



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:22 AM UTC

PDB ID : 1VQP / pdb_00001vqp
Title : The structure of the transition state analogue "RAP" bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.25 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

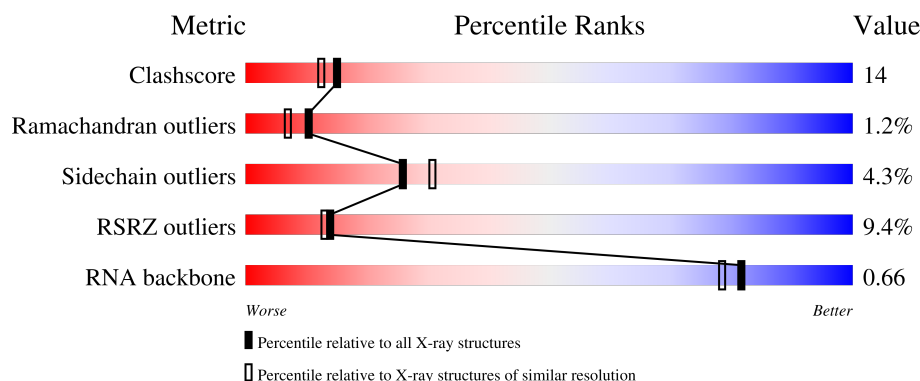
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

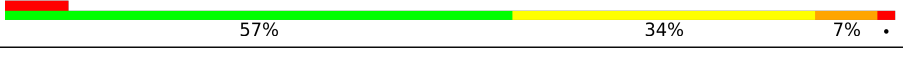
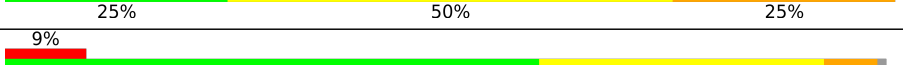
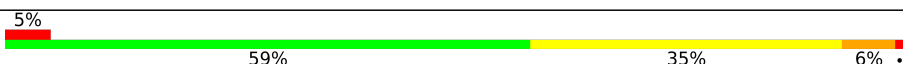
The reported resolution of this entry is 2.25 Å.

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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)
RNA backbone	3983	1005 (2.56-1.96)

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

Mol	Chain	Length	Quality of chain
1	0	2922	
2	9	122	
3	4	8	
4	A	240	
5	B	338	

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

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8022	-	-	-	X
33	MG	0	8024	-	-	-	X
37	SR	0	9500	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99070 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			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	GB 3377779

- 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*(DC)P*(DC)P*(PPU)*(LOF)P*(PO2)P*AP*C*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	8	Total	C	N	O	P	0	0	0
			132	67	23	37	5			

- 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	S	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	0	0	0
			735	450	141	144			

- 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	0	0	0
			1149	713	209	223	4			

- 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	0	0	0
			641	389	111	138	3			

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

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

- 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	0	0	0
			410	244	75	86	5			

- 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	0	0	0
			499	304	94	100	1			

- 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	0	0	0
			1196	737	209	244	6			

- 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	A	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	3	Total	K	0	0
			3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	64	Total	Na	0	0
			64	64		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	9	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	D	1	Total 1	Na 1	0	0
35	H	1	Total 1	Na 1	0	0
35	J	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	R	3	Total 3	Na 3	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	3	1	Total	Cl	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total	Sr	0	0
			98	98		
37	9	3	Total	Sr	0	0
			3	3		
37	A	3	Total	Sr	0	0
			3	3		
37	B	2	Total	Sr	0	0
			2	2		
37	F	1	Total	Sr	0	0
			1	1		
37	H	1	Total	Sr	0	0
			1	1		
37	L	1	Total	Sr	0	0
			1	1		
37	R	1	Total	Sr	0	0
			1	1		
37	S	1	Total	Sr	0	0
			1	1		
37	1	2	Total	Sr	0	0
			2	2		
37	3	1	Total	Sr	0	0
			1	1		

- Molecule 38 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total	Cd	0	0
			1	1		
38	U	1	Total	Cd	0	0
			1	1		
38	Z	1	Total	Cd	0	0
			1	1		
38	1	1	Total	Cd	0	0
			1	1		
38	3	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	0	5757	Total O 5757 5757	0	0
39	9	139	Total O 139 139	0	0
39	4	6	Total O 6 6	0	0
39	A	124	Total O 124 124	0	0
39	B	140	Total O 140 140	0	0
39	C	172	Total O 172 172	0	0
39	D	50	Total O 50 50	0	0
39	E	40	Total O 40 40	0	0
39	F	25	Total O 25 25	0	0
39	G	16	Total O 16 16	0	0
39	H	69	Total O 69 69	0	0
39	J	52	Total O 52 52	0	0
39	K	59	Total O 59 59	0	0
39	L	83	Total O 83 83	0	0
39	M	131	Total O 131 131	0	0
39	N	58	Total O 58 58	0	0
39	O	39	Total O 39 39	0	0
39	P	57	Total O 57 57	0	0
39	Q	51	Total O 51 51	0	0
39	R	87	Total O 87 87	0	0
39	S	32	Total O 32 32	0	0

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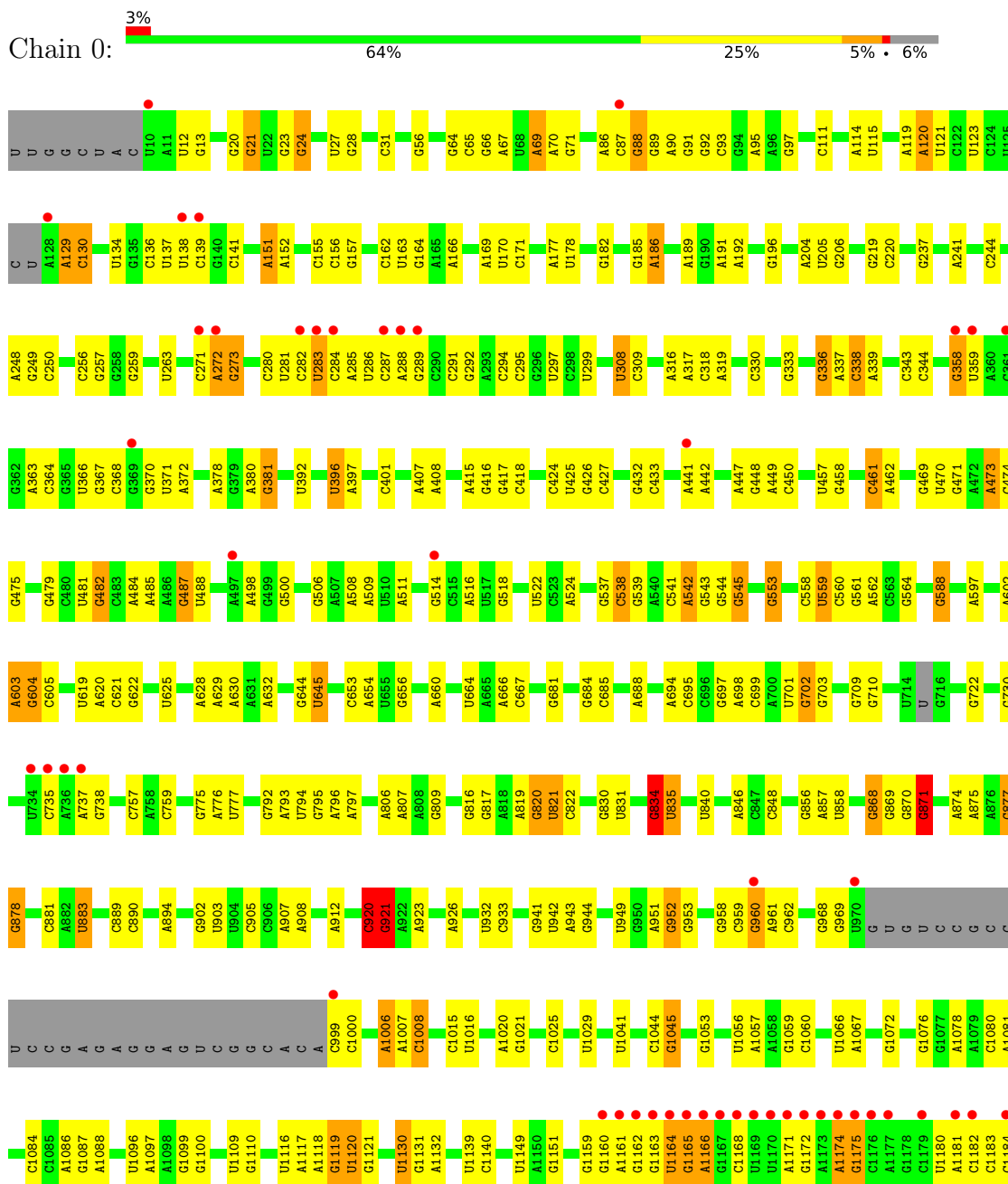
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	T	36	Total 36	O 36	0	0
39	U	30	Total 30	O 30	0	0
39	V	11	Total 11	O 11	0	0
39	W	72	Total 72	O 72	0	0
39	X	24	Total 24	O 24	0	0
39	Y	88	Total 88	O 88	0	0
39	Z	31	Total 31	O 31	0	0
39	1	49	Total 49	O 49	0	0
39	2	38	Total 38	O 38	0	0
39	3	66	Total 66	O 66	0	0
39	I	9	Total 9	O 9	0	0

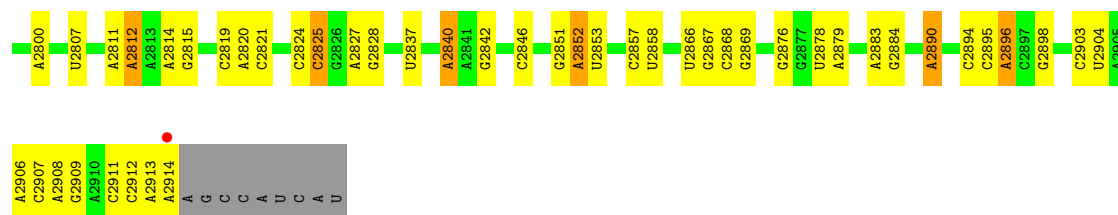
3 Residue-property plots

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

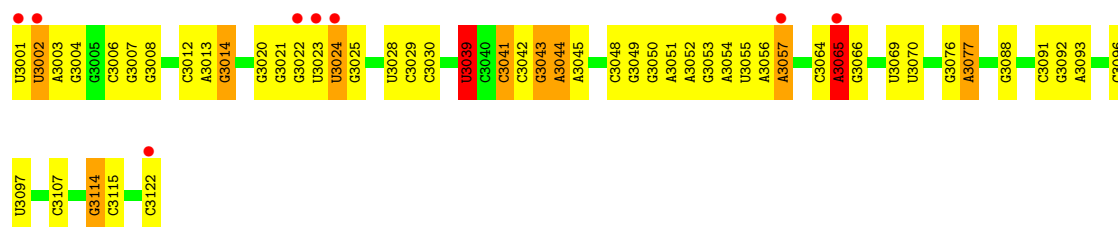
- Molecule 1: 23S ribosomal rna



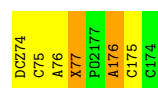




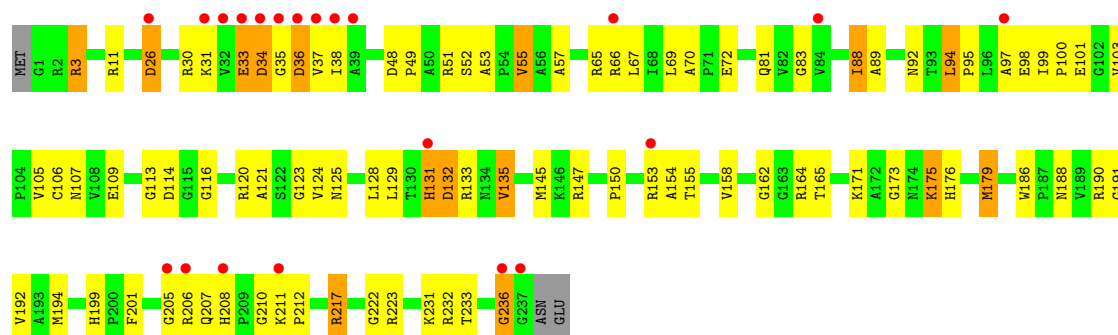
• Molecule 2: 5S ribosomal RNA



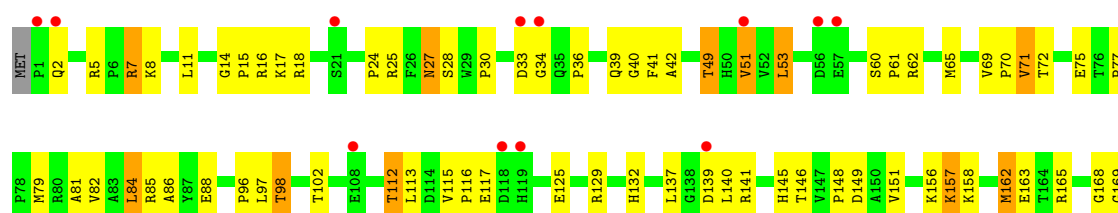
• Molecule 3: 5'-R*(DC)P*(DC)P*(PPU)*(LOF)P*(PO2)P*AP*C*C)-3'

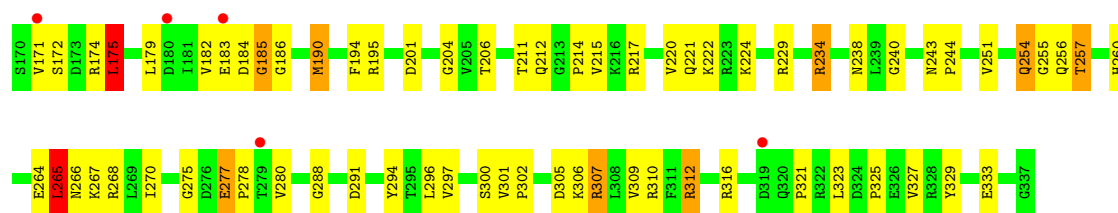


• Molecule 4: 50S ribosomal protein L2P

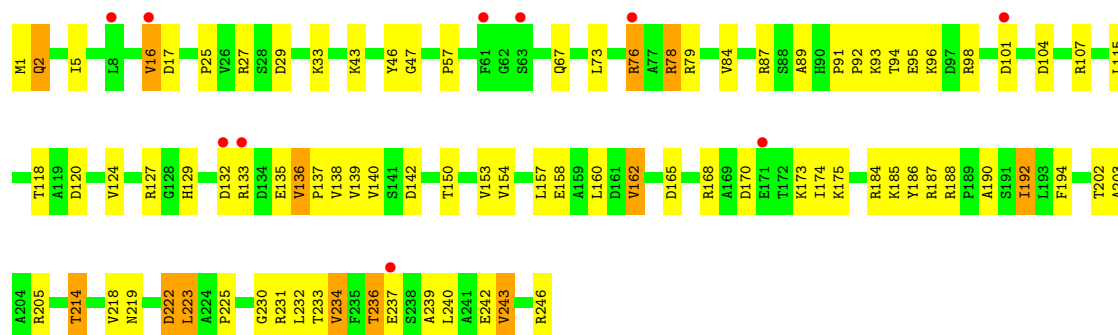


• Molecule 5: 50S ribosomal protein L3P

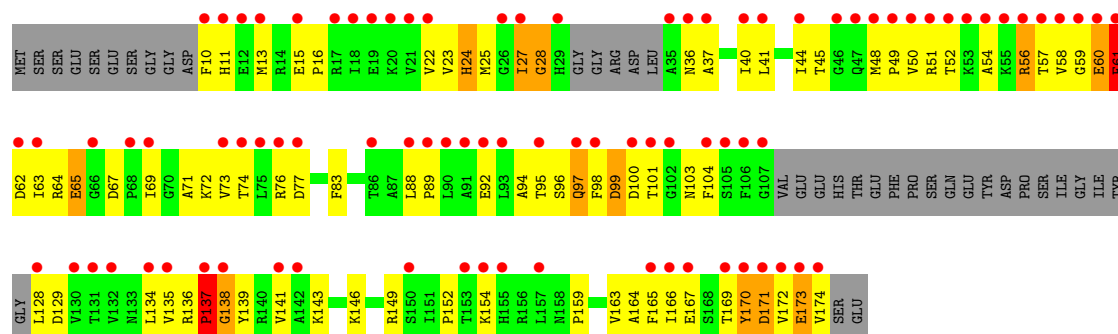




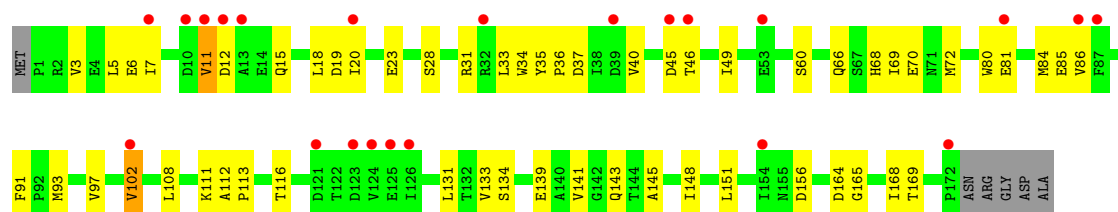
• Molecule 6: 50S ribosomal protein L4E



• Molecule 7: 50S ribosomal protein L5P



• Molecule 8: 50S ribosomal protein L6P

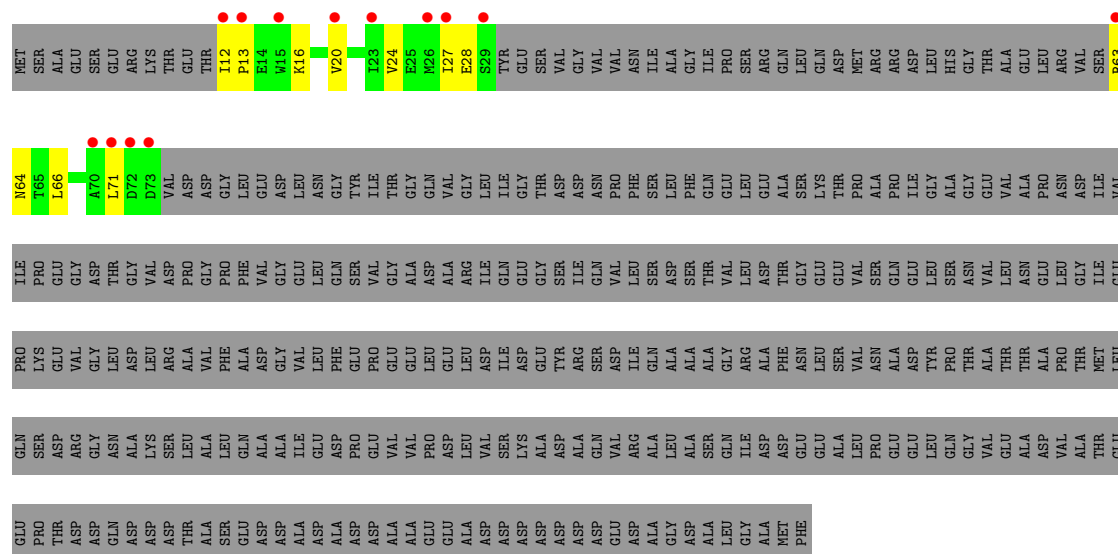


• Molecule 9: 50S ribosomal protein L7AE

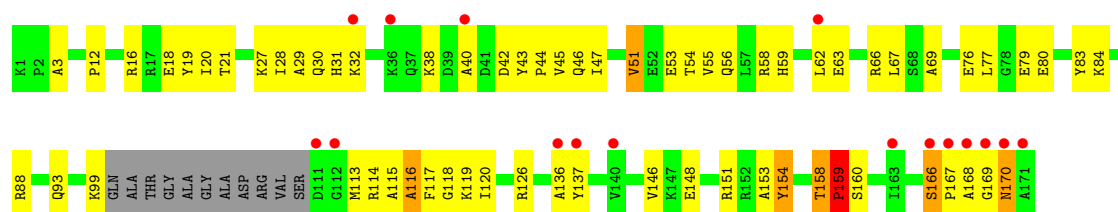




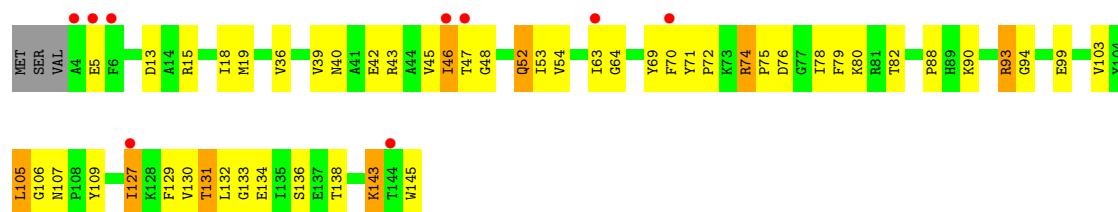
- Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



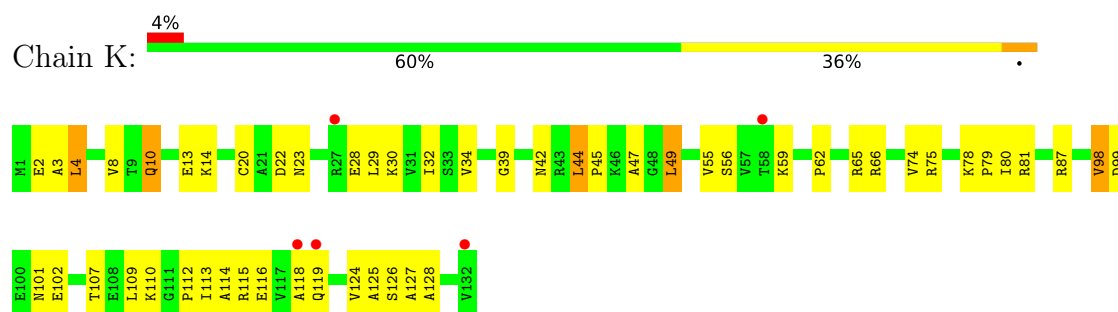
- Molecule 11: 50S RIBOSOMAL PROTEIN L10E



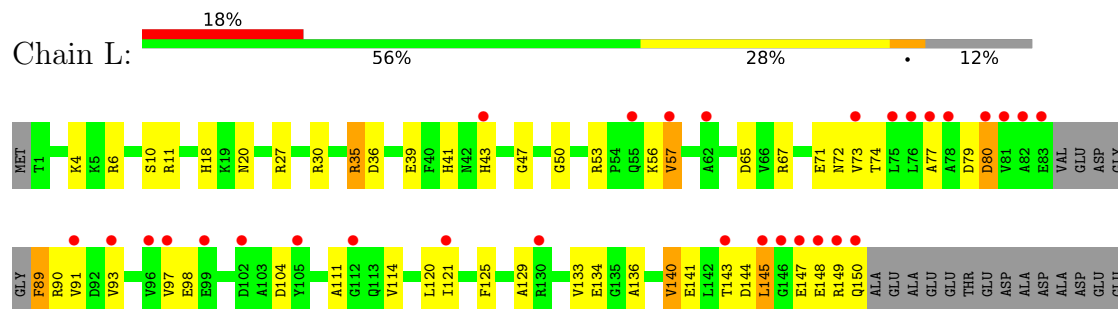
- Molecule 12: 50S ribosomal protein L13P



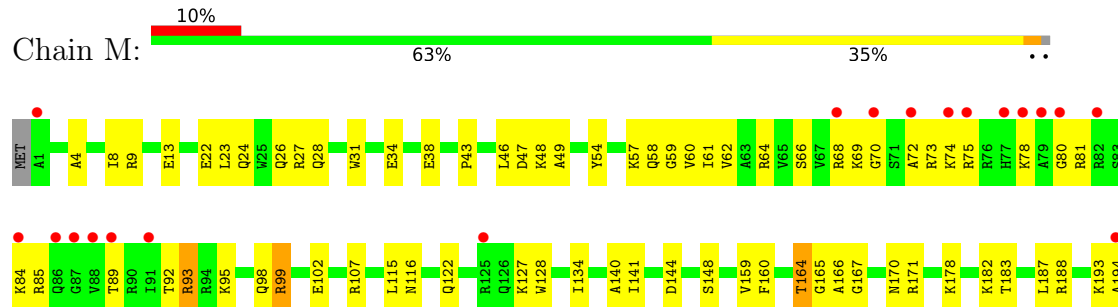
- Molecule 13: 50S ribosomal protein L14P



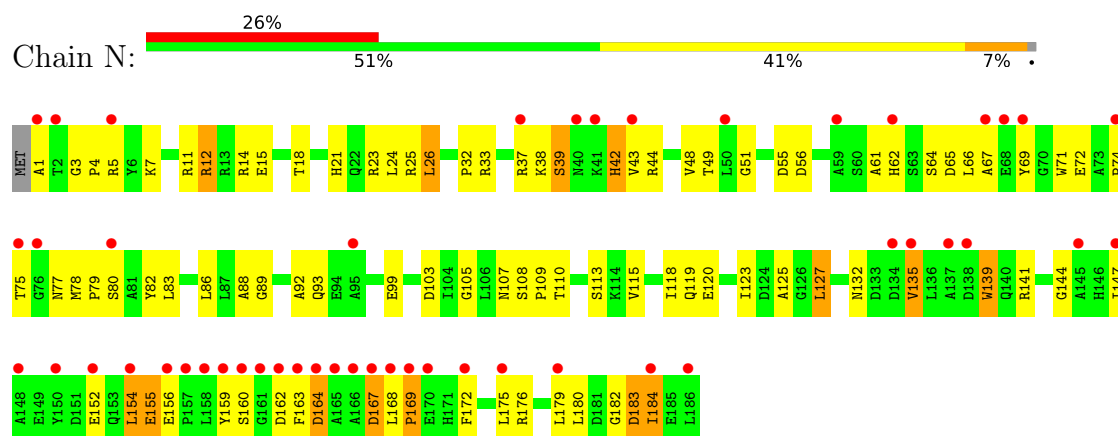
• Molecule 14: 50S ribosomal protein L15P



• Molecule 15: 50S Ribosomal Protein L15E

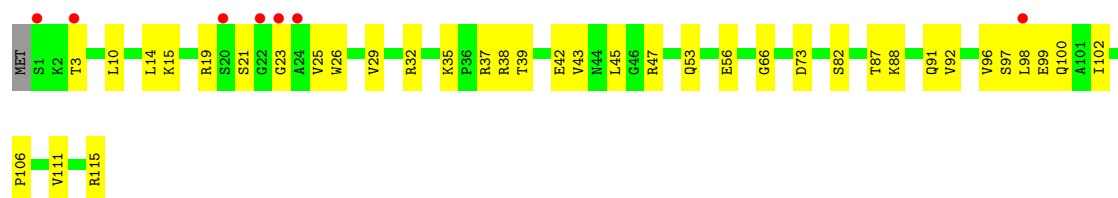


• Molecule 16: 50S ribosomal protein L18P

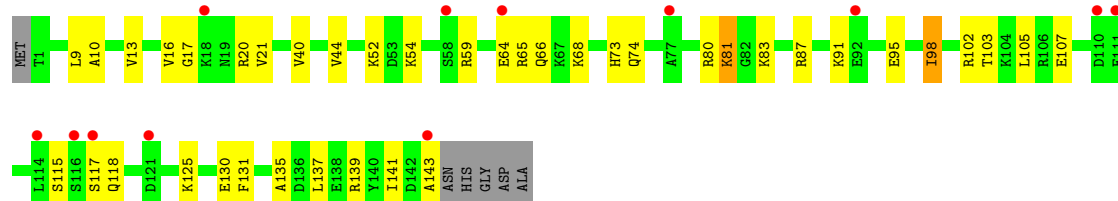


• Molecule 17: 50S ribosomal protein L18e

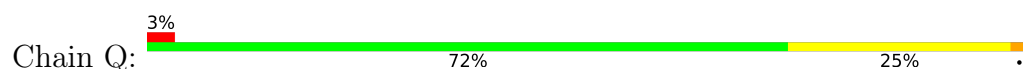




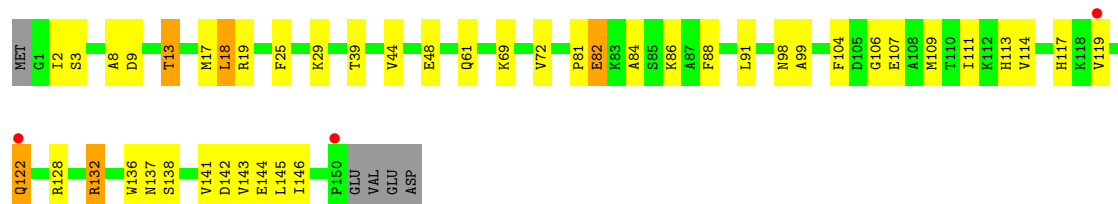
- Molecule 18: 50S ribosomal protein L19E



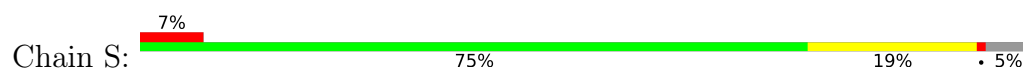
- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P



- Molecule 22: 50S ribosomal protein L24P





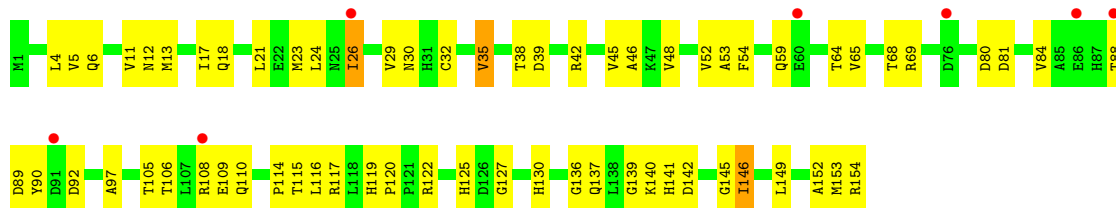
- Molecule 23: 50S ribosomal protein L24E



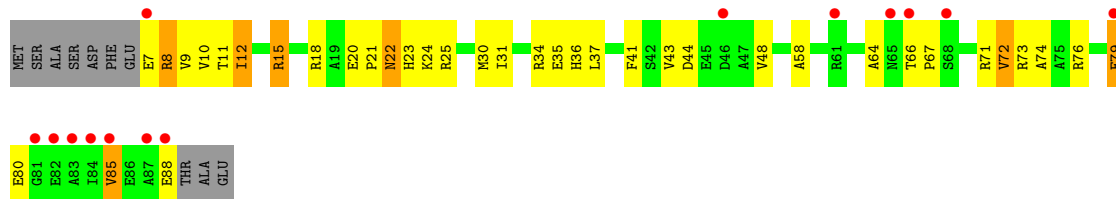
- Molecule 24: 50S ribosomal protein L29P



