLY:C	2.42	0.45
19:Q:91:LEU:C	19:Q:92:ARG:HG2	2.41	0.45
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.25	0.45
31:3:38:ARG:CB	31:3:42:ARG:HH12	2.25	0.45
1:0:1056:U:H2'	1:0:1057:A:O4'	2.16	0.44
1:0:1603:A:C5'	1:0:1605:G:H5'	2.47	0.44
1:0:1942:A:H3'	40:0:7797:HOH:O	2.17	0.44
1:0:2415:A:H2'	1:0:2416:G:H5'	1.98	0.44
1:0:2591:C:H2'	1:0:2592:G:O4'	2.17	0.44
6:C:157:LEU:HD22	6:C:162:VAL:HG11	1.98	0.44
9:F:109:GLU:HG2	9:F:113:ASP:OD2	2.17	0.44
13:K:87:ARG:NH1	40:K:4066:HOH:O	2.49	0.44
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.52	0.44
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.47	0.44
18:P:18:LYS:O	18:P:21:VAL:HG13	2.17	0.44
26:X:25:ARG:HD3	26:X:64:ALA:O	2.17	0.44
32:I:75:THR:O	32:I:76:ALA:C	2.60	0.44
1:0:1250:C:O2'	1:0:1251:C:H5'	2.16	0.44
1:0:1435:U:H5'	40:0:3201:HOH:O	2.16	0.44
1:0:1835:U:C5	1:0:1840:A:N7	2.69	0.44
2:9:3051:A:H5'	16:N:160:SER:HB2	1.99	0.44
2:9:3052:A:H2'	2:9:3053:G:O4'	2.17	0.44
2:9:3064:C:C2'	2:9:3065:A:H5'	2.48	0.44
5:B:60:SER:HA	5:B:61:PRO:HD3	1.86	0.44
5:B:168:GLY:O	5:B:169:GLY:O	2.36	0.44
5:B:183:GLU:O	5:B:184:ASP:C	2.60	0.44
5:B:277:GLU:N	5:B:278:PRO:HD2	2.32	0.44
6:C:49:ASP:HB3	6:C:52:ALA:HB2	1.99	0.44
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.16	0.44
7:D:91:ALA:HB2	7:D:106:PHE:CD2	2.52	0.44
7:D:154:LYS:HD2	7:D:154:LYS:N	2.26	0.44
10:G:19:GLU:HG2	10:G:66:LEU:HD13	1.99	0.44
22:T:53:GLY:HA3	40:T:6384:HOH:O	2.17	0.44
26:X:12:ILE:HD12	26:X:36:HIS:CG	2.52	0.44
1:0:1166:A:N6	1:0:1180:U:H3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.83	0.44
1:0:1768:C:H2'	1:0:1769:C:O4'	2.17	0.44
1:0:1972:U:H2'	1:0:1973:A:H5''	1.98	0.44
1:0:2456:A:H2'	1:0:2457:U:H6	1.83	0.44
2:9:3108:C:O2'	2:9:3109:G:H5'	2.16	0.44
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.32	0.44
7:D:68:PRO:C	7:D:69:ILE:HG13	2.42	0.44
8:E:116:THR:CG2	8:E:151:LEU:HD22	2.47	0.44
10:G:68:GLU:O	10:G:72:ASP:HB2	2.18	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.82	0.44
27:Y:107:PRO:HD3	27:Y:182:PHE:CE1	2.52	0.44
31:3:91:GLN:O	31:3:92:GLU:HB2	2.17	0.44
1:0:177:A:H2'	1:0:178:U:O4'	2.16	0.44
1:0:447:A:OP1	22:T:1:SER:HB2	2.17	0.44
1:0:2073:G:H3'	40:0:4398:HOH:O	2.18	0.44
1:0:2361:A:H2'	1:0:2362:A:C8	2.51	0.44
2:9:3056:A:C6	7:D:13:MET:HE3	2.52	0.44
4:A:99:ILE:O	4:A:131:HIS:CE1	2.70	0.44
4:A:164:ARG:NE	40:A:9572:HOH:O	2.50	0.44
7:D:66:GLY:O	7:D:67:ASP:HB3	2.17	0.44
7:D:173:GLU:OE1	7:D:174:VAL:HG23	2.18	0.44
12:J:63:ILE:CG2	12:J:64:GLY:N	2.79	0.44
15:M:95:LYS:HD2	15:M:99:ARG:HG2	1.98	0.44
16:N:67:ALA:C	16:N:69:TYR:N	2.75	0.44
17:O:38:ARG:NH1	40:O:7674:HOH:O	2.50	0.44
1:0:794:U:H3	1:0:819:A:H61	1.64	0.44
1:0:2364:A:H5''	19:Q:15:LYS:HD3	2.00	0.44
40:0:9644:HOH:O	14:L:30:ARG:HD2	2.16	0.44
8:E:101:GLU:HB3	8:E:117:THR:HA	2.00	0.44
11:H:154:TYR:CD1	11:H:154:TYR:C	2.95	0.44
15:M:86:GLN:O	15:M:88:VAL:HG23	2.16	0.44
16:N:112:GLY:HA2	16:N:137:ALA:N	2.32	0.44
17:O:32:ARG:HH21	17:O:35:LYS:NZ	2.15	0.44
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.83	0.44
1:0:602:A:O2'	1:0:605:C:H4'	2.17	0.44
2:9:3092:G:H2'	2:9:3093:A:C8	2.53	0.44
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.44
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.47	0.44
5:B:74:ILE:HD13	5:B:309:VAL:HG21	2.00	0.44
6:C:7:ASP:OD1	6:C:11:ASN:N	2.50	0.44
11:H:76:GLU:O	11:H:77:LEU:HD23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:168:LEU:HA	16:N:169:PRO:HD3	1.77	0.44
23:U:4:ARG:HG2	23:U:4:ARG:NH1	2.31	0.44
25:W:119:HIS:HD2	25:W:120:PRO:O	2.00	0.44
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.53	0.44
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.83	0.44
1:O:220:C:H1'	40:O:6282:HOH:O	2.17	0.44
1:O:236:A:H8	1:O:236:A:OP1	2.01	0.44
1:O:1025:C:H5'	25:W:23:MET:O	2.17	0.44
1:O:1098:A:O3'	25:W:129:LYS:HE2	2.18	0.44
1:O:1120:U:H5''	1:O:1120:U:C6	2.53	0.44
1:O:2791:U:H1'	1:O:2792:A:H5''	1.99	0.44
5:B:225:GLY:HA3	40:B:9567:HOH:O	2.18	0.44
11:H:66:ARG:HD3	40:H:9545:HOH:O	2.18	0.44
18:P:63:ARG:NH2	40:P:190:HOH:O	2.51	0.44
20:R:39:THR:CG2	20:R:107:GLU:O	2.66	0.44
21:S:57:THR:HG22	21:S:59:ASP:H	1.81	0.44
24:V:20:LEU:HD11	24:V:53:ILE:HG23	2.00	0.44
1:O:1182:C:H1'	1:O:1192:A:C8	2.50	0.44
1:O:1476:A:O2'	1:O:1868:G:H5'	2.18	0.44
1:O:1751:G:C2'	1:O:1752:G:H5''	2.42	0.44
4:A:135:VAL:HG13	4:A:135:VAL:O	2.17	0.44
8:E:101:GLU:OE2	8:E:115:ARG:HD3	2.17	0.44
1:O:90:A:H2'	1:O:91:G:O4'	2.18	0.44
1:O:335:U:H4'	22:T:92:ASP:OD2	2.18	0.44
1:O:407:A:H5'	40:O:6540:HOH:O	2.17	0.44
1:O:926:A:O2'	14:L:41:HIS:CD2	2.71	0.44
1:O:1852:A:H5''	4:A:232:ARG:O	2.18	0.44
1:O:1926:G:H2'	1:O:1927:A:H8	1.82	0.44
1:O:2506:A:O2'	1:O:2507:G:P	2.76	0.44
40:O:5826:HOH:O	25:W:119:HIS:CG	2.71	0.44
11:H:96:ARG:NH2	40:H:9498:HOH:O	2.50	0.44
11:H:114:ARG:O	11:H:115:ALA:C	2.61	0.44
14:L:34:GLY:HA3	14:L:38:HIS:CE1	2.53	0.44
19:Q:75:ILE:HD13	19:Q:84:ILE:CD1	2.48	0.44
21:S:57:THR:HG23	40:S:9487:HOH:O	2.17	0.44
27:Y:209:VAL:HG12	27:Y:214:ARG:HG3	1.99	0.44
1:O:1203:G:O2'	1:O:1204:C:H5'	2.17	0.43
1:O:1252:A:H2'	1:O:1253:C:O4'	2.17	0.43
1:O:2254:G:O2'	1:O:2255:A:H5'	2.18	0.43
40:O:5006:HOH:O	30:2:39:ARG:HG2	2.18	0.43
4:A:26:ASP:OD1	4:A:26:ASP:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:162:MET:HG3	5:B:310:ARG:HD3	2.00	0.43
9:F:11:ASP:O	9:F:14:ASP:HB2	2.17	0.43
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.98	0.43
15:M:36:ALA:HB1	40:M:9353:HOH:O	2.17	0.43
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.98	0.43
20:R:95:ALA:HB2	20:R:145:LEU:HD23	2.00	0.43
20:R:104:PHE:HB3	20:R:109:MET:HE2	1.99	0.43
24:V:12:THR:HG23	24:V:14:ALA:H	1.82	0.43
30:2:48:ASP:O	30:2:49:GLU:CB	2.65	0.43
1:0:262:A:OP2	9:F:91:VAL:HG11	2.18	0.43
1:0:263:U:C2	9:F:59:ILE:HD12	2.53	0.43
1:0:1163:G:H2'	1:0:1164:U:C5	2.52	0.43
1:0:1306:U:OP1	6:C:184:ARG:HD2	2.18	0.43
1:0:2491:G:H1'	40:0:7345:HOH:O	2.17	0.43
40:9:3472:HOH:O	16:N:41:LYS:HD3	2.17	0.43
4:A:204:GLY:O	4:A:205:GLY:C	2.60	0.43
6:C:21:VAL:C	6:C:23:GLU:H	2.26	0.43
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.86	0.43
7:D:51:ARG:NH1	7:D:68:PRO:HB3	2.32	0.43
12:J:132:LEU:HD23	12:J:132:LEU:HA	1.89	0.43
20:R:96:VAL:HG13	20:R:106:GLY:HA3	2.00	0.43
25:W:141:HIS:HB2	25:W:146:ILE:HG12	2.00	0.43
26:X:43:VAL:CG1	26:X:44:ASP:N	2.81	0.43
1:0:137:U:H2'	1:0:139:C:C5	2.53	0.43
1:0:196:G:H1'	1:0:198:A:N7	2.34	0.43
1:0:449:A:N7	6:C:43:LYS:HG2	2.33	0.43
1:0:699:C:H2'	1:0:744:G:O4'	2.18	0.43
1:0:1972:U:C2'	1:0:1973:A:H5''	2.48	0.43
5:B:205:VAL:O	5:B:307:ARG:NE	2.49	0.43
9:F:32:GLY:N	40:F:3111:HOH:O	2.50	0.43
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.84	0.43
1:0:371:U:H2'	1:0:372:A:C8	2.53	0.43
1:0:921:G:H4'	1:0:924:G:N1	2.33	0.43
1:0:1015:C:H2'	1:0:1016:U:C6	2.53	0.43
1:0:1132:A:N6	1:0:1229:C:H2'	2.33	0.43
1:0:1218:U:H2'	1:0:1219:U:H6	1.82	0.43
1:0:1342:C:O2'	1:0:1343:C:H5'	2.18	0.43
1:0:1406:A:H5'	1:0:1407:A:C8	2.54	0.43
1:0:2649:A:O4'	1:0:2650:U:H5	2.01	0.43
13:K:30:LYS:O	13:K:55:VAL:HG13	2.18	0.43
16:N:161:GLY:O	16:N:162:ASP:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.34	0.43
1:0:93:C:H5''	24:V:1:THR:CB	2.43	0.43
1:0:308:U:C2	22:T:52:ARG:NH2	2.87	0.43
1:0:830:G:O2'	1:0:831:U:H5'	2.18	0.43
1:0:1206:U:H5'	1:0:1206:U:C6	2.33	0.43
1:0:1211:G:H2'	1:0:1212:C:H6	1.83	0.43
1:0:1503:U:H2'	1:0:1504:A:O4'	2.19	0.43
1:0:1838:U:H1'	1:0:2644:C:O4'	2.18	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.54	0.43
1:0:2515:C:C2'	1:0:2516:G:H5'	2.48	0.43
40:0:3297:HOH:O	15:M:82:ARG:HA	2.17	0.43
4:A:65:ARG:HG2	4:A:65:ARG:HH11	1.83	0.43
4:A:201:PHE:HB3	40:A:9617:HOH:O	2.18	0.43
8:E:84:MET:HE1	8:E:148:ILE:HD13	2.01	0.43
12:J:54:VAL:O	12:J:58:GLU:HG3	2.18	0.43
13:K:125:ALA:C	13:K:127:ALA:N	2.76	0.43
14:L:94:ARG:NH1	14:L:143:THR:HG21	2.34	0.43
21:S:18:MET:HE3	21:S:75:GLN:HG2	2.00	0.43
1:0:544:G:C3'	1:0:545:G:H5''	2.49	0.43
1:0:945:U:H2'	1:0:946:C:H6	1.83	0.43
1:0:1268:C:O2'	1:0:1269:G:H5'	2.18	0.43
1:0:2676:C:H4'	12:J:70:PHE:HD1	1.83	0.43
6:C:184:ARG:HB3	40:C:9167:HOH:O	2.18	0.43
11:H:56:GLN:NE2	11:H:93:GLN:HG2	2.31	0.43
23:U:35:LYS:HE2	23:U:51:TRP:CZ2	2.53	0.43
25:W:106:THR:OG1	25:W:109:GLU:HB2	2.19	0.43
32:I:75:THR:N	32:I:112:LYS:HZ1	2.16	0.43
32:I:92:PRO:C	32:I:94:GLU:N	2.74	0.43
1:0:1189:A:H1'	1:0:1209:C:H1'	1.99	0.43
1:0:1201:C:C2'	1:0:1202:A:H5'	2.44	0.43
1:0:1439:C:OP1	30:2:41:HIS:HE1	2.02	0.43
1:0:1482:A:O2'	1:0:1483:C:H5'	2.19	0.43
1:0:1603:A:H5'	1:0:1605:G:C4'	2.48	0.43
1:0:2645:U:OP2	1:0:2645:U:H6	2.00	0.43
2:9:3044:A:H2'	2:9:3045:A:O4'	2.19	0.43
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.99	0.43
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.54	0.43
5:B:248:ARG:NH2	40:B:9527:HOH:O	2.44	0.43
8:E:18:LEU:HD13	8:E:34:TRP:CG	2.53	0.43
9:F:86:ALA:C	9:F:88:GLY:H	2.27	0.43
12:J:43:ARG:NH1	40:J:5361:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:38:ALA:O	21:S:42:GLU:HG3	2.18	0.43
25:W:11:VAL:O	25:W:12:ASN:HB2	2.18	0.43
1:0:10:U:O4	1:0:532:A:OP2	2.37	0.43
1:0:271:C:H41	1:0:378:A:H2	1.62	0.43
1:0:559:U:H5'	1:0:559:U:C6	2.44	0.43
1:0:1213:C:O2'	1:0:1214:G:H5'	2.19	0.43
1:0:2250:G:OP1	4:A:31:LYS:HD3	2.19	0.43
1:0:2346:C:O3'	7:D:52:THR:HG23	2.19	0.43
40:0:7250:HOH:O	16:N:4:PRO:HD2	2.18	0.43
6:C:45:ASP:OD2	6:C:98:ARG:HD2	2.19	0.43
13:K:125:ALA:O	13:K:127:ALA:N	2.47	0.43
16:N:143:ARG:HE	16:N:143:ARG:HB3	1.65	0.43
19:Q:30:VAL:HG12	19:Q:30:VAL:O	2.18	0.43
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.49	0.43
25:W:26:ILE:O	25:W:26:ILE:HG12	2.17	0.43
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.53	0.43
1:0:329:A:OP2	6:C:206:ASN:HB2	2.19	0.43
1:0:812:A:H2'	1:0:813:C:C6	2.54	0.43
1:0:1175:G:H2'	1:0:1176:C:O4'	2.19	0.43
1:0:1206:U:H6	1:0:1206:U:C5'	2.21	0.43
1:0:2032:U:C2'	1:0:2033:G:H5''	2.49	0.43
40:0:4961:HOH:O	4:A:11:ARG:CZ	2.66	0.43
2:9:3006:C:OP1	16:N:37:ARG:CZ	2.67	0.43
4:A:66:ARG:CB	4:A:66:ARG:NH1	2.81	0.43
5:B:112:THR:HG23	5:B:158:LYS:HZ1	1.81	0.43
7:D:25:MET:HE1	7:D:37:ALA:O	2.18	0.43
7:D:172:VAL:CG1	7:D:173:GLU:H	2.26	0.43
22:T:20:HIS:HB3	22:T:41:ARG:HD2	2.00	0.43
22:T:78:THR:HB	22:T:87:VAL:O	2.19	0.43
22:T:88:PRO:HB3	40:T:6320:HOH:O	2.19	0.43
1:0:1044:C:H3'	1:0:1045:G:H5''	2.01	0.43
1:0:1755:A:H2'	1:0:1756:G:O4'	2.19	0.43
4:A:217:ARG:CG	4:A:217:ARG:NH1	2.79	0.43
6:C:98:ARG:NH1	40:C:9161:HOH:O	2.51	0.43
8:E:105:GLU:HG2	8:E:113:PRO:HB3	2.01	0.43
12:J:39:VAL:CG1	12:J:40:ASN:N	2.82	0.43
13:K:13:GLU:OE1	13:K:44:LEU:HD12	2.19	0.43
14:L:92:ASP:OD1	14:L:94:ARG:HB2	2.18	0.43
15:M:61:ILE:HD12	15:M:61:ILE:N	2.33	0.43
16:N:43:VAL:HG13	16:N:118:ILE:HD11	2.01	0.43
22:T:49:GLU:HB3	22:T:59:GLU:CG	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:151:SER:HB3	27:Y:154:ARG:CB	2.49	0.43
30:2:19:SER:O	30:2:36:ASN:ND2	2.43	0.43
1:0:111:C:HO2'	29:1:20:ARG:HG2	1.79	0.42
1:0:603:A:H5''	1:0:604:G:OP1	2.18	0.42
1:0:793:A:C5'	18:P:83:LYS:HG2	2.49	0.42
1:0:1196:C:H2'	1:0:1197:G:O4'	2.18	0.42
1:0:1377:C:H1'	40:0:7728:HOH:O	2.18	0.42
1:0:2435:U:H1'	40:0:5968:HOH:O	2.19	0.42
2:9:3001:U:O3'	2:9:3003:A:H5''	2.19	0.42
5:B:101:TRP:HB2	5:B:119:HIS:CD2	2.54	0.42
7:D:164:ALA:O	7:D:165:PHE:C	2.61	0.42
12:J:130:VAL:HG12	12:J:131:THR:H	1.84	0.42
13:K:34:VAL:HG21	13:K:47:ALA:HB2	2.00	0.42
13:K:63:GLU:HB2	40:K:6344:HOH:O	2.19	0.42
22:T:75:GLU:O	22:T:76:ASP:HB2	2.19	0.42
28:Z:75:GLY:O	28:Z:78:THR:HB	2.18	0.42
31:3:65:THR:HG23	31:3:88:LEU:HD22	2.00	0.42
32:I:80:LYS:HD3	32:I:86:GLU:O	2.18	0.42
1:0:565:A:OP2	1:0:592:G:N1	2.49	0.42
1:0:1186:C:H5''	32:I:119:TYR:CE1	2.54	0.42
1:0:1226:G:H5'	40:0:5079:HOH:O	2.19	0.42
1:0:2428:G:N7	31:3:60:LYS:NZ	2.65	0.42
7:D:62:ASP:HA	40:D:4233:HOH:O	2.17	0.42
9:F:28:ALA:HB3	9:F:99:THR:O	2.19	0.42
9:F:40:ILE:HD11	9:F:48:VAL:HG11	2.00	0.42
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.84	0.42
16:N:67:ALA:O	16:N:69:TYR:N	2.52	0.42
20:R:109:MET:HE3	20:R:109:MET:HB2	1.93	0.42
21:S:37:VAL:O	21:S:41:VAL:HG23	2.18	0.42
31:3:70:ARG:HG3	31:3:77:ALA:HB2	2.01	0.42
1:0:1174:A:C5	1:0:1201:C:H4'	2.54	0.42
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.42
1:0:2251:G:H2'	1:0:2252:A:C8	2.54	0.42
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.42
40:0:7872:HOH:O	22:T:9:LYS:HB2	2.18	0.42
4:A:192:VAL:HG12	4:A:207:GLN:CB	2.41	0.42
5:B:175:LEU:HD23	5:B:175:LEU:C	2.45	0.42
7:D:23:VAL:O	7:D:23:VAL:HG23	2.19	0.42
9:F:5:ASP:O	9:F:119:ARG:NH1	2.52	0.42
11:H:16:ARG:HH21	11:H:18:GLU:CD	2.26	0.42
13:K:49:LEU:HD12	13:K:80:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:46:LEU:HD22	15:M:50:ARG:HG3	2.02	0.42
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.50	0.42
25:W:73:LEU:HD12	25:W:73:LEU:HA	1.89	0.42
26:X:7:GLU:HA	26:X:75:ALA:HA	2.01	0.42
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.54	0.42
1:O:362:G:H2'	1:O:363:A:C8	2.54	0.42
1:O:1925:G:O2'	1:O:1926:G:H5'	2.20	0.42
1:O:2478:U:O2'	1:O:2479:A:H5'	2.20	0.42
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.45	0.42
4:A:94:LEU:HG	4:A:99:ILE:HD11	2.00	0.42
5:B:190:MET:CE	5:B:194:PHE:CD1	2.96	0.42
14:L:77:ALA:C	14:L:79:ASP:H	2.28	0.42
14:L:143:THR:CG2	14:L:144:ASP:H	2.32	0.42
16:N:35:VAL:HG12	16:N:37:ARG:HD3	2.01	0.42
22:T:115:GLU:CG	22:T:116:ASP:N	2.79	0.42
25:W:48:VAL:O	25:W:48:VAL:CG1	2.67	0.42
26:X:74:ALA:HB2	26:X:85:VAL:HG22	2.02	0.42
1:O:137:U:OP1	1:O:259:G:O2'	2.37	0.42
1:O:1476:A:H1'	1:O:1867:G:O2'	2.19	0.42
1:O:2587:OMU:H2'	1:O:2589:U:H5''	2.01	0.42
5:B:11:LEU:C	40:B:9610:HOH:O	2.62	0.42
7:D:67:ASP:O	7:D:69:ILE:HG13	2.20	0.42
12:J:45:VAL:CG2	12:J:129:PHE:CD1	3.03	0.42
14:L:12:THR:HG21	14:L:16:GLY:O	2.18	0.42
15:M:49:ALA:C	15:M:54:TYR:HB3	2.45	0.42
24:V:1:THR:OG1	24:V:2:VAL:N	2.52	0.42
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.35	0.42
30:2:19:SER:HB3	40:2:4479:HOH:O	2.20	0.42
31:3:20:HIS:HA	31:3:70:ARG:O	2.20	0.42
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.82	0.42
2:9:3107:C:H5	40:9:3167:HOH:O	2.02	0.42
7:D:10:PHE:CG	7:D:11:HIS:N	2.87	0.42
7:D:173:GLU:O	7:D:174:VAL:C	2.63	0.42
9:F:106:ALA:HB3	40:F:6617:HOH:O	2.18	0.42
17:O:18:ALA:HB2	17:O:26:TRP:HB2	2.01	0.42
17:O:49:GLU:OE1	17:O:70:LEU:HD12	2.19	0.42
20:R:114:VAL:HA	20:R:144:GLU:O	2.19	0.42
21:S:6:LYS:O	21:S:7:HIS:HB3	2.20	0.42
24:V:16:ARG:NH1	24:V:65:ASP:O	2.53	0.42
24:V:42:ASN:O	24:V:44:GLY:N	2.52	0.42
25:W:34:LEU:HD12	25:W:107:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:49:GLU:HB2	40:2:131:HOH:O	2.20	0.42
32:I:92:PRO:HB2	32:I:134:SER:C	2.45	0.42
1:0:87:C:C2	30:2:30:ASP:OD2	2.73	0.42
