



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:31 PM UTC

PDB ID : 1VQ5 / pdb_00001vq5
Title : The structure of the transition state analogue "RAA" bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.60 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

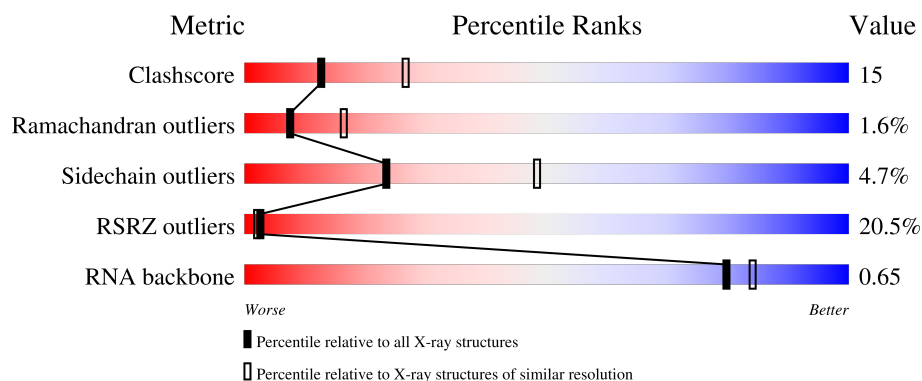
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)
RNA backbone	3983	1014 (2.84-2.36)

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	15% 61% 28% 5% • 6%
2	9	122	14% 58% 32% 10%
3	4	8	38% 38% 25%
4	A	240	8% 58% 35% 5% •
5	B	338	46% 48% 45% 7%

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Mol	Chain	Length	Quality of chain
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	

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Mol	Chain	Length	Quality of chain
31	3	92	8% 72% 24%
32	I	162	35% 12% 31% 57%

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99060 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'-D*(DC)P*(DC)P*(5AA)P*(2OP)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
			126	61	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	106	Total	Mg	0	0
			106	106		
33	9	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	B	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	3	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 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	71	Total Na 71 71	0	0
35	9	2	Total Na 2 2	0	0
35	A	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	H	2	Total Na 2 2	0	0
35	J	1	Total Na 1 1	0	0
35	L	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	S	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	L	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	M	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	O	1	Total 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0
37	3	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5820	Total 5820	O 5820	0	0
38	9	133	Total 133	O 133	0	0
38	4	8	Total 8	O 8	0	0
38	A	117	Total 117	O 117	0	0
38	B	150	Total 150	O 150	0	0
38	C	165	Total 165	O 165	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	D	49	Total 49	O 49	0	0
38	E	47	Total 47	O 47	0	0
38	F	21	Total 21	O 21	0	0
38	G	16	Total 16	O 16	0	0
38	H	66	Total 66	O 66	0	0
38	J	52	Total 52	O 52	0	0
38	K	54	Total 54	O 54	0	0
38	L	83	Total 83	O 83	0	0
38	M	118	Total 118	O 118	0	0
38	N	66	Total 66	O 66	0	0
38	O	39	Total 39	O 39	0	0
38	P	65	Total 65	O 65	0	0
38	Q	52	Total 52	O 52	0	0
38	R	85	Total 85	O 85	0	0
38	S	31	Total 31	O 31	0	0
38	T	39	Total 39	O 39	0	0
38	U	25	Total 25	O 25	0	0
38	V	13	Total 13	O 13	0	0
38	W	68	Total 68	O 68	0	0
38	X	27	Total 27	O 27	0	0
38	Y	92	Total 92	O 92	0	0

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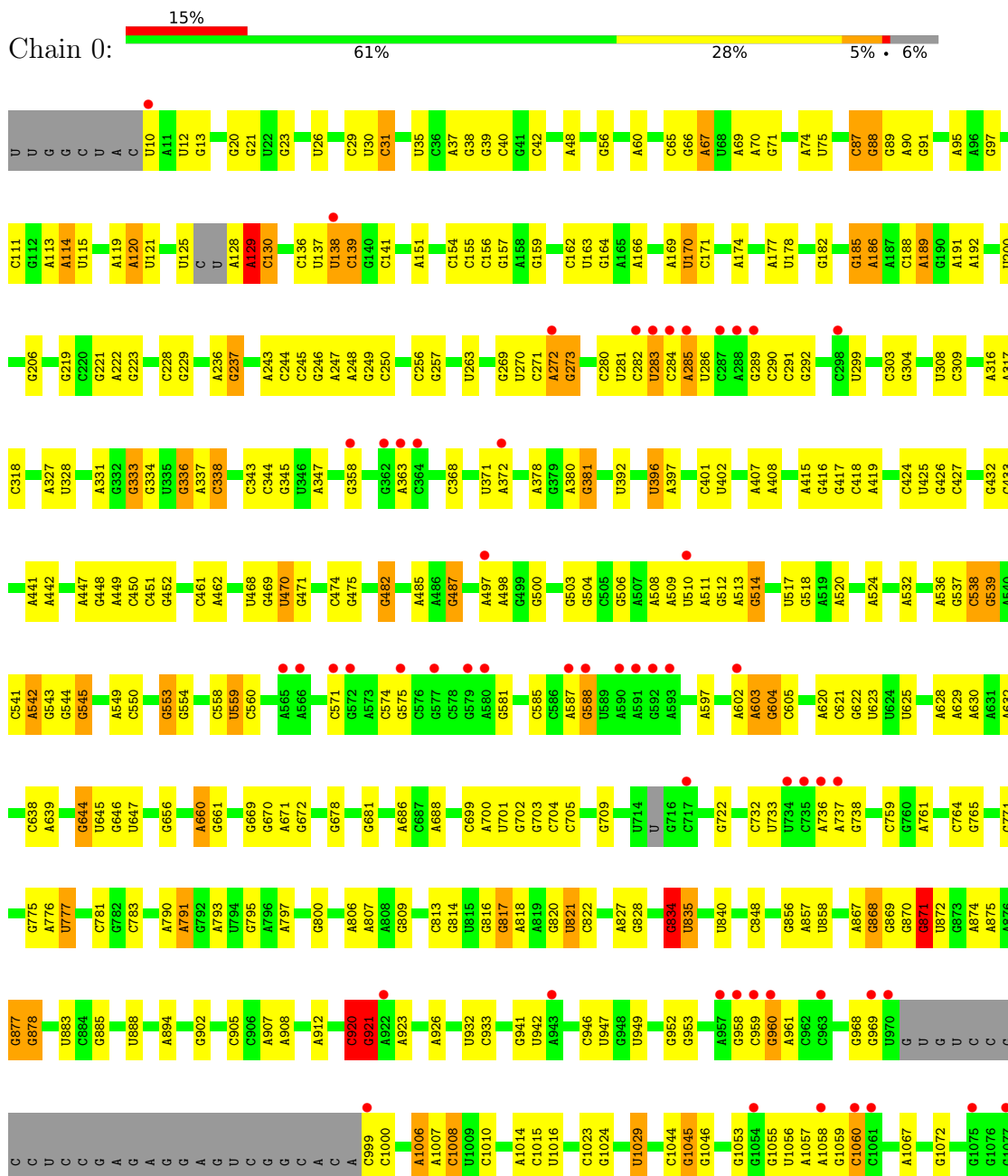
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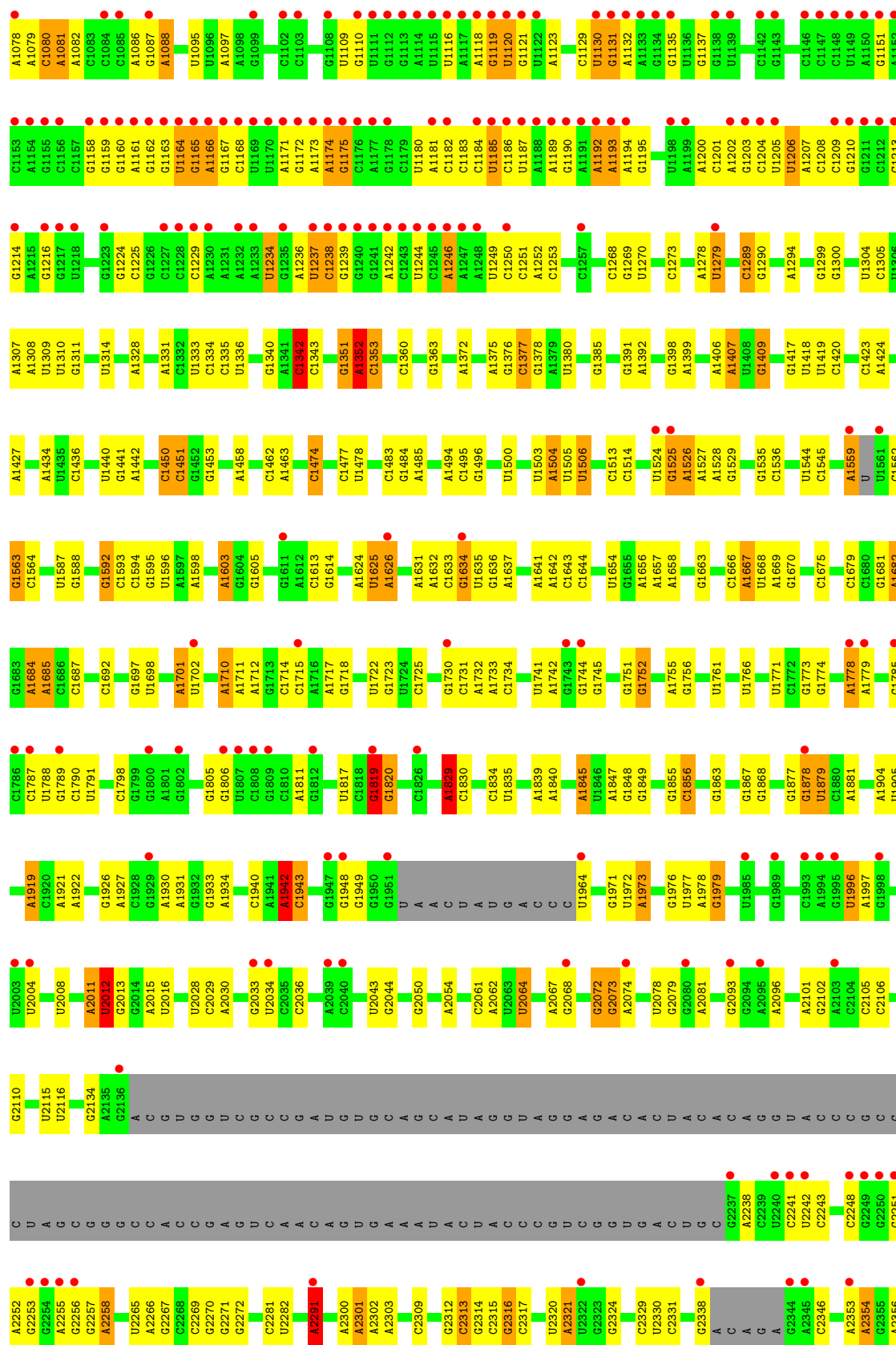
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	Z	30	Total 30	O 30	0	0
38	1	59	Total 59	O 59	0	0
38	2	42	Total 42	O 42	0	0
38	3	74	Total 74	O 74	0	0
38	I	10	Total 10	O 10	0	0

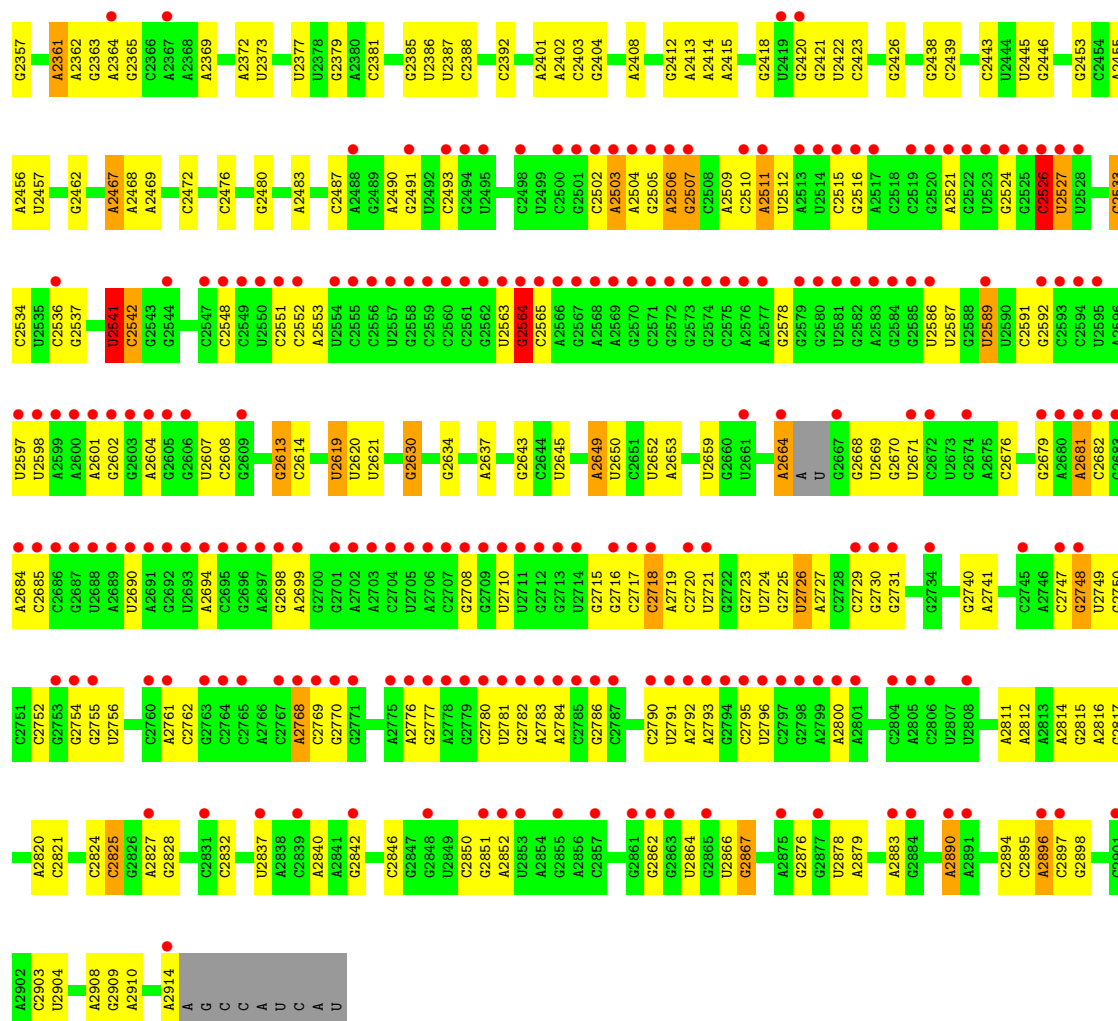
3 Residue-property plots

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.

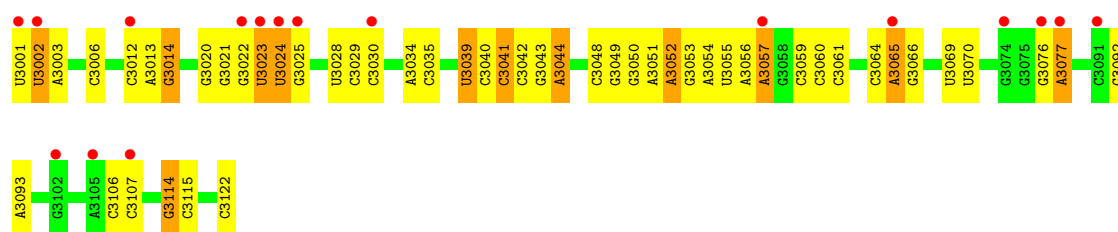
- Molecule 1: 23S ribosomal rna







• Molecule 2: 5S ribosomal RNA

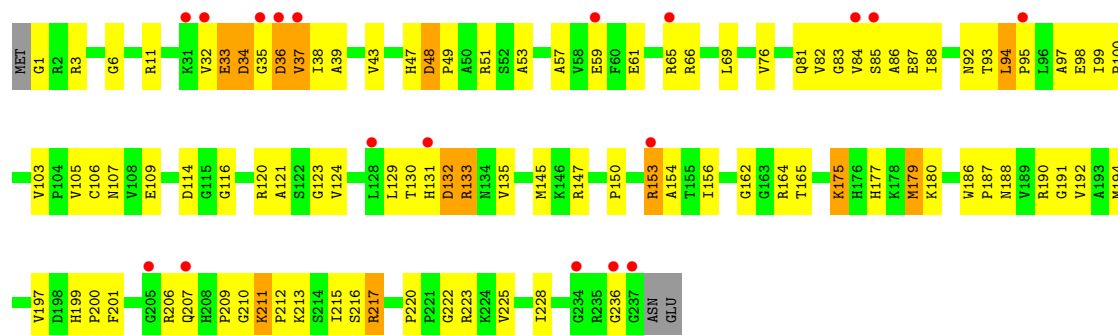


• Molecule 3: 5'-D*(DC)P*(DC)P*(5AA)P*(2OP)P*(PO2)P*AP*C*C)-3'



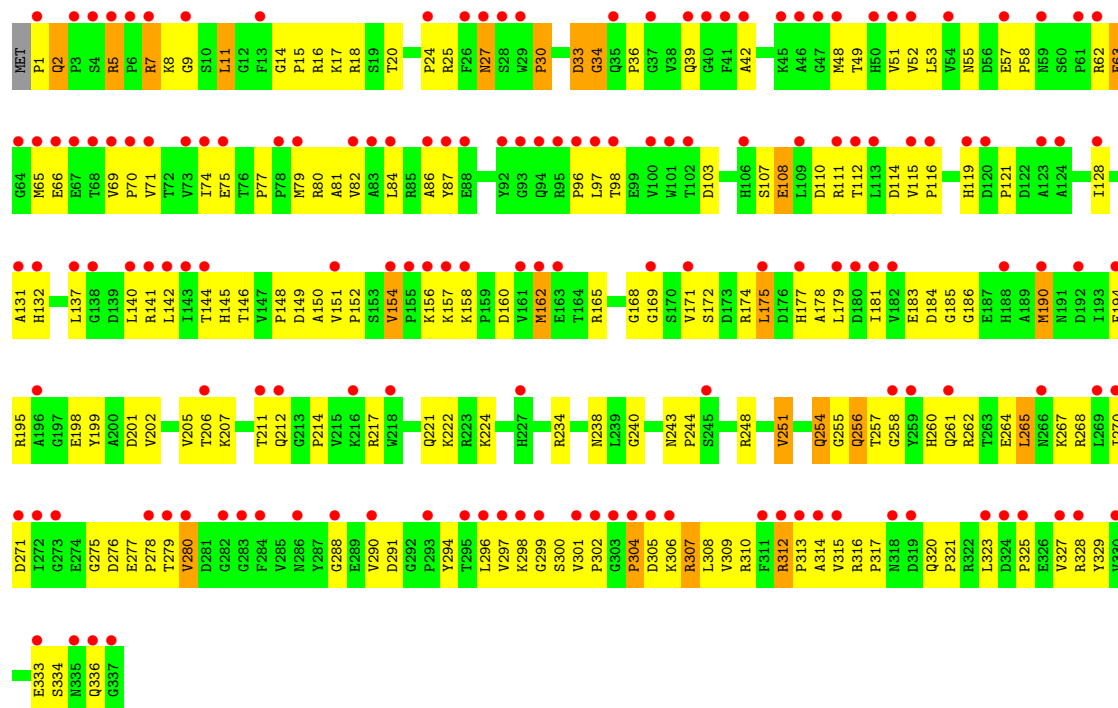
• Molecule 4: 50S ribosomal protein L2P

Chain A: 



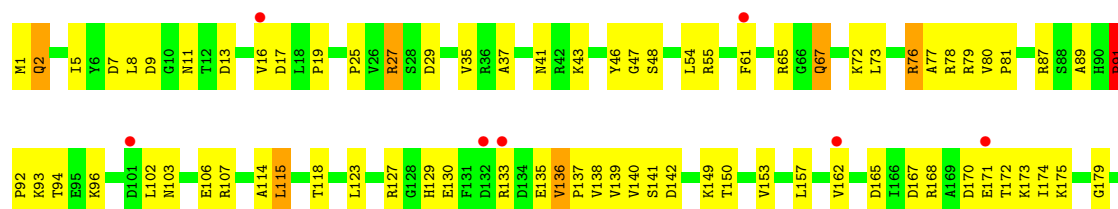
• Molecule 5: 50S ribosomal protein L3P

Chain B: 



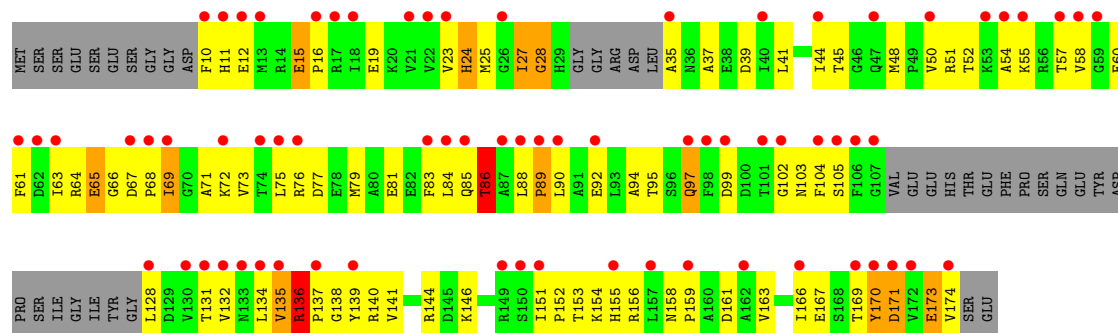
• Molecule 6: 50S ribosomal protein L4E

Chain C: 

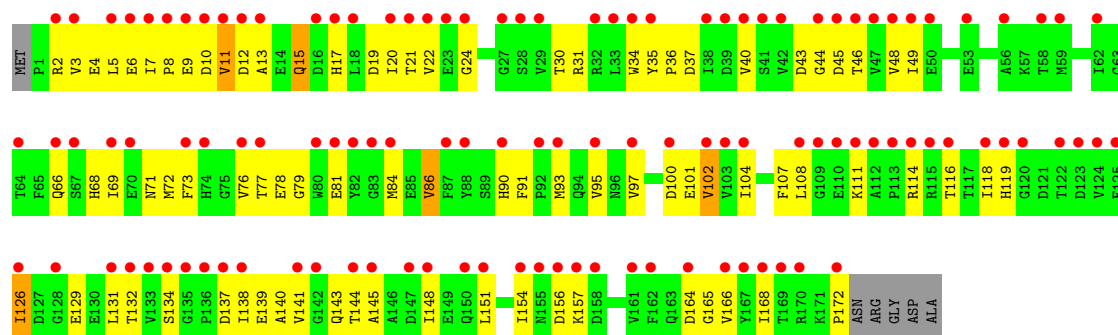




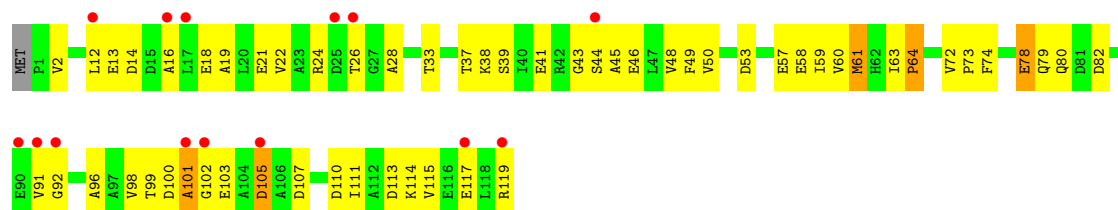
• Molecule 7: 50S ribosomal protein L5P



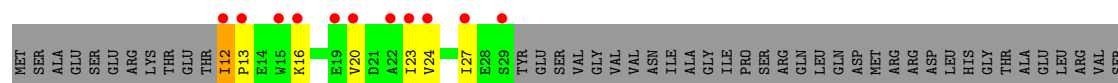
• Molecule 8: 50S ribosomal protein L6P

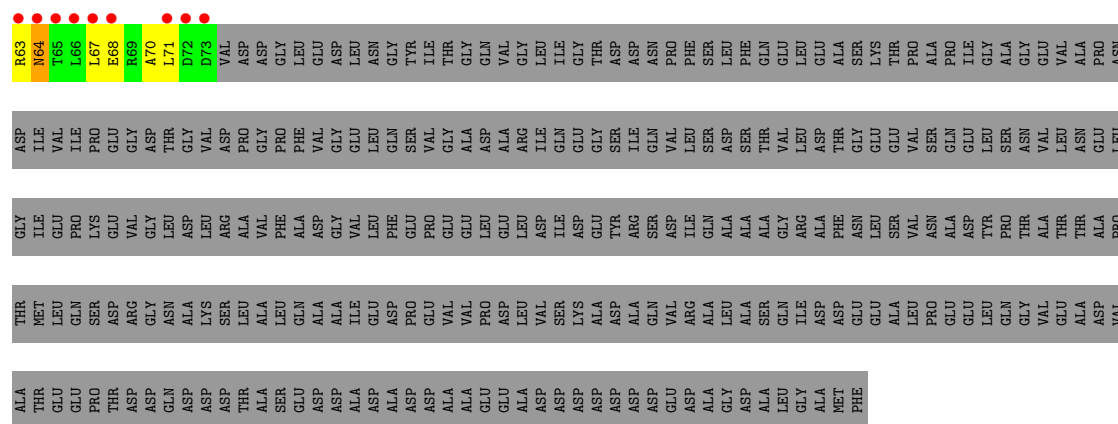


• Molecule 9: 50S ribosomal protein L7AE

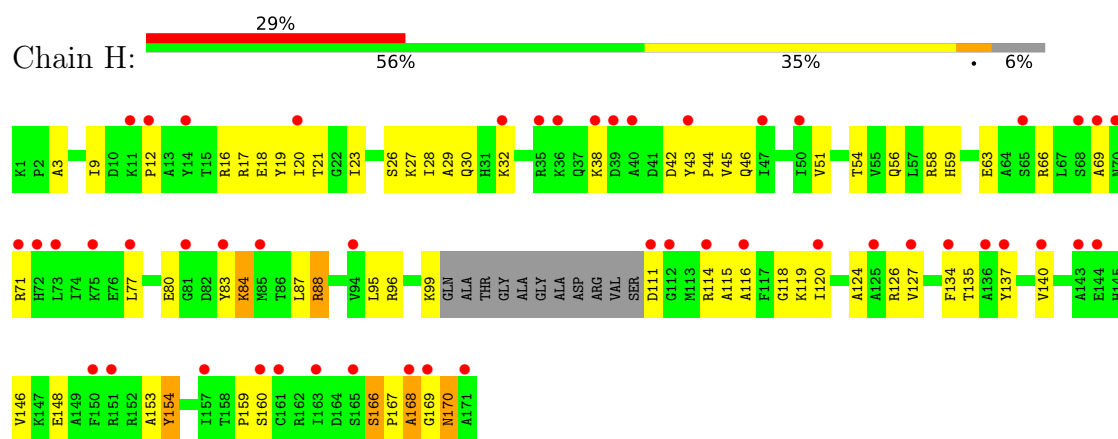


• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

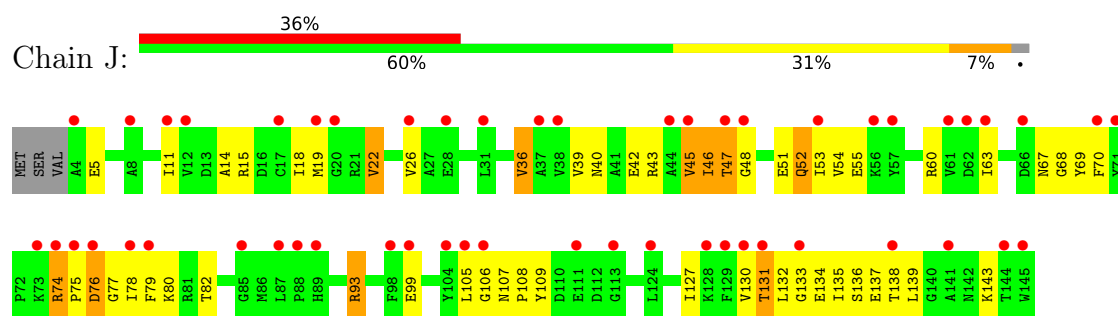




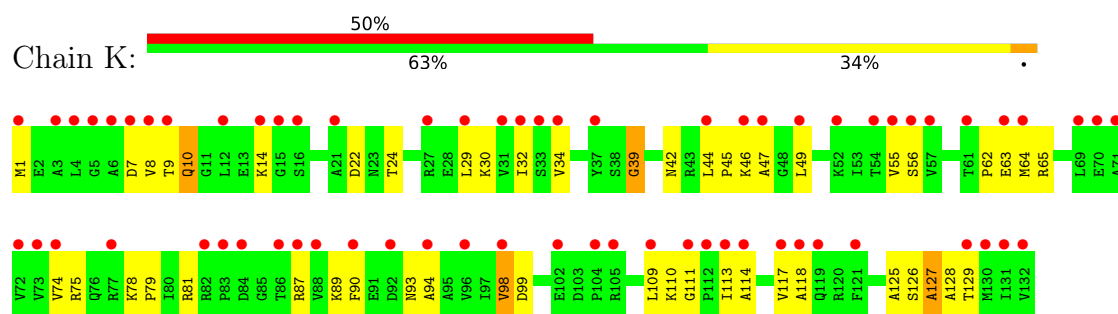
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E



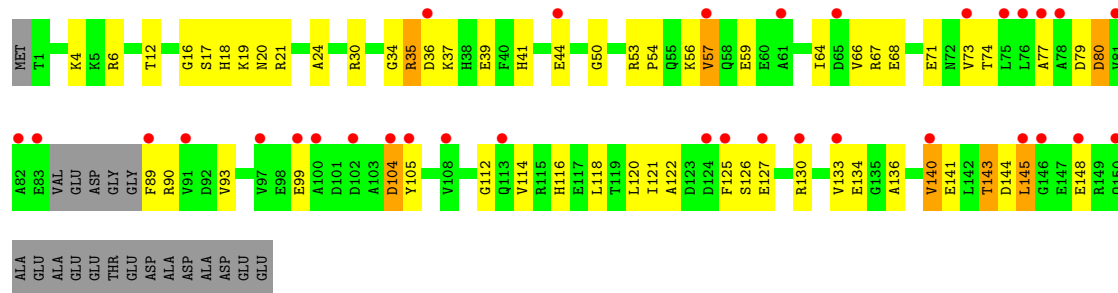
• Molecule 12: 50S ribosomal protein L13P



• Molecule 13: 50S ribosomal protein L14P



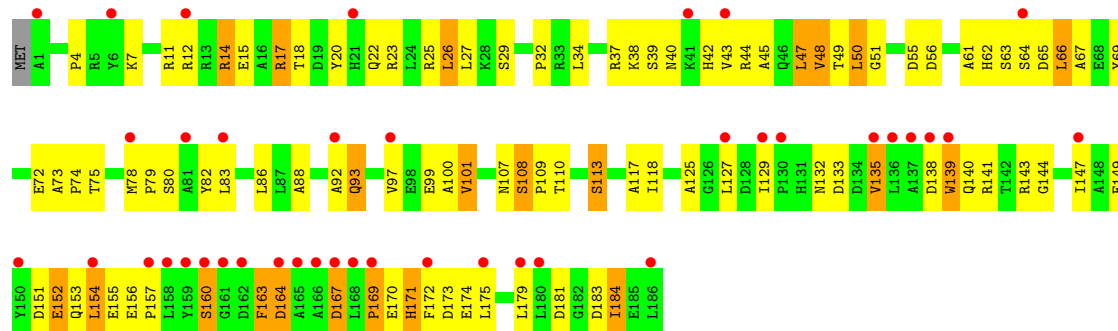
• Molecule 14: 50S ribosomal protein L15P



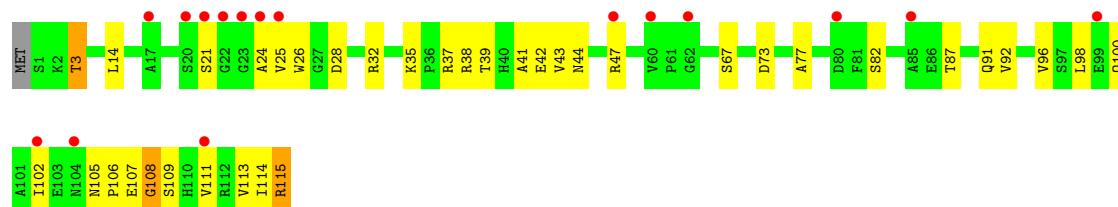
• Molecule 15: 50S Ribosomal Protein L15E



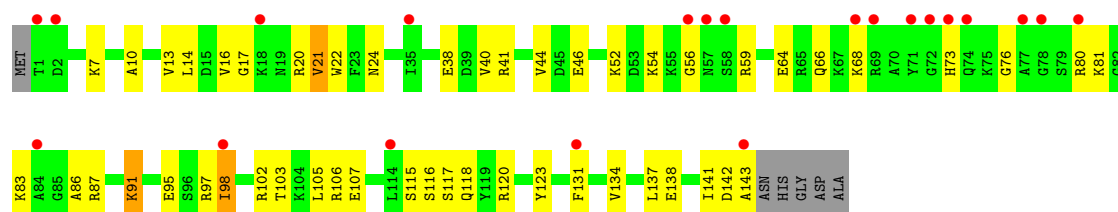
• Molecule 16: 50S ribosomal protein L18P



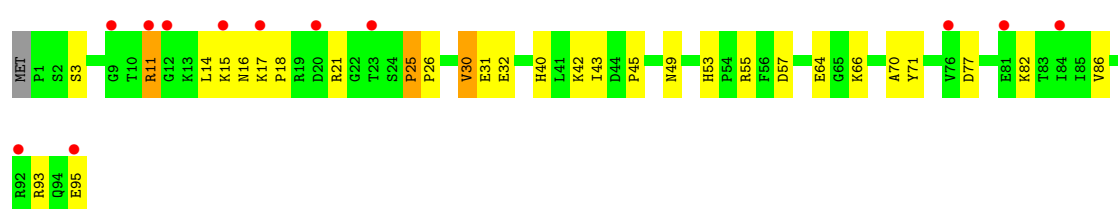
• Molecule 17: 50S ribosomal protein L18e



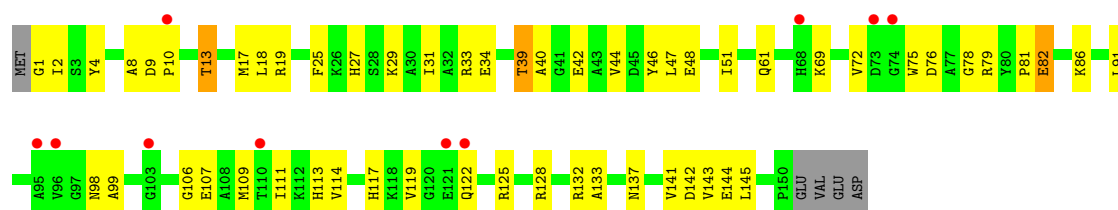
• Molecule 18: 50S ribosomal protein L19E



- Molecule 19: 50S ribosomal protein L21e



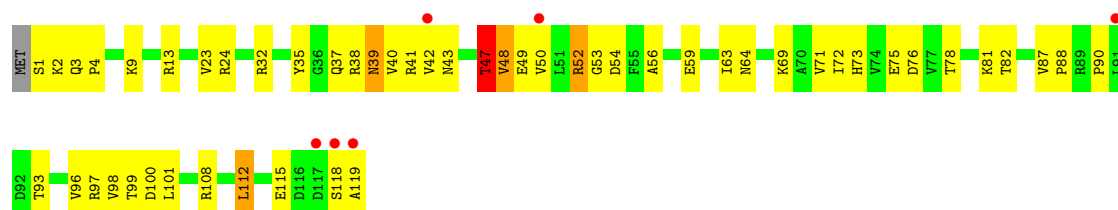
- Molecule 20: 50S ribosomal protein L22P



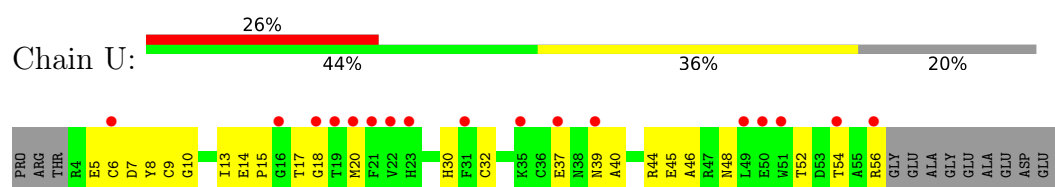
- Molecule 21: 50S ribosomal protein L23P



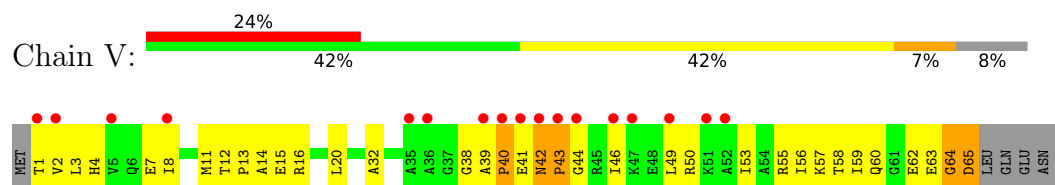
- Molecule 22: 50S ribosomal protein L24P