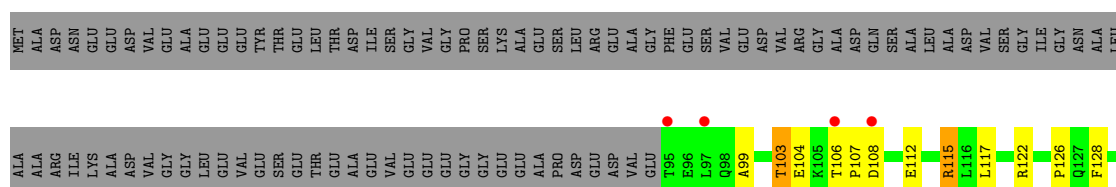
- Molecule 25: 50S ribosomal protein L30P

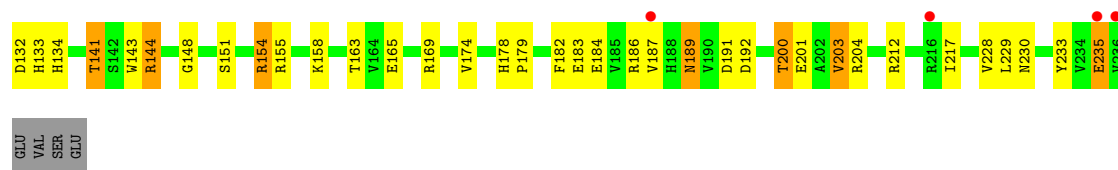


- Molecule 26: 50S ribosomal protein L31e

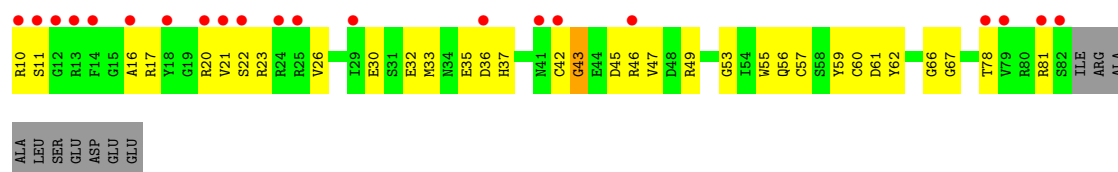


- Molecule 27: 50S ribosomal protein L32E

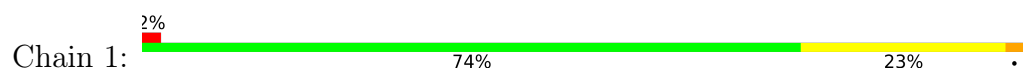




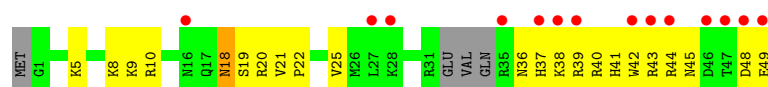
- Molecule 28: 50S ribosomal protein L37Ae



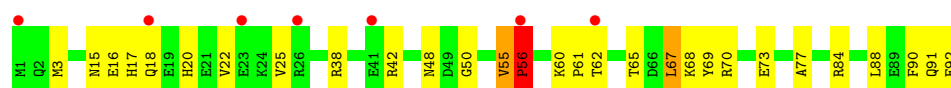
- Molecule 29: 50S ribosomal protein L37e



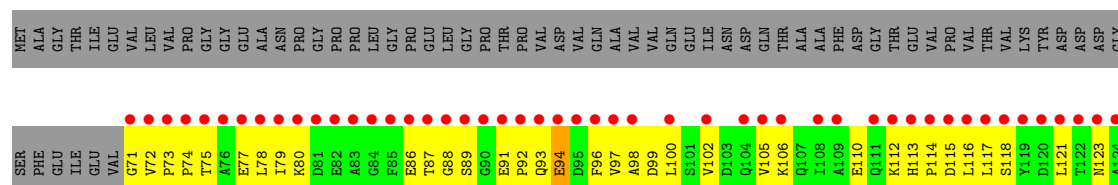
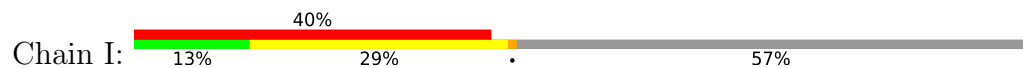
- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



A125	K126	E127	V128	V129	G130	T131	C132	T133	S134	L135	G136	V137	T138	I139	E140	GLY	GLU	ASN	PRO	ARG	GLU	PHE	LYS	GLU	ARG	ILE	ASP	ALA	GLY	GLU	TYR	ASP	ASP	VAL	PHE	ALA	ALA	GLU	ALA	GLN	ALA
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.61Å 298.19Å 574.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 50.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.25) 90.5 (50.00-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.247 0.212 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99070	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% 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: DCZ, K, PO2, PSU, PPU, CL, HFA, OMU, NA, OMG, CD, UR3, MG, SR, 1MA

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	0.38	1/65959 (0.0%)	0.62	37/102870 (0.0%)
2	9	0.37	0/2905	0.60	2/4528 (0.0%)
3	4	0.42	0/83	1.02	1/119 (0.8%)
4	A	0.42	0/1786	0.99	5/2408 (0.2%)
5	B	0.42	0/2690	0.98	11/3652 (0.3%)
6	C	0.44	0/1884	0.97	7/2551 (0.3%)
7	D	0.33	0/1111	0.84	5/1498 (0.3%)
8	E	0.35	0/1382	0.85	3/1880 (0.2%)
9	F	0.37	0/901	0.86	0/1224
10	G	0.34	0/241	0.74	0/324
11	H	0.36	0/1287	0.95	6/1725 (0.3%)
12	J	0.39	0/1136	0.91	2/1530 (0.1%)
13	K	0.41	0/1001	0.98	2/1347 (0.1%)
14	L	0.37	0/1130	0.99	4/1509 (0.3%)
15	M	0.41	0/1584	0.89	5/2119 (0.2%)
16	N	0.35	0/1474	1.02	9/1999 (0.5%)
17	O	0.39	0/874	0.89	3/1181 (0.3%)
18	P	0.39	0/1147	0.85	0/1528
19	Q	0.41	0/749	1.04	1/1005 (0.1%)
20	R	0.43	0/1172	0.95	5/1578 (0.3%)
21	S	0.35	0/648	0.90	2/875 (0.2%)
22	T	0.36	0/958	0.95	7/1289 (0.5%)
23	U	0.38	0/417	0.85	1/562 (0.2%)
24	V	0.34	0/502	0.88	2/675 (0.3%)
25	W	0.48	0/1219	0.95	2/1655 (0.1%)
26	X	0.41	0/664	0.92	3/895 (0.3%)
27	Y	0.43	0/1146	0.96	4/1536 (0.3%)
28	Z	0.34	0/589	0.89	0/787
29	1	0.49	0/438	0.91	1/578 (0.2%)
30	2	0.41	0/401	0.80	0/529
31	3	0.38	0/771	0.86	3/1024 (0.3%)
32	I	0.35	0/526	0.87	3/716 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	1/98775 (0.0%)	0.72	136/147696 (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	0	45
2	9	0	2
All	All	0	47

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2619	UR3	O3'-P	5.47	1.61	1.56

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1979	G	C2'-C3'-O3'	9.93	124.40	109.50
16	N	163	PHE	N-CA-C	-9.52	102.18	113.88
19	Q	17	LYS	N-CA-C	-9.40	97.89	109.83
14	L	47	GLY	N-CA-C	8.37	120.73	111.85
1	0	1942	A	C5'-C4'-C3'	8.16	128.23	116.00
5	B	222	LYS	N-CA-C	-7.84	98.92	110.52
1	0	1819	G	C5'-C4'-C3'	7.56	127.34	116.00
4	A	70	ALA	N-CA-C	7.47	119.07	109.65
14	L	57	VAL	N-CA-C	-7.46	105.56	112.43
7	D	100	ASP	N-CA-C	-7.43	103.34	113.30
21	S	27	ALA	N-CA-C	-7.38	97.22	109.46
2	9	3039	U	N1-C1'-C2'	7.32	122.98	112.00
1	0	871	G	C5'-C4'-O4'	-7.25	98.93	109.80
15	M	89	THR	N-CA-C	7.07	118.64	111.07
1	0	920	C	C2'-C3'-O3'	-7.05	103.13	113.70
11	H	160	SER	N-CA-C	-6.99	101.11	110.55
16	N	135	VAL	N-CA-C	-6.92	106.56	113.20
5	B	323	LEU	N-CA-C	6.89	119.20	110.24
16	N	169	PRO	N-CA-C	-6.84	104.67	114.18
1	0	1592	G	N9-C1'-C2'	6.84	122.26	112.00
6	C	205	ARG	N-CA-C	6.82	119.58	111.33
5	B	157	LYS	N-CA-C	-6.69	105.68	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	4	176	A	C1'-C2'-O2'	-6.63	101.86	111.80
1	0	1080	C	C2'-C3'-O3'	-6.62	103.77	113.70
20	R	141	VAL	N-CA-C	6.58	117.32	108.11
26	X	12	ILE	N-CA-C	6.51	114.34	107.76
27	Y	183	GLU	N-CA-C	-6.39	99.28	109.76
17	O	66	GLY	N-CA-C	6.38	126.00	115.34
4	A	222	GLY	N-CA-C	-6.37	106.35	114.37
27	Y	143	TRP	N-CA-C	6.35	119.44	110.23
20	R	137	ASN	N-CA-C	6.34	120.24	110.42
15	M	8	ILE	N-CA-C	-6.31	104.35	110.72
4	A	88	ILE	N-CA-C	6.29	112.94	106.21
16	N	51	GLY	CA-C-N	6.28	126.48	119.32
16	N	51	GLY	C-N-CA	6.28	126.48	119.32
1	0	2291	A	N9-C1'-C2'	6.28	121.42	112.00
5	B	175	LEU	N-CA-C	-6.16	104.49	111.14
26	X	22	ASN	N-CA-C	6.14	117.98	111.28
16	N	42	HIS	N-CA-C	6.14	118.75	109.41
7	D	170	TYR	N-CA-C	6.07	120.24	111.56
7	D	48	MET	N-CA-C	6.06	116.57	109.60
22	T	3	GLN	CA-C-N	6.02	126.19	119.32
22	T	3	GLN	C-N-CA	6.02	126.19	119.32
1	0	2726	U	N1-C1'-C2'	6.00	121.00	112.00
1	0	1684	A	C2'-C3'-O3'	5.93	118.40	109.50
1	0	883	U	N1-C1'-C2'	5.92	120.89	112.00
22	T	52	ARG	N-CA-C	5.92	123.40	110.80
27	Y	230	ASN	CA-C-N	5.92	125.89	120.03
27	Y	230	ASN	C-N-CA	5.92	125.89	120.03
1	0	1352	A	C4'-C3'-O3'	5.87	118.21	109.40
25	W	35	VAL	N-CA-C	5.85	114.57	107.61
6	C	84	VAL	N-CA-C	-5.85	101.99	109.30
1	0	1701	A	C5'-C4'-C3'	5.79	123.89	115.20
1	0	206	G	C5'-C4'-C3'	-5.79	107.31	116.00
12	J	36	VAL	N-CA-C	5.77	116.79	108.48
1	0	1819	G	C4'-C3'-C2'	-5.76	96.84	102.60
1	0	2301	A	N9-C1'-C2'	5.75	120.62	112.00
26	X	79	GLU	N-CA-C	5.74	117.54	111.28
1	0	874	A	C4'-C3'-O3'	-5.72	104.42	113.00
5	B	265	LEU	N-CA-C	5.71	118.25	110.55
1	0	2467	A	O4'-C4'-C3'	-5.69	100.41	106.10
1	0	1878	G	O4'-C1'-C2'	-5.68	101.92	107.60
1	0	1120	U	C5'-C4'-C3'	-5.68	107.48	116.00
8	E	11	VAL	N-CA-C	5.65	117.96	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1504	A	N9-C1'-C2'	5.64	120.45	112.00
1	0	1615	A	C5'-C4'-C3'	5.63	124.44	116.00
29	1	21	ARG	N-CA-C	5.62	118.26	111.40
23	U	50	GLU	N-CA-C	5.59	118.10	111.33
31	3	55	VAL	CA-C-N	5.59	126.83	119.84
31	3	55	VAL	C-N-CA	5.59	126.83	119.84
6	C	192	ILE	N-CA-C	5.57	116.79	109.21
7	D	15	GLU	CA-C-N	5.54	126.77	119.84
7	D	15	GLU	C-N-CA	5.54	126.77	119.84
11	H	118	GLY	N-CA-C	5.53	119.62	112.54
2	9	3039	U	C4'-C3'-O3'	-5.53	104.71	113.00
1	0	134	U	C5'-C4'-C3'	-5.52	107.72	116.00
20	R	3	SER	N-CA-C	-5.52	100.97	109.52
22	T	89	ARG	CA-C-N	5.51	125.52	119.90
22	T	89	ARG	C-N-CA	5.51	125.52	119.90
13	K	8	VAL	N-CA-C	5.49	116.38	108.48
15	M	4	ALA	N-CA-C	-5.48	105.47	111.82
16	N	3	GLY	CA-C-N	5.45	125.54	119.32
16	N	3	GLY	C-N-CA	5.45	125.54	119.32
11	H	159	PRO	N-CA-C	5.45	119.59	111.41
1	0	921	G	N9-C1'-C2'	5.45	120.17	112.00
17	O	43	VAL	N-CA-C	5.44	116.42	108.53
6	C	89	ALA	N-CA-C	5.42	116.86	111.07
5	B	117	GLU	N-CA-C	-5.38	107.37	114.04
16	N	39	SER	N-CA-C	-5.36	101.15	109.14
1	0	473	A	C5'-C4'-C3'	5.35	124.02	116.00
1	0	2664	A	N9-C1'-C2'	5.34	120.01	112.00
32	I	91	GLU	CA-C-N	5.34	125.31	120.03
32	I	91	GLU	C-N-CA	5.34	125.31	120.03
1	0	2012	U	N1-C1'-C2'	5.32	119.97	112.00
6	C	188	ARG	N-CA-C	5.30	112.99	108.22
20	R	18	LEU	N-CA-C	-5.29	101.53	109.95
1	0	1452	G	C5'-C4'-C3'	-5.29	108.07	116.00
15	M	70	GLY	N-CA-C	5.28	120.64	112.45
5	B	151	VAL	CA-C-N	5.28	124.91	119.05
5	B	151	VAL	C-N-CA	5.28	124.91	119.05
6	C	78	ARG	N-CA-C	5.28	115.51	108.38
5	B	49	THR	N-CA-C	-5.28	101.25	108.38
4	A	188	ASN	N-CA-C	5.27	117.00	108.41
5	B	224	LYS	N-CA-C	5.27	118.33	109.95
8	E	156	ASP	N-CA-C	5.25	117.68	111.33
5	B	266	ASN	N-CA-C	5.25	118.57	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	158	THR	N-CA-C	5.24	121.40	109.81
13	K	124	VAL	N-CA-C	-5.23	105.43	110.72
32	I	94	GLU	N-CA-C	-5.23	107.03	113.41
1	0	2313	C	C5'-C4'-C3'	5.23	123.84	116.00
11	H	88	ARG	N-CA-C	5.22	119.49	113.18
31	3	67	LEU	N-CA-C	5.21	118.08	109.85
6	C	175	LYS	N-CA-C	5.20	117.42	110.35
1	0	1261	A	N9-C1'-C2'	5.19	119.79	112.00
15	M	13	GLU	N-CA-C	-5.16	106.49	112.89
14	L	145	LEU	N-CA-C	-5.15	105.67	111.28
12	J	105	LEU	N-CA-C	-5.15	101.58	109.76
11	H	116	ALA	N-CA-C	5.11	119.23	112.89
25	W	115	THR	N-CA-C	5.11	117.82	109.59
8	E	37	ASP	N-CA-C	5.11	119.09	112.86
1	0	2726	U	C2'-C3'-O3'	-5.10	106.05	113.70
14	L	20	ASN	N-CA-C	5.10	117.81	111.24
1	0	820	G	N9-C1'-C2'	5.09	119.63	112.00
1	0	1752	G	C5'-C4'-C3'	5.09	122.83	115.20
22	T	92	ASP	N-CA-C	-5.08	101.68	109.76
21	S	10	VAL	N-CA-C	5.08	114.89	107.37
22	T	16	LEU	N-CA-C	5.08	117.21	111.11
1	0	1006	A	N9-C1'-C2'	5.08	119.62	112.00
17	O	82	SER	N-CA-C	-5.08	103.70	110.55
1	0	2526	C	N1-C1'-C2'	5.07	119.60	112.00
1	0	834	G	C2'-C3'-O3'	-5.05	106.12	113.70
24	V	42	ASN	CA-C-N	5.04	126.14	119.84
24	V	42	ASN	C-N-CA	5.04	126.14	119.84
4	A	135	VAL	N-CA-C	5.04	115.00	108.35
1	0	129	A	C2'-C3'-O3'	5.03	121.25	113.70
20	R	122	GLN	N-CA-C	-5.01	100.34	108.41

There are no chirality outliers.

All (47) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1132	A	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1458	A	Sidechain
1	0	1744	G	Sidechain
1	0	1809	G	Sidechain