1:0:204:A:H2'	1:0:205:U:H5'	2.01	0.42
1:0:646:G:H2'	1:0:647:U:C6	2.55	0.42
1:0:1159:G:H1	1:0:1208:C:N4	2.16	0.42
1:0:1185:U:H4'	32:I:123:ASN:HB3	2.01	0.42
1:0:1588:G:C6	1:0:1589:G:N1	2.88	0.42
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.55	0.42
1:0:2577:A:H5'	40:0:8264:HOH:O	2.18	0.42
1:0:2667:G:H1'	1:0:2914:A:N3	2.34	0.42
1:0:2809:G:H2'	1:0:2810:G:O4'	2.19	0.42
5:B:16:ARG:NE	40:B:9557:HOH:O	2.28	0.42
7:D:128:LEU:C	7:D:128:LEU:HD23	2.45	0.42
8:E:7:ILE:HD11	8:E:11:VAL:C	2.44	0.42
8:E:22:VAL:O	8:E:28:SER:HA	2.20	0.42
9:F:28:ALA:C	9:F:99:THR:HG23	2.44	0.42
22:T:102:ASP:C	22:T:102:ASP:OD1	2.62	0.42
25:W:38:THR:HG22	25:W:39:ASP:H	1.84	0.42
1:0:171:C:OP2	15:M:84:LYS:HG3	2.19	0.42
1:0:1185:U:H5'	40:0:7910:HOH:O	2.20	0.42
1:0:1603:A:H5''	1:0:1604:G:H3'	2.02	0.42
1:0:2324:G:N2	1:0:2377:U:H1'	2.35	0.42
1:0:2780:C:C1'	8:E:143:GLN:HE21	2.25	0.42
40:0:6241:HOH:O	13:K:87:ARG:CZ	2.68	0.42
4:A:81:GLN:N	4:A:92:ASN:OD1	2.42	0.42
5:B:234:ARG:NH1	40:B:9612:HOH:O	2.52	0.42
15:M:76:ARG:HG3	15:M:88:VAL:HG21	2.02	0.42
15:M:164:THR:HG22	15:M:167:GLY:H	1.85	0.42
18:P:89:ASN:OD1	18:P:92:GLU:HB2	2.19	0.42
18:P:115:SER:C	18:P:117:SER:N	2.76	0.42
26:X:43:VAL:HG12	26:X:47:ALA:HB3	2.00	0.42
27:Y:122:ARG:NH2	40:Y:9336:HOH:O	2.52	0.42
30:2:18:ASN:ND2	30:2:40:ARG:H	2.17	0.42
31:3:6:ARG:HA	31:3:20:HIS:O	2.20	0.42
1:0:1573:A:H2'	1:0:1574:C:O4'	2.19	0.42
1:0:1759:A:N3	1:0:1818:C:H2'	2.35	0.42
1:0:2011:A:H4'	1:0:2012:U:O5'	2.20	0.42
40:0:3426:HOH:O	5:B:252:PRO:HD3	2.20	0.42
2:9:3039:U:H3'	2:9:3040:C:H5''	2.01	0.42
4:A:93:THR:C	4:A:94:LEU:HD23	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:294:TYR:CD1	5:B:294:TYR:C	2.97	0.42
11:H:88:ARG:HG2	11:H:133:LEU:O	2.20	0.42
13:K:74:VAL:O	13:K:74:VAL:HG12	2.18	0.42
13:K:118:ALA:HB1	13:K:125:ALA:CB	2.50	0.42
15:M:182:LYS:C	15:M:194:ALA:HB2	2.45	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.85	0.42
1:O:295:C:H2'	1:O:296:G:O4'	2.19	0.42
1:O:737:A:C8	1:O:737:A:H3'	2.55	0.42
1:O:879:C:H5	40:O:3763:HOH:O	2.03	0.42
1:O:2034:U:H4'	40:O:6439:HOH:O	2.20	0.42
4:A:95:PRO:HA	4:A:153:ARG:HA	2.02	0.42
4:A:207:GLN:O	4:A:208:HIS:HB3	2.20	0.42
4:A:223:ARG:NE	40:A:9559:HOH:O	2.52	0.42
7:D:35:ALA:C	7:D:37:ALA:N	2.78	0.42
7:D:99:ASP:HB3	7:D:103:ASN:H	1.85	0.42
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.20	0.42
16:N:154:LEU:CG	16:N:155:GLU:H	2.25	0.42
23:U:44:ARG:HB3	40:U:3805:HOH:O	2.19	0.42
27:Y:133:HIS:HD2	40:Y:9384:HOH:O	2.03	0.42
29:1:28:HIS:O	29:1:32:LYS:N	2.45	0.42
1:O:944:G:H21	25:W:44:MET:HE2	1.85	0.41
1:O:1174:A:C6	1:O:1201:C:H4'	2.55	0.41
1:O:2089:A:O2'	1:O:2090:G:H5'	2.20	0.41
1:O:2523:U:O2'	1:O:2524:G:H5'	2.20	0.41
5:B:1:PRO:O	5:B:2:GLN:HB2	2.20	0.41
7:D:15:GLU:HA	7:D:16:PRO:HD3	1.83	0.41
11:H:146:VAL:HG22	40:H:9542:HOH:O	2.20	0.41
15:M:120:VAL:HG11	15:M:130:GLU:HG3	2.01	0.41
18:P:55:LYS:HG2	18:P:56:GLY:N	2.34	0.41
21:S:11:THR:H	21:S:14:ALA:HB3	1.83	0.41
22:T:102:ASP:OD1	22:T:104:GLU:HG3	2.20	0.41
25:W:5:VAL:C	25:W:52:VAL:HG23	2.45	0.41
1:O:304:G:H1'	1:O:347:A:N6	2.34	0.41
1:O:941:G:C5	1:O:942:U:C4	3.09	0.41
1:O:1257:C:H2'	1:O:1258:G:O4'	2.20	0.41
1:O:1507:C:H4'	40:O:4185:HOH:O	2.20	0.41
1:O:1748:U:H4'	40:O:7963:HOH:O	2.19	0.41
1:O:2768:A:O2'	1:O:2769:C:O4'	2.33	0.41
1:O:2869:G:H2'	1:O:2870:C:O4'	2.20	0.41
40:O:4417:HOH:O	11:H:11:LYS:HE2	2.20	0.41
4:A:112:PRO:HD3	4:A:152:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:20:ILE:O	8:E:30:THR:HA	2.20	0.41
12:J:143:LYS:HG3	12:J:145:TRP:CE2	2.55	0.41
18:P:14:LEU:O	18:P:16:VAL:HG23	2.20	0.41
20:R:61:GLN:NE2	40:R:9451:HOH:O	2.53	0.41
20:R:114:VAL:HG13	20:R:114:VAL:O	2.20	0.41
24:V:59:ILE:O	24:V:63:GLU:HG2	2.20	0.41
26:X:79:GLU:CD	26:X:80:GLU:N	2.78	0.41
1:O:271:C:O2	1:O:273:G:H5''	2.19	0.41
1:O:380:A:H2'	40:O:7686:HOH:O	2.19	0.41
1:O:2363:G:O2'	19:Q:11:ARG:HG3	2.20	0.41
1:O:2637:A:H5''	38:4:9701:SPS:O3	2.19	0.41
2:9:3004:G:O2'	16:N:44:ARG:NH2	2.53	0.41
2:9:3056:A:C3'	2:9:3057:A:H5''	2.50	0.41
4:A:43:VAL:O	4:A:44:ASP:HB2	2.20	0.41
6:C:27:ARG:HD2	17:O:5:PRO:HD2	2.02	0.41
7:D:167:GLU:OE2	7:D:173:GLU:HB3	2.20	0.41
8:E:1:PRO:HD2	8:E:53:GLU:O	2.20	0.41
11:H:51:VAL:CG1	11:H:53:GLU:O	2.68	0.41
11:H:78:GLY:C	11:H:80:GLU:H	2.27	0.41
18:P:55:LYS:CG	18:P:56:GLY:N	2.82	0.41
22:T:45:GLY:C	40:T:3851:HOH:O	2.63	0.41
22:T:79:LEU:HG	22:T:89:ARG:HB2	2.02	0.41
23:U:19:THR:HG22	23:U:20:MET:N	2.35	0.41
26:X:72:VAL:CG1	26:X:85:VAL:CG1	2.98	0.41
29:1:28:HIS:HD2	29:1:30:LYS:H	1.68	0.41
1:O:447:A:O2'	1:O:448:G:H5'	2.20	0.41
1:O:522:U:O2'	1:O:1366:C:H5'	2.19	0.41
1:O:1236:A:H2'	1:O:1237:U:O4'	2.20	0.41
1:O:1741:U:O2'	1:O:2723:G:H4'	2.20	0.41
1:O:1849:G:H1'	1:O:2011:A:N1	2.35	0.41
1:O:2338:G:OP1	7:D:97:GLN:HG2	2.20	0.41
1:O:2580:G:N3	1:O:2600:A:H2	2.18	0.41
1:O:2769:C:C2'	1:O:2770:G:C5'	2.98	0.41
1:O:2784:A:H1'	8:E:60:SER:OG	2.20	0.41
7:D:27:ILE:HB	40:D:5858:HOH:O	2.19	0.41
7:D:35:ALA:C	7:D:37:ALA:H	2.27	0.41
8:E:81:GLU:HA	8:E:133:VAL:O	2.20	0.41
15:M:183:THR:CG2	15:M:194:ALA:HB1	2.46	0.41
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.20	0.41
18:P:15:ASP:OD1	18:P:15:ASP:O	2.39	0.41
18:P:98:ILE:CD1	18:P:102:ARG:NE	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.41
1:0:697:G:H4'	1:0:730:G:O3'	2.21	0.41
1:0:899:C:H5'	40:0:3789:HOH:O	2.21	0.41
1:0:1020:A:H2'	1:0:1021:G:C8	2.56	0.41
1:0:1565:C:O4'	1:0:2738:G:H1'	2.20	0.41
1:0:1657:A:H2'	1:0:1658:A:C8	2.55	0.41
1:0:1666:C:C2'	1:0:1667:A:H5''	2.50	0.41
1:0:1675:C:H5''	30:2:5:LYS:HD2	2.03	0.41
1:0:1773:G:C8	28:Z:16:ALA:HA	2.56	0.41
4:A:30:ARG:HE	4:A:30:ARG:HB3	1.69	0.41
4:A:43:VAL:HG21	4:A:59:GLU:HG3	2.01	0.41
4:A:114:ASP:C	4:A:114:ASP:OD1	2.63	0.41
5:B:154:VAL:HA	5:B:155:PRO:HD3	1.88	0.41
10:G:12:ILE:HG22	10:G:17:GLN:NE2	2.36	0.41
15:M:74:LYS:HE3	15:M:75:ARG:O	2.20	0.41
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.49	0.41
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.35	0.41
1:0:290:C:O2'	1:0:291:C:H5'	2.20	0.41
1:0:625:U:H5''	1:0:1044:C:H41	1.86	0.41
1:0:1318:A:H4'	1:0:1343:C:H4'	2.02	0.41
1:0:2253:G:O2'	1:0:2254:G:H5'	2.21	0.41
1:0:2351:C:H2'	1:0:2352:G:O4'	2.20	0.41
1:0:2428:G:H5'	40:0:7132:HOH:O	2.21	0.41
40:0:6789:HOH:O	27:Y:158:LYS:HD3	2.19	0.41
12:J:42:GLU:O	12:J:131:THR:HG23	2.20	0.41
15:M:47:ASP:CG	15:M:48:LYS:N	2.79	0.41
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	2.03	0.41
22:T:115:GLU:HG3	22:T:116:ASP:H	1.81	0.41
27:Y:102:LEU:HD11	27:Y:225:GLY:HA2	2.02	0.41
27:Y:213:LYS:HE3	27:Y:213:LYS:HB2	1.85	0.41
31:3:7:PHE:CE1	31:3:9:THR:HB	2.56	0.41
1:0:695:C:H2'	1:0:696:C:C6	2.55	0.41
1:0:1299:G:N2	40:0:5231:HOH:O	2.53	0.41
1:0:2299:G:O6	19:Q:1:PRO:HA	2.21	0.41
1:0:2388:C:H2'	1:0:2389:U:O4'	2.21	0.41
1:0:2517:A:H2'	1:0:2518:C:O4'	2.21	0.41
40:0:5826:HOH:O	25:W:69:ARG:NH2	2.54	0.41
40:0:9728:HOH:O	5:B:229:ARG:HD2	2.20	0.41
5:B:276:ASP:O	5:B:279:THR:HG22	2.20	0.41
5:B:280:VAL:HG13	5:B:333:GLU:O	2.21	0.41
7:D:60:GLU:O	7:D:60:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:135:VAL:HG22	7:D:136:ARG:H	1.86	0.41
7:D:166:ILE:O	7:D:169:THR:N	2.54	0.41
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.51	0.41
11:H:17:ARG:HD3	11:H:23:ILE:HD12	2.03	0.41
11:H:36:LYS:HA	11:H:84:LYS:NZ	2.36	0.41
14:L:130:ARG:O	14:L:131:GLU:C	2.64	0.41
15:M:82:ARG:O	15:M:84:LYS:N	2.53	0.41
16:N:64:SER:C	16:N:66:LEU:N	2.79	0.41
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.18	0.41
26:X:73:ARG:NH1	26:X:73:ARG:HB2	2.35	0.41
1:O:359:U:H3'	40:O:6290:HOH:O	2.20	0.41
1:O:1173:A:H4'	1:O:1174:A:C8	2.56	0.41
1:O:1505:U:H1'	40:O:8100:HOH:O	2.20	0.41
1:O:1556:G:O2'	1:O:1557:G:H5'	2.21	0.41
1:O:1636:G:O2'	1:O:1637:A:H5'	2.20	0.41
1:O:2515:C:H2'	1:O:2516:G:C5'	2.51	0.41
4:A:223:ARG:CZ	40:A:9559:HOH:O	2.69	0.41
8:E:20:ILE:HD12	8:E:33:LEU:CD1	2.49	0.41
12:J:95:ARG:HG2	12:J:99:GLU:OE2	2.21	0.41
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.54	0.41
13:K:82:ARG:NH2	13:K:115:ARG:HG2	2.36	0.41
14:L:80:ASP:HB3	14:L:90:ARG:HB3	2.02	0.41
16:N:71:TRP:HB2	40:N:9335:HOH:O	2.19	0.41
21:S:57:THR:HG22	21:S:59:ASP:N	2.34	0.41
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.21	0.41
28:Z:49:ARG:HB2	28:Z:55:TRP:CZ3	2.56	0.41
31:3:38:ARG:HB3	31:3:42:ARG:NH1	2.31	0.41
1:O:255:A:H2'	1:O:256:C:C6	2.56	0.41
1:O:721:A:H4'	17:O:51:TYR:CD1	2.55	0.41
1:O:1095:U:O2	25:W:120:PRO:HG2	2.21	0.41
1:O:2281:C:C2'	1:O:2282:U:H5'	2.50	0.41
2:9:3118:C:H4'	16:N:56:ASP:OD1	2.21	0.41
3:4:76:DA:H8	38:4:9701:SPS:H81	1.85	0.41
4:A:104:PRO:HG3	4:A:127:GLN:OE1	2.21	0.41
5:B:141:ARG:HD2	5:B:163:GLU:OE2	2.21	0.41
5:B:171:VAL:HG23	5:B:172:SER:N	2.36	0.41
6:C:133:ARG:NH1	40:C:9214:HOH:O	2.53	0.41
6:C:162:VAL:HG13	6:C:192:ILE:HD11	2.02	0.41
9:F:57:GLU:O	9:F:61:MET:HG3	2.21	0.41
11:H:9:ILE:HD12	11:H:54:THR:HG22	2.03	0.41
11:H:54:THR:HG23	11:H:128:GLN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:167:PRO:O	11:H:168:ALA:HB2	2.21	0.41
13:K:118:ALA:HB1	13:K:125:ALA:HB2	2.03	0.41
14:L:34:GLY:C	14:L:36:ASP:H	2.29	0.41
14:L:59:GLU:HB3	40:L:9465:HOH:O	2.20	0.41
16:N:38:LYS:HD3	16:N:107:ASN:ND2	2.36	0.41
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.21	0.41
22:T:32:ARG:HH12	22:T:38:ARG:HH12	1.66	0.41
28:Z:39:CYS:HA	28:Z:40:PRO:HD3	1.95	0.41
30:2:11:LEU:HD23	30:2:11:LEU:HA	1.90	0.41
32:I:118:SER:CB	32:I:123:ASN:HB2	2.50	0.41
1:0:1132:A:N3	1:0:2521:A:O2'	2.49	0.41
1:0:2016:U:H2'	1:0:2017:U:C6	2.55	0.41
1:0:2553:A:H2'	1:0:2553:A:N3	2.35	0.41
2:9:3011:A:P	19:Q:19:ARG:HH21	2.43	0.41
5:B:84:LEU:O	5:B:99:GLU:HA	2.21	0.41
7:D:88:LEU:N	7:D:89:PRO:CD	2.84	0.41
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.56	0.41
17:O:44:ASN:CG	17:O:67:SER:HB2	2.46	0.41
22:T:81:LYS:HD2	22:T:87:VAL:CG1	2.52	0.41
25:W:6:GLN:CB	25:W:26:ILE:HD11	2.27	0.41
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.51	0.41
1:0:526:U:H2'	1:0:527:U:C6	2.56	0.40
1:0:819:A:H5''	40:Z:9220:HOH:O	2.20	0.40
1:0:1163:G:H5'	32:I:115:ASP:O	2.21	0.40
1:0:2094:G:O6	1:0:2649:A:H2	2.04	0.40
5:B:320:GLN:HA	5:B:321:PRO:HD3	1.95	0.40
6:C:57:PRO:O	6:C:58:ALA:C	2.63	0.40
7:D:28:GLY:O	7:D:29:HIS:HB3	2.21	0.40
12:J:49:ARG:O	12:J:50:GLU:C	2.64	0.40
17:O:15:LYS:HD3	17:O:19:ARG:NH2	2.36	0.40
20:R:99:ALA:HB1	20:R:109:MET:CE	2.30	0.40
27:Y:144:ARG:NH2	40:Y:9411:HOH:O	2.51	0.40
28:Z:39:CYS:O	28:Z:42:CYS:O	2.40	0.40
31:3:70:ARG:CG	31:3:77:ALA:HB2	2.51	0.40
1:0:27:U:H2'	1:0:28:G:O4'	2.21	0.40
1:0:1176:C:H3'	40:0:5396:HOH:O	2.22	0.40
1:0:1797:A:H2'	1:0:1799:G:O5'	2.22	0.40
1:0:2421:G:H2'	40:0:4646:HOH:O	2.20	0.40
1:0:2515:C:H2'	1:0:2516:G:H5'	2.03	0.40
1:0:2821:C:H4'	5:B:116:PRO:HG3	2.03	0.40
1:0:2908:A:H2'	1:0:2909:G:C4'	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3044:A:O4'	7:D:76:ARG:NE	2.55	0.40
5:B:24:PRO:HG3	5:B:204:GLY:HA2	2.03	0.40
9:F:86:ALA:C	9:F:88:GLY:N	2.79	0.40
11:H:54:THR:O	11:H:55:VAL:HG13	2.21	0.40
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.57	0.40
16:N:23:ARG:HG2	16:N:23:ARG:NH1	2.34	0.40
17:O:81:PHE:N	17:O:81:PHE:CD1	2.89	0.40
18:P:94:TRP:CZ2	18:P:98:ILE:HG13	2.56	0.40
1:0:338:C:H4'	6:C:174:ILE:HD11	2.02	0.40
1:0:432:G:H2'	1:0:433:C:H6	1.86	0.40
1:0:1077:G:H2'	1:0:1080:C:H42	1.86	0.40
1:0:1342:C:C2'	1:0:1343:C:H5'	2.51	0.40
1:0:1596:U:OP2	18:P:123:TYR:OH	2.35	0.40
1:0:2070:G:H2'	1:0:2072:G:OP1	2.22	0.40
1:0:2612:A:H4'	40:0:4260:HOH:O	2.21	0.40
2:9:3028:U:P	16:N:39:SER:OG	2.80	0.40
4:A:109:GLU:CD	4:A:153:ARG:NH1	2.79	0.40
5:B:149:ASP:HB2	40:B:9579:HOH:O	2.21	0.40
6:C:123:LEU:HA	6:C:123:LEU:HD23	1.84	0.40
7:D:165:PHE:O	7:D:168:SER:HB3	2.22	0.40
9:F:58:GLU:CG	9:F:61:MET:HE2	2.50	0.40
11:H:140:VAL:O	11:H:140:VAL:HG12	2.21	0.40
11:H:165:SER:OG	11:H:168:ALA:HB3	2.21	0.40
24:V:12:THR:OG1	24:V:13:PRO:HD2	2.20	0.40
27:Y:170:SER:OG	27:Y:175:ARG:HG3	2.21	0.40
1:0:920:C:H5'	1:0:921:G:C4	2.56	0.40
1:0:956:G:H2'	1:0:957:A:O4'	2.21	0.40
1:0:1242:A:O3'	12:J:20:GLY:HA3	2.22	0.40
1:0:2326:U:H4'	1:0:2412:G:H4'	2.04	0.40
2:9:3095:C:O2'	2:9:3096:C:H5'	2.22	0.40
4:A:36:ASP:O	4:A:38:ILE:N	2.48	0.40
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.51	0.40
8:E:7:ILE:HA	8:E:8:PRO:HD3	1.95	0.40
13:K:2:GLU:O	13:K:3:ALA:C	2.64	0.40
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.57	0.40
14:L:145:LEU:C	14:L:147:GLU:N	2.78	0.40
14:L:145:LEU:C	14:L:145:LEU:CD2	2.94	0.40
24:V:12:THR:HG23	24:V:14:ALA:N	2.36	0.40
25:W:126:ASP:HB3	25:W:135:GLY:O	2.21	0.40
31:3:17:HIS:O	31:3:18:GLN:HG3	2.22	0.40
32:I:78:LEU:CD1	32:I:112:LYS:HZ2	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:401:C:O2'	15:M:92:THR:HB	2.22	0.40
1:0:559:U:H2'	1:0:560:C:O4'	2.22	0.40
1:0:816:G:C6	1:0:817:G:N1	2.90	0.40
1:0:1380:U:O4	1:0:2748:G:H1'	2.22	0.40
1:0:1504:A:H5'	40:0:4966:HOH:O	2.20	0.40
1:0:2896:A:N3	1:0:2896:A:C2'	2.84	0.40
40:0:4664:HOH:O	5:B:216:LYS:HE2	2.20	0.40
4:A:32:VAL:HG12	4:A:34:ASP:N	2.36	0.40
6:C:194:PHE:CE2	6:C:234:VAL:HG11	2.56	0.40
11:H:70:ASN:O	11:H:74:ILE:HG13	2.21	0.40
20:R:109:MET:HG2	20:R:148:GLU:C	2.46	0.40
22:T:43:ASN:C	22:T:45:GLY:H	2.30	0.40
23:U:52:THR:HG21	23:U:54:THR:HB	2.03	0.40
31:3:48:ASN:ND2	31:3:50:GLY:H	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	210 (89%)	21 (9%)	4 (2%)	7	5
5	B	335/338 (99%)	312 (93%)	19 (6%)	4 (1%)	10	8
6	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
7	D	134/177 (76%)	103 (77%)	23 (17%)	8 (6%)	1	0
8	E	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
9	F	117/120 (98%)	102 (87%)	13 (11%)	2 (2%)	7	5
10	G	25/348 (7%)	25 (100%)	0	0	100	100
11	H	156/171 (91%)	140 (90%)	13 (8%)	3 (2%)	6	4
12	J	140/145 (97%)	132 (94%)	6 (4%)	2 (1%)	9	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	K	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	16	16
14	L	141/165 (86%)	118 (84%)	21 (15%)	2 (1%)	9	7
15	M	192/194 (99%)	181 (94%)	9 (5%)	2 (1%)	12	11
16	N	184/187 (98%)	161 (88%)	13 (7%)	10 (5%)	1	0
17	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
18	P	141/149 (95%)	134 (95%)	7 (5%)	0	100	100
19	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
22	T	117/120 (98%)	111 (95%)	5 (4%)	1 (1%)	14	14
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	57 (90%)	3 (5%)	3 (5%)	2	0
25	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
26	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	62 (87%)	6 (8%)	3 (4%)	2	1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	11	10
32	I	68/162 (42%)	54 (79%)	11 (16%)	3 (4%)	2	1
All	All	3705/4430 (84%)	3410 (92%)	246 (7%)	49 (1%)	9	8