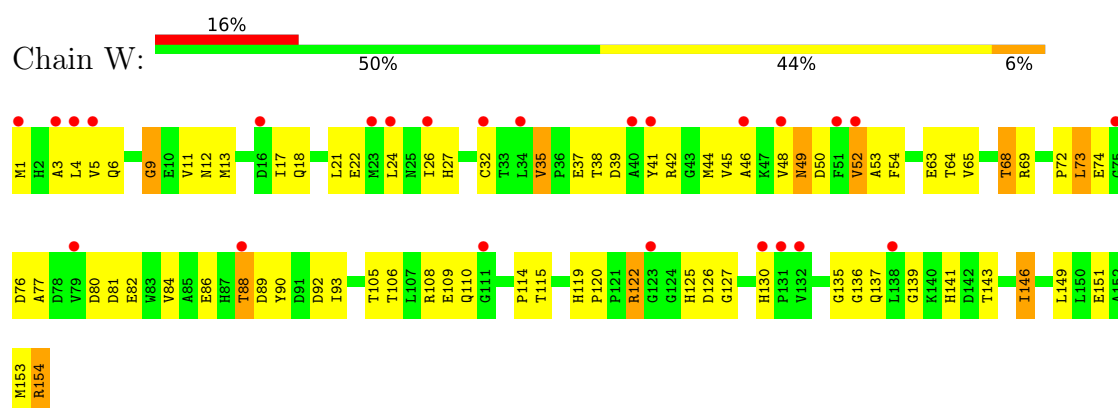
- Molecule 23: 50S ribosomal protein L24E



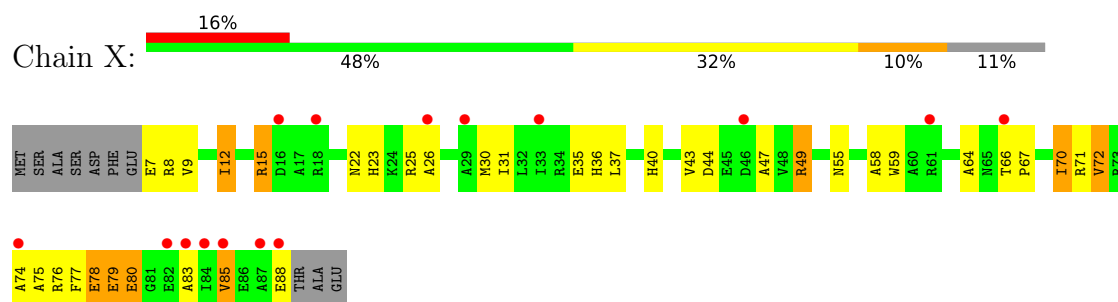
• Molecule 24: 50S ribosomal protein L29P



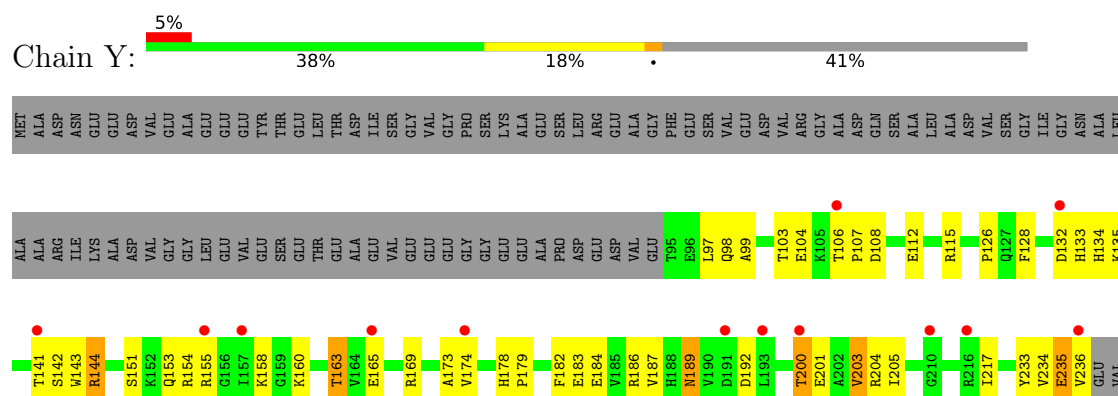
• Molecule 25: 50S ribosomal protein L30P



• Molecule 26: 50S ribosomal protein L31e

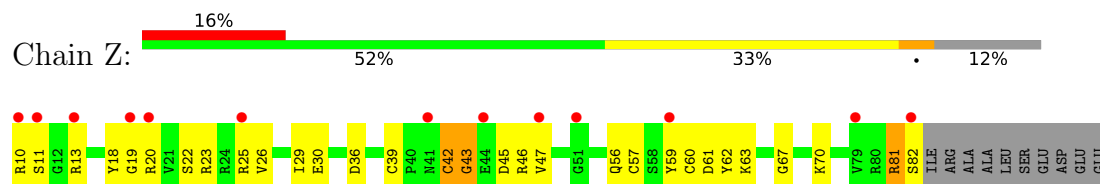


• Molecule 27: 50S ribosomal protein L32E

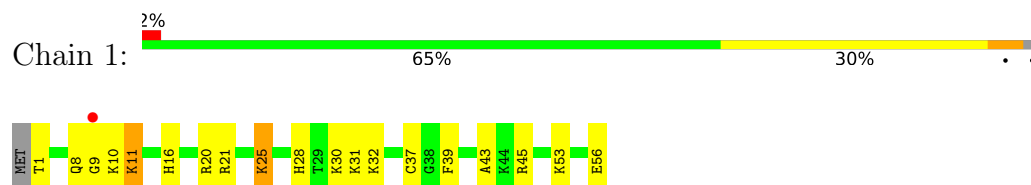


SER
GLU

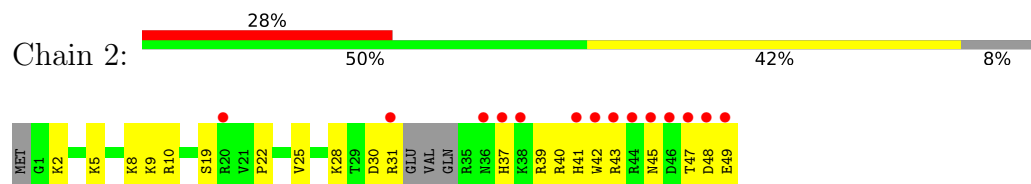
- Molecule 28: 50S ribosomal protein L37Ae



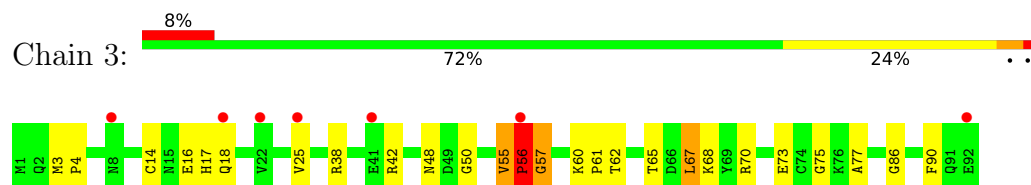
- Molecule 29: 50S ribosomal protein L37e



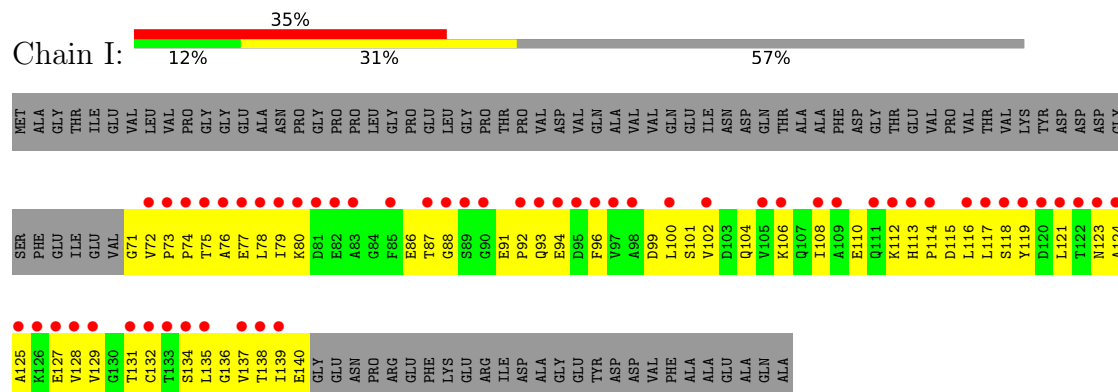
- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.79Å 300.61Å 573.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.60) 94.1 (50.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.237 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	99060	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: MG, OMU, PO2, CD, CL, UR3, NA, 5AA, PSU, K, 2OP, OMG, 1MA, DCZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.39	0/65959	0.61	29/102870 (0.0%)
2	9	0.38	0/2905	0.60	2/4528 (0.0%)
3	4	0.44	0/83	0.99	1/119 (0.8%)
4	A	0.43	0/1786	1.00	7/2408 (0.3%)
5	B	0.41	0/2690	0.99	9/3652 (0.2%)
6	C	0.48	0/1884	1.01	7/2551 (0.3%)
7	D	0.33	0/1111	0.87	5/1498 (0.3%)
8	E	0.38	0/1382	0.89	3/1880 (0.2%)
9	F	0.37	0/901	0.87	0/1224
10	G	0.36	0/241	0.72	0/324
11	H	0.39	0/1287	0.95	4/1725 (0.2%)
12	J	0.42	0/1136	0.94	5/1530 (0.3%)
13	K	0.44	0/1001	1.03	3/1347 (0.2%)
14	L	0.38	0/1130	0.96	4/1509 (0.3%)
15	M	0.42	0/1584	0.90	5/2119 (0.2%)
16	N	0.37	0/1474	1.05	15/1999 (0.8%)
17	O	0.43	0/874	0.93	1/1181 (0.1%)
18	P	0.40	0/1147	0.89	3/1528 (0.2%)
19	Q	0.44	0/749	1.03	5/1005 (0.5%)
20	R	0.45	0/1172	0.94	3/1578 (0.2%)
21	S	0.37	0/648	0.88	3/875 (0.3%)
22	T	0.39	0/958	0.97	3/1289 (0.2%)
23	U	0.39	0/417	0.86	0/562
24	V	0.36	0/502	0.94	3/675 (0.4%)
25	W	0.45	0/1219	0.99	4/1655 (0.2%)
26	X	0.44	0/664	1.00	3/895 (0.3%)
27	Y	0.45	0/1146	0.99	3/1536 (0.2%)
28	Z	0.42	0/589	0.94	1/787 (0.1%)
29	1	0.47	0/438	0.94	2/578 (0.3%)
30	2	0.40	0/401	0.76	0/529
31	3	0.42	0/771	0.89	3/1024 (0.3%)
32	I	0.35	0/526	0.91	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	0/98775	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	1	52
25	W	0	1
All	All	1	53

There are no bond length outliers.

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	13.94	130.40	109.50
4	A	222	GLY	N-CA-C	-9.56	103.11	114.48
16	N	163	PHE	N-CA-C	-9.01	102.42	113.41
1	0	1563	G	C4'-C3'-O3'	8.84	122.66	109.40
19	Q	17	LYS	N-CA-C	-8.54	97.77	110.24
1	0	1942	A	C5'-C4'-C3'	8.39	128.58	116.00
16	N	135	VAL	N-CA-C	-8.36	104.87	112.90
12	J	68	GLY	N-CA-C	8.02	122.19	112.48
5	B	157	LYS	N-CA-C	-7.87	103.81	113.41
17	O	82	SER	N-CA-C	-7.38	100.78	110.53
11	H	160	SER	N-CA-C	-7.23	98.82	110.32
2	9	3039	U	N1-C1'-C2'	7.23	122.84	112.00
7	D	136	ARG	CA-C-N	7.10	128.71	119.84
7	D	136	ARG	C-N-CA	7.10	128.71	119.84
26	X	22	ASN	N-CA-C	7.09	119.91	111.33
27	Y	143	TRP	N-CA-C	6.94	120.29	110.23
20	R	141	VAL	N-CA-C	6.82	118.30	108.48
15	M	89	THR	N-CA-C	6.80	118.69	111.28
19	Q	49	ASN	N-CA-C	6.78	118.75	110.41
16	N	133	ASP	N-CA-C	6.77	119.53	111.33
5	B	175	LEU	N-CA-C	-6.75	103.85	111.14
26	X	80	GLU	N-CA-C	-6.74	106.94	114.62
1	0	1819	G	C5'-C4'-C3'	6.63	125.94	116.00
22	T	52	ARG	N-CA-C	6.62	124.91	110.80
8	E	11	VAL	N-CA-C	6.53	119.09	108.97
18	P	56	GLY	N-CA-C	-6.48	100.98	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	3	55	VAL	CA-C-N	6.48	127.94	119.84
31	3	55	VAL	C-N-CA	6.48	127.94	119.84
16	N	153	GLN	N-CA-C	-6.43	105.81	113.21
1	0	834	G	C2'-C3'-O3'	-6.42	104.08	113.70
5	B	154	VAL	CA-C-N	6.41	125.64	118.97
5	B	154	VAL	C-N-CA	6.41	125.64	118.97
13	K	46	LYS	N-CA-C	6.37	120.08	109.95
21	S	59	ASP	N-CA-C	-6.36	104.77	113.30
1	0	1504	A	N9-C1'-C2'	6.33	121.49	112.00
20	R	137	ASN	N-CA-C	6.32	119.82	110.46
1	0	2291	A	N9-C1'-C2'	6.29	121.43	112.00
4	A	48	ASP	CA-C-N	6.22	126.68	119.47
4	A	48	ASP	C-N-CA	6.22	126.68	119.47
1	0	920	C	C2'-C3'-O3'	-6.21	104.39	113.70
1	0	1120	U	C5'-C4'-C3'	-6.16	106.77	116.00
8	E	17	HIS	CB-CA-C	-6.08	109.58	116.63
25	W	68	THR	N-CA-C	6.08	117.99	111.36
16	N	66	LEU	N-CA-C	-6.02	105.01	112.90
5	B	265	LEU	N-CA-C	6.01	118.46	110.53
16	N	51	GLY	CA-C-N	5.99	125.67	119.56
16	N	51	GLY	C-N-CA	5.99	125.67	119.56
14	L	57	VAL	N-CA-C	-5.98	107.16	112.90
24	V	64	GLY	N-CA-C	-5.94	106.75	115.72
4	A	133	ARG	N-CA-C	-5.94	105.80	113.16
22	T	78	THR	N-CA-C	5.92	117.96	109.14
2	9	3039	U	C4'-C3'-O3'	-5.89	104.17	113.00
1	0	871	G	C5'-C4'-O4'	-5.88	100.98	109.80
6	C	175	LYS	N-CA-C	5.88	117.88	110.24
25	W	50	ASP	N-CA-C	5.84	120.41	113.16
20	R	122	GLN	N-CA-C	-5.81	99.67	108.67
1	0	2316	G	C5'-C4'-C3'	-5.76	106.56	115.20
24	V	42	ASN	CA-C-N	5.75	127.03	119.84
24	V	42	ASN	C-N-CA	5.75	127.03	119.84
1	0	206	G	C5'-C4'-C3'	-5.75	107.38	116.00
29	1	43	ALA	N-CA-C	-5.74	105.10	111.36
6	C	91	PRO	N-CA-C	5.74	117.70	110.70
3	4	176	A	C1'-C2'-O2'	-5.72	103.22	111.80
1	0	129	A	C2'-C3'-O3'	5.70	122.25	113.70
16	N	108	SER	CA-C-N	5.68	126.95	119.84
16	N	108	SER	C-N-CA	5.68	126.95	119.84
1	0	2012	U	N1-C1'-C2'	5.64	120.47	112.00
18	P	97	ARG	N-CA-C	5.64	117.43	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Y	183	GLU	N-CA-C	-5.64	100.51	109.76
16	N	169	PRO	N-CA-C	-5.62	107.11	114.03
28	Z	18	TYR	N-CA-C	5.62	122.77	110.80
12	J	67	ASN	N-CA-C	-5.61	105.16	111.28
16	N	117	ALA	N-CA-C	-5.57	105.12	111.14
14	L	44	GLU	N-CA-C	-5.57	102.57	109.64
1	0	921	G	N9-C1'-C2'	5.53	120.30	112.00
25	W	9	GLY	N-CA-C	5.52	119.65	112.25
15	M	70	GLY	N-CA-C	5.52	121.01	112.45
26	X	12	ILE	N-CA-C	5.48	113.29	107.76
15	M	18	GLY	N-CA-C	5.45	121.00	111.78
1	0	2301	A	N9-C1'-C2'	5.45	120.17	112.00
29	1	11	LYS	N-CA-C	5.45	118.01	108.52
15	M	13	GLU	N-CA-C	-5.45	106.13	112.89
1	0	2526	C	N1-C1'-C2'	5.45	120.17	112.00
6	C	89	ALA	N-CA-C	5.41	117.62	111.02
1	0	2313	C	C5'-C4'-C3'	5.41	124.11	116.00
4	A	188	ASN	N-CA-C	5.41	117.33	108.52
5	B	151	VAL	CA-C-N	5.40	125.05	119.05
5	B	151	VAL	C-N-CA	5.40	125.05	119.05
1	0	2291	A	C4'-C3'-O3'	-5.39	104.92	113.00
4	A	228	ILE	N-CA-C	5.37	116.17	108.93
14	L	20	ASN	N-CA-C	5.33	119.31	111.04
16	N	14	ARG	N-CA-C	-5.33	105.37	111.07
21	S	27	ALA	N-CA-C	-5.32	100.06	108.73
13	K	127	ALA	N-CA-C	-5.31	106.56	114.64
21	S	57	THR	N-CA-C	5.30	117.71	110.55
31	3	67	LEU	N-CA-C	5.27	118.17	109.85
1	0	2726	U	N1-C1'-C2'	5.26	119.89	112.00
16	N	171	HIS	N-CA-C	-5.25	105.73	111.82
1	0	1352	A	C2'-C3'-O3'	-5.23	105.86	113.70
6	C	205	ARG	N-CA-C	5.23	117.66	111.33
1	0	874	A	C4'-C3'-O3'	-5.23	105.16	113.00
1	0	2664	A	N9-C1'-C2'	5.22	119.83	112.00
1	0	2541	U	C2'-C3'-O3'	5.21	121.51	113.70
6	C	192	ILE	N-CA-C	5.20	116.28	109.21
19	Q	86	VAL	N-CA-C	5.20	115.22	108.35
12	J	45	VAL	N-CA-C	5.20	117.52	108.95
25	W	24	LEU	N-CA-C	-5.19	106.81	112.72
16	N	48	VAL	N-CA-C	5.17	116.75	108.89
6	C	167	ASP	N-CA-C	-5.17	106.48	112.89
5	B	222	LYS	N-CA-C	-5.16	101.86	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	T	47	THR	N-CA-C	-5.16	101.74	109.95
13	K	8	VAL	N-CA-C	5.15	115.90	108.48
15	M	121	GLY	N-CA-C	5.15	119.38	112.17
1	0	883	U	N1-C1'-C2'	5.14	119.72	112.00
11	H	159	PRO	N-CA-C	5.14	118.42	111.22
1	0	1942	A	C4'-C3'-C2'	-5.14	97.46	102.60
16	N	20	TYR	N-CA-C	5.14	117.62	111.71
14	L	145	LEU	N-CA-C	-5.12	105.59	111.07
27	Y	173	ALA	N-CA-C	5.12	118.30	111.75
8	E	37	ASP	N-CA-C	5.09	119.07	112.86
11	H	118	GLY	N-CA-C	5.08	117.92	112.33
19	Q	25	PRO	CA-C-N	5.07	124.73	119.56
19	Q	25	PRO	C-N-CA	5.07	124.73	119.56
12	J	36	VAL	N-CA-C	5.07	115.77	108.48
11	H	116	ALA	N-CA-C	5.06	119.31	113.18
6	C	179	GLY	N-CA-C	-5.06	106.54	113.27
1	0	138	U	C2'-C3'-O3'	-5.05	106.12	113.70
12	J	22	VAL	N-CA-C	-5.05	106.14	110.74
1	0	1592	G	N9-C1'-C2'	5.04	119.56	112.00
1	0	1006	A	N9-C1'-C2'	5.04	119.56	112.00
7	D	170	TYR	N-CA-C	5.04	118.76	111.56
4	A	156	ILE	N-CA-C	5.03	115.59	109.30
7	D	15	GLU	CA-C-N	5.03	126.12	119.84
7	D	15	GLU	C-N-CA	5.03	126.12	119.84
18	P	46	GLU	N-CA-C	-5.00	107.14	113.20
5	B	108	GLU	N-CA-C	5.00	119.10	112.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (53) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1055	G	Sidechain
1	0	1078	A	Sidechain
1	0	1340	G	Sidechain
1	0	1342	C	Sidechain
1	0	1351	G	Sidechain
1	0	1417	G	Sidechain
1	0	1458	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1718	G	Sidechain
1	0	174	A	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1839	A	Sidechain
1	0	1845	A	Sidechain
1	0	1848	G	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	189	A	Sidechain
1	0	2312	G	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2551	C	Sidechain
1	0	2552	C	Sidechain
1	0	2564	G	Sidechain
1	0	26	U	Sidechain
1	0	2607	U	Sidechain
1	0	2620	U	Sidechain
1	0	2630	G	Sidechain
1	0	2643	G	Sidechain
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	48	A	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	554	G	Sidechain
1	0	722	G	Sidechain
1	0	771	G	Sidechain
1	0	781	C	Sidechain
1	0	791	A	Sidechain
1	0	817	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
25	W	90	TYR	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	781	1
2	9	2600	0	1326	52	1
3	4	126	0	75	5	0
4	A	1753	0	1766	109	0
5	B	2625	0	2533	165	1
6	C	1859	0	1816	114	0
7	D	1094	0	1085	99	0
8	E	1357	0	1266	79	0
9	F	890	0	843	55	0
10	G	240	0	231	11	0
11	H	1266	0	1268	60	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	52	1
14	L	1118	0	1076	59	0
15	M	1560	0	1568	65	0
16	N	1445	0	1401	114	0
17	O	865	0	873	31	0
18	P	1136	0	1123	53	0
19	Q	735	0	729	24	0
20	R	1149	0	1122	55	0
21	S	641	0	605	19	0
22	T	950	0	923	51	0
23	U	410	0	364	23	0
24	V	499	0	511	37	0
25	W	1196	0	1137	98	0
26	X	654	0	653	45	0
27	Y	1130	0	1133	54	0
28	Z	578	0	539	23	0
29	1	431	0	426	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	2	396	0	413	29	0
31	3	755	0	728	19	0
32	I	519	0	500	59	0
33	0	106	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	3	0	0	0	0
35	0	71	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	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	1	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	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	0	5820	0	0	111	0
38	1	59	0	0	2	0
38	2	42	0	0	2	0
38	3	74	0	0	4	0
38	4	8	0	0	0	0
38	9	133	0	0	3	0
38	A	117	0	0	10	0
38	B	150	0	0	16	0
38	C	165	0	0	15	0
38	D	49	0	0	11	0
38	E	47	0	0	7	0
38	F	21	0	0	3	0
38	G	16	0	0	0	0
38	H	66	0	0	6	0
38	I	10	0	0	2	0
38	J	52	0	0	1	0
38	K	54	0	0	3	0
38	L	83	0	0	10	0
38	M	118	0	0	3	0
38	N	66	0	0	8	0
38	O	39	0	0	4	0
38	P	65	0	0	3	0
38	Q	52	0	0	5	0
38	R	85	0	0	5	0
38	S	31	0	0	3	0
38	T	39	0	0	1	0
38	U	25	0	0	0	0
38	V	13	0	0	2	0
38	W	68	0	0	6	0
38	X	27	0	0	2	0
38	Y	92	0	0	5	0
38	Z	30	0	0	2	0
All	All	99060	0	59975	2299	3

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 15.