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Mol	Chain	Res	Type	Group
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	1979	G	Sidechain
1	0	2036	C	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	2599	A	Sidechain
1	0	2607	U	Sidechain
1	0	2616	G	Sidechain
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2679	G	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	469	G	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	792	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	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	29813	689	0
2	9	2600	0	1326	57	0
3	4	132	0	79	4	0
4	A	1753	0	1766	114	0
5	B	2625	0	2531	135	0
6	C	1859	0	1816	95	0
7	D	1094	0	1085	91	0
8	E	1357	0	1266	62	0
9	F	890	0	843	48	0
10	G	240	0	231	10	0
11	H	1266	0	1268	65	0
12	J	1120	0	1098	72	0
13	K	992	0	1031	58	0
14	L	1118	0	1076	50	0
15	M	1560	0	1568	65	0
16	N	1445	0	1401	90	0
17	O	865	0	873	33	0
18	P	1136	0	1123	35	0
19	Q	735	0	729	22	0
20	R	1149	0	1122	42	0
21	S	641	0	605	17	0
22	T	950	0	923	56	0
23	U	410	0	364	17	0
24	V	499	0	511	35	0
25	W	1196	0	1137	88	0
26	X	654	0	653	40	0
27	Y	1130	0	1133	51	0
28	Z	578	0	539	22	0
29	1	431	0	426	22	0
30	2	396	0	413	32	0
31	3	755	0	728	25	0
32	I	519	0	500	57	0
33	0	88	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Y	1	0	0	0	0
34	0	3	0	0	0	0
35	0	64	0	0	0	0
35	9	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	H	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	3	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	2	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	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
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	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5757	0	0	89	0
39	1	49	0	0	1	0
39	2	38	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	3	66	0	0	2	0
39	4	6	0	0	0	0
39	9	139	0	0	7	0
39	A	124	0	0	16	0
39	B	140	0	0	18	0
39	C	172	0	0	16	0
39	D	50	0	0	12	0
39	E	40	0	0	3	0
39	F	25	0	0	2	0
39	G	16	0	0	1	0
39	H	69	0	0	6	0
39	I	9	0	0	0	0
39	J	52	0	0	3	0
39	K	59	0	0	3	0
39	L	83	0	0	9	0
39	M	131	0	0	5	0
39	N	58	0	0	4	0
39	O	39	0	0	5	0
39	P	57	0	0	1	0
39	Q	51	0	0	5	0
39	R	87	0	0	3	0
39	S	32	0	0	0	0
39	T	36	0	0	6	0
39	U	30	0	0	3	0
39	V	11	0	0	1	0
39	W	72	0	0	3	0
39	X	24	0	0	4	0
39	Y	88	0	0	7	0
39	Z	31	0	0	2	0
All	All	99070	0	59977	2063	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 (2063) 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)
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.29	1.14
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.29	1.11
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.27	1.09
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.28	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.31	1.06
6:C:236:THR:HG22	6:C:239:ALA:H	1.19	1.06
7:D:25:MET:HE2	7:D:41:LEU:HG	1.37	1.03
9:F:91:VAL:HG12	9:F:92:GLY:H	1.24	1.03
1:O:1160:G:H5'	1:O:1161:A:H5'	1.40	1.02
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.25	1.01
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.40	1.01
2:9:3076:G:H3'	2:9:3077:A:H5''	1.42	1.00
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.09	0.99
1:O:156:C:H5''	15:M:171:ARG:HD3	1.40	0.99
30:2:18:ASN:HD21	30:2:40:ARG:H	1.09	0.99
1:O:871:G:C8	1:O:871:G:H5'	1.98	0.99
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.46	0.98
1:O:21:G:H5'	20:R:2:ILE:HA	1.46	0.97
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.47	0.96
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.45	0.96
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.49	0.94
24:V:8:ILE:HA	24:V:11:MET:HE3	1.49	0.94
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.82	0.94
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.50	0.94
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.03	0.93
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.50	0.93
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.50	0.93
1:O:1372:A:H3'	39:O:7674:HOH:O	1.69	0.93
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.92
5:B:238:ASN:HD22	5:B:240:GLY:H	1.18	0.92
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.52	0.92
1:O:2840:A:OP1	5:B:211:THR:HG23	1.70	0.92
13:K:10:GLN:H	13:K:10:GLN:NE2	1.68	0.91
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.17	0.91
1:O:2717:C:H2'	1:O:2718:C:H5''	1.52	0.91
25:W:149:LEU:HG	25:W:153:MET:HE2	1.53	0.91
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.70	0.91
1:O:542:A:H5'	1:O:542:A:H8	1.35	0.90
13:K:10:GLN:HE21	13:K:10:GLN:N	1.69	0.90
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.37	0.90
6:C:1:MET:HG2	6:C:2:GLN:H	1.34	0.90
1:O:2506:A:HO2'	1:O:2507:G:H8	0.94	0.90
18:P:115:SER:H	18:P:118:GLN:HE21	1.11	0.90
16:N:113:SER:HB2	39:N:9352:HOH:O	1.73	0.89
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.52	0.89
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.56	0.88
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.55	0.88
5:B:140:LEU:HA	39:B:9578:HOH:O	1.72	0.88
1:O:871:G:H5'	1:O:871:G:H8	1.39	0.88
16:N:144:GLY:O	16:N:147:ILE:HG22	1.73	0.88
1:O:2896:A:H5''	39:O:6619:HOH:O	1.74	0.87
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.36	0.87
1:O:2717:C:C2'	1:O:2718:C:H5''	2.03	0.87
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.56	0.87
1:O:870:G:H2'	1:O:871:G:H5''	1.54	0.87
1:O:2812:A:H2	1:O:2814:A:H62	1.19	0.87
9:F:58:GLU:HA	9:F:61:MET:HE2	1.54	0.86
4:A:179:MET:HA	4:A:179:MET:HE3	1.58	0.86
2:9:3056:A:H2'	2:9:3057:A:H5''	1.54	0.86
30:2:41:HIS:H	30:2:45:ASN:HD22	1.18	0.86
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.41	0.86
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.76	0.86
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.58	0.86
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.55	0.86
5:B:86:ALA:HA	39:B:9578:HOH:O	1.75	0.85
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.58	0.85
25:W:88:THR:HB	39:W:6679:HOH:O	1.75	0.85
1:O:1242:A:H5'	12:J:82:THR:HG23	1.57	0.85
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.58	0.85
1:O:1041:U:H5'	39:L:9491:HOH:O	1.74	0.85
6:C:104:ASP:HA	6:C:107:ARG:NH1	1.91	0.85
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.59	0.85
1:O:2716:G:H5''	5:B:206:THR:HG21	1.59	0.84
25:W:122:ARG:HG2	25:W:152:ALA:O	1.77	0.84
4:A:199:HIS:HD2	4:A:201:PHE:H	1.23	0.84
4:A:192:VAL:HG22	39:A:9621:HOH:O	1.76	0.83
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.42	0.83
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.61	0.83
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.13	0.83
39:O:5401:HOH:O	12:J:47:THR:HB	1.78	0.83
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.60	0.83
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.58	0.83
1:O:1973:A:H5'	1:O:1973:A:H8	1.44	0.83
1:O:1474:C:H6	1:O:1474:C:H5'	1.43	0.83
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1835:U:H5	1:0:1840:A:N7	1.77	0.82
24:V:1:THR:HG23	24:V:2:VAL:H	1.45	0.82
4:A:192:VAL:HB	39:A:9584:HOH:O	1.78	0.82
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.94	0.82
27:Y:235:GLU:CD	27:Y:235:GLU:H	1.84	0.82
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.95	0.82
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.43	0.82
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.60	0.82
25:W:137:GLN:HE21	25:W:141:HIS:CE1	1.96	0.82
25:W:125:HIS:HD2	25:W:127:GLY:H	1.28	0.81
1:0:541:C:H2'	1:0:542:A:H5''	1.62	0.81
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.62	0.81
25:W:13:MET:HE2	25:W:18:GLN:HA	1.63	0.81
12:J:93:ARG:HB3	12:J:93:ARG:HH11	1.45	0.81
1:0:1116:U:O2'	1:0:1118:A:H2	1.64	0.81
20:R:99:ALA:HB1	20:R:109:MET:CE	2.11	0.81
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.63	0.80
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.46	0.80
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.97	0.80
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.11	0.80
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.64	0.80
12:J:74:ARG:NH1	12:J:76:ASP:HB2	1.97	0.80
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.47	0.80
32:I:78:LEU:HD12	32:I:112:LYS:NZ	1.95	0.80
1:0:2851:G:C2'	1:0:2852:A:H5'	2.12	0.80
1:0:1667:A:H8	1:0:1667:A:H5'	1.46	0.79
1:0:1751:G:H2'	1:0:1752:G:H5''	1.64	0.79
6:C:236:THR:HG22	6:C:239:ALA:N	1.96	0.79
4:A:191:GLY:HA2	4:A:194:MET:CE	2.11	0.79
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.65	0.79
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.64	0.79
7:D:57:THR:HG23	7:D:63:ILE:HA	1.63	0.79
25:W:13:MET:HE2	25:W:18:GLN:CA	2.13	0.79
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.65	0.79
1:0:2054:A:N3	20:R:128:ARG:NH2	2.31	0.78
1:0:1160:G:C5'	1:0:1161:A:H5'	2.14	0.78
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.65	0.78
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.45	0.78
1:0:2541:U:H4'	1:0:2542:C:OP1	1.82	0.78
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.64	0.77
13:K:10:GLN:H	13:K:10:GLN:HE21	0.87	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1116:U:HO2'	1:0:1118:A:H2	0.81	0.77
1:0:281:U:H2'	1:0:282:C:O4'	1.84	0.77
1:0:289:G:H22	1:0:363:A:H2	1.31	0.77
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.67	0.77
1:0:288:A:H61	1:0:364:C:H42	1.30	0.77
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.15	0.77
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.66	0.77
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.15	0.77
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.19	0.77
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.67	0.77
5:B:162:MET:HE3	5:B:310:ARG:HD3	1.68	0.76
1:0:871:G:C8	1:0:871:G:C5'	2.69	0.76
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.19	0.76
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.67	0.76
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.01	0.76
1:0:871:G:H8	1:0:871:G:C5'	1.97	0.76
18:P:115:SER:OG	18:P:118:GLN:HG3	1.85	0.76
6:C:236:THR:CG2	6:C:239:ALA:H	1.98	0.76
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.13	0.76
2:9:3039:U:H1'	2:9:3044:A:H61	1.49	0.76
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.51	0.76
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.21	0.76
11:H:27:LYS:H	11:H:59:HIS:HD2	1.33	0.76
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.66	0.76
1:0:541:C:C2'	1:0:542:A:H5''	2.16	0.76
1:0:1119:G:N2	1:0:1246:A:C2	2.53	0.76
16:N:37:ARG:HG3	36:N:9307:CL:CL	2.23	0.76
29:1:25:LYS:HD2	30:2:49:GLU:H	1.51	0.76
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.66	0.75
2:9:3014:G:H5'	2:9:3014:G:H8	1.51	0.75
25:W:88:THR:HG22	25:W:89:ASP:H	1.50	0.75
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.86	0.75
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.68	0.75
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.68	0.75
1:0:1603:A:H5'	1:0:1605:G:O4'	1.87	0.75
16:N:80:SER:HB2	39:N:9333:HOH:O	1.87	0.75
1:0:1162:G:H1'	32:I:117:LEU:HD11	1.69	0.75
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.86	0.75
25:W:122:ARG:NH2	25:W:154:ARG:HG2	2.02	0.75
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.32	0.75
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.69	0.74
11:H:21:THR:O	11:H:120:ILE:HD12	1.87	0.74
25:W:137:GLN:NE2	25:W:141:HIS:HE1	1.85	0.74
1:O:506:G:H22	1:O:509:A:C5'	2.00	0.74
1:O:1159:G:H21	1:O:1189:A:H8	1.35	0.74
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.02	0.74
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.85	0.74
1:O:2506:A:O2'	1:O:2507:G:H8	1.69	0.74
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.17	0.74
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.03	0.74
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.69	0.74
1:O:481:U:H5''	39:O:6187:HOH:O	1.87	0.74
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.18	0.73
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.69	0.73
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.03	0.73
1:O:2534:C:H1'	39:O:4094:HOH:O	1.89	0.73
18:P:115:SER:H	18:P:118:GLN:NE2	1.85	0.73
1:O:470:U:O2'	29:1:16:HIS:HD2	1.72	0.73
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.19	0.73
24:V:39:ALA:N	24:V:40:PRO:HD2	2.04	0.73
5:B:16:ARG:NH1	39:B:9613:HOH:O	2.22	0.73
1:O:111:C:O2'	29:1:20:ARG:HG2	1.89	0.72
1:O:560:C:H42	1:O:597:A:H61	1.35	0.72
1:O:1118:A:H62	1:O:1244:U:H3	1.37	0.72
1:O:2533:C:H5'	1:O:2533:C:H6	1.54	0.72
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.54	0.72
1:O:545:G:H5'	1:O:545:G:H8	1.54	0.72
1:O:559:U:H6	1:O:559:U:H5'	1.54	0.72
1:O:1562:C:H42	1:O:2738:G:H1	1.37	0.72
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.19	0.72
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.38	0.72
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.72	0.72
25:W:88:THR:HG22	25:W:89:ASP:N	2.05	0.72
28:Z:17:ARG:HD3	39:Z:9220:HOH:O	1.89	0.72
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.70	0.71
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.05	0.71
25:W:52:VAL:HG22	25:W:53:ALA:H	1.55	0.71
1:O:1701:A:H4'	1:O:1702:U:H5''	1.73	0.71
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.55	0.71
9:F:91:VAL:HG12	9:F:92:GLY:N	2.03	0.71
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:870:G:C2'	1:0:871:G:H5''	2.20	0.71
7:D:99:ASP:HB2	7:D:103:ASN:H	1.54	0.71
1:0:1700:C:H5''	1:0:1701:A:OP2	1.91	0.71
5:B:179:LEU:O	5:B:183:GLU:HG2	1.89	0.71
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.72	0.71
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.72	0.71
1:0:2468:A:H61	31:3:48:ASN:HD21	1.38	0.71
4:A:199:HIS:CD2	4:A:201:PHE:H	2.07	0.71
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.09	0.71
2:9:3051:A:H5'	16:N:160:SER:HB3	1.71	0.71
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.04	0.71
1:0:544:G:H2'	1:0:545:G:H5''	1.72	0.71
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.54	0.71
9:F:37:THR:O	9:F:41:GLU:HG3	1.91	0.70
12:J:19:MET:HE2	12:J:79:PHE:HA	1.72	0.70
4:A:153:ARG:HB2	4:A:153:ARG:HH11	1.55	0.70
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.72	0.70
2:9:3039:U:H1'	2:9:3044:A:N6	2.05	0.70
17:O:32:ARG:O	17:O:32:ARG:HD3	1.91	0.70
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.91	0.70
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.72	0.70
15:M:99:ARG:NH2	15:M:170:ASN:HD22	1.90	0.70
4:A:48:ASP:HB3	39:A:9596:HOH:O	1.90	0.70
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.73	0.70
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.72	0.70
25:W:80:ASP:O	25:W:84:VAL:HG23	1.90	0.70
1:0:1593:C:OP1	18:P:117:SER:HB3	1.91	0.70
39:O:7918:HOH:O	5:B:211:THR:HG21	1.91	0.70
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.73	0.70
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.90	0.70
1:0:282:C:O2'	1:0:283:U:H5'	1.90	0.70
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.22	0.70
1:0:1206:U:H5'	1:0:1206:U:H6	1.57	0.69
5:B:51:VAL:HG23	5:B:329:TYR:O	1.92	0.69
1:0:1641:A:H2'	1:0:1642:A:H5'	1.73	0.69
1:0:2073:G:OP2	1:0:2490:A:H5'	1.93	0.69
22:T:26:THR:HA	22:T:39:ASN:HB3	1.74	0.69
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.72	0.69
4:A:33:GLU:H	4:A:33:GLU:CD	2.00	0.69
1:0:542:A:H5'	1:0:542:A:C8	2.23	0.69
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:96:ALA:HA	39:F:3111:HOH:O	1.91	0.69
24:V:12:THR:HG22	24:V:15:GLU:CG	2.21	0.69
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.75	0.69
30:2:20:ARG:HG3	30:2:39:ARG:HH21	1.57	0.69
1:0:2005:G:H3'	1:0:2005:G:OP2	1.92	0.69
5:B:162:MET:CE	5:B:310:ARG:HD3	2.22	0.69
11:H:170:ASN:HD22	11:H:170:ASN:N	1.91	0.69
1:0:2491:G:H1'	39:0:7359:HOH:O	1.91	0.69
16:N:164:ASP:CG	16:N:167:ASP:HA	2.17	0.69
1:0:1166:A:H1'	1:0:1192:A:C2	2.28	0.69
1:0:2749:U:H5'	39:0:8460:HOH:O	1.92	0.69
39:0:6651:HOH:O	30:2:20:ARG:HB3	1.93	0.69
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.74	0.69
1:0:282:C:H1'	1:0:368:C:N4	2.07	0.69
1:0:1165:G:H4'	1:0:1174:A:O2'	1.93	0.69
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.27	0.69
6:C:1:MET:HG2	6:C:2:GLN:N	2.07	0.69
10:G:12:ILE:N	10:G:13:PRO:HD3	2.08	0.69
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.75	0.69
6:C:246:ARG:HB3	6:C:246:ARG:NH1	2.06	0.69
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.93	0.69
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.91	0.69
18:P:91:LYS:O	18:P:95:GLU:HG3	1.91	0.69
1:0:1474:C:H5'	1:0:1474:C:C6	2.27	0.69
4:A:35:GLY:O	4:A:36:ASP:HB3	1.92	0.68
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.56	0.68
1:0:2291:A:C8	1:0:2309:C:H5'	2.28	0.68
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.73	0.68
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.73	0.68
32:I:87:THR:HG22	32:I:88:GLY:H	1.58	0.68
8:E:84:MET:HE1	8:E:148:ILE:CD1	2.24	0.68
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.23	0.68
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.75	0.68
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.75	0.68
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.57	0.68
1:0:1118:A:C8	1:0:1118:A:H3'	2.28	0.68
1:0:1118:A:H3'	1:0:1118:A:H8	1.58	0.68
1:0:1377:C:H5'	1:0:1377:C:H6	1.58	0.68
7:D:170:TYR:O	7:D:171:ASP:HB3	1.93	0.68
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.75	0.68
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.07	0.68
27:Y:144:ARG:CZ	39:Y:9404:HOH:O	2.42	0.68
1:0:280:C:H2'	1:0:281:U:O4'	1.94	0.68
4:A:51:ARG:HB2	39:A:9596:HOH:O	1.91	0.68
12:J:45:VAL:HG23	12:J:130:VAL:O	1.94	0.68
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.22	0.68
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.93	0.68
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.22	0.68
1:0:1878:G:H1'	39:0:6641:HOH:O	1.93	0.68
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.24	0.68
16:N:38:LYS:HE2	16:N:107:ASN:HD21	1.59	0.68
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.08	0.68
1:0:506:G:H22	1:0:509:A:H5''	1.58	0.68
1:0:1175:G:H1'	1:0:1193:A:H2'	1.74	0.67
1:0:380:A:OP2	15:M:9:ARG:HD2	1.95	0.67
1:0:2851:G:H2'	1:0:2852:A:H5'	1.75	0.67
3:4:176:A:O4'	3:4:175:C:H2'	1.94	0.67
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.25	0.67
1:0:121:U:OP2	30:2:10:ARG:NH2	2.27	0.67
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.59	0.67
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.16	0.67
8:E:34:TRP:O	12:J:127:ILE:HD11	1.94	0.67
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.58	0.67
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.77	0.67
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.25	0.67
1:0:541:C:H2'	1:0:542:A:C5'	2.25	0.67
1:0:709:G:O2'	17:O:25:VAL:HG12	1.93	0.67
1:0:1116:U:H3	1:0:1246:A:H62	1.42	0.67
25:W:139:GLY:O	25:W:141:HIS:HD2	1.77	0.67
39:0:7000:HOH:O	27:Y:141:THR:HG23	1.94	0.67
5:B:254:GLN:HG2	5:B:255:GLY:N	2.09	0.67
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.09	0.67
24:V:56:ILE:O	24:V:60:GLN:HG3	1.95	0.67
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.30	0.67
2:9:3013:A:O2'	2:9:3014:G:H5''	1.94	0.67
11:H:166:SER:CB	11:H:167:PRO:HD3	2.25	0.66
30:2:18:ASN:ND2	30:2:40:ARG:H	1.88	0.66
32:I:89:SER:HB3	32:I:97:VAL:HG23	1.77	0.66
1:0:2420:G:O2'	1:0:2421:G:H5'	1.96	0.66
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.96	0.66
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.93	0.66
14:L:133:VAL:HA	39:L:9471:HOH:O	1.94	0.66
27:Y:165:GLU:HB3	39:Y:9387:HOH:O	1.94	0.66
1:O:93:C:H5''	24:V:1:THR:HB	1.76	0.66
6:C:107:ARG:NE	39:C:9258:HOH:O	2.28	0.66
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.30	0.66
1:O:1244:U:OP1	12:J:18:ILE:HD13	1.95	0.66
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.61	0.66
14:L:67:ARG:O	14:L:71:GLU:HG3	1.96	0.66
15:M:80:GLY:O	15:M:81:ARG:HD2	1.95	0.66
11:H:166:SER:CB	11:H:167:PRO:CD	2.74	0.66
1:O:1184:C:H1'	39:O:7928:HOH:O	1.95	0.66
1:O:2908:A:H2'	1:O:2909:G:O4'	1.96	0.66
2:9:3020:G:O2'	2:9:3021:G:H5'	1.96	0.66
20:R:99:ALA:CB	20:R:109:MET:HE1	2.15	0.66
1:O:1189:A:H1'	1:O:1209:C:O4'	1.96	0.65
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.76	0.65
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.11	0.65
1:O:1666:C:O2'	1:O:1667:A:H5''	1.95	0.65
39:O:4349:HOH:O	22:T:9:LYS:HD3	1.97	0.65
1:O:2890:A:H1'	23:U:56:ARG:NH2	2.11	0.65
25:W:48:VAL:O	25:W:48:VAL:HG12	1.95	0.65
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.95	0.65
4:A:153:ARG:HB2	4:A:153:ARG:NH1	2.11	0.65
1:O:2578:G:H5'	1:O:2578:G:H8	1.61	0.65
4:A:33:GLU:O	4:A:34:ASP:HB2	1.96	0.65
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.77	0.65
1:O:960:G:H4'	39:O:7894:HOH:O	1.97	0.65
1:O:2270:G:H4'	4:A:223:ARG:HH12	1.62	0.65
1:O:2878:U:H2'	1:O:2879:A:O4'	1.95	0.65
5:B:275:GLY:O	5:B:291:ASP:HA	1.97	0.65
7:D:25:MET:HE2	7:D:41:LEU:CG	2.22	0.65
32:I:87:THR:HG22	32:I:88:GLY:N	2.12	0.65
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.77	0.65
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.27	0.65
29:1:25:LYS:HD2	30:2:49:GLU:N	2.12	0.65
1:O:396:U:O2'	1:O:418:C:H4'	1.97	0.65
2:9:3056:A:C2'	2:9:3057:A:H5''	2.27	0.65
14:L:143:THR:HG22	14:L:144:ASP:N	2.12	0.65
15:M:164:THR:HG22	15:M:166:ALA:H	1.60	0.65
1:O:1160:G:H5'	1:O:1161:A:C5'	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3069:U:OP1	16:N:4:PRO:HG3	1.97	0.65
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.97	0.65
30:2:36:ASN:HB3	30:2:39:ARG:HG3	1.79	0.65
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.27	0.65
1:0:877:G:H5'	1:0:878:G:OP1	1.96	0.64
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.79	0.64
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.79	0.64
25:W:125:HIS:CD2	25:W:127:GLY:H	2.11	0.64
1:0:220:C:H1'	39:0:6292:HOH:O	1.96	0.64
1:0:381:G:H5''	39:M:9377:HOH:O	1.96	0.64
1:0:1666:C:H2'	1:0:1667:A:H5'	1.79	0.64
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.27	0.64
29:1:10:LYS:HG3	39:1:9488:HOH:O	1.96	0.64
1:0:1182:C:H1'	1:0:1192:A:H8	1.61	0.64
1:0:1299:G:O6	14:L:6:ARG:HD3	1.98	0.64
1:0:2586:U:H3	1:0:2592:G:H22	1.45	0.64
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.27	0.64
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.97	0.64
1:0:1973:A:H5'	1:0:1973:A:C8	2.31	0.64
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.12	0.64
7:D:159:PRO:O	7:D:163:VAL:HG23	1.97	0.64
23:U:14:GLU:O	23:U:17:THR:HB	1.97	0.64
7:D:135:VAL:HG22	7:D:136:ARG:H	1.62	0.64
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.80	0.64
7:D:49:PRO:HA	7:D:73:VAL:HG22	1.79	0.64
6:C:115:LEU:O	6:C:118:THR:HB	1.97	0.64
39:0:9974:HOH:O	29:1:1:THR:HA	1.97	0.64
1:0:2426:G:H1'	39:0:6612:HOH:O	1.96	0.64
4:A:179:MET:HG2	4:A:186:TRP:CB	2.27	0.64
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.98	0.64
25:W:13:MET:CE	25:W:17:ILE:HG22	2.27	0.64
1:0:338:C:H4'	6:C:174:ILE:CD1	2.28	0.63
1:0:1183:C:N4	1:0:1184:C:H41	1.95	0.63
8:E:68:HIS:O	8:E:72:MET:HG3	1.98	0.63
1:0:69:A:H5'	1:0:69:A:C8	2.34	0.63
1:0:544:G:C2'	1:0:545:G:H5''	2.28	0.63
2:9:3014:G:H5'	2:9:3014:G:C8	2.32	0.63
25:W:84:VAL:HG12	39:W:6679:HOH:O	1.97	0.63
32:I:106:LYS:O	32:I:110:GLU:HG3	1.99	0.63
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.63	0.63
24:V:55:ARG:O	24:V:59:ILE:HG12	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:154:TYR:HB2	39:H:9555:HOH:O	1.97	0.63
20:R:17:MET:HE1	20:R:19:ARG:NH2	2.12	0.63
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.65	0.63
32:I:125:ALA:O	32:I:129:VAL:HG23	1.98	0.63
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.79	0.63
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.28	0.63
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.63	0.63
1:O:1201:C:H2'	1:O:1202:A:H5'	1.79	0.63
1:O:2661:U:H3	1:O:2812:A:H62	1.47	0.63
1:O:2748:G:H2'	39:O:8000:HOH:O	1.98	0.63
6:C:246:ARG:HB3	6:C:246:ARG:HH11	1.64	0.63
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.98	0.63
1:O:447:A:P	22:T:1:SER:HB2	2.39	0.63
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.32	0.63
20:R:9:ASP:O	20:R:13:THR:HB	1.99	0.63
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.64	0.63
5:B:212:GLN:CB	5:B:257:THR:HG21	2.15	0.63
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.81	0.63
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.62	0.63
1:O:2346:C:O2'	7:D:52:THR:HG21	1.97	0.62
4:A:131:HIS:O	4:A:132:ASP:HB2	1.99	0.62
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.62	0.62
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.81	0.62
1:O:291:C:H2'	1:O:292:G:O4'	1.99	0.62
5:B:102:THR:HG23	5:B:182:VAL:HG12	1.81	0.62
5:B:125:GLU:O	5:B:129:ARG:HG3	2.00	0.62
6:C:242:GLU:HG3	39:C:9185:HOH:O	1.99	0.62
12:J:74:ARG:O	12:J:78:ILE:HG12	1.99	0.62
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.82	0.62
9:F:58:GLU:HG3	9:F:61:MET:HE2	1.80	0.62
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.14	0.62
11:H:76:GLU:O	11:H:77:LEU:HD23	1.99	0.62
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.82	0.62
22:T:71:VAL:HG12	22:T:72:ILE:N	2.13	0.62
32:I:113:HIS:N	32:I:114:PRO:HD2	2.14	0.62
1:O:2507:G:H2'	1:O:2510:C:H42	1.64	0.62
11:H:166:SER:HB2	11:H:167:PRO:CD	2.29	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.62	0.62
32:I:92:PRO:C	32:I:94:GLU:H	2.06	0.62
1:O:558:C:C2'	1:O:559:U:H5''	2.30	0.62
1:O:796:A:HO2'	28:Z:10:ARG:N	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.29	0.62
12:J:19:MET:CE	12:J:132:LEU:HD11	2.27	0.62
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.79	0.62
14:L:143:THR:HG22	14:L:144:ASP:H	1.64	0.62
18:P:115:SER:N	18:P:118:GLN:HE21	1.91	0.62
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.86	0.62
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.98	0.62
1:O:834:G:H4'	1:O:835:U:OP2	2.00	0.62
21:S:77:VAL:O	21:S:80:ARG:HG2	1.99	0.62
1:O:263:U:O4'	9:F:59:ILE:HD13	1.98	0.62
4:A:179:MET:HA	4:A:179:MET:CE	2.29	0.62
12:J:39:VAL:HG13	12:J:106:GLY:O	2.00	0.62
12:J:75:PRO:HD3	12:J:136:SER:OG	1.99	0.62
1:O:2064:U:H5'	1:O:2652:U:O3'	2.00	0.62
5:B:307:ARG:HG3	5:B:307:ARG:NH1	2.07	0.62
10:G:24:VAL:O	10:G:28:GLU:HB2	1.99	0.62
22:T:47:THR:HB	22:T:100:ASP:HB3	1.80	0.62
24:V:12:THR:HG23	24:V:14:ALA:H	1.64	0.62
32:I:99:ASP:OD1	32:I:138:THR:HB	2.00	0.62
1:O:138:U:H5''	1:O:139:C:OP2	2.00	0.62
1:O:516:A:H5'	39:O:6187:HOH:O	2.00	0.62
1:O:1119:G:H22	1:O:1246:A:H2	1.43	0.62
17:O:97:SER:OG	17:O:100:GLN:HG3	2.00	0.62
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.82	0.62
1:O:553:G:P	27:Y:204:ARG:HH22	2.22	0.61
1:O:2064:U:H5'	1:O:2652:U:H4'	1.80	0.61
2:9:3029:C:H2'	2:9:3030:C:H5'	1.82	0.61
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.00	0.61
7:D:154:LYS:H	7:D:154:LYS:HD2	1.65	0.61
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.29	0.61
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.64	0.61
1:O:2676:C:H4'	12:J:70:PHE:CE1	2.35	0.61
6:C:132:ASP:HB3	39:C:9165:HOH:O	1.98	0.61
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.81	0.61
7:D:50:VAL:O	7:D:71:ALA:HA	2.00	0.61
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.46	0.61
1:O:1730:G:H5'	1:O:1731:C:C5	2.35	0.61
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.81	0.61
4:A:153:ARG:HH11	4:A:153:ARG:CB	2.12	0.61
6:C:236:THR:HG21	39:C:9177:HOH:O	1.99	0.61
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:65:THR:CG2	31:3:67:LEU:HG	2.30	0.61
4:A:36:ASP:HB2	4:A:83:GLY:HA3	1.81	0.61
5:B:41:PHE:HB3	5:B:190:MET:HE1	1.83	0.61
5:B:297:VAL:HB	39:B:9602:HOH:O	2.00	0.61
9:F:60:VAL:O	9:F:60:VAL:HG12	2.00	0.61
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.66	0.61
13:K:49:LEU:HD12	13:K:80:ILE:HG21	1.83	0.61
17:O:21:SER:OG	17:O:106:PRO:HB2	1.99	0.61
1:0:120:A:H5'	29:1:20:ARG:HH21	1.66	0.61
1:0:272:A:H5'	1:0:273:G:OP2	1.99	0.61
1:0:316:A:H5'	22:T:54:ASP:OD2	1.99	0.61
1:0:757:C:OP1	14:L:27:ARG:HD2	2.00	0.61
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.34	0.61
24:V:1:THR:HG23	24:V:2:VAL:N	2.16	0.61
1:0:1205:U:H2'	1:0:1206:U:H5''	1.81	0.61
1:0:1209:C:H2'	1:0:1210:G:H8	1.66	0.61
5:B:40:GLY:HA3	39:B:9642:HOH:O	2.00	0.61
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.31	0.61
13:K:125:ALA:C	13:K:127:ALA:H	2.08	0.61
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.00	0.61
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.15	0.61
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.73	0.61
1:0:1819:G:H2'	1:0:1820:G:H4'	1.82	0.61
1:0:2073:G:H5''	39:0:4416:HOH:O	2.00	0.61
1:0:2718:C:H6	1:0:2718:C:H5'	1.66	0.61
1:0:2807:U:P	5:B:27:ASN:HD21	2.24	0.61
39:0:8062:HOH:O	31:3:60:LYS:HG3	2.01	0.61
9:F:46:GLU:OE1	9:F:100:ASP:HA	2.01	0.61
16:N:115:VAL:HG22	39:N:9352:HOH:O	2.00	0.61
5:B:62:ARG:HA	5:B:65:MET:CE	2.30	0.61
5:B:81:ALA:O	5:B:186:GLY:HA3	2.01	0.61
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.35	0.61
15:M:107:ARG:HG3	15:M:107:ARG:NH1	2.11	0.61
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.01	0.61
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.30	0.61
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.16	0.61
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	2.00	0.61
1:0:12:U:H2'	1:0:13:G:H5'	1.83	0.60
1:0:244:C:OP2	9:F:38:LYS:HE3	2.02	0.60
1:0:775:G:OP1	29:1:16:HIS:HE1	1.84	0.60
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.36	0.60
16:N:110:THR:HB	16:N:113:SER:OG	2.01	0.60
30:2:41:HIS:HD2	30:2:44:ARG:H	1.48	0.60
1:0:506:G:H22	1:0:509:A:H5'	1.67	0.60
1:0:558:C:O2'	1:0:559:U:H5''	2.02	0.60
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.82	0.60
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.66	0.60
7:D:172:VAL:HG12	7:D:173:GLU:N	2.16	0.60
27:Y:144:ARG:HG3	27:Y:144:ARG:HH11	1.65	0.60
32:I:75:THR:HA	32:I:112:LYS:HZ3	1.66	0.60
1:0:123:U:H5'	39:0:7153:HOH:O	2.00	0.60
1:0:558:C:H2'	1:0:559:U:C5'	2.31	0.60
1:0:2851:G:H4'	5:B:157:LYS:NZ	2.16	0.60
6:C:236:THR:H	6:C:239:ALA:HB3	1.67	0.60
15:M:60:VAL:C	15:M:61:ILE:HD12	2.26	0.60
26:X:25:ARG:HD3	26:X:64:ALA:O	2.01	0.60
1:0:681:G:N3	1:0:681:G:H5'	2.17	0.60
1:0:797:A:C4'	28:Z:10:ARG:N	2.64	0.60
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.84	0.60
16:N:169:PRO:O	16:N:172:PHE:HB3	2.02	0.60
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.49	0.60
1:0:2502:C:H2'	1:0:2503:A:H5'	1.84	0.60
5:B:238:ASN:HD22	5:B:240:GLY:N	1.93	0.60
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.31	0.60
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.64	0.60
1:0:2533:C:H5'	1:0:2533:C:C6	2.35	0.60
20:R:39:THR:HG22	20:R:107:GLU:O	2.00	0.60
1:0:69:A:H5'	1:0:69:A:H8	1.67	0.59
1:0:1206:U:H2'	1:0:1207:A:O4'	2.02	0.59
1:0:1528:A:H2'	1:0:1529:G:O4'	2.02	0.59
39:0:3157:HOH:O	18:P:81:LYS:HG2	2.02	0.59
39:0:7365:HOH:O	15:M:178:LYS:HB2	2.02	0.59
32:I:134:SER:O	32:I:135:LEU:HD23	2.02	0.59
1:0:902:G:N7	14:L:18:HIS:HD2	2.00	0.59
8:E:15:GLN:HG2	8:E:19:ASP:O	2.02	0.59
1:0:485:A:N3	1:0:487:G:H5''	2.17	0.59
1:0:949:U:H4'	19:Q:95:GLU:HA	1.82	0.59
1:0:1426:C:H2'	39:0:3210:HOH:O	2.00	0.59
6:C:107:ARG:HB3	6:C:107:ARG:HH11	1.66	0.59
13:K:115:ARG:HG3	13:K:116:GLU:N	2.17	0.59
15:M:164:THR:HG22	15:M:166:ALA:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:55:VAL:HG12	13:K:56:SER:N	2.17	0.59
15:M:57:LYS:HE2	15:M:140:ALA:O	2.02	0.59
26:X:31:ILE:O	26:X:35:GLU:HG3	2.02	0.59
1:O:289:G:N2	1:O:363:A:H2	2.00	0.59
1:O:2851:G:O2'	1:O:2852:A:H5'	2.01	0.59
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.68	0.59
12:J:52:GLN:HG3	12:J:53:ILE:N	2.16	0.59
28:Z:10:ARG:HA	39:Z:9214:HOH:O	2.02	0.59
1:O:1595:G:O2'	1:O:1596:U:H5'	2.02	0.59
1:O:2565:C:H4'	39:O:5400:HOH:O	2.03	0.59
16:N:154:LEU:O	16:N:155:GLU:HB3	2.03	0.59
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.83	0.59
22:T:38:ARG:NH1	39:T:6217:HOH:O	2.36	0.59
1:O:1183:C:H2'	39:O:6764:HOH:O	2.03	0.59
4:A:36:ASP:C	4:A:38:ILE:H	2.11	0.59
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.32	0.59
8:E:102:VAL:HG11	8:E:148:ILE:HG12	1.84	0.59
23:U:17:THR:HG22	23:U:18:GLY:N	2.18	0.59
1:O:2502:C:C2'	1:O:2503:A:H5'	2.33	0.59
7:D:95:THR:OG1	7:D:174:VAL:HG22	2.03	0.59
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.31	0.59
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.85	0.59
14:L:73:VAL:HG23	14:L:74:THR:H	1.68	0.59
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.84	0.59
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.59
1:O:1766:U:O2	1:O:1778:A:H5'	2.03	0.59
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.68	0.59
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.14	0.59
1:O:538:C:OP2	27:Y:134:HIS:HE1	1.86	0.58
17:O:73:ASP:HA	17:O:92:VAL:O	2.03	0.58
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.99	0.58
25:W:130:HIS:O	25:W:136:GLY:HA3	2.04	0.58
1:O:1116:U:O2'	1:O:1118:A:C2	2.46	0.58
1:O:1201:C:H5''	39:O:6753:HOH:O	2.03	0.58
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.85	0.58
25:W:38:THR:HG22	25:W:39:ASP:N	2.18	0.58
25:W:52:VAL:HG22	25:W:53:ALA:N	2.17	0.58
1:O:2333:G:P	7:D:56:ARG:HH22	2.26	0.58
6:C:139:VAL:HG13	39:C:9248:HOH:O	2.04	0.58
8:E:7:ILE:HG22	8:E:45:ASP:O	2.03	0.58
11:H:30:GLN:H	11:H:66:ARG:NH1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.33	0.58
25:W:13:MET:HE3	25:W:17:ILE:CG2	2.33	0.58
30:2:18:ASN:HD21	30:2:40:ARG:N	1.92	0.58
1:0:1119:G:H8	12:J:52:GLN:NE2	2.01	0.58
4:A:26:ASP:OD1	4:A:26:ASP:O	2.22	0.58
5:B:162:MET:HE3	5:B:310:ARG:CD	2.33	0.58
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.32	0.58
25:W:122:ARG:HG2	25:W:122:ARG:HH11	1.69	0.58
1:0:1119:G:H8	12:J:52:GLN:HE22	1.52	0.58
4:A:194:MET:HE3	4:A:199:HIS:CB	2.34	0.58
32:I:128:VAL:C	32:I:130:GLY:H	2.11	0.58
1:0:441:A:H1'	1:0:442:A:N7	2.18	0.58
1:0:1205:U:H2'	1:0:1206:U:C5'	2.34	0.58
5:B:72:THR:HB	39:B:9602:HOH:O	2.04	0.58