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	37	VAL
5	B	139	ASP
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	183	ASP
16	N	184	ILE

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Mol	Chain	Res	Type
28	Z	81	ARG
4	A	34	ASP
5	B	169	GLY
7	D	16	PRO
7	D	60	GLU
7	D	61	PHE
15	M	83	SER
16	N	155	GLU
16	N	162	ASP
28	Z	20	ARG
32	I	132	CYS
5	B	185	GLY
7	D	56	ARG
7	D	137	PRO
7	D	164	ALA
7	D	171	ASP
12	J	143	LYS
16	N	65	ASP
16	N	68	GLU
24	V	43	PRO
28	Z	41	ASN
13	K	126	SER
14	L	82	ALA
31	3	56	PRO
32	I	114	PRO
4	A	132	ASP
4	A	205	GLY
12	J	5	GLU
22	T	53	GLY
7	D	69	ILE
9	F	71	GLY
24	V	40	PRO
32	I	129	VAL
5	B	182	VAL
16	N	157	PRO
16	N	161	GLY
11	H	167	PRO
15	M	88	VAL
24	V	2	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%)	163 (91%)	16 (9%)	9	10
5	B	282/283 (100%)	264 (94%)	18 (6%)	16	19
6	C	193/193 (100%)	178 (92%)	15 (8%)	11	13
7	D	117/148 (79%)	112 (96%)	5 (4%)	26	35
8	E	152/156 (97%)	147 (97%)	5 (3%)	33	45
9	F	93/94 (99%)	90 (97%)	3 (3%)	34	47
10	G	27/283 (10%)	26 (96%)	1 (4%)	30	41
11	H	132/138 (96%)	126 (96%)	6 (4%)	24	33
12	J	118/121 (98%)	112 (95%)	6 (5%)	21	27
13	K	106/106 (100%)	101 (95%)	5 (5%)	23	31
14	L	113/127 (89%)	109 (96%)	4 (4%)	32	43
15	M	158/158 (100%)	155 (98%)	3 (2%)	50	66
16	N	149/150 (99%)	141 (95%)	8 (5%)	20	25
17	O	93/94 (99%)	90 (97%)	3 (3%)	34	47
18	P	113/117 (97%)	110 (97%)	3 (3%)	39	53
19	Q	79/80 (99%)	76 (96%)	3 (4%)	29	40
20	R	117/122 (96%)	115 (98%)	2 (2%)	53	69
21	S	71/74 (96%)	70 (99%)	1 (1%)	59	75
22	T	105/106 (99%)	100 (95%)	5 (5%)	23	30
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	48	64
25	W	130/130 (100%)	126 (97%)	4 (3%)	35	48
26	X	66/74 (89%)	61 (92%)	5 (8%)	12	14
27	Y	120/196 (61%)	110 (92%)	10 (8%)	10	11
28	Z	60/68 (88%)	58 (97%)	2 (3%)	33	45
29	1	46/47 (98%)	45 (98%)	1 (2%)	45	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	2	42/46 (91%)	41 (98%)	1 (2%)	43	58
31	3	79/79 (100%)	77 (98%)	2 (2%)	42	56
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2955 (96%)	138 (4%)	24	33