All (2299) 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)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:62:ARG:HA	5:B:65:MET:HE3	1.31	1.10
15:M:164:THR:HG22	15:M:167:GLY:H	1.13	1.09
1:0:156:C:H5''	15:M:171:ARG:HD3	1.35	1.08
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.30	1.08
11:H:166:SER:HB2	11:H:167:PRO:HD3	1.35	1.07
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.31	1.07
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.36	1.06
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.37	1.06
7:D:25:MET:HE2	7:D:41:LEU:HG	1.42	1.02
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.75	1.02
2:9:3076:G:H3'	2:9:3077:A:H5''	1.39	1.02
6:C:236:THR:HG22	6:C:239:ALA:H	1.24	1.01
1:0:1242:A:H5'	12:J:82:THR:HG23	1.41	1.01
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.43	0.99
1:0:2717:C:H2'	1:0:2718:C:H5''	1.42	0.99
1:0:1119:G:H2'	12:J:52:GLN:NE2	1.77	0.98
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.41	0.97
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.29	0.97
30:2:41:HIS:H	30:2:45:ASN:HD22	0.98	0.97
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.48	0.95
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.32	0.95
4:A:211:LYS:HB3	4:A:212:PRO:HD2	1.49	0.94
1:0:2717:C:C2'	1:0:2718:C:H5''	1.98	0.93
1:0:870:G:H2'	1:0:871:G:H5''	1.48	0.93
1:0:871:G:C8	1:0:871:G:H5'	2.02	0.93
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.51	0.93
13:K:10:GLN:NE2	13:K:10:GLN:H	1.66	0.92
1:0:541:C:H2'	1:0:542:A:H5''	1.52	0.92
1:0:1474:C:H6	1:0:1474:C:H5'	1.34	0.92
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.50	0.92
25:W:5:VAL:HG11	25:W:153:MET:HE1	1.50	0.92
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.49	0.91
16:N:17:ARG:HB3	16:N:17:ARG:HH11	1.34	0.91
13:K:10:GLN:H	13:K:10:GLN:HE21	0.94	0.90
1:0:2812:A:H2	1:0:2814:A:H62	1.17	0.89
1:0:871:G:H5'	1:0:871:G:H8	1.36	0.89
18:P:115:SER:H	18:P:118:GLN:HE21	0.93	0.89
1:0:1667:A:H8	1:0:1667:A:H5'	1.38	0.89
6:C:236:THR:HG22	6:C:239:ALA:N	1.87	0.88
2:9:3056:A:H2'	2:9:3057:A:H5''	1.54	0.88
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.53	0.88
4:A:179:MET:HA	4:A:179:MET:HE3	1.53	0.88
1:O:1835:U:H5	1:O:1840:A:N7	1.72	0.88
25:W:149:LEU:HG	25:W:153:MET:HE2	1.54	0.88
28:Z:10:ARG:HA	38:Z:9215:HOH:O	1.74	0.88
22:T:101:LEU:HD13	22:T:112:LEU:HD11	1.54	0.87
1:O:1751:G:H2'	1:O:1752:G:H5''	1.54	0.87
1:O:2364:A:H5''	19:Q:15:LYS:HD3	1.56	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.37	0.87
13:K:10:GLN:HE21	13:K:10:GLN:N	1.71	0.87
24:V:1:THR:HG23	24:V:2:VAL:H	1.40	0.86
1:O:1160:G:C5'	1:O:1161:A:H5'	2.04	0.86
1:O:2506:A:HO2'	1:O:2507:G:H8	0.87	0.86
5:B:264:GLU:HG2	5:B:267:LYS:HE2	1.57	0.86
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.57	0.86
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.89	0.86
5:B:307:ARG:HH11	5:B:307:ARG:HB2	1.39	0.85
4:A:35:GLY:O	4:A:36:ASP:HB3	1.76	0.85
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.57	0.85
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.06	0.85
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.57	0.85
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.59	0.85
1:O:542:A:H5'	1:O:542:A:H8	1.41	0.85
1:O:545:G:H5'	1:O:545:G:H8	1.42	0.84
4:A:153:ARG:HB2	4:A:153:ARG:HH11	1.41	0.84
18:P:115:SER:N	18:P:118:GLN:HE21	1.75	0.84
16:N:144:GLY:O	16:N:147:ILE:HG22	1.77	0.84
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.56	0.84
1:O:2586:U:H3	1:O:2592:G:H22	1.25	0.84
15:M:166:ALA:HA	15:M:169:ARG:NH1	1.93	0.84
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.58	0.84
7:D:57:THR:HG23	7:D:63:ILE:HA	1.60	0.83
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.43	0.83
18:P:115:SER:H	18:P:118:GLN:NE2	1.76	0.83
15:M:164:THR:HG22	15:M:167:GLY:N	1.91	0.83
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.59	0.83
2:9:3006:C:H5''	16:N:37:ARG:NH1	1.94	0.83
4:A:191:GLY:HA2	4:A:194:MET:CE	2.09	0.82
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.79	0.82
24:V:12:THR:HG23	24:V:14:ALA:H	1.42	0.82
27:Y:235:GLU:CD	27:Y:235:GLU:H	1.86	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.27	0.82
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.25	0.82
1:0:21:G:H5'	20:R:2:ILE:HA	1.61	0.82
1:0:1159:G:H21	1:0:1189:A:H8	1.27	0.82
1:0:2904:U:H4'	26:X:8:ARG:NH1	1.95	0.82
23:U:9:CYS:HA	23:U:52:THR:HG23	1.62	0.82
11:H:166:SER:HB2	11:H:167:PRO:CD	2.10	0.82
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.60	0.82
30:2:41:HIS:N	30:2:45:ASN:HD22	1.77	0.82
1:0:282:C:H1'	1:0:368:C:N4	1.94	0.81
1:0:381:G:H5''	38:0:4610:HOH:O	1.79	0.81
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.62	0.81
1:0:2506:A:O2'	1:0:2507:G:H8	1.64	0.81
12:J:107:ASN:ND2	12:J:109:TYR:H	1.79	0.81
1:0:21:G:C5'	20:R:2:ILE:HA	2.12	0.80
25:W:88:THR:HB	38:W:6679:HOH:O	1.80	0.80
7:D:154:LYS:H	7:D:154:LYS:HD2	1.46	0.80
20:R:39:THR:HG22	20:R:42:GLU:H	1.46	0.80
20:R:17:MET:HE1	20:R:19:ARG:NH2	1.96	0.80
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.62	0.80
1:0:2533:C:H5'	1:0:2533:C:H6	1.46	0.80
1:0:506:G:H22	1:0:509:A:H5''	1.47	0.79
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.63	0.79
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.63	0.79
1:0:541:C:C2'	1:0:542:A:H5''	2.10	0.79
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.61	0.79
1:0:1160:G:H5'	1:0:1161:A:C5'	2.10	0.79
5:B:27:ASN:HD22	5:B:27:ASN:H	1.30	0.79
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.47	0.79
1:0:1165:G:H4'	1:0:1174:A:O2'	1.83	0.79
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.64	0.79
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.82	0.79
25:W:38:THR:HG22	25:W:39:ASP:H	1.47	0.79
18:P:115:SER:OG	18:P:118:GLN:HG3	1.83	0.78
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.65	0.78
1:0:1450:C:H4'	1:0:1451:C:OP2	1.82	0.78
16:N:93:GLN:HA	16:N:93:GLN:HE21	1.47	0.78
6:C:236:THR:H	6:C:239:ALA:HB3	1.49	0.78
7:D:25:MET:HE3	7:D:37:ALA:HB1	1.64	0.78
4:A:36:ASP:OD2	4:A:85:SER:HB2	1.84	0.77
24:V:8:ILE:HA	24:V:11:MET:HE3	1.63	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2291:A:C8	1:0:2309:C:H5'	2.19	0.77
12:J:45:VAL:HG23	12:J:130:VAL:O	1.83	0.77
7:D:136:ARG:HD2	7:D:155:HIS:O	1.83	0.77
25:W:80:ASP:O	25:W:84:VAL:HG23	1.84	0.77
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.83	0.77
9:F:91:VAL:HG12	9:F:92:GLY:H	1.49	0.77
1:0:559:U:H6	1:0:559:U:H5'	1.49	0.77
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.15	0.77
25:W:13:MET:HE2	25:W:18:GLN:HA	1.67	0.76
1:0:2748:G:H2'	38:0:7745:HOH:O	1.84	0.76
4:A:131:HIS:O	4:A:132:ASP:HB2	1.86	0.76
1:0:877:G:H5'	1:0:878:G:OP1	1.85	0.76
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.85	0.76
5:B:238:ASN:HD22	5:B:240:GLY:H	1.33	0.76
6:C:115:LEU:HD21	6:C:243:VAL:HG13	1.64	0.76
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.66	0.76
1:0:871:G:H8	1:0:871:G:C5'	1.99	0.76
1:0:1162:G:H1'	32:I:117:LEU:HD11	1.67	0.76
1:0:870:G:C2'	1:0:871:G:H5''	2.16	0.76
1:0:56:G:H5''	24:V:50:ARG:HH12	1.49	0.76
7:D:135:VAL:HG22	7:D:136:ARG:H	1.51	0.76
21:S:57:THR:HG22	21:S:59:ASP:H	1.52	0.75
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.67	0.75
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.67	0.75
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.66	0.75
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.50	0.75
25:W:122:ARG:HG2	25:W:122:ARG:HH11	1.51	0.75
5:B:179:LEU:O	5:B:183:GLU:HG2	1.87	0.75
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.69	0.75
6:C:139:VAL:HG13	38:C:9244:HOH:O	1.85	0.75
1:0:1641:A:H2'	1:0:1642:A:H5'	1.69	0.75
25:W:88:THR:HG22	25:W:89:ASP:H	1.49	0.75
1:0:1372:A:H3'	38:0:7407:HOH:O	1.87	0.74
1:0:2862:G:H4'	5:B:336:GLN:O	1.87	0.74
11:H:166:SER:CB	11:H:167:PRO:HD3	2.13	0.74
24:V:39:ALA:N	24:V:40:PRO:HD2	2.02	0.74
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.69	0.74
38:0:6419:HOH:O	4:A:223:ARG:HG3	1.86	0.74
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.70	0.74
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.18	0.74
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3006:C:OP1	16:N:37:ARG:NH1	2.21	0.74
1:0:2908:A:H2'	1:0:2909:G:O4'	1.88	0.74
26:X:25:ARG:HD3	26:X:64:ALA:O	1.88	0.74
29:1:10:LYS:HG3	38:1:9236:HOH:O	1.87	0.74
1:0:2904:U:H4'	26:X:8:ARG:HH12	1.50	0.74
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.88	0.74
1:0:1116:U:HO2'	1:0:1118:A:H2	1.34	0.74
1:0:2756:U:H3	1:0:2896:A:H2	1.34	0.73
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.85	0.73
20:R:99:ALA:HB1	20:R:109:MET:CE	2.17	0.73
11:H:46:GLN:HB3	11:H:167:PRO:CD	2.15	0.73
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.68	0.73
1:0:1299:G:O6	14:L:6:ARG:HD3	1.89	0.73
9:F:91:VAL:HG12	9:F:92:GLY:N	2.03	0.73
16:N:17:ARG:HB3	16:N:17:ARG:NH1	2.03	0.73
2:9:3014:G:H5'	2:9:3014:G:H8	1.54	0.73
16:N:164:ASP:CG	16:N:167:ASP:HA	2.14	0.73
2:9:3029:C:H2'	2:9:3030:C:H5'	1.70	0.73
16:N:151:ASP:O	16:N:154:LEU:HB2	1.88	0.73
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.70	0.73
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.70	0.73
11:H:58:ARG:HH11	11:H:58:ARG:HG3	1.53	0.73
12:J:131:THR:HG22	12:J:134:GLU:H	1.53	0.73
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.70	0.73
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.23	0.72
22:T:63:ILE:HD11	22:T:75:GLU:HB2	1.70	0.72
1:0:2716:G:H5''	5:B:206:THR:HG21	1.71	0.72
7:D:146:LYS:NZ	16:N:107:ASN:HD21	1.87	0.72
1:0:793:A:H5''	18:P:83:LYS:HG2	1.71	0.72
1:0:281:U:H2'	1:0:282:C:O4'	1.89	0.72
11:H:27:LYS:H	11:H:59:HIS:HD2	1.37	0.72
1:0:182:G:H5'	38:0:5431:HOH:O	1.90	0.72
4:A:199:HIS:HD2	4:A:201:PHE:H	1.34	0.72
14:L:133:VAL:HA	38:L:9371:HOH:O	1.88	0.72
1:0:1116:U:O2'	1:0:1118:A:H2	1.72	0.72
1:0:1119:G:N2	1:0:1246:A:C2	2.58	0.72
1:0:2270:G:H4'	4:A:223:ARG:HH12	1.54	0.72
1:0:506:G:H22	1:0:509:A:C5'	2.03	0.72
26:X:43:VAL:HG12	26:X:44:ASP:H	1.55	0.72
5:B:195:ARG:HG2	5:B:323:LEU:HD22	1.71	0.72
2:9:3039:U:H1'	2:9:3044:A:H61	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:9:ILE:HD12	11:H:54:THR:HG22	1.71	0.71
22:T:49:GLU:OE2	22:T:97:ARG:HD2	1.90	0.71
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.72	0.71
1:O:1184:C:H1'	38:O:7672:HOH:O	1.89	0.71
1:O:1701:A:H4'	1:O:1702:U:H5''	1.72	0.71
20:R:99:ALA:CB	20:R:109:MET:HE1	2.20	0.71
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.72	0.71
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.06	0.71
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.06	0.71
30:2:41:HIS:H	30:2:45:ASN:ND2	1.82	0.71
20:R:17:MET:HE1	20:R:19:ARG:CZ	2.20	0.71
1:O:1116:U:H3	1:O:1246:A:H62	1.35	0.71
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.25	0.71
1:O:871:G:C8	1:O:871:G:C5'	2.74	0.71
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.73	0.71
12:J:74:ARG:HH11	12:J:74:ARG:CB	2.01	0.71
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.20	0.71
5:B:168:GLY:H	5:B:174:ARG:HD3	1.56	0.71
1:O:272:A:H5'	1:O:273:G:OP2	1.90	0.71
1:O:380:A:H2'	38:O:7446:HOH:O	1.90	0.71
1:O:188:C:H5''	15:M:163:LEU:HD21	1.73	0.70
16:N:113:SER:HB2	38:N:9360:HOH:O	1.89	0.70
32:I:99:ASP:OD1	32:I:138:THR:HB	1.90	0.70
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.89	0.70
12:J:93:ARG:HB3	12:J:93:ARG:HH11	1.55	0.70
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.72	0.70
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.21	0.70
16:N:47:LEU:HD11	16:N:127:LEU:HD21	1.74	0.70
26:X:43:VAL:HG12	26:X:44:ASP:N	2.05	0.70
1:O:2054:A:N3	20:R:128:ARG:NH2	2.39	0.70
1:O:2533:C:H5'	1:O:2533:C:C6	2.25	0.70
7:D:99:ASP:HA	38:D:5675:HOH:O	1.92	0.70
16:N:169:PRO:O	16:N:172:PHE:HB3	1.91	0.70
28:Z:26:VAL:O	28:Z:30:GLU:HG3	1.91	0.70
4:A:33:GLU:O	4:A:34:ASP:HB2	1.90	0.70
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.72	0.70
6:C:162:VAL:HG12	6:C:192:ILE:HD11	1.72	0.70
6:C:246:ARG:HB3	6:C:246:ARG:HH11	1.56	0.70
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.74	0.70
1:O:1118:A:H8	1:O:1118:A:H3'	1.56	0.70
1:O:450:C:OP1	6:C:184:ARG:NH2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2256:G:H2'	1:0:2257:G:H5'	1.74	0.70
4:A:153:ARG:HB2	4:A:153:ARG:NH1	2.07	0.70
8:E:93:MET:HE1	8:E:165:GLY:N	2.07	0.69
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.38	0.69
2:9:3006:C:H5''	16:N:37:ARG:HH12	1.57	0.69
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.55	0.69
7:D:99:ASP:HB3	7:D:103:ASN:H	1.55	0.69
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.90	0.69
18:P:103:THR:HA	18:P:106:ARG:NH1	2.06	0.69
8:E:3:VAL:HG22	8:E:49:ILE:HB	1.75	0.69
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.56	0.69
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.75	0.69
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.73	0.69
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.22	0.69
1:0:1118:A:H3'	1:0:1118:A:C8	2.28	0.69
1:0:1559:A:H1'	38:0:6128:HOH:O	1.93	0.69
1:0:1667:A:H5'	1:0:1667:A:C8	2.25	0.69
5:B:258:GLY:H	5:B:260:HIS:CE1	2.11	0.69
25:W:13:MET:HE2	25:W:18:GLN:CA	2.22	0.69
1:0:474:C:O3'	6:C:73:LEU:HD21	1.93	0.69
4:A:121:ALA:O	4:A:124:VAL:HG22	1.92	0.69
7:D:86:THR:C	7:D:89:PRO:HD2	2.17	0.69
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.41	0.69
1:0:1209:C:H2'	1:0:1210:G:H8	1.56	0.69
1:0:1603:A:H5'	1:0:1605:G:O4'	1.93	0.68
1:0:2679:G:H2'	1:0:2681:A:OP2	1.93	0.68
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.90	0.68
17:O:32:ARG:O	17:O:32:ARG:HD3	1.92	0.68
23:U:52:THR:HG22	23:U:54:THR:H	1.58	0.68
1:0:1979:G:H2'	38:0:3601:HOH:O	1.92	0.68
4:A:153:ARG:HH11	4:A:153:ARG:CB	2.05	0.68
8:E:97:VAL:HG12	38:E:4191:HOH:O	1.93	0.68
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.75	0.68
25:W:84:VAL:HG12	38:W:6679:HOH:O	1.93	0.68
1:0:2851:G:O2'	1:0:2852:A:H5'	1.92	0.68
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.73	0.68
5:B:320:GLN:NE2	5:B:321:PRO:HD2	2.09	0.68
7:D:25:MET:CE	7:D:37:ALA:HB1	2.23	0.68
38:0:3542:HOH:O	32:I:92:PRO:HD2	1.93	0.68
1:0:603:A:H5''	1:0:604:G:OP1	1.94	0.68
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.93	0.68
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.75	0.68
1:0:2426:G:H1'	38:0:6350:HOH:O	1.92	0.67
1:0:2769:C:C2'	1:0:2770:G:H5'	2.23	0.67
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.23	0.67
4:A:200:PRO:HG2	4:A:225:VAL:HG21	1.76	0.67
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.76	0.67
1:0:56:G:H5''	24:V:50:ARG:NH1	2.07	0.67
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.75	0.67
25:W:119:HIS:HD2	25:W:120:PRO:O	1.77	0.67
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.76	0.67
12:J:19:MET:HE3	12:J:132:LEU:CD1	2.21	0.67
1:0:2840:A:OP1	5:B:211:THR:HG23	1.94	0.67
5:B:140:LEU:HA	38:B:9380:HOH:O	1.95	0.67
5:B:7:ARG:NH1	5:B:11:LEU:HD21	2.09	0.67
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.95	0.67
27:Y:112:GLU:CD	27:Y:115:ARG:HH12	2.01	0.67
5:B:108:GLU:HB3	5:B:111:ARG:HD2	1.75	0.67
1:0:1751:G:C2'	1:0:1752:G:H5''	2.24	0.67
1:0:2827:A:H2'	1:0:2828:G:O4'	1.95	0.67
7:D:95:THR:OG1	7:D:174:VAL:HG22	1.95	0.67
1:0:1474:C:H5'	1:0:1474:C:C6	2.23	0.66
2:9:3056:A:C2'	2:9:3057:A:H5''	2.24	0.66
1:0:1441:G:H1'	38:0:7965:HOH:O	1.96	0.66
4:A:179:MET:HG2	4:A:186:TRP:CB	2.25	0.66
5:B:62:ARG:CA	5:B:65:MET:HE3	2.18	0.66
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.77	0.66
6:C:140:VAL:HB	38:C:9247:HOH:O	1.95	0.66
14:L:37:LYS:HG2	38:L:9335:HOH:O	1.95	0.66
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.77	0.66
16:N:152:GLU:C	16:N:154:LEU:H	2.04	0.66
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.25	0.66
1:0:1205:U:H2'	1:0:1206:U:H5''	1.78	0.66
1:0:1377:C:H5'	1:0:1377:C:H6	1.61	0.66
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.09	0.66
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.77	0.66
32:I:92:PRO:C	32:I:94:GLU:H	2.02	0.66
1:0:1328:A:OP1	27:Y:169:ARG:HD2	1.95	0.66
1:0:1189:A:H1'	1:0:1209:C:O4'	1.95	0.66
3:4:176:A:O4'	3:4:175:C:H2'	1.95	0.66
14:L:79:ASP:HB3	38:L:9356:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:560:C:H42	1:0:597:A:H61	1.41	0.66
1:0:88:G:H8	1:0:88:G:H5'	1.61	0.66
21:S:57:THR:HG22	21:S:59:ASP:N	2.11	0.66
23:U:14:GLU:O	23:U:17:THR:HB	1.96	0.66
1:0:2578:G:H5'	1:0:2578:G:H8	1.60	0.65
15:M:164:THR:CG2	15:M:167:GLY:H	2.00	0.65
1:0:21:G:H5''	20:R:1:GLY:O	1.96	0.65
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.25	0.65
25:W:38:THR:HG22	25:W:39:ASP:N	2.12	0.65
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.78	0.65
8:E:7:ILE:HG22	8:E:45:ASP:O	1.95	0.65
13:K:74:VAL:HG12	13:K:75:ARG:HG3	1.79	0.65
1:0:447:A:OP2	22:T:1:SER:HB2	1.96	0.65
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.78	0.65
29:1:25:LYS:HG3	30:2:49:GLU:H	1.60	0.65
32:I:101:SER:H	32:I:104:GLN:NE2	1.94	0.65
1:0:2878:U:H2'	1:0:2879:A:O4'	1.95	0.65
9:F:58:GLU:HA	9:F:61:MET:HG3	1.78	0.65
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.61	0.65
24:V:12:THR:HG22	24:V:15:GLU:CG	2.17	0.65
26:X:78:GLU:HG2	26:X:79:GLU:H	1.60	0.65
1:0:545:G:H5'	1:0:545:G:C8	2.30	0.65
4:A:210:GLY:HA3	38:A:9379:HOH:O	1.97	0.65
5:B:275:GLY:O	5:B:291:ASP:HA	1.97	0.65
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.62	0.65
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.79	0.65
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.36	0.65
6:C:16:VAL:HG12	6:C:17:ASP:H	1.61	0.65
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.79	0.65
16:N:100:ALA:O	16:N:129:ILE:HG23	1.98	0.65
25:W:65:VAL:HA	25:W:68:THR:HG22	1.79	0.65
1:0:21:G:H4'	20:R:2:ILE:HG22	1.80	0.64
11:H:51:VAL:HG21	11:H:127:VAL:HG11	1.79	0.64
1:0:1667:A:H2'	1:0:1668:U:C6	2.32	0.64
4:A:192:VAL:HG13	38:A:9350:HOH:O	1.96	0.64
1:0:777:U:O2'	29:1:11:LYS:HG2	1.97	0.64
1:0:1666:C:O2'	1:0:1667:A:H5''	1.96	0.64
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.11	0.64
11:H:21:THR:O	11:H:120:ILE:HD12	1.98	0.64
16:N:38:LYS:HE2	16:N:107:ASN:HD21	1.63	0.64
1:0:544:G:H2'	1:0:545:G:H5''	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:106:THR:OG1	25:W:109:GLU:HG3	1.98	0.64
1:O:1654:U:H2'	4:A:47:HIS:HD2	1.61	0.64
38:O:4899:HOH:O	17:O:39:THR:HB	1.97	0.64
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.79	0.64
8:E:69:ILE:HA	8:E:72:MET:CE	2.27	0.64
18:P:64:GLU:HG2	38:P:169:HOH:O	1.98	0.64
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.63	0.64
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.31	0.64
6:C:16:VAL:HG12	6:C:17:ASP:N	2.12	0.64
5:B:297:VAL:HB	38:B:9407:HOH:O	1.97	0.64
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.80	0.64
1:O:2073:G:H5''	38:O:4124:HOH:O	1.98	0.64
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.79	0.64
32:I:125:ALA:O	32:I:129:VAL:HG23	1.97	0.64
1:O:2676:C:H4'	12:J:70:PHE:CE1	2.32	0.63
1:O:1189:A:H1'	1:O:1209:C:C1'	2.27	0.63
4:A:32:VAL:HG22	4:A:38:ILE:HG13	1.80	0.63
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.81	0.63
6:C:246:ARG:HB3	6:C:246:ARG:NH1	2.13	0.63
10:G:16:LYS:O	10:G:20:VAL:HG23	1.98	0.63
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.44	0.63
2:9:3051:A:H5'	16:N:160:SER:HB3	1.81	0.63
14:L:143:THR:HG22	14:L:144:ASP:N	2.11	0.63
24:V:64:GLY:O	24:V:65:ASP:HB2	1.96	0.63
2:9:3039:U:H1'	2:9:3044:A:N6	2.13	0.63
1:O:338:C:H4'	6:C:174:ILE:CD1	2.29	0.63
5:B:81:ALA:O	5:B:186:GLY:HA3	1.99	0.63
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.97	0.63
1:O:282:C:O2'	1:O:283:U:H5'	1.98	0.63
1:O:1116:U:O2'	1:O:1118:A:C2	2.51	0.63
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.45	0.63
10:G:64:ASN:HD22	10:G:64:ASN:N	1.94	0.63
11:H:27:LYS:H	11:H:59:HIS:CD2	2.16	0.63
2:9:3041:C:H4'	7:D:48:MET:HB2	1.80	0.63
7:D:25:MET:HE2	7:D:41:LEU:CG	2.24	0.63
12:J:52:GLN:HG3	12:J:53:ILE:N	2.13	0.63
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.29	0.63
1:O:1058:A:H2'	1:O:1060:C:H5''	1.79	0.63
30:2:40:ARG:HA	30:2:45:ASN:ND2	2.14	0.63
1:O:542:A:H5'	1:O:542:A:C8	2.29	0.62
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:110:THR:HB	16:N:113:SER:OG	1.98	0.62
23:U:5:GLU:HG3	23:U:10:GLY:O	1.99	0.62
25:W:21:LEU:CD2	25:W:26:ILE:HD11	2.28	0.62
27:Y:189:ASN:C	27:Y:189:ASN:HD22	2.07	0.62
4:A:36:ASP:C	4:A:38:ILE:H	2.07	0.62
15:M:60:VAL:C	15:M:61:ILE:HD12	2.23	0.62
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.45	0.62
1:O:2256:G:C2'	1:O:2257:G:H5'	2.30	0.62
8:E:84:MET:HE1	8:E:148:ILE:CD1	2.29	0.62
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.35	0.62
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.64	0.62
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.28	0.62
30:2:40:ARG:HD2	30:2:47:THR:HG22	1.80	0.62
1:O:111:C:O2'	29:1:20:ARG:HG2	1.99	0.62
2:9:3054:A:O2'	2:9:3055:U:H5'	1.99	0.62
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.82	0.62
12:J:19:MET:HE2	12:J:79:PHE:HA	1.81	0.62
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	1.98	0.62
1:O:1625:U:H4'	38:0:4948:HOH:O	1.97	0.62
9:F:2:VAL:HG22	9:F:57:GLU:OE1	2.00	0.62
1:O:2534:C:H1'	38:0:3800:HOH:O	1.99	0.62
1:O:1206:U:H5'	1:O:1206:U:H6	1.65	0.62
1:O:1634:G:H3'	38:0:4189:HOH:O	2.00	0.62
1:O:2251:G:H2'	1:O:2252:A:C8	2.34	0.62
5:B:145:HIS:HD2	5:B:146:THR:O	1.81	0.62
12:J:130:VAL:HG12	12:J:131:THR:N	2.15	0.62
1:O:31:C:H2'	38:0:7888:HOH:O	1.99	0.62
1:O:299:U:H5'	38:0:7546:HOH:O	1.99	0.62
1:O:2780:C:H1'	8:E:143:GLN:HE21	1.65	0.62
2:9:3001:U:H5''	2:9:3003:A:OP1	2.00	0.62
21:S:11:THR:H	21:S:14:ALA:HB3	1.65	0.62
23:U:52:THR:HG22	23:U:54:THR:N	2.15	0.62
1:O:1819:G:H2'	1:O:1820:G:H4'	1.82	0.62
4:A:199:HIS:CD2	4:A:201:PHE:H	2.16	0.62
11:H:169:GLY:C	11:H:170:ASN:HD22	2.08	0.62
15:M:28:GLN:O	15:M:32:ARG:HG3	2.00	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.64	0.62
16:N:23:ARG:HG2	16:N:23:ARG:HH11	1.65	0.61
23:U:20:MET:HE2	23:U:30:HIS:NE2	2.14	0.61
1:O:541:C:H2'	1:O:542:A:C5'	2.26	0.61
1:O:1684:A:H1'	30:2:43:ARG:HH22	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2256:G:H2'	1:0:2257:G:C5'	2.30	0.61
5:B:62:ARG:HA	5:B:65:MET:CE	2.21	0.61
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.36	0.61
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.80	0.61
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.82	0.61
1:0:470:U:O2'	29:1:16:HIS:HD2	1.83	0.61
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.30	0.61
1:0:1166:A:H1'	1:0:1192:A:C2	2.36	0.61
5:B:84:LEU:HD23	5:B:142:LEU:HD23	1.82	0.61
1:0:119:A:H2'	1:0:120:A:H5''	1.81	0.61
7:D:138:GLY:N	38:D:7597:HOH:O	2.33	0.61
21:S:33:SER:O	21:S:37:VAL:HG23	1.99	0.61
32:I:76:ALA:O	32:I:80:LYS:HG3	2.01	0.61
1:0:20:G:H21	20:R:117:HIS:HD2	1.48	0.61
1:0:2491:G:H1'	38:0:7098:HOH:O	1.99	0.61
2:9:3014:G:H5'	2:9:3014:G:C8	2.34	0.61
16:N:154:LEU:O	16:N:155:GLU:HB3	2.00	0.61
27:Y:144:ARG:CZ	38:Y:9407:HOH:O	2.48	0.61
1:0:656:G:OP2	17:O:37:ARG:HD2	2.01	0.61
16:N:80:SER:HB2	38:N:9335:HOH:O	2.01	0.61
1:0:1527:A:H1'	1:0:1528:A:C8	2.35	0.61
38:0:4951:HOH:O	5:B:300:SER:HB3	1.99	0.61
5:B:144:THR:HB	38:B:9426:HOH:O	2.00	0.61
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.31	0.61
1:0:969:G:H1	1:0:999:C:H42	1.49	0.61
1:0:1080:C:H4'	1:0:1081:A:OP1	2.00	0.61
1:0:2649:A:H5'	1:0:2649:A:H8	1.66	0.61
5:B:254:GLN:HG2	5:B:255:GLY:N	2.14	0.61
8:E:81:GLU:HG2	8:E:134:SER:CB	2.30	0.61
9:F:38:LYS:HZ3	15:M:3:SER:HA	1.64	0.61
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.81	0.61
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.84	0.60
4:A:211:LYS:HB3	4:A:212:PRO:CD	2.27	0.60
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.63	0.60
1:0:247:A:H2'	38:0:4218:HOH:O	2.01	0.60
1:0:285:A:H2'	1:0:286:U:O4'	2.00	0.60
1:0:797:A:H4'	28:Z:10:ARG:N	2.16	0.60
1:0:902:G:N7	14:L:18:HIS:HD2	2.00	0.60
1:0:1180:U:H4'	32:I:91:GLU:HG2	1.82	0.60
1:0:1182:C:H1'	1:0:1192:A:H8	1.64	0.60
1:0:1535:G:H2'	1:0:1536:C:C6	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2346:C:H6	1:0:2346:C:O5'	1.84	0.60
4:A:179:MET:HA	4:A:179:MET:CE	2.28	0.60
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.83	0.60
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.98	0.60
38:0:5117:HOH:O	12:J:47:THR:HB	2.01	0.60
16:N:132:ASN:O	16:N:135:VAL:HG12	2.01	0.60
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.32	0.60
1:0:157:G:H4'	15:M:95:LYS:HE3	1.84	0.60
1:0:2896:A:H5''	38:0:6357:HOH:O	2.01	0.60
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.31	0.60
11:H:9:ILE:HG23	11:H:126:ARG:CZ	2.32	0.60
1:0:1118:A:H62	1:0:1244:U:H3	1.48	0.60
1:0:1741:U:H5'	1:0:1742:A:OP1	2.01	0.60
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.67	0.60
18:P:105:LEU:HD21	18:P:137:LEU:HD21	1.84	0.60
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.84	0.60
6:C:27:ARG:HG3	6:C:29:ASP:OD1	2.02	0.60
17:O:105:ASN:HD21	17:O:109:SER:H	1.49	0.60
25:W:35:VAL:HG23	25:W:41:TYR:CD2	2.36	0.60
8:E:13:ALA:HB2	8:E:22:VAL:HG22	1.84	0.60
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.32	0.60
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.02	0.60
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.14	0.60
5:B:168:GLY:N	5:B:174:ARG:HD3	2.16	0.60
6:C:162:VAL:HG13	6:C:232:LEU:HD21	1.83	0.60
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.84	0.60
1:0:447:A:P	22:T:1:SER:HB2	2.42	0.60
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.37	0.60
1:0:1500:U:P	18:P:41:ARG:HH22	2.24	0.59
1:0:2524:G:H21	1:0:2526:C:N4	2.00	0.59
1:0:2720:C:O2	13:K:87:ARG:NH2	2.35	0.59
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.02	0.59
5:B:103:ASP:HB2	38:B:9394:HOH:O	2.02	0.59
7:D:23:VAL:HG23	7:D:23:VAL:O	2.02	0.59
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.14	0.59
1:0:2505:G:O2'	1:0:2506:A:H5'	2.02	0.59
38:0:7663:HOH:O	5:B:211:THR:HG21	2.01	0.59
2:9:3013:A:O2'	2:9:3014:G:H5''	2.03	0.59
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.84	0.59
4:A:105:VAL:HG11	4:A:154:ALA:HB1	1.83	0.59
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2769:C:H2'	1:0:2770:G:H5'	1.82	0.59
20:R:119:VAL:HG12	20:R:119:VAL:O	2.00	0.59
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.82	0.59
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.84	0.59
30:2:40:ARG:HG3	30:2:45:ASN:HB3	1.82	0.59
1:0:1972:U:H2'	1:0:1973:A:H5'	1.83	0.59
2:9:3114:G:O6	16:N:11:ARG:HD3	2.02	0.59
1:0:820:G:H5''	38:0:3356:HOH:O	2.01	0.59
1:0:2414:A:H2'	1:0:2415:A:C8	2.37	0.59
1:0:2851:G:C2'	1:0:2852:A:H5'	2.32	0.59
1:0:558:C:C2'	1:0:559:U:H5''	2.33	0.59
6:C:236:THR:HA	38:C:9247:HOH:O	2.03	0.59
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.50	0.59
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.85	0.59
22:T:69:LYS:O	22:T:71:VAL:HG23	2.03	0.59
32:I:102:VAL:CG1	32:I:106:LYS:HE3	2.30	0.59
5:B:305:ASP:O	5:B:306:LYS:HB2	2.01	0.59
7:D:135:VAL:HG22	7:D:136:ARG:N	2.17	0.59
9:F:61:MET:HB3	15:M:19:GLN:OE1	2.01	0.59
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.02	0.59
1:0:407:A:H2'	1:0:408:A:C8	2.38	0.59
1:0:2630:G:O6	4:A:206:ARG:NH2	2.36	0.59
2:9:3092:G:H2'	2:9:3093:A:C8	2.38	0.59
8:E:93:MET:HE1	8:E:165:GLY:H	1.65	0.59
12:J:107:ASN:HD22	12:J:108:PRO:N	2.01	0.59
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.84	0.59
1:0:681:G:N3	1:0:681:G:H5'	2.18	0.58
1:0:1187:U:O2'	1:0:1189:A:H2	1.86	0.58
1:0:2241:C:H2'	1:0:2242:U:C6	2.38	0.58
1:0:2502:C:C2'	1:0:2503:A:H5'	2.33	0.58
5:B:175:LEU:C	5:B:175:LEU:HD23	2.28	0.58
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.38	0.58
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.83	0.58
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.85	0.58
14:L:143:THR:HG22	14:L:145:LEU:H	1.67	0.58
1:0:952:G:OP1	19:Q:42:LYS:HE2	2.03	0.58
5:B:137:LEU:HD11	5:B:140:LEU:HD21	1.85	0.58
7:D:86:THR:O	7:D:90:LEU:HG	2.04	0.58
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.68	0.58
18:P:134:VAL:O	18:P:138:GLU:HG3	2.03	0.58
18:P:141:ILE:C	18:P:143:ALA:H	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.85	0.58
26:X:80:GLU:HB3	38:X:5564:HOH:O	2.02	0.58
1:O:1594:C:OP2	18:P:120:ARG:HD2	2.02	0.58
5:B:154:VAL:HG12	5:B:156:LYS:HG2	1.85	0.58
14:L:54:PRO:HG2	14:L:57:VAL:HG21	1.85	0.58
1:O:2812:A:C2	1:O:2814:A:N6	2.69	0.58
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.85	0.58
20:R:9:ASP:O	20:R:13:THR:HB	2.02	0.58
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.85	0.58
1:O:449:A:N7	6:C:43:LYS:HG2	2.19	0.58
1:O:1175:G:H1'	1:O:1193:A:H2'	1.85	0.58
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	1.85	0.58
11:H:45:VAL:HA	11:H:167:PRO:O	2.03	0.58
11:H:56:GLN:HE21	11:H:126:ARG:NE	2.00	0.58
23:U:17:THR:HG22	23:U:18:GLY:N	2.18	0.58
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.85	0.58
1:O:1060:C:H6	1:O:1060:C:H5'	1.69	0.58
1:O:1835:U:C5	1:O:1840:A:N7	2.64	0.58
5:B:307:ARG:HH11	5:B:307:ARG:CB	2.12	0.58
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.52	0.58
1:O:130:C:H2'	38:O:3467:HOH:O	2.02	0.58
1:O:1593:C:OP1	18:P:117:SER:HB3	2.04	0.58
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.34	0.58
13:K:98:VAL:HG13	13:K:99:ASP:N	2.18	0.58
16:N:170:GLU:O	16:N:174:GLU:HG3	2.03	0.58
23:U:13:ILE:HG12	23:U:32:CYS:HB3	1.84	0.58
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.86	0.58
1:O:280:C:H2'	1:O:281:U:O4'	2.03	0.58
13:K:125:ALA:C	13:K:127:ALA:H	2.12	0.58
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.86	0.58
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.85	0.58
26:X:31:ILE:O	26:X:35:GLU:HG3	2.03	0.58
27:Y:98:GLN:HG3	27:Y:236:VAL:HB	1.84	0.58
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.86	0.57
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.68	0.57
24:V:58:THR:O	24:V:62:GLU:HG3	2.03	0.57
1:O:1342:C:C2'	1:O:1343:C:H5'	2.34	0.57
2:9:3029:C:C2'	2:9:3030:C:H5'	2.34	0.57
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.33	0.57
17:O:96:VAL:HA	38:O:4258:HOH:O	2.03	0.57
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:144:ARG:HH11	27:Y:144:ARG:HG3	1.69	0.57
1:0:95:A:H5''	1:0:97:G:O4'	2.03	0.57
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.84	0.57
1:0:1377:C:H5'	1:0:1377:C:C6	2.39	0.57
2:9:3076:G:C3'	2:9:3077:A:H5''	2.25	0.57
17:O:42:GLU:HB2	38:O:2176:HOH:O	2.05	0.57
1:0:1118:A:H8	1:0:1119:G:H5''	1.70	0.57
1:0:2541:U:H5'	38:O:9721:HOH:O	2.04	0.57
1:0:316:A:N3	1:0:336:G:O2'	2.37	0.57
1:0:1189:A:H3'	38:O:7881:HOH:O	2.03	0.57
4:A:109:GLU:HG2	4:A:116:GLY:N	2.19	0.57
5:B:52:VAL:C	5:B:53:LEU:HD12	2.30	0.57
5:B:58:PRO:HA	5:B:63:GLU:OE1	2.05	0.57
24:V:55:ARG:O	24:V:59:ILE:HG12	2.02	0.57
32:I:139:ILE:C	32:I:140:GLU:HG3	2.28	0.57
1:0:558:C:H2'	1:0:559:U:C5'	2.34	0.57
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.70	0.57
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.87	0.57
17:O:87:THR:O	17:O:91:GLN:HG3	2.03	0.57
21:S:33:SER:OG	21:S:36:GLU:HG3	2.05	0.57
32:I:93:GLN:HA	32:I:96:PHE:CE2	2.40	0.57
1:0:558:C:O2'	1:0:559:U:H5''	2.05	0.57
2:9:3028:U:H5''	16:N:40:ASN:ND2	2.20	0.57
8:E:6:GLU:HA	8:E:46:THR:HG22	1.85	0.57
1:0:2769:C:H2'	1:0:2770:G:C5'	2.35	0.57
21:S:57:THR:CG2	21:S:58:MET:N	2.67	0.57
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.78	0.57
5:B:321:PRO:HA	38:B:9461:HOH:O	2.05	0.57
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.32	0.57
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.87	0.57
1:0:1185:U:H2'	1:0:1186:C:C6	2.40	0.57
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.40	0.57
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.68	0.57
20:R:132:ARG:HG2	20:R:133:ALA:N	2.20	0.57
32:I:113:HIS:N	32:I:114:PRO:HD2	2.20	0.57
1:0:90:A:H2'	1:0:91:G:O4'	2.04	0.56
1:0:1205:U:H2'	1:0:1206:U:C5'	2.35	0.56
7:D:65:GLU:HG3	38:D:6752:HOH:O	2.05	0.56
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.19	0.56
14:L:136:ALA:HB3	38:L:9371:HOH:O	2.05	0.56
24:V:39:ALA:N	24:V:40:PRO:CD	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:39:ALA:C	24:V:41:GLU:H	2.13	0.56
27:Y:132:ASP:OD1	27:Y:135:LYS:HD2	2.05	0.56
1:0:1352:A:H5''	1:0:1353:C:OP2	2.05	0.56
1:0:2420:G:O2'	1:0:2421:G:H5'	2.06	0.56
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.33	0.56
6:C:170:ASP:O	6:C:171:GLU:HG3	2.05	0.56
29:1:45:ARG:HB3	38:1:9223:HOH:O	2.05	0.56
1:0:328:U:O4'	6:C:202:THR:HG22	2.04	0.56
1:0:1209:C:H2'	1:0:1210:G:C8	2.40	0.56
1:0:2502:C:H2'	1:0:2503:A:H5'	1.85	0.56
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.86	0.56
7:D:88:LEU:C	7:D:90:LEU:H	2.13	0.56
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.86	0.56
10:G:12:ILE:N	10:G:13:PRO:HD3	2.20	0.56
13:K:55:VAL:HG12	13:K:56:SER:N	2.20	0.56
18:P:103:THR:O	18:P:107:GLU:HG3	2.05	0.56
20:R:39:THR:HG23	20:R:107:GLU:O	2.05	0.56
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.18	0.56
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.87	0.56
1:0:138:U:H5''	1:0:139:C:OP2	2.05	0.56
10:G:20:VAL:O	10:G:24:VAL:HG23	2.05	0.56
12:J:130:VAL:HG12	12:J:131:THR:H	1.71	0.56
1:0:200:U:H2'	38:0:3748:HOH:O	2.05	0.56
1:0:1687:C:O2	29:1:9:GLY:HA2	2.06	0.56
1:0:2468:A:H61	31:3:48:ASN:HD21	1.52	0.56
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.20	0.56
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.05	0.56
32:I:129:VAL:HG13	32:I:139:ILE:HD11	1.88	0.56
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.36	0.56
1:0:1679:C:H5'	38:0:9638:HOH:O	2.06	0.56
1:0:2649:A:H5'	1:0:2649:A:C8	2.41	0.56
2:9:3020:G:O2'	2:9:3021:G:H5'	2.06	0.56
6:C:153:VAL:O	6:C:157:LEU:HG	2.06	0.56
20:R:44:VAL:O	20:R:48:GLU:HG3	2.06	0.56
1:0:1667:A:H2'	1:0:1668:U:H6	1.69	0.56
20:R:39:THR:HB	20:R:42:GLU:HG3	1.86	0.56
30:2:41:HIS:O	30:2:45:ASN:HB2	2.06	0.56
1:0:65:C:O2'	1:0:66:G:H5'	2.05	0.56
1:0:462:A:C2	30:2:37:HIS:HB3	2.41	0.56
1:0:1086:A:N6	25:W:11:VAL:HG11	2.21	0.56
1:0:1163:G:H5'	32:I:115:ASP:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2320:U:H4'	1:0:2321:A:O4'	2.05	0.56
7:D:153:THR:O	7:D:156:ARG:HB2	2.06	0.56
16:N:37:ARG:NE	38:N:9333:HOH:O	2.35	0.56
5:B:30:PRO:HB2	5:B:39:GLN:NE2	2.21	0.56
14:L:93:VAL:HG21	14:L:122:ALA:HB2	1.88	0.56
21:S:43:GLU:HB3	38:S:7106:HOH:O	2.05	0.56
25:W:122:ARG:HH21	25:W:154:ARG:HD2	1.70	0.56
1:0:1834:C:H2'	1:0:1840:A:N6	2.20	0.56
8:E:126:ILE:HB	8:E:131:LEU:HD23	1.88	0.56
1:0:317:A:H5''	22:T:52:ARG:HD2	1.88	0.55
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.05	0.55
1:0:1167:G:H4'	32:I:135:LEU:HD22	1.88	0.55
1:0:2690:U:O2'	8:E:111:LYS:HE3	2.06	0.55
1:0:2909:G:H2'	1:0:2910:A:H8	1.70	0.55
38:0:7252:HOH:O	4:A:211:LYS:HG2	2.05	0.55
4:A:88:ILE:O	4:A:88:ILE:HG22	2.06	0.55
4:A:192:VAL:HB	38:A:9388:HOH:O	2.06	0.55
23:U:6:CYS:C	23:U:8:TYR:H	2.14	0.55
1:0:2795:C:O2'	1:0:2796:U:H5'	2.05	0.55
38:0:5492:HOH:O	13:K:39:GLY:HA2	2.06	0.55
16:N:34:LEU:HA	16:N:47:LEU:HD23	1.86	0.55
25:W:26:ILE:O	25:W:26:ILE:HG13	2.06	0.55
26:X:9:VAL:HG22	26:X:88:GLU:OE2	2.05	0.55
32:I:138:THR:HG22	32:I:139:ILE:N	2.22	0.55
1:0:1213:C:O2'	1:0:1214:G:H5'	2.07	0.55
1:0:1441:G:O2'	1:0:1442:A:H5'	2.06	0.55
6:C:1:MET:HG2	6:C:2:GLN:N	2.12	0.55
7:D:84:LEU:C	7:D:86:THR:H	2.13	0.55
8:E:45:ASP:OD2	8:E:46:THR:HG23	2.06	0.55
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.36	0.55
31:3:17:HIS:O	31:3:18:GLN:HG3	2.07	0.55
4:A:105:VAL:CG1	4:A:154:ALA:HB1	2.37	0.55
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.21	0.55
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.21	0.55
19:Q:11:ARG:HD3	38:Q:5620:HOH:O	2.05	0.55
31:3:62:THR:HG23	31:3:86:GLY:HA2	1.88	0.55
1:0:2812:A:H2	1:0:2814:A:N6	1.97	0.55
38:0:4281:HOH:O	22:T:82:THR:HA	2.05	0.55
5:B:57:GLU:O	5:B:63:GLU:HB2	2.06	0.55
5:B:214:PRO:HD2	38:B:9320:HOH:O	2.06	0.55
14:L:133:VAL:HB	38:L:9355:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:503:G:H2'	1:0:504:G:H8	1.72	0.55
1:0:1189:A:H1'	1:0:1209:C:H1'	1.87	0.55
1:0:2533:C:H6	1:0:2533:C:C5'	2.18	0.55
8:E:81:GLU:O	8:E:172:PRO:HD3	2.07	0.55
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.87	0.55
1:0:820:G:H3'	38:0:3356:HOH:O	2.05	0.55
1:0:1342:C:O2'	1:0:1343:C:H5'	2.05	0.55
1:0:1506:U:H6	1:0:1506:U:H5'	1.71	0.55
1:0:2526:C:O2'	1:0:2527:U:H5'	2.07	0.55
1:0:2896:A:OP1	26:X:15:ARG:NH1	2.40	0.55
6:C:25:PRO:HG2	38:C:9123:HOH:O	2.06	0.55
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.62	0.55
1:0:2241:C:H2'	1:0:2242:U:H6	1.70	0.55
1:0:2824:C:H5''	1:0:2825:C:H5'	1.88	0.55
38:0:6533:HOH:O	27:Y:158:LYS:HD3	2.06	0.55
6:C:218:VAL:HG12	38:C:9220:HOH:O	2.04	0.55
25:W:88:THR:HG22	25:W:89:ASP:N	2.21	0.55
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.72	0.55
1:0:2909:G:H2'	1:0:2910:A:C8	2.42	0.55
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.42	0.55
1:0:316:A:H5'	22:T:54:ASP:OD2	2.06	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.89	0.55
1:0:816:G:H5'	1:0:1598:A:H4'	1.89	0.55
1:0:2694:A:H4'	8:E:91:PHE:CE1	2.41	0.55
11:H:83:TYR:CD1	11:H:83:TYR:C	2.85	0.55
24:V:38:GLY:C	24:V:40:PRO:HD2	2.32	0.55
25:W:1:MET:N	25:W:37:GLU:HG3	2.22	0.55
1:0:159:G:OP1	15:M:74:LYS:HE3	2.07	0.54
1:0:1778:A:H2'	1:0:1779:A:H5'	1.89	0.54
1:0:2781:U:H2'	1:0:2782:G:H5'	1.88	0.54
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.22	0.54
11:H:170:ASN:HD22	11:H:170:ASN:N	2.04	0.54
17:O:106:PRO:HG2	17:O:107:GLU:OE1	2.07	0.54
25:W:52:VAL:HG22	25:W:53:ALA:H	1.72	0.54
25:W:82:GLU:O	25:W:86:GLU:HG3	2.07	0.54
2:9:3006:C:C5'	16:N:37:ARG:NH1	2.69	0.54
5:B:36:PRO:HA	5:B:168:GLY:CA	2.33	0.54
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.90	0.54
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.37	0.54
4:A:97:ALA:HB2	4:A:150:PRO:HB2	1.90	0.54
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.62	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1120:U:H5'	1:0:1121:G:OP2	2.07	0.54
1:0:2506:A:O2'	1:0:2507:G:O5'	2.26	0.54
1:0:544:G:C2'	1:0:545:G:H5''	2.37	0.54
1:0:969:G:H1	1:0:999:C:N4	2.05	0.54
8:E:95:VAL:O	8:E:126:ILE:HD12	2.08	0.54
15:M:57:LYS:HE2	15:M:140:ALA:O	2.07	0.54
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.89	0.54
16:N:44:ARG:HG3	16:N:45:ALA:N	2.22	0.54
1:0:10:U:O4	1:0:532:A:OP2	2.25	0.54
1:0:1202:A:H2'	1:0:1203:G:H5'	1.88	0.54
1:0:2248:C:H3'	38:0:5709:HOH:O	2.07	0.54
1:0:2504:A:H4'	11:H:71:ARG:HH11	1.72	0.54
7:D:51:ARG:HD3	38:D:7636:HOH:O	2.07	0.54
8:E:69:ILE:HA	8:E:72:MET:HE3	1.88	0.54
9:F:21:GLU:O	9:F:24:ARG:HG2	2.08	0.54
24:V:39:ALA:O	24:V:41:GLU:N	2.36	0.54
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.43	0.54
5:B:71:VAL:HG11	5:B:296:LEU:HB3	1.89	0.54
6:C:35:VAL:HG21	6:C:227:GLY:HA2	1.90	0.54
8:E:77:THR:OG1	8:E:78:GLU:N	2.40	0.54
26:X:78:GLU:HG2	26:X:79:GLU:N	2.22	0.54
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.90	0.54
9:F:38:LYS:NZ	15:M:3:SER:HA	2.22	0.54
14:L:35:ARG:C	14:L:35:ARG:HD3	2.33	0.54
25:W:139:GLY:O	25:W:141:HIS:HD2	1.90	0.54
1:0:1596:U:H2'	1:0:1598:A:OP2	2.08	0.54
1:0:2755:G:H1'	38:0:4963:HOH:O	2.08	0.54
13:K:62:PRO:CG	13:K:65:ARG:HH21	2.17	0.54
22:T:35:TYR:CG	22:T:112:LEU:HD22	2.43	0.54
31:3:62:THR:HB	38:3:9351:HOH:O	2.08	0.54
1:0:396:U:O2'	1:0:418:C:H4'	2.08	0.54
1:0:1666:C:H2'	1:0:1667:A:H5'	1.89	0.54
1:0:2064:U:H5'	1:0:2652:U:O3'	2.08	0.54
7:D:50:VAL:O	7:D:71:ALA:HA	2.08	0.54
21:S:77:VAL:O	21:S:80:ARG:HG2	2.07	0.54
25:W:13:MET:CE	25:W:17:ILE:HG22	2.38	0.54
25:W:41:TYR:HA	25:W:44:MET:HE3	1.89	0.54
25:W:137:GLN:NE2	25:W:141:HIS:HE1	2.02	0.54
1:0:1787:C:H4'	1:0:2883:A:O4'	2.08	0.53
1:0:2385:G:H2'	1:0:2386:U:C6	2.43	0.53
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:132:THR:HG23	8:E:132:THR:O	2.08	0.53
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.25	0.53
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.36	0.53
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.09	0.53
1:O:625:U:H5''	1:O:1044:C:N4	2.22	0.53
1:O:1351:G:OP1	6:C:96:LYS:NZ	2.38	0.53
1:O:1943:C:H4'	4:A:211:LYS:O	2.08	0.53
1:O:2443:C:O3'	14:L:56:LYS:HE3	2.08	0.53
38:O:4905:HOH:O	4:A:6:GLY:HA3	2.08	0.53
2:9:3064:C:H2'	2:9:3065:A:H5'	1.90	0.53
5:B:112:THR:OG1	5:B:158:LYS:HG2	2.09	0.53
8:E:11:VAL:HG12	8:E:12:ASP:N	2.22	0.53
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.90	0.53
1:O:960:G:N3	1:O:960:G:H2'	2.23	0.53
1:O:1418:U:OP1	30:2:42:TRP:HB3	2.08	0.53
6:C:233:THR:HG22	6:C:234:VAL:N	2.24	0.53
8:E:84:MET:HG2	8:E:168:ILE:HD13	1.90	0.53
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.09	0.53
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.39	0.53
24:V:1:THR:HG23	24:V:2:VAL:N	2.17	0.53
26:X:30:MET:CE	26:X:55:ASN:HA	2.37	0.53
1:O:380:A:OP2	15:M:9:ARG:HD2	2.09	0.53
1:O:1166:A:H61	1:O:1180:U:H3	1.56	0.53
1:O:2241:C:O2'	1:O:2242:U:H5'	2.09	0.53
1:O:2768:A:H2'	1:O:2769:C:O4'	2.07	0.53
5:B:280:VAL:HG13	5:B:334:SER:HA	1.89	0.53
17:O:73:ASP:HA	17:O:92:VAL:O	2.07	0.53
31:3:73:GLU:HB3	38:3:9363:HOH:O	2.07	0.53
1:O:396:U:OP2	31:3:38:ARG:HD2	2.07	0.53
1:O:818:A:O2'	28:Z:13:ARG:HD3	2.08	0.53
38:O:5796:HOH:O	15:M:58:GLN:HG3	2.08	0.53
4:A:32:VAL:HG12	4:A:34:ASP:H	1.72	0.53
4:A:36:ASP:O	4:A:38:ILE:N	2.40	0.53
4:A:194:MET:HE3	4:A:199:HIS:CB	2.38	0.53
12:J:47:THR:HG22	12:J:48:GLY:H	1.74	0.53
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.39	0.53
18:P:143:ALA:HA	38:P:190:HOH:O	2.08	0.53
1:O:121:U:OP2	30:2:10:ARG:NH2	2.28	0.53
2:9:3044:A:O4'	7:D:76:ARG:NE	2.41	0.53
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.23	0.53
18:P:20:ARG:NH1	18:P:54:LYS:HD3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2265:U:H2'	1:0:2266:A:C8	2.44	0.53
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.39	0.53
10:G:67:LEU:O	10:G:71:LEU:HG	2.08	0.53
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.09	0.53
1:0:588:G:O6	25:W:154:ARG:NH1	2.42	0.53
1:0:1766:U:O2	1:0:1778:A:H5'	2.09	0.53
5:B:175:LEU:HD23	5:B:175:LEU:O	2.07	0.53
5:B:248:ARG:O	5:B:251:VAL:HG13	2.08	0.53
9:F:96:ALA:HA	38:F:3111:HOH:O	2.08	0.53
1:0:790:A:H2'	1:0:791:A:O4'	2.09	0.53
4:A:132:ASP:OD1	4:A:133:ARG:N	2.42	0.53
5:B:75:GLU:C	5:B:77:PRO:HD3	2.34	0.53
8:E:69:ILE:HA	8:E:72:MET:HE2	1.90	0.53
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.09	0.53
23:U:9:CYS:CA	23:U:52:THR:HG23	2.36	0.53
1:0:644:G:H5'	1:0:644:G:N3	2.23	0.53
1:0:1299:G:N7	14:L:6:ARG:NH1	2.56	0.53
1:0:1477:C:H5'	1:0:1868:G:C5'	2.39	0.53
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.08	0.53
1:0:2073:G:OP2	1:0:2490:A:H5'	2.09	0.53
3:4:74:DCZ:C2'	3:4:75:DC:H5'	2.38	0.53
7:D:27:ILE:HD11	7:D:37:ALA:HB2	1.90	0.53
7:D:167:GLU:OE2	7:D:173:GLU:HG2	2.09	0.53
8:E:13:ALA:CB	8:E:22:VAL:HG22	2.39	0.53
22:T:50:VAL:HG12	22:T:56:ALA:HA	1.91	0.53
26:X:30:MET:HE3	26:X:55:ASN:OD1	2.08	0.53
32:I:131:THR:O	32:I:131:THR:HG22	2.09	0.53
1:0:185:G:O3'	1:0:186:A:H4'	2.09	0.52
1:0:244:C:OP2	9:F:38:LYS:HE3	2.09	0.52
1:0:797:A:C4'	28:Z:10:ARG:N	2.71	0.52
1:0:1029:U:O2'	1:0:1273:C:OP1	2.27	0.52
1:0:1406:A:H4'	1:0:1407:A:H5''	1.90	0.52
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.09	0.52
25:W:108:ARG:HE	25:W:114:PRO:CG	2.23	0.52
1:0:1477:C:H5'	1:0:1868:G:H5'	1.90	0.52
1:0:1741:U:O2'	1:0:2723:G:H4'	2.09	0.52
1:0:2423:C:H5''	38:0:7262:HOH:O	2.08	0.52
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.24	0.52
24:V:42:ASN:HB3	38:V:7247:HOH:O	2.09	0.52
1:0:2781:U:C2'	1:0:2782:G:H5'	2.40	0.52
7:D:170:TYR:O	7:D:171:ASP:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:133:HIS:HD2	38:Y:9379:HOH:O	1.93	0.52
1:O:468:U:H3'	38:O:7773:HOH:O	2.10	0.52
1:O:1632:A:H2'	1:O:1633:C:H5'	1.91	0.52
5:B:87:TYR:CE2	5:B:96:PRO:HG3	2.44	0.52
8:E:84:MET:HE1	8:E:148:ILE:HD13	1.91	0.52
9:F:19:ALA:O	9:F:22:VAL:HG22	2.09	0.52
12:J:107:ASN:HD22	12:J:107:ASN:C	2.16	0.52
14:L:114:VAL:HG11	38:L:9371:HOH:O	2.08	0.52
16:N:179:LEU:HD23	16:N:184:ILE:CD1	2.39	0.52
25:W:88:THR:CG2	25:W:110:GLN:NE2	2.73	0.52
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.40	0.52
1:O:1130:U:H2'	1:O:1131:G:O4'	2.09	0.52
1:O:2072:G:C6	1:O:2533:C:H1'	2.45	0.52
1:O:2769:C:O2'	1:O:2770:G:H5'	2.08	0.52
2:9:3051:A:H5'	16:N:160:SER:CB	2.39	0.52
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.92	0.52
17:O:77:ALA:HB1	17:O:98:LEU:HD12	1.89	0.52
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.44	0.52
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.92	0.52
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.92	0.52
7:D:85:GLN:O	7:D:86:THR:HG23	2.09	0.52
8:E:137:ASP:O	8:E:141:VAL:HG23	2.09	0.52
21:S:56:ASN:O	30:2:8:LYS:NZ	2.35	0.52
4:A:1:GLY:HA2	4:A:197:VAL:HG23	1.91	0.52
4:A:194:MET:HE3	4:A:199:HIS:HB2	1.91	0.52
5:B:162:MET:HE1	5:B:308:LEU:HD21	1.91	0.52
5:B:177:HIS:O	5:B:181:ILE:HG13	2.09	0.52
6:C:140:VAL:HG12	6:C:141:SER:N	2.24	0.52
12:J:45:VAL:HG22	12:J:46:ILE:N	2.24	0.52
14:L:21:ARG:N	38:L:9329:HOH:O	2.43	0.52
16:N:72:GLU:O	16:N:72:GLU:HG2	2.10	0.52
23:U:17:THR:CG2	23:U:18:GLY:N	2.72	0.52
25:W:4:LEU:O	25:W:32:CYS:HA	2.10	0.52
27:Y:155:ARG:NH1	38:Y:9358:HOH:O	2.42	0.52
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.57	0.52
31:3:14:CYS:HB3	31:3:16:GLU:HG2	1.90	0.52
1:O:958:G:H2'	1:O:959:C:C6	2.45	0.52
5:B:320:GLN:HE21	5:B:321:PRO:HD2	1.75	0.52
7:D:146:LYS:HZ1	16:N:107:ASN:HD21	1.58	0.52
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.25	0.52
20:R:39:THR:HB	20:R:42:GLU:CD	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:64:GLY:O	24:V:65:ASP:CB	2.57	0.52
1:0:1669:A:H2'	1:0:1670:G:C8	2.45	0.52
1:0:1701:A:H5'	38:0:6532:HOH:O	2.10	0.52
7:D:67:ASP:O	7:D:69:ILE:HG13	2.10	0.52
7:D:163:VAL:HA	38:D:6326:HOH:O	2.10	0.52
8:E:107:PHE:CE2	8:E:108:LEU:HD13	2.44	0.52
11:H:154:TYR:CD1	11:H:154:TYR:C	2.87	0.52
18:P:105:LEU:CD2	18:P:137:LEU:HD21	2.39	0.52
30:2:39:ARG:HG2	38:2:3143:HOH:O	2.09	0.52
1:0:447:A:OP1	22:T:2:LYS:HG2	2.10	0.52
1:0:447:A:O2'	1:0:448:G:H5'	2.10	0.52
1:0:1234:U:N3	5:B:244:PRO:HB3	2.25	0.52
4:A:86:ALA:HB3	4:A:94:LEU:HD13	1.92	0.52
5:B:148:PRO:HB2	5:B:156:LYS:O	2.10	0.52
9:F:113:ASP:O	9:F:117:GLU:HG3	2.10	0.52
12:J:26:VAL:HG13	12:J:36:VAL:HG11	1.92	0.52
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.25	0.52
1:0:2054:A:H2	20:R:128:ARG:HH22	1.51	0.51
1:0:2769:C:H2'	1:0:2770:G:O4'	2.10	0.51
12:J:74:ARG:O	12:J:78:ILE:HG12	2.11	0.51
31:3:3:MET:O	31:3:90:PHE:HA	2.09	0.51
1:0:524:A:H5''	20:R:29:LYS:HD3	1.93	0.51
1:0:848:C:H5'	38:0:7491:HOH:O	2.09	0.51
3:4:74:DCZ:H2'1	3:4:75:DC:O4'	2.10	0.51
4:A:76:VAL:CG2	28:Z:63:LYS:HB3	2.40	0.51
5:B:217:ARG:CG	5:B:257:THR:HG22	2.37	0.51
16:N:47:LEU:HD12	16:N:92:ALA:HB1	1.92	0.51
21:S:81:ILE:HG12	38:S:4527:HOH:O	2.10	0.51
22:T:48:VAL:HG23	22:T:98:VAL:HA	1.93	0.51
1:0:2252:A:C6	1:0:2253:G:H1'	2.45	0.51
25:W:149:LEU:CG	25:W:153:MET:HE2	2.35	0.51
26:X:43:VAL:HG12	26:X:47:ALA:HB3	1.91	0.51
1:0:2717:C:O2'	1:0:2718:C:H5''	2.11	0.51
2:9:3049:G:O2'	2:9:3050:G:H5'	2.10	0.51
5:B:162:MET:HE2	5:B:310:ARG:CD	2.39	0.51
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.76	0.51
16:N:32:PRO:HD2	16:N:99:GLU:O	2.10	0.51
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.92	0.51
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.26	0.51
26:X:78:GLU:CG	26:X:79:GLU:H	2.23	0.51
1:0:669:G:O2'	1:0:670:G:H5'	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1375:A:H2'	1:0:1376:G:H5'	1.93	0.51
1:0:2597:U:H2'	1:0:2598:U:H5'	1.93	0.51
8:E:95:VAL:HG22	8:E:104:ILE:HG12	1.92	0.51
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.41	0.51
12:J:108:PRO:HG2	12:J:109:TYR:CD1	2.45	0.51
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.46	0.51
22:T:41:ARG:HG2	22:T:41:ARG:NH1	2.25	0.51
1:0:512:G:O3'	1:0:513:A:H8	1.94	0.51
1:0:1641:A:C2'	1:0:1642:A:H5'	2.39	0.51
5:B:108:GLU:HA	5:B:110:ASP:OD1	2.11	0.51
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.92	0.51
16:N:149:GLU:O	16:N:152:GLU:HB2	2.10	0.51
25:W:126:ASP:HB3	25:W:135:GLY:O	2.10	0.51
32:I:134:SER:O	32:I:135:LEU:HD23	2.11	0.51
1:0:474:C:O3'	6:C:73:LEU:CD2	2.59	0.51
1:0:553:G:OP2	27:Y:204:ARG:NH2	2.37	0.51
1:0:1119:G:H22	1:0:1246:A:H2	1.50	0.51
1:0:1787:C:H2'	1:0:1788:U:H6	1.75	0.51
2:9:3057:A:C8	7:D:141:VAL:HG21	2.46	0.51
5:B:42:ALA:HB1	5:B:308:LEU:HD11	1.92	0.51
12:J:51:GLU:O	12:J:55:GLU:HG3	2.10	0.51
28:Z:81:ARG:O	28:Z:82:SER:C	2.53	0.51
32:I:131:THR:O	32:I:135:LEU:HG	2.10	0.51
1:0:517:U:H1'	38:0:7782:HOH:O	2.10	0.51
1:0:1559:A:OP2	1:0:1559:A:H8	1.94	0.51
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.10	0.51
4:A:43:VAL:HG21	4:A:59:GLU:HG3	1.93	0.51
9:F:79:GLN:HG3	9:F:82:ASP:OD2	2.11	0.51
11:H:167:PRO:O	11:H:168:ALA:HB2	2.11	0.51
26:X:43:VAL:CG1	26:X:47:ALA:HB3	2.40	0.51
1:0:834:G:H4'	1:0:835:U:OP2	2.11	0.51
1:0:920:C:H4'	1:0:921:G:C2	2.45	0.51
1:0:1123:A:C6	1:0:1238:C:H5'	2.46	0.51
5:B:150:ALA:O	5:B:152:PRO:HD3	2.10	0.51
8:E:166:VAL:HG12	38:E:3134:HOH:O	2.10	0.51
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.93	0.51
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.26	0.51
20:R:33:ARG:NH1	38:R:9345:HOH:O	2.44	0.51
24:V:4:HIS:HB3	38:V:6622:HOH:O	2.10	0.51
25:W:46:ALA:O	25:W:49:ASN:HB2	2.10	0.51
1:0:289:G:H22	1:0:363:A:H2	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1086:A:C6	25:W:11:VAL:HG11	2.45	0.51
1:0:2591:C:OP1	5:B:1:PRO:HG3	2.11	0.51
38:0:7104:HOH:O	15:M:178:LYS:HB2	2.09	0.51
4:A:212:PRO:HB2	38:A:9353:HOH:O	2.10	0.51
6:C:79:ARG:O	6:C:87:ARG:HG2	2.10	0.51
8:E:131:LEU:HD12	8:E:166:VAL:HG11	1.92	0.51
11:H:154:TYR:C	11:H:154:TYR:HD1	2.18	0.51
19:Q:77:ASP:HB3	19:Q:82:LYS:HE3	1.91	0.51
1:0:1123:A:C2	1:0:1129:C:H4'	2.46	0.50
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.10	0.50
1:0:1236:A:H2'	1:0:1237:U:O4'	2.12	0.50
1:0:1289:C:H3'	38:0:6650:HOH:O	2.10	0.50
4:A:37:VAL:HG22	38:A:9391:HOH:O	2.11	0.50
12:J:93:ARG:HB3	12:J:93:ARG:NH1	2.23	0.50
19:Q:32:GLU:O	19:Q:93:ARG:NH2	2.44	0.50
21:S:6:LYS:O	21:S:7:HIS:HB3	2.11	0.50
1:0:1044:C:H3'	1:0:1045:G:H5''	1.93	0.50
1:0:1940:C:H4'	38:0:7555:HOH:O	2.11	0.50
1:0:2717:C:H2'	1:0:2718:C:C5'	2.29	0.50
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.38	0.50
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.46	0.50
1:0:702:G:O2'	1:0:703:G:H5'	2.11	0.50
2:9:3002:U:OP2	2:9:3003:A:H5'	2.12	0.50
4:A:131:HIS:O	4:A:132:ASP:CB	2.59	0.50
6:C:236:THR:HG21	38:C:9171:HOH:O	2.11	0.50
8:E:137:ASP:OD1	8:E:139:GLU:HB2	2.11	0.50
9:F:91:VAL:CG1	9:F:92:GLY:H	2.21	0.50
11:H:28:ILE:HG23	38:H:9179:HOH:O	2.11	0.50
14:L:73:VAL:HG11	14:L:118:LEU:HD21	1.93	0.50
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.92	0.50
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.46	0.50
1:0:343:C:O2'	1:0:344:C:H5'	2.11	0.50
1:0:1132:A:N6	1:0:1229:C:H2'	2.27	0.50
1:0:1423:C:O2'	1:0:1424:A:H5'	2.11	0.50
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.27	0.50
9:F:37:THR:O	9:F:41:GLU:HG3	2.10	0.50
11:H:148:GLU:OE1	11:H:148:GLU:HA	2.12	0.50
15:M:164:THR:HG23	15:M:165:GLY:N	2.25	0.50
18:P:134:VAL:O	18:P:137:LEU:HB3	2.11	0.50
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.93	0.50
38:9:7568:HOH:O	16:N:107:ASN:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:143:THR:CG2	14:L:144:ASP:N	2.74	0.50
18:P:120:ARG:NH2	18:P:123:TYR:CD2	2.79	0.50
25:W:21:LEU:CD1	25:W:26:ILE:HD11	2.40	0.50
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.47	0.50
1:O:441:A:H1'	1:O:442:A:N7	2.27	0.50
1:O:2898:G:H4'	5:B:288:GLY:HA2	1.94	0.50
5:B:7:ARG:HG2	5:B:7:ARG:HH11	1.77	0.50
8:E:101:GLU:HB2	8:E:116:THR:O	2.11	0.50
14:L:34:GLY:C	14:L:36:ASP:H	2.20	0.50
15:M:46:LEU:HG	38:M:9416:HOH:O	2.10	0.50
21:S:52:VAL:C	21:S:53:ASN:HD22	2.20	0.50
29:1:28:HIS:O	29:1:32:LYS:N	2.44	0.50
30:2:40:ARG:CD	30:2:47:THR:HG22	2.42	0.50
1:O:920:C:H5'	1:O:921:G:C4	2.46	0.50
1:O:2668:G:H2'	1:O:2669:U:C6	2.47	0.50
38:O:3205:HOH:O	12:J:46:ILE:HA	2.12	0.50
4:A:36:ASP:CG	4:A:85:SER:HB2	2.36	0.50
7:D:81:GLU:C	7:D:83:PHE:H	2.20	0.50
8:E:84:MET:HE1	8:E:148:ILE:HG21	1.94	0.50
16:N:47:LEU:HD13	16:N:97:VAL:HG11	1.93	0.50
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.47	0.50
21:S:57:THR:HG22	21:S:58:MET:N	2.26	0.50
1:O:475:G:C5'	6:C:73:LEU:HD23	2.42	0.50
1:O:1201:C:H5''	38:O:6487:HOH:O	2.12	0.50
1:O:1375:A:C2'	1:O:1376:G:H5'	2.41	0.50
2:9:3049:G:H2'	2:9:3050:G:O4'	2.12	0.50
5:B:279:THR:OG1	5:B:290:VAL:HB	2.12	0.50
16:N:143:ARG:NH1	16:N:173:ASP:OD1	2.45	0.50
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.28	0.50
1:O:2064:U:H4'	1:O:2653:A:OP1	2.11	0.50
5:B:132:HIS:HB2	5:B:137:LEU:HD22	1.94	0.50
7:D:146:LYS:HZ3	16:N:107:ASN:ND2	2.07	0.50
20:R:27:HIS:O	20:R:31:ILE:HG13	2.12	0.50
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.25	0.50
25:W:63:GLU:HG2	25:W:93:ILE:HG22	1.93	0.50
9:F:46:GLU:OE2	9:F:100:ASP:HA	2.12	0.49
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.33	0.49
1:O:2036:C:O4'	13:K:44:LEU:HG	2.12	0.49
4:A:36:ASP:HB2	4:A:85:SER:H	1.77	0.49
5:B:66:GLU:OE1	5:B:328:ARG:HD2	2.12	0.49
5:B:294:TYR:HE2	38:B:9454:HOH:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.93	0.49
7:D:94:ALA:HB3	7:D:97:GLN:HG3	1.94	0.49
8:E:119:HIS:O	8:E:140:ALA:HB1	2.12	0.49
26:X:43:VAL:HG22	26:X:76:ARG:NH1	2.27	0.49
30:2:5:LYS:O	30:2:9:LYS:HG3	2.12	0.49
1:0:1014:A:H2'	1:0:1015:C:H5'	1.93	0.49
1:0:2521:A:OP2	11:H:3:ALA:HB3	2.12	0.49
1:0:2710:U:H1'	38:0:7824:HOH:O	2.12	0.49