9:F:13:GLU:OE2	9:F:78:GLU:HG2	2.04	0.58
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.86	0.58
1:0:1189:A:H3'	39:0:8221:HOH:O	2.04	0.58
1:0:2591:C:H2'	1:0:2592:G:O4'	2.03	0.58
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.34	0.58
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.60	0.58
5:B:102:THR:HG21	5:B:182:VAL:O	2.04	0.58
6:C:236:THR:HG22	6:C:239:ALA:CB	2.34	0.58
11:H:27:LYS:N	11:H:59:HIS:HD2	2.00	0.58
24:V:64:GLY:O	24:V:65:ASP:HB2	2.03	0.58
23:U:17:THR:CG2	23:U:18:GLY:N	2.67	0.58
1:0:1189:A:O2'	1:0:1208:C:H2'	2.04	0.57
5:B:305:ASP:O	5:B:306:LYS:HB2	2.04	0.57
17:O:39:THR:O	17:O:115:ARG:NH2	2.37	0.57
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.12	0.57
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.85	0.57
1:0:475:G:H5'	6:C:73:LEU:HD23	1.86	0.57
32:I:102:VAL:O	32:I:106:LYS:HG3	2.04	0.57
15:M:99:ARG:HH21	15:M:170:ASN:ND2	1.94	0.57
1:0:737:A:H2'	1:0:738:G:O4'	2.04	0.57
1:0:1462:C:H2'	1:0:1463:A:C8	2.40	0.57
15:M:115:LEU:HD13	15:M:116:ASN:HB2	1.86	0.57
23:U:52:THR:HG22	23:U:54:THR:N	2.19	0.57
1:0:447:A:OP2	22:T:1:SER:HB2	2.05	0.57
1:0:656:G:OP2	17:O:37:ARG:HD2	2.05	0.57
1:0:962:C:H1'	16:N:5:ARG:NH1	2.20	0.57
1:0:1943:C:H4'	4:A:211:LYS:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:158:THR:HB	11:H:159:PRO:HD3	1.87	0.57
21:S:57:THR:HG22	21:S:59:ASP:H	1.70	0.57
18:P:9:LEU:O	18:P:13:VAL:HG12	2.04	0.57
1:O:710:G:H5'	17:O:25:VAL:CG1	2.35	0.57
1:O:1634:G:H3'	39:O:4484:HOH:O	2.02	0.57
1:O:2643:G:H5''	39:O:4516:HOH:O	2.05	0.57
1:O:2644:C:O2'	1:O:2645:U:H5'	2.04	0.57
6:C:142:ASP:CG	6:C:237:GLU:HB3	2.30	0.57
16:N:132:ASN:O	16:N:135:VAL:HG12	2.04	0.57
22:T:40:VAL:HG22	22:T:41:ARG:N	2.20	0.57
26:X:25:ARG:HG2	39:X:5356:HOH:O	2.03	0.57
1:O:90:A:H2'	1:O:91:G:O4'	2.04	0.57
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.18	0.57
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.34	0.57
1:O:475:G:OP1	6:C:73:LEU:HD22	2.04	0.57
1:O:1853:C:OP1	4:A:231:LYS:HG3	2.05	0.57
4:A:52:SER:HB2	4:A:164:ARG:HH11	1.70	0.57
5:B:62:ARG:HA	5:B:65:MET:HE2	1.87	0.57
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.34	0.57
1:O:1625:U:H4'	39:O:5235:HOH:O	2.03	0.56
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.87	0.56
1:O:20:G:H21	20:R:117:HIS:HD2	1.53	0.56
1:O:1377:C:H5'	1:O:1377:C:C6	2.40	0.56
1:O:2103:A:H5'	1:O:2103:A:H8	1.70	0.56
32:I:138:THR:HG22	32:I:139:ILE:H	1.69	0.56
1:O:1878:G:O2'	1:O:1879:U:OP2	2.23	0.56
1:O:2645:U:C6	1:O:2645:U:OP2	2.58	0.56
1:O:2649:A:H5'	1:O:2649:A:H8	1.69	0.56
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.70	0.56
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.38	0.56
5:B:145:HIS:HD2	5:B:146:THR:O	1.89	0.56
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.19	0.56
6:C:16:VAL:HG12	6:C:17:ASP:H	1.70	0.56
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.23	0.56
24:V:39:ALA:C	24:V:41:GLU:H	2.13	0.56
32:I:75:THR:OG1	32:I:112:LYS:HE2	2.05	0.56
32:I:138:THR:HG22	32:I:139:ILE:N	2.20	0.56
1:O:343:C:O2'	1:O:344:C:H5'	2.05	0.56
1:O:1159:G:H1	1:O:1208:C:H42	1.53	0.56
1:O:1701:A:H4'	1:O:1702:U:C5'	2.35	0.56
1:O:2081:A:H4'	12:J:69:TYR:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.87	0.56
32:I:129:VAL:O	32:I:129:VAL:HG12	2.05	0.56
1:O:1333:U:H2'	1:O:1334:C:C6	2.41	0.56
1:O:1552:G:N2	1:O:1634:G:H1'	2.20	0.56
7:D:99:ASP:HB3	7:D:101:THR:H	1.71	0.56
15:M:107:ARG:NH1	39:M:9384:HOH:O	2.38	0.56
22:T:89:ARG:HG3	22:T:89:ARG:O	2.06	0.56
1:O:88:G:H2'	1:O:89:G:C8	2.40	0.56
1:O:1165:G:H4'	1:O:1174:A:HO2'	1.70	0.56
1:O:1787:C:OP1	18:P:68:LYS:HE2	2.06	0.56
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.35	0.56
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.06	0.56
1:O:2795:C:O2'	1:O:2796:U:H5'	2.06	0.56
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.88	0.56
1:O:2505:G:O2'	1:O:2506:A:H5'	2.06	0.56
4:A:105:VAL:HG12	4:A:106:CYS:N	2.21	0.56
25:W:122:ARG:HH22	25:W:154:ARG:HG2	1.71	0.56
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.41	0.56
1:O:1979:G:O2'	1:O:1980:U:OP1	2.21	0.56
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.21	0.56
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.21	0.56
18:P:40:VAL:O	18:P:44:VAL:HG23	2.06	0.56
1:O:248:A:H5'	1:O:249:G:OP2	2.06	0.56
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.30	0.56
27:Y:154:ARG:HB3	27:Y:154:ARG:HH11	1.71	0.56
1:O:185:G:H4'	1:O:186:A:H4'	1.87	0.55
1:O:1555:G:H4'	1:O:1630:A:H2	1.71	0.55
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.41	0.55
1:O:1118:A:H8	1:O:1119:G:H5'	1.71	0.55
27:Y:112:GLU:HA	27:Y:112:GLU:OE1	2.06	0.55
1:O:2837:U:H2'	39:O:7329:HOH:O	2.06	0.55
9:F:57:GLU:O	9:F:61:MET:HG3	2.07	0.55
1:O:894:A:N1	6:C:87:ARG:NH2	2.54	0.55
1:O:2866:U:H4'	1:O:2867:G:H5'	1.87	0.55
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.87	0.55
5:B:156:LYS:HE2	39:B:9627:HOH:O	2.05	0.55
8:E:84:MET:HE2	8:E:133:VAL:CG2	2.35	0.55
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.18	0.55
13:K:23:ASN:HD21	13:K:107:THR:HB	1.71	0.55
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.06	0.55
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.89	0.55
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.22	0.55
1:O:2670:G:O2'	1:O:2671:U:H5'	2.07	0.55
4:A:113:GLY:HA2	4:A:153:ARG:NH2	2.21	0.55
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.88	0.55
16:N:162:ASP:HA	39:N:9329:HOH:O	2.07	0.55
1:O:1187:U:O2'	1:O:1189:A:H2	1.90	0.55
1:O:2338:G:OP1	7:D:97:GLN:HG2	2.06	0.55
5:B:185:GLY:HA2	39:B:9630:HOH:O	2.07	0.55
7:D:138:GLY:N	39:D:7597:HOH:O	2.38	0.55
11:H:170:ASN:N	11:H:170:ASN:ND2	2.52	0.55
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.54	0.55
32:I:75:THR:HA	32:I:112:LYS:NZ	2.22	0.55
32:I:112:LYS:C	32:I:114:PRO:HD2	2.31	0.55
1:O:2827:A:H2'	1:O:2828:G:O4'	2.07	0.55
2:9:3054:A:H2	39:9:3535:HOH:O	1.88	0.55
5:B:85:ARG:NH1	39:B:9631:HOH:O	2.39	0.55
12:J:93:ARG:HB3	12:J:93:ARG:NH1	2.18	0.55
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.05	0.55
1:O:558:C:H2'	1:O:559:U:H5'	1.89	0.55
1:O:2521:A:OP2	11:H:3:ALA:HB3	2.07	0.55
7:D:59:GLY:O	7:D:61:PHE:N	2.40	0.55
11:H:63:GLU:HA	39:H:9544:HOH:O	2.07	0.55
12:J:47:THR:HG22	12:J:48:GLY:N	2.22	0.55
13:K:75:ARG:HD3	13:K:112:PRO:O	2.06	0.55
19:Q:75:ILE:HD13	19:Q:84:ILE:HD11	1.89	0.55
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.88	0.55
22:T:71:VAL:HG13	22:T:91:LEU:O	2.07	0.55
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.89	0.55
1:O:2896:A:N3	1:O:2896:A:H2'	2.23	0.55
4:A:89:ALA:HB3	39:A:9613:HOH:O	2.07	0.55
9:F:91:VAL:CG1	9:F:92:GLY:H	2.07	0.55
25:W:13:MET:HE2	25:W:18:GLN:N	2.22	0.55
26:X:30:MET:HE1	26:X:58:ALA:CB	2.30	0.55
29:I:25:LYS:CD	30:2:49:GLU:H	2.20	0.55
32:I:75:THR:HG22	32:I:79:ILE:HD11	1.88	0.55
1:O:162:C:H2'	1:O:163:U:H5'	1.89	0.54
6:C:140:VAL:HB	39:C:9251:HOH:O	2.04	0.54
7:D:103:ASN:ND2	7:D:134:LEU:H	2.04	0.54
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.06	0.54
20:R:106:GLY:HA2	20:R:109:MET:CE	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:25:LYS:HE2	39:2:7213:HOH:O	2.07	0.54
1:0:1406:A:H4'	1:0:1407:A:H5''	1.89	0.54
1:0:2769:C:C2'	1:0:2770:G:H5'	2.37	0.54
2:9:3064:C:H2'	2:9:3065:A:H5'	1.89	0.54
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.70	0.54
9:F:107:ASP:O	9:F:111:ILE:HG13	2.07	0.54
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.32	0.54
14:L:35:ARG:C	14:L:35:ARG:HD3	2.32	0.54
18:P:103:THR:O	18:P:107:GLU:HG3	2.06	0.54
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.42	0.54
1:0:830:G:O2'	1:0:831:U:H5'	2.08	0.54
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.89	0.54
18:P:141:ILE:C	18:P:143:ALA:H	2.15	0.54
22:T:115:GLU:HG3	22:T:116:ASP:N	2.22	0.54
1:0:1163:G:H2'	1:0:1164:U:C5	2.42	0.54
1:0:2480:G:H3'	39:0:4767:HOH:O	2.08	0.54
1:0:656:G:H5'	17:O:3:THR:HB	1.90	0.54
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.08	0.54
1:0:1667:A:H5'	1:0:1667:A:C8	2.35	0.54
1:0:1838:U:O2'	1:0:2644:C:H5'	2.08	0.54
21:S:57:THR:HG22	21:S:59:ASP:N	2.22	0.54
32:I:102:VAL:HG23	32:I:140:GLU:O	2.08	0.54
1:0:1687:C:O2	29:1:9:GLY:HA2	2.08	0.54
1:0:2563:U:H2'	1:0:2565:C:O5'	2.08	0.54
2:9:3050:G:H5''	16:N:159:TYR:HE1	1.73	0.54
2:9:3057:A:C8	7:D:141:VAL:HG21	2.42	0.54
5:B:137:LEU:HD21	5:B:140:LEU:HD21	1.90	0.54
11:H:76:GLU:C	11:H:77:LEU:HD23	2.33	0.54
18:P:16:VAL:HG12	18:P:17:GLY:N	2.21	0.54
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.37	0.54
26:X:43:VAL:HG12	26:X:44:ASP:N	2.22	0.54
1:0:1666:C:H2'	1:0:1667:A:C5'	2.37	0.54
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.88	0.54
1:0:2481:G:H5''	39:0:5116:HOH:O	2.07	0.54
6:C:79:ARG:O	6:C:87:ARG:HG2	2.07	0.54
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.89	0.54
8:E:69:ILE:HA	8:E:72:MET:HE3	1.89	0.54
10:G:20:VAL:O	10:G:24:VAL:HG23	2.08	0.54
15:M:182:LYS:O	15:M:194:ALA:HB2	2.08	0.54
20:R:44:VAL:O	20:R:48:GLU:HG3	2.08	0.54
1:0:2649:A:H5'	1:0:2649:A:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:246:ARG:NH1	39:C:9173:HOH:O	2.39	0.54
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.90	0.54
9:F:77:VAL:HG21	9:F:83:LEU:HD13	1.89	0.54
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.40	0.54
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.90	0.54
25:W:26:ILE:O	25:W:26:ILE:HG13	2.07	0.54
1:O:475:G:C5'	6:C:73:LEU:HD23	2.38	0.54
1:O:1751:G:C2'	1:O:1752:G:H5''	2.36	0.54
1:O:2821:C:H4'	5:B:116:PRO:HG3	1.90	0.54
5:B:25:ARG:HA	5:B:310:ARG:HH21	1.72	0.54
5:B:96:PRO:HG3	39:B:9631:HOH:O	2.07	0.54
11:H:66:ARG:HD3	39:H:9544:HOH:O	2.08	0.54
30:2:36:ASN:HB3	30:2:39:ARG:NE	2.23	0.54
32:I:139:ILE:HG22	32:I:140:GLU:N	2.22	0.54
1:O:1418:U:OP1	30:2:42:TRP:HB3	2.08	0.54
6:C:218:VAL:HG12	39:C:9225:HOH:O	2.07	0.54
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.90	0.54
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.90	0.54
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.48	0.54
1:O:949:U:O2'	19:Q:40:HIS:HE1	1.92	0.53
8:E:84:MET:HE2	8:E:133:VAL:HG23	1.90	0.53
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.23	0.53
30:2:41:HIS:CD2	30:2:44:ARG:H	2.26	0.53
1:O:171:C:OP2	15:M:84:LYS:HG3	2.08	0.53
1:O:545:G:H5'	1:O:545:G:C8	2.41	0.53
1:O:926:A:H5'	14:L:39:GLU:OE2	2.08	0.53
1:O:2694:A:H4'	8:E:91:PHE:CE1	2.43	0.53
2:9:3049:G:O2'	2:9:3050:G:H5'	2.07	0.53
7:D:135:VAL:HG22	7:D:136:ARG:N	2.23	0.53
7:D:166:ILE:HB	39:D:6326:HOH:O	2.08	0.53
16:N:77:ASN:OD1	16:N:79:PRO:HD2	2.08	0.53
1:O:1120:U:H5''	1:O:1120:U:C6	2.43	0.53
1:O:2032:U:H2'	1:O:2033:G:C5'	2.37	0.53
14:L:80:ASP:HB2	14:L:90:ARG:O	2.08	0.53
22:T:69:LYS:O	22:T:71:VAL:HG23	2.09	0.53
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.89	0.53
1:O:1878:G:H4'	39:O:4700:HOH:O	2.08	0.53
1:O:2015:A:H2'	1:O:2016:U:O4'	2.08	0.53
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.91	0.53
6:C:214:THR:HG23	39:C:9238:HOH:O	2.09	0.53
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.23	0.53
1:O:299:U:H5'	39:O:7810:HOH:O	2.08	0.53
1:O:1789:G:O6	18:P:73:HIS:HE1	1.91	0.53
1:O:1878:G:O2'	1:O:1879:U:C6	2.59	0.53
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.44	0.53
1:O:308:U:H5'	22:T:97:ARG:NH2	2.23	0.53
1:O:1384:C:H5'	26:X:30:MET:HG2	1.89	0.53
12:J:130:VAL:HG12	12:J:131:THR:N	2.24	0.53
17:O:25:VAL:HG23	17:O:26:TRP:N	2.24	0.53
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	2.09	0.53
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.66	0.53
1:O:625:U:H5''	1:O:1044:C:N4	2.24	0.53
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.38	0.53
6:C:25:PRO:HG2	39:C:9122:HOH:O	2.08	0.53
8:E:69:ILE:HA	8:E:72:MET:CE	2.39	0.53
13:K:30:LYS:O	13:K:55:VAL:HG13	2.08	0.53
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.07	0.53
24:V:29:ASN:O	24:V:33:VAL:HG23	2.09	0.53
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.90	0.53
1:O:870:G:OP2	4:A:3:ARG:HD3	2.09	0.53
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.91	0.53
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.39	0.53
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.91	0.53
1:O:449:A:N7	6:C:43:LYS:HG2	2.23	0.53
1:O:776:A:OP1	29:1:28:HIS:HE1	1.92	0.53
1:O:1205:U:C2'	1:O:1206:U:H5''	2.38	0.53
1:O:1730:G:C5'	1:O:1731:C:C6	2.92	0.53
1:O:1981:A:H1'	1:O:1983:C:N4	2.24	0.53
7:D:25:MET:CE	7:D:37:ALA:HB1	2.38	0.53
7:D:172:VAL:HG12	7:D:173:GLU:H	1.74	0.53
8:E:15:GLN:NE2	8:E:40:VAL:O	2.41	0.53
9:F:46:GLU:O	9:F:73:PRO:HD2	2.08	0.53
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.05	0.53
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.08	0.53
39:O:7264:HOH:O	16:N:4:PRO:HD2	2.08	0.53
8:E:11:VAL:HG12	8:E:12:ASP:N	2.23	0.53
17:O:15:LYS:HD3	17:O:19:ARG:NH2	2.23	0.53
17:O:87:THR:O	17:O:91:GLN:HG3	2.08	0.53
1:O:137:U:H2'	1:O:139:C:C5	2.44	0.52
1:O:151:A:H2'	1:O:152:A:O4'	2.09	0.52
1:O:653:C:H2'	1:O:654:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1328:A:C8	27:Y:169:ARG:HD3	2.44	0.52
1:0:1730:G:H5''	1:0:1731:C:H6	1.75	0.52
1:0:1942:A:H3'	39:0:7817:HOH:O	2.08	0.52
39:0:6869:HOH:O	4:A:205:GLY:HA3	2.09	0.52
5:B:41:PHE:CG	5:B:79:MET:HE2	2.44	0.52
5:B:148:PRO:HB3	5:B:156:LYS:HG2	1.90	0.52
16:N:32:PRO:HD2	16:N:99:GLU:O	2.10	0.52
16:N:33:ARG:NH1	16:N:103:ASP:OD2	2.41	0.52
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.39	0.52
1:0:603:A:H5''	1:0:604:G:OP1	2.08	0.52
6:C:2:GLN:HB3	39:C:9188:HOH:O	2.07	0.52
7:D:51:ARG:HD3	39:D:7636:HOH:O	2.09	0.52
26:X:20:GLU:HG3	26:X:21:PRO:HD2	1.90	0.52
1:0:95:A:H5''	1:0:97:G:O4'	2.10	0.52
1:0:1506:U:H6	1:0:1506:U:H5'	1.74	0.52
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.10	0.52
7:D:146:LYS:NZ	16:N:107:ASN:HD21	2.07	0.52
39:9:5071:HOH:O	16:N:23:ARG:HD3	2.09	0.52
17:O:32:ARG:HH21	17:O:35:LYS:NZ	2.08	0.52
1:0:2769:C:H2'	1:0:2770:G:O4'	2.09	0.52
4:A:223:ARG:NE	39:A:9561:HOH:O	2.41	0.52
6:C:107:ARG:HH11	6:C:107:ARG:CB	2.22	0.52
7:D:13:MET:HA	7:D:137:PRO:HG2	1.91	0.52
11:H:28:ILE:HG23	39:H:9544:HOH:O	2.08	0.52
12:J:70:PHE:CG	12:J:70:PHE:O	2.63	0.52
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.19	0.52
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.90	0.52
16:N:67:ALA:HA	16:N:71:TRP:HB3	1.89	0.52
18:P:64:GLU:HG2	39:P:163:HOH:O	2.09	0.52
1:0:164:G:H4'	14:L:30:ARG:HD3	1.91	0.52
1:0:1119:G:N2	1:0:1246:A:N1	2.57	0.52
1:0:2320:U:H4'	1:0:2321:A:O4'	2.10	0.52
39:0:9697:HOH:O	5:B:214:PRO:HD2	2.09	0.52
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.58	0.52
12:J:42:GLU:O	12:J:131:THR:HG23	2.10	0.52
15:M:24:GLN:O	15:M:28:GLN:HG3	2.10	0.52
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.17	0.52
1:0:316:A:N3	1:0:336:G:O2'	2.40	0.52
1:0:2824:C:H5''	1:0:2825:C:H5'	1.91	0.52
2:9:3049:G:H5''	39:9:4707:HOH:O	2.09	0.52
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.36	0.52
25:W:4:LEU:O	25:W:32:CYS:HA	2.09	0.52
25:W:5:VAL:O	25:W:52:VAL:HG23	2.09	0.52
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.90	0.52
1:0:241:A:C2	1:0:378:A:H4'	2.45	0.52
1:0:2072:G:H4'	39:0:4390:HOH:O	2.10	0.52
4:A:105:VAL:HG13	4:A:155:THR:O	2.10	0.52
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.90	0.52
8:E:93:MET:HE1	8:E:165:GLY:N	2.25	0.52
14:L:72:ASN:HB2	39:L:9479:HOH:O	2.10	0.52
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.92	0.52
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.10	0.52
1:0:470:U:O2'	29:1:16:HIS:CD2	2.60	0.52
1:0:2419:U:H5''	1:0:2420:G:H5'	1.91	0.52
4:A:94:LEU:HD23	4:A:94:LEU:N	2.25	0.52
11:H:148:GLU:OE1	11:H:148:GLU:HA	2.10	0.52
1:0:1189:A:H1'	1:0:1209:C:C1'	2.40	0.52
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.09	0.52
39:0:6800:HOH:O	27:Y:158:LYS:HD3	2.10	0.52
2:9:3004:G:H21	16:N:44:ARG:NH1	2.08	0.52
13:K:14:LYS:HG3	13:K:32:ILE:O	2.09	0.52
22:T:41:ARG:HG2	22:T:41:ARG:NH1	2.25	0.52
1:0:380:A:H2'	39:0:7710:HOH:O	2.10	0.51
1:0:848:C:H5'	39:0:7752:HOH:O	2.10	0.51
1:0:1250:C:O2'	1:0:1251:C:H5'	2.10	0.51
1:0:2748:G:H1'	39:0:8436:HOH:O	2.09	0.51
4:A:36:ASP:O	4:A:38:ILE:N	2.43	0.51
1:0:2769:C:O2'	1:0:2770:G:H5'	2.10	0.51
1:0:2815:G:N7	12:J:80:LYS:NZ	2.56	0.51
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.92	0.51
14:L:97:VAL:HG12	14:L:98:GLU:O	2.10	0.51
14:L:148:GLU:HB2	39:L:9487:HOH:O	2.09	0.51
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.09	0.51
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.76	0.51
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.93	0.51
1:0:1441:G:O2'	1:0:1442:A:H5'	2.10	0.51
4:A:164:ARG:CZ	39:A:9577:HOH:O	2.58	0.51
10:G:12:ILE:N	10:G:13:PRO:CD	2.73	0.51
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.10	0.51
1:0:524:A:H5''	20:R:29:LYS:HD3	1.92	0.51
1:0:926:A:O2'	14:L:41:HIS:HD2	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1164:U:OP1	32:I:74:PRO:HA	2.10	0.51
1:0:2103:A:H5'	1:0:2103:A:C8	2.45	0.51
1:0:2717:C:O2'	1:0:2718:C:H5''	2.10	0.51
4:A:210:GLY:N	39:A:9576:HOH:O	2.42	0.51
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.39	0.51
32:I:93:GLN:HA	32:I:96:PHE:CE2	2.44	0.51
1:0:1218:U:H2'	1:0:1219:U:C6	2.45	0.51
1:0:2508:C:H2'	39:O:7246:HOH:O	2.10	0.51
2:9:3114:G:O6	16:N:11:ARG:HD3	2.11	0.51
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.92	0.51
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.44	0.51
7:D:94:ALA:HA	7:D:174:VAL:HA	1.92	0.51
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.26	0.51
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.92	0.51
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.93	0.51
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.93	0.51
1:0:1503:U:H2'	1:0:1504:A:O4'	2.09	0.51
1:0:2779:G:H21	8:E:143:GLN:NE2	2.08	0.51
2:9:3064:C:C2'	2:9:3065:A:H5'	2.39	0.51
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.39	0.51
14:L:134:GLU:HG3	39:L:9453:HOH:O	2.10	0.51
22:T:40:VAL:HG22	22:T:41:ARG:H	1.75	0.51
1:0:317:A:OP1	22:T:52:ARG:O	2.29	0.51
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.93	0.51
17:O:98:LEU:O	17:O:102:ILE:HG13	2.11	0.51
25:W:122:ARG:NH2	39:W:5817:HOH:O	2.43	0.51
1:0:2414:A:H2'	1:0:2415:A:C8	2.46	0.51
5:B:17:LYS:O	5:B:260:HIS:HD2	1.93	0.51
6:C:154:VAL:O	6:C:158:GLU:HG3	2.11	0.51
1:0:482:G:H4'	1:0:508:A:N1	2.26	0.51
1:0:920:C:H4'	1:0:921:G:C2	2.46	0.51
1:0:1180:U:H2'	1:0:1181:A:C8	2.46	0.51
1:0:2524:G:H21	1:0:2526:C:N4	2.08	0.51
2:9:3024:U:H3'	2:9:3025:G:H5'	1.92	0.51
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.41	0.51
4:A:128:LEU:HD21	4:A:131:HIS:HE1	1.75	0.51
25:W:119:HIS:HD2	25:W:120:PRO:O	1.94	0.51
31:3:3:MET:O	31:3:90:PHE:HA	2.11	0.51
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.75	0.51
39:9:4707:HOH:O	16:N:147:ILE:HB	2.11	0.51
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.38	0.51
7:D:25:MET:SD	7:D:40:ILE:HD11	2.51	0.51
12:J:130:VAL:HG12	12:J:131:THR:H	1.76	0.51
22:T:61:GLU:HG3	39:T:3851:HOH:O	2.11	0.51
23:U:49:LEU:HG	39:U:3805:HOH:O	2.10	0.51
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.09	0.51
1:0:542:A:H2'	1:0:543:G:O4'	2.11	0.50
1:0:2541:U:O2	3:4:77:HFA:HA	2.10	0.50
1:0:2726:U:O2	1:0:2749:U:O5'	2.28	0.50
11:H:116:ALA:O	11:H:117:PHE:C	2.55	0.50
14:L:145:LEU:HD23	14:L:145:LEU:O	2.11	0.50
7:D:56:ARG:N	39:D:6752:HOH:O	2.44	0.50
21:S:57:THR:CG2	21:S:58:MET:N	2.74	0.50
1:0:196:G:H2'	39:0:7154:HOH:O	2.10	0.50
1:0:969:G:H1	1:0:999:C:H42	1.58	0.50
1:0:2541:U:H5'	39:0:3027:HOH:O	2.11	0.50
2:9:3051:A:H5'	16:N:160:SER:CB	2.39	0.50
4:A:109:GLU:HG2	4:A:116:GLY:N	2.26	0.50
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.41	0.50
1:0:2361:A:H2'	1:0:2362:A:C8	2.45	0.50
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.80	0.50
14:L:129:ALA:O	14:L:133:VAL:HG23	2.11	0.50
16:N:11:ARG:O	16:N:15:GLU:HG3	2.11	0.50
26:X:7:GLU:HA	26:X:74:ALA:O	2.11	0.50
32:I:100:LEU:O	32:I:139:ILE:HG23	2.10	0.50
1:0:558:C:H2'	1:0:559:U:H5''	1.92	0.50
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.75	0.50
9:F:117:GLU:C	9:F:119:ARG:H	2.18	0.50
1:0:1626:A:H2'	1:0:1627:G:O4'	2.11	0.50
1:0:2883:A:H2'	1:0:2884:G:O4'	2.12	0.50
5:B:243:ASN:HA	5:B:244:PRO:C	2.35	0.50
6:C:236:THR:HA	39:C:9251:HOH:O	2.10	0.50
12:J:131:THR:HG22	12:J:134:GLU:H	1.75	0.50
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.41	0.50
1:0:1166:A:H61	1:0:1180:U:H3	1.59	0.50
1:0:1476:A:O2'	1:0:1477:C:H5'	2.12	0.50
1:0:1527:A:H1'	1:0:1528:A:C8	2.47	0.50
39:0:3173:HOH:O	25:W:119:HIS:HE1	1.94	0.50
4:A:135:VAL:HG11	4:A:147:ARG:NH1	2.27	0.50
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.92	0.50
11:H:58:ARG:HH11	11:H:58:ARG:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.26	0.50
15:M:78:LYS:HD3	39:M:9447:HOH:O	2.11	0.50
21:S:33:SER:O	21:S:37:VAL:HG23	2.12	0.50
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.87	0.50
1:0:1406:A:H4'	1:0:1407:A:C5'	2.41	0.50
4:A:53:ALA:HB3	39:A:9596:HOH:O	2.12	0.50
12:J:45:VAL:HG22	12:J:46:ILE:N	2.26	0.50
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.93	0.50
21:S:57:THR:HG22	21:S:58:MET:N	2.26	0.50
1:0:119:A:H2'	1:0:120:A:H5''	1.93	0.50
1:0:407:A:H2'	1:0:408:A:C8	2.47	0.50
1:0:793:A:H5''	18:P:83:LYS:HG2	1.94	0.50
1:0:1299:G:H5'	39:0:4657:HOH:O	2.11	0.50
1:0:2768:A:O2'	1:0:2769:C:H5'	2.12	0.50
39:0:4807:HOH:O	30:2:38:LYS:HE3	2.12	0.50
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.12	0.50
5:B:234:ARG:HB3	5:B:234:ARG:HH11	1.76	0.50
8:E:85:GLU:HG3	8:E:169:THR:OG1	2.12	0.50
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.93	0.50
12:J:74:ARG:HH11	12:J:74:ARG:CB	2.22	0.50
19:Q:11:ARG:HD3	39:Q:5620:HOH:O	2.10	0.50
20:R:114:VAL:HA	20:R:144:GLU:O	2.12	0.50
25:W:5:VAL:HG11	25:W:153:MET:HE1	1.92	0.50
32:I:80:LYS:HD3	32:I:86:GLU:O	2.12	0.50
1:0:204:A:C2'	1:0:205:U:H5'	2.42	0.49
1:0:432:G:O2'	1:0:433:C:H5'	2.12	0.49
1:0:603:A:H1'	1:0:605:C:C2	2.47	0.49
1:0:1972:U:H2'	1:0:1973:A:C5'	2.42	0.49
1:0:2812:A:C2	1:0:2814:A:N6	2.69	0.49
5:B:42:ALA:HB2	5:B:162:MET:HE2	1.94	0.49
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.42	0.49
24:V:1:THR:CG2	24:V:2:VAL:H	2.14	0.49
32:I:113:HIS:N	32:I:114:PRO:CD	2.75	0.49
1:0:1730:G:C5'	1:0:1731:C:H6	2.24	0.49
1:0:2456:A:H2'	1:0:2457:U:C6	2.48	0.49
2:9:3039:U:HO2'	2:9:3042:C:H5	1.52	0.49
5:B:254:GLN:HG3	39:B:9532:HOH:O	2.12	0.49
5:B:264:GLU:CG	5:B:267:LYS:HE2	2.36	0.49
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.43	0.49
22:T:20:HIS:HB3	22:T:41:ARG:HD2	1.94	0.49
25:W:65:VAL:HA	25:W:68:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:55:VAL:HG22	39:3:9444:HOH:O	2.11	0.49
1:0:960:G:N3	1:0:960:G:H2'	2.25	0.49
4:A:132:ASP:OD1	4:A:133:ARG:N	2.45	0.49
6:C:246:ARG:NE	39:C:9225:HOH:O	2.35	0.49
7:D:36:ASN:HA	39:D:7500:HOH:O	2.12	0.49
11:H:27:LYS:H	11:H:59:HIS:CD2	2.23	0.49
13:K:13:GLU:OE1	13:K:44:LEU:HD12	2.12	0.49
26:X:20:GLU:HG3	26:X:21:PRO:CD	2.42	0.49
1:0:558:C:C2'	1:0:559:U:C5'	2.90	0.49
1:0:794:U:H3	1:0:819:A:H61	1.59	0.49
4:A:194:MET:HE3	4:A:199:HIS:HB2	1.92	0.49
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.95	0.49
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.77	0.49
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.76	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
1:0:1118:A:C8	1:0:1118:A:C3'	2.91	0.49
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.95	0.49
25:W:64:THR:O	25:W:68:THR:HG22	2.13	0.49
1:0:1163:G:H5'	32:I:115:ASP:O	2.12	0.49
1:0:1946:C:H2'	1:0:1971:G:C8	2.48	0.49
1:0:2852:A:H5''	39:0:5781:HOH:O	2.13	0.49
6:C:98:ARG:NH1	39:C:9158:HOH:O	2.46	0.49
24:V:12:THR:HG23	24:V:14:ALA:N	2.26	0.49
25:W:88:THR:CG2	25:W:89:ASP:H	2.20	0.49
1:0:1921:A:O2'	1:0:1922:A:H5'	2.12	0.49
1:0:2568:A:H2'	1:0:2569:A:O4'	2.13	0.49
2:9:3028:U:H2'	2:9:3029:C:C6	2.47	0.49
2:9:3041:C:C6	7:D:50:VAL:HG21	2.47	0.49
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.95	0.49
10:G:64:ASN:HD22	10:G:64:ASN:N	2.09	0.49
12:J:19:MET:CE	12:J:132:LEU:HD21	2.43	0.49
1:0:1666:C:C2'	1:0:1667:A:C5'	2.91	0.49
8:E:84:MET:HG2	8:E:168:ILE:HD13	1.95	0.49
20:R:122:GLN:HB3	20:R:138:SER:HB2	1.93	0.49
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.76	0.49
24:V:64:GLY:O	24:V:65:ASP:CB	2.61	0.49
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.92	0.49
27:Y:212:ARG:HD2	39:Y:9395:HOH:O	2.12	0.49
1:0:256:C:H2'	1:0:257:G:O4'	2.12	0.49
1:0:602:A:O2'	1:0:605:C:H4'	2.12	0.49
1:0:625:U:H5'	39:0:3785:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1666:C:C2'	1:0:1667:A:H5''	2.43	0.49
9:F:21:GLU:O	9:F:24:ARG:HG3	2.13	0.49
22:T:38:ARG:NH1	22:T:38:ARG:HG3	2.26	0.49
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.27	0.49
26:X:18:ARG:NH1	39:X:4132:HOH:O	2.42	0.49
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.93	0.49
1:0:155:C:OP2	15:M:188:ARG:HD3	2.12	0.49
1:0:462:A:C2	30:2:37:HIS:HB3	2.48	0.49
1:0:1172:G:H1'	39:0:5534:HOH:O	2.13	0.49
1:0:1198:U:H2'	1:0:1200:A:OP2	2.12	0.49
1:0:1218:U:H2'	1:0:1219:U:H6	1.78	0.49
1:0:1786:C:OP1	18:P:74:GLN:HG2	2.13	0.49
18:P:125:LYS:HB3	18:P:130:GLU:HG3	1.94	0.49
1:0:500:G:H21	20:R:98:ASN:HD21	1.60	0.48
1:0:951:A:C2'	1:0:952:G:H5'	2.42	0.48
1:0:1209:C:H2'	1:0:1210:G:C8	2.47	0.48
1:0:2768:A:H2'	1:0:2769:C:O4'	2.13	0.48
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.95	0.48
11:H:30:GLN:H	11:H:66:ARG:HH11	1.59	0.48
11:H:63:GLU:O	11:H:67:LEU:HB2	2.13	0.48
12:J:76:ASP:HA	39:J:5907:HOH:O	2.13	0.48
27:Y:115:ARG:HB3	27:Y:115:ARG:HH11	1.78	0.48
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.13	0.48
1:0:1119:G:C8	12:J:52:GLN:NE2	2.81	0.48
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.94	0.48
1:0:1753:C:O2	5:B:229:ARG:NH2	2.40	0.48
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.14	0.48
1:0:2626:C:H2'	1:0:2627:G:C8	2.48	0.48
2:9:3006:C:H5''	16:N:37:ARG:HE	1.78	0.48
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.39	0.48
1:0:1667:A:H2'	1:0:1668:U:C6	2.48	0.48
4:A:129:LEU:CD1	4:A:145:MET:HE1	2.43	0.48
5:B:301:VAL:HG11	5:B:309:VAL:HG11	1.95	0.48
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.43	0.48
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.46	0.48
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.95	0.48
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.13	0.48
26:X:41:PHE:O	26:X:43:VAL:HG23	2.13	0.48
1:0:21:G:H4'	20:R:2:ILE:HG22	1.93	0.48
1:0:447:A:O2'	1:0:448:G:H5'	2.14	0.48
1:0:629:A:H2'	1:0:630:A:O4'	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1192:A:H3'	1:0:1193:A:H5'	1.95	0.48
4:A:194:MET:CE	4:A:199:HIS:HB2	2.42	0.48
8:E:6:GLU:HA	8:E:46:THR:HG22	1.94	0.48
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.34	0.48
29:1:25:LYS:HG3	30:2:49:GLU:H	1.78	0.48
31:3:65:THR:HG22	31:3:67:LEU:HG	1.95	0.48
1:0:319:A:H4'	1:0:338:C:C5	2.48	0.48
1:0:1183:C:H5	1:0:1192:A:OP1	1.97	0.48
1:0:2472:C:O2'	1:0:2634:G:H4'	2.13	0.48
1:0:2866:U:C4	23:U:50:GLU:HB3	2.49	0.48
5:B:41:PHE:HA	5:B:79:MET:CE	2.43	0.48
10:G:12:ILE:HD12	39:G:692:HOH:O	2.13	0.48
17:O:32:ARG:HH21	17:O:35:LYS:HZ1	1.59	0.48
22:T:71:VAL:CG1	22:T:72:ILE:N	2.76	0.48
25:W:122:ARG:NH1	25:W:152:ALA:O	2.46	0.48
1:0:588:G:O6	25:W:154:ARG:NH1	2.47	0.48
1:0:932:U:H2'	1:0:933:C:C6	2.49	0.48
2:9:3091:C:H2'	2:9:3092:G:O4'	2.13	0.48
4:A:206:ARG:NH1	39:A:9499:HOH:O	2.47	0.48
15:M:98:GLN:O	15:M:102:GLU:HG3	2.13	0.48
17:O:25:VAL:HG23	17:O:26:TRP:H	1.79	0.48
20:R:132:ARG:CZ	39:R:9497:HOH:O	2.61	0.48
22:T:23:VAL:HG23	22:T:41:ARG:HG3	1.94	0.48
1:0:447:A:OP1	22:T:2:LYS:HG2	2.14	0.48
6:C:233:THR:HG22	6:C:234:VAL:N	2.28	0.48
10:G:16:LYS:O	10:G:20:VAL:HG23	2.14	0.48
12:J:88:PRO:O	12:J:94:GLY:HA3	2.14	0.48
14:L:145:LEU:HD23	14:L:145:LEU:C	2.38	0.48
22:T:19:ARG:HD3	22:T:67:LEU:O	2.14	0.48
23:U:9:CYS:O	23:U:52:THR:HG23	2.12	0.48
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.49	0.48
1:0:450:C:OP1	6:C:184:ARG:NH2	2.44	0.48
1:0:622:G:P	27:Y:148:GLY:HA3	2.53	0.48
1:0:1745:G:H22	1:0:2033:G:H5'	1.79	0.48
1:0:2748:G:H8	39:O:8000:HOH:O	1.95	0.48
6:C:168:ARG:NH2	6:C:190:ALA:O	2.47	0.48
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.79	0.48
11:H:3:ALA:CA	11:H:58:ARG:HH12	2.25	0.48
25:W:5:VAL:C	25:W:52:VAL:HG23	2.39	0.48
25:W:11:VAL:O	25:W:12:ASN:HB2	2.13	0.48
1:0:474:C:O3'	6:C:73:LEU:HD21	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2072:G:H3'	1:0:2073:G:C5'	2.44	0.48
2:9:3008:G:O6	16:N:11:ARG:NH1	2.45	0.48
3:4:176:A:OP1	3:4:175:C:H5''	2.14	0.48
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.49	0.48
14:L:149:ARG:O	14:L:150:GLN:HB2	2.13	0.48
15:M:61:ILE:HD12	15:M:61:ILE:N	2.28	0.48
1:0:136:C:H2'	1:0:137:U:O4'	2.13	0.48
1:0:2090:G:H2'	1:0:2091:G:C8	2.49	0.48
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.14	0.48
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.14	0.48
6:C:118:THR:O	6:C:136:VAL:HG13	2.13	0.48
15:M:69:LYS:O	15:M:73:ARG:NH2	2.44	0.48
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.27	0.48
1:0:883:U:H2'	1:0:883:U:O2	2.14	0.47
1:0:1462:C:H2'	1:0:1463:A:H8	1.78	0.47
5:B:51:VAL:HG23	5:B:327:VAL:HG13	1.94	0.47
5:B:238:ASN:ND2	5:B:240:GLY:H	1.99	0.47
6:C:246:ARG:HH11	6:C:246:ARG:CB	2.27	0.47
13:K:118:ALA:O	13:K:119:GLN:C	2.56	0.47
15:M:183:THR:CG2	15:M:194:ALA:HB1	2.41	0.47
18:P:98:ILE:O	18:P:98:ILE:HD13	2.14	0.47
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.29	0.47
31:3:91:GLN:O	31:3:92:GLU:HB2	2.14	0.47
1:0:1056:U:H2'	1:0:1057:A:O4'	2.14	0.47
2:9:3012:C:H5'	2:9:3070:U:O4'	2.15	0.47
5:B:14:GLY:HA2	5:B:15:PRO:C	2.39	0.47
12:J:39:VAL:CG1	12:J:40:ASN:N	2.76	0.47
16:N:154:LEU:HG	16:N:155:GLU:H	1.79	0.47
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.95	0.47
1:0:1168:C:H5''	32:I:87:THR:CG2	2.45	0.47
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.47	0.47
5:B:146:THR:C	5:B:148:PRO:HD3	2.39	0.47
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.96	0.47
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.44	0.47
4:A:65:ARG:C	4:A:66:ARG:HG3	2.40	0.47
5:B:16:ARG:NH2	39:B:9555:HOH:O	2.41	0.47
8:E:108:LEU:HD11	8:E:164:ASP:HB2	1.96	0.47
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.44	0.47
12:J:131:THR:HG22	12:J:133:GLY:N	2.30	0.47
14:L:57:VAL:HG12	14:L:57:VAL:O	2.14	0.47
16:N:183:ASP:O	16:N:184:ILE:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:3:SER:HB3	39:Q:5998:HOH:O	2.14	0.47
23:U:44:ARG:HB3	39:U:3805:HOH:O	2.14	0.47
31:3:3:MET:HB2	31:3:88:LEU:HD11	1.97	0.47
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.44	0.47
1:0:1736:A:H1'	39:0:8130:HOH:O	2.15	0.47
1:0:2265:U:H2'	1:0:2266:A:C8	2.50	0.47
12:J:107:ASN:C	12:J:107:ASN:HD22	2.23	0.47
14:L:93:VAL:HG12	14:L:97:VAL:HG23	1.97	0.47
27:Y:133:HIS:HD2	39:Y:9377:HOH:O	1.97	0.47
1:0:1025:C:H5'	25:W:23:MET:O	2.15	0.47
1:0:2769:C:H2'	1:0:2770:G:C5'	2.44	0.47
2:9:3002:U:OP2	2:9:3003:A:H5'	2.14	0.47
6:C:16:VAL:HG12	6:C:17:ASP:N	2.29	0.47
8:E:80:TRP:O	8:E:134:SER:HA	2.14	0.47
15:M:58:GLN:HG3	39:M:9414:HOH:O	2.12	0.47
18:P:115:SER:HG	18:P:118:GLN:HG3	1.78	0.47
25:W:108:ARG:HE	25:W:114:PRO:CG	2.27	0.47
26:X:34:ARG:NH1	26:X:48:VAL:O	2.47	0.47
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.50	0.47
31:3:16:GLU:HG3	31:3:18:GLN:HE21	1.79	0.47
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.97	0.47
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.96	0.47
1:0:93:C:H5''	24:V:1:THR:CB	2.43	0.47
1:0:286:U:H2'	1:0:287:C:C6	2.50	0.47
1:0:797:A:O4'	28:Z:10:ARG:N	2.47	0.47
1:0:1972:U:H2'	1:0:1973:A:H5'	1.97	0.47
1:0:2329:C:O2'	1:0:2330:U:H5'	2.15	0.47
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.13	0.47
1:0:2676:C:H6	1:0:2676:C:H5''	1.79	0.47
39:9:4707:HOH:O	16:N:147:ILE:HD12	2.15	0.47
5:B:53:LEU:HD21	5:B:270:ILE:HD12	1.96	0.47
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.96	0.47
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.97	0.47
16:N:154:LEU:O	16:N:155:GLU:CB	2.63	0.47
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.96	0.47
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.49	0.47
1:0:1211:G:O2'	1:0:1212:C:H5'	2.15	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.73	0.47
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.14	0.47
1:0:2911:C:O2'	1:0:2912:C:H5'	2.15	0.47
2:9:3049:G:C2'	2:9:3050:G:H5'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:36:ASP:C	4:A:38:ILE:N	2.71	0.47
14:L:89:PHE:CD1	14:L:89:PHE:N	2.83	0.47
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.50	0.47
1:0:27:U:H2'	1:0:28:G:O4'	2.15	0.47
1:0:204:A:H2'	1:0:205:U:H5'	1.96	0.47
1:0:1236:A:H2'	1:0:1237:U:O4'	2.15	0.47
1:0:1778:A:H2'	1:0:1779:A:H5'	1.96	0.47
4:A:69:LEU:HD23	4:A:107:ASN:CB	2.45	0.47
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.30	0.47
6:C:127:ARG:HD3	6:C:129:HIS:CE1	2.48	0.47
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.45	0.47
12:J:45:VAL:CG2	12:J:129:PHE:CD1	2.98	0.47
31:3:22:VAL:HG11	31:3:67:LEU:HD13	1.97	0.47
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.40	0.47
1:0:392:U:H5''	15:M:193:LYS:HB3	1.96	0.47
1:0:1234:U:N3	5:B:244:PRO:HB3	2.30	0.47
4:A:69:LEU:HD23	4:A:107:ASN:CG	2.40	0.47
5:B:41:PHE:CZ	5:B:79:MET:HG3	2.49	0.47
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.50	0.47
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.45	0.47
22:T:48:VAL:CG2	22:T:96:VAL:HG13	2.45	0.47
26:X:66:THR:HG22	26:X:67:PRO:O	2.14	0.47
1:0:407:A:H5'	39:0:6549:HOH:O	2.14	0.46
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.15	0.46
1:0:2587:OMU:O5'	1:0:2587:OMU:H6	2.15	0.46
1:0:2712:G:H5'	39:K:4183:HOH:O	2.15	0.46
39:0:5296:HOH:O	16:N:21:HIS:HD2	1.98	0.46
5:B:41:PHE:HA	5:B:79:MET:HE1	1.98	0.46
5:B:321:PRO:HG3	39:B:9597:HOH:O	2.15	0.46
12:J:143:LYS:HG3	12:J:145:TRP:CE2	2.50	0.46
1:0:710:G:H5'	17:O:25:VAL:HG13	1.98	0.46
1:0:1252:A:H2'	1:0:1253:C:O4'	2.15	0.46
1:0:1441:G:H1'	39:0:8302:HOH:O	2.15	0.46
1:0:1641:A:C2'	1:0:1642:A:H5'	2.43	0.46