All (138) 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	55	VAL
4	A	62	ASP
4	A	68	ILE
4	A	94	LEU
4	A	131	HIS
4	A	144	GLU
4	A	151	GLN
4	A	153	ARG
4	A	165	THR
4	A	175	LYS
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	190	MET
5	B	195	ARG
5	B	234	ARG
5	B	251	VAL
5	B	254	GLN
5	B	264	GLU
5	B	265	LEU
5	B	307	ARG

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Mol	Chain	Res	Type
5	B	312	ARG
6	C	2	GLN
6	C	16	VAL
6	C	76	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	240	LEU
6	C	243	VAL
7	D	24	HIS
7	D	50	VAL
7	D	52	THR
7	D	61	PHE
7	D	137	PRO
8	E	3	VAL
8	E	86	VAL
8	E	102	VAL
8	E	108	LEU
8	E	155	ASN
9	F	12	LEU
9	F	46	GLU
9	F	99	THR
10	G	72	ASP
11	H	18	GLU
11	H	68	SER
11	H	84	LYS
11	H	154	TYR
11	H	159	PRO
11	H	170	ASN
12	J	39	VAL
12	J	70	PHE
12	J	74	ARG
12	J	93	ARG
12	J	127	ILE
12	J	131	THR

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Mol	Chain	Res	Type
13	K	4	LEU
13	K	10	GLN
13	K	84	ASP
13	K	98	VAL
13	K	107	THR
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
14	L	140	VAL
15	M	46	LEU
15	M	93	ARG
15	M	164	THR
16	N	12	ARG
16	N	26	LEU
16	N	38	LYS
16	N	56	ASP
16	N	65	ASP
16	N	127	LEU
16	N	135	VAL
16	N	139	TRP
17	O	3	THR
17	O	25	VAL
17	O	96	VAL
18	P	21	VAL
18	P	52	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	16	ASN
19	Q	57	ASP
20	R	13	THR
20	R	143	VAL
21	S	10	VAL
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
22	T	96	VAL
22	T	117	ASP
24	V	65	ASP
25	W	26	ILE
25	W	35	VAL
25	W	142	ASP
25	W	146	ILE