2:9:3023:U:O2'	2:9:3024:U:H4'	2.12	0.49
6:C:61:PHE:HB3	38:C:9242:HOH:O	2.13	0.49
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.94	0.49
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.94	0.49
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.94	0.49
19:Q:16:ASN:HB2	38:Q:6597:HOH:O	2.11	0.49
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.12	0.49
1:0:327:A:OP1	6:C:149:LYS:NZ	2.41	0.49
1:0:1503:U:H2'	1:0:1504:A:O4'	2.12	0.49
38:0:3592:HOH:O	13:K:9:THR:HA	2.11	0.49
4:A:94:LEU:HD23	4:A:94:LEU:N	2.27	0.49
4:A:179:MET:HG2	4:A:186:TRP:CG	2.47	0.49
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.27	0.49
8:E:24:GLY:HA3	8:E:76:VAL:HB	1.94	0.49
16:N:34:LEU:HD22	16:N:129:ILE:HD13	1.94	0.49
27:Y:106:THR:CG2	27:Y:107:PRO:HD2	2.43	0.49
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.27	0.49
30:2:40:ARG:HG2	30:2:40:ARG:HH11	1.77	0.49
14:L:73:VAL:HG23	14:L:74:THR:N	2.28	0.49
16:N:47:LEU:CD1	16:N:97:VAL:HG11	2.42	0.49
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.12	0.49
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.45	0.49
27:Y:200:THR:HG22	27:Y:201:GLU:CG	2.42	0.49
1:0:263:U:O4'	9:F:59:ILE:HD13	2.12	0.49
1:0:1462:C:H2'	1:0:1463:A:C8	2.48	0.49
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.13	0.49
1:0:1820:G:C6	1:0:2030:A:C2	3.00	0.49
1:0:2392:C:H4'	38:Q:2875:HOH:O	2.13	0.49
7:D:154:LYS:H	7:D:154:LYS:CD	2.19	0.49
9:F:16:ALA:HA	9:F:111:ILE:HD13	1.94	0.49
9:F:101:ALA:HA	38:F:5413:HOH:O	2.13	0.49
11:H:63:GLU:HA	38:H:9179:HOH:O	2.12	0.49
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:71:ARG:HD3	38:X:2171:HOH:O	2.12	0.49
1:0:256:C:H2'	1:0:257:G:O4'	2.12	0.49
1:0:705:C:O2	1:0:705:C:H2'	2.13	0.49
1:0:1733:A:H4'	5:B:212:GLN:HA	1.94	0.49
1:0:1845:A:O3'	4:A:187:PRO:HB2	2.12	0.49
31:3:55:VAL:HB	31:3:56:PRO:HD2	1.94	0.49
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.94	0.49
32:I:132:CYS:C	32:I:134:SER:H	2.19	0.49
1:0:661:G:C5	1:0:686:A:C2	3.01	0.49
5:B:221:GLN:HE22	13:K:42:ASN:ND2	2.10	0.49
22:T:48:VAL:HG22	22:T:97:ARG:O	2.13	0.49
25:W:26:ILE:HG22	38:W:5420:HOH:O	2.12	0.49
1:0:1202:A:H2'	1:0:1203:G:C5'	2.43	0.49
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.78	0.49
1:0:2894:C:O2'	1:0:2895:C:H5'	2.12	0.49
38:0:9532:HOH:O	4:A:11:ARG:HD3	2.12	0.49
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.13	0.49
2:9:3064:C:C2'	2:9:3065:A:H5'	2.42	0.49
4:A:220:PRO:HD2	4:A:223:ARG:HD3	1.95	0.49
6:C:7:ASP:OD2	6:C:9:ASP:HB2	2.12	0.49
25:W:139:GLY:O	25:W:141:HIS:CD2	2.66	0.49
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.48	0.49
29:1:28:HIS:HD2	29:1:30:LYS:H	1.60	0.49
1:0:585:C:H5''	38:0:5151:HOH:O	2.13	0.49
1:0:1118:A:C8	1:0:1118:A:C3'	2.91	0.49
1:0:2252:A:C5	1:0:2253:G:H1'	2.47	0.49
38:0:5676:HOH:O	4:A:164:ARG:CZ	2.60	0.49
5:B:314:ALA:CB	5:B:317:PRO:HG3	2.43	0.49
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.24	0.49
22:T:48:VAL:HG22	22:T:97:ARG:C	2.38	0.49
1:0:1878:G:H1'	38:0:6378:HOH:O	2.11	0.48
7:D:173:GLU:O	7:D:174:VAL:C	2.56	0.48
9:F:107:ASP:O	9:F:111:ILE:HG13	2.12	0.48
9:F:111:ILE:O	9:F:115:VAL:HG23	2.13	0.48
15:M:78:LYS:HD3	38:M:9434:HOH:O	2.13	0.48
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.76	0.48
17:O:113:VAL:O	17:O:114:ILE:HD13	2.13	0.48
22:T:71:VAL:HG12	22:T:72:ILE:N	2.27	0.48
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.48	0.48
30:2:10:ARG:HH11	30:2:49:GLU:CD	2.21	0.48
1:0:221:G:H2'	1:0:222:A:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:926:A:H5'	14:L:39:GLU:OE2	2.13	0.48
1:0:1427:A:H61	1:0:1440:U:C1'	2.25	0.48
1:0:1701:A:H4'	1:0:1702:U:C5'	2.42	0.48
4:A:32:VAL:HG12	4:A:34:ASP:N	2.27	0.48
4:A:215:ILE:HG13	4:A:216:SER:N	2.28	0.48
8:E:9:GLU:HG3	8:E:10:ASP:N	2.28	0.48
10:G:64:ASN:N	10:G:64:ASN:ND2	2.59	0.48
14:L:104:ASP:O	14:L:105:TYR:HB3	2.12	0.48
15:M:166:ALA:HA	15:M:169:ARG:HH12	1.73	0.48
16:N:64:SER:C	16:N:66:LEU:H	2.21	0.48
16:N:154:LEU:C	16:N:156:GLU:H	2.19	0.48
17:O:77:ALA:HA	17:O:96:VAL:O	2.13	0.48
32:I:75:THR:OG1	32:I:112:LYS:NZ	2.45	0.48
1:0:74:A:H2'	1:0:75:U:C6	2.48	0.48
1:0:282:C:H1'	1:0:368:C:H42	1.74	0.48
1:0:800:G:H4'	38:0:7283:HOH:O	2.13	0.48
1:0:941:G:C5	1:0:942:U:C4	3.01	0.48
1:0:1135:G:H5'	38:0:6188:HOH:O	2.12	0.48
1:0:1904:A:H2'	1:0:1905:U:O4'	2.13	0.48
1:0:2762:C:H3'	38:0:3673:HOH:O	2.13	0.48
8:E:15:GLN:HG2	8:E:19:ASP:O	2.13	0.48
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.12	0.48
20:R:39:THR:HB	20:R:42:GLU:CG	2.43	0.48
21:S:23:LYS:HE2	38:S:3430:HOH:O	2.12	0.48
22:T:41:ARG:NH1	22:T:42:VAL:O	2.46	0.48
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.43	0.48
1:0:1165:G:H1'	1:0:1174:A:H1'	1.96	0.48
1:0:1352:A:N1	6:C:48:SER:HB3	2.27	0.48
1:0:2730:G:O2'	1:0:2731:G:H5'	2.13	0.48
6:C:136:VAL:HA	6:C:137:PRO:C	2.39	0.48
8:E:2:ARG:HH21	8:E:48:VAL:HG21	1.77	0.48
9:F:14:ASP:O	9:F:18:GLU:HG3	2.13	0.48
15:M:59:GLY:C	15:M:141:ILE:HD11	2.39	0.48
19:Q:14:LEU:HD21	19:Q:43:ILE:HD12	1.95	0.48
24:V:56:ILE:O	24:V:60:GLN:HG3	2.14	0.48
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.48	0.48
32:I:96:PHE:HA	32:I:136:GLY:CA	2.44	0.48
1:0:536:A:H3'	38:0:5327:HOH:O	2.12	0.48
1:0:602:A:O2'	1:0:605:C:H4'	2.13	0.48
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.96	0.48
1:0:2356:A:H2'	1:0:2357:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:254:GLN:NE2	38:B:9390:HOH:O	2.46	0.48
8:E:15:GLN:NE2	8:E:40:VAL:O	2.46	0.48
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.94	0.48
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.79	0.48
22:T:75:GLU:O	22:T:76:ASP:HB2	2.12	0.48
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.13	0.48
1:O:317:A:OP1	22:T:52:ARG:O	2.30	0.48
1:O:827:A:H2'	1:O:828:G:O4'	2.14	0.48
1:O:1363:G:OP1	6:C:76:ARG:NH2	2.45	0.48
1:O:1666:C:H2'	1:O:1667:A:C5'	2.44	0.48
5:B:84:LEU:HD23	5:B:142:LEU:CD2	2.42	0.48
11:H:88:ARG:NH1	11:H:135:THR:OG1	2.40	0.48
12:J:133:GLY:O	12:J:137:GLU:HG3	2.14	0.48
14:L:54:PRO:HG2	14:L:57:VAL:CG2	2.42	0.48
1:O:777:U:HO2'	29:1:11:LYS:HG2	1.77	0.48
1:O:1201:C:H2'	1:O:1202:A:H5'	1.95	0.48
1:O:1829:A:H2'	1:O:1830:C:H5'	1.96	0.48
4:A:105:VAL:HG12	4:A:106:CYS:N	2.28	0.48
7:D:27:ILE:HD11	7:D:37:ALA:CB	2.44	0.48
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.32	0.48
21:S:37:VAL:O	21:S:41:VAL:HG23	2.13	0.48
27:Y:144:ARG:CG	27:Y:144:ARG:NH1	2.76	0.48
32:I:87:THR:HG22	32:I:88:GLY:N	2.28	0.48
32:I:96:PHE:HD2	32:I:136:GLY:HA2	1.79	0.48
1:O:1785:G:OP1	18:P:76:GLY:HA3	2.13	0.48
6:C:138:VAL:O	6:C:234:VAL:HA	2.13	0.48
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.43	0.48
17:O:38:ARG:NH1	38:O:7674:HOH:O	2.47	0.48
19:Q:3:SER:HB3	38:Q:5998:HOH:O	2.13	0.48
27:Y:112:GLU:CD	27:Y:115:ARG:NH1	2.70	0.48
1:O:1087:G:H4'	1:O:1088:A:OP1	2.14	0.48
1:O:1333:U:H2'	1:O:1334:C:C6	2.49	0.48
1:O:1380:U:O4	1:O:2043:U:H4'	2.13	0.48
1:O:1544:U:H2'	1:O:1545:C:H6	1.79	0.48
1:O:1790:C:H2'	1:O:1791:U:H6	1.79	0.48
1:O:2685:C:H1'	38:O:3745:HOH:O	2.13	0.48
1:O:2718:C:H6	1:O:2718:C:H5'	1.78	0.48
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.95	0.48
12:J:39:VAL:HG12	12:J:40:ASN:ND2	2.29	0.48
14:L:6:ARG:NH2	38:L:9347:HOH:O	2.45	0.48
14:L:59:GLU:HG2	14:L:104:ASP:CG	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:80:ASP:HB2	14:L:90:ARG:O	2.14	0.48
26:X:49:ARG:O	26:X:49:ARG:HG3	2.09	0.48
1:0:1130:U:H5'	38:0:7873:HOH:O	2.13	0.48
1:0:1300:G:H1'	38:0:4964:HOH:O	2.14	0.48
1:0:2613:G:O2'	1:0:2614:C:H5'	2.14	0.48
38:0:6937:HOH:O	27:Y:165:GLU:HB3	2.13	0.48
4:A:114:ASP:C	4:A:114:ASP:OD1	2.56	0.48
7:D:10:PHE:CD1	7:D:11:HIS:N	2.82	0.48
24:V:49:LEU:O	24:V:53:ILE:HG13	2.14	0.48
1:0:170:U:H2'	1:0:171:C:H5'	1.95	0.47
1:0:1202:A:C2'	1:0:1203:G:H5'	2.43	0.47
1:0:2255:A:O2'	1:0:2256:G:H5'	2.14	0.47
1:0:2256:G:O2'	1:0:2257:G:H5'	2.14	0.47
8:E:100:ASP:HB2	38:E:2789:HOH:O	2.13	0.47
1:0:378:A:OP1	15:M:9:ARG:NH2	2.45	0.47
1:0:1681:G:H5''	1:0:1682:A:H5'	1.95	0.47
2:9:3039:U:H3'	2:9:3040:C:H5''	1.96	0.47
5:B:82:VAL:O	5:B:82:VAL:HG12	2.13	0.47
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.44	0.47
6:C:236:THR:CG2	6:C:239:ALA:H	2.12	0.47
9:F:91:VAL:CG1	9:F:92:GLY:N	2.74	0.47
12:J:135:ILE:O	12:J:139:LEU:HG	2.13	0.47
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.96	0.47
1:0:2361:A:H2'	1:0:2362:A:C8	2.49	0.47
4:A:36:ASP:C	4:A:38:ILE:N	2.69	0.47
5:B:14:GLY:HA2	5:B:15:PRO:C	2.40	0.47
5:B:79:MET:HE2	5:B:144:THR:HG22	1.96	0.47
5:B:195:ARG:CZ	5:B:323:LEU:HD13	2.44	0.47
5:B:310:ARG:HD2	38:B:9452:HOH:O	2.14	0.47
1:0:415:A:O2'	1:0:416:G:H5'	2.15	0.47
1:0:1097:A:H5''	25:W:125:HIS:NE2	2.30	0.47
1:0:1180:U:H2'	1:0:1181:A:C8	2.49	0.47
1:0:2782:G:O6	1:0:2790:C:H5''	2.14	0.47
4:A:105:VAL:HG11	4:A:154:ALA:CB	2.44	0.47
5:B:79:MET:C	5:B:80:ARG:HG3	2.39	0.47
5:B:128:ILE:O	5:B:131:ALA:HB3	2.14	0.47
6:C:37:ALA:O	6:C:41:ASN:ND2	2.48	0.47
12:J:46:ILE:O	12:J:46:ILE:HG12	2.13	0.47
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.49	0.47
18:P:83:LYS:O	18:P:86:ALA:HB3	2.13	0.47
19:Q:18:PRO:O	19:Q:21:ARG:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:821:U:H2'	1:0:822:C:H6	1.79	0.47
1:0:1919:A:H4'	38:0:5131:HOH:O	2.13	0.47
1:0:2403:C:H3'	38:0:5482:HOH:O	2.15	0.47
1:0:2507:G:H2'	1:0:2510:C:H42	1.78	0.47
1:0:2541:U:H4'	1:0:2542:C:OP1	2.13	0.47
38:0:9672:HOH:O	29:1:1:THR:HA	2.13	0.47
6:C:2:GLN:HB3	38:C:9181:HOH:O	2.14	0.47
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.96	0.47
16:N:27:LEU:HD22	16:N:50:LEU:HD13	1.96	0.47
16:N:73:ALA:HB1	16:N:74:PRO:HD2	1.97	0.47
32:I:75:THR:HA	32:I:112:LYS:HZ1	1.79	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
1:0:2897:C:H2'	1:0:2898:G:H8	1.79	0.47
6:C:234:VAL:O	6:C:234:VAL:HG22	2.14	0.47
7:D:39:ASP:HB2	38:D:5583:HOH:O	2.15	0.47
7:D:173:GLU:HG3	7:D:174:VAL:N	2.30	0.47
9:F:101:ALA:HB3	9:F:105:ASP:OD1	2.15	0.47
16:N:22:GLN:HG2	16:N:26:LEU:HD22	1.97	0.47
16:N:37:ARG:NH2	38:N:9333:HOH:O	2.47	0.47
18:P:10:ALA:O	18:P:13:VAL:HG12	2.14	0.47
21:S:39:ASP:HB3	21:S:43:GLU:OE2	2.15	0.47
1:0:37:A:H2'	1:0:38:G:C8	2.49	0.47
1:0:177:A:H2'	1:0:178:U:O4'	2.14	0.47
1:0:587:A:H5''	38:0:7501:HOH:O	2.15	0.47
1:0:1406:A:H4'	1:0:1407:A:C5'	2.44	0.47
1:0:1654:U:H2'	4:A:47:HIS:CD2	2.46	0.47
1:0:1666:C:C2'	1:0:1667:A:H5''	2.45	0.47
3:4:74:DCZ:H2'1	3:4:75:DC:H5'	1.96	0.47
5:B:162:MET:CE	5:B:308:LEU:HD21	2.44	0.47
6:C:236:THR:O	6:C:237:GLU:C	2.58	0.47
7:D:81:GLU:C	7:D:83:PHE:N	2.73	0.47
8:E:79:GLY:HA3	38:E:7046:HOH:O	2.15	0.47
8:E:86:VAL:CG1	8:E:129:GLU:HA	2.44	0.47
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.45	0.47
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.15	0.47
28:Z:25:ARG:O	28:Z:29:ILE:HG13	2.15	0.47
32:I:113:HIS:NE2	32:I:121:LEU:HD22	2.29	0.47
1:0:475:G:OP1	6:C:73:LEU:HD22	2.15	0.47
1:0:660:A:H4'	1:0:661:G:O5'	2.15	0.47
1:0:1495:C:H2'	1:0:1496:G:C8	2.50	0.47
5:B:16:ARG:NH1	38:B:9418:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:238:ASN:HD22	5:B:240:GLY:N	2.07	0.47
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.15	0.47
24:V:42:ASN:O	24:V:44:GLY:N	2.48	0.47
1:0:12:U:H2'	1:0:13:G:H5'	1.96	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.45	0.47
38:0:5785:HOH:O	5:B:298:LYS:HD3	2.14	0.47
2:9:3055:U:H4'	2:9:3056:A:C8	2.50	0.47
5:B:277:GLU:N	5:B:278:PRO:HD2	2.29	0.47
6:C:55:ARG:NH2	29:1:56:GLU:OE2	2.39	0.47
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.97	0.47
9:F:13:GLU:OE2	9:F:78:GLU:HG2	2.14	0.47
12:J:22:VAL:O	12:J:26:VAL:HG23	2.15	0.47
12:J:75:PRO:HD3	12:J:136:SER:OG	2.15	0.47
31:3:57:GLY:HA2	38:3:9327:HOH:O	2.15	0.47
1:0:1183:C:N4	1:0:1184:C:H41	2.13	0.47
1:0:2361:A:H5''	38:0:9323:HOH:O	2.15	0.47
2:9:3055:U:H4'	2:9:3056:A:H8	1.79	0.47
18:P:103:THR:HB	38:P:180:HOH:O	2.15	0.47
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.96	0.47
25:W:13:MET:HE3	25:W:17:ILE:CG2	2.44	0.47
1:0:553:G:P	27:Y:204:ARG:HH22	2.38	0.46
1:0:558:C:C2'	1:0:559:U:C5'	2.92	0.46
1:0:1118:A:C8	1:0:1119:G:H5''	2.49	0.46
1:0:2011:A:H4'	1:0:2012:U:O5'	2.15	0.46
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.79	0.46
5:B:25:ARG:HA	5:B:310:ARG:HH21	1.80	0.46
5:B:258:GLY:H	5:B:260:HIS:HE1	1.56	0.46
6:C:130:GLU:OE1	6:C:130:GLU:HA	2.15	0.46
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.50	0.46
7:D:35:ALA:N	38:D:5576:HOH:O	2.47	0.46
8:E:73:PHE:O	8:E:76:VAL:HG22	2.14	0.46
9:F:26:THR:HG21	9:F:103:GLU:HG3	1.97	0.46
15:M:61:ILE:HD12	15:M:61:ILE:N	2.29	0.46
16:N:34:LEU:HD13	16:N:47:LEU:HD21	1.97	0.46
18:P:59:ARG:HH22	18:P:66:GLN:NE2	2.09	0.46
25:W:11:VAL:O	25:W:12:ASN:HB2	2.14	0.46
32:I:112:LYS:C	32:I:114:PRO:HD2	2.40	0.46
32:I:138:THR:HG22	32:I:139:ILE:H	1.79	0.46
1:0:485:A:N3	1:0:487:G:H5''	2.30	0.46
1:0:1172:G:H1'	38:0:5254:HOH:O	2.15	0.46
1:0:1427:A:H61	1:0:1440:U:H1'	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2548:C:OP2	5:B:5:ARG:NH2	2.48	0.46
1:O:2846:C:H4'	5:B:156:LYS:HB3	1.98	0.46
4:A:35:GLY:O	4:A:36:ASP:CB	2.56	0.46
12:J:39:VAL:HG13	12:J:106:GLY:O	2.15	0.46
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.46	0.46
16:N:69:TYR:CE2	16:N:184:ILE:HD11	2.50	0.46
18:P:13:VAL:HG13	18:P:14:LEU:N	2.31	0.46
25:W:130:HIS:O	25:W:136:GLY:HA3	2.14	0.46
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.80	0.46
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.15	0.46
32:I:132:CYS:C	32:I:134:SER:N	2.73	0.46
1:O:2694:A:H5''	8:E:90:HIS:CE1	2.51	0.46
1:O:2748:G:H1'	38:O:8206:HOH:O	2.14	0.46
38:O:3949:HOH:O	17:O:3:THR:HG21	2.15	0.46
2:9:3050:G:H2'	2:9:3051:A:C8	2.50	0.46
8:E:114:ARG:HB3	8:E:151:LEU:HD11	1.97	0.46
25:W:108:ARG:HE	25:W:114:PRO:HG2	1.80	0.46
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.97	0.46
32:I:106:LYS:O	32:I:110:GLU:HG3	2.15	0.46
1:O:29:C:O2'	1:O:30:U:H5'	2.16	0.46
1:O:424:C:H2'	1:O:425:U:C6	2.50	0.46
1:O:776:A:OP1	29:1:28:HIS:HE1	1.99	0.46
1:O:1385:G:O3'	26:X:49:ARG:NH1	2.48	0.46
1:O:2301:A:H5''	1:O:2302:A:H5'	1.98	0.46
1:O:2866:U:H4'	1:O:2867:G:H5'	1.97	0.46
38:O:9868:HOH:O	25:W:119:HIS:HE1	1.97	0.46
4:A:129:LEU:CD1	4:A:145:MET:HE1	2.46	0.46
6:C:242:GLU:HG3	38:C:9178:HOH:O	2.15	0.46
10:G:64:ASN:O	10:G:68:GLU:HG3	2.16	0.46
11:H:9:ILE:HG12	11:H:56:GLN:CG	2.46	0.46
16:N:67:ALA:C	16:N:69:TYR:N	2.74	0.46
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.40	0.46
1:O:236:A:H4'	1:O:237:G:H5'	1.97	0.46
1:O:775:G:OP1	29:1:16:HIS:HE1	1.99	0.46
1:O:1119:G:H8	12:J:52:GLN:NE2	2.13	0.46
1:O:2487:C:H5	38:O:5168:HOH:O	1.98	0.46
1:O:2708:G:N2	13:K:1:MET:O	2.47	0.46
6:C:200:PRO:HB3	6:C:212:VAL:CG2	2.45	0.46
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.98	0.46
11:H:170:ASN:N	11:H:170:ASN:ND2	2.59	0.46
17:O:21:SER:HB3	17:O:107:GLU:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:9:CYS:HA	23:U:52:THR:CG2	2.39	0.46
1:0:482:G:H4'	1:0:508:A:N1	2.31	0.46
1:0:1278:A:H4'	1:0:1279:U:C4	2.50	0.46
1:0:2064:U:H5'	1:0:2652:U:H4'	1.98	0.46
13:K:9:THR:O	13:K:10:GLN:C	2.58	0.46
14:L:145:LEU:O	14:L:148:GLU:HG3	2.15	0.46
18:P:40:VAL:O	18:P:44:VAL:HG23	2.15	0.46
20:R:113:HIS:O	20:R:145:LEU:HD12	2.15	0.46
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.98	0.46
24:V:1:THR:O	24:V:4:HIS:CE1	2.69	0.46
24:V:57:LYS:HA	24:V:60:GLN:HE21	1.81	0.46
1:0:87:C:H2'	30:2:28:LYS:O	2.16	0.46
1:0:558:C:H2'	1:0:559:U:H5''	1.97	0.46
1:0:1205:U:C2'	1:0:1206:U:H5''	2.45	0.46
1:0:1427:A:N6	1:0:1440:U:H1'	2.31	0.46
1:0:2269:C:C2'	1:0:2270:G:H5'	2.46	0.46
1:0:2324:G:H4'	1:0:2418:G:O2'	2.15	0.46
1:0:2415:A:N3	16:N:26:LEU:HD13	2.31	0.46
5:B:145:HIS:HA	5:B:160:ASP:O	2.15	0.46
5:B:154:VAL:CG1	5:B:156:LYS:HG2	2.45	0.46
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.16	0.46
13:K:22:ASP:HB2	38:K:5264:HOH:O	2.14	0.46
1:0:21:G:H5''	20:R:2:ILE:HA	1.96	0.46
1:0:1086:A:OP1	25:W:9:GLY:N	2.43	0.46
1:0:1236:A:C8	12:J:63:ILE:HD11	2.51	0.46
1:0:2445:U:H2'	1:0:2446:G:C8	2.51	0.46
1:0:2670:G:O2'	1:0:2671:U:H5'	2.16	0.46
15:M:64:ARG:HD2	38:M:9383:HOH:O	2.15	0.46
28:Z:39:CYS:HA	28:Z:47:VAL:HG21	1.97	0.46
1:0:88:G:H2'	1:0:89:G:C8	2.51	0.46
1:0:1878:G:O2'	1:0:1879:U:C6	2.67	0.46
1:0:2832:C:H5	38:0:7432:HOH:O	1.98	0.46
36:0:9303:CL:CL	30:2:2:LYS:HE3	2.52	0.46
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.98	0.46
4:A:165:THR:O	4:A:165:THR:HG22	2.15	0.46
6:C:162:VAL:CG1	6:C:192:ILE:HD11	2.44	0.46
9:F:48:VAL:HG23	9:F:74:PHE:HB2	1.97	0.46
9:F:57:GLU:HB2	15:M:23:LEU:HD11	1.97	0.46
12:J:52:GLN:HG3	12:J:53:ILE:H	1.80	0.46
29:1:25:LYS:HD2	30:2:49:GLU:N	2.30	0.46
1:0:793:A:C5'	18:P:83:LYS:HG2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:960:G:N3	1:0:960:G:C2'	2.79	0.46
1:0:1613:C:H2'	1:0:1614:G:O4'	2.15	0.46
1:0:2365:G:H4'	19:Q:45:PRO:O	2.16	0.46
5:B:243:ASN:HA	5:B:244:PRO:C	2.39	0.46
7:D:140:ARG:O	7:D:144:ARG:HG2	2.16	0.46
9:F:33:THR:HG21	9:F:59:ILE:O	2.16	0.46
20:R:119:VAL:O	20:R:119:VAL:CG1	2.63	0.46
22:T:35:TYR:CD2	22:T:112:LEU:HD22	2.51	0.46
25:W:21:LEU:HD21	25:W:48:VAL:HG13	1.98	0.46
30:2:40:ARG:HG3	30:2:45:ASN:CB	2.44	0.46
1:0:2472:C:O2'	1:0:2634:G:H4'	2.16	0.45
38:0:4054:HOH:O	22:T:9:LYS:HD3	2.16	0.45
2:9:3013:A:HO2'	2:9:3014:G:H5''	1.80	0.45
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.98	0.45
22:T:23:VAL:C	22:T:93:THR:HG21	2.41	0.45
25:W:65:VAL:HA	25:W:68:THR:CG2	2.45	0.45
32:I:96:PHE:HA	32:I:136:GLY:HA3	1.97	0.45
1:0:289:G:N2	1:0:363:A:H2	2.15	0.45
5:B:175:LEU:C	5:B:175:LEU:CD2	2.89	0.45
7:D:166:ILE:HB	38:D:6326:HOH:O	2.15	0.45
8:E:102:VAL:HG11	8:E:148:ILE:HG12	1.98	0.45
13:K:75:ARG:CZ	38:K:4172:HOH:O	2.63	0.45
15:M:69:LYS:HG2	15:M:127:LYS:HG3	1.98	0.45
16:N:34:LEU:HD22	16:N:129:ILE:CD1	2.45	0.45
18:P:141:ILE:C	18:P:143:ALA:N	2.73	0.45
26:X:43:VAL:CG1	26:X:44:ASP:H	2.24	0.45
32:I:102:VAL:O	32:I:106:LYS:HG3	2.17	0.45
1:0:500:G:H21	20:R:98:ASN:HD21	1.62	0.45
1:0:894:A:C2	6:C:87:ARG:NH2	2.84	0.45
1:0:1120:U:H5''	1:0:1120:U:C6	2.51	0.45
1:0:1168:C:H4'	38:I:5128:HOH:O	2.15	0.45
1:0:2372:A:H2'	1:0:2373:U:C6	2.52	0.45
5:B:97:LEU:HD21	38:B:9444:HOH:O	2.17	0.45
8:E:154:ILE:HD11	8:E:157:LYS:HE2	1.97	0.45
22:T:32:ARG:CZ	22:T:38:ARG:NH1	2.80	0.45
25:W:153:MET:O	25:W:154:ARG:C	2.59	0.45
1:0:156:C:H5''	15:M:171:ARG:CD	2.24	0.45
1:0:1309:U:O2'	1:0:1310:U:H5'	2.15	0.45
1:0:2300:A:H4'	1:0:2301:A:O5'	2.16	0.45
1:0:2415:A:C2	16:N:25:ARG:HB3	2.52	0.45
5:B:202:VAL:HG11	5:B:301:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:75:ARG:O	13:K:93:ASN:HA	2.16	0.45
20:R:132:ARG:CZ	38:R:9383:HOH:O	2.65	0.45
22:T:49:GLU:HG3	22:T:97:ARG:HB3	1.97	0.45
32:I:112:LYS:O	32:I:116:LEU:HG	2.16	0.45
1:0:270:U:H1'	38:0:4020:HOH:O	2.16	0.45
1:0:952:G:N3	1:0:2302:A:H2'	2.31	0.45
1:0:1095:U:O2	25:W:120:PRO:HG2	2.16	0.45
1:0:2467:A:H1'	38:0:5014:HOH:O	2.17	0.45
1:0:2563:U:H2'	1:0:2565:C:O5'	2.16	0.45
7:D:159:PRO:O	7:D:163:VAL:HG23	2.16	0.45
12:J:47:THR:O	12:J:53:ILE:HD11	2.17	0.45
26:X:7:GLU:HA	26:X:74:ALA:O	2.16	0.45
1:0:290:C:O2'	1:0:291:C:H5'	2.15	0.45
1:0:678:G:OP2	6:C:107:ARG:NH2	2.50	0.45
1:0:2385:G:H2'	1:0:2386:U:H6	1.80	0.45
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.17	0.45
5:B:79:MET:HE2	5:B:144:THR:CG2	2.47	0.45
6:C:165:ASP:O	6:C:168:ARG:HB3	2.17	0.45
9:F:46:GLU:O	9:F:73:PRO:HD2	2.17	0.45
15:M:98:GLN:O	15:M:102:GLU:HG3	2.17	0.45
26:X:75:ALA:O	26:X:83:ALA:HA	2.16	0.45
1:0:136:C:H2'	1:0:137:U:O4'	2.17	0.45
1:0:1079:A:N1	1:0:2068:G:O2'	2.46	0.45
1:0:1314:U:H2'	38:0:6137:HOH:O	2.15	0.45
1:0:1711:A:O2'	1:0:1712:A:H5'	2.17	0.45
1:0:2004:U:H4'	38:0:5579:HOH:O	2.16	0.45
1:0:2729:C:O2'	1:0:2730:G:H5'	2.17	0.45
1:0:2816:A:H5''	1:0:2817:G:H5'	1.99	0.45
38:0:3990:HOH:O	8:E:143:GLN:HG2	2.16	0.45
4:A:192:VAL:HG12	4:A:192:VAL:O	2.17	0.45
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.99	0.45
6:C:214:THR:HG23	38:C:9234:HOH:O	2.15	0.45
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.86	0.45
15:M:167:GLY:O	15:M:171:ARG:HG3	2.17	0.45
16:N:183:ASP:O	16:N:184:ILE:C	2.59	0.45
27:Y:97:LEU:C	27:Y:98:GLN:HG2	2.42	0.45
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.52	0.45
1:0:559:U:H2'	1:0:560:C:O4'	2.17	0.45
1:0:703:G:O2'	1:0:704:C:H5'	2.17	0.45
1:0:907:A:H2'	1:0:908:A:H8	1.81	0.45
1:0:2281:C:C2'	1:0:2282:U:H5'	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:O:7005:HOH:O	16:N:4:PRO:HD2	2.16	0.45
5:B:51:VAL:O	5:B:51:VAL:HG13	2.16	0.45
5:B:86:ALA:HA	38:B:9380:HOH:O	2.16	0.45
6:C:172:THR:HG22	6:C:188:ARG:CZ	2.47	0.45
8:E:43:ASP:O	8:E:45:ASP:N	2.47	0.45
8:E:118:ILE:HG23	8:E:144:THR:HG21	1.99	0.45
11:H:114:ARG:O	11:H:115:ALA:C	2.60	0.45
14:L:66:VAL:HG23	14:L:67:ARG:N	2.32	0.45
16:N:93:GLN:HA	16:N:93:GLN:NE2	2.23	0.45
16:N:140:GLN:HA	16:N:143:ARG:HD3	1.99	0.45
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.31	0.45
26:X:66:THR:HG22	26:X:67:PRO:O	2.17	0.45
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.46	0.45
1:O:23:G:H1'	1:O:520:A:N6	2.32	0.45
1:O:243:A:H61	1:O:269:G:H1'	1.81	0.45
1:O:1007:A:H2'	11:H:19:TYR:CZ	2.52	0.45
1:O:1163:G:H2'	1:O:1164:U:C5	2.52	0.45
5:B:276:ASP:HB3	5:B:291:ASP:OD1	2.17	0.45
12:J:47:THR:HG22	12:J:48:GLY:N	2.31	0.45
12:J:107:ASN:HD22	12:J:108:PRO:CD	2.29	0.45
13:K:22:ASP:C	13:K:22:ASP:OD1	2.60	0.45
13:K:30:LYS:O	13:K:55:VAL:HG13	2.17	0.45
18:P:142:ASP:O	18:P:143:ALA:O	2.35	0.45
24:V:46:ILE:HA	24:V:49:LEU:HD12	1.99	0.45
26:X:30:MET:HE1	26:X:55:ASN:HA	1.99	0.45
1:O:451:C:O2'	1:O:452:G:H5'	2.17	0.45
1:O:920:C:H5''	1:O:921:G:O5'	2.17	0.45
1:O:2698:G:H2'	1:O:2699:A:O4'	2.16	0.45
38:O:5725:HOH:O	10:G:12:ILE:HA	2.16	0.45
2:9:3106:C:O2'	2:9:3107:C:H5'	2.16	0.45
6:C:133:ARG:HG2	6:C:135:GLU:O	2.17	0.45
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.46	0.45
7:D:81:GLU:O	7:D:85:GLN:HG3	2.17	0.45
8:E:34:TRP:HA	38:E:4572:HOH:O	2.17	0.45
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.82	0.45
14:L:64:ILE:HG13	14:L:68:GLU:OE1	2.15	0.45
14:L:145:LEU:HD23	14:L:145:LEU:C	2.42	0.45
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.32	0.45
25:W:76:ASP:O	25:W:77:ALA:C	2.60	0.45
1:O:249:G:O2'	1:O:250:C:H5'	2.16	0.44
1:O:432:G:O2'	1:O:433:C:H5'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1289:C:O2'	1:0:1290:G:H5'	2.16	0.44
1:0:1304:U:H2'	1:0:1305:C:C6	2.52	0.44
8:E:15:GLN:CG	8:E:20:ILE:HG12	2.47	0.44
12:J:99:GLU:HA	38:J:9371:HOH:O	2.17	0.44
14:L:12:THR:HG21	14:L:16:GLY:O	2.17	0.44
16:N:39:SER:HB3	16:N:42:HIS:H	1.82	0.44
16:N:63:SER:HB2	16:N:75:THR:HB	1.99	0.44
19:Q:25:PRO:HB2	38:Q:4350:HOH:O	2.16	0.44
31:3:65:THR:CG2	31:3:67:LEU:HG	2.47	0.44
1:0:816:G:C6	1:0:817:G:N1	2.85	0.44
1:0:1056:U:H2'	1:0:1057:A:O4'	2.16	0.44
1:0:1200:A:H4'	38:0:7550:HOH:O	2.17	0.44
1:0:1657:A:H2'	1:0:1658:A:C8	2.52	0.44
1:0:1942:A:O2'	1:0:1943:C:H5'	2.17	0.44
1:0:2781:U:H2'	1:0:2782:G:C5'	2.47	0.44
38:0:9851:HOH:O	18:P:81:LYS:HG2	2.18	0.44
38:0:9937:HOH:O	9:F:38:LYS:HE2	2.17	0.44
4:A:135:VAL:HG21	4:A:147:ARG:HG2	2.00	0.44
5:B:198:GLU:HA	38:B:9461:HOH:O	2.15	0.44
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.99	0.44
8:E:43:ASP:HA	38:E:5864:HOH:O	2.16	0.44
25:W:38:THR:O	25:W:42:ARG:HB2	2.17	0.44
29:1:37:CYS:SG	29:1:39:PHE:HB2	2.57	0.44
1:0:35:U:H5'	6:C:47:GLY:O	2.17	0.44
1:0:1943:C:O4'	4:A:212:PRO:HA	2.17	0.44
1:0:2061:C:C2'	1:0:2062:A:H5'	2.48	0.44
1:0:2438:G:H2'	1:0:2439:C:O4'	2.17	0.44
1:0:2715:G:O2'	5:B:262:ARG:HD2	2.17	0.44
4:A:53:ALA:HB3	38:A:9400:HOH:O	2.17	0.44
4:A:100:PRO:HG2	4:A:103:VAL:CG2	2.45	0.44
6:C:133:ARG:NE	6:C:135:GLU:O	2.50	0.44
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.86	0.44
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.99	0.44
19:Q:31:GLU:CD	19:Q:93:ARG:HH12	2.25	0.44
22:T:64:ASN:HB3	22:T:73:HIS:HB2	1.98	0.44
1:0:1167:G:H2'	1:0:1168:C:O4'	2.17	0.44
1:0:1174:A:C5	1:0:1201:C:H4'	2.52	0.44
1:0:1249:U:H2'	1:0:1250:C:C6	2.52	0.44
1:0:2036:C:C4'	13:K:44:LEU:HG	2.47	0.44
38:0:7568:HOH:O	4:A:177:HIS:HE1	2.01	0.44
5:B:301:VAL:HG13	5:B:302:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:158:ASN:HB2	7:D:161:ASP:OD2	2.16	0.44
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.98	0.44
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.15	0.44
12:J:39:VAL:HG11	12:J:107:ASN:HB2	1.99	0.44
13:K:90:PHE:N	13:K:90:PHE:CD1	2.86	0.44
16:N:18:THR:HG21	38:N:9348:HOH:O	2.17	0.44
22:T:53:GLY:HA3	38:T:6384:HOH:O	2.16	0.44
27:Y:112:GLU:OE1	27:Y:115:ARG:NH1	2.50	0.44
32:I:92:PRO:O	32:I:94:GLU:HG3	2.16	0.44
1:O:113:A:OP2	1:O:114:A:H2'	2.18	0.44
1:O:1544:U:H2'	1:O:1545:C:C6	2.53	0.44
1:O:2061:C:H2'	1:O:2062:A:H5'	2.00	0.44
1:O:2403:C:H2'	1:O:2404:G:O5'	2.17	0.44
1:O:2453:G:H4'	14:L:50:GLY:C	2.42	0.44
5:B:146:THR:C	5:B:148:PRO:HD3	2.43	0.44
6:C:246:ARG:NE	38:C:9220:HOH:O	2.51	0.44
8:E:21:THR:HG23	8:E:30:THR:OG1	2.17	0.44
9:F:50:VAL:HG11	9:F:60:VAL:HG11	1.99	0.44
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.52	0.44
14:L:77:ALA:HB3	38:L:9328:HOH:O	2.18	0.44
16:N:15:GLU:HB3	16:N:17:ARG:HG3	1.99	0.44
16:N:67:ALA:C	16:N:69:TYR:H	2.25	0.44
16:N:154:LEU:HD12	16:N:156:GLU:O	2.17	0.44
18:P:141:ILE:O	18:P:143:ALA:N	2.41	0.44
20:R:114:VAL:HG13	20:R:114:VAL:O	2.18	0.44
25:W:88:THR:CG2	25:W:110:GLN:HE21	2.22	0.44
26:X:70:ILE:HG23	26:X:70:ILE:O	2.17	0.44
32:I:101:SER:OG	32:I:104:GLN:HG3	2.18	0.44
32:I:110:GLU:HA	32:I:113:HIS:CD2	2.52	0.44
1:O:656:G:H5'	17:O:3:THR:CG2	2.48	0.44
1:O:968:G:H1'	11:H:32:LYS:HD2	2.00	0.44
1:O:968:G:O2'	1:O:969:G:H5'	2.17	0.44
1:O:1067:A:H5'	38:O:4638:HOH:O	2.18	0.44
1:O:1632:A:C2'	1:O:1633:C:H5'	2.47	0.44
6:C:16:VAL:CG1	6:C:17:ASP:N	2.80	0.44
7:D:64:ARG:CD	7:D:67:ASP:HB3	2.47	0.44
11:H:38:LYS:HE2	11:H:42:ASP:CB	2.47	0.44
16:N:11:ARG:NH2	38:N:9316:HOH:O	2.51	0.44
20:R:40:ALA:O	20:R:44:VAL:HG23	2.18	0.44
23:U:6:CYS:C	23:U:8:TYR:N	2.76	0.44
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:926:A:O2'	14:L:41:HIS:CD2	2.70	0.44
1:0:1307:A:H2'	1:0:1308:A:C8	2.53	0.44
1:0:1811:A:C2	1:0:2752:C:H1'	2.52	0.44
1:0:2015:A:H2'	1:0:2016:U:O4'	2.17	0.44
4:A:130:THR:HG22	4:A:131:HIS:N	2.32	0.44
5:B:212:GLN:HG2	5:B:257:THR:OG1	2.17	0.44
6:C:65:ARG:HG3	6:C:67:GLN:HB2	2.00	0.44
6:C:102:LEU:HD12	38:C:9117:HOH:O	2.16	0.44
6:C:129:HIS:HD2	6:C:165:ASP:OD2	2.01	0.44
7:D:44:ILE:HG12	7:D:83:PHE:CE1	2.49	0.44
7:D:76:ARG:O	7:D:77:ASP:HB2	2.16	0.44
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.99	0.44
13:K:114:ALA:HB3	13:K:117:VAL:HG23	2.00	0.44
16:N:82:TYR:C	16:N:82:TYR:CD2	2.96	0.44
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.22	0.44
25:W:122:ARG:HG2	25:W:122:ARG:NH1	2.25	0.44
1:0:425:U:H4'	38:0:7160:HOH:O	2.17	0.44
1:0:1587:U:H2'	1:0:1588:G:O4'	2.18	0.44
1:0:1829:A:H5''	38:0:3389:HOH:O	2.16	0.44
2:9:3042:C:O2	7:D:76:ARG:NH1	2.50	0.44
5:B:14:GLY:HA3	38:B:9410:HOH:O	2.17	0.44
6:C:19:PRO:HD2	6:C:240:LEU:HD21	2.00	0.44
6:C:233:THR:HG22	6:C:234:VAL:H	1.83	0.44
15:M:182:LYS:C	15:M:194:ALA:HB2	2.43	0.44
16:N:15:GLU:OE1	16:N:17:ARG:HD2	2.17	0.44
16:N:63:SER:O	16:N:66:LEU:HB2	2.17	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.75	0.44
23:U:52:THR:CG2	23:U:54:THR:HB	2.48	0.44
25:W:73:LEU:O	25:W:74:GLU:HG2	2.18	0.44
28:Z:56:GLN:HA	28:Z:62:TYR:O	2.17	0.44
1:0:248:A:H5'	1:0:249:G:OP2	2.18	0.44
1:0:1204:C:H1'	38:0:5023:HOH:O	2.18	0.44
1:0:2329:C:O2'	1:0:2330:U:H5'	2.17	0.44
1:0:2511:A:H2'	1:0:2512:U:O4'	2.18	0.44
5:B:7:ARG:HD3	5:B:9:GLY:O	2.18	0.44
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.33	0.44
5:B:312:ARG:HD3	5:B:315:VAL:HG13	2.00	0.44
8:E:71:ASN:HD22	8:E:138:ILE:HD13	1.83	0.44
12:J:39:VAL:HG12	12:J:40:ASN:CG	2.43	0.44
16:N:37:ARG:HA	16:N:37:ARG:HD3	1.75	0.44
18:P:91:LYS:O	18:P:95:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:43:ASN:HD22	22:T:108:ARG:NH2	2.15	0.44
25:W:143:THR:N	38:W:3520:HOH:O	2.51	0.44
26:X:76:ARG:HG3	26:X:76:ARG:NH1	2.31	0.44
1:0:958:G:H2'	1:0:959:C:H6	1.82	0.43
1:0:999:C:H2'	1:0:1000:C:O4'	2.18	0.43
1:0:1224:G:H2'	1:0:1225:C:C6	2.52	0.43
1:0:1926:G:H2'	1:0:1927:A:C8	2.53	0.43
1:0:2684:A:H2'	1:0:2685:C:C6	2.53	0.43
5:B:24:PRO:HA	5:B:261:GLN:OE1	2.18	0.43
5:B:304:PRO:HD2	5:B:307:ARG:NH1	2.32	0.43
6:C:5:ILE:CD1	6:C:16:VAL:HG23	2.40	0.43
6:C:72:LYS:HG2	6:C:77:ALA:HA	1.99	0.43
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.00	0.43
9:F:117:GLU:C	9:F:119:ARG:H	2.26	0.43
13:K:14:LYS:HG3	13:K:32:ILE:O	2.18	0.43
16:N:154:LEU:HD11	16:N:157:PRO:HA	1.99	0.43
17:O:96:VAL:HG12	17:O:100:GLN:HB2	1.99	0.43
25:W:64:THR:O	25:W:68:THR:HG22	2.18	0.43
25:W:105:THR:HG23	25:W:106:THR:N	2.31	0.43
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.53	0.43
1:0:162:C:H2'	1:0:163:U:H5'	2.01	0.43
1:0:806:A:H2'	1:0:807:A:O4'	2.18	0.43
1:0:1666:C:C2'	1:0:1667:A:C5'	2.96	0.43
2:9:3049:G:C2'	2:9:3050:G:H5'	2.48	0.43
4:A:43:VAL:HG21	4:A:59:GLU:OE2	2.18	0.43
5:B:175:LEU:O	5:B:178:ALA:HB3	2.18	0.43
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.48	0.43
9:F:110:ASP:O	9:F:114:LYS:HG3	2.18	0.43
16:N:42:HIS:CB	16:N:62:HIS:HE1	2.31	0.43
16:N:154:LEU:O	16:N:155:GLU:CB	2.65	0.43
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.43
22:T:81:LYS:HD2	22:T:87:VAL:HG11	1.99	0.43
1:0:333:G:O2'	1:0:334:G:H5'	2.18	0.43
1:0:946:C:H2'	1:0:947:U:C6	2.53	0.43
1:0:1015:C:H2'	1:0:1016:U:C6	2.53	0.43
1:0:1168:C:H5''	32:I:87:THR:HG23	2.00	0.43
1:0:1398:G:H2'	1:0:1399:A:C8	2.53	0.43
1:0:1504:A:H5'	38:O:4704:HOH:O	2.17	0.43
1:0:1682:A:H2'	38:O:3108:HOH:O	2.18	0.43
1:0:1849:G:H1'	1:0:2011:A:N1	2.33	0.43
1:0:2684:A:H1'	38:O:3235:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2724:U:H2'	1:0:2725:G:O4'	2.18	0.43
5:B:51:VAL:HG13	5:B:53:LEU:CD1	2.48	0.43
6:C:168:ARG:NH2	6:C:190:ALA:O	2.51	0.43
7:D:58:VAL:HG12	7:D:60:GLU:HG2	2.00	0.43
9:F:43:GLY:C	9:F:45:ALA:H	2.26	0.43
14:L:130:ARG:O	14:L:134:GLU:HG3	2.18	0.43
20:R:114:VAL:HA	20:R:144:GLU:O	2.18	0.43
1:0:574:C:H2'	1:0:575:G:O4'	2.19	0.43
1:0:1250:C:O2'	1:0:1251:C:H5'	2.18	0.43
1:0:1450:C:O2'	1:0:1494:A:H5'	2.17	0.43
1:0:1528:A:H2'	1:0:1529:G:O4'	2.18	0.43
1:0:1595:G:O2'	1:0:1596:U:H5'	2.19	0.43
1:0:1973:A:H5'	1:0:1973:A:H8	1.83	0.43
1:0:2338:G:H1'	7:D:105:SER:OG	2.18	0.43
1:0:2455:A:H2'	1:0:2456:A:O4'	2.18	0.43
1:0:2717:C:OP1	5:B:207:LYS:HG3	2.18	0.43
1:0:2756:U:N3	1:0:2896:A:H2	2.08	0.43
5:B:51:VAL:HG13	5:B:53:LEU:HD11	2.00	0.43
13:K:55:VAL:CG1	13:K:56:SER:N	2.81	0.43
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.54	0.43
16:N:23:ARG:HG2	16:N:23:ARG:NH1	2.33	0.43
24:V:12:THR:HG23	24:V:14:ALA:N	2.21	0.43
1:0:926:A:O2'	14:L:41:HIS:HD2	2.01	0.43
1:0:2504:A:H2'	1:0:2505:G:O4'	2.18	0.43
6:C:7:ASP:OD1	6:C:11:ASN:O	2.37	0.43
7:D:35:ALA:C	7:D:37:ALA:N	2.76	0.43
17:O:44:ASN:CG	17:O:67:SER:HB2	2.43	0.43
20:R:47:LEU:O	20:R:51:ILE:HG13	2.18	0.43
1:0:2365:G:P	19:Q:15:LYS:HG3	2.59	0.43
38:O:7762:HOH:O	31:3:60:LYS:HG3	2.17	0.43
4:A:51:ARG:NH1	4:A:120:ARG:O	2.51	0.43
5:B:79:MET:O	5:B:80:ARG:HG3	2.19	0.43
7:D:128:LEU:C	7:D:128:LEU:HD23	2.44	0.43
8:E:145:ALA:HB1	8:E:168:ILE:HD11	2.01	0.43
11:H:87:LEU:HD13	11:H:134:PHE:CE2	2.53	0.43
20:R:4:TYR:HA	20:R:144:GLU:OE2	2.19	0.43
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.63	0.43
29:1:8:GLN:NE2	29:1:11:LYS:NZ	2.59	0.43
1:0:120:A:H2'	1:0:120:A:N3	2.34	0.43
1:0:475:G:H5'	6:C:73:LEU:HD23	2.00	0.43
1:0:622:G:O2'	1:0:623:U:H5'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1878:G:O2'	1:0:1879:U:OP2	2.35	0.43
1:0:2456:A:H2'	1:0:2457:U:C6	2.54	0.43
5:B:27:ASN:HD22	5:B:27:ASN:N	2.01	0.43
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.37	0.43
8:E:156:ASP:OD1	8:E:156:ASP:N	2.51	0.43
12:J:107:ASN:ND2	12:J:107:ASN:C	2.77	0.43
15:M:182:LYS:HD2	15:M:193:LYS:HB2	1.99	0.43
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.84	0.43
1:0:392:U:O2'	15:M:182:LYS:HE2	2.18	0.43
1:0:644:G:H1'	38:0:6645:HOH:O	2.19	0.43
1:0:1189:A:O2'	1:0:1208:C:H2'	2.18	0.43
1:0:1419:U:H5'	1:0:1420:C:OP2	2.18	0.43
1:0:1636:G:O2'	1:0:1637:A:H5'	2.18	0.43
1:0:1930:A:H2'	1:0:1931:A:C8	2.53	0.43
1:0:2379:G:H5'	1:0:2381:C:O4'	2.18	0.43
1:0:2587:OMU:HM23	1:0:2589:U:C6	2.54	0.43
5:B:52:VAL:O	5:B:53:LEU:HD12	2.19	0.43
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.86	0.43
5:B:183:GLU:O	5:B:184:ASP:C	2.61	0.43
6:C:150:THR:HA	6:C:203:ALA:O	2.18	0.43
7:D:152:PRO:O	7:D:156:ARG:HG2	2.18	0.43
10:G:23:ILE:O	10:G:27:ILE:HG13	2.19	0.43
14:L:93:VAL:CG2	14:L:122:ALA:HB2	2.48	0.43
18:P:38:GLU:HA	18:P:41:ARG:HH11	1.83	0.43
1:0:154:C:P	15:M:188:ARG:HH12	2.41	0.43
1:0:245:C:H2'	1:0:246:G:H5'	2.01	0.43
2:9:3003:A:H2	2:9:3021:G:N3	2.17	0.43
5:B:313:PRO:O	5:B:314:ALA:C	2.62	0.43
6:C:7:ASP:C	6:C:9:ASP:H	2.27	0.43
6:C:236:THR:O	6:C:239:ALA:N	2.51	0.43
7:D:170:TYR:CD1	7:D:170:TYR:N	2.86	0.43
13:K:113:ILE:HG22	13:K:114:ALA:O	2.19	0.43
15:M:182:LYS:O	15:M:194:ALA:HB2	2.18	0.43
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.47	0.43
1:0:222:A:H2'	1:0:223:G:O4'	2.18	0.43
1:0:303:C:H2'	1:0:304:G:O4'	2.19	0.43
1:0:709:G:O2'	17:O:25:VAL:CG1	2.67	0.43
1:0:912:A:C4	1:0:1294:A:C2	3.07	0.43
1:0:1817:U:O2	18:P:81:LYS:NZ	2.47	0.43
1:0:2134:G:C6	1:0:2258:A:C8	3.07	0.43
1:0:2715:G:N2	5:B:264:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2780:C:H2'	1:0:2781:U:C6	2.54	0.43
38:0:9991:HOH:O	27:Y:163:THR:HG23	2.19	0.43
5:B:17:LYS:O	5:B:260:HIS:HD2	2.02	0.43
7:D:169:THR:C	7:D:170:TYR:HD1	2.27	0.43
11:H:80:GLU:HA	38:H:9183:HOH:O	2.18	0.43
13:K:113:ILE:HD12	13:K:128:ALA:HB2	2.01	0.43
15:M:31:TRP:HA	15:M:34:GLU:HG3	2.01	0.43
18:P:22:TRP:CH2	18:P:24:ASN:HA	2.54	0.43
18:P:38:GLU:HA	18:P:41:ARG:NH1	2.34	0.43
26:X:76:ARG:O	26:X:77:PHE:HB3	2.18	0.43
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.59	0.43
1:0:737:A:H2'	1:0:738:G:O4'	2.19	0.42
1:0:1008:C:H5''	11:H:16:ARG:HH12	1.84	0.42
1:0:1675:C:H5''	30:2:5:LYS:HD2	2.01	0.42
4:A:94:LEU:HG	4:A:99:ILE:CD1	2.49	0.42
6:C:91:PRO:O	6:C:93:LYS:HG3	2.19	0.42
8:E:145:ALA:O	8:E:148:ILE:HB	2.19	0.42
9:F:28:ALA:HB3	9:F:99:THR:HG23	2.01	0.42
14:L:24:ALA:HB2	14:L:30:ARG:HD2	2.01	0.42
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.48	0.42
32:I:92:PRO:HG3	38:I:6825:HOH:O	2.18	0.42
32:I:124:ALA:O	32:I:128:VAL:HG23	2.19	0.42
32:I:132:CYS:CB	32:I:137:VAL:HB	2.35	0.42
1:0:638:C:H2'	1:0:639:A:C8	2.54	0.42
1:0:795:G:N3	1:0:817:G:C2	2.87	0.42
1:0:1309:U:H2'	1:0:1310:U:O4'	2.19	0.42
1:0:2067:A:H2'	1:0:2068:G:O4'	2.19	0.42
1:0:2251:G:H2'	1:0:2252:A:H8	1.81	0.42
1:0:2815:G:N7	12:J:80:LYS:NZ	2.65	0.42
1:0:2820:A:H2'	1:0:2821:C:O4'	2.18	0.42
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.20	0.42
7:D:23:VAL:O	7:D:23:VAL:CG2	2.66	0.42
8:E:3:VAL:CG2	8:E:49:ILE:HB	2.47	0.42
38:E:2512:HOH:O	12:J:127:ILE:HD11	2.18	0.42
14:L:77:ALA:C	14:L:79:ASP:H	2.27	0.42
15:M:43:PRO:HG3	15:M:62:VAL:HG21	2.01	0.42
24:V:7:GLU:O	24:V:11:MET:HG3	2.18	0.42
24:V:12:THR:OG1	24:V:13:PRO:HD2	2.19	0.42
1:0:920:C:H4'	1:0:921:G:N2	2.33	0.42
1:0:2467:A:O2'	1:0:2468:A:H2'	2.19	0.42
5:B:207:LYS:HG2	5:B:304:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:35:TYR:CD2	8:E:36:PRO:HD2	2.54	0.42
11:H:20:ILE:HG23	11:H:120:ILE:HD11	2.00	0.42
12:J:130:VAL:CG1	12:J:131:THR:N	2.82	0.42
14:L:59:GLU:HG2	14:L:104:ASP:OD2	2.19	0.42
16:N:34:LEU:HA	16:N:47:LEU:CD2	2.49	0.42
19:Q:64:GLU:OE1	19:Q:64:GLU:HA	2.19	0.42
20:R:17:MET:CE	20:R:19:ARG:CZ	2.94	0.42
27:Y:108:ASP:OD1	27:Y:108:ASP:N	2.53	0.42
1:O:2255:A:C6	1:O:2256:G:C5	3.08	0.42
1:O:2314:G:C2'	1:O:2315:C:H5'	2.49	0.42
1:O:2564:G:OP2	1:O:2565:C:H5''	2.19	0.42
2:9:3034:A:H2'	2:9:3035:C:O4'	2.19	0.42
5:B:305:ASP:O	5:B:306:LYS:CB	2.66	0.42
7:D:104:PHE:CE2	7:D:132:VAL:HB	2.55	0.42
13:K:22:ASP:O	13:K:110:LYS:HE3	2.20	0.42
15:M:24:GLN:O	15:M:28:GLN:HG3	2.19	0.42
20:R:72:VAL:CG1	20:R:75:TRP:HB3	2.49	0.42
23:U:37:GLU:O	23:U:40:ALA:HB3	2.20	0.42
1:O:764:C:H2'	1:O:765:G:O4'	2.20	0.42
1:O:2346:C:O2'	7:D:52:THR:HG21	2.19	0.42
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.45	0.42
5:B:277:GLU:N	5:B:278:PRO:CD	2.83	0.42
6:C:13:ASP:OD1	6:C:13:ASP:O	2.37	0.42
6:C:16:VAL:CG1	6:C:17:ASP:H	2.30	0.42
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.79	0.42
18:P:7:LYS:HD3	18:P:21:VAL:CG2	2.49	0.42
20:R:125:ARG:HG2	38:R:9344:HOH:O	2.19	0.42
25:W:38:THR:CG2	25:W:39:ASP:N	2.82	0.42
32:I:71:GLY:O	32:I:72:VAL:C	2.62	0.42
1:O:37:A:H2'	1:O:38:G:H8	1.84	0.42
1:O:67:A:H5''	1:O:69:A:C8	2.55	0.42
1:O:514:G:OP1	1:O:514:G:H2'	2.20	0.42
1:O:1151:G:OP1	10:G:63:ARG:NH1	2.53	0.42
1:O:2044:G:OP1	26:X:23:HIS:HE1	2.03	0.42
1:O:2524:G:H21	1:O:2526:C:H41	1.68	0.42
1:O:2761:A:H2'	38:O:5903:HOH:O	2.18	0.42
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.42
5:B:55:ASN:HB3	5:B:63:GLU:HA	2.01	0.42
5:B:84:LEU:HD13	5:B:84:LEU:C	2.44	0.42
7:D:66:GLY:O	7:D:67:ASP:HB3	2.18	0.42
7:D:99:ASP:CB	7:D:103:ASN:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:108:LEU:HD11	8:E:164:ASP:HB2	2.02	0.42
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.00	0.42
19:Q:93:ARG:HG3	19:Q:93:ARG:NH1	2.35	0.42
22:T:71:VAL:CG1	22:T:72:ILE:N	2.82	0.42
24:V:39:ALA:C	24:V:41:GLU:N	2.78	0.42
27:Y:144:ARG:NH2	38:Y:9407:HOH:O	2.51	0.42
28:Z:39:CYS:HA	28:Z:47:VAL:CG2	2.50	0.42
1:O:347:A:O2'	6:C:205:ARG:NH2	2.53	0.42
1:O:371:U:H2'	1:O:372:A:H8	1.84	0.42
1:O:783:C:OP1	4:A:180:LYS:HE3	2.19	0.42
1:O:820:G:O2'	1:O:856:G:H4'	2.19	0.42
1:O:1160:G:O2'	1:O:1190:G:H1'	2.19	0.42
1:O:1206:U:H2'	1:O:1207:A:O4'	2.19	0.42
1:O:1380:U:H5'	38:O:9533:HOH:O	2.20	0.42
1:O:1409:G:H5'	38:O:4024:HOH:O	2.19	0.42
1:O:1483:C:O2'	1:O:1484:G:H5'	2.19	0.42
1:O:1771:U:O2	28:Z:19:GLY:HA2	2.19	0.42
5:B:307:ARG:HH11	5:B:307:ARG:CG	2.33	0.42
7:D:88:LEU:O	7:D:90:LEU:N	2.53	0.42
12:J:39:VAL:CG1	12:J:107:ASN:HB2	2.50	0.42
16:N:42:HIS:CG	16:N:62:HIS:HE1	2.37	0.42
26:X:15:ARG:NH1	26:X:15:ARG:HB3	2.34	0.42
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.85	0.42
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.49	0.42
1:O:236:A:H8	1:O:236:A:OP1	2.03	0.42
1:O:1058:A:H2'	1:O:1060:C:C5'	2.48	0.42
1:O:1525:G:H5'	1:O:1526:A:OP2	2.20	0.42
1:O:1634:G:H2'	1:O:1635:U:C6	2.54	0.42
1:O:1881:A:OP1	4:A:199:HIS:HE1	2.02	0.42
4:A:109:GLU:HG2	4:A:116:GLY:H	1.83	0.42
4:A:130:THR:HG22	4:A:131:HIS:O	2.19	0.42
4:A:213:LYS:NZ	38:A:9357:HOH:O	2.52	0.42
6:C:237:GLU:HB2	38:C:9226:HOH:O	2.18	0.42
7:D:60:GLU:O	7:D:61:PHE:C	2.62	0.42
10:G:27:ILE:HD12	10:G:70:ALA:HB1	2.01	0.42
11:H:66:ARG:HD3	38:H:9179:HOH:O	2.19	0.42
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.84	0.42
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.45	0.42
26:X:30:MET:CE	26:X:58:ALA:HB3	2.44	0.42
26:X:36:HIS:CE1	26:X:40:HIS:CD2	3.08	0.42
32:I:99:ASP:O	32:I:100:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:42:C:H1'	38:0:4957:HOH:O	2.19	0.42
1:0:125:U:H2'	38:0:4064:HOH:O	2.18	0.42
1:0:164:G:O3'	14:L:30:ARG:HB2	2.20	0.42
1:0:475:G:OP1	6:C:73:LEU:CD2	2.68	0.42
1:0:645:U:O2	1:0:761:A:H2	2.03	0.42
1:0:1331:A:OP2	27:Y:142:SER:OG	2.34	0.42
1:0:1335:C:H2'	1:0:1336:U:C6	2.55	0.42
1:0:1697:G:O2'	1:0:1698:U:H5'	2.20	0.42
1:0:2105:C:H2'	1:0:2106:C:C6	2.54	0.42
1:0:2266:A:H2'	1:0:2267:G:C8	2.55	0.42
4:A:87:GLU:HB3	38:A:9415:HOH:O	2.20	0.42
5:B:329:TYR:HE2	23:U:15:PRO:HG2	1.81	0.42
6:C:27:ARG:HH11	6:C:27:ARG:CG	2.32	0.42
12:J:42:GLU:O	12:J:131:THR:HG23	2.20	0.42
13:K:24:THR:HB	13:K:64:MET:HE2	2.02	0.42
14:L:120:LEU:HD12	14:L:133:VAL:HG21	2.01	0.42
25:W:13:MET:CE	25:W:18:GLN:HA	2.45	0.42
32:I:129:VAL:HG13	32:I:139:ILE:CD1	2.49	0.42
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.20	0.42
1:0:700:A:C2	14:L:71:GLU:HG2	2.55	0.42
1:0:813:C:H2'	1:0:814:G:O4'	2.20	0.42
1:0:1184:C:O2'	1:0:1185:U:OP2	2.31	0.42
1:0:2837:U:H1'	5:B:307:ARG:HH12	1.85	0.42
5:B:280:VAL:HG22	5:B:333:GLU:O	2.19	0.42
9:F:99:THR:HA	38:F:3461:HOH:O	2.19	0.42
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.85	0.42
12:J:107:ASN:HD22	12:J:108:PRO:HD2	1.85	0.42
25:W:21:LEU:O	25:W:26:ILE:HG12	2.20	0.42
26:X:78:GLU:CG	26:X:79:GLU:N	2.82	0.42
27:Y:153:GLN:HG3	27:Y:160:LYS:O	2.20	0.42
1:0:704:C:H2'	1:0:705:C:H6	1.85	0.41
1:0:1181:A:N1	1:0:1192:A:O2'	2.50	0.41
1:0:1252:A:H2'	1:0:1253:C:O4'	2.19	0.41
1:0:2269:C:H2'	1:0:2270:G:C5'	2.50	0.41
1:0:2330:U:H4'	1:0:2331:C:OP1	2.20	0.41
4:A:65:ARG:C	4:A:66:ARG:HG3	2.45	0.41
8:E:4:GLU:HG2	8:E:48:VAL:HG22	2.02	0.41
11:H:166:SER:HB3	38:H:9143:HOH:O	2.20	0.41
12:J:77:GLY:O	12:J:78:ILE:C	2.60	0.41
16:N:73:ALA:HB2	16:N:163:PHE:CE2	2.55	0.41
20:R:61:GLN:CD	38:R:9342:HOH:O	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:82:GLU:O	20:R:86:LYS:HG3	2.20	0.41
30:2:19:SER:HB3	38:2:4479:HOH:O	2.20	0.41
1:0:39:G:H2'	1:0:40:C:O4'	2.20	0.41
1:0:401:C:H2'	1:0:402:U:C6	2.55	0.41
1:0:419:A:H1'	1:0:1921:A:C2	2.55	0.41
1:0:629:A:H2'	1:0:630:A:O4'	2.20	0.41
1:0:1046:G:N3	1:0:1082:A:H2	2.18	0.41
1:0:1453:G:N2	1:0:1675:C:C2	2.87	0.41
1:0:1921:A:C6	1:0:1922:A:C2	3.08	0.41
1:0:1948:G:O2'	1:0:1949:G:H5'	2.21	0.41
1:0:2028:U:H2'	1:0:2029:C:C6	2.55	0.41
1:0:2604:A:H5'	38:0:6052:HOH:O	2.19	0.41
1:0:2821:C:O2'	5:B:114:ASP:O	2.36	0.41
38:0:7650:HOH:O	4:A:211:LYS:NZ	2.51	0.41
4:A:48:ASP:HA	4:A:49:PRO:HD3	1.83	0.41
6:C:27:ARG:CG	6:C:27:ARG:NH1	2.83	0.41
6:C:54:LEU:HD23	6:C:79:ARG:HG3	2.01	0.41
6:C:140:VAL:CG1	6:C:141:SER:N	2.83	0.41
7:D:23:VAL:HG22	7:D:73:VAL:HB	2.02	0.41
7:D:95:THR:HG1	7:D:174:VAL:HG22	1.80	0.41
11:H:17:ARG:HD3	11:H:23:ILE:CD1	2.50	0.41
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.68	0.41
14:L:67:ARG:O	14:L:71:GLU:HG3	2.20	0.41
16:N:157:PRO:HA	38:N:9323:HOH:O	2.21	0.41
18:P:16:VAL:HG12	18:P:17:GLY:N	2.35	0.41
21:S:29:ASP:OD1	21:S:31:ARG:HG3	2.21	0.41
1:0:128:A:O2'	1:0:129:A:H5'	2.20	0.41
1:0:138:U:OP2	1:0:139:C:H5	2.03	0.41
1:0:1377:C:H6	1:0:1377:C:C5'	2.32	0.41
1:0:1398:G:O2'	1:0:1399:A:H5'	2.20	0.41
1:0:1701:A:H5''	1:0:1702:U:H3'	2.01	0.41
1:0:2363:G:O3'	19:Q:11:ARG:NH1	2.53	0.41
4:A:82:VAL:HG13	4:A:93:THR:HB	2.01	0.41
5:B:258:GLY:N	5:B:260:HIS:CE1	2.85	0.41
6:C:27:ARG:NH1	6:C:27:ARG:HG2	2.34	0.41
15:M:181:GLU:OE1	15:M:181:GLU:N	2.48	0.41
20:R:9:ASP:HA	20:R:10:PRO:HD2	1.92	0.41
22:T:43:ASN:ND2	22:T:108:ARG:CZ	2.83	0.41
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.35	0.41
29:1:53:LYS:HD3	29:1:53:LYS:HA	1.92	0.41
1:0:671:A:O2'	1:0:672:G:H2'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:932:U:H2'	1:0:933:C:C6	2.56	0.41
1:0:1023:C:O2'	1:0:1024:G:H5'	2.20	0.41
1:0:1333:U:H2'	1:0:1334:C:H6	1.85	0.41
1:0:1641:A:H2'	1:0:1642:A:C5'	2.45	0.41
1:0:2270:G:H4'	4:A:223:ARG:NH1	2.29	0.41
4:A:217:ARG:HG3	38:A:9325:HOH:O	2.20	0.41
5:B:119:HIS:O	5:B:121:PRO:HD3	2.20	0.41
5:B:270:ILE:O	5:B:271:ASP:HB2	2.19	0.41
7:D:151:ILE:HA	7:D:152:PRO:HD3	1.95	0.41
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.27	0.41
17:O:21:SER:OG	17:O:106:PRO:HB2	2.20	0.41
25:W:115:THR:HG23	38:W:5420:HOH:O	2.21	0.41
25:W:125:HIS:CD2	25:W:127:GLY:H	2.38	0.41
30:2:30:ASP:O	30:2:31:ARG:HB2	2.20	0.41
1:0:426:G:H2'	1:0:427:C:O4'	2.21	0.41
1:0:538:C:H5''	1:0:539:G:C8	2.55	0.41
1:0:870:G:C3'	1:0:871:G:H5''	2.50	0.41
1:0:1734:C:OP1	5:B:234:ARG:NH1	2.50	0.41
1:0:2269:C:H2'	1:0:2270:G:H5'	2.01	0.41
1:0:2401:A:H2'	1:0:2402:A:C8	2.55	0.41
1:0:2821:C:H4'	5:B:116:PRO:HG3	2.01	0.41
6:C:170:ASP:C	6:C:171:GLU:HG3	2.45	0.41
8:E:11:VAL:HG13	8:E:76:VAL:HG21	2.03	0.41
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.50	0.41
9:F:99:THR:O	9:F:100:ASP:HB2	2.19	0.41
13:K:75:ARG:HE	13:K:94:ALA:HB3	1.85	0.41
13:K:113:ILE:HG22	13:K:114:ALA:N	2.34	0.41
16:N:143:ARG:HH12	16:N:173:ASP:CG	2.28	0.41
16:N:183:ASP:O	16:N:184:ILE:O	2.38	0.41
25:W:122:ARG:NH1	25:W:122:ARG:CG	2.82	0.41
1:0:137:U:H2'	1:0:139:C:C5	2.56	0.41
1:0:470:U:O2'	29:1:16:HIS:CD2	2.69	0.41
1:0:485:A:O2'	1:0:487:G:H5'	2.21	0.41
1:0:820:G:H5'	1:0:821:U:H5'	2.03	0.41
1:0:946:C:H2'	1:0:947:U:H6	1.84	0.41
1:0:1080:C:O5'	1:0:1080:C:H6	2.04	0.41
1:0:1528:A:H62	1:0:1663:G:H21	1.67	0.41
1:0:2078:U:O2'	1:0:2079:G:H5'	2.21	0.41
1:0:2768:A:O2'	1:0:2769:C:H5'	2.21	0.41
1:0:2783:A:H2'	1:0:2784:A:C8	2.56	0.41
5:B:255:GLY:O	5:B:257:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.85	0.41
6:C:236:THR:HG22	6:C:239:ALA:CB	2.50	0.41
8:E:68:HIS:O	8:E:72:MET:HG3	2.20	0.41
9:F:26:THR:HB	9:F:102:GLY:HA3	2.03	0.41
12:J:42:GLU:HG2	12:J:43:ARG:HG3	2.03	0.41
16:N:101:VAL:HG12	38:N:9328:HOH:O	2.19	0.41
17:O:107:GLU:O	17:O:108:GLY:C	2.63	0.41
25:W:48:VAL:CG1	25:W:48:VAL:O	2.68	0.41
1:O:736:A:H2'	1:O:737:A:O4'	2.21	0.41
1:O:1185:U:H2'	1:O:1186:C:H6	1.84	0.41
1:O:1269:G:H2'	1:O:1270:U:C6	2.56	0.41
1:O:1391:G:H2'	1:O:1392:A:H5'	2.02	0.41
1:O:1744:G:H2'	1:O:1745:G:H5'	2.02	0.41
1:O:2377:U:H6	1:O:2377:U:O5'	2.03	0.41
1:O:2754:G:O2'	1:O:2755:G:H5'	2.21	0.41
5:B:16:ARG:HD3	38:B:9410:HOH:O	2.19	0.41
6:C:114:ALA:HB1	6:C:223:LEU:HB3	2.03	0.41
9:F:60:VAL:O	9:F:61:MET:C	2.63	0.41
19:Q:53:HIS:ND1	19:Q:55:ARG:HB2	2.36	0.41
1:O:821:U:H2'	1:O:822:C:C6	2.56	0.41
1:O:958:G:O2'	1:O:959:C:H5'	2.20	0.41
1:O:1016:U:O2'	1:O:2303:A:N7	2.49	0.41
1:O:1268:C:O2'	27:Y:169:ARG:HB2	2.20	0.41
1:O:1500:U:OP2	18:P:41:ARG:NH2	2.54	0.41
1:O:2353:A:H4'	1:O:2354:A:O5'	2.20	0.41
1:O:2413:A:H2'	1:O:2414:A:O4'	2.20	0.41
5:B:51:VAL:O	5:B:53:LEU:HD13	2.21	0.41
7:D:92:GLU:HB2	38:D:3862:HOH:O	2.19	0.41
11:H:9:ILE:O	11:H:9:ILE:HG22	2.20	0.41
11:H:95:LEU:HD11	11:H:124:ALA:HB2	2.03	0.41
16:N:29:SER:OG	16:N:101:VAL:HG21	2.20	0.41
18:P:16:VAL:CG1	18:P:17:GLY:N	2.84	0.41
24:V:1:THR:C	24:V:3:LEU:N	2.78	0.41
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.86	0.41
31:3:48:ASN:ND2	31:3:50:GLY:H	2.17	0.41
1:O:189:A:OP1	15:M:171:ARG:NH2	2.53	0.41
1:O:281:U:O2'	1:O:282:C:H5'	2.20	0.41
1:O:542:A:H2'	1:O:543:G:O4'	2.21	0.41
1:O:907:A:H2'	1:O:908:A:C8	2.54	0.41
1:O:926:A:C4'	14:L:39:GLU:HG2	2.51	0.41
1:O:1180:U:H4'	32:I:91:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1194:A:O2'	1:0:1195:G:H5'	2.21	0.41
1:0:1755:A:H2'	1:0:1756:G:O4'	2.20	0.41
1:0:2387:U:H2'	1:0:2388:C:C6	2.56	0.41
2:9:3060:C:O2'	2:9:3061:C:H5'	2.20	0.41
2:9:3107:C:H5	38:9:3167:HOH:O	2.03	0.41
2:9:3114:G:H2'	2:9:3115:C:C6	2.56	0.41
4:A:33:GLU:O	4:A:34:ASP:CB	2.61	0.41
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.86	0.41
5:B:199:TYR:CE2	5:B:268:ARG:HB2	2.56	0.41
5:B:224:LYS:HA	5:B:224:LYS:HD3	1.94	0.41
6:C:46:TYR:CE1	6:C:92:PRO:HB3	2.56	0.41
6:C:123:LEU:HD23	6:C:123:LEU:HA	1.94	0.41
6:C:133:ARG:HD2	38:C:9206:HOH:O	2.20	0.41
6:C:223:LEU:HD12	6:C:223:LEU:HA	1.94	0.41
7:D:102:GLY:C	7:D:103:ASN:HD22	2.28	0.41
7:D:105:SER:HB2	7:D:131:THR:HG23	2.01	0.41
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.24	0.41
11:H:38:LYS:O	11:H:84:LYS:HE2	2.21	0.41
11:H:146:VAL:HG22	38:H:9176:HOH:O	2.21	0.41
12:J:14:ALA:O	12:J:15:ARG:C	2.64	0.41
12:J:131:THR:HG22	12:J:133:GLY:N	2.35	0.41
14:L:34:GLY:C	14:L:36:ASP:N	2.78	0.41
15:M:47:ASP:CG	15:M:48:LYS:N	2.79	0.41
15:M:59:GLY:HA3	15:M:141:ILE:HD11	2.03	0.41
17:O:24:ALA:O	17:O:28:ASP:HB2	2.20	0.41
17:O:32:ARG:HH11	17:O:115:ARG:HH21	1.69	0.41
17:O:41:ALA:HA	38:O:5104:HOH:O	2.21	0.41
22:T:40:VAL:HG22	22:T:41:ARG:N	2.36	0.41
22:T:40:VAL:HG23	22:T:119:ALA:C	2.46	0.41
22:T:47:THR:HB	22:T:100:ASP:HB3	2.01	0.41
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.36	0.41
25:W:3:ALA:O	25:W:54:PHE:HA	2.21	0.41
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.50	0.41
27:Y:187:VAL:CG1	27:Y:205:ILE:HA	2.51	0.41
28:Z:67:GLY:N	28:Z:70:LYS:O	2.53	0.41
31:3:75:GLY:C	38:3:9374:HOH:O	2.64	0.41
32:I:92:PRO:C	32:I:94:GLU:N	2.70	0.41
32:I:113:HIS:N	32:I:114:PRO:CD	2.83	0.41
1:0:155:C:OP2	15:M:188:ARG:HD3	2.20	0.41
1:0:1173:A:H4'	1:0:1174:A:C8	2.56	0.41
1:0:1419:U:H2'	1:0:1685:A:C2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1477:C:O2'	1:0:1478:U:H5'	2.21	0.41
1:0:1773:G:N2	1:0:1774:G:C8	2.88	0.41
1:0:1976:G:O2'	1:0:1977:U:H5'	2.21	0.41
1:0:2265:U:H2'	1:0:2266:A:H8	1.86	0.41
1:0:2365:G:OP1	19:Q:15:LYS:HG3	2.21	0.41
7:D:10:PHE:CG	7:D:11:HIS:N	2.89	0.41
16:N:110:THR:HB	16:N:113:SER:HG	1.84	0.41
21:S:17:ASP:HB3	21:S:23:LYS:HB2	2.02	0.41
28:Z:13:ARG:NH1	38:Z:9218:HOH:O	2.53	0.41
32:I:78:LEU:HD13	32:I:108:ILE:HG23	2.03	0.41
1:0:228:C:H2'	1:0:229:G:H5'	2.03	0.40
1:0:380:A:C2	15:M:13:GLU:HB3	2.56	0.40
1:0:571:C:H6	1:0:571:C:O5'	2.03	0.40
1:0:732:C:O2'	1:0:733:U:H5'	2.21	0.40
1:0:1158:G:O2'	1:0:1159:G:H5'	2.21	0.40
1:0:1714:C:O2'	1:0:1715:C:H5'	2.21	0.40
1:0:1761:U:H5'	18:P:81:LYS:O	2.22	0.40
1:0:1789:G:O6	18:P:73:HIS:HE1	2.04	0.40
1:0:1933:G:O2'	1:0:1934:A:H5'	2.20	0.40
38:0:9988:HOH:O	6:C:214:THR:HB	2.20	0.40
2:9:3059:C:H5'	38:9:5233:HOH:O	2.21	0.40
4:A:165:THR:O	4:A:165:THR:CG2	2.69	0.40
4:A:211:LYS:HB2	38:A:9413:HOH:O	2.21	0.40
5:B:48:MET:HE3	5:B:299:GLY:O	2.21	0.40
7:D:55:LYS:HA	38:D:6752:HOH:O	2.21	0.40
7:D:57:THR:HG23	7:D:63:ILE:CA	2.42	0.40
7:D:68:PRO:C	7:D:69:ILE:HG13	2.47	0.40
13:K:44:LEU:HA	13:K:45:PRO:HD2	1.96	0.40
13:K:89:LYS:HA	38:K:7064:HOH:O	2.21	0.40
15:M:9:ARG:HB2	15:M:47:ASP:OD2	2.20	0.40
15:M:134:ILE:O	15:M:136:PRO:HD3	2.21	0.40
16:N:181:ASP:O	16:N:184:ILE:HG22	2.21	0.40
22:T:47:THR:HG22	22:T:99:THR:OG1	2.21	0.40
25:W:72:PRO:CG	25:W:77:ALA:HB3	2.39	0.40
1:0:1311:G:O6	6:C:173:LYS:HE3	2.22	0.40
1:0:1513:C:O2'	1:0:1514:C:H5'	2.21	0.40
1:0:1562:C:N4	38:0:6128:HOH:O	2.55	0.40
1:0:1643:C:O2'	1:0:1644:C:H5'	2.22	0.40
1:0:1741:U:H3'	38:0:3074:HOH:O	2.21	0.40
1:0:1855:G:H4'	1:0:1856:C:O5'	2.21	0.40
1:0:1943:C:H5''	4:A:209:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1996:U:O2'	1:0:1997:A:H5'	2.21	0.40
1:0:2619:UR3:H5'	3:4:76:5AA:H103	2.03	0.40
1:0:2740:G:H2'	1:0:2741:A:O4'	2.21	0.40
38:0:7751:HOH:O	5:B:2:GLN:HG3	2.21	0.40
5:B:80:ARG:HA	5:B:186:GLY:O	2.21	0.40
5:B:171:VAL:HG23	5:B:172:SER:N	2.35	0.40
6:C:187:ARG:NH2	38:C:9162:HOH:O	2.51	0.40
14:L:89:PHE:CD1	14:L:89:PHE:N	2.89	0.40
26:X:26:ALA:HB1	26:X:59:TRP:CE2	2.56	0.40
32:I:77:GLU:C	32:I:79:ILE:N	2.78	0.40
32:I:119:TYR:N	32:I:119:TYR:CD1	2.89	0.40
1:0:291:C:H2'	1:0:292:G:O4'	2.21	0.40
1:0:646:G:H2'	1:0:647:U:C6	2.56	0.40
1:0:790:A:H1'	1:0:1710:A:O2'	2.22	0.40
1:0:949:U:O2'	19:Q:40:HIS:HE1	2.03	0.40
1:0:1167:G:H4'	32:I:135:LEU:CD2	2.51	0.40
1:0:1434:A:H2'	1:0:1436:C:C5	2.56	0.40
1:0:1631:A:H2'	1:0:1632:A:C8	2.56	0.40
1:0:2050:G:OP1	20:R:79:ARG:HB3	2.21	0.40
1:0:2115:U:H2'	1:0:2116:U:C6	2.56	0.40
1:0:2266:A:OP2	15:M:90:ARG:NH2	2.52	0.40
1:0:2379:G:N7	1:0:2408:A:N1	2.70	0.40
2:9:3029:C:H2'	2:9:3030:C:C5'	2.45	0.40
5:B:205:VAL:O	5:B:307:ARG:NE	2.54	0.40
6:C:118:THR:O	6:C:136:VAL:HG13	2.21	0.40
7:D:75:LEU:HD22	7:D:79:MET:HB3	2.02	0.40
8:E:144:THR:O	8:E:148:ILE:HG13	2.21	0.40
9:F:99:THR:HG23	9:F:99:THR:O	2.21	0.40
11:H:26:SER:HA	11:H:59:HIS:HD2	1.85	0.40
11:H:54:THR:HA	11:H:127:VAL:O	2.22	0.40
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.95	0.40
14:L:122:ALA:HB3	14:L:125:PHE:CZ	2.56	0.40
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.57	0.40
23:U:39:ASN:HD22	23:U:44:ARG:HH11	1.68	0.40
25:W:48:VAL:O	25:W:48:VAL:HG12	2.21	0.40
25:W:125:HIS:HE1	38:W:3071:HOH:O	2.05	0.40
1:0:549:A:O2'	1:0:550:C:H5'	2.21	0.40
1:0:1167:G:H3'	38:0:7702:HOH:O	2.20	0.40
1:0:1624:A:H4'	1:0:1626:A:H5''	2.03	0.40
1:0:1744:G:C2'	1:0:1745:G:H5'	2.51	0.40
1:0:1805:G:O2'	1:0:1806:G:H5'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2314:G:O2'	1:0:2315:C:H5'	2.22	0.40
1:0:2776:A:H2'	1:0:2777:G:O4'	2.20	0.40
2:9:3012:C:H5'	2:9:3070:U:O4'	2.21	0.40
4:A:186:TRP:CD1	4:A:187:PRO:HA	2.56	0.40
5:B:33:ASP:HB3	5:B:34:GLY:H	1.57	0.40
5:B:183:GLU:OE1	5:B:183:GLU:HA	2.21	0.40
7:D:19:GLU:HG3	38:D:6165:HOH:O	2.21	0.40
7:D:64:ARG:HG2	7:D:67:ASP:HB3	2.04	0.40
7:D:99:ASP:HB2	7:D:103:ASN:HB2	2.04	0.40
14:L:17:SER:C	14:L:19:LYS:H	2.28	0.40
14:L:53:ARG:NH2	14:L:57:VAL:CG1	2.84	0.40
14:L:68:GLU:HG3	38:L:9342:HOH:O	2.22	0.40
14:L:126:SER:O	14:L:127:GLU:C	2.64	0.40
16:N:152:GLU:C	16:N:154:LEU:N	2.73	0.40
18:P:115:SER:O	18:P:116:SER:C	2.65	0.40
20:R:69:LYS:HE2	20:R:78:GLY:O	2.21	0.40
20:R:132:ARG:NH1	38:R:9383:HOH:O	2.54	0.40
22:T:37:GLN:OE1	22:T:118:SER:HA	2.21	0.40
24:V:59:ILE:O	24:V:63:GLU:HG2	2.21	0.40
25:W:73:LEU:HA	25:W:73:LEU:HD12	1.74	0.40
25:W:137:GLN:HG3	25:W:137:GLN:O	2.21	0.40
32:I:74:PRO:HG2	32:I:77:GLU:CD	2.46	0.40
1:0:56:G:C5'	24:V:50:ARG:HH12	2.27	0.40
1:0:2093:G:H5''	38:B:9327:HOH:O	2.21	0.40
1:0:2515:C:H2'	1:0:2516:G:O4'	2.21	0.40
1:0:2659:U:H4'	20:R:76:ASP:HB3	2.03	0.40
38:O:9429:HOH:O	6:C:103:ASN:HB3	2.20	0.40
5:B:115:VAL:HA	5:B:116:PRO:HD3	1.88	0.40
6:C:80:VAL:HA	6:C:81:PRO:HD3	1.95	0.40
6:C:173:LYS:O	6:C:186:TYR:HA	2.22	0.40
7:D:12:GLU:HA	7:D:15:GLU:CD	2.46	0.40
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.51	0.40
12:J:11:ILE:HD11	12:J:109:TYR:CD2	2.57	0.40
12:J:107:ASN:HD22	12:J:109:TYR:H	1.64	0.40
15:M:40:ILE:HG21	15:M:64:ARG:NH2	2.36	0.40
15:M:69:LYS:HG3	15:M:126:GLN:CA	2.52	0.40
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.04	0.40
16:N:138:ASP:O	16:N:139:TRP:C	2.64	0.40
22:T:24:ARG:HH21	22:T:39:ASN:ND2	2.14	0.40
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.18	0.40
27:Y:144:ARG:NH1	38:Y:9373:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:28:HIS:CD2	29:1:31:LYS:H	2.39	0.40
30:2:40:ARG:HG2	30:2:40:ARG:NH1	2.37	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3020:G:OP1	5:B:195:ARG:NH2[7_545]	1.98	0.22
1:0:1171:A:N3	1:0:1964:U:O5'[3_655]	2.13	0.07
13:K:63:GLU:CB	13:K:63:GLU:CB[3_655]	2.13	0.07