1:0:2435:U:H1'	39:0:5974:HOH:O	2.15	0.46
1:0:2443:C:H5'	14:L:57:VAL:HG21	1.97	0.46
7:D:99:ASP:N	7:D:103:ASN:O	2.43	0.46
8:E:97:VAL:HG12	39:E:4191:HOH:O	2.15	0.46
1:0:1477:C:H5'	1:0:1868:G:C5'	2.45	0.46
4:A:34:ASP:OD1	4:A:35:GLY:N	2.48	0.46
6:C:57:PRO:HG2	6:C:73:LEU:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:35:TYR:HB2	39:E:5715:HOH:O	2.16	0.46
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.97	0.46
15:M:68:ARG:O	15:M:68:ARG:HD3	2.15	0.46
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.97	0.46
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.16	0.46
1:0:292:G:H2'	1:0:358:G:N2	2.30	0.46
1:0:666:A:H2'	1:0:667:C:O4'	2.15	0.46
1:0:797:A:H4'	28:Z:10:ARG:N	2.30	0.46
1:0:1182:C:H1'	1:0:1192:A:C8	2.47	0.46
1:0:1730:G:H5'	1:0:1731:C:C6	2.50	0.46
4:A:33:GLU:OE1	4:A:33:GLU:N	2.38	0.46
5:B:171:VAL:HG23	5:B:172:SER:N	2.31	0.46
6:C:162:VAL:HG13	6:C:192:ILE:HD11	1.97	0.46
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.46	0.46
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.50	0.46
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.97	0.46
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.95	0.46
32:I:131:THR:O	32:I:135:LEU:HG	2.16	0.46
1:0:249:G:O2'	1:0:250:C:H5'	2.15	0.46
1:0:1268:C:O2'	1:0:1269:G:H5'	2.15	0.46
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.45	0.46
11:H:83:TYR:CD1	11:H:83:TYR:C	2.93	0.46
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.16	0.46
22:T:53:GLY:HA3	39:T:6384:HOH:O	2.14	0.46
27:Y:122:ARG:NH2	39:Y:9335:HOH:O	2.48	0.46
30:2:39:ARG:HG2	39:2:3143:HOH:O	2.16	0.46
1:0:1044:C:H5''	39:0:9648:HOH:O	2.16	0.46
1:0:1118:A:C8	1:0:1119:G:H5''	2.50	0.46
1:0:2064:U:H4'	1:0:2653:A:OP1	2.15	0.46
5:B:51:VAL:HG22	5:B:53:LEU:HD13	1.98	0.46
7:D:173:GLU:HG3	7:D:174:VAL:N	2.31	0.46
25:W:142:ASP:HB3	25:W:145:GLY:H	1.81	0.46
1:0:285:A:H2'	1:0:286:U:O4'	2.16	0.46
1:0:1299:G:N2	39:0:5251:HOH:O	2.49	0.46
1:0:1615:A:H5'	39:0:4766:HOH:O	2.15	0.46
4:A:207:GLN:O	4:A:208:HIS:HB3	2.15	0.46
5:B:277:GLU:N	5:B:278:PRO:HD2	2.31	0.46
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.31	0.46
23:U:4:ARG:HG2	23:U:4:ARG:HH11	1.80	0.46
24:V:1:THR:O	24:V:2:VAL:C	2.58	0.46
4:A:88:ILE:O	4:A:88:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:62:ASP:HA	39:D:4233:HOH:O	2.16	0.46
12:J:103:VAL:HG12	39:J:5907:HOH:O	2.15	0.46
13:K:125:ALA:C	13:K:127:ALA:N	2.74	0.46
15:M:164:THR:CG2	15:M:165:GLY:N	2.78	0.46
24:V:42:ASN:O	24:V:44:GLY:N	2.49	0.46
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.16	0.46
26:X:72:VAL:CG2	26:X:85:VAL:HG12	2.44	0.46
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.56	0.46
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.60	0.46
1:0:177:A:H2'	1:0:178:U:O4'	2.16	0.46
1:0:1755:A:H2'	1:0:1756:G:O4'	2.16	0.46
1:0:2044:G:OP1	26:X:23:HIS:HE1	1.99	0.46
7:D:25:MET:HE1	7:D:37:ALA:O	2.16	0.46
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.30	0.46
13:K:55:VAL:CG1	13:K:56:SER:N	2.78	0.46
14:L:114:VAL:HB	39:L:9471:HOH:O	2.15	0.46
1:0:189:A:OP1	15:M:171:ARG:NH2	2.49	0.46
1:0:1171:A:H2'	1:0:1172:G:H5'	1.97	0.46
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.16	0.46
1:0:1926:G:H2'	1:0:1927:A:C8	2.51	0.46
1:0:2415:A:N3	16:N:26:LEU:HD13	2.30	0.46
4:A:81:GLN:HB2	4:A:92:ASN:HD21	1.80	0.46
4:A:121:ALA:O	4:A:124:VAL:HG22	2.16	0.46
5:B:16:ARG:NE	39:B:9555:HOH:O	2.34	0.46
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.46	0.46
7:D:65:GLU:HG3	39:D:6752:HOH:O	2.15	0.46
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.46	0.46
11:H:47:ILE:HG21	39:H:9541:HOH:O	2.14	0.46
32:I:128:VAL:C	32:I:130:GLY:N	2.74	0.46
1:0:65:C:O2'	1:0:66:G:H5'	2.16	0.45
1:0:92:G:H4'	24:V:44:GLY:HA3	1.98	0.45
1:0:834:G:H3'	1:0:835:U:H4'	1.99	0.45
1:0:1603:A:H5''	1:0:1605:G:H5'	1.97	0.45
1:0:2032:U:H2'	1:0:2033:G:H5'	1.97	0.45
2:9:3052:A:H2'	2:9:3053:G:O4'	2.16	0.45
5:B:221:GLN:NE2	13:K:42:ASN:HD22	2.07	0.45
9:F:117:GLU:C	9:F:119:ARG:N	2.73	0.45
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.98	0.45
16:N:67:ALA:C	16:N:69:TYR:H	2.23	0.45
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.82	0.45
1:0:820:G:O2'	1:0:856:G:H4'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:944:G:C8	25:W:23:MET:HE1	2.51	0.45
1:0:2453:G:H4'	14:L:50:GLY:C	2.41	0.45
1:0:2904:U:H4'	26:X:8:ARG:NH1	2.32	0.45
2:9:3042:C:O2	7:D:76:ARG:NH1	2.49	0.45
5:B:305:ASP:O	5:B:306:LYS:CB	2.63	0.45
6:C:133:ARG:NH1	39:C:9213:HOH:O	2.49	0.45
7:D:60:GLU:O	7:D:61:PHE:C	2.58	0.45
14:L:136:ALA:HB3	39:L:9471:HOH:O	2.16	0.45
15:M:49:ALA:C	15:M:54:TYR:HB3	2.41	0.45
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.45
20:R:114:VAL:HG13	20:R:114:VAL:O	2.16	0.45
25:W:105:THR:HA	25:W:109:GLU:OE1	2.16	0.45
26:X:12:ILE:HD12	26:X:36:HIS:CG	2.51	0.45
2:9:3050:G:H5''	16:N:159:TYR:CE1	2.52	0.45
2:9:3114:G:H2'	2:9:3115:C:C6	2.51	0.45
5:B:183:GLU:O	5:B:184:ASP:C	2.60	0.45
7:D:128:LEU:C	7:D:128:LEU:HD23	2.41	0.45
8:E:66:GLN:O	8:E:70:GLU:HG3	2.16	0.45
9:F:57:GLU:HB2	15:M:23:LEU:HD11	1.97	0.45
20:R:119:VAL:O	20:R:119:VAL:HG12	2.16	0.45
27:Y:115:ARG:NE	39:Y:9350:HOH:O	2.49	0.45
1:0:2299:G:O6	19:Q:1:PRO:HA	2.17	0.45
4:A:30:ARG:HE	4:A:30:ARG:HB3	1.59	0.45
5:B:84:LEU:HD13	5:B:84:LEU:O	2.17	0.45
1:0:603:A:H4'	1:0:604:G:O5'	2.16	0.45
1:0:1525:G:H5'	1:0:1526:A:OP2	2.17	0.45
1:0:1902:G:H2'	1:0:1903:U:O4'	2.16	0.45
1:0:1947:G:H2'	1:0:1948:G:H8	1.81	0.45
1:0:2717:C:H5'	5:B:302:PRO:HA	1.97	0.45
39:O:9644:HOH:O	14:L:30:ARG:HD2	2.17	0.45
2:9:3049:G:H2'	2:9:3050:G:O4'	2.17	0.45
2:9:3076:G:C3'	2:9:3077:A:H5''	2.30	0.45
4:A:135:VAL:HG11	4:A:147:ARG:HH12	1.81	0.45
5:B:62:ARG:HA	5:B:65:MET:HE3	1.99	0.45
1:0:366:U:H2'	1:0:367:G:O4'	2.17	0.45
1:0:2906:A:H5'	1:0:2907:C:O4'	2.16	0.45
11:H:29:ALA:C	11:H:30:GLN:HG3	2.42	0.45
15:M:74:LYS:HG2	15:M:75:ARG:N	2.31	0.45
16:N:155:GLU:O	16:N:156:GLU:HG3	2.16	0.45
16:N:183:ASP:O	16:N:184:ILE:C	2.59	0.45
17:O:23:GLY:C	39:O:3062:HOH:O	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.49	0.45
1:O:952:G:OP1	19:Q:42:LYS:HE2	2.17	0.45
1:O:1724:U:H5''	39:O:4327:HOH:O	2.16	0.45
16:N:37:ARG:CZ	16:N:105:GLY:HA3	2.46	0.45
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.52	0.45
22:T:81:LYS:HD2	22:T:87:VAL:HG11	1.98	0.45
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.17	0.45
1:O:288:A:H2'	1:O:289:G:C8	2.51	0.45
1:O:1184:C:H4'	32:I:126:LYS:HB3	1.98	0.45
1:O:2316:G:OP1	1:O:2317:C:H1'	2.16	0.45
39:9:5851:HOH:O	16:N:38:LYS:HD3	2.16	0.45
4:A:201:PHE:HB3	39:A:9621:HOH:O	2.15	0.45
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.99	0.45
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.98	0.45
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.52	0.45
1:O:137:U:OP1	1:O:259:G:O2'	2.35	0.45
1:O:2568:A:H5''	1:O:2702:A:O2'	2.16	0.45
1:O:2748:G:OP1	1:O:2749:U:H5''	2.17	0.45
2:9:3054:A:O2'	2:9:3055:U:H5'	2.17	0.45
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.52	0.45
7:D:23:VAL:CG2	7:D:73:VAL:HB	2.45	0.45
7:D:167:GLU:C	7:D:169:THR:H	2.24	0.45
13:K:99:ASP:OD1	13:K:101:ASN:N	2.49	0.45
16:N:64:SER:C	16:N:66:LEU:H	2.24	0.45
16:N:72:GLU:O	16:N:72:GLU:HG2	2.16	0.45
22:T:78:THR:HB	22:T:87:VAL:O	2.17	0.45
1:O:1185:U:H2'	1:O:1186:C:C6	2.51	0.45
1:O:2252:A:C5	1:O:2253:G:H1'	2.51	0.45
1:O:2681:A:H4'	1:O:2682:C:H5'	1.99	0.45
1:O:2907:C:H2'	1:O:2908:A:O4'	2.17	0.45
4:A:99:ILE:O	4:A:131:HIS:CE1	2.70	0.45
4:A:192:VAL:HG11	4:A:207:GLN:HB3	1.98	0.45
5:B:254:GLN:NE2	39:B:9589:HOH:O	2.50	0.45
9:F:26:THR:HG21	9:F:102:GLY:C	2.42	0.45
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.21	0.45
9:F:99:THR:O	9:F:100:ASP:HB2	2.17	0.45
13:K:2:GLU:O	13:K:3:ALA:C	2.60	0.45
15:M:59:GLY:C	15:M:141:ILE:HD11	2.41	0.45
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.99	0.45
16:N:152:GLU:C	16:N:154:LEU:H	2.25	0.45
1:O:1573:A:H2'	1:O:1574:C:O4'	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1773:G:C8	28:Z:16:ALA:HA	2.50	0.44
1:0:1942:A:H5'	4:A:233:THR:HB	1.98	0.44
2:9:3029:C:C2'	2:9:3030:C:H5'	2.47	0.44
5:B:215:VAL:HB	5:B:234:ARG:NH1	2.26	0.44
11:H:45:VAL:HA	11:H:167:PRO:O	2.17	0.44
15:M:22:GLU:HG2	15:M:26:GLN:NE2	2.32	0.44
15:M:43:PRO:HG3	15:M:62:VAL:HG21	1.98	0.44
22:T:79:LEU:HG	22:T:89:ARG:HB2	1.99	0.44
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.97	0.44
27:Y:155:ARG:NH1	39:Y:9352:HOH:O	2.49	0.44
1:0:958:G:H2'	1:0:959:C:C6	2.52	0.44
1:0:1120:U:H5''	1:0:1120:U:H6	1.82	0.44
1:0:1748:U:H4'	39:0:7981:HOH:O	2.16	0.44
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.44
6:C:150:THR:HA	6:C:203:ALA:O	2.17	0.44
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.99	0.44
7:D:49:PRO:HB3	39:D:5828:HOH:O	2.18	0.44
16:N:82:TYR:HE1	16:N:120:GLU:HG2	1.82	0.44
1:0:484:A:N1	1:0:506:G:H4'	2.31	0.44
1:0:2541:U:C2	1:0:2620:U:O4	2.71	0.44
4:A:51:ARG:HH21	4:A:55:VAL:HG23	1.83	0.44
7:D:163:VAL:HA	39:D:6326:HOH:O	2.17	0.44
8:E:23:GLU:HG2	8:E:28:SER:CB	2.46	0.44
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.55	0.44
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.52	0.44
23:U:20:MET:CG	23:U:28:THR:HG23	2.47	0.44
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.82	0.44
1:0:426:G:H2'	1:0:427:C:O4'	2.18	0.44
1:0:821:U:H2'	1:0:822:C:H6	1.82	0.44
1:0:1163:G:H5''	32:I:115:ASP:HB3	1.99	0.44
1:0:1226:G:H5'	39:0:5101:HOH:O	2.18	0.44
1:0:1768:C:H2'	1:0:1769:C:O4'	2.17	0.44
1:0:1878:G:O2'	1:0:1879:U:C5	2.63	0.44
6:C:236:THR:HG22	6:C:239:ALA:HB2	1.99	0.44
6:C:236:THR:O	6:C:237:GLU:C	2.60	0.44
11:H:56:GLN:NE2	11:H:93:GLN:HG2	2.31	0.44
11:H:58:ARG:O	11:H:62:LEU:HD22	2.18	0.44
19:Q:30:VAL:HG12	19:Q:30:VAL:O	2.17	0.44
19:Q:75:ILE:HD13	19:Q:84:ILE:CD1	2.47	0.44
25:W:5:VAL:O	25:W:52:VAL:CG2	2.66	0.44
25:W:29:VAL:O	25:W:30:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:113:HIS:CE1	32:I:121:LEU:HD22	2.53	0.44
1:0:1213:C:O2'	1:0:1214:G:H5'	2.18	0.44
1:0:1419:U:H2'	1:0:1685:A:C2	2.52	0.44
1:0:2003:U:H4'	1:0:2004:U:H5	1.83	0.44
1:0:2104:C:O2	1:0:2485:A:N1	2.50	0.44
1:0:2346:C:H4'	7:D:52:THR:CG2	2.48	0.44
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.49	0.44
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.15	0.44
6:C:129:HIS:HD2	6:C:165:ASP:OD2	2.01	0.44
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.00	0.44
22:T:88:PRO:HB3	39:T:6320:HOH:O	2.18	0.44
1:0:461:C:N3	1:0:479:G:H5'	2.33	0.44
1:0:488:U:O2'	22:T:82:THR:HG21	2.17	0.44
1:0:564:G:H1'	39:0:6825:HOH:O	2.16	0.44
1:0:1139:U:H2'	1:0:1140:C:C6	2.52	0.44
1:0:2478:U:O2'	1:0:2479:A:H5'	2.18	0.44
1:0:2531:U:O2'	1:0:2532:A:H5'	2.17	0.44
5:B:88:GLU:HB3	5:B:97:LEU:HD12	1.98	0.44
5:B:190:MET:HA	5:B:190:MET:HE3	2.00	0.44
6:C:219:ASN:O	6:C:222:ASP:OD1	2.36	0.44
9:F:102:GLY:O	9:F:103:GLU:HB2	2.18	0.44
21:S:57:THR:C	21:S:59:ASP:H	2.26	0.44
30:2:20:ARG:NE	30:2:39:ARG:NH2	2.66	0.44
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.18	0.44
1:0:920:C:H5'	1:0:921:G:C4	2.52	0.44
1:0:968:G:H1'	11:H:32:LYS:HD2	1.98	0.44
1:0:1592:G:O2'	1:0:1593:C:O4'	2.34	0.44
4:A:36:ASP:CB	4:A:83:GLY:HA3	2.45	0.44
4:A:232:ARG:NH2	4:A:236:GLY:O	2.43	0.44
9:F:60:VAL:O	9:F:60:VAL:CG1	2.66	0.44
11:H:51:VAL:CG1	11:H:53:GLU:O	2.66	0.44
14:L:143:THR:CG2	14:L:144:ASP:N	2.81	0.44
16:N:103:ASP:C	16:N:103:ASP:OD1	2.60	0.44
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.18	0.44
31:3:69:TYR:O	31:3:77:ALA:HA	2.17	0.44
1:0:1066:U:H2'	1:0:1067:A:C8	2.52	0.44
1:0:1067:A:H5'	39:0:4922:HOH:O	2.17	0.44
1:0:1130:U:H2'	1:0:1131:G:O4'	2.18	0.44
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.50	0.44
1:0:1884:G:O6	4:A:190:ARG:HD2	2.17	0.44
7:D:23:VAL:O	7:D:23:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:42:HIS:CE1	16:N:75:THR:OG1	2.71	0.44
16:N:119:GLN:O	16:N:123:ILE:HG13	2.18	0.44
16:N:167:ASP:C	16:N:168:LEU:HG	2.43	0.44
17:O:10:LEU:HD13	17:O:99:GLU:HG3	1.99	0.44
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.76	0.44
32:I:110:GLU:HA	32:I:113:HIS:CD2	2.53	0.44
1:O:1919:A:H4'	39:O:5415:HOH:O	2.17	0.44
4:A:179:MET:HG2	4:A:186:TRP:HB3	1.99	0.44
8:E:84:MET:HE1	8:E:148:ILE:HD13	2.00	0.44
16:N:182:GLY:O	16:N:183:ASP:C	2.61	0.44
20:R:18:LEU:HG	20:R:91:LEU:HD13	2.00	0.44
21:S:56:ASN:O	30:2:8:LYS:NZ	2.44	0.44
26:X:73:ARG:NH1	26:X:88:GLU:HG2	2.33	0.44
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.18	0.44
30:2:41:HIS:N	30:2:45:ASN:HD22	1.99	0.44
32:I:87:THR:CG2	32:I:88:GLY:N	2.81	0.44
1:O:960:G:N3	1:O:960:G:C2'	2.81	0.43
1:O:1422:U:H2'	1:O:1423:C:C6	2.53	0.43
4:A:223:ARG:O	4:A:223:ARG:HG2	2.18	0.43
5:B:49:THR:HG22	5:B:280:VAL:CG2	2.48	0.43
5:B:175:LEU:O	5:B:175:LEU:HD23	2.18	0.43
5:B:217:ARG:HG3	5:B:257:THR:HB	2.00	0.43
5:B:254:GLN:HG2	5:B:255:GLY:H	1.80	0.43
8:E:7:ILE:HD11	8:E:11:VAL:C	2.42	0.43
9:F:11:ASP:O	9:F:14:ASP:HB2	2.18	0.43
15:M:81:ARG:HG3	15:M:85:ARG:HB2	2.00	0.43
15:M:187:LEU:HD22	15:M:194:ALA:HB3	1.99	0.43
16:N:176:ARG:HG3	16:N:180:LEU:HD13	2.00	0.43
1:O:1588:G:C6	1:O:1589:G:N1	2.87	0.43
1:O:1681:G:H5''	1:O:1682:A:H5'	2.00	0.43
1:O:1684:A:H1'	30:2:43:ARG:HH22	1.83	0.43
1:O:1992:U:OP2	13:K:66:ARG:HD2	2.18	0.43
1:O:2083:A:N6	12:J:90:LYS:HE2	2.32	0.43
1:O:2363:G:O2'	19:Q:11:ARG:HG3	2.17	0.43
16:N:108:SER:HA	16:N:109:PRO:HD3	1.81	0.43
1:O:1096:U:O2'	1:O:1097:A:H5'	2.18	0.43
1:O:1131:G:C6	1:O:1230:A:C4	3.06	0.43
1:O:2032:U:H2'	1:O:2033:G:H5''	1.99	0.43
1:O:2506:A:O2'	1:O:2507:G:O5'	2.36	0.43
1:O:2846:C:H4'	39:O:5633:HOH:O	2.18	0.43
5:B:41:PHE:HB3	5:B:190:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:149:ARG:HH12	16:N:15:GLU:HA	1.83	0.43
8:E:81:GLU:HA	8:E:133:VAL:O	2.18	0.43
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.18	0.43
25:W:65:VAL:HG12	25:W:116:LEU:HD13	2.01	0.43
27:Y:189:ASN:HD22	27:Y:191:ASP:N	2.16	0.43
31:3:17:HIS:O	31:3:18:GLN:HG3	2.19	0.43
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.18	0.43
1:0:185:G:O3'	1:0:186:A:H4'	2.19	0.43
1:0:702:G:O2'	1:0:703:G:H5'	2.18	0.43
1:0:2526:C:C6	1:0:2526:C:H5'	2.53	0.43
1:0:2549:C:OP1	5:B:7:ARG:NH1	2.51	0.43
14:L:73:VAL:HG23	14:L:74:THR:N	2.33	0.43
16:N:67:ALA:C	16:N:69:TYR:N	2.76	0.43
24:V:5:VAL:HG11	24:V:9:ARG:NH1	2.32	0.43
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.48	0.43
26:X:20:GLU:CG	26:X:21:PRO:HD2	2.47	0.43
1:0:1741:U:O2'	1:0:2723:G:H4'	2.18	0.43
1:0:2239:C:H2'	1:0:2240:U:C6	2.54	0.43
1:0:2323:G:H5'	39:0:7509:HOH:O	2.18	0.43
1:0:2533:C:H6	1:0:2533:C:C5'	2.26	0.43
39:0:7490:HOH:O	19:Q:9:GLY:HA2	2.17	0.43
4:A:36:ASP:O	4:A:36:ASP:CG	2.61	0.43
7:D:92:GLU:HB2	39:D:3862:HOH:O	2.18	0.43
11:H:146:VAL:HG22	39:H:9541:HOH:O	2.18	0.43
11:H:169:GLY:C	11:H:170:ASN:HD22	2.25	0.43
12:J:99:GLU:HA	39:J:7377:HOH:O	2.18	0.43
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.51	0.43
20:R:84:ALA:O	20:R:88:PHE:HD1	2.02	0.43
1:0:2506:A:O2'	1:0:2507:G:P	2.77	0.43
14:L:77:ALA:C	14:L:79:ASP:H	2.27	0.43
17:O:42:GLU:HB2	39:O:2176:HOH:O	2.19	0.43
22:T:49:GLU:OE2	22:T:51:LEU:HD21	2.19	0.43
26:X:23:HIS:CD2	26:X:24:LYS:HG3	2.53	0.43
1:0:1406:A:H5'	1:0:1407:A:C8	2.54	0.43
1:0:2456:A:H2'	1:0:2457:U:H6	1.84	0.43
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.19	0.43
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.84	0.43
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.48	0.43
27:Y:107:PRO:HD3	27:Y:182:PHE:CE1	2.54	0.43
1:0:23:G:C6	1:0:24:G:N1	2.87	0.43
1:0:338:C:H4'	6:C:174:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:697:G:H4'	1:0:730:G:O3'	2.18	0.43
1:0:1760:G:H5'	1:0:1818:C:O2'	2.17	0.43
4:A:223:ARG:NH1	39:A:9507:HOH:O	2.51	0.43
5:B:267:LYS:HE3	5:B:300:SER:O	2.18	0.43
12:J:132:LEU:HD23	12:J:132:LEU:HA	1.82	0.43
15:M:144:ASP:O	15:M:148:SER:HB3	2.19	0.43
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.48	0.43
22:T:75:GLU:O	22:T:76:ASP:HB2	2.19	0.43
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.49	0.43
25:W:139:GLY:O	25:W:141:HIS:CD2	2.65	0.43
1:0:294:C:H2'	1:0:295:C:O4'	2.19	0.43
1:0:522:U:O2'	1:0:1366:C:H5'	2.18	0.43
1:0:2408:A:H4'	31:3:15:ASN:O	2.19	0.43
1:0:2676:C:H4'	12:J:70:PHE:HD1	1.78	0.43
1:0:2699:A:H2'	1:0:2700:G:O4'	2.18	0.43
4:A:206:ARG:HH11	4:A:206:ARG:HG3	1.83	0.43
8:E:133:VAL:HG12	8:E:141:VAL:HG13	2.01	0.43
9:F:101:ALA:HA	39:F:5413:HOH:O	2.18	0.43
14:L:10:SER:O	14:L:11:ARG:HB3	2.19	0.43
15:M:47:ASP:CG	15:M:48:LYS:N	2.77	0.43
22:T:106:GLU:HG3	39:T:4913:HOH:O	2.18	0.43
23:U:47:ARG:HG3	39:U:4381:HOH:O	2.18	0.43
32:I:132:CYS:O	32:I:135:LEU:N	2.49	0.43
1:0:263:U:C2	9:F:59:ILE:HD12	2.54	0.43
1:0:999:C:H2'	1:0:1000:C:O4'	2.19	0.43
1:0:2072:G:N2	39:0:7359:HOH:O	2.52	0.43
2:9:3044:A:O4'	7:D:76:ARG:NE	2.52	0.43
5:B:171:VAL:HG23	5:B:172:SER:H	1.84	0.43
8:E:20:ILE:HD12	8:E:33:LEU:CD1	2.48	0.43
11:H:114:ARG:O	11:H:115:ALA:C	2.62	0.43
13:K:20:CYS:HB2	13:K:29:LEU:HG	2.01	0.43
16:N:93:GLN:HE21	16:N:127:LEU:CD1	2.32	0.43
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.49	0.43
24:V:11:MET:HB3	24:V:15:GLU:HB2	2.00	0.43
30:2:19:SER:O	30:2:36:ASN:ND2	2.52	0.43
1:0:370:G:O2'	1:0:371:U:H5'	2.19	0.42
1:0:1163:G:H1	1:0:1184:C:N4	2.17	0.42
1:0:1185:U:H5'	39:0:7928:HOH:O	2.19	0.42
1:0:1236:A:C8	12:J:63:ILE:HD11	2.54	0.42
1:0:1473:U:O2'	1:0:1474:C:H5''	2.19	0.42
1:0:1819:G:H2'	1:0:1820:G:C4'	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2365:G:H4'	19:Q:45:PRO:O	2.19	0.42
1:0:2372:A:H2'	1:0:2373:U:C6	2.54	0.42
1:0:2379:G:N3	1:0:2418:G:H2'	2.33	0.42
1:0:2690:U:H4'	8:E:111:LYS:HE3	2.01	0.42
1:0:2717:C:H2'	1:0:2718:C:C5'	2.36	0.42
1:0:2720:C:O2	13:K:87:ARG:NH2	2.52	0.42
2:9:3045:A:H4'	7:D:143:LYS:O	2.19	0.42
4:A:105:VAL:CG1	4:A:106:CYS:N	2.82	0.42
4:A:114:ASP:C	4:A:114:ASP:OD1	2.62	0.42
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.49	0.42
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.49	0.42
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.99	0.42
12:J:45:VAL:CG2	12:J:129:PHE:HD1	2.32	0.42
15:M:64:ARG:HD2	39:M:9392:HOH:O	2.19	0.42
15:M:159:VAL:HG13	15:M:160:PHE:N	2.34	0.42
20:R:61:GLN:NE2	39:R:9452:HOH:O	2.52	0.42
20:R:69:LYS:HB2	20:R:72:VAL:HG23	2.01	0.42
23:U:4:ARG:HG2	23:U:4:ARG:NH1	2.34	0.42
29:1:18:LYS:HD3	30:2:10:ARG:HD3	2.01	0.42
1:0:138:U:OP2	1:0:139:C:H5	2.02	0.42
1:0:359:U:H3'	39:0:6300:HOH:O	2.18	0.42
1:0:1044:C:H3'	1:0:1045:G:H5''	2.00	0.42
1:0:1174:A:C5	1:0:1201:C:H4'	2.54	0.42
1:0:1797:A:H2'	1:0:1799:G:O5'	2.19	0.42
1:0:2642:G:H2'	1:0:2643:G:O4'	2.20	0.42
1:0:2769:C:H2'	1:0:2770:G:H5'	1.99	0.42
1:0:2851:G:H4'	5:B:157:LYS:HZ1	1.84	0.42
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.18	0.42
5:B:17:LYS:O	5:B:260:HIS:CD2	2.72	0.42
6:C:120:ASP:OD1	6:C:120:ASP:C	2.62	0.42
8:E:36:PRO:HD3	12:J:127:ILE:CD1	2.43	0.42
8:E:81:GLU:HG2	8:E:134:SER:CB	2.50	0.42
11:H:20:ILE:HG23	11:H:120:ILE:CD1	2.48	0.42
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.01	0.42
16:N:89:GLY:O	16:N:92:ALA:HB3	2.19	0.42
24:V:39:ALA:O	24:V:41:GLU:N	2.47	0.42
1:0:64:G:H2'	1:0:65:C:O4'	2.19	0.42
1:0:645:U:OP2	14:L:4:LYS:HE2	2.19	0.42
1:0:1730:G:H5'	1:0:1731:C:H5	1.81	0.42
1:0:2032:U:C2'	1:0:2033:G:H5''	2.49	0.42
1:0:2374:A:H2'	1:0:2375:G:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:192:VAL:HG12	4:A:207:GLN:CB	2.48	0.42
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.94	0.42
6:C:33:LYS:HE2	39:C:9162:HOH:O	2.19	0.42
10:G:63:ARG:HB2	10:G:66:LEU:HG	2.01	0.42
17:O:29:VAL:HG11	17:O:98:LEU:HD21	2.00	0.42
25:W:59:GLN:NE2	25:W:97:ALA:HB3	2.34	0.42
1:0:21:G:C5'	20:R:2:ILE:HA	2.32	0.42
1:0:903:U:O4	14:L:18:HIS:HB2	2.19	0.42
1:0:941:G:C5	1:0:942:U:C4	3.08	0.42
1:0:1162:G:H1'	32:I:117:LEU:CD1	2.46	0.42
1:0:2314:G:C2'	1:0:2315:C:H5'	2.49	0.42
1:0:2587:OMU:H2'	1:0:2589:U:H5''	2.00	0.42
1:0:2679:G:H2'	1:0:2681:A:OP2	2.19	0.42
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.83	0.42
1:0:2820:A:H2'	1:0:2821:C:C6	2.54	0.42
1:0:2820:A:OP1	5:B:98:THR:HG22	2.20	0.42
5:B:221:GLN:HE22	13:K:42:ASN:ND2	2.07	0.42
5:B:321:PRO:HA	39:B:9650:HOH:O	2.18	0.42
6:C:95:GLU:H	6:C:95:GLU:CD	2.26	0.42
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.49	0.42
19:Q:47:VAL:HB	19:Q:90:HIS:CE1	2.55	0.42
19:Q:75:ILE:CD1	19:Q:84:ILE:HD11	2.49	0.42
20:R:119:VAL:O	20:R:119:VAL:CG1	2.66	0.42
22:T:12:ARG:NH1	39:T:3035:HOH:O	2.43	0.42
1:0:943:A:C5	25:W:23:MET:HE2	2.54	0.42
1:0:1020:A:H2'	1:0:1021:G:C8	2.55	0.42
1:0:1714:C:O2'	1:0:1715:C:H5'	2.19	0.42
1:0:1739:G:H1'	1:0:2726:U:O4	2.19	0.42
1:0:2784:A:H1'	8:E:60:SER:OG	2.19	0.42
4:A:223:ARG:CZ	39:A:9561:HOH:O	2.68	0.42
7:D:96:SER:C	7:D:98:PHE:H	2.27	0.42
7:D:99:ASP:HB2	7:D:103:ASN:N	2.29	0.42
9:F:58:GLU:HG3	9:F:61:MET:CE	2.47	0.42
13:K:22:ASP:O	13:K:110:LYS:HE3	2.19	0.42
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.49	0.42
20:R:82:GLU:O	20:R:86:LYS:HG3	2.20	0.42
1:0:664:U:O4	1:0:681:G:H5''	2.19	0.42
1:0:2133:U:H4'	1:0:2134:G:H5'	2.02	0.42
3:4:74:DCZ:C2'	3:4:75:DC:H5'	2.49	0.42
6:C:153:VAL:O	6:C:157:LEU:HG	2.20	0.42
9:F:99:THR:O	9:F:99:THR:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.50	0.42
15:M:182:LYS:C	15:M:194:ALA:HB2	2.44	0.42
22:T:48:VAL:HG21	22:T:96:VAL:CG1	2.49	0.42
31:3:16:GLU:HG3	31:3:18:GLN:NE2	2.35	0.42
31:3:20:HIS:HA	31:3:70:ARG:O	2.20	0.42
31:3:48:ASN:ND2	31:3:50:GLY:H	2.18	0.42
1:0:401:C:O2'	15:M:92:THR:HB	2.19	0.42
1:0:952:G:N3	1:0:2302:A:H2'	2.35	0.42
1:0:1117:A:C2	1:0:1244:U:C2	3.07	0.42
1:0:1311:G:O6	6:C:173:LYS:HE3	2.19	0.42
1:0:2053:G:H4'	20:R:136:TRP:CE2	2.55	0.42
1:0:2898:G:H4'	5:B:288:GLY:HA2	2.01	0.42
4:A:36:ASP:HB2	4:A:83:GLY:CA	2.49	0.42
4:A:179:MET:HG2	4:A:186:TRP:HB2	2.01	0.42
7:D:57:THR:HG23	7:D:63:ILE:HG22	2.02	0.42
9:F:70:LYS:C	9:F:72:VAL:H	2.28	0.42
13:K:113:ILE:HG22	13:K:114:ALA:N	2.34	0.42
13:K:113:ILE:HD12	13:K:128:ALA:HB2	2.01	0.42
25:W:65:VAL:CG1	25:W:116:LEU:HD13	2.49	0.42
32:I:98:ALA:O	32:I:137:VAL:HA	2.19	0.42
1:0:424:C:H2'	1:0:425:U:C6	2.54	0.42
1:0:1086:A:C6	25:W:11:VAL:HG11	2.55	0.42
1:0:1165:G:O2'	1:0:1174:A:H1'	2.20	0.42
1:0:1203:G:O2'	1:0:1204:C:H5'	2.19	0.42
1:0:2547:C:OP2	5:B:5:ARG:NH1	2.53	0.42
1:0:2748:G:H4'	1:0:2749:U:H5'	2.01	0.42
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.42
2:9:3057:A:H8	7:D:141:VAL:HG21	1.85	0.42
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.50	0.42
5:B:280:VAL:HG13	5:B:333:GLU:O	2.19	0.42
5:B:294:TYR:HE2	39:B:9644:HOH:O	2.02	0.42
13:K:4:LEU:CD2	13:K:116:GLU:HB3	2.40	0.42
25:W:4:LEU:CD1	25:W:24:LEU:HD13	2.50	0.42
30:2:20:ARG:CG	30:2:21:VAL:N	2.83	0.42
32:I:71:GLY:O	32:I:72:VAL:C	2.63	0.42
1:0:130:C:H2'	39:0:3760:HOH:O	2.19	0.42
1:0:559:U:H2'	1:0:560:C:O4'	2.20	0.42
1:0:912:A:C4	1:0:1294:A:C2	3.06	0.42
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.51	0.42
1:0:2351:C:H2'	1:0:2352:G:O4'	2.19	0.42
1:0:2511:A:H2'	1:0:2512:U:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2726:U:O2'	26:X:22:ASN:ND2	2.53	0.42
1:0:2894:C:O2'	1:0:2895:C:H5'	2.19	0.42
39:0:6168:HOH:O	5:B:2:GLN:CD	2.62	0.42
5:B:277:GLU:N	5:B:278:PRO:CD	2.83	0.42
12:J:107:ASN:ND2	12:J:109:TYR:H	2.18	0.42
15:M:107:ARG:NH1	15:M:107:ARG:CG	2.77	0.42
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.55	0.42
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	2.02	0.42
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.84	0.42
32:I:79:ILE:HG23	32:I:100:LEU:HD11	2.02	0.42
32:I:139:ILE:CG2	32:I:140:GLU:N	2.83	0.42
1:0:12:U:C2'	1:0:13:G:H5'	2.49	0.42
1:0:441:A:H8	1:0:441:A:O5'	2.03	0.42
1:0:907:A:H2'	1:0:908:A:C8	2.54	0.42
1:0:1120:U:H5'	1:0:1121:G:OP2	2.20	0.42
1:0:1482:A:O2'	1:0:1483:C:H5'	2.20	0.42
1:0:1594:C:O2'	1:0:1607:A:H4'	2.19	0.42
1:0:2645:U:H1'	39:0:9923:HOH:O	2.19	0.42
2:9:3096:C:H2'	2:9:3097:U:C6	2.55	0.42
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.55	0.42
11:H:30:GLN:N	11:H:66:ARG:NH1	2.68	0.42
14:L:36:ASP:HB2	39:L:9429:HOH:O	2.18	0.42
21:S:37:VAL:O	21:S:41:VAL:HG23	2.19	0.42
1:0:157:G:H4'	15:M:95:LYS:HE2	2.00	0.41
1:0:1972:U:C2'	1:0:1973:A:H5''	2.50	0.41
1:0:2011:A:H4'	1:0:2012:U:O5'	2.20	0.41
1:0:2326:U:H4'	1:0:2412:G:C4'	2.49	0.41
39:0:4982:HOH:O	4:A:11:ARG:CZ	2.68	0.41
2:9:3042:C:H5'	2:9:3043:G:OP2	2.20	0.41
2:9:3076:G:H3'	2:9:3077:A:C5'	2.31	0.41
6:C:194:PHE:CE2	6:C:234:VAL:HG11	2.55	0.41
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.20	0.41
11:H:79:GLU:C	11:H:80:GLU:HG3	2.44	0.41
16:N:82:TYR:OH	16:N:176:ARG:NH1	2.53	0.41
17:O:26:TRP:N	39:O:3062:HOH:O	2.53	0.41
17:O:45:LEU:CD1	17:O:88:LYS:HD2	2.50	0.41
25:W:45:VAL:HG23	25:W:46:ALA:N	2.35	0.41
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.85	0.41
26:X:80:GLU:O	26:X:80:GLU:HG2	2.20	0.41
1:0:415:A:O2'	1:0:416:G:H5'	2.21	0.41
1:0:816:G:H5'	1:0:1598:A:H4'	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1076:G:C2	1:0:1084:C:C2	3.08	0.41
1:0:1613:C:H2'	1:0:1614:G:O4'	2.19	0.41
1:0:1741:U:H3'	39:0:3376:HOH:O	2.18	0.41
1:0:1947:G:H2'	1:0:1948:G:C8	2.55	0.41
1:0:2065:C:O2'	1:0:2066:C:H5'	2.20	0.41
2:9:3008:G:OP1	16:N:23:ARG:NH1	2.53	0.41
4:A:192:VAL:HG13	39:A:9547:HOH:O	2.19	0.41
5:B:75:GLU:C	5:B:77:PRO:HD3	2.45	0.41
5:B:255:GLY:O	5:B:257:THR:HG22	2.20	0.41
6:C:133:ARG:HE	6:C:138:VAL:HG22	1.84	0.41
7:D:136:ARG:HB3	7:D:137:PRO:HD2	2.01	0.41
10:G:27:ILE:HD13	10:G:71:LEU:HD23	2.02	0.41
16:N:39:SER:HB3	16:N:42:HIS:H	1.85	0.41
17:O:26:TRP:HB2	39:O:3062:HOH:O	2.19	0.41
18:P:16:VAL:CG1	18:P:17:GLY:N	2.82	0.41
20:R:61:GLN:CD	39:R:9452:HOH:O	2.62	0.41
24:V:43:PRO:O	24:V:46:ILE:HG22	2.20	0.41
25:W:38:THR:O	25:W:42:ARG:HB2	2.20	0.41
27:Y:108:ASP:OD1	27:Y:108:ASP:N	2.52	0.41
27:Y:184:GLU:HG2	27:Y:229:LEU:HD11	2.02	0.41
32:I:75:THR:HG22	32:I:79:ILE:CD1	2.51	0.41
4:A:103:VAL:O	4:A:105:VAL:HG23	2.20	0.41
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.56	0.41
23:U:52:THR:HG22	23:U:55:ALA:H	1.85	0.41
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.35	0.41
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.56	0.41
1:0:56:G:H5''	24:V:50:ARG:NH1	2.35	0.41
1:0:553:G:O4'	1:0:1325:G:H5'	2.20	0.41
1:0:1099:G:H2'	1:0:1100:G:O4'	2.21	0.41
1:0:1149:U:H5''	1:0:1151:G:O4'	2.19	0.41
1:0:1432:U:H5'	39:0:9820:HOH:O	2.20	0.41
1:0:2112:A:H2'	1:0:2113:G:C8	2.56	0.41
39:0:6253:HOH:O	13:K:87:ARG:CZ	2.68	0.41
2:9:3092:G:H2'	2:9:3093:A:C8	2.55	0.41
2:9:3107:C:H5	39:9:3167:HOH:O	2.03	0.41
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.19	0.41
12:J:64:GLY:HA3	36:J:9321:CL:CL	2.57	0.41
13:K:98:VAL:HG11	13:K:102:GLU:HA	2.02	0.41
15:M:102:GLU:CD	15:M:164:THR:HG21	2.43	0.41
19:Q:59:GLN:HB3	39:Q:6286:HOH:O	2.20	0.41
31:3:62:THR:HB	39:3:9483:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:297:U:H1'	39:0:4524:HOH:O	2.20	0.41
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.55	0.41
1:0:1659:A:H2'	1:0:1660:G:O4'	2.20	0.41
7:D:172:VAL:CG1	7:D:173:GLU:N	2.82	0.41
12:J:107:ASN:HD22	12:J:109:TYR:H	1.68	0.41
25:W:108:ARG:CG	25:W:114:PRO:HG3	2.43	0.41
1:0:330:C:H5	6:C:170:ASP:OD2	2.04	0.41
1:0:870:G:C3'	1:0:871:G:H5''	2.51	0.41
1:0:1555:G:H4'	1:0:1630:A:C2	2.54	0.41
1:0:1733:A:H4'	5:B:212:GLN:HA	2.02	0.41
1:0:1909:A:N1	1:0:2128:G:H1'	2.36	0.41
1:0:2326:U:H4'	1:0:2412:G:H4'	2.02	0.41
1:0:2724:U:H2'	1:0:2725:G:O4'	2.20	0.41
1:0:2819:C:O4'	5:B:96:PRO:HB2	2.19	0.41
4:A:36:ASP:O	4:A:36:ASP:OD1	2.38	0.41
5:B:60:SER:HA	5:B:61:PRO:HD3	1.92	0.41
5:B:139:ASP:HB3	39:B:9550:HOH:O	2.21	0.41
6:C:104:ASP:CA	6:C:107:ARG:HH12	2.12	0.41
6:C:138:VAL:HG11	6:C:160:LEU:HD13	2.03	0.41
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.90	0.41
15:M:167:GLY:O	15:M:171:ARG:HG3	2.20	0.41
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	2.02	0.41
16:N:38:LYS:HE3	16:N:38:LYS:HB2	1.80	0.41
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.21	0.41
1:0:806:A:H2'	1:0:807:A:O4'	2.20	0.41
1:0:2072:G:C6	1:0:2533:C:H1'	2.56	0.41
4:A:217:ARG:HG3	39:A:9520:HOH:O	2.19	0.41
6:C:133:ARG:NE	6:C:135:GLU:O	2.53	0.41
8:E:18:LEU:HD13	8:E:34:TRP:CG	2.55	0.41
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.77	0.41
11:H:154:TYR:CD1	11:H:154:TYR:C	2.99	0.41
12:J:13:ASP:OD1	12:J:15:ARG:HB3	2.21	0.41
13:K:66:ARG:HG2	13:K:66:ARG:HH11	1.84	0.41
20:R:113:HIS:O	20:R:145:LEU:HD12	2.21	0.41
1:0:371:U:H2'	1:0:372:A:H8	1.86	0.41
1:0:889:C:H2'	1:0:890:C:C6	2.56	0.41
1:0:907:A:H2'	1:0:908:A:H8	1.86	0.41
1:0:1881:A:OP1	4:A:199:HIS:HE1	2.04	0.41
1:0:2504:A:H2'	1:0:2505:G:O4'	2.21	0.41
6:C:93:LYS:O	6:C:98:ARG:NH2	2.54	0.41
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Z:49:ARG:HB2	28:Z:55:TRP:CZ3	2.56	0.41
1:0:396:U:O2'	1:0:418:C:C4'	2.68	0.41
1:0:1008:C:H5''	11:H:16:ARG:HH12	1.86	0.41
1:0:1794:G:N2	1:0:1796:A:H3'	2.36	0.41
1:0:2102:G:H5''	1:0:2538:A:C2	2.55	0.41
1:0:2365:G:H5''	39:Q:6597:HOH:O	2.19	0.41
1:0:2398:A:H2'	1:0:2399:G:O4'	2.20	0.41
1:0:2748:G:H4'	1:0:2749:U:C5'	2.50	0.41
1:0:2857:C:H2'	1:0:2858:U:C6	2.56	0.41
1:0:2868:C:H2'	1:0:2869:G:O4'	2.21	0.41
4:A:55:VAL:HG12	4:A:67:LEU:HD22	2.02	0.41
6:C:133:ARG:HH11	6:C:133:ARG:HG3	1.85	0.41
7:D:76:ARG:O	7:D:77:ASP:HB2	2.21	0.41
8:E:11:VAL:HG13	8:E:23:GLU:O	2.20	0.41
8:E:108:LEU:CD1	8:E:164:ASP:HB2	2.51	0.41
9:F:52:GLU:HG3	9:F:77:VAL:O	2.21	0.41
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.91	0.41
14:L:67:ARG:HG2	14:L:67:ARG:HH11	1.85	0.41
15:M:80:GLY:O	15:M:81:ARG:CD	2.66	0.41
16:N:37:ARG:NH2	16:N:105:GLY:HA3	2.35	0.41
20:R:104:PHE:HB3	20:R:109:MET:HE2	2.03	0.41
22:T:32:ARG:CZ	22:T:38:ARG:NH1	2.84	0.41
22:T:48:VAL:HG21	22:T:96:VAL:HG13	2.02	0.41
24:V:39:ALA:C	24:V:41:GLU:N	2.79	0.41
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.56	0.41
30:2:5:LYS:O	30:2:9:LYS:HG3	2.20	0.41
1:0:1181:A:N1	1:0:1192:A:O2'	2.53	0.41
1:0:1257:C:H2'	1:0:1258:G:O4'	2.21	0.41
1:0:1287:A:O4'	25:W:117:ARG:HD3	2.21	0.41
1:0:2912:C:H2'	1:0:2913:A:O4'	2.21	0.41
2:9:3001:U:H5''	2:9:3003:A:OP1	2.21	0.41
2:9:3056:A:C6	7:D:13:MET:HE3	2.56	0.41
4:A:48:ASP:HA	4:A:49:PRO:HD3	1.94	0.41
7:D:173:GLU:O	7:D:174:VAL:C	2.63	0.41
11:H:54:THR:O	11:H:55:VAL:HG13	2.20	0.41
12:J:47:THR:CG2	12:J:48:GLY:N	2.84	0.41
14:L:145:LEU:C	14:L:147:GLU:N	2.77	0.41
22:T:85:GLU:CG	22:T:86:GLU:N	2.83	0.41
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.56	0.41
30:2:48:ASP:O	30:2:49:GLU:HB2	2.21	0.41
1:0:684:G:H2'	1:0:685:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2718:C:H5'	1:0:2718:C:C6	2.51	0.40
1:0:2820:A:H2'	1:0:2821:C:O4'	2.20	0.40
5:B:112:THR:HG23	5:B:158:LYS:HE3	2.03	0.40
7:D:164:ALA:O	7:D:165:PHE:C	2.63	0.40
8:E:31:ARG:NH1	39:E:5919:HOH:O	2.53	0.40
15:M:69:LYS:HG2	15:M:127:LYS:HG3	2.03	0.40
20:R:145:LEU:HD12	20:R:146:ILE:N	2.36	0.40
26:X:10:VAL:HG12	26:X:11:THR:N	2.35	0.40
1:0:2243:C:H5''	39:0:4344:HOH:O	2.22	0.40
4:A:97:ALA:HB2	4:A:150:PRO:HB2	2.03	0.40
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.45	0.40
6:C:57:PRO:HG2	6:C:73:LEU:CD1	2.50	0.40
7:D:65:GLU:HA	39:D:6752:HOH:O	2.21	0.40
21:S:29:ASP:CG	21:S:31:ARG:NH1	2.80	0.40
1:0:561:G:O2'	1:0:562:A:H5'	2.21	0.40
1:0:881:C:H5''	39:0:4234:HOH:O	2.20	0.40
1:0:1873:G:H2'	1:0:1874:U:H5'	2.03	0.40
2:9:3088:G:OP1	25:W:130:HIS:NE2	2.48	0.40
5:B:175:LEU:C	5:B:175:LEU:CD2	2.93	0.40
11:H:28:ILE:HG21	11:H:31:HIS:CE1	2.56	0.40
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.51	0.40
25:W:38:THR:CG2	25:W:39:ASP:N	2.84	0.40
26:X:25:ARG:HD2	39:X:3861:HOH:O	2.20	0.40
1:0:1706:G:OP1	18:P:65:ARG:HD2	2.21	0.40
1:0:2250:G:OP1	4:A:31:LYS:HD3	2.22	0.40
1:0:2445:U:H2'	1:0:2446:G:C8	2.56	0.40
1:0:2509:A:H2'	1:0:2510:C:O4'	2.21	0.40
39:0:6200:HOH:O	22:T:68:ASP:HB2	2.20	0.40
4:A:94:LEU:HD12	4:A:98:GLU:HB2	2.02	0.40
7:D:128:LEU:HB2	39:D:6007:HOH:O	2.20	0.40
8:E:112:ALA:HA	8:E:113:PRO:HD3	1.86	0.40
13:K:115:ARG:O	13:K:118:ALA:HB3	2.21	0.40
13:K:125:ALA:O	13:K:127:ALA:N	2.54	0.40
19:Q:46:SER:O	19:Q:48:PRO:HD3	2.22	0.40
1:0:694:A:H2'	1:0:695:C:H5'	2.03	0.40
1:0:1015:C:H2'	1:0:1016:U:C6	2.56	0.40
1:0:1386:G:O2'	1:0:1387:G:H5'	2.22	0.40
1:0:1679:C:H5'	39:0:9941:HOH:O	2.22	0.40
1:0:2283:G:C6	11:H:113:MET:HB3	2.56	0.40
1:0:2507:G:H2'	1:0:2510:C:N4	2.33	0.40
4:A:171:LYS:NZ	39:A:9514:HOH:O	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:173:GLY:O	4:A:176:HIS:HB3	2.21	0.40
6:C:124:VAL:HA	6:C:230:GLY:O	2.22	0.40
7:D:27:ILE:HG22	7:D:28:GLY:N	2.35	0.40
7:D:57:THR:HG23	7:D:63:ILE:CA	2.41	0.40
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.69	0.40
8:E:84:MET:HE3	8:E:131:LEU:HD13	2.03	0.40
9:F:1:PRO:H3	9:F:4:VAL:HG23	1.86	0.40
14:L:6:ARG:NH2	39:L:9441:HOH:O	2.53	0.40
29:1:28:HIS:HD2	29:1:30:LYS:H	1.69	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%)	212 (90%)	19 (8%)	4 (2%)	7	3
5	B	335/338 (99%)	316 (94%)	16 (5%)	3 (1%)	14	12
6	C	244/246 (99%)	224 (92%)	20 (8%)	0	100	100
7	D	134/177 (76%)	108 (81%)	14 (10%)	12 (9%)	0	0
8	E	170/178 (96%)	166 (98%)	4 (2%)	0	100	100
9	F	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	7	3
10	G	25/348 (7%)	25 (100%)	0	0	100	100
11	H	156/171 (91%)	143 (92%)	11 (7%)	2 (1%)	9	6
12	J	140/145 (97%)	132 (94%)	6 (4%)	2 (1%)	9	5
13	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	16	14
14	L	141/165 (86%)	123 (87%)	17 (12%)	1 (1%)	18	17
15	M	192/195 (98%)	183 (95%)	9 (5%)	0	100	100
16	N	184/187 (98%)	165 (90%)	13 (7%)	6 (3%)	3	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
18	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
19	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	R	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	18	17
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
22	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	14	12
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	3	1
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%)	140 (100%)	0	0	100	100
28	Z	71/83 (86%)	59 (83%)	8 (11%)	4 (6%)	1	0
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%)	89 (99%)	0	1 (1%)	11	8
32	I	68/162 (42%)	53 (78%)	14 (21%)	1 (2%)	8	4
All	All	3705/4431 (84%)	3451 (93%)	211 (6%)	43 (1%)	10	7