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Mol	Chain	Res	Type
26	X	8	ARG
26	X	15	ARG
26	X	72	VAL
26	X	79	GLU
26	X	80	GLU
27	Y	103	THR
27	Y	108	ASP
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG
27	Y	172	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	231	PRO
27	Y	235	GLU
28	Z	44	GLU
28	Z	78	THR
29	1	29	THR
30	2	46	ASP
31	3	56	PRO
31	3	65	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	29	HIS
4	A	134	ASN
4	A	199	HIS
4	A	218	ASN
5	B	27	ASN
5	B	145	HIS
5	B	177	HIS
5	B	238	ASN
5	B	260	HIS
5	B	318	ASN
5	B	320	GLN
5	B	332	ASN
6	C	39	GLN
6	C	67	GLN
6	C	129	HIS
6	C	163	HIS
6	C	178	GLN

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Mol	Chain	Res	Type
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	30	GLN
11	H	37	GLN
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	155	ASN
11	H	170	ASN
12	J	25	GLN
12	J	107	ASN
13	K	10	GLN
13	K	42	ASN
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	137	ASN
15	M	143	ASN
15	M	170	ASN
16	N	22	GLN
16	N	107	ASN
17	O	53	GLN
17	O	100	GLN
18	P	50	GLN
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

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Mol	Chain	Res	Type
20	R	98	ASN
20	R	102	GLN
20	R	113	HIS
20	R	117	HIS
20	R	122	GLN
21	S	44	GLN
21	S	53	ASN
21	S	55	GLN
22	T	11	GLN
22	T	39	ASN
22	T	43	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	29	ASN
24	V	60	GLN
25	W	12	ASN
25	W	28	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
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	18	GLN
31	3	30	GLN
31	3	48	ASN
32	I	93	GLN
32	I	104	GLN
32	I	113	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	251 (9%)	36 (1%)
2	9	121/122 (99%)	18 (14%)	2 (1%)
3	4	1/5 (20%)	0	0
All	All	2867/3049 (94%)	269 (9%)	38 (1%)

All (269) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	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	169	A
1	0	170	U
1	0	186	A
1	0	187	A
1	0	191	A
1	0	192	A
1	0	219	G
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	338	C
1	0	339	A

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Mol	Chain	Res	Type
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	473	A
1	0	487	G
1	0	498	A
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	620	A
1	0	632	A
1	0	644	G
1	0	645	U
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	702	G
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

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Mol	Chain	Res	Type
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	1151	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
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

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Mol	Chain	Res	Type
1	0	1279	U
1	0	1287	A
1	0	1289	C
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
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	1731	C
1	0	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G

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Mol	Chain	Res	Type
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	1971	G
1	0	1973	A
1	0	1974	G
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	2063	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
1	0	2103	A
1	0	2110	G
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	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G

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Mol	Chain	Res	Type
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2536	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	2645	U
1	0	2646	G
1	0	2649	A
1	0	2650	U
1	0	2664	A
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	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2852	A

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Mol	Chain	Res	Type
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	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3039	U
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3055	U
2	9	3056	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	87	C
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
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	1232	A
1	0	1237	U

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Mol	Chain	Res	Type
1	0	1246	A
1	0	1352	A
1	0	1506	U
1	0	1563	G
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1730	G
1	0	1856	C
1	0	1942	A
1	0	1973	A
1	0	1979	G
1	0	2011	A
1	0	2313	C
1	0	2467	A
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	3055	U
2	9	3065	A

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

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	$\# Z > 2$
3	ACA	4	78	3	3,3,8	0.54	0	1,2,8	0.63	0
1	UR3	0	2619	1	19,22,23	0.47	0	26,32,35	0.70	1 (3%)
1	1MA	0	628	1,35	21,25,26	0.76	1 (4%)	30,37,40	0.81	2 (6%)
1	OMG	0	2588	1	23,26,27	0.27	0	32,38,41	0.34	0

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	0.25	0	25,31,34	0.44	0
1	PSU	0	2621	1	18,21,22	1.55	2 (11%)	21,30,33	1.39	3 (14%)

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
3	ACA	4	78	3	-	0/0/1/6	-
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,35	-	2/7/25/26	0/3/3/3
1	OMG	0	2588	1	-	0/9/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.11	1.43	1.36
1	0	2621	PSU	C6-C5	3.15	1.38	1.35
1	0	628	1MA	C6-N6	2.62	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	3.46	120.51	118.17
1	0	2621	PSU	C6-N1-C2	-3.28	119.65	122.69
1	0	2621	PSU	O2-C2-N1	2.92	125.80	122.79
1	0	628	1MA	N1-C2-N3	2.76	129.27	126.00
1	0	2619	UR3	C4-N3-C2	2.68	126.74	124.58
1	0	628	1MA	CM1-N1-C6	2.08	123.37	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	2619	UR3	1	0
1	0	2587	OMU	2	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	1.96	5 (21%)

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	4.46	1.53	1.45
38	4	9701	SPS	C9-C10	-2.99	1.41	1.48
38	4	9701	SPS	O15-S15	-2.06	1.43	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	9701	SPS	C7-C5-N4	4.63	118.81	113.42
38	4	9701	SPS	N4-C3-N2	3.80	121.71	115.74
38	4	9701	SPS	C7-C5-C6	-3.70	121.67	126.47
38	4	9701	SPS	C1-N2-C3	-3.65	121.34	126.37
38	4	9701	SPS	C6-C1-N2	2.32	118.51	114.45

There are no chirality outliers.

All (5) torsion outliers are listed below:

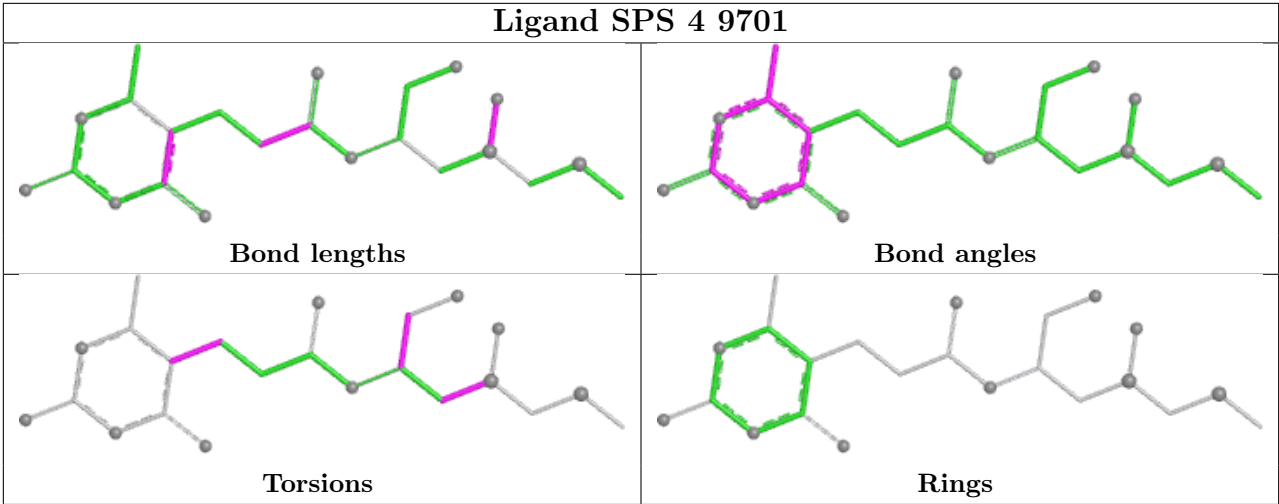
Mol	Chain	Res	Type	Atoms
38	4	9701	SPS	C14-C12-C13-O13
38	4	9701	SPS	C12-C14-S15-O15
38	4	9701	SPS	C12-C14-S15-C16
38	4	9701	SPS	N11-C12-C13-O13
38	4	9701	SPS	C5-C6-C8-C9

There are no ring outliers.

1 monomer is involved in 4 short contacts:

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

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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:DA	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%)	-0.26	85 (3%)	51	48	19, 43, 76, 127	0
2	9	122/122 (100%)	0.43	6 (4%)	35	31	39, 58, 76, 127	0
3	4	4/5 (80%)	0.96	1 (25%)	2	1	52, 54, 55, 58	0
4	A	237/240 (98%)	0.58	20 (8%)	17	14	26, 45, 70, 85	0
5	B	337/338 (99%)	0.56	15 (4%)	38	35	27, 47, 65, 73	0
6	C	246/246 (100%)	0.52	11 (4%)	38	35	26, 44, 61, 69	0
7	D	140/177 (79%)	2.20	63 (45%)	0	0	51, 74, 102, 109	0
8	E	172/178 (96%)	0.94	16 (9%)	14	12	40, 57, 69, 74	0
9	F	119/120 (99%)	1.20	19 (15%)	5	3	45, 62, 82, 87	0
10	G	29/348 (8%)	1.96	10 (34%)	1	0	59, 77, 83, 86	0
11	H	160/171 (93%)	0.94	15 (9%)	14	11	41, 54, 79, 83	0
12	J	142/145 (97%)	0.55	9 (6%)	26	23	36, 45, 58, 71	0
13	K	132/132 (100%)	0.40	4 (3%)	52	49	32, 43, 59, 64	0
14	L	145/165 (87%)	1.04	24 (16%)	4	3	26, 56, 90, 100	0
15	M	194/194 (100%)	0.75	27 (13%)	6	5	32, 42, 65, 70	0
16	N	186/187 (99%)	1.25	35 (18%)	3	2	42, 56, 89, 94	0
17	O	115/116 (99%)	0.82	6 (5%)	33	29	37, 50, 60, 65	0
18	P	143/149 (95%)	0.62	7 (4%)	35	31	35, 47, 57, 66	0
19	Q	95/96 (98%)	0.56	7 (7%)	20	18	39, 45, 56, 67	0
20	R	150/155 (96%)	0.15	1 (0%)	84	82	29, 41, 56, 64	0
21	S	81/85 (95%)	0.64	2 (2%)	58	55	39, 52, 66, 79	0
22	T	119/120 (99%)	0.85	8 (6%)	24	21	38, 50, 70, 92	0
23	U	53/66 (80%)	0.62	4 (7%)	20	17	38, 47, 61, 69	0
24	V	65/71 (91%)	1.52	12 (18%)	3	2	46, 64, 93, 97	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.58	6 (3%) 43 40	36, 47, 60, 68	0
26	X	82/92 (89%)	0.83	12 (14%) 6 4	39, 50, 69, 85	0
27	Y	142/241 (58%)	0.39	4 (2%) 55 52	28, 41, 59, 73	0
28	Z	73/83 (87%)	1.28	16 (21%) 2 1	43, 58, 70, 76	0
29	1	56/57 (98%)	-0.07	1 (1%) 67 64	25, 32, 39, 48	0
30	2	46/50 (92%)	0.86	7 (15%) 5 4	31, 49, 62, 71	0
31	3	92/92 (100%)	0.66	4 (4%) 40 36	34, 51, 60, 70	0
32	I	70/162 (43%)	3.91	66 (94%) 0 0	90, 102, 117, 118	0
All	All	6650/7479 (88%)	0.38	523 (7%) 18 16	19, 47, 79, 127	0

All (523) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	V	1	THR	10.2
7	D	10	PHE	9.7
32	I	133	THR	9.6
16	N	166	ALA	9.3
15	M	70	GLY	8.6
7	D	63	ILE	8.3
32	I	90	GLY	7.8
7	D	174	VAL	7.0
32	I	117	LEU	7.0
32	I	118	SER	6.9
17	O	22	GLY	6.9
16	N	165	ALA	6.9
7	D	107	GLY	6.8
32	I	79	ILE	6.6
16	N	154	LEU	6.6
32	I	76	ALA	6.4
32	I	121	LEU	6.3
7	D	61	PHE	6.3
2	9	3001	U	6.2
32	I	85	PHE	6.2
15	M	74	LYS	6.0
12	J	70	PHE	6.0
32	I	137	VAL	5.9
5	B	1	PRO	5.7
4	A	37	VAL	5.7
30	2	49	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
32	I	88	GLY	5.6
24	V	40	PRO	5.5
32	I	105	VAL	5.4
24	V	39	ALA	5.4
7	D	172	VAL	5.4
32	I	135	LEU	5.4
32	I	129	VAL	5.4
24	V	2	VAL	5.4
32	I	139	ILE	5.3
16	N	168	LEU	5.3
7	D	57	THR	5.2
15	M	80	GLY	5.2
4	A	36	ASP	5.2
32	I	134	SER	5.2
22	T	117	ASP	5.1
1	0	1161	A	5.1
1	0	1173	A	5.1
11	H	168	ALA	5.0
11	H	111	ASP	5.0
7	D	55	LYS	5.0
32	I	116	LEU	5.0
8	E	45	ASP	4.9
7	D	135	VAL	4.9
26	X	88	GLU	4.8
32	I	132	CYS	4.8
32	I	89	SER	4.8
32	I	96	PHE	4.7
32	I	125	ALA	4.7
4	A	237	GLY	4.7
7	D	171	ASP	4.7
2	9	3002	U	4.7
10	G	12	ILE	4.7
28	Z	82	SER	4.6
14	L	82	ALA	4.6
14	L	148	GLU	4.6
32	I	93	GLN	4.5
32	I	83	ALA	4.5
10	G	26	MET	4.5
32	I	78	LEU	4.4
15	M	88	VAL	4.4
8	E	10	ASP	4.4
1	0	138	U	4.4