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	206 (88%)	24 (10%)	5 (2%)	5	11
5	B	335/338 (99%)	294 (88%)	35 (10%)	6 (2%)	6	14
6	C	244/246 (99%)	217 (89%)	26 (11%)	1 (0%)	30	51
7	D	134/177 (76%)	97 (72%)	25 (19%)	12 (9%)	0	0
8	E	170/178 (96%)	156 (92%)	13 (8%)	1 (1%)	21	42
9	F	117/120 (98%)	106 (91%)	7 (6%)	4 (3%)	3	4
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
11	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	6	13
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	9	19
13	K	130/132 (98%)	119 (92%)	8 (6%)	3 (2%)	5	9
14	L	141/165 (86%)	120 (85%)	19 (14%)	2 (1%)	9	19
15	M	192/194 (99%)	178 (93%)	14 (7%)	0	100	100
16	N	184/187 (98%)	167 (91%)	11 (6%)	6 (3%)	3	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	O	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	14	30
18	P	141/149 (95%)	135 (96%)	6 (4%)	0	100	100
19	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	R	148/155 (96%)	138 (93%)	8 (5%)	2 (1%)	9	19
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	107 (92%)	10 (8%)	0	100	100
23	U	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	6	12
24	V	63/71 (89%)	55 (87%)	6 (10%)	2 (3%)	3	5
25	W	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	18	38
26	X	80/92 (87%)	70 (88%)	8 (10%)	2 (2%)	4	8
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	1	1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	88 (98%)	0	2 (2%)	5	10
32	I	68/162 (42%)	51 (75%)	17 (25%)	0	100	100
All	All	3705/4430 (84%)	3350 (90%)	295 (8%)	60 (2%)	7	16