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	H	166	SER
14	L	80	ASP
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG
4	A	34	ASP
4	A	37	VAL
5	B	34	GLY
5	B	169	GLY
7	D	27	ILE
7	D	60	GLU
7	D	137	PRO
7	D	171	ASP
7	D	173	GLU
9	F	101	ALA

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Mol	Chain	Res	Type
11	H	168	ALA
12	J	143	LYS
4	A	132	ASP
5	B	185	GLY
7	D	16	PRO
7	D	28	GLY
7	D	56	ARG
12	J	5	GLU
13	K	126	SER
16	N	164	ASP
16	N	167	ASP
16	N	183	ASP
22	T	53	GLY
24	V	43	PRO
7	D	65	GLU
7	D	97	GLN
28	Z	20	ARG
28	Z	43	GLY
7	D	61	PHE
16	N	155	GLU
4	A	236	GLY
9	F	71	GLY
31	3	56	PRO
32	I	129	VAL
24	V	2	VAL
28	Z	21	VAL
7	D	138	GLY
20	R	81	PRO

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%)	168 (94%)	11 (6%)	17	17
5	B	282/283 (100%)	256 (91%)	26 (9%)	8	6
6	C	193/193 (100%)	175 (91%)	18 (9%)	8	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	D	117/148 (79%)	113 (97%)	4 (3%)	32	40
8	E	152/156 (97%)	150 (99%)	2 (1%)	61	72
9	F	93/94 (99%)	91 (98%)	2 (2%)	45	56
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	24	29
12	J	118/121 (98%)	112 (95%)	6 (5%)	21	23
13	K	106/106 (100%)	101 (95%)	5 (5%)	23	26
14	L	113/127 (89%)	108 (96%)	5 (4%)	25	29
15	M	158/159 (99%)	154 (98%)	4 (2%)	42	52
16	N	149/150 (99%)	145 (97%)	4 (3%)	39	49
17	O	93/94 (99%)	92 (99%)	1 (1%)	65	75
18	P	113/117 (97%)	109 (96%)	4 (4%)	32	39
19	Q	79/80 (99%)	74 (94%)	5 (6%)	16	16
20	R	117/122 (96%)	114 (97%)	3 (3%)	40	50
21	S	71/74 (96%)	70 (99%)	1 (1%)	59	70
22	T	105/106 (99%)	101 (96%)	4 (4%)	29	36
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	48	59
25	W	130/130 (100%)	127 (98%)	3 (2%)	44	55
26	X	66/74 (89%)	61 (92%)	5 (8%)	12	10
27	Y	120/196 (61%)	110 (92%)	10 (8%)	10	8
28	Z	60/68 (88%)	59 (98%)	1 (2%)	53	65
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	43	54
31	3	79/79 (100%)	78 (99%)	1 (1%)	61	72
32	I	58/130 (45%)	57 (98%)	1 (2%)	53	65
All	All	3093/3612 (86%)	2959 (96%)	134 (4%)	26	31