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Mol	Chain	Res	Type	RSRZ
22	T	119	ALA	4.4
32	I	75	THR	4.4
32	I	138	THR	4.4
7	D	35	ALA	4.3
15	M	79	ALA	4.3
7	D	170	TYR	4.3
24	V	43	PRO	4.3
15	M	82	ARG	4.3
2	9	3024	U	4.2
1	0	2748	G	4.2
14	L	77	ALA	4.2
14	L	150	GLN	4.2
14	L	149	ARG	4.2
1	0	10	U	4.2
1	0	2345	A	4.2
13	K	118	ALA	4.2
16	N	163	PHE	4.2
15	M	86	GLN	4.1
14	L	78	ALA	4.1
10	G	71	LEU	4.1
15	M	89	THR	4.1
32	I	128	VAL	4.1
7	D	90	LEU	4.1
12	J	4	ALA	4.1
15	M	78	LYS	4.0
15	M	71	SER	4.0
7	D	11	HIS	4.0
1	0	1192	A	4.0
15	M	75	ARG	4.0
32	I	98	ALA	4.0
32	I	119	TYR	3.9
32	I	109	ALA	3.9
26	X	65	ASN	3.9
14	L	83	GLU	3.9
4	A	35	GLY	3.9
16	N	164	ASP	3.8
7	D	59	GLY	3.8
28	Z	10	ARG	3.8
7	D	44	ILE	3.8
14	L	145	LEU	3.8
15	M	83	SER	3.8
28	Z	11	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	0	2645	U	3.8
21	S	81	ILE	3.8
11	H	169	GLY	3.8
32	I	102	VAL	3.8
2	9	3023	U	3.7
9	F	102	GLY	3.7
1	0	1172	G	3.7
1	0	1175	G	3.7
15	M	72	ALA	3.7
17	O	23	GLY	3.7
10	G	73	ASP	3.7
15	M	194	ALA	3.7
26	X	85	VAL	3.7
32	I	94	GLU	3.6
16	N	167	ASP	3.6
32	I	114	PRO	3.6
15	M	81	ARG	3.6
32	I	81	ASP	3.6
22	T	118	SER	3.6
7	D	69	ILE	3.6
32	I	77	GLU	3.6
22	T	116	ASP	3.6
32	I	123	ASN	3.6
22	T	82	THR	3.6
16	N	95	ALA	3.6
6	C	63	SER	3.5
1	0	282	C	3.5
14	L	75	LEU	3.5
32	I	80	LYS	3.5
32	I	131	THR	3.5
11	H	40	ALA	3.5
26	X	87	ALA	3.5
32	I	82	GLU	3.5
1	0	737	A	3.5
7	D	62	ASP	3.5
10	G	29	SER	3.5
15	M	84	LYS	3.5
27	Y	216	ARG	3.5
4	A	31	LYS	3.4
14	L	81	VAL	3.4
18	P	18	LYS	3.4
18	P	143	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
32	I	92	PRO	3.4
16	N	1	ALA	3.4
1	0	2747	C	3.4
16	N	134	ASP	3.4
32	I	100	LEU	3.4
8	E	87	PHE	3.4
1	0	1165	G	3.4
7	D	36	ASN	3.4
7	D	134	LEU	3.4
1	0	1162	G	3.4
15	M	87	GLY	3.4
32	I	84	GLY	3.4
1	0	1168	C	3.3
7	D	137	PRO	3.3
1	0	960	G	3.3
28	Z	22	SER	3.3
7	D	12	GLU	3.3
1	0	1951	G	3.3
15	M	76	ARG	3.3
1	0	441	A	3.2
1	0	1202	A	3.2
15	M	77	HIS	3.2
32	I	87	THR	3.2
9	F	101	ALA	3.2
7	D	17	ARG	3.2
3	4	77	PHE	3.2
15	M	73	ARG	3.2
10	G	70	ALA	3.2
5	B	57	GLU	3.2
8	E	12	ASP	3.2
32	I	108	ILE	3.2
1	0	2769	C	3.2
1	0	1164	U	3.2
1	0	1169	U	3.2
32	I	124	ALA	3.1
32	I	97	VAL	3.1
16	N	159	TYR	3.1
1	0	2237	G	3.1
8	E	154	ILE	3.1
1	0	1967	U	3.1
7	D	93	LEU	3.1
1	0	1167	G	3.1

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Mol	Chain	Res	Type	RSRZ
32	I	140	GLU	3.1
8	E	100	ASP	3.1
7	D	58	VAL	3.1
7	D	56	ARG	3.1
30	2	35	ARG	3.1
16	N	162	ASP	3.1
1	0	288	A	3.0
7	D	169	THR	3.0
7	D	54	ALA	3.0
32	I	72	VAL	3.0
1	0	1171	A	3.0
5	B	2	GLN	3.0
32	I	111	GLN	3.0
11	H	167	PRO	3.0
19	Q	18	PRO	3.0
27	Y	236	VAL	3.0
26	X	66	THR	3.0
14	L	146	GLY	3.0
9	F	8	VAL	3.0
32	I	113	HIS	3.0
1	0	1170	U	3.0
1	0	1524	U	3.0
1	0	514	G	3.0
19	Q	95	GLU	3.0
1	0	1184	C	2.9
7	D	37	ALA	2.9
16	N	158	LEU	2.9
5	B	119	HIS	2.9
32	I	126	LYS	2.9
10	G	27	ILE	2.9
12	J	46	ILE	2.9
1	0	2511	A	2.9
17	O	1	SER	2.9
4	A	205	GLY	2.9
9	F	118	LEU	2.9
16	N	180	LEU	2.9
32	I	112	LYS	2.9
30	2	44	ARG	2.9
14	L	55	GLN	2.9
32	I	104	GLN	2.9
16	N	147	ILE	2.9
27	Y	235	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
32	I	73	PRO	2.9
6	C	16	VAL	2.9
7	D	131	THR	2.9
16	N	68	GLU	2.9
1	0	497	A	2.9
22	T	114	SER	2.9
16	N	186	LEU	2.9
1	0	1929	G	2.9
24	V	41	GLU	2.9
1	0	1166	A	2.8
1	0	1174	A	2.8
16	N	179	LEU	2.8
1	0	271	C	2.8
31	3	41	GLU	2.8
4	A	38	ILE	2.8
7	D	27	ILE	2.8
10	G	23	ILE	2.8
32	I	120	ASP	2.8
26	X	61	ARG	2.8
7	D	89	PRO	2.8
7	D	91	ALA	2.8
7	D	104	PHE	2.8
7	D	106	PHE	2.8
1	0	1176	C	2.8
14	L	147	GLU	2.8
28	Z	16	ALA	2.8
1	0	1181	A	2.8
14	L	99	GLU	2.8
14	L	105	TYR	2.8
30	2	39	ARG	2.8
14	L	91	VAL	2.8
1	0	1160	G	2.7
7	D	153	THR	2.7
9	F	105	ASP	2.7
5	B	21	SER	2.7
32	I	130	GLY	2.7
7	D	128	LEU	2.7
11	H	171	ALA	2.7
23	U	47	ARG	2.7
1	0	1964	U	2.7
28	Z	14	PHE	2.7
9	F	91	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
24	V	37	GLY	2.7
16	N	169	PRO	2.7
32	I	74	PRO	2.7
5	B	183	GLU	2.7
1	0	1193	A	2.7
1	0	1199	A	2.7
11	H	137	TYR	2.7
7	D	155	HIS	2.7
1	0	284	C	2.7
11	H	112	GLY	2.7
22	T	36	GLY	2.7
4	A	33	GLU	2.7
7	D	29	HIS	2.7
14	L	62	ALA	2.7
9	F	60	VAL	2.7
7	D	173	GLU	2.7
8	E	126	ILE	2.7
24	V	38	GLY	2.7
14	L	100	ALA	2.6
15	M	1	ALA	2.6
32	I	107	GLN	2.6
32	I	122	THR	2.6
8	E	172	PRO	2.6
20	R	150	PRO	2.6
1	0	2344	G	2.6
1	0	1177	A	2.6
8	E	6	GLU	2.6
25	W	86	GLU	2.6
25	W	88	THR	2.6
7	D	105	SER	2.6
8	E	20	ILE	2.6
1	0	1197	G	2.6
1	0	1200	A	2.6
32	I	106	LYS	2.6
32	I	91	GLU	2.6
16	N	137	ALA	2.6
24	V	36	ALA	2.6
16	N	172	PHE	2.6
16	N	76	GLY	2.6
16	N	175	LEU	2.6
1	0	1190	G	2.6
1	0	1203	G	2.6

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Mol	Chain	Res	Type	RSRZ
4	A	203	GLY	2.6
19	Q	84	ILE	2.6
2	9	3122	C	2.6
19	Q	17	LYS	2.6
7	D	88	LEU	2.5
7	D	157	LEU	2.5
22	T	115	GLU	2.5
15	M	85	ARG	2.5
28	Z	20	ARG	2.5
1	0	1523	G	2.5
5	B	123	ALA	2.5
13	K	132	VAL	2.5
24	V	46	ILE	2.5
1	0	999	C	2.5
26	X	79	GLU	2.5
17	O	24	ALA	2.5
26	X	83	ALA	2.5
24	V	44	GLY	2.5
14	L	93	VAL	2.5
15	M	68	ARG	2.5
1	0	1189	A	2.5
9	F	104	ALA	2.5
7	D	141	VAL	2.5
14	L	97	VAL	2.5
14	L	98	GLU	2.5
18	P	64	GLU	2.5
28	Z	24	ARG	2.5
1	0	970	U	2.5
7	D	154	LYS	2.5
5	B	56	ASP	2.5
30	2	17	GLN	2.5
32	I	71	GLY	2.5
9	F	78	GLU	2.4
9	F	119	ARG	2.4
6	C	61	PHE	2.4
10	G	20	VAL	2.4
1	0	2004	U	2.4
5	B	33	ASP	2.4
8	E	39	ASP	2.4
11	H	39	ASP	2.4
24	V	42	ASN	2.4
9	F	99	THR	2.4