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	34	ASP
4	A	132	ASP
9	F	101	ALA
11	H	168	ALA
12	J	5	GLU
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG
4	A	37	VAL
5	B	34	GLY
5	B	169	GLY
6	C	8	LEU
7	D	65	GLU
7	D	137	PRO
7	D	173	GLU

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Mol	Chain	Res	Type
9	F	44	SER
11	H	166	SER
24	V	43	PRO
5	B	107	SER
7	D	86	THR
11	H	140	VAL
13	K	126	SER
14	L	80	ASP
14	L	143	THR
16	N	113	SER
16	N	164	ASP
23	U	7	ASP
26	X	78	GLU
28	Z	42	CYS
5	B	185	GLY
7	D	171	ASP
8	E	44	GLY
9	F	61	MET
9	F	64	PRO
12	J	143	LYS
16	N	167	ASP
26	X	70	ILE
31	3	56	PRO
5	B	2	GLN
7	D	89	PRO
16	N	160	SER
25	W	49	ASN
28	Z	20	ARG
31	3	57	GLY
7	D	16	PRO
7	D	97	GLN
28	Z	43	GLY
4	A	211	LYS
4	A	236	GLY
7	D	28	GLY
24	V	40	PRO
7	D	27	ILE
17	O	108	GLY
20	R	106	GLY
7	D	69	ILE
7	D	135	VAL
13	K	39	GLY