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	26	ASP

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Mol	Chain	Res	Type
4	A	33	GLU
4	A	36	ASP
4	A	55	VAL
4	A	94	LEU
4	A	131	HIS
4	A	165	THR
4	A	175	LYS
4	A	179	MET
4	A	217	ARG
5	B	7	ARG
5	B	11	LEU
5	B	27	ASN
5	B	28	SER
5	B	33	ASP
5	B	51	VAL
5	B	53	LEU
5	B	71	VAL
5	B	82	VAL
5	B	84	LEU
5	B	98	THR
5	B	112	THR
5	B	113	LEU
5	B	149	ASP
5	B	162	MET
5	B	175	LEU
5	B	190	MET
5	B	195	ARG
5	B	234	ARG
5	B	251	VAL
5	B	254	GLN
5	B	257	THR
5	B	265	LEU
5	B	277	GLU
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	16	VAL
6	C	67	GLN
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	101	ASP

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Mol	Chain	Res	Type
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	202	THR
6	C	214	THR
6	C	222	ASP
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	61	PHE
7	D	99	ASP
7	D	137	PRO
8	E	86	VAL
8	E	102	VAL
9	F	12	LEU
9	F	46	GLU
11	H	18	GLU
11	H	51	VAL
11	H	84	LYS
11	H	154	TYR
11	H	159	PRO
11	H	170	ASN
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	93	ARG
12	J	127	ILE
12	J	131	THR
13	K	4	LEU
13	K	10	GLN
13	K	44	LEU
13	K	49	LEU
13	K	98	VAL
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
14	L	104	ASP
14	L	140	VAL
15	M	46	LEU

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Mol	Chain	Res	Type
15	M	93	ARG
15	M	99	ARG
15	M	164	THR
16	N	12	ARG
16	N	26	LEU
16	N	127	LEU
16	N	139	TRP
17	O	111	VAL
18	P	21	VAL
18	P	52	LYS
18	P	81	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	16	ASN
19	Q	18	PRO
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	82	GLU
20	R	132	ARG
21	S	10	VAL
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
22	T	96	VAL
24	V	65	ASP
25	W	26	ILE
25	W	35	VAL
25	W	146	ILE
26	X	8	ARG
26	X	15	ARG
26	X	72	VAL
26	X	79	GLU
26	X	85	VAL
27	Y	103	THR
27	Y	115	ARG
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	200	THR

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Mol	Chain	Res	Type
27	Y	203	VAL
27	Y	235	GLU
28	Z	78	THR
30	2	18	ASN
31	3	56	PRO
32	I	77	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	188	ASN
4	A	199	HIS
4	A	218	ASN
5	B	27	ASN
5	B	94	GLN
5	B	145	HIS
5	B	177	HIS
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
6	C	151	GLN
6	C	163	HIS
6	C	178	GLN
7	D	103	ASN
7	D	133	ASN
8	E	106	ASN
8	E	119	HIS
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	132	GLN
11	H	170	ASN
12	J	25	GLN

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Mol	Chain	Res	Type
12	J	52	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
14	L	58	GLN
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	77	HIS
15	M	143	ASN
15	M	170	ASN
16	N	22	GLN
16	N	93	GLN
16	N	107	ASN
16	N	140	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	88	GLN
18	P	101	GLN
18	P	118	GLN
19	Q	40	HIS
20	R	22	GLN
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
20	R	122	GLN
20	R	140	GLN
21	S	9	HIS
21	S	53	ASN
21	S	55	GLN
22	T	7	GLN
22	T	11	GLN
22	T	37	GLN
22	T	39	ASN
22	T	43	ASN

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Mol	Chain	Res	Type
22	T	73	HIS
23	U	30	HIS
23	U	39	ASN
23	U	48	ASN
24	V	6	GLN
24	V	60	GLN
25	W	14	HIS
25	W	27	HIS
25	W	59	GLN
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
27	Y	119	GLN
27	Y	127	GLN
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	153	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	36	ASN
30	2	41	HIS
30	2	45	ASN
31	3	18	GLN
31	3	30	GLN
31	3	48	ASN
32	I	104	GLN
32	I	113	HIS
32	I	123	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	246 (8%)	34 (1%)
2	9	121/122 (99%)	14 (11%)	1 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	4	0/8	-	-
All	All	2866/3052 (93%)	260 (9%)	35 (1%)

All (260) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	21	G
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	170	U
1	0	186	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
1	0	358	G

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Mol	Chain	Res	Type
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	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	735	C
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	846	A
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	875	A
1	0	877	G

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Mol	Chain	Res	Type
1	0	878	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	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1246	A
1	0	1247	A
1	0	1279	U
1	0	1289	C
1	0	1331	A
1	0	1342	C

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Mol	Chain	Res	Type
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	1692	C
1	0	1693	A
1	0	1701	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	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

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Mol	Chain	Res	Type
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2526	C
1	0	2527	U

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Mol	Chain	Res	Type
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
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	2613	G
1	0	2634	G
1	0	2637	A
1	0	2644	C
1	0	2645	U
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	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2840	A
1	0	2852	A
1	0	2853	U
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A

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Mol	Chain	Res	Type
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
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	1232	A
1	0	1237	U
1	0	1246	A
1	0	1351	G
1	0	1352	A
1	0	1506	U
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1730	G
1	0	1856	C
1	0	1979	G
1	0	2011	A

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Mol	Chain	Res	Type
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2541	U
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2852	A
2	9	3065	A

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

8 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	HFA	4	77	3	10,11,12	1.27	1 (10%)	11,13,15	0.64	0
1	UR3	0	2619	1	19,22,23	0.43	0	26,32,35	0.69	1 (3%)
1	1MA	0	628	1,35	21,25,26	0.70	1 (4%)	30,37,40	0.84	2 (6%)
1	PSU	0	2621	1	18,21,22	1.65	2 (11%)	21,30,33	1.34	3 (14%)
3	PPU	4	76	1,3	23,26,41	0.38	0	29,38,60	0.80	1 (3%)
1	OMG	0	2588	1,3	23,26,27	0.30	0	32,38,41	0.40	0
1	OMU	0	2587	1	19,22,23	0.32	0	25,31,34	0.42	0
3	DCZ	4	74	3	17,17,17	0.27	0	24,24,24	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HFA	4	77	3	-	1/5/6/8	0/1/1/1
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	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
3	PPU	4	76	1,3	-	0/11/29/44	0/3/3/4
1	OMG	0	2588	1,3	-	0/9/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
3	DCZ	4	74	3	-	0/6/18/18	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.31	1.43	1.36
1	0	2621	PSU	C6-C5	3.54	1.39	1.35
3	4	77	HFA	OA-CA	3.36	1.49	1.43
1	0	628	1MA	C6-N6	2.38	1.33	1.28

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.37	120.45	118.17
1	0	2621	PSU	C6-N1-C2	-3.20	119.72	122.69
3	4	76	PPU	C2-N1-C6	2.89	118.89	111.83
1	0	2621	PSU	O2-C2-N1	2.78	125.65	122.79
1	0	628	1MA	N1-C2-N3	2.75	129.26	126.00
1	0	2619	UR3	C4-N3-C2	2.69	126.75	124.58
1	0	628	1MA	CM1-N1-C6	2.28	123.69	120.15

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	4	77	HFA	C-CA-CB-CG
1	0	628	1MA	C2'-C1'-N9-C8
1	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	4	77	HFA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2619	UR3	1	0
1	0	2587	OMU	2	0
3	4	74	DCZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 313 ligands modelled in this entry, 313 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.18	96 (3%) 47 47	23, 45, 88, 147	0
2	9	122/122 (100%)	0.58	8 (6%) 24 23	40, 63, 89, 149	0
3	4	4/8 (50%)	-0.35	0 100 100	40, 45, 47, 48	0
4	A	237/240 (98%)	0.65	21 (8%) 15 14	27, 48, 83, 102	0
5	B	337/338 (99%)	0.58	17 (5%) 34 33	27, 50, 76, 88	0
6	C	246/246 (100%)	0.54	10 (4%) 41 41	24, 45, 68, 79	0
7	D	140/177 (79%)	2.65	87 (62%) 0 0	55, 93, 121, 129	0
8	E	172/178 (96%)	1.14	22 (12%) 7 7	41, 63, 83, 88	0
9	F	119/120 (99%)	1.37	24 (20%) 3 2	46, 69, 94, 106	0
10	G	29/348 (8%)	2.13	13 (44%) 0 0	67, 89, 97, 100	0
11	H	160/171 (93%)	0.99	16 (10%) 12 12	40, 58, 91, 98	0
12	J	142/145 (97%)	0.55	9 (6%) 26 24	34, 47, 69, 90	0
13	K	132/132 (100%)	0.34	5 (3%) 44 44	33, 44, 68, 78	0
14	L	145/165 (87%)	1.18	30 (20%) 2 2	26, 62, 107, 117	0
15	M	194/195 (99%)	0.54	19 (9%) 13 12	32, 44, 60, 69	0
16	N	186/187 (99%)	1.49	48 (25%) 1 1	44, 61, 107, 115	0
17	O	115/116 (99%)	0.92	7 (6%) 27 25	38, 53, 68, 77	0
18	P	143/149 (95%)	0.70	12 (8%) 17 15	36, 50, 63, 75	0
19	Q	95/96 (98%)	0.43	3 (3%) 50 50	37, 46, 61, 72	0
20	R	150/155 (96%)	0.16	3 (2%) 65 65	30, 43, 62, 71	0
21	S	81/85 (95%)	0.74	6 (7%) 20 19	39, 55, 75, 90	0
22	T	119/120 (99%)	0.96	10 (8%) 17 15	39, 53, 79, 104	0
23	U	53/66 (80%)	0.66	4 (7%) 20 18	40, 50, 69, 78	0
24	V	65/71 (91%)	1.80	17 (26%) 1 1	52, 72, 109, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.64	7 (4%) 38 37	37, 49, 69, 78	0
26	X	82/92 (89%)	0.97	14 (17%) 4 3	39, 54, 81, 98	0
27	Y	142/241 (58%)	0.40	8 (5%) 30 28	28, 42, 64, 84	0
28	Z	73/83 (87%)	1.44	21 (28%) 1 1	46, 63, 80, 91	0
29	1	56/57 (98%)	-0.06	1 (1%) 67 68	28, 33, 40, 48	0
30	2	46/50 (92%)	1.53	14 (30%) 1 0	34, 60, 89, 96	0
31	3	92/92 (100%)	0.75	7 (7%) 20 18	34, 54, 68, 80	0
32	I	70/162 (43%)	4.07	64 (91%) 0 0	105, 117, 137, 138	0
All	All	6650/7483 (88%)	0.46	623 (9%) 14 13	23, 50, 95, 149	0

All (623) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	V	1	THR	13.3
16	N	166	ALA	10.0
32	I	133	THR	9.5
7	D	10	PHE	9.3
32	I	88	GLY	7.9
32	I	90	GLY	7.8
7	D	107	GLY	7.8
2	9	3001	U	7.6
16	N	154	LEU	7.3
32	I	76	ALA	7.3
5	B	1	PRO	7.3
32	I	79	ILE	7.3
24	V	2	VAL	7.0
16	N	168	LEU	7.0
14	L	82	ALA	6.9
1	0	2645	U	6.8
32	I	121	LEU	6.6
22	T	119	ALA	6.5
7	D	174	VAL	6.5
24	V	43	PRO	6.4
32	I	85	PHE	6.3
22	T	117	ASP	6.3
32	I	138	THR	6.2
32	I	96	PHE	6.1
32	I	129	VAL	6.1
32	I	117	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
7	D	55	LYS	6.0
32	I	139	ILE	6.0
16	N	165	ALA	5.9
4	A	37	VAL	5.9
30	2	49	GLU	5.9
32	I	137	VAL	5.8
10	G	12	ILE	5.8
7	D	57	THR	5.6
17	O	22	GLY	5.6
11	H	111	ASP	5.6
12	J	70	PHE	5.6
21	S	81	ILE	5.5
32	I	105	VAL	5.5
24	V	40	PRO	5.5
8	E	10	ASP	5.5
24	V	39	ALA	5.5
1	0	1161	A	5.4
32	I	87	THR	5.4
32	I	135	LEU	5.4
7	D	90	LEU	5.3
32	I	78	LEU	5.3
1	0	1173	A	5.3
26	X	88	GLU	5.3
28	Z	82	SER	5.2
32	I	109	ALA	5.2
32	I	72	VAL	5.2
32	I	132	CYS	5.2
7	D	135	VAL	5.1
11	H	168	ALA	5.1
32	I	118	SER	5.1
28	Z	10	ARG	5.0
7	D	63	ILE	5.0
1	0	1175	G	5.0
28	Z	11	SER	5.0
22	T	118	SER	4.9
7	D	61	PHE	4.9
8	E	45	ASP	4.9
32	I	125	ALA	4.9
15	M	70	GLY	4.9
32	I	128	VAL	4.9
14	L	146	GLY	4.9
32	I	102	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
14	L	78	ALA	4.8
15	M	74	LYS	4.8
14	L	77	ALA	4.8
7	D	172	VAL	4.8
11	H	112	GLY	4.7
32	I	97	VAL	4.6
1	0	2748	G	4.6
1	0	10	U	4.6
2	9	3002	U	4.6
14	L	148	GLU	4.6
18	P	143	ALA	4.5
10	G	71	LEU	4.5
4	A	36	ASP	4.5
32	I	116	LEU	4.5
32	I	92	PRO	4.5
1	0	2345	A	4.5
4	A	35	GLY	4.5
32	I	89	SER	4.5
7	D	171	ASP	4.5
30	2	37	HIS	4.4
30	2	44	ARG	4.4
12	J	4	ALA	4.4
32	I	131	THR	4.4
10	G	26	MET	4.4
16	N	186	LEU	4.4
7	D	11	HIS	4.4
16	N	167	ASP	4.4
16	N	37	ARG	4.3
7	D	105	SER	4.3
7	D	106	PHE	4.3
14	L	91	VAL	4.3
30	2	38	LYS	4.2
7	D	35	ALA	4.2
7	D	54	ALA	4.2
16	N	163	PHE	4.2
7	D	157	LEU	4.1
7	D	69	ILE	4.1
26	X	87	ALA	4.1
14	L	150	GLN	4.1
1	0	138	U	4.1
7	D	134	LEU	4.1
32	I	75	THR	4.1

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Mol	Chain	Res	Type	RSRZ
7	D	50	VAL	4.1
26	X	85	VAL	4.1
16	N	169	PRO	4.0
9	F	102	GLY	4.0
16	N	164	ASP	4.0
30	2	48	ASP	4.0
7	D	73	VAL	4.0
32	I	100	LEU	4.0
4	A	38	ILE	4.0
7	D	44	ILE	4.0
1	0	2769	C	3.9
15	M	79	ALA	3.9
14	L	99	GLU	3.9
7	D	36	ASN	3.9
10	G	73	ASP	3.9
32	I	114	PRO	3.9
11	H	169	GLY	3.9
14	L	81	VAL	3.9
9	F	8	VAL	3.8
1	0	1192	A	3.8
7	D	62	ASP	3.8
22	T	116	ASP	3.8
24	V	42	ASN	3.8
8	E	154	ILE	3.8
14	L	143	THR	3.8
1	0	1169	U	3.8
17	O	23	GLY	3.8
1	0	1176	C	3.7
5	B	2	GLN	3.7
19	Q	95	GLU	3.7
32	I	119	TYR	3.7
26	X	65	ASN	3.7
16	N	158	LEU	3.7
16	N	95	ALA	3.7
8	E	12	ASP	3.7
14	L	149	ARG	3.7
7	D	18	ILE	3.6
7	D	12	GLU	3.6
7	D	88	LEU	3.6
30	2	35	ARG	3.6
1	0	737	A	3.6
7	D	59	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
7	D	128	LEU	3.6
14	L	75	LEU	3.6
7	D	89	PRO	3.6
11	H	40	ALA	3.6
32	I	80	LYS	3.6
1	0	1193	A	3.6
1	0	2004	U	3.6
1	0	1165	G	3.6
16	N	134	ASP	3.6
6	C	16	VAL	3.6
9	F	101	ALA	3.6
32	I	93	GLN	3.5
8	E	20	ILE	3.5
32	I	84	GLY	3.5
32	I	106	LYS	3.5
31	3	41	GLU	3.5
32	I	74	PRO	3.5
1	0	514	G	3.5
32	I	134	SER	3.5
1	0	288	A	3.5
7	D	170	TYR	3.5
1	0	960	G	3.5
7	D	131	THR	3.5
16	N	137	ALA	3.5
32	I	98	ALA	3.5
10	G	27	ILE	3.5
16	N	179	LEU	3.5
1	0	1525	G	3.5
1	0	1964	U	3.5
14	L	83	GLU	3.4
7	D	17	ARG	3.4
7	D	137	PRO	3.4
16	N	157	PRO	3.4
32	I	73	PRO	3.4
14	L	145	LEU	3.4
2	9	3024	U	3.4
32	I	82	GLU	3.4
7	D	29	HIS	3.4
16	N	1	ALA	3.4
1	0	1168	C	3.3
18	P	116	SER	3.3
27	Y	236	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
4	A	31	LYS	3.3
16	N	147	ILE	3.3
16	N	172	PHE	3.3
32	I	122	THR	3.3
32	I	113	HIS	3.3
1	0	1162	G	3.3
1	0	1172	G	3.3
22	T	114	SER	3.3
5	B	56	ASP	3.3
24	V	46	ILE	3.3
4	A	237	GLY	3.3
7	D	40	ILE	3.3
13	K	119	GLN	3.3
24	V	44	GLY	3.2
7	D	49	PRO	3.2
32	I	140	GLU	3.2
7	D	104	PHE	3.2
16	N	159	TYR	3.2
7	D	58	VAL	3.2
32	I	83	ALA	3.2
1	0	1524	U	3.2
7	D	154	LYS	3.2
22	T	115	GLU	3.2
24	V	41	GLU	3.2
7	D	155	HIS	3.2
15	M	80	GLY	3.2
11	H	170	ASN	3.2
8	E	126	ILE	3.2
10	G	29	SER	3.2
32	I	112	LYS	3.2
16	N	162	ASP	3.2
9	F	118	LEU	3.2
1	0	1929	G	3.2
1	0	497	A	3.2
1	0	2747	C	3.1
8	E	87	PHE	3.1
24	V	36	ALA	3.1
1	0	736	A	3.1
10	G	63	ARG	3.1
22	T	36	GLY	3.1
1	0	1166	A	3.1
4	A	211	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
7	D	153	THR	3.1
1	0	735	C	3.1
1	0	128	A	3.1
5	B	57	GLU	3.1
1	0	1951	G	3.1
1	0	2237	G	3.1
7	D	86	THR	3.1
30	2	47	THR	3.1
1	0	1170	U	3.1
15	M	1	ALA	3.1
1	0	1171	A	3.0
1	0	1981	A	3.0
7	D	52	THR	3.0
26	X	83	ALA	3.0
28	Z	16	ALA	3.0
4	A	32	VAL	3.0
7	D	93	LEU	3.0
7	D	74	THR	3.0
7	D	101	THR	3.0
1	0	1197	G	3.0
10	G	23	ILE	3.0
32	I	108	ILE	3.0
1	0	1167	G	3.0
7	D	26	GLY	3.0
1	0	284	C	3.0
11	H	167	PRO	3.0
7	D	37	ALA	3.0
7	D	21	VAL	3.0
1	0	1164	U	3.0
4	A	34	ASP	3.0
7	D	66	GLY	3.0
7	D	13	MET	3.0
1	0	271	C	2.9
5	B	171	VAL	2.9
9	F	119	ARG	2.9
18	P	117	SER	2.9
7	D	60	GLU	2.9
8	E	53	GLU	2.9
26	X	79	GLU	2.9
27	Y	235	GLU	2.9
32	I	71	GLY	2.9
1	0	999	C	2.9

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Mol	Chain	Res	Type	RSRZ
1	0	1204	C	2.9
5	B	119	HIS	2.9
7	D	56	ARG	2.9
25	W	108	ARG	2.9
27	Y	216	ARG	2.9
28	Z	78	THR	2.9
32	I	77	GLU	2.9
32	I	94	GLU	2.9
8	E	123	ASP	2.9
1	0	87	C	2.9
9	F	104	ALA	2.9
9	F	112	ALA	2.9
13	K	118	ALA	2.9
9	F	60	VAL	2.9
1	0	2511	A	2.9
8	E	172	PRO	2.9
6	C	8	LEU	2.9
9	F	22	VAL	2.9
9	F	111	ILE	2.9
18	P	18	LYS	2.8
26	X	81	GLY	2.8
7	D	75	LEU	2.8
1	0	2344	G	2.8
16	N	170	GLU	2.8
22	T	82	THR	2.8
10	G	70	ALA	2.8
7	D	53	LYS	2.8
7	D	166	ILE	2.8
12	J	46	ILE	2.8
14	L	130	ARG	2.8
16	N	160	SER	2.8
17	O	1	SER	2.8
22	T	53	GLY	2.8
1	0	1160	G	2.8
15	M	75	ARG	2.8
8	E	39	ASP	2.8
30	2	42	TRP	2.8
28	Z	42	CYS	2.8
1	0	1174	A	2.8
1	0	1177	A	2.8
1	0	2508	C	2.8
28	Z	12	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
20	R	150	PRO	2.7
1	0	272	A	2.7
32	I	126	LYS	2.7
7	D	132	VAL	2.7
15	M	77	HIS	2.7
7	D	47	GLN	2.7
32	I	120	ASP	2.7
1	0	358	G	2.7
4	A	236	GLY	2.7
16	N	76	GLY	2.7
16	N	175	LEU	2.7
28	Z	20	ARG	2.7
7	D	91	ALA	2.7
7	D	22	VAL	2.7
26	X	84	ILE	2.7
9	F	9	PRO	2.7
1	0	441	A	2.7
28	Z	24	ARG	2.7
1	0	970	U	2.7
1	0	1205	U	2.7
7	D	142	ALA	2.7
16	N	67	ALA	2.7
1	0	1184	C	2.7
26	X	66	THR	2.7
4	A	206	ARG	2.7
23	U	47	ARG	2.7
17	O	24	ALA	2.6
32	I	111	GLN	2.6
9	F	91	VAL	2.6
27	Y	108	ASP	2.6
28	Z	22	SER	2.6
1	0	2506	A	2.6
1	0	1561	U	2.6
2	9	3023	U	2.6
5	B	183	GLU	2.6
9	F	103	GLU	2.6
5	B	180	ASP	2.6
16	N	161	GLY	2.6
1	0	1188	A	2.6
26	X	7	GLU	2.6
9	F	105	ASP	2.6
5	B	34	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
7	D	102	GLY	2.6
7	D	169	THR	2.6
11	H	137	TYR	2.6
14	L	57	VAL	2.6
19	Q	76	VAL	2.6
11	H	32	LYS	2.6
11	H	62	LEU	2.6
26	X	61	ARG	2.6
6	C	132	ASP	2.6
25	W	91	ASP	2.6
23	U	52	THR	2.6
8	E	11	VAL	2.6
14	L	93	VAL	2.6
4	A	208	HIS	2.6
4	A	33	GLU	2.5
7	D	19	GLU	2.5
24	V	3	LEU	2.5
26	X	82	GLU	2.5
30	2	27	LEU	2.5
1	0	1523	G	2.5
32	I	95	ASP	2.5
15	M	78	LYS	2.5
28	Z	79	VAL	2.5
7	D	27	ILE	2.5
14	L	121	ILE	2.5
28	Z	29	ILE	2.5
1	0	1179	C	2.5
2	9	3122	C	2.5
7	D	92	GLU	2.5
14	L	147	GLU	2.5
25	W	86	GLU	2.5
6	C	133	ARG	2.5
18	P	114	LEU	2.5
1	0	1202	A	2.5
1	0	2768	A	2.5
2	9	3057	A	2.5
11	H	171	ALA	2.5
23	U	10	GLY	2.5
11	H	166	SER	2.5
5	B	108	GLU	2.5
7	D	167	GLU	2.5
7	D	173	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
6	C	76	ARG	2.5
1	0	1191	A	2.5
15	M	194	ALA	2.5
32	I	124	ALA	2.5
9	F	1	PRO	2.5
7	D	98	PHE	2.5
8	E	102	VAL	2.5
9	F	90	GLU	2.5
14	L	73	VAL	2.5
16	N	68	GLU	2.5
28	Z	81	ARG	2.5
1	0	1182	C	2.5
8	E	81	GLU	2.4
12	J	5	GLU	2.4
32	I	86	GLU	2.4
18	P	58	SER	2.4
1	0	282	C	2.4
7	D	41	LEU	2.4
32	I	123	ASN	2.4
21	S	12	GLU	2.4
24	V	13	PRO	2.4
7	D	165	PHE	2.4
15	M	91	ILE	2.4
28	Z	18	TYR	2.4
30	2	46	ASP	2.4
6	C	237	GLU	2.4
32	I	130	GLY	2.4
2	9	3022	G	2.4
1	0	1206	U	2.4
22	T	40	VAL	2.4
17	O	98	LEU	2.4
1	0	1199	A	2.4
16	N	40	ASN	2.4
16	N	156	GLU	2.4
32	I	81	ASP	2.4
16	N	74	PRO	2.4
14	L	62	ALA	2.4
24	V	38	GLY	2.4
1	0	1950	G	2.4
1	0	1967	U	2.4
5	B	51	VAL	2.4
7	D	48	MET	2.4