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Mol	Chain	Res	Type	RSRZ
9	F	22	VAL	2.4
15	M	91	ILE	2.4
4	A	34	ASP	2.4
11	H	170	ASN	2.4
28	Z	36	ASP	2.4
6	C	171	GLU	2.4
16	N	157	PRO	2.4
1	0	1279	U	2.4
1	0	2512	U	2.4
7	D	166	ILE	2.4
16	N	184	ILE	2.4
18	P	141	ILE	2.4
4	A	26	ASP	2.4
9	F	103	GLU	2.4
13	K	100	GLU	2.4
6	C	237	GLU	2.4
32	I	86	GLU	2.4
11	H	41	ASP	2.3
4	A	211	LYS	2.3
1	0	1198	U	2.3
1	0	2419	U	2.3
7	D	73	VAL	2.3
4	A	65	ARG	2.3
28	Z	42	CYS	2.3
7	D	60	GLU	2.3
7	D	92	GLU	2.3
1	0	1201	C	2.3
6	C	132	ASP	2.3
1	0	128	A	2.3
9	F	28	ALA	2.3
6	C	133	ARG	2.3
16	N	37	ARG	2.3
12	J	63	ILE	2.3
1	0	735	C	2.3
16	N	148	ALA	2.3
4	A	206	ARG	2.3
14	L	121	ILE	2.3
7	D	132	VAL	2.3
5	B	120	ASP	2.3
1	0	2508	C	2.3
7	D	68	PRO	2.3
11	H	34	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
28	Z	23	ARG	2.3
18	P	58	SER	2.3
4	A	32	VAL	2.3
7	D	41	LEU	2.2
12	J	130	VAL	2.3
6	C	101	ASP	2.2
1	0	1182	C	2.2
1	0	1196	C	2.2
1	0	1204	C	2.2
16	N	74	PRO	2.2
1	0	1476	A	2.2
28	Z	27	ALA	2.2
7	D	95	THR	2.2
8	E	11	VAL	2.2
12	J	45	VAL	2.2
17	O	98	LEU	2.2
28	Z	21	VAL	2.2
10	G	63	ARG	2.2
16	N	5	ARG	2.2
1	0	1188	A	2.2
16	N	170	GLU	2.2
18	P	111	GLU	2.2
16	N	2	THR	2.2
23	U	52	THR	2.2
16	N	160	SER	2.2
21	S	1	SER	2.2
32	I	101	SER	2.2
5	B	118	ASP	2.2
25	W	76	ASP	2.2
9	F	9	PRO	2.2
5	B	168	GLY	2.2
6	C	135	GLU	2.2
1	0	272	A	2.2
1	0	1966	U	2.2
8	E	13	ALA	2.2
9	F	112	ALA	2.2
27	Y	106	THR	2.2
11	H	83	TYR	2.2
7	D	40	ILE	2.2
25	W	26	ILE	2.2
9	F	24	ARG	2.2
18	P	110	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
32	I	95	ASP	2.2
15	M	15	PRO	2.2
23	U	37	GLU	2.2
16	N	161	GLY	2.2
32	I	136	GLY	2.2
1	0	283	U	2.2
2	9	3065	A	2.2
12	J	47	THR	2.2
16	N	145	ALA	2.2
31	3	62	THR	2.2
8	E	7	ILE	2.1
26	X	84	ILE	2.1
7	D	22	VAL	2.1
9	F	7	ASP	2.1
28	Z	26	VAL	2.1
12	J	5	GLU	2.1
26	X	82	GLU	2.1
5	B	34	GLY	2.1
1	0	734	U	2.1
1	0	1206	U	2.1
1	0	1163	G	2.1
4	A	85	SER	2.1
4	A	86	ALA	2.1
6	C	76	ARG	2.1
6	C	246	ARG	2.1
15	M	90	ARG	2.1
28	Z	18	TYR	2.1
12	J	127	ILE	2.1
15	M	69	LYS	2.1
5	B	108	GLU	2.1
8	E	43	ASP	2.1
5	B	51	VAL	2.1
26	X	77	PHE	2.1
31	3	56	PRO	2.1
1	0	1625	U	2.1
1	0	1965	C	2.1
23	U	4	ARG	2.1
7	D	142	ALA	2.1
14	L	60	GLU	2.1
19	Q	20	ASP	2.1
26	X	22	ASN	2.1
30	2	16	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
30	2	46	ASP	2.1
4	A	236	GLY	2.1
1	0	1561	U	2.1
1	0	361	C	2.1
1	0	1947	G	2.1
7	D	53	LYS	2.1
4	A	68	ILE	2.1
7	D	66	GLY	2.1
7	D	165	PHE	2.1
1	0	1185	U	2.1
1	0	2749	U	2.1
16	N	139	TRP	2.1
11	H	36	LYS	2.0
7	D	86	THR	2.0
14	L	143	THR	2.0
17	O	21	SER	2.0
1	0	2538	A	2.0
7	D	167	GLU	2.0
31	3	92	GLU	2.0
1	0	1525	G	2.0
1	0	1950	G	2.0
9	F	25	ASP	2.0
25	W	142	ASP	2.0
7	D	18	ILE	2.0
4	A	153	ARG	2.0
11	H	146	VAL	2.0
19	Q	92	ARG	2.0
19	Q	12	GLY	2.0
7	D	74	THR	2.0
25	W	74	GLU	2.0
28	Z	78	THR	2.0
29	1	47	ASP	2.0
32	I	115	ASP	2.0
8	E	32	ARG	2.0
13	K	27	ARG	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($\text{\AA}^2$)	Q<0.9
3	ACA	4	78	4/9	0.73	0.31	57,57,58,58	0
1	UR3	0	2619	21/22	0.95	0.08	34,38,41,43	0
1	OMG	0	2588	24/25	0.96	0.08	30,34,36,38	0
1	PSU	0	2621	20/21	0.97	0.07	31,33,38,38	0
1	1MA	0	628	23/24	0.98	0.06	28,32,33,34	0
1	OMU	0	2587	21/22	0.98	0.07	30,35,36,37	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
33	MG	0	8092	1/1	0.60	0.39	80,80,80,80	0
33	MG	0	8014	1/1	0.63	0.27	67,67,67,67	0
35	NA	S	9112	1/1	0.65	0.20	75,75,75,75	0
35	NA	0	9122	1/1	0.66	0.39	77,77,77,77	0
33	MG	0	8050	1/1	0.66	0.24	88,88,88,88	0
37	SR	B	9521	1/1	0.67	0.51	185,185,185,185	0
33	MG	0	8045	1/1	0.71	0.23	84,84,84,84	0
35	NA	0	9185	1/1	0.72	0.35	52,52,52,52	0
35	NA	0	9129	1/1	0.73	0.35	74,74,74,74	0
37	SR	0	9500	1/1	0.73	0.41	197,197,197,197	0
33	MG	0	8055	1/1	0.73	0.22	83,83,83,83	0
35	NA	0	9169	1/1	0.75	0.41	90,90,90,90	0
35	NA	0	9179	1/1	0.76	0.37	89,89,89,89	0
37	SR	0	9547	1/1	0.77	0.33	166,166,166,166	0
35	NA	0	9184	1/1	0.77	0.32	73,73,73,73	0
35	NA	0	9164	1/1	0.79	0.27	60,60,60,60	0
39	CD	O	9205	1/1	0.79	0.48	197,197,197,197	0
35	NA	9	9183	1/1	0.80	0.21	77,77,77,77	0
35	NA	0	9172	1/1	0.80	0.48	76,76,76,76	0
35	NA	D	9151	1/1	0.81	0.15	62,62,62,62	0
35	NA	0	9111	1/1	0.81	0.18	59,59,59,59	0
33	MG	0	8065	1/1	0.81	0.20	93,93,93,93	0
33	MG	0	8061	1/1	0.82	0.18	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8094	1/1	0.82	0.27	83,83,83,83	0
35	NA	0	9140	1/1	0.82	0.24	63,63,63,63	0
33	MG	0	8082	1/1	0.82	0.37	82,82,82,82	0
35	NA	0	9170	1/1	0.83	0.27	72,72,72,72	0
33	MG	0	8052	1/1	0.83	0.16	74,74,74,74	0
35	NA	0	9173	1/1	0.84	0.14	59,59,59,59	0
35	NA	0	9124	1/1	0.84	0.29	53,53,53,53	0
37	SR	0	9501	1/1	0.84	0.24	196,196,196,196	0
35	NA	0	9171	1/1	0.85	0.37	66,66,66,66	0
33	MG	0	8047	1/1	0.85	0.28	85,85,85,85	0
33	MG	0	8090	1/1	0.85	0.19	68,68,68,68	0
35	NA	0	9186	1/1	0.85	0.16	67,67,67,67	0
33	MG	0	8040	1/1	0.86	0.20	69,69,69,69	0
35	NA	0	9163	1/1	0.86	0.15	58,58,58,58	0
37	SR	0	9484	1/1	0.86	0.13	134,134,134,134	0
35	NA	0	9118	1/1	0.86	0.18	49,49,49,49	0
35	NA	0	9168	1/1	0.86	0.31	66,66,66,66	0
33	MG	0	8099	1/1	0.86	0.14	62,62,62,62	0
37	SR	0	9601	1/1	0.86	0.24	191,191,191,191	0
33	MG	0	8107	1/1	0.86	0.27	70,70,70,70	0
34	K	0	9001	1/1	0.86	0.38	84,84,84,84	0
35	NA	0	9175	1/1	0.87	0.21	47,47,47,47	0
35	NA	0	9152	1/1	0.87	0.24	64,64,64,64	0
35	NA	0	9139	1/1	0.87	0.14	57,57,57,57	0
35	NA	0	9125	1/1	0.87	0.23	93,93,93,93	0
35	NA	0	9174	1/1	0.87	0.21	61,61,61,61	0
33	MG	0	8103	1/1	0.88	0.20	62,62,62,62	0
33	MG	0	8022	1/1	0.88	0.28	63,63,63,63	0
35	NA	0	9177	1/1	0.88	0.30	71,71,71,71	0
35	NA	0	9178	1/1	0.88	0.30	52,52,52,52	0
33	MG	A	8066	1/1	0.88	0.13	53,53,53,53	0
35	NA	0	9127	1/1	0.88	0.19	57,57,57,57	0
33	MG	0	8113	1/1	0.89	0.14	49,49,49,49	0
37	SR	0	9529	1/1	0.89	0.18	136,136,136,136	0
33	MG	0	8114	1/1	0.89	0.15	71,71,71,71	0
33	MG	0	8024	1/1	0.89	0.35	74,74,74,74	0
37	SR	0	9626	1/1	0.89	0.56	127,127,127,127	0
33	MG	0	8102	1/1	0.89	0.07	66,66,66,66	0
38	SPS	4	9701	23/23	0.89	0.15	49,53,67,71	0
33	MG	0	8108	1/1	0.89	0.19	81,81,81,81	0
33	MG	9	8095	1/1	0.90	0.22	48,48,48,48	0
35	NA	0	9120	1/1	0.90	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8021	1/1	0.90	0.15	56,56,56,56	0
35	NA	0	9181	1/1	0.90	0.12	52,52,52,52	0
36	CL	B	9319	1/1	0.90	0.33	53,53,53,53	0
37	SR	9	9588	1/1	0.90	0.11	118,118,118,118	0
37	SR	0	9482	1/1	0.90	0.41	115,115,115,115	0
33	MG	0	8084	1/1	0.90	0.47	61,61,61,61	0
33	MG	0	8101	1/1	0.90	0.12	59,59,59,59	0
35	NA	0	9154	1/1	0.91	0.20	57,57,57,57	0
35	NA	0	9158	1/1	0.91	0.22	55,55,55,55	0
35	NA	0	9101	1/1	0.91	0.11	45,45,45,45	0
33	MG	0	8042	1/1	0.91	0.07	57,57,57,57	0
37	SR	0	9537	1/1	0.91	0.14	136,136,136,136	0
35	NA	B	9161	1/1	0.91	0.19	62,62,62,62	0
33	MG	0	8091	1/1	0.91	0.10	64,64,64,64	0
33	MG	T	8073	1/1	0.91	0.16	41,41,41,41	0
36	CL	0	9316	1/1	0.91	0.38	69,69,69,69	0
33	MG	0	8072	1/1	0.91	0.21	70,70,70,70	0
37	SR	0	9459	1/1	0.91	0.09	95,95,95,95	0
34	K	0	9002	1/1	0.91	0.20	78,78,78,78	0
33	MG	0	8060	1/1	0.92	0.15	76,76,76,76	0
37	SR	0	9468	1/1	0.92	0.09	97,97,97,97	0
33	MG	0	8115	1/1	0.92	0.10	55,55,55,55	0
33	MG	0	8085	1/1	0.92	0.18	67,67,67,67	0
33	MG	0	8088	1/1	0.92	0.07	43,43,43,43	0
35	NA	0	9182	1/1	0.92	0.11	63,63,63,63	0
35	NA	0	9166	1/1	0.92	0.27	68,68,68,68	0
33	MG	0	8089	1/1	0.92	0.14	54,54,54,54	0
37	SR	0	9539	1/1	0.92	0.60	145,145,145,145	0
35	NA	0	9126	1/1	0.92	0.12	52,52,52,52	0
33	MG	0	8057	1/1	0.92	0.13	77,77,77,77	0
33	MG	0	8063	1/1	0.92	0.10	64,64,64,64	0
33	MG	0	8083	1/1	0.92	0.07	53,53,53,53	0
35	NA	0	9102	1/1	0.92	0.38	61,61,61,61	0
35	NA	0	9141	1/1	0.92	0.15	70,70,70,70	0
33	MG	0	8093	1/1	0.92	0.10	45,45,45,45	0
37	SR	0	9532	1/1	0.93	0.12	115,115,115,115	0
33	MG	0	8059	1/1	0.93	0.15	48,48,48,48	0
33	MG	0	8097	1/1	0.93	0.11	57,57,57,57	0
35	NA	0	9107	1/1	0.93	0.11	54,54,54,54	0
37	SR	0	9581	1/1	0.93	0.10	110,110,110,110	0
37	SR	0	9590	1/1	0.93	0.13	117,117,117,117	0
33	MG	0	8039	1/1	0.93	0.07	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	4	8118	1/1	0.93	0.06	45,45,45,45	0
35	NA	M	9147	1/1	0.93	0.07	43,43,43,43	0
35	NA	0	9150	1/1	0.93	0.10	47,47,47,47	0
35	NA	0	9167	1/1	0.93	0.08	49,49,49,49	0
37	SR	0	9530	1/1	0.93	0.10	102,102,102,102	0
33	MG	0	8043	1/1	0.94	0.06	50,50,50,50	0
37	SR	0	9452	1/1	0.94	0.10	105,105,105,105	0
35	NA	0	9113	1/1	0.94	0.20	64,64,64,64	0
35	NA	0	9165	1/1	0.94	0.27	44,44,44,44	0
35	NA	0	9116	1/1	0.94	0.12	46,46,46,46	0
33	MG	0	8104	1/1	0.94	0.08	49,49,49,49	0
35	NA	C	9104	1/1	0.94	0.12	31,31,31,31	0
33	MG	0	8054	1/1	0.94	0.07	55,55,55,55	0
35	NA	0	9155	1/1	0.94	0.19	52,52,52,52	0
33	MG	0	8080	1/1	0.94	0.16	46,46,46,46	0
35	NA	0	9159	1/1	0.94	0.17	46,46,46,46	0
33	MG	0	8067	1/1	0.95	0.10	33,33,33,33	0
33	MG	0	8117	1/1	0.95	0.06	39,39,39,39	0
37	SR	0	9490	1/1	0.95	0.18	101,101,101,101	0
33	MG	0	8058	1/1	0.95	0.08	39,39,39,39	0
35	NA	0	9106	1/1	0.95	0.20	35,35,35,35	0
37	SR	0	9505	1/1	0.95	0.26	97,97,97,97	0
37	SR	0	9515	1/1	0.95	0.30	88,88,88,88	0
35	NA	0	9157	1/1	0.95	0.22	37,37,37,37	0
33	MG	0	8076	1/1	0.95	0.08	51,51,51,51	0
35	NA	J	9146	1/1	0.95	0.06	51,51,51,51	0
33	MG	0	8112	1/1	0.95	0.05	45,45,45,45	0
33	MG	0	8041	1/1	0.95	0.06	51,51,51,51	0
36	CL	0	9311	1/1	0.95	0.11	61,61,61,61	0
37	SR	0	9566	1/1	0.95	0.16	92,92,92,92	0
36	CL	0	9315	1/1	0.95	0.09	53,53,53,53	0
35	NA	0	9114	1/1	0.95	0.16	56,56,56,56	0
35	NA	0	9132	1/1	0.95	0.10	54,54,54,54	0
36	CL	3	9304	1/1	0.95	0.08	65,65,65,65	0
37	SR	9	9503	1/1	0.95	0.09	102,102,102,102	0
37	SR	0	9425	1/1	0.95	0.09	108,108,108,108	0
35	NA	0	9115	1/1	0.95	0.19	35,35,35,35	0
37	SR	H	9486	1/1	0.95	0.30	107,107,107,107	0
33	MG	0	8046	1/1	0.95	0.05	37,37,37,37	0
35	NA	0	9117	1/1	0.95	0.06	32,32,32,32	0
33	MG	0	8116	1/1	0.96	0.05	51,51,51,51	0
37	SR	0	9504	1/1	0.96	0.06	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CL	J	9301	1/1	0.96	0.14	46,46,46,46	0
36	CL	J	9302	1/1	0.96	0.09	54,54,54,54	0
36	CL	J	9321	1/1	0.96	0.09	64,64,64,64	0
36	CL	L	9310	1/1	0.96	0.14	47,47,47,47	0
36	CL	N	9307	1/1	0.96	0.07	60,60,60,60	0
36	CL	O	9308	1/1	0.96	0.15	59,59,59,59	0
33	MG	0	8019	1/1	0.96	0.05	47,47,47,47	0
33	MG	0	8051	1/1	0.96	0.07	23,23,23,23	0
35	NA	0	9160	1/1	0.96	0.10	36,36,36,36	0
35	NA	0	9162	1/1	0.96	0.11	49,49,49,49	0
37	SR	0	9465	1/1	0.96	0.07	98,98,98,98	0
35	NA	Q	9148	1/1	0.96	0.07	51,51,51,51	0
37	SR	0	9477	1/1	0.96	0.06	75,75,75,75	0
35	NA	0	9128	1/1	0.96	0.11	39,39,39,39	0
37	SR	0	9483	1/1	0.96	0.06	69,69,69,69	0
33	MG	0	8037	1/1	0.96	0.08	39,39,39,39	0
37	SR	0	9489	1/1	0.96	0.09	85,85,85,85	0
35	NA	0	9131	1/1	0.96	0.09	45,45,45,45	0
35	NA	0	9110	1/1	0.96	0.12	45,45,45,45	0
35	NA	R	9137	1/1	0.97	0.06	33,33,33,33	0
37	SR	0	9506	1/1	0.97	0.18	74,74,74,74	0
37	SR	0	9509	1/1	0.97	0.06	83,83,83,83	0
35	NA	R	9138	1/1	0.97	0.09	58,58,58,58	0
37	SR	0	9517	1/1	0.97	0.07	92,92,92,92	0
37	SR	0	9522	1/1	0.97	0.07	98,98,98,98	0
37	SR	0	9433	1/1	0.97	0.08	68,68,68,68	0
33	MG	0	8106	1/1	0.97	0.04	47,47,47,47	0
33	MG	0	8036	1/1	0.97	0.06	56,56,56,56	0
37	SR	0	9534	1/1	0.97	0.27	95,95,95,95	0
36	CL	0	9314	1/1	0.97	0.16	43,43,43,43	0
33	MG	0	8098	1/1	0.97	0.07	45,45,45,45	0
37	SR	0	9545	1/1	0.97	0.08	72,72,72,72	0
37	SR	0	9475	1/1	0.97	0.07	76,76,76,76	0
37	SR	0	9560	1/1	0.97	0.06	88,88,88,88	0
33	MG	0	8110	1/1	0.97	0.22	44,44,44,44	0
37	SR	0	9568	1/1	0.97	0.06	70,70,70,70	0
37	SR	0	9570	1/1	0.97	0.07	92,92,92,92	0
37	SR	0	9480	1/1	0.97	0.05	82,82,82,82	0
37	SR	0	9585	1/1	0.97	0.06	83,83,83,83	0
33	MG	0	8075	1/1	0.97	0.04	43,43,43,43	0
35	NA	0	9143	1/1	0.97	0.05	37,37,37,37	0
33	MG	0	8044	1/1	0.97	0.05	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	9629	1/1	0.97	0.05	68,68,68,68	0
33	MG	0	8031	1/1	0.97	0.07	51,51,51,51	0
33	MG	0	8068	1/1	0.97	0.14	41,41,41,41	0
37	SR	A	9497	1/1	0.97	0.05	78,78,78,78	0
37	SR	0	9495	1/1	0.97	0.05	85,85,85,85	0
37	SR	F	9595	1/1	0.97	0.10	92,92,92,92	0
33	MG	0	8096	1/1	0.97	0.06	40,40,40,40	0
35	NA	0	9156	1/1	0.97	0.10	55,55,55,55	0
36	CL	Y	9320	1/1	0.97	0.07	40,40,40,40	0
36	CL	A	9309	1/1	0.98	0.20	56,56,56,56	0
37	SR	0	9488	1/1	0.98	0.04	72,72,72,72	0
35	NA	0	9130	1/1	0.98	0.06	47,47,47,47	0
33	MG	0	8013	1/1	0.98	0.22	14,14,14,14	0
33	MG	0	8025	1/1	0.98	0.19	24,24,24,24	0
35	NA	0	9134	1/1	0.98	0.05	42,42,42,42	0
35	NA	0	9135	1/1	0.98	0.07	39,39,39,39	0
36	CL	M	9318	1/1	0.98	0.04	40,40,40,40	0
35	NA	0	9136	1/1	0.98	0.07	30,30,30,30	0
35	NA	0	9123	1/1	0.98	0.10	39,39,39,39	0
37	SR	0	9508	1/1	0.98	0.06	78,78,78,78	0
36	CL	R	9306	1/1	0.98	0.05	43,43,43,43	0
33	MG	0	8027	1/1	0.98	0.13	35,35,35,35	0
33	MG	0	8056	1/1	0.98	0.08	54,54,54,54	0
37	SR	0	9417	1/1	0.98	0.04	53,53,53,53	0
37	SR	0	9420	1/1	0.98	0.08	65,65,65,65	0
37	SR	0	9421	1/1	0.98	0.04	65,65,65,65	0
33	MG	0	8029	1/1	0.98	0.09	26,26,26,26	0
37	SR	0	9426	1/1	0.98	0.04	64,64,64,64	0
37	SR	0	9427	1/1	0.98	0.05	54,54,54,54	0
37	SR	0	9431	1/1	0.98	0.04	56,56,56,56	0
37	SR	0	9432	1/1	0.98	0.09	61,61,61,61	0
36	CL	0	9303	1/1	0.98	0.09	43,43,43,43	0
37	SR	0	9438	1/1	0.98	0.04	61,61,61,61	0
37	SR	0	9445	1/1	0.98	0.03	55,55,55,55	0
37	SR	0	9447	1/1	0.98	0.04	62,62,62,62	0
36	CL	0	9305	1/1	0.98	0.06	50,50,50,50	0
37	SR	0	9454	1/1	0.98	0.06	71,71,71,71	0
35	NA	0	9149	1/1	0.98	0.11	43,43,43,43	0
37	SR	0	9461	1/1	0.98	0.08	71,71,71,71	0
37	SR	0	9464	1/1	0.98	0.06	79,79,79,79	0
36	CL	0	9312	1/1	0.98	0.07	47,47,47,47	0
37	SR	0	9466	1/1	0.98	0.10	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	9467	1/1	0.98	0.06	71,71,71,71	0
36	CL	0	9313	1/1	0.98	0.07	47,47,47,47	0
37	SR	A	9437	1/1	0.98	0.06	61,61,61,61	0
37	SR	0	9469	1/1	0.98	0.07	83,83,83,83	0
37	SR	B	9458	1/1	0.98	0.04	64,64,64,64	0
33	MG	0	8009	1/1	0.98	0.06	31,31,31,31	0
33	MG	0	8015	1/1	0.98	0.03	29,29,29,29	0
35	NA	0	9108	1/1	0.98	0.04	31,31,31,31	0
37	SR	S	9470	1/1	0.98	0.06	91,91,91,91	0
37	SR	1	9460	1/1	0.98	0.04	51,51,51,51	0
37	SR	3	9439	1/1	0.98	0.04	64,64,64,64	0
36	CL	0	9317	1/1	0.98	0.08	48,48,48,48	0
36	CL	0	9322	1/1	0.98	0.30	51,51,51,51	0
37	SR	0	9416	1/1	0.99	0.05	47,47,47,47	0
33	MG	0	8008	1/1	0.99	0.11	16,16,16,16	0
33	MG	0	8026	1/1	0.99	0.04	28,28,28,28	0
33	MG	0	8079	1/1	0.99	0.04	28,28,28,28	0
37	SR	0	9422	1/1	0.99	0.03	55,55,55,55	0
37	SR	0	9423	1/1	0.99	0.03	51,51,51,51	0
33	MG	0	8017	1/1	0.99	0.07	23,23,23,23	0
33	MG	0	8028	1/1	0.99	0.02	31,31,31,31	0
33	MG	0	8001	1/1	0.99	0.11	23,23,23,23	0
37	SR	0	9428	1/1	0.99	0.03	49,49,49,49	0
37	SR	0	9429	1/1	0.99	0.04	64,64,64,64	0
33	MG	K	8069	1/1	0.99	0.09	24,24,24,24	0
33	MG	0	8030	1/1	0.99	0.04	37,37,37,37	0
33	MG	Y	8109	1/1	0.99	0.06	35,35,35,35	0
37	SR	0	9434	1/1	0.99	0.04	59,59,59,59	0
37	SR	0	9435	1/1	0.99	0.03	68,68,68,68	0
33	MG	0	8020	1/1	0.99	0.04	36,36,36,36	0
37	SR	0	9440	1/1	0.99	0.03	61,61,61,61	0
37	SR	0	9441	1/1	0.99	0.04	57,57,57,57	0
37	SR	0	9442	1/1	0.99	0.03	59,59,59,59	0
37	SR	0	9443	1/1	0.99	0.03	54,54,54,54	0
33	MG	0	8032	1/1	0.99	0.05	33,33,33,33	0
37	SR	0	9446	1/1	0.99	0.05	78,78,78,78	0
33	MG	0	8012	1/1	0.99	0.11	37,37,37,37	0
37	SR	0	9448	1/1	0.99	0.03	59,59,59,59	0
37	SR	0	9450	1/1	0.99	0.04	60,60,60,60	0
37	SR	0	9451	1/1	0.99	0.04	64,64,64,64	0
33	MG	0	8002	1/1	0.99	0.02	29,29,29,29	0
37	SR	0	9453	1/1	0.99	0.04	68,68,68,68	0