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Mol	Chain	Res	Type
20	R	81	PRO
5	B	30	PRO
13	K	111	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	169 (94%)	10 (6%)	19	40
5	B	282/283 (100%)	263 (93%)	19 (7%)	15	33
6	C	193/193 (100%)	176 (91%)	17 (9%)	9	21
7	D	117/148 (79%)	114 (97%)	3 (3%)	40	68
8	E	152/156 (97%)	148 (97%)	4 (3%)	40	68
9	F	93/94 (99%)	91 (98%)	2 (2%)	45	72
10	G	27/283 (10%)	25 (93%)	2 (7%)	13	29
11	H	132/138 (96%)	124 (94%)	8 (6%)	17	37
12	J	118/121 (98%)	111 (94%)	7 (6%)	18	38
13	K	106/106 (100%)	101 (95%)	5 (5%)	23	48
14	L	113/127 (89%)	108 (96%)	5 (4%)	25	50
15	M	158/158 (100%)	151 (96%)	7 (4%)	25	50
16	N	149/150 (99%)	141 (95%)	8 (5%)	20	42
17	O	93/94 (99%)	89 (96%)	4 (4%)	26	51
18	P	113/117 (97%)	109 (96%)	4 (4%)	32	59
19	Q	79/80 (99%)	75 (95%)	4 (5%)	21	45
20	R	117/122 (96%)	114 (97%)	3 (3%)	40	68
21	S	71/74 (96%)	70 (99%)	1 (1%)	59	81
22	T	105/106 (99%)	99 (94%)	6 (6%)	18	40
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	28	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	W	130/130 (100%)	122 (94%)	8 (6%)	16	36
26	X	66/74 (89%)	61 (92%)	5 (8%)	12	27
27	Y	120/196 (61%)	112 (93%)	8 (7%)	15	33
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	45 (98%)	1 (2%)	45	72
30	2	42/46 (91%)	42 (100%)	0	100	100
31	3	79/79 (100%)	77 (98%)	2 (2%)	42	69
32	I	58/130 (45%)	57 (98%)	1 (2%)	53	78
All	All	3093/3611 (86%)	2947 (95%)	146 (5%)	23	48

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU
4	A	36	ASP
4	A	69	LEU
4	A	84	VAL
4	A	94	LEU
4	A	153	ARG
4	A	175	LYS
4	A	179	MET
4	A	217	ARG
5	B	5	ARG
5	B	7	ARG
5	B	11	LEU
5	B	20	THR
5	B	27	ASN
5	B	33	ASP
5	B	49	THR
5	B	63	GLU
5	B	98	THR
5	B	149	ASP
5	B	162	MET
5	B	190	MET
5	B	251	VAL
5	B	254	GLN
5	B	256	GLN
5	B	280	VAL

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Mol	Chain	Res	Type
5	B	304	PRO
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	27	ARG
6	C	67	GLN
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	106	GLU
6	C	115	LEU
6	C	136	VAL
6	C	187	ARG
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	246	ARG
7	D	24	HIS
7	D	86	THR
7	D	136	ARG
8	E	15	GLN
8	E	86	VAL
8	E	102	VAL
8	E	126	ILE
9	F	78	GLU
9	F	105	ASP
10	G	12	ILE
10	G	64	ASN
11	H	18	GLU
11	H	30	GLN
11	H	84	LYS
11	H	88	ARG
11	H	96	ARG
11	H	111	ASP
11	H	154	TYR
11	H	170	ASN
12	J	46	ILE
12	J	47	THR
12	J	52	GLN

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Mol	Chain	Res	Type
12	J	74	ARG
12	J	76	ASP
12	J	93	ARG
12	J	131	THR
13	K	7	ASP
13	K	10	GLN
13	K	49	LEU
13	K	98	VAL
13	K	129	THR
14	L	4	LYS
14	L	35	ARG
14	L	99	GLU
14	L	104	ASP
14	L	140	VAL
15	M	46	LEU
15	M	74	LYS
15	M	84	LYS
15	M	93	ARG
15	M	99	ARG
15	M	130	GLU
15	M	164	THR
16	N	17	ARG
16	N	26	LEU
16	N	47	LEU
16	N	50	LEU
16	N	93	GLN
16	N	101	VAL
16	N	139	TRP
16	N	152	GLU
17	O	3	THR
17	O	43	VAL
17	O	111	VAL
17	O	115	ARG
18	P	21	VAL
18	P	52	LYS
18	P	91	LYS
18	P	98	ILE
19	Q	11	ARG
19	Q	30	VAL
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR

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Mol	Chain	Res	Type
20	R	39	THR
20	R	82	GLU
21	S	10	VAL
22	T	39	ASN
22	T	47	THR
22	T	48	VAL
22	T	96	VAL
22	T	112	LEU
22	T	115	GLU
24	V	43	PRO
24	V	65	ASP
25	W	35	VAL
25	W	52	VAL
25	W	73	LEU
25	W	88	THR
25	W	122	ARG
25	W	146	ILE
25	W	151	GLU
25	W	154	ARG
26	X	15	ARG
26	X	49	ARG
26	X	72	VAL
26	X	79	GLU
26	X	85	VAL
27	Y	141	THR
27	Y	144	ARG
27	Y	163	THR
27	Y	174	VAL
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	235	GLU
29	1	25	LYS
31	3	42	ARG
31	3	56	PRO
32	I	86	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	29	HIS
4	A	199	HIS

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Mol	Chain	Res	Type
5	B	27	ASN
5	B	94	GLN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	67	GLN
6	C	129	HIS
6	C	163	HIS
6	C	178	GLN
7	D	47	GLN
7	D	97	GLN
7	D	103	ASN
7	D	133	ASN
8	E	71	ASN
8	E	90	HIS
8	E	106	ASN
8	E	143	GLN
9	F	55	GLN
10	G	64	ASN
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	72	HIS
11	H	128	GLN
11	H	132	GLN
11	H	145	HIS
11	H	170	ASN
12	J	25	GLN
12	J	29	GLN
12	J	52	GLN
12	J	107	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
15	M	24	GLN
15	M	26	GLN

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Mol	Chain	Res	Type
15	M	58	GLN
15	M	129	HIS
15	M	143	ASN
15	M	170	ASN
16	N	22	GLN
16	N	53	ASN
16	N	93	GLN
16	N	107	ASN
16	N	153	GLN
18	P	28	GLN
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
19	Q	59	GLN
20	R	22	GLN
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
20	R	122	GLN
21	S	16	ASN
21	S	25	GLN
21	S	53	ASN
21	S	55	GLN
22	T	11	GLN
22	T	39	ASN
22	T	43	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	4	HIS
24	V	29	ASN
24	V	60	GLN
25	W	2	HIS
25	W	27	HIS
25	W	110	GLN
25	W	119	HIS
25	W	141	HIS

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Mol	Chain	Res	Type
26	X	23	HIS
27	Y	119	GLN
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN
28	Z	37	HIS
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	45	ASN
31	3	2	GLN
31	3	30	GLN
31	3	39	GLN
31	3	48	ASN
32	I	93	GLN
32	I	104	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	245 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	0/8	-	-
All	All	2866/3052 (93%)	260 (9%)	33 (1%)

All (260) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	70	A
1	0	71	G
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A

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Mol	Chain	Res	Type
1	0	130	C
1	0	139	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	170	U
1	0	185	G
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	285	A
1	0	308	U
1	0	309	C
1	0	318	C
1	0	331	A
1	0	336	G
1	0	337	A
1	0	345	G
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	461	C
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G

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Mol	Chain	Res	Type
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A

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Mol	Chain	Res	Type
1	0	1088	A
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1131	G
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1234	U
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1451	C
1	0	1474	C
1	0	1485	A
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1559	A
1	0	1564	C
1	0	1592	G
1	0	1603	A

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Mol	Chain	Res	Type
1	0	1625	U
1	0	1626	A
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	1701	A
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1943	C
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1996	U
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

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Mol	Chain	Res	Type
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
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	2291	A
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
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
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	2637	A
1	0	2645	U
1	0	2649	A
1	0	2650	U

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Mol	Chain	Res	Type
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	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
1	0	2864	U
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	129	A
1	0	169	A
1	0	338	C
1	0	603	A
1	0	699	C
1	0	834	G
1	0	857	A
1	0	869	G
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1450	C
1	0	1563	G
1	0	1667	A
1	0	1692	C
1	0	1856	C
1	0	1942	A
1	0	2011	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2541	U
1	0	2637	A
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2791	U
2	9	3065	A

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

7 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	DCZ	4	74	3	17,17,17	0.30	0	24,24,24	0.28	0
1	PSU	0	2621	1	18,21,22	1.59	2 (11%)	21,30,33	1.39	3 (14%)
1	1MA	0	628	1	21,25,26	0.77	1 (4%)	30,37,40	0.81	1 (3%)
1	OMU	0	2587	1,35	19,22,23	0.22	0	25,31,34	0.37	0
1	UR3	0	2619	1	19,22,23	0.33	0	26,32,35	0.67	1 (3%)
1	OMG	0	2588	1,3	23,26,27	0.33	0	32,38,41	0.33	0
3	5AA	4	76	1,3	23,26,27	0.27	0	29,38,41	0.79	1 (3%)

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	DCZ	4	74	3	-	0/6/18/18	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	2/7/25/26	0/3/3/3
1	OMU	0	2587	1,35	-	0/9/27/28	0/2/2/2
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1,3	-	0/9/27/28	0/3/3/3
3	5AA	4	76	1,3	-	0/11/29/30	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.20	1.43	1.36
1	0	2621	PSU	C6-C5	3.27	1.38	1.35
1	0	628	1MA	C6-N6	2.73	1.34	1.28

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.49	120.53	118.17
1	0	2621	PSU	C6-N1-C2	-3.39	119.54	122.69
1	0	628	1MA	N1-C2-N3	2.88	129.42	126.00
3	4	76	5AA	C2-N1-C6	2.87	118.83	111.83
1	0	2621	PSU	O2-C2-N1	2.72	125.59	122.79
1	0	2619	UR3	C4-N3-C2	2.66	126.72	124.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	4	74	DCZ	3	0
1	0	2587	OMU	2	0
1	0	2619	UR3	2	0
3	4	76	5AA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 234 ligands modelled in this entry, 234 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%)	1.01	449 (16%) 4 3	24, 51, 98, 161	0
2	9	122/122 (100%)	1.45	17 (13%) 6 5	46, 68, 96, 153	0
3	4	4/8 (50%)	0.76	0 100 100	42, 42, 46, 46	0
4	A	237/240 (98%)	0.86	18 (7%) 20 16	31, 55, 94, 120	0
5	B	337/338 (99%)	2.02	157 (46%) 0 0	33, 65, 94, 103	0
6	C	246/246 (100%)	0.69	11 (4%) 38 32	26, 51, 75, 86	0
7	D	140/177 (79%)	2.27	71 (50%) 0 0	64, 110, 134, 141	0
8	E	172/178 (96%)	2.56	116 (67%) 0 0	50, 81, 105, 115	0
9	F	119/120 (99%)	1.12	14 (11%) 9 7	57, 81, 107, 122	0
10	G	29/348 (8%)	2.57	20 (68%) 0 0	74, 95, 105, 107	0
11	H	160/171 (93%)	1.69	49 (30%) 1 1	42, 63, 94, 101	0
12	J	142/145 (97%)	1.85	52 (36%) 1 0	42, 59, 82, 97	0
13	K	132/132 (100%)	2.09	66 (50%) 0 0	37, 62, 86, 90	0
14	L	145/165 (87%)	1.22	33 (22%) 2 2	28, 74, 118, 131	0
15	M	194/194 (100%)	0.39	2 (1%) 79 76	33, 48, 64, 72	0
16	N	186/187 (99%)	1.43	40 (21%) 2 2	43, 69, 118, 124	0
17	O	115/116 (99%)	1.05	16 (13%) 6 5	43, 61, 79, 89	0
18	P	143/149 (95%)	1.25	21 (14%) 6 4	46, 62, 75, 81	0
19	Q	95/96 (98%)	1.07	12 (12%) 8 6	40, 50, 66, 77	0
20	R	150/155 (96%)	0.91	10 (6%) 24 19	36, 51, 72, 82	0
21	S	81/85 (95%)	0.85	5 (6%) 26 21	48, 65, 85, 94	0
22	T	119/120 (99%)	0.80	6 (5%) 34 28	44, 61, 90, 111	0
23	U	53/66 (80%)	1.76	17 (32%) 1 1	48, 63, 80, 88	0
24	V	65/71 (91%)	1.45	17 (26%) 1 1	59, 83, 117, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	1.32	25 (16%) 4 3	41, 57, 78, 88	0
26	X	82/92 (89%)	1.43	15 (18%) 3 3	49, 66, 89, 106	0
27	Y	142/241 (58%)	1.02	13 (9%) 14 11	32, 51, 74, 95	0
28	Z	73/83 (87%)	1.32	13 (17%) 4 3	45, 64, 78, 96	0
29	1	56/57 (98%)	0.30	1 (1%) 67 63	31, 38, 46, 61	0
30	2	46/50 (92%)	1.73	14 (30%) 1 1	40, 70, 123, 128	0
31	3	92/92 (100%)	0.84	7 (7%) 20 16	37, 60, 74, 89	0
32	I	70/162 (43%)	3.14	56 (80%) 0 0	108, 129, 152, 155	0
All	All	6650/7482 (88%)	1.22	1363 (20%) 2 2	24, 58, 109, 161	0

All (1363) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	133	THR	8.6
24	V	1	THR	6.4
7	D	10	PHE	6.3
16	N	168	LEU	6.2
32	I	132	CYS	5.9
1	0	10	U	5.8
8	E	102	VAL	5.7
7	D	135	VAL	5.6
2	9	3001	U	5.6
8	E	83	GLY	5.4
1	0	138	U	5.3
30	2	38	LYS	5.3
24	V	43	PRO	5.2
7	D	134	LEU	5.2
32	I	137	VAL	5.2
8	E	22	VAL	5.2
1	0	1190	G	5.1
30	2	43	ARG	5.0
7	D	44	ILE	5.0
5	B	196	ALA	4.9
28	Z	59	TYR	4.9
32	I	125	ALA	4.9
30	2	49	GLU	4.9
8	E	82	TYR	4.8
32	I	118	SER	4.8
1	0	1175	G	4.8

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Mol	Chain	Res	Type	RSRZ
7	D	17	ARG	4.8
24	V	39	ALA	4.7
7	D	172	VAL	4.7
32	I	85	PHE	4.7
1	0	2797	C	4.7
30	2	47	THR	4.7
30	2	48	ASP	4.7
32	I	121	LEU	4.7
32	I	117	LEU	4.6
7	D	11	HIS	4.6
32	I	90	GLY	4.6
1	0	1173	A	4.6
7	D	104	PHE	4.5
1	0	1185	U	4.5
1	0	2786	G	4.5
8	E	145	ALA	4.5
5	B	73	VAL	4.5
7	D	88	LEU	4.5
5	B	98	THR	4.5
30	2	37	HIS	4.5
8	E	10	ASP	4.5
8	E	95	VAL	4.5
32	I	93	GLN	4.4
10	G	23	ILE	4.4
16	N	1	ALA	4.4
8	E	11	VAL	4.4
1	0	1176	C	4.4
32	I	78	LEU	4.3
8	E	126	ILE	4.3
32	I	108	ILE	4.3
7	D	106	PHE	4.3
8	E	144	THR	4.3
30	2	42	TRP	4.3
32	I	135	LEU	4.3
14	L	82	ALA	4.3
12	J	57	TYR	4.3
13	K	132	VAL	4.3
26	X	85	VAL	4.3
8	E	134	SER	4.3
7	D	55	LYS	4.2
16	N	158	LEU	4.2
7	D	107	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
32	I	128	VAL	4.2
5	B	112	THR	4.2
1	0	2004	U	4.2
2	9	3002	U	4.2
12	J	48	GLY	4.2
10	G	27	ILE	4.2
32	I	139	ILE	4.2
11	H	40	ALA	4.1
5	B	93	GLY	4.1
1	0	1188	A	4.1
1	0	2692	G	4.1
8	E	104	ILE	4.1
5	B	296	LEU	4.1
1	0	2567	G	4.1
32	I	106	LYS	4.1
8	E	29	VAL	4.1
32	I	129	VAL	4.1
13	K	47	ALA	4.0
5	B	283	GLY	4.0
1	0	2768	A	4.0
8	E	67	SER	4.0
32	I	116	LEU	4.0
8	E	111	LYS	4.0
8	E	138	ILE	4.0
11	H	47	ILE	4.0
18	P	114	LEU	4.0
10	G	64	ASN	4.0
4	A	37	VAL	4.0
24	V	2	VAL	4.0
13	K	3	ALA	4.0
32	I	119	TYR	4.0
8	E	100	ASP	4.0
5	B	71	VAL	4.0
1	0	1130	U	4.0
28	Z	82	SER	3.9
4	A	237	GLY	3.9
8	E	135	GLY	3.9
32	I	89	SER	3.9
8	E	80	TRP	3.9
1	0	1184	C	3.9
5	B	336	GLN	3.9
1	0	1121	G	3.9

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Mol	Chain	Res	Type	RSRZ
8	E	45	ASP	3.9
12	J	47	THR	3.9
24	V	40	PRO	3.9
32	I	131	THR	3.9
32	I	138	THR	3.8
5	B	86	ALA	3.8
23	U	51	TRP	3.8
1	0	2793	A	3.8
28	Z	10	ARG	3.8
5	B	61	PRO	3.8
10	G	20	VAL	3.8
1	0	2558	G	3.8
1	0	2574	G	3.8
1	0	2576	A	3.8
27	Y	141	THR	3.8
1	0	2693	U	3.8
7	D	128	LEU	3.8
10	G	67	LEU	3.8
12	J	105	LEU	3.8
1	0	960	G	3.7
7	D	63	ILE	3.7
11	H	68	SER	3.7
18	P	58	SER	3.7
1	0	735	C	3.7
5	B	51	VAL	3.7
1	0	1525	G	3.7
1	0	2344	G	3.7
1	0	2790	C	3.7
16	N	154	LEU	3.7
18	P	77	ALA	3.7
32	I	76	ALA	3.7
32	I	112	LYS	3.7
2	9	3024	U	3.7
1	0	2254	G	3.7
1	0	2585	G	3.7
28	Z	20	ARG	3.7
7	D	35	ALA	3.7
5	B	74	ILE	3.6
1	0	1165	G	3.6
1	0	2501	G	3.6
30	2	44	ARG	3.6
8	E	56	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
16	N	81	ALA	3.6
8	E	59	MET	3.6
8	E	162	PHE	3.6
1	0	2684	A	3.6
13	K	111	GLY	3.6
1	0	1160	G	3.6
1	0	1204	C	3.6
8	E	172	PRO	3.6
8	E	42	VAL	3.6
14	L	140	VAL	3.6
8	E	108	LEU	3.6
10	G	71	LEU	3.6
11	H	73	LEU	3.6
30	2	41	HIS	3.6
10	G	63	ARG	3.6
8	E	156	ASP	3.6
2	9	3023	U	3.6
5	B	337	GLY	3.6
1	0	1186	C	3.6
1	0	1167	G	3.6
32	I	114	PRO	3.6
1	0	1171	A	3.6
11	H	150	PHE	3.6
1	0	2565	C	3.5
13	K	15	GLY	3.5
5	B	97	LEU	3.5
5	B	119	HIS	3.5
8	E	119	HIS	3.5
1	0	1118	A	3.5
1	0	1189	A	3.5
1	0	2568	A	3.5
32	I	75	THR	3.5
14	L	102	ASP	3.5
5	B	138	GLY	3.5
5	B	314	ALA	3.5
8	E	13	ALA	3.5
16	N	169	PRO	3.5
1	0	1210	G	3.5
1	0	2579	G	3.5
1	0	2584	G	3.5
8	E	124	VAL	3.5
1	0	2577	A	3.5

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Mol	Chain	Res	Type	RSRZ
8	E	122	THR	3.5
13	K	86	THR	3.5
5	B	83	ALA	3.5
13	K	71	ALA	3.5
7	D	84	LEU	3.5
1	0	2686	C	3.5
1	0	2769	C	3.5
1	0	1143	G	3.5
1	0	2570	G	3.5
1	0	2566	A	3.5
11	H	111	ASP	3.5
8	E	97	VAL	3.5
25	W	79	VAL	3.5
32	I	72	VAL	3.5
32	I	79	ILE	3.4
1	0	1102	C	3.4
1	0	2502	C	3.4
1	0	2720	C	3.4
1	0	1162	G	3.4
1	0	1230	A	3.4
9	F	91	VAL	3.4
12	J	45	VAL	3.4
11	H	83	TYR	3.4
1	0	2575	C	3.4
13	K	92	ASP	3.4
1	0	1561	U	3.4
5	B	161	VAL	3.4
8	E	40	VAL	3.4
1	0	1163	G	3.4
11	H	112	GLY	3.4
32	I	124	ALA	3.4
5	B	266	ASN	3.4
6	C	101	ASP	3.4
1	0	1212	C	3.4
1	0	2787	C	3.4
7	D	21	VAL	3.4
7	D	174	VAL	3.4
1	0	1172	G	3.4
1	0	1809	G	3.4
1	0	2798	G	3.4
1	0	2503	A	3.4
1	0	2513	A	3.4

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Mol	Chain	Res	Type	RSRZ
7	D	89	PRO	3.4
12	J	4	ALA	3.4
13	K	5	GLY	3.4
8	E	158	ASP	3.4
14	L	124	ASP	3.4
7	D	58	VAL	3.4
8	E	48	VAL	3.4
13	K	46	LYS	3.3
1	0	1209	C	3.3
1	0	2695	C	3.3
5	B	70	PRO	3.3
1	0	1152	A	3.3
1	0	2691	A	3.3
1	0	2702	A	3.3
11	H	69	ALA	3.3
5	B	27	ASN	3.3
32	I	105	VAL	3.3
13	K	131	ILE	3.3
1	0	1187	U	3.3
8	E	35	TYR	3.3
5	B	163	GLU	3.3
13	K	83	PRO	3.3
14	L	130	ARG	3.3
32	I	73	PRO	3.3
19	Q	20	ASP	3.3
1	0	1161	A	3.3
1	0	1246	A	3.3
1	0	2506	A	3.3
1	0	2852	A	3.3
8	E	118	ILE	3.3
7	D	131	THR	3.3
5	B	155	PRO	3.3
8	E	155	ASN	3.3
13	K	98	VAL	3.3
13	K	113	ILE	3.3
10	G	15	TRP	3.3
1	0	1155	G	3.3
1	0	1211	G	3.3
1	0	1730	G	3.3
1	0	2771	G	3.3
1	0	1169	U	3.3
8	E	73	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
7	D	18	ILE	3.3
13	K	96	VAL	3.3
1	0	2556	C	3.2
1	0	2560	C	3.2
1	0	2345	A	3.2
1	0	2599	A	3.2
1	0	2694	A	3.2
1	0	2890	A	3.2
5	B	113	LEU	3.2
5	B	142	LEU	3.2
8	E	132	THR	3.2
12	J	113	GLY	3.2
26	X	74	ALA	3.2
1	0	2249	G	3.2
1	0	2580	G	3.2
14	L	97	VAL	3.2
32	I	102	VAL	3.2
8	E	33	LEU	3.2
5	B	96	PRO	3.2
13	K	14	LYS	3.2
32	I	87	THR	3.2
13	K	16	SER	3.2
1	0	1150	A	3.2
1	0	2569	A	3.2
26	X	29	ALA	3.2
32	I	109	ALA	3.2
12	J	11	ILE	3.2
10	G	73	ASP	3.2
1	0	2250	G	3.2
1	0	2712	G	3.2
1	0	1139	U	3.2
10	G	66	LEU	3.2
5	B	94	GLN	3.2
5	B	279	THR	3.2
1	0	2498	C	3.2
7	D	87	ALA	3.2
7	D	139	TYR	3.2
5	B	26	PHE	3.2
13	K	72	VAL	3.2
1	0	2800	A	3.2
5	B	175	LEU	3.2
26	X	88	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	0	1108	G	3.2
1	0	2683	G	3.2
5	B	64	GLY	3.2
12	J	78	ILE	3.2
7	D	61	PHE	3.2
30	2	46	ASP	3.1
5	B	162	MET	3.1
1	0	1133	A	3.1
1	0	1174	A	3.1
1	0	1193	A	3.1
8	E	18	LEU	3.1
8	E	116	THR	3.1
1	0	1111	U	3.1
1	0	1279	U	3.1
1	0	1524	U	3.1
8	E	168	ILE	3.1
18	P	35	ILE	3.1
5	B	69	VAL	3.1
5	B	280	VAL	3.1
16	N	172	PHE	3.1
1	0	1203	G	3.1
1	0	2754	G	3.1
1	0	2779	G	3.1
5	B	95	ARG	3.1
1	0	1228	C	3.1
32	I	100	LEU	3.1
5	B	67	GLU	3.1
19	Q	81	GLU	3.1
23	U	37	GLU	3.1
16	N	157	PRO	3.1
1	0	1191	A	3.1
9	F	17	LEU	3.1
16	N	186	LEU	3.1
1	0	2522	G	3.1
1	0	2696	G	3.1
13	K	63	GLU	3.1
5	B	325	PRO	3.1
1	0	1229	C	3.1
17	O	23	GLY	3.1
9	F	16	ALA	3.1
6	C	16	VAL	3.1
8	E	3	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
17	O	25	VAL	3.1
6	C	132	ASP	3.1
26	X	82	GLU	3.1
8	E	92	PRO	3.1
1	0	2507	G	3.1
1	0	2564	G	3.1
5	B	40	GLY	3.1
7	D	57	THR	3.1
10	G	12	ILE	3.1
10	G	16	LYS	3.1
11	H	11	LYS	3.1
16	N	165	ALA	3.1
24	V	51	LYS	3.1
5	B	65	MET	3.1
5	B	101	TRP	3.1
1	0	1182	C	3.1
1	0	1213	C	3.1
12	J	70	PHE	3.1
12	J	130	VAL	3.1
13	K	121	PHE	3.1
13	K	56	SER	3.1
1	0	1154	A	3.0
1	0	1181	A	3.0
1	0	2805	A	3.0
4	A	36	ASP	3.0
7	D	69	ILE	3.0
8	E	38	ILE	3.0
25	W	123	GLY	3.0
8	E	93	MET	3.0
11	H	35	ARG	3.0
32	I	98	ALA	3.0
7	D	130	VAL	3.0
13	K	74	VAL	3.0
1	0	1217	G	3.0
1	0	1951	G	3.0
1	0	2572	G	3.0
5	B	140	LEU	3.0
16	N	179	LEU	3.0
1	0	2897	C	3.0
12	J	111	GLU	3.0
19	Q	95	GLU	3.0
1	0	2706	A	3.0

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Mol	Chain	Res	Type	RSRZ
12	J	62	ASP	3.0
7	D	102	GLY	3.0
8	E	84	MET	3.0
17	O	24	ALA	3.0
14	L	99	GLU	3.0
14	L	148	GLU	3.0
32	I	113	HIS	3.0
16	N	159	TYR	3.0
1	0	2865	G	3.0
5	B	306	LYS	3.0
25	W	16	ASP	3.0
1	0	2707	C	3.0
1	0	2664	A	3.0
5	B	288	GLY	3.0
1	0	2514	U	3.0
12	J	87	LEU	3.0
7	D	47	GLN	3.0
7	D	26	GLY	3.0
1	0	1138	G	3.0
1	0	1241	G	3.0
1	0	2674	G	3.0
1	0	2708	G	3.0
1	0	2770	G	3.0
1	0	1227	C	3.0
1	0	2780	C	3.0
18	P	84	ALA	3.0
1	0	288	A	3.0
1	0	1192	A	3.0
1	0	2600	A	3.0
1	0	2601	A	3.0
1	0	1164	U	2.9
1	0	2554	U	2.9
1	0	2690	U	2.9
1	0	2781	U	2.9
20	R	121	GLU	2.9
16	N	161	GLY	2.9
26	X	83	ALA	2.9
5	B	54	VAL	2.9
5	B	151	VAL	2.9
5	B	311	PHE	2.9
7	D	75	LEU	2.9
1	0	1929	G	2.9

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Mol	Chain	Res	Type	RSRZ
1	0	2755	G	2.9
5	B	333	GLU	2.9
1	0	2883	A	2.9
11	H	85	MET	2.9
5	B	62	ARG	2.9
8	E	114	ARG	2.9
8	E	147	ASP	2.9
12	J	71	TYR	2.9
12	J	76	ASP	2.9
16	N	167	ASP	2.9
8	E	142	GLY	2.9
8	E	131	LEU	2.9
23	U	50	GLU	2.9
1	0	287	C	2.9
1	0	1177	A	2.9
1	0	2681	A	2.9
1	0	2573	G	2.9
1	0	2581	U	2.9
1	0	2687	G	2.9
1	0	2688	U	2.9
1	0	2713	G	2.9
5	B	335	ASN	2.9
5	B	319	ASP	2.9
11	H	20	ILE	2.9
11	H	169	GLY	2.9
13	K	21	ALA	2.9
5	B	100	VAL	2.9
16	N	135	VAL	2.9
28	Z	79	VAL	2.9
8	E	6	GLU	2.9
13	K	70	GLU	2.9
12	J	74	ARG	2.9
12	J	145	TRP	2.9
18	P	80	ARG	2.9
7	D	150	SER	2.9
1	0	734	U	2.9
5	B	282	GLY	2.9
1	0	2748	G	2.9
5	B	179	LEU	2.9
16	N	97	VAL	2.9
25	W	4	LEU	2.9
7	D	83	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
7	D	98	PHE	2.9
5	B	106	HIS	2.9
8	E	81	GLU	2.8
5	B	313	PRO	2.8
13	K	130	MET	2.8
5	B	111	ARG	2.8
32	I	134	SER	2.8
21	S	81	ILE	2.8
8	E	12	ASP	2.8
18	P	56	GLY	2.8
5	B	137	LEU	2.8
5	B	144	THR	2.8
11	H	168	ALA	2.8
1	0	272	A	2.8
1	0	2557	U	2.8
5	B	315	VAL	2.8
14	L	81	VAL	2.8
1	0	2697	A	2.8
1	0	2783	A	2.8
1	0	2526	C	2.8
5	B	1	PRO	2.8
1	0	1112	G	2.8
12	J	53	ILE	2.8
16	N	147	ILE	2.8
5	B	298	LYS	2.8
5	B	102	THR	2.8
5	B	297	VAL	2.8
6	C	162	VAL	2.8
13	K	34	VAL	2.8
31	3	22	VAL	2.8
32	I	127	GLU	2.8
1	0	1115	U	2.8
1	0	1964	U	2.8
1	0	2705	U	2.8
10	G	13	PRO	2.8
1	0	1117	A	2.8
1	0	1166	A	2.8
1	0	2511	A	2.8
8	E	150	GLN	2.8
19	Q	15	LYS	2.8
19	Q	84	ILE	2.8
1	0	969	G	2.8