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Mol	Chain	Res	Type	RSRZ
8	E	7	ILE	2.4
13	K	132	VAL	2.4
16	N	184	ILE	2.4
24	V	45	ARG	2.4
16	N	150	TYR	2.3
1	0	734	U	2.3
1	0	2419	U	2.3
4	A	84	VAL	2.3
12	J	6	PHE	2.3
21	S	20	PHE	2.3
15	M	68	ARG	2.3
32	I	104	GLN	2.3
14	L	102	ASP	2.3
29	1	47	ASP	2.3
7	D	138	GLY	2.3
4	A	39	ALA	2.3
8	E	13	ALA	2.3
18	P	77	ALA	2.3
12	J	47	THR	2.3
15	M	89	THR	2.3
26	X	68	SER	2.3
7	D	51	ARG	2.3
28	Z	25	ARG	2.3
1	0	1195	G	2.3
6	C	171	GLU	2.3
9	F	98	VAL	2.3
18	P	92	GLU	2.3
18	P	111	GLU	2.3
31	3	18	GLN	2.3
9	F	89	LEU	2.3
4	A	205	GLY	2.3
16	N	69	TYR	2.3
11	H	136	ALA	2.3
16	N	2	THR	2.3
25	W	88	THR	2.3
21	S	1	SER	2.3
7	D	15	GLU	2.3
25	W	60	GLU	2.3
25	W	26	ILE	2.3
7	D	141	VAL	2.3
9	F	2	VAL	2.3
16	N	43	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
20	R	119	VAL	2.3
1	0	1203	G	2.3
5	B	33	ASP	2.3
1	0	2644	C	2.3
7	D	68	PRO	2.3
10	G	13	PRO	2.3
1	0	1189	A	2.3
1	0	1200	A	2.3
32	I	136	GLY	2.3
9	F	99	THR	2.3
16	N	80	SER	2.3
17	O	20	SER	2.3
14	L	96	VAL	2.3
15	M	88	VAL	2.3
24	V	20	LEU	2.2
1	0	289	G	2.2
5	B	118	ASP	2.2
15	M	82	ARG	2.2
28	Z	46	ARG	2.2
30	2	43	ARG	2.2
1	0	1279	U	2.2
12	J	144	THR	2.2
5	B	21	SER	2.2
21	S	2	TRP	2.2
21	S	75	GLN	2.2
6	C	61	PHE	2.2
14	L	97	VAL	2.2
27	Y	187	VAL	2.2
28	Z	14	PHE	2.2
5	B	139	ASP	2.2
9	F	24	ARG	2.2
5	B	279	THR	2.2
9	F	106	ALA	2.2
17	O	3	THR	2.2
16	N	50	LEU	2.2
7	D	130	VAL	2.2
14	L	80	ASP	2.2
15	M	87	GLY	2.2
1	0	287	C	2.2
2	9	3065	A	2.2
27	Y	95	THR	2.2
27	Y	106	THR	2.2

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Mol	Chain	Res	Type	RSRZ
14	L	105	TYR	2.2
4	A	153	ARG	2.2
6	C	101	ASP	2.2
10	G	72	ASP	2.2
16	N	135	VAL	2.2
16	N	138	ASP	2.2
26	X	46	ASP	2.2
9	F	117	GLU	2.2
11	H	36	LYS	2.2
15	M	86	GLN	2.2
20	R	122	GLN	2.2
1	0	283	U	2.2
1	0	1163	G	2.2
1	0	2914	A	2.2
4	A	97	ALA	2.2
7	D	150	SER	2.2
13	K	58	THR	2.2
16	N	75	THR	2.2
16	N	145	ALA	2.2
31	3	26	ARG	2.1
12	J	127	ILE	2.1
4	A	26	ASP	2.1
8	E	86	VAL	2.1
11	H	140	VAL	2.1
24	V	65	ASP	2.1
8	E	125	GLU	2.1
31	3	23	GLU	2.1
32	I	91	GLU	2.1
7	D	97	GLN	2.1
14	L	43	HIS	2.1
1	0	139	C	2.1
8	E	46	THR	2.1
16	N	148	ALA	2.1
16	N	5	ARG	2.1
30	2	39	ARG	2.1
11	H	163	ILE	2.1
14	L	76	LEU	2.1
7	D	77	ASP	2.1
18	P	110	ASP	2.1
19	Q	20	ASP	2.1
8	E	124	VAL	2.1
10	G	15	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
31	3	56	PRO	2.1
1	0	1625	U	2.1
1	0	1201	C	2.1
1	0	1190	G	2.1
7	D	95	THR	2.1
8	E	32	ARG	2.1
15	M	125	ARG	2.1
6	C	63	SER	2.1
16	N	41	LYS	2.1
18	P	64	GLU	2.1
12	J	63	ILE	2.1
4	A	131	HIS	2.1
14	L	55	GLN	2.1
10	G	20	VAL	2.1
7	D	46	GLY	2.1
1	0	361	C	2.1
1	0	369	G	2.1
15	M	72	ALA	2.1
16	N	59	ALA	2.1
31	3	1	MET	2.1
16	N	152	GLU	2.1
8	E	121	ASP	2.1
16	N	62	HIS	2.1
18	P	121	ASP	2.1
28	Z	36	ASP	2.1
28	Z	41	ASN	2.1
30	2	16	ASN	2.1
28	Z	21	VAL	2.1
14	L	112	GLY	2.1
4	A	66	ARG	2.1
23	U	56	ARG	2.1
31	3	62	THR	2.0
1	0	1181	A	2.0
1	0	1207	A	2.0
1	0	1947	G	2.0
1	0	2355	G	2.0
5	B	319	ASP	2.0
7	D	100	ASP	2.0
25	W	76	ASP	2.0
27	Y	97	LEU	2.0
32	I	115	ASP	2.0
1	0	359	U	2.0

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Mol	Chain	Res	Type	RSRZ
9	F	93	SER	2.0
24	V	6	GLN	2.0
1	0	2507	G	2.0
7	D	76	ARG	2.0
13	K	27	ARG	2.0
28	Z	13	ARG	2.0
7	D	20	LYS	2.0
15	M	84	LYS	2.0
30	2	28	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	DCZ	4	74	16/16	0.93	0.11	46,50,55,60	0
3	HFA	4	77	11/12	0.95	0.11	37,39,42,43	0
1	OMG	0	2588	24/25	0.97	0.07	28,32,36,37	0
1	UR3	0	2619	21/22	0.97	0.07	34,37,39,41	0
3	PPU	4	76	24/38	0.97	0.07	35,39,41,43	0
1	1MA	0	628	23/24	0.97	0.07	30,32,34,39	0
1	OMU	0	2587	21/22	0.97	0.07	28,35,37,37	0
1	PSU	0	2621	20/21	0.98	0.06	28,31,38,39	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(Å ²)	Q<0.9
33	MG	0	8055	1/1	0.67	0.23	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8108	1/1	0.68	0.28	111,111,111,111	0
33	MG	0	8058	1/1	0.69	0.16	79,79,79,79	0
33	MG	0	8052	1/1	0.70	0.29	88,88,88,88	0
33	MG	0	8022	1/1	0.73	0.45	103,103,103,103	0
33	MG	0	8024	1/1	0.73	0.62	92,92,92,92	0
35	NA	0	9164	1/1	0.73	0.26	59,59,59,59	0
35	NA	9	9183	1/1	0.74	0.36	73,73,73,73	0
35	NA	0	9184	1/1	0.75	0.25	75,75,75,75	0
33	MG	0	8092	1/1	0.77	0.33	68,68,68,68	0
35	NA	0	9171	1/1	0.77	0.20	56,56,56,56	0
35	NA	0	9129	1/1	0.78	0.23	70,70,70,70	0
37	SR	0	9500	1/1	0.78	0.46	179,179,179,179	0
35	NA	0	9182	1/1	0.79	0.18	78,78,78,78	0
35	NA	0	9185	1/1	0.79	0.27	50,50,50,50	0
33	MG	0	8045	1/1	0.80	0.17	66,66,66,66	0
35	NA	0	9140	1/1	0.80	0.16	55,55,55,55	0
33	MG	0	8082	1/1	0.80	0.52	89,89,89,89	0
35	NA	0	9173	1/1	0.81	0.18	66,66,66,66	0
35	NA	0	9168	1/1	0.81	0.29	63,63,63,63	0
33	MG	0	8059	1/1	0.81	0.24	61,61,61,61	0
37	SR	0	9547	1/1	0.81	0.38	194,194,194,194	0
35	NA	0	9169	1/1	0.82	0.33	96,96,96,96	0
33	MG	0	8101	1/1	0.82	0.15	78,78,78,78	0
33	MG	A	8065	1/1	0.82	0.13	79,79,79,79	0
35	NA	D	9151	1/1	0.83	0.13	61,61,61,61	0
35	NA	S	9112	1/1	0.83	0.21	68,68,68,68	0
35	NA	0	9157	1/1	0.84	0.16	44,44,44,44	0
33	MG	0	8014	1/1	0.84	0.28	78,78,78,78	0
38	CD	O	9205	1/1	0.84	0.23	183,183,183,183	0
35	NA	0	9111	1/1	0.85	0.17	66,66,66,66	0
35	NA	0	9118	1/1	0.85	0.21	60,60,60,60	0
35	NA	0	9174	1/1	0.85	0.27	62,62,62,62	0
35	NA	0	9170	1/1	0.85	0.48	82,82,82,82	0
35	NA	H	9122	1/1	0.86	0.36	80,80,80,80	0
35	NA	0	9125	1/1	0.86	0.32	93,93,93,93	0
33	MG	0	8050	1/1	0.86	0.13	74,74,74,74	0
35	NA	0	9181	1/1	0.86	0.14	52,52,52,52	0
33	MG	0	8025	1/1	0.86	0.17	29,29,29,29	0
35	NA	0	9152	1/1	0.87	0.24	66,66,66,66	0
35	NA	0	9124	1/1	0.87	0.25	53,53,53,53	0
34	K	0	9001	1/1	0.87	0.45	78,78,78,78	0
33	MG	0	8094	1/1	0.87	0.22	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	9	9588	1/1	0.87	0.11	126,126,126,126	0
37	SR	B	9521	1/1	0.87	0.51	165,165,165,165	0
33	MG	0	8072	1/1	0.87	0.12	69,69,69,69	0
35	NA	0	9179	1/1	0.88	0.30	107,107,107,107	0
33	MG	9	8095	1/1	0.89	0.21	49,49,49,49	0
35	NA	0	9172	1/1	0.89	0.35	71,71,71,71	0
33	MG	0	8039	1/1	0.89	0.12	80,80,80,80	0
33	MG	0	8040	1/1	0.89	0.14	69,69,69,69	0
33	MG	0	8042	1/1	0.89	0.07	53,53,53,53	0
33	MG	0	8114	1/1	0.89	0.15	76,76,76,76	0
35	NA	0	9163	1/1	0.90	0.12	59,59,59,59	0
33	MG	0	8089	1/1	0.90	0.14	58,58,58,58	0
35	NA	0	9167	1/1	0.90	0.12	50,50,50,50	0
33	MG	0	8047	1/1	0.90	0.16	89,89,89,89	0
35	NA	0	9116	1/1	0.90	0.19	44,44,44,44	0
35	NA	0	9126	1/1	0.90	0.15	54,54,54,54	0
33	MG	0	8057	1/1	0.91	0.14	69,69,69,69	0
33	MG	A	8066	1/1	0.91	0.10	56,56,56,56	0
35	NA	0	9127	1/1	0.91	0.11	45,45,45,45	0
33	MG	0	8084	1/1	0.91	0.34	76,76,76,76	0
33	MG	0	8107	1/1	0.91	0.21	63,63,63,63	0
35	NA	0	9141	1/1	0.91	0.10	60,60,60,60	0
37	SR	0	9452	1/1	0.91	0.12	107,107,107,107	0
37	SR	0	9459	1/1	0.91	0.11	97,97,97,97	0
35	NA	0	9150	1/1	0.91	0.14	42,42,42,42	0
37	SR	0	9532	1/1	0.91	0.12	123,123,123,123	0
35	NA	0	9113	1/1	0.91	0.07	61,61,61,61	0
33	MG	0	8063	1/1	0.91	0.14	60,60,60,60	0
33	MG	0	8090	1/1	0.91	0.26	84,84,84,84	0
33	MG	0	8051	1/1	0.91	0.07	35,35,35,35	0
36	CL	B	9319	1/1	0.92	0.20	55,55,55,55	0
35	NA	0	9107	1/1	0.92	0.08	63,63,63,63	0
33	MG	0	8061	1/1	0.92	0.08	60,60,60,60	0
37	SR	0	9484	1/1	0.92	0.10	123,123,123,123	0
33	MG	0	8046	1/1	0.92	0.07	41,41,41,41	0
33	MG	T	8073	1/1	0.92	0.15	40,40,40,40	0
35	NA	0	9177	1/1	0.92	0.17	62,62,62,62	0
33	MG	0	8093	1/1	0.92	0.13	41,41,41,41	0
35	NA	0	9158	1/1	0.92	0.16	66,66,66,66	0
36	CL	0	9316	1/1	0.92	0.20	71,71,71,71	0
34	K	0	9003	1/1	0.93	0.21	80,80,80,80	0
37	SR	0	9517	1/1	0.93	0.14	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	9165	1/1	0.93	0.18	42,42,42,42	0
37	SR	0	9537	1/1	0.93	0.09	119,119,119,119	0
36	CL	J	9301	1/1	0.93	0.13	51,51,51,51	0
37	SR	0	9581	1/1	0.93	0.13	106,106,106,106	0
37	SR	0	9626	1/1	0.93	0.45	114,114,114,114	0
35	NA	0	9114	1/1	0.93	0.09	42,42,42,42	0
33	MG	0	8080	1/1	0.93	0.15	48,48,48,48	0
33	MG	0	8085	1/1	0.93	0.16	65,65,65,65	0
33	MG	0	8104	1/1	0.94	0.14	50,50,50,50	0
35	NA	0	9166	1/1	0.94	0.17	59,59,59,59	0
33	MG	0	8097	1/1	0.94	0.13	56,56,56,56	0
33	MG	0	8099	1/1	0.94	0.09	62,62,62,62	0
34	K	0	9002	1/1	0.94	0.16	61,61,61,61	0
35	NA	0	9120	1/1	0.94	0.11	53,53,53,53	0
35	NA	0	9154	1/1	0.94	0.21	46,46,46,46	0
37	SR	0	9539	1/1	0.94	0.55	134,134,134,134	0
33	MG	0	8060	1/1	0.94	0.11	76,76,76,76	0
35	NA	R	9186	1/1	0.94	0.12	67,67,67,67	0
35	NA	0	9102	1/1	0.94	0.25	58,58,58,58	0
33	MG	0	8102	1/1	0.94	0.06	61,61,61,61	0
35	NA	0	9175	1/1	0.94	0.19	51,51,51,51	0
33	MG	0	8103	1/1	0.94	0.13	63,63,63,63	0
38	CD	Z	9203	1/1	0.94	0.07	57,57,57,57	0
36	CL	N	9307	1/1	0.95	0.17	55,55,55,55	0
33	MG	0	8083	1/1	0.95	0.06	50,50,50,50	0
35	NA	0	9101	1/1	0.95	0.09	46,46,46,46	0
37	SR	0	9465	1/1	0.95	0.06	93,93,93,93	0
37	SR	0	9468	1/1	0.95	0.10	108,108,108,108	0
37	SR	0	9482	1/1	0.95	0.40	93,93,93,93	0
35	NA	0	9155	1/1	0.95	0.17	52,52,52,52	0
33	MG	0	8041	1/1	0.95	0.07	53,53,53,53	0
37	SR	0	9509	1/1	0.95	0.07	84,84,84,84	0
35	NA	0	9130	1/1	0.95	0.08	44,44,44,44	0
35	NA	0	9159	1/1	0.95	0.18	55,55,55,55	0
35	NA	0	9162	1/1	0.95	0.14	49,49,49,49	0
35	NA	J	9146	1/1	0.95	0.07	43,43,43,43	0
35	NA	Q	9148	1/1	0.95	0.05	48,48,48,48	0
35	NA	R	9138	1/1	0.95	0.06	59,59,59,59	0
37	SR	0	9590	1/1	0.95	0.11	91,91,91,91	0
33	MG	0	8115	1/1	0.95	0.06	51,51,51,51	0
33	MG	0	8116	1/1	0.95	0.11	49,49,49,49	0
35	NA	0	9149	1/1	0.95	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	F	9595	1/1	0.95	0.07	99,99,99,99	0
37	SR	H	9486	1/1	0.95	0.27	97,97,97,97	0
35	NA	0	9178	1/1	0.95	0.17	51,51,51,51	0
33	MG	0	8043	1/1	0.95	0.07	49,49,49,49	0
35	NA	0	9106	1/1	0.96	0.15	37,37,37,37	0
37	SR	0	9475	1/1	0.96	0.07	76,76,76,76	0
37	SR	0	9477	1/1	0.96	0.06	83,83,83,83	0
35	NA	M	9147	1/1	0.96	0.06	39,39,39,39	0
33	MG	0	8017	1/1	0.96	0.05	31,31,31,31	0
37	SR	0	9495	1/1	0.96	0.07	90,90,90,90	0
33	MG	0	8021	1/1	0.96	0.12	53,53,53,53	0
37	SR	0	9505	1/1	0.96	0.24	79,79,79,79	0
33	MG	0	8088	1/1	0.96	0.04	36,36,36,36	0
33	MG	0	8013	1/1	0.96	0.05	37,37,37,37	0
36	CL	0	9311	1/1	0.96	0.09	60,60,60,60	0
36	CL	0	9313	1/1	0.96	0.07	51,51,51,51	0
36	CL	0	9315	1/1	0.96	0.08	50,50,50,50	0
35	NA	0	9115	1/1	0.96	0.11	36,36,36,36	0
37	SR	0	9560	1/1	0.96	0.08	91,91,91,91	0
36	CL	A	9309	1/1	0.96	0.16	57,57,57,57	0
33	MG	0	8110	1/1	0.96	0.21	43,43,43,43	0
35	NA	0	9134	1/1	0.96	0.11	48,48,48,48	0
36	CL	L	9310	1/1	0.96	0.12	49,49,49,49	0
35	NA	0	9135	1/1	0.96	0.08	43,43,43,43	0
36	CL	Y	9320	1/1	0.96	0.08	39,39,39,39	0
35	NA	C	9104	1/1	0.96	0.09	27,27,27,27	0
35	NA	0	9139	1/1	0.96	0.12	41,41,41,41	0
33	MG	0	8113	1/1	0.96	0.12	43,43,43,43	0
33	MG	0	8031	1/1	0.97	0.08	44,44,44,44	0
35	NA	0	9143	1/1	0.97	0.08	36,36,36,36	0
37	SR	0	9467	1/1	0.97	0.06	74,74,74,74	0
33	MG	0	8067	1/1	0.97	0.12	38,38,38,38	0
33	MG	0	8009	1/1	0.97	0.04	32,32,32,32	0
33	MG	0	8096	1/1	0.97	0.06	42,42,42,42	0
35	NA	0	9108	1/1	0.97	0.06	33,33,33,33	0
37	SR	0	9483	1/1	0.97	0.05	68,68,68,68	0
35	NA	0	9110	1/1	0.97	0.07	44,44,44,44	0
37	SR	0	9490	1/1	0.97	0.19	89,89,89,89	0
35	NA	0	9156	1/1	0.97	0.11	53,53,53,53	0
35	NA	0	9128	1/1	0.97	0.06	40,40,40,40	0
37	SR	0	9504	1/1	0.97	0.07	90,90,90,90	0
36	CL	0	9314	1/1	0.97	0.12	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	9508	1/1	0.97	0.08	82,82,82,82	0
33	MG	0	8076	1/1	0.97	0.06	56,56,56,56	0
37	SR	0	9515	1/1	0.97	0.27	81,81,81,81	0
33	MG	0	8098	1/1	0.97	0.05	43,43,43,43	0
37	SR	0	9522	1/1	0.97	0.06	103,103,103,103	0
37	SR	0	9529	1/1	0.97	0.17	89,89,89,89	0
36	CL	0	9322	1/1	0.97	0.28	53,53,53,53	0
37	SR	0	9534	1/1	0.97	0.31	90,90,90,90	0
35	NA	0	9161	1/1	0.97	0.15	59,59,59,59	0
35	NA	0	9131	1/1	0.97	0.12	44,44,44,44	0
35	NA	0	9132	1/1	0.97	0.12	45,45,45,45	0
36	CL	J	9321	1/1	0.97	0.07	57,57,57,57	0
37	SR	0	9566	1/1	0.97	0.14	76,76,76,76	0
37	SR	0	9568	1/1	0.97	0.04	70,70,70,70	0
33	MG	0	8112	1/1	0.97	0.07	41,41,41,41	0
37	SR	0	9585	1/1	0.97	0.09	77,77,77,77	0
33	MG	0	8029	1/1	0.97	0.10	35,35,35,35	0
37	SR	0	9601	1/1	0.97	0.11	107,107,107,107	0
36	CL	O	9308	1/1	0.97	0.14	61,61,61,61	0
37	SR	9	9503	1/1	0.97	0.05	104,104,104,104	0
33	MG	0	8044	1/1	0.97	0.04	41,41,41,41	0
37	SR	A	9437	1/1	0.97	0.04	59,59,59,59	0
36	CL	3	9304	1/1	0.97	0.06	54,54,54,54	0
37	SR	0	9405	1/1	0.97	0.05	67,67,67,67	0
37	SR	0	9431	1/1	0.97	0.04	61,61,61,61	0
37	SR	S	9470	1/1	0.97	0.05	87,87,87,87	0
37	SR	0	9433	1/1	0.97	0.06	64,64,64,64	0
35	NA	0	9117	1/1	0.97	0.06	43,43,43,43	0
36	CL	0	9303	1/1	0.98	0.09	44,44,44,44	0
36	CL	R	9306	1/1	0.98	0.05	44,44,44,44	0
36	CL	0	9305	1/1	0.98	0.06	52,52,52,52	0
33	MG	0	8106	1/1	0.98	0.07	43,43,43,43	0
37	SR	0	9506	1/1	0.98	0.12	61,61,61,61	0
33	MG	0	8002	1/1	0.98	0.07	45,45,45,45	0
37	SR	0	9420	1/1	0.98	0.04	59,59,59,59	0
37	SR	0	9421	1/1	0.98	0.04	66,66,66,66	0
37	SR	0	9427	1/1	0.98	0.04	50,50,50,50	0
33	MG	0	8117	1/1	0.98	0.07	39,39,39,39	0
37	SR	0	9432	1/1	0.98	0.05	61,61,61,61	0
37	SR	0	9530	1/1	0.98	0.04	66,66,66,66	0
33	MG	0	8056	1/1	0.98	0.05	46,46,46,46	0
37	SR	0	9442	1/1	0.98	0.05	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	9447	1/1	0.98	0.05	64,64,64,64	0
33	MG	0	8027	1/1	0.98	0.08	33,33,33,33	0
37	SR	0	9545	1/1	0.98	0.10	70,70,70,70	0
37	SR	0	9455	1/1	0.98	0.05	78,78,78,78	0
37	SR	0	9457	1/1	0.98	0.06	56,56,56,56	0
36	CL	0	9317	1/1	0.98	0.06	45,45,45,45	0
37	SR	0	9461	1/1	0.98	0.07	69,69,69,69	0
37	SR	0	9570	1/1	0.98	0.11	86,86,86,86	0
33	MG	0	8032	1/1	0.98	0.06	41,41,41,41	0
33	MG	0	8037	1/1	0.98	0.07	37,37,37,37	0
35	NA	0	9123	1/1	0.98	0.12	38,38,38,38	0
37	SR	0	9469	1/1	0.98	0.06	81,81,81,81	0
37	SR	0	9474	1/1	0.98	0.05	57,57,57,57	0
37	SR	0	9629	1/1	0.98	0.04	71,71,71,71	0
37	SR	9	9481	1/1	0.98	0.07	80,80,80,80	0
35	NA	R	9137	1/1	0.98	0.03	38,38,38,38	0
36	CL	J	9302	1/1	0.98	0.06	51,51,51,51	0
37	SR	0	9480	1/1	0.98	0.04	85,85,85,85	0
37	SR	A	9497	1/1	0.98	0.04	78,78,78,78	0
37	SR	B	9458	1/1	0.98	0.07	68,68,68,68	0
33	MG	Y	8109	1/1	0.98	0.09	38,38,38,38	0
35	NA	0	9136	1/1	0.98	0.08	33,33,33,33	0
36	CL	M	9318	1/1	0.98	0.05	39,39,39,39	0
37	SR	0	9488	1/1	0.98	0.03	69,69,69,69	0
37	SR	0	9489	1/1	0.98	0.07	80,80,80,80	0
33	MG	0	8054	1/1	0.98	0.05	39,39,39,39	0
35	NA	0	9105	1/1	0.99	0.04	38,38,38,38	0
33	MG	0	8028	1/1	0.99	0.03	35,35,35,35	0
37	SR	0	9473	1/1	0.99	0.10	69,69,69,69	0
33	MG	0	8005	1/1	0.99	0.02	28,28,28,28	0
33	MG	0	8030	1/1	0.99	0.05	34,34,34,34	0
33	MG	0	8019	1/1	0.99	0.04	45,45,45,45	0
37	SR	0	9478	1/1	0.99	0.03	71,71,71,71	0
33	MG	0	8091	1/1	0.99	0.14	47,47,47,47	0
33	MG	0	8020	1/1	0.99	0.07	34,34,34,34	0
33	MG	0	8036	1/1	0.99	0.05	56,56,56,56	0
37	SR	0	9407	1/1	0.99	0.03	41,41,41,41	0
37	SR	0	9410	1/1	0.99	0.02	36,36,36,36	0
37	SR	0	9411	1/1	0.99	0.06	42,42,42,42	0
37	SR	0	9412	1/1	0.99	0.02	38,38,38,38	0
37	SR	0	9414	1/1	0.99	0.03	57,57,57,57	0
37	SR	0	9498	1/1	0.99	0.05	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	9416	1/1	0.99	0.04	45,45,45,45	0
37	SR	0	9501	1/1	0.99	0.04	64,64,64,64	0
37	SR	0	9417	1/1	0.99	0.03	55,55,55,55	0
33	MG	0	8068	1/1	0.99	0.13	46,46,46,46	0
33	MG	0	8118	1/1	0.99	0.03	33,33,33,33	0
37	SR	0	9422	1/1	0.99	0.04	52,52,52,52	0
37	SR	0	9423	1/1	0.99	0.05	56,56,56,56	0
37	SR	0	9425	1/1	0.99	0.03	54,54,54,54	0
37	SR	0	9426	1/1	0.99	0.04	61,61,61,61	0
33	MG	0	8070	1/1	0.99	0.04	27,27,27,27	0
37	SR	0	9429	1/1	0.99	0.03	59,59,59,59	0
36	CL	0	9312	1/1	0.99	0.05	48,48,48,48	0
33	MG	0	8008	1/1	0.99	0.03	23,23,23,23	0
33	MG	0	8074	1/1	0.99	0.10	31,31,31,31	0
37	SR	0	9434	1/1	0.99	0.04	60,60,60,60	0
37	SR	0	9435	1/1	0.99	0.04	67,67,67,67	0
37	SR	0	9438	1/1	0.99	0.03	59,59,59,59	0
37	SR	0	9440	1/1	0.99	0.06	69,69,69,69	0
37	SR	0	9441	1/1	0.99	0.06	62,62,62,62	0
33	MG	K	8069	1/1	0.99	0.10	22,22,22,22	0
37	SR	0	9443	1/1	0.99	0.05	54,54,54,54	0
37	SR	0	9445	1/1	0.99	0.04	55,55,55,55	0
37	SR	0	9446	1/1	0.99	0.04	77,77,77,77	0
33	MG	0	8075	1/1	0.99	0.03	37,37,37,37	0
37	SR	0	9449	1/1	0.99	0.06	60,60,60,60	0
37	SR	0	9450	1/1	0.99	0.06	65,65,65,65	0
37	SR	0	9451	1/1	0.99	0.05	62,62,62,62	0
33	MG	0	8038	1/1	0.99	0.12	27,27,27,27	0
37	SR	0	9453	1/1	0.99	0.05	66,66,66,66	0
37	SR	0	9454	1/1	0.99	0.06	65,65,65,65	0
33	MG	0	8079	1/1	0.99	0.03	30,30,30,30	0
37	SR	A	9436	1/1	0.99	0.06	47,47,47,47	0
37	SR	0	9456	1/1	0.99	0.06	57,57,57,57	0
33	MG	0	8001	1/1	0.99	0.05	23,23,23,23	0
35	NA	0	9160	1/1	0.99	0.09	35,35,35,35	0
33	MG	0	8012	1/1	0.99	0.09	40,40,40,40	0
37	SR	0	9462	1/1	0.99	0.03	64,64,64,64	0
37	SR	0	9464	1/1	0.99	0.06	73,73,73,73	0
37	SR	R	9418	1/1	0.99	0.02	50,50,50,50	0
33	MG	0	8003	1/1	0.99	0.03	33,33,33,33	0
37	SR	1	9419	1/1	0.99	0.02	41,41,41,41	0
37	SR	1	9460	1/1	0.99	0.04	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	3	9439	1/1	0.99	0.05	57,57,57,57	0
37	SR	0	9466	1/1	0.99	0.14	80,80,80,80	0
33	MG	0	8004	1/1	0.99	0.02	33,33,33,33	0
38	CD	1	9202	1/1	0.99	0.11	50,50,50,50	0
38	CD	3	9204	1/1	0.99	0.05	57,57,57,57	0
37	SR	0	9428	1/1	1.00	0.06	49,49,49,49	0
37	SR	0	9413	1/1	1.00	0.02	43,43,43,43	0
37	SR	L	9409	1/1	1.00	0.02	36,36,36,36	0
37	SR	0	9430	1/1	1.00	0.03	47,47,47,47	0
37	SR	0	9408	1/1	1.00	0.02	36,36,36,36	0
37	SR	0	9444	1/1	1.00	0.06	51,51,51,51	0
37	SR	0	9415	1/1	1.00	0.02	50,50,50,50	0
37	SR	0	9424	1/1	1.00	0.02	45,45,45,45	0
33	MG	0	8026	1/1	1.00	0.07	33,33,33,33	0
38	CD	U	9201	1/1	1.00	0.03	58,58,58,58	0
37	SR	0	9448	1/1	1.00	0.04	52,52,52,52	0
37	SR	0	9406	1/1	1.00	0.01	32,32,32,32	0
33	MG	0	8015	1/1	1.00	0.02	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.