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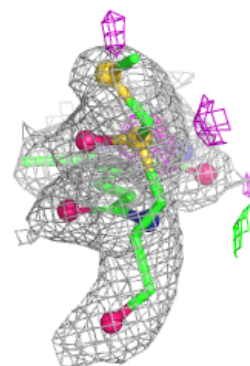
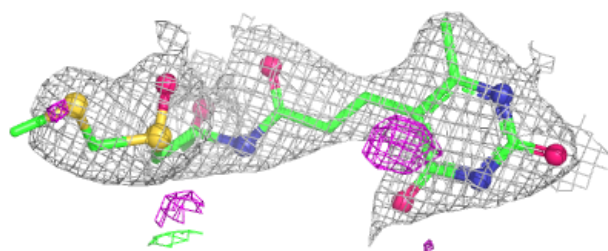
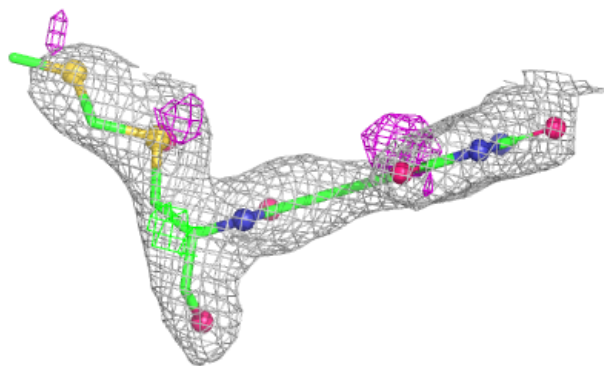
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	9105	1/1	0.99	0.03	33,33,33,33	0
37	SR	0	9455	1/1	0.99	0.03	61,61,61,61	0
37	SR	0	9456	1/1	0.99	0.06	64,64,64,64	0
37	SR	0	9457	1/1	0.99	0.03	49,49,49,49	0
33	MG	0	8038	1/1	0.99	0.13	18,18,18,18	0
33	MG	0	8070	1/1	0.99	0.06	21,21,21,21	0
37	SR	9	9481	1/1	0.99	0.05	82,82,82,82	0
37	SR	0	9462	1/1	0.99	0.03	64,64,64,64	0
33	MG	0	8003	1/1	0.99	0.05	26,26,26,26	0
37	SR	A	9436	1/1	0.99	0.12	68,68,68,68	0
33	MG	0	8074	1/1	0.99	0.14	20,20,20,20	0
37	SR	0	9405	1/1	0.99	0.05	80,80,80,80	0
37	SR	0	9407	1/1	0.99	0.06	46,46,46,46	0
37	SR	0	9410	1/1	0.99	0.09	45,45,45,45	0
37	SR	0	9412	1/1	0.99	0.06	48,48,48,48	0
37	SR	0	9473	1/1	0.99	0.05	69,69,69,69	0
37	SR	R	9418	1/1	0.99	0.06	54,54,54,54	0
37	SR	0	9474	1/1	0.99	0.03	71,71,71,71	0
37	SR	1	9419	1/1	0.99	0.06	43,43,43,43	0
37	SR	0	9413	1/1	0.99	0.04	49,49,49,49	0
37	SR	0	9414	1/1	0.99	0.04	54,54,54,54	0
37	SR	0	9478	1/1	0.99	0.04	69,69,69,69	0
37	SR	0	9415	1/1	0.99	0.03	54,54,54,54	0
39	CD	Z	9203	1/1	0.99	0.05	59,59,59,59	0
39	CD	1	9202	1/1	0.99	0.06	55,55,55,55	0
39	CD	3	9204	1/1	0.99	0.04	59,59,59,59	0
37	SR	L	9409	1/1	1.00	0.10	49,49,49,49	0
33	MG	0	8005	1/1	1.00	0.03	29,29,29,29	0
37	SR	0	9498	1/1	1.00	0.07	61,61,61,61	0
37	SR	0	9444	1/1	1.00	0.03	50,50,50,50	0
37	SR	0	9408	1/1	1.00	0.09	45,45,45,45	0
33	MG	0	8004	1/1	1.00	0.02	26,26,26,26	0
37	SR	0	9411	1/1	1.00	0.09	46,46,46,46	0
37	SR	0	9430	1/1	1.00	0.05	46,46,46,46	0
39	CD	U	9201	1/1	1.00	0.03	59,59,59,59	0
37	SR	0	9449	1/1	1.00	0.02	57,57,57,57	0
37	SR	0	9424	1/1	1.00	0.05	46,46,46,46	0
37	SR	0	9406	1/1	1.00	0.10	43,43,43,43	0

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

Electron density around SPS 4 9701:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.