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Mol	Chain	Res	Type	RSRZ
1	0	1119	G	2.8
1	0	2516	G	2.8
8	E	109	GLY	2.8
9	F	26	THR	2.8
8	E	110	GLU	2.8
13	K	55	VAL	2.8
14	L	83	GLU	2.8
1	0	2563	U	2.8
1	0	2598	U	2.8
11	H	75	LYS	2.8
24	V	47	LYS	2.8
1	0	2896	A	2.8
2	9	3091	C	2.8
5	B	269	LEU	2.8
8	E	5	LEU	2.8
16	N	127	LEU	2.8
10	G	65	THR	2.8
8	E	87	PHE	2.8
8	E	166	VAL	2.8
8	E	169	THR	2.8
20	R	110	THR	2.8
24	V	52	ALA	2.8
1	0	2420	G	2.8
1	0	2562	G	2.8
1	0	2603	G	2.8
1	0	2709	G	2.8
1	0	2731	G	2.8
1	0	2851	G	2.8
5	B	7	ARG	2.8
27	Y	216	ARG	2.8
30	2	20	ARG	2.8
5	B	212	GLN	2.7
4	A	31	LYS	2.7
8	E	148	ILE	2.7
25	W	26	ILE	2.7
1	0	2796	U	2.7
5	B	218	TRP	2.7
23	U	49	LEU	2.7
1	0	497	A	2.7
1	0	737	A	2.7
1	0	2775	A	2.7
8	E	39	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
8	E	47	VAL	2.7
14	L	65	ASP	2.7
1	0	2717	C	2.7
23	U	54	THR	2.7
32	I	94	GLU	2.7
16	N	6	TYR	2.7
1	0	1159	G	2.7
1	0	2667	G	2.7
1	0	2794	G	2.7
2	9	3025	G	2.7
16	N	175	LEU	2.7
5	B	273	GLY	2.7
8	E	120	GLY	2.7
25	W	111	GLY	2.7
32	I	88	GLY	2.7
7	D	62	ASP	2.7
7	D	162	ALA	2.7
8	E	170	ARG	2.7
12	J	38	VAL	2.7
13	K	8	VAL	2.7
16	N	137	ALA	2.7
24	V	35	ALA	2.7
32	I	96	PHE	2.7
1	0	2103	A	2.7
1	0	2488	A	2.7
11	H	12	PRO	2.7
14	L	105	TYR	2.7
14	L	150	GLN	2.7
1	0	2593	C	2.7
1	0	2831	C	2.7
12	J	63	ILE	2.7
7	D	90	LEU	2.7
1	0	588	G	2.7
1	0	1802	G	2.7
1	0	2520	G	2.7
1	0	2524	G	2.7
1	0	2701	G	2.7
1	0	2763	G	2.7
8	E	27	GLY	2.7
23	U	39	ASN	2.7
11	H	94	VAL	2.7
7	D	171	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
12	J	79	PHE	2.7
13	K	73	VAL	2.7
25	W	51	PHE	2.7
5	B	24	PRO	2.7
13	K	32	ILE	2.7
1	0	1148	C	2.7
1	0	1250	C	2.7
1	0	1787	C	2.7
5	B	48	MET	2.7
25	W	138	LEU	2.7
13	K	77	ARG	2.7
10	G	19	GLU	2.7
16	N	64	SER	2.7
32	I	77	GLU	2.7
7	D	169	THR	2.7
11	H	125	ALA	2.7
32	I	126	LYS	2.7
10	G	72	ASP	2.7
16	N	138	ASP	2.7
1	0	1995	G	2.6
32	I	111	GLN	2.6
1	0	2523	U	2.6
1	0	2837	U	2.6
13	K	37	TYR	2.6
11	H	161	CYS	2.6
1	0	1248	A	2.6
5	B	5	ARG	2.6
27	Y	155	ARG	2.6
5	B	169	GLY	2.6
8	E	44	GLY	2.6
8	E	53	GLU	2.6
1	0	1153	C	2.6
30	2	36	ASN	2.6
30	2	45	ASN	2.6
5	B	171	VAL	2.6
8	E	161	VAL	2.6
9	F	101	ALA	2.6
12	J	141	ALA	2.6
9	F	105	ASP	2.6
13	K	84	ASP	2.6
31	3	18	GLN	2.6
32	I	95	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	0	1744	G	2.6
26	X	61	ARG	2.6
7	D	59	GLY	2.6
8	E	9	GLU	2.6
8	E	70	GLU	2.6
1	0	285	A	2.6
1	0	2367	A	2.6
5	B	28	SER	2.6
10	G	24	VAL	2.6
8	E	113	PRO	2.6
13	K	114	ALA	2.6
14	L	73	VAL	2.6
22	T	50	VAL	2.6
27	Y	236	VAL	2.6
13	K	54	THR	2.6
18	P	74	GLN	2.6
1	0	2718	C	2.6
1	0	2747	C	2.6
5	B	192	ASP	2.6
8	E	88	TYR	2.6
13	K	29	LEU	2.6
13	K	69	LEU	2.6
13	K	109	LEU	2.6
16	N	136	LEU	2.6
1	0	970	U	2.6
1	0	2240	U	2.6
7	D	53	LYS	2.6
24	V	44	GLY	2.6
1	0	579	G	2.6
1	0	2494	G	2.6
7	D	50	VAL	2.6
10	G	22	ALA	2.6
16	N	92	ALA	2.6
32	I	92	PRO	2.6
14	L	104	ASP	2.6
8	E	62	ILE	2.6
17	O	102	ILE	2.6
1	0	282	C	2.6
1	0	2559	C	2.6
1	0	2561	C	2.6
5	B	109	LEU	2.6
26	X	18	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
7	D	72	LYS	2.6
12	J	128	LYS	2.6
32	I	82	GLU	2.6
1	0	2721	U	2.6
5	B	82	VAL	2.6
18	P	1	THR	2.5
1	0	1087	G	2.5
1	0	1151	G	2.5
1	0	2606	G	2.5
1	0	2855	G	2.5
15	M	154	ASP	2.5
1	0	736	A	2.5
1	0	2776	A	2.5
1	0	2827	A	2.5
12	J	31	LEU	2.5
12	J	124	LEU	2.5
6	C	133	ARG	2.5
9	F	119	ARG	2.5
13	K	87	ARG	2.5
18	P	18	LYS	2.5
1	0	2551	C	2.5
1	0	2685	C	2.5
12	J	85	GLY	2.5
5	B	3	PRO	2.5
5	B	327	VAL	2.5
7	D	16	PRO	2.5
7	D	23	VAL	2.5
8	E	112	ALA	2.5
11	H	171	ALA	2.5
5	B	59	ASN	2.5
13	K	119	GLN	2.5
5	B	68	THR	2.5
1	0	1122	U	2.5
1	0	2586	U	2.5
7	D	13	MET	2.5
13	K	7	ASP	2.5
12	J	56	LYS	2.5
16	N	180	LEU	2.5
5	B	227	HIS	2.5
8	E	74	HIS	2.5
1	0	572	G	2.5
1	0	1785	G	2.5

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Mol	Chain	Res	Type	RSRZ
1	0	1878	G	2.5
1	0	2730	G	2.5
1	0	580	A	2.5
1	0	1078	A	2.5
5	B	302	PRO	2.5
5	B	301	VAL	2.5
11	H	140	VAL	2.5
32	I	97	VAL	2.5
23	U	21	PHE	2.5
32	I	83	ALA	2.5
1	0	1142	C	2.5
1	0	2493	C	2.5
1	0	2500	C	2.5
5	B	79	MET	2.5
23	U	20	MET	2.5
12	J	17	CYS	2.5
28	Z	11	SER	2.5
5	B	45	LYS	2.5
7	D	40	ILE	2.5
8	E	90	HIS	2.5
18	P	71	TYR	2.5
20	R	74	GLY	2.5
1	0	591	A	2.5
1	0	1110	G	2.5
1	0	1158	G	2.5
1	0	1819	G	2.5
1	0	2253	G	2.5
1	0	2255	A	2.5
1	0	2680	A	2.5
6	C	61	PHE	2.5
12	J	98	PHE	2.5
11	H	36	LYS	2.5
4	A	128	LEU	2.5
7	D	157	LEU	2.5
8	E	151	LEU	2.5
11	H	157	ILE	2.5
13	K	82	ARG	2.5
22	T	118	SER	2.5
1	0	1808	C	2.5
1	0	2853	U	2.5
12	J	104	TYR	2.5
8	E	133	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
7	D	54	ALA	2.5
12	J	37	ALA	2.5
14	L	125	PHE	2.5
23	U	31	PHE	2.5
7	D	74	THR	2.4
1	0	1202	A	2.4
1	0	1559	A	2.4
1	0	1626	A	2.4
1	0	2353	A	2.4
1	0	2801	A	2.4
8	E	115	ARG	2.4
15	M	125	ARG	2.4
25	W	24	LEU	2.4
1	0	1239	G	2.4
1	0	2093	G	2.4
8	E	41	SER	2.4
17	O	80	ASP	2.4
22	T	117	ASP	2.4
1	0	2682	C	2.4
1	0	2806	C	2.4
1	0	2791	U	2.4
7	D	159	PRO	2.4
12	J	75	PRO	2.4
25	W	75	GLY	2.4
32	I	74	PRO	2.4
5	B	92	TYR	2.4
5	B	259	TYR	2.4
5	B	154	VAL	2.4
5	B	330	VAL	2.4
7	D	132	VAL	2.4
16	N	41	LYS	2.4
19	Q	76	VAL	2.4
20	R	96	VAL	2.4
25	W	5	VAL	2.4
5	B	13	PHE	2.4
18	P	131	PHE	2.4
18	P	143	ALA	2.4
7	D	101	THR	2.4
13	K	9	THR	2.4
5	B	188	HIS	2.4
16	N	160	SER	2.4
1	0	2517	A	2.4

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Mol	Chain	Res	Type	RSRZ
14	L	36	ASP	2.4
8	E	50	GLU	2.4
1	0	2251	G	2.4
1	0	2582	G	2.4
1	0	2609	G	2.4
13	K	64	MET	2.4
29	1	9	GLY	2.4
13	K	52	LYS	2.4
32	I	80	LYS	2.4
5	B	290	VAL	2.4
13	K	88	VAL	2.4
27	Y	174	VAL	2.4
1	0	2550	U	2.4
5	B	131	ALA	2.4
22	T	119	ALA	2.4
5	B	272	ILE	2.4
13	K	4	LEU	2.4
14	L	145	LEU	2.4
32	I	122	THR	2.4
5	B	4	SER	2.4
5	B	75	GLU	2.4
16	N	162	ASP	2.4
25	W	1	MET	2.4
1	0	590	A	2.4
1	0	1132	A	2.4
1	0	1199	A	2.4
1	0	2504	A	2.4
1	0	2778	A	2.4
5	B	158	LYS	2.4
4	A	32	VAL	2.4
8	E	76	VAL	2.4
14	L	91	VAL	2.4
17	O	60	VAL	2.4
1	0	1131	G	2.4
1	0	2862	G	2.4
5	B	312	ARG	2.4
12	J	129	PHE	2.4
13	K	90	PHE	2.4
23	U	56	ARG	2.4
1	0	1993	C	2.4
5	B	132	HIS	2.4
7	D	105	SER	2.4

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Mol	Chain	Res	Type	RSRZ
11	H	65	SER	2.4
11	H	160	SER	2.4
17	O	20	SER	2.4
7	D	99	ASP	2.4
32	I	81	ASP	2.4
13	K	1	MET	2.4
4	A	205	GLY	2.4
4	A	234	GLY	2.4
11	H	81	GLY	2.4
20	R	103	GLY	2.4
5	B	115	VAL	2.4
17	O	111	VAL	2.4
1	0	2792	A	2.4
13	K	6	ALA	2.4
13	K	118	ALA	2.4
26	X	87	ALA	2.4
8	E	49	ILE	2.3
12	J	144	THR	2.3
25	W	88	THR	2.3
11	H	70	ASN	2.3
31	3	8	ASN	2.3
1	0	1235	G	2.3
1	0	1947	G	2.3
1	0	2419	U	2.3
1	0	2698	G	2.3
1	0	2716	G	2.3
1	0	2753	G	2.3
1	0	2863	G	2.3
2	9	3022	G	2.3
4	A	59	GLU	2.3
6	C	237	GLU	2.3
1	0	959	C	2.3
1	0	963	C	2.3
1	0	1168	C	2.3
9	F	25	ASP	2.3
17	O	21	SER	2.3
5	B	29	TRP	2.3
25	W	32	CYS	2.3
30	2	31	ARG	2.3
6	C	243	VAL	2.3
14	L	76	LEU	2.3
14	L	77	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
14	L	78	ALA	2.3
16	N	166	ALA	2.3
25	W	3	ALA	2.3
26	X	33	ILE	2.3
5	B	87	TYR	2.3
7	D	170	TYR	2.3
11	H	14	TYR	2.3
1	0	1247	A	2.3
1	0	2761	A	2.3
2	9	3077	A	2.3
5	B	295	THR	2.3
8	E	58	THR	2.3
5	B	216	LYS	2.3
8	E	23	GLU	2.3
9	F	44	SER	2.3
1	0	1120	U	2.3
1	0	1237	U	2.3
1	0	289	G	2.3
1	0	1054	G	2.3
1	0	1214	G	2.3
1	0	2080	G	2.3
1	0	2777	G	2.3
7	D	137	PRO	2.3
1	0	284	C	2.3
1	0	999	C	2.3
1	0	1257	C	2.3
1	0	2760	C	2.3
1	0	2804	C	2.3
13	K	27	ARG	2.3
5	B	52	VAL	2.3
21	S	52	VAL	2.3
11	H	143	ALA	2.3
13	K	49	LEU	2.3
24	V	49	LEU	2.3
8	E	7	ILE	2.3
8	E	20	ILE	2.3
16	N	129	ILE	2.3
5	B	211	THR	2.3
7	D	12	GLU	2.3
1	0	2291	A	2.3
1	0	2699	A	2.3
1	0	2703	A	2.3

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Mol	Chain	Res	Type	RSRZ
2	9	3105	A	2.3
4	A	95	PRO	2.3
7	D	67	ASP	2.3
26	X	16	ASP	2.3
13	K	105	ARG	2.3
5	B	9	GLY	2.3
23	U	16	GLY	2.3
27	Y	210	GLY	2.3
1	0	1807	U	2.3
1	0	2527	U	2.3
1	0	2595	U	2.3
1	0	2710	U	2.3
8	E	103	VAL	2.3
12	J	12	VAL	2.3
14	L	133	VAL	2.3
23	U	22	VAL	2.3
24	V	5	VAL	2.3
16	N	83	LEU	2.3
7	D	151	ILE	2.3
7	D	166	ILE	2.3
12	J	44	ALA	2.3
1	0	571	C	2.3
1	0	575	G	2.3
1	0	1146	C	2.3
1	0	1245	C	2.3
1	0	1806	G	2.3
1	0	1812	G	2.3
1	0	1948	G	2.3
1	0	1989	G	2.3
1	0	1998	G	2.3
1	0	2237	G	2.3
1	0	2338	G	2.3
1	0	2519	C	2.3
1	0	2552	C	2.3
1	0	2571	C	2.3
1	0	2679	G	2.3
1	0	2767	C	2.3
1	0	2782	G	2.3
2	9	3012	C	2.3
23	U	23	HIS	2.3
25	W	130	HIS	2.3
8	E	21	THR	2.3

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Mol	Chain	Res	Type	RSRZ
12	J	131	THR	2.3
23	U	19	THR	2.3
16	N	150	TYR	2.3
24	V	41	GLU	2.3
28	Z	44	GLU	2.3
4	A	85	SER	2.3
8	E	16	ASP	2.3
27	Y	132	ASP	2.3
1	0	922	A	2.3
1	0	943	A	2.3
1	0	1233	A	2.3
1	0	2914	A	2.3
2	9	3057	A	2.3
4	A	35	GLY	2.3
5	B	303	GLY	2.3
8	E	141	VAL	2.3
13	K	31	VAL	2.3
13	K	57	VAL	2.3
25	W	52	VAL	2.3
27	Y	193	LEU	2.3
5	B	181	ILE	2.2
20	R	68	HIS	2.2
25	W	23	MET	2.2
8	E	77	THR	2.2
6	C	245	GLU	2.2
14	L	127	GLU	2.2
1	0	1061	C	2.2
1	0	1156	C	2.2
1	0	1238	C	2.2
1	0	1243	C	2.2
1	0	2594	C	2.2
1	0	2785	C	2.2
2	9	3107	C	2.2
1	0	577	G	2.2
1	0	1075	G	2.2
1	0	2256	G	2.2
6	C	246	ARG	2.2
8	E	2	ARG	2.2
19	Q	92	ARG	2.2
5	B	6	PRO	2.2
7	D	68	PRO	2.2
5	B	39	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
11	H	39	ASP	2.2
27	Y	191	ASP	2.2
13	K	12	LEU	2.2
13	K	117	VAL	2.2
1	0	587	A	2.2
1	0	1778	A	2.2
1	0	2521	A	2.2
5	B	41	PHE	2.2
5	B	124	ALA	2.2
5	B	128	ILE	2.2
5	B	177	HIS	2.2
23	U	35	LYS	2.2
1	0	1116	U	2.2
1	0	1205	U	2.2
8	E	125	GLU	2.2
8	E	167	TYR	2.2
21	S	45	TYR	2.2
25	W	41	TYR	2.2
8	E	32	ARG	2.2
25	W	131	PRO	2.2
31	3	56	PRO	2.2
1	0	1085	C	2.2
1	0	2548	C	2.2
1	0	2704	C	2.2
1	0	2765	C	2.2
1	0	2795	C	2.2
8	E	164	ASP	2.2
1	0	1216	G	2.2
1	0	2033	G	2.2
1	0	2602	G	2.2
1	0	2605	G	2.2
1	0	2842	G	2.2
1	0	2861	G	2.2
1	0	2884	G	2.2
12	J	20	GLY	2.2
19	Q	12	GLY	2.2
25	W	34	LEU	2.2
5	B	157	LYS	2.2
8	E	157	LYS	2.2
28	Z	47	VAL	2.2
11	H	136	ALA	2.2
1	0	372	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	0	1114	A	2.2
1	0	2689	A	2.2
8	E	46	THR	2.2
8	E	64	THR	2.2
12	J	138	THR	2.2
19	Q	23	THR	2.2
27	Y	106	THR	2.2
1	0	510	U	2.2
1	0	1149	U	2.2
1	0	2589	U	2.2
1	0	2808	U	2.2
12	J	88	PRO	2.2
5	B	261	GLN	2.2
5	B	120	ASP	2.2
5	B	180	ASP	2.2
5	B	324	ASP	2.2
8	E	123	ASP	2.2
9	F	12	LEU	2.2
11	H	38	LYS	2.2
13	K	44	LEU	2.2
16	N	78	MET	2.2
1	0	1103	C	2.2
1	0	2241	C	2.2
1	0	2248	C	2.2
1	0	2536	C	2.2
1	0	2549	C	2.2
1	0	2729	C	2.2
5	B	284	PHE	2.2
11	H	116	ALA	2.2
13	K	94	ALA	2.2
1	0	592	G	2.2
1	0	1789	G	2.2
1	0	2544	G	2.2
5	B	66	GLU	2.2
7	D	92	GLU	2.2
9	F	90	GLU	2.2
23	U	6	CYS	2.2
1	0	363	A	2.2
1	0	1779	A	2.2
1	0	2784	A	2.2
1	0	2875	A	2.2
1	0	2891	A	2.2

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Mol	Chain	Res	Type	RSRZ
5	B	304	PRO	2.2
8	E	8	PRO	2.2
1	0	1170	U	2.2
1	0	1702	U	2.2
1	0	2322	U	2.2
1	0	2528	U	2.2
5	B	37	GLY	2.2
5	B	47	GLY	2.2
17	O	22	GLY	2.2
18	P	78	GLY	2.2
20	R	73	ASP	2.2
10	G	29	SER	2.2
5	B	123	ALA	2.1
17	O	17	ALA	2.1
20	R	95	ALA	2.1
25	W	40	ALA	2.1
26	X	26	ALA	2.1
5	B	88	GLU	2.1
12	J	28	GLU	2.1
27	Y	165	GLU	2.1
1	0	1060	C	2.1
1	0	1826	C	2.1
1	0	2745	C	2.1
1	0	2764	C	2.1
4	A	153	ARG	2.1
1	0	1240	G	2.1
1	0	2068	G	2.1
1	0	2136	G	2.1
1	0	2525	G	2.1
2	9	3074	G	2.1
2	9	3076	G	2.1
8	E	136	PRO	2.1
5	B	35	GLN	2.1
11	H	137	TYR	2.1
20	R	122	GLN	2.1
5	B	323	LEU	2.1
12	J	19	MET	2.1
14	L	75	LEU	2.1
1	0	566	A	2.1
1	0	1194	A	2.1
1	0	2095	A	2.1
2	9	3065	A	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	236	GLY	2.1
5	B	258	GLY	2.1
8	E	24	GLY	2.1
12	J	133	GLY	2.1
14	L	146	GLY	2.1
1	0	1198	U	2.1
1	0	2003	U	2.1
5	B	50	HIS	2.1
5	B	270	ILE	2.1
5	B	305	ASP	2.1
7	D	22	VAL	2.1
8	E	137	ASP	2.1
8	E	28	SER	2.1
11	H	165	SER	2.1
12	J	26	VAL	2.1
16	N	164	ASP	2.1
22	T	42	VAL	2.1
5	B	194	PHE	2.1
5	B	46	ALA	2.1
8	E	34	TRP	2.1
11	H	144	GLU	2.1
13	K	102	GLU	2.1
21	S	12	GLU	2.1
4	A	65	ARG	2.1
7	D	149	ARG	2.1
17	O	47	ARG	2.1
28	Z	13	ARG	2.1
13	K	112	PRO	2.1
19	Q	17	LYS	2.1
1	0	2515	C	2.1
1	0	2901	C	2.1
5	B	318	ASN	2.1
7	D	133	ASN	2.1
8	E	66	GLN	2.1
14	L	113	GLN	2.1
18	P	57	ASN	2.1
11	H	43	TYR	2.1
18	P	72	GLY	2.1
28	Z	51	GLY	2.1
1	0	362	G	2.1
1	0	1134	G	2.1
1	0	1178	G	2.1

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Mol	Chain	Res	Type	RSRZ
1	0	1223	G	2.1
1	0	1634	G	2.1
1	0	1743	G	2.1
1	0	2592	G	2.1
1	0	2734	G	2.1
1	0	2848	G	2.1
1	0	2877	G	2.1
5	B	271	ASP	2.1
8	E	69	ILE	2.1
8	E	154	ILE	2.1
26	X	84	ILE	2.1
5	B	245	SER	2.1
13	K	33	SER	2.1
1	0	1218	U	2.1
1	0	1985	U	2.1
1	0	2364	A	2.1
1	0	2604	A	2.1
12	J	8	ALA	2.1
14	L	61	ALA	2.1
17	O	85	ALA	2.1
9	F	117	GLU	2.1
12	J	99	GLU	2.1
18	P	69	ARG	2.1
4	A	207	GLN	2.1
5	B	286	ASN	2.1
4	A	131	HIS	2.1
7	D	155	HIS	2.1
8	E	128	GLY	2.1
16	N	21	HIS	2.1
28	Z	19	GLY	2.1
1	0	1147	C	2.1
1	0	1786	C	2.1
1	0	2040	C	2.1
1	0	2672	C	2.1
1	0	2839	C	2.1
5	B	143	ILE	2.1
11	H	50	ILE	2.1
11	H	127	VAL	2.1
16	N	43	VAL	2.1
25	W	48	VAL	2.1
14	L	89	PHE	2.1
32	I	120	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
5	B	42	ALA	2.1
5	B	57	GLU	2.1
14	L	100	ALA	2.1
1	0	958	G	2.1
1	0	1099	G	2.1
1	0	1800	G	2.1
1	0	2491	G	2.1
2	9	3102	G	2.1
1	0	602	A	2.1
1	0	957	A	2.1
1	0	2583	A	2.1
1	0	2714	U	2.1
11	H	32	LYS	2.1
12	J	73	LYS	2.1
18	P	68	LYS	2.1
26	X	66	THR	2.1
27	Y	200	THR	2.1
5	B	190	MET	2.1
11	H	77	LEU	2.1
22	T	91	LEU	2.1
24	V	42	ASN	2.1
32	I	123	ASN	2.1
9	F	92	GLY	2.1
18	P	73	HIS	2.1
27	Y	157	ILE	2.1
14	L	108	VAL	2.1
25	W	132	VAL	2.1
11	H	134	PHE	2.1
5	B	141	ARG	2.0
10	G	68	GLU	2.0
11	H	151	ARG	2.0
12	J	66	ASP	2.0
16	N	12	ARG	2.0
18	P	2	ASP	2.0
6	C	171	GLU	2.0
31	3	41	GLU	2.0
1	0	1084	C	2.0
1	0	1715	C	2.0
1	0	2547	C	2.0
1	0	2555	C	2.0
16	N	139	TRP	2.0
5	B	78	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
5	B	116	PRO	2.0
5	B	278	PRO	2.0
5	B	293	PRO	2.0
13	K	104	PRO	2.0
1	0	283	U	2.0
1	0	2495	U	2.0
1	0	2597	U	2.0
1	0	2661	U	2.0
1	0	2711	U	2.0
5	B	84	LEU	2.0
7	D	85	GLN	2.0
1	0	358	G	2.0
1	0	593	A	2.0
1	0	1077	G	2.0
1	0	1113	G	2.0
1	0	1135	G	2.0
1	0	1611	G	2.0
1	0	1994	A	2.0
1	0	2074	A	2.0
1	0	2505	G	2.0
1	0	2799	A	2.0
8	E	17	HIS	2.0
11	H	72	HIS	2.0
17	O	104	ASN	2.0
28	Z	41	ASN	2.0
5	B	299	GLY	2.0
11	H	120	ILE	2.0
18	P	98	ILE	2.0
23	U	18	GLY	2.0
5	B	182	VAL	2.0
12	J	61	VAL	2.0
31	3	25	VAL	2.0
5	B	328	ARG	2.0
7	D	76	ARG	2.0
11	H	71	ARG	2.0
19	Q	11	ARG	2.0
28	Z	25	ARG	2.0
14	L	44	GLU	2.0
17	O	99	GLU	2.0
24	V	36	ALA	2.0
25	W	46	ALA	2.0
26	X	46	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
31	3	92	GLU	2.0
5	B	156	LYS	2.0
21	S	78	ALA	2.0
5	B	206	THR	2.0
13	K	61	THR	2.0
13	K	129	THR	2.0
16	N	130	PRO	2.0
20	R	10	PRO	2.0
1	0	298	C	2.0
1	0	364	C	2.0
1	0	717	C	2.0
1	0	2510	C	2.0
1	0	2857	C	2.0
2	9	3030	C	2.0
7	D	97	GLN	2.0
12	J	89	HIS	2.0
1	0	1244	U	2.0
1	0	2034	U	2.0
1	0	2242	U	2.0
1	0	2671	U	2.0
9	F	102	GLY	2.0
11	H	163	ILE	2.0
12	J	106	GLY	2.0
17	O	62	GLY	2.0
19	Q	9	GLY	2.0
24	V	8	ILE	2.0
24	V	46	ILE	2.0
1	0	565	A	2.0
1	0	1058	A	2.0
1	0	1232	A	2.0
1	0	1242	A	2.0
1	0	2039	A	2.0
4	A	84	VAL	2.0
11	H	114	ARG	2.0
14	L	57	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	DCZ	4	74	16/16	0.81	0.17	48,52,56,60	0
1	OMG	0	2588	24/25	0.88	0.15	30,33,38,40	0
1	1MA	0	628	23/24	0.90	0.14	28,34,37,38	0
1	OMU	0	2587	21/22	0.90	0.15	31,35,40,41	0
3	5AA	4	76	24/25	0.91	0.14	40,44,46,47	0
1	UR3	0	2619	21/22	0.91	0.14	33,38,39,42	0
1	PSU	0	2621	20/21	0.94	0.09	31,34,40,41	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	9124	1/1	0.52	0.33	66,66,66,66	0
35	NA	0	9182	1/1	0.53	0.32	81,81,81,81	0
35	NA	0	9164	1/1	0.62	0.24	53,53,53,53	0
35	NA	0	9110	1/1	0.62	0.21	43,43,43,43	0
35	NA	0	9129	1/1	0.64	0.16	57,57,57,57	0
35	NA	0	9102	1/1	0.65	0.17	45,45,45,45	0
35	NA	R	9186	1/1	0.68	0.26	78,78,78,78	0
35	NA	0	9157	1/1	0.69	0.18	73,73,73,73	0
35	NA	0	9170	1/1	0.69	0.18	49,49,49,49	0
35	NA	9	9151	1/1	0.70	0.23	64,64,64,64	0
33	MG	0	8117	1/1	0.71	0.13	37,37,37,37	0
35	NA	0	9121	1/1	0.71	0.36	55,55,55,55	0
33	MG	0	8053	1/1	0.72	0.17	57,57,57,57	0
35	NA	0	9176	1/1	0.73	0.20	49,49,49,49	0
35	NA	0	9156	1/1	0.74	0.24	49,49,49,49	0
35	NA	S	9112	1/1	0.74	0.15	73,73,73,73	0
35	NA	0	9181	1/1	0.75	0.14	56,56,56,56	0
33	MG	0	8050	1/1	0.76	0.14	69,69,69,69	0
35	NA	0	9155	1/1	0.77	0.24	79,79,79,79	0
33	MG	0	8101	1/1	0.77	0.20	72,72,72,72	0
35	NA	0	9184	1/1	0.77	0.17	83,83,83,83	0
33	MG	9	8095	1/1	0.78	0.17	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	9139	1/1	0.78	0.12	31,31,31,31	0
35	NA	0	9166	1/1	0.79	0.16	69,69,69,69	0
36	CL	N	9307	1/1	0.79	0.24	72,72,72,72	0
35	NA	H	9109	1/1	0.80	0.11	34,34,34,34	0
33	MG	0	8063	1/1	0.80	0.13	71,71,71,71	0
33	MG	0	8023	1/1	0.80	0.15	52,52,52,52	0
33	MG	0	8047	1/1	0.80	0.17	86,86,86,86	0
35	NA	0	9105	1/1	0.81	0.16	44,44,44,44	0
35	NA	0	9133	1/1	0.81	0.15	34,34,34,34	0
36	CL	J	9321	1/1	0.81	0.18	55,55,55,55	0
35	NA	0	9113	1/1	0.81	0.17	67,67,67,67	0
33	MG	0	8049	1/1	0.82	0.16	81,81,81,81	0
36	CL	0	9315	1/1	0.83	0.24	80,80,80,80	0
33	MG	0	8087	1/1	0.83	0.18	59,59,59,59	0
35	NA	0	9141	1/1	0.83	0.10	45,45,45,45	0
35	NA	0	9144	1/1	0.84	0.10	33,33,33,33	0
35	NA	0	9150	1/1	0.84	0.13	42,42,42,42	0
35	NA	0	9175	1/1	0.84	0.28	52,52,52,52	0
33	MG	0	8113	1/1	0.84	0.10	52,52,52,52	0
33	MG	0	8041	1/1	0.84	0.12	79,79,79,79	0
36	CL	J	9301	1/1	0.84	0.19	78,78,78,78	0
33	MG	0	8072	1/1	0.84	0.15	60,60,60,60	0
35	NA	0	9125	1/1	0.84	0.15	59,59,59,59	0
36	CL	0	9312	1/1	0.85	0.16	59,59,59,59	0
35	NA	0	9123	1/1	0.85	0.33	44,44,44,44	0
33	MG	0	8092	1/1	0.85	0.23	90,90,90,90	0
33	MG	0	8082	1/1	0.85	0.19	76,76,76,76	0
35	NA	0	9162	1/1	0.85	0.25	64,64,64,64	0
36	CL	0	9311	1/1	0.86	0.14	53,53,53,53	0
35	NA	0	9163	1/1	0.86	0.18	65,65,65,65	0
35	NA	0	9108	1/1	0.86	0.12	49,49,49,49	0
36	CL	0	9316	1/1	0.86	0.18	66,66,66,66	0
35	NA	0	9177	1/1	0.86	0.23	68,68,68,68	0
36	CL	J	9302	1/1	0.86	0.19	79,79,79,79	0
33	MG	0	8100	1/1	0.86	0.18	70,70,70,70	0
35	NA	0	9131	1/1	0.86	0.13	41,41,41,41	0
36	CL	3	9304	1/1	0.86	0.14	61,61,61,61	0
35	NA	0	9135	1/1	0.87	0.15	52,52,52,52	0
35	NA	0	9159	1/1	0.87	0.21	50,50,50,50	0
33	MG	0	8099	1/1	0.87	0.12	53,53,53,53	0
33	MG	0	8057	1/1	0.87	0.12	42,42,42,42	0
35	NA	0	9117	1/1	0.87	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	9106	1/1	0.87	0.27	38,38,38,38	0
35	NA	B	9158	1/1	0.87	0.38	70,70,70,70	0
33	MG	0	8064	1/1	0.87	0.09	30,30,30,30	0
35	NA	R	9137	1/1	0.87	0.10	44,44,44,44	0
35	NA	0	9134	1/1	0.87	0.13	41,41,41,41	0
35	NA	Q	9148	1/1	0.88	0.11	38,38,38,38	0
35	NA	0	9120	1/1	0.88	0.17	52,52,52,52	0
35	NA	0	9171	1/1	0.88	0.15	52,52,52,52	0
33	MG	0	8045	1/1	0.88	0.17	73,73,73,73	0
35	NA	0	9111	1/1	0.88	0.17	61,61,61,61	0
35	NA	0	9101	1/1	0.88	0.12	40,40,40,40	0
35	NA	0	9136	1/1	0.88	0.14	55,55,55,55	0
35	NA	0	9115	1/1	0.88	0.12	37,37,37,37	0
35	NA	0	9126	1/1	0.88	0.15	41,41,41,41	0
33	MG	0	8103	1/1	0.88	0.14	65,65,65,65	0
35	NA	9	9183	1/1	0.88	0.11	60,60,60,60	0
35	NA	0	9165	1/1	0.88	0.16	47,47,47,47	0
35	NA	0	9149	1/1	0.88	0.10	38,38,38,38	0
37	CD	U	9201	1/1	0.88	0.09	74,74,74,74	0
33	MG	0	8090	1/1	0.89	0.18	65,65,65,65	0
33	MG	0	8115	1/1	0.89	0.09	57,57,57,57	0
35	NA	0	9185	1/1	0.89	0.17	51,51,51,51	0
33	MG	0	8116	1/1	0.89	0.10	62,62,62,62	0
33	MG	0	8059	1/1	0.89	0.12	51,51,51,51	0
33	MG	0	8046	1/1	0.89	0.10	59,59,59,59	0
33	MG	Y	8109	1/1	0.89	0.09	44,44,44,44	0
36	CL	0	9322	1/1	0.90	0.27	77,77,77,77	0
36	CL	A	9309	1/1	0.90	0.18	61,61,61,61	0
36	CL	B	9319	1/1	0.90	0.22	55,55,55,55	0
33	MG	0	8119	1/1	0.90	0.11	62,62,62,62	0
35	NA	A	9145	1/1	0.90	0.10	48,48,48,48	0
34	K	0	9002	1/1	0.90	0.10	48,48,48,48	0
35	NA	0	9143	1/1	0.90	0.10	33,33,33,33	0
33	MG	0	8068	1/1	0.90	0.09	60,60,60,60	0
35	NA	0	9178	1/1	0.90	0.24	57,57,57,57	0
33	MG	0	8081	1/1	0.91	0.07	52,52,52,52	0
33	MG	0	8111	1/1	0.91	0.08	52,52,52,52	0
35	NA	C	9104	1/1	0.91	0.07	40,40,40,40	0
35	NA	0	9114	1/1	0.91	0.22	64,64,64,64	0
35	NA	H	9122	1/1	0.91	0.17	72,72,72,72	0
35	NA	0	9152	1/1	0.91	0.29	61,61,61,61	0
33	MG	3	8078	1/1	0.91	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	9169	1/1	0.91	0.15	60,60,60,60	0
33	MG	0	8102	1/1	0.91	0.07	58,58,58,58	0
35	NA	0	9119	1/1	0.91	0.07	44,44,44,44	0
33	MG	0	8114	1/1	0.91	0.07	56,56,56,56	0
33	MG	T	8073	1/1	0.92	0.07	59,59,59,59	0
33	MG	0	8088	1/1	0.92	0.09	38,38,38,38	0
36	CL	0	9313	1/1	0.92	0.12	60,60,60,60	0
33	MG	0	8075	1/1	0.92	0.07	57,57,57,57	0
33	MG	0	8084	1/1	0.92	0.09	38,38,38,38	0
36	CL	0	9317	1/1	0.92	0.09	61,61,61,61	0
35	NA	0	9173	1/1	0.92	0.08	62,62,62,62	0
33	MG	9	8052	1/1	0.92	0.08	54,54,54,54	0
33	MG	0	8044	1/1	0.92	0.08	55,55,55,55	0
35	NA	0	9161	1/1	0.92	0.14	56,56,56,56	0
35	NA	0	9142	1/1	0.92	0.12	47,47,47,47	0
35	NA	0	9103	1/1	0.92	0.11	43,43,43,43	0
36	CL	L	9310	1/1	0.92	0.19	63,63,63,63	0
33	MG	B	8055	1/1	0.92	0.12	62,62,62,62	0
36	CL	Y	9320	1/1	0.92	0.13	52,52,52,52	0
35	NA	0	9118	1/1	0.92	0.17	62,62,62,62	0
36	CL	0	9303	1/1	0.92	0.14	53,53,53,53	0
33	MG	0	8037	1/1	0.93	0.07	45,45,45,45	0
35	NA	0	9168	1/1	0.93	0.11	49,49,49,49	0
33	MG	0	8106	1/1	0.93	0.07	54,54,54,54	0
33	MG	0	8021	1/1	0.93	0.08	32,32,32,32	0
33	MG	B	8056	1/1	0.93	0.11	47,47,47,47	0
35	NA	0	9172	1/1	0.93	0.18	62,62,62,62	0
33	MG	0	8093	1/1	0.93	0.08	66,66,66,66	0
35	NA	0	9174	1/1	0.93	0.15	62,62,62,62	0
35	NA	0	9140	1/1	0.93	0.09	47,47,47,47	0
35	NA	L	9180	1/1	0.93	0.19	51,51,51,51	0
33	MG	0	8094	1/1	0.93	0.10	73,73,73,73	0
33	MG	0	8085	1/1	0.93	0.13	72,72,72,72	0
33	MG	0	8086	1/1	0.93	0.07	50,50,50,50	0
36	CL	O	9308	1/1	0.93	0.20	79,79,79,79	0
35	NA	0	9179	1/1	0.93	0.15	70,70,70,70	0
33	MG	0	8051	1/1	0.93	0.10	72,72,72,72	0
33	MG	0	8025	1/1	0.93	0.07	46,46,46,46	0
34	K	0	9003	1/1	0.94	0.17	64,64,64,64	0
33	MG	0	8009	1/1	0.94	0.06	30,30,30,30	0
33	MG	0	8070	1/1	0.94	0.10	57,57,57,57	0
33	MG	0	8058	1/1	0.94	0.07	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	R	9138	1/1	0.94	0.08	63,63,63,63	0
33	MG	0	8108	1/1	0.94	0.10	58,58,58,58	0
33	MG	0	8110	1/1	0.94	0.07	32,32,32,32	0
33	MG	0	8096	1/1	0.94	0.06	53,53,53,53	0
35	NA	0	9160	1/1	0.94	0.16	46,46,46,46	0
33	MG	0	8097	1/1	0.94	0.08	40,40,40,40	0
33	MG	0	8039	1/1	0.94	0.06	52,52,52,52	0
33	MG	0	8026	1/1	0.94	0.07	24,24,24,24	0
37	CD	O	9205	1/1	0.94	0.15	143,143,143,143	0
33	MG	0	8043	1/1	0.94	0.06	47,47,47,47	0
33	MG	0	8098	1/1	0.95	0.07	47,47,47,47	0
35	NA	0	9167	1/1	0.95	0.08	52,52,52,52	0
35	NA	0	9107	1/1	0.95	0.07	46,46,46,46	0
33	MG	0	8077	1/1	0.95	0.05	28,28,28,28	0
33	MG	0	8015	1/1	0.95	0.06	33,33,33,33	0
35	NA	0	9127	1/1	0.95	0.08	42,42,42,42	0
35	NA	0	9153	1/1	0.95	0.14	21,21,21,21	0
33	MG	0	8091	1/1	0.95	0.06	79,79,79,79	0
33	MG	0	8032	1/1	0.95	0.07	41,41,41,41	0
34	K	0	9001	1/1	0.95	0.19	71,71,71,71	0
33	MG	0	8042	1/1	0.95	0.06	44,44,44,44	0
35	NA	0	9116	1/1	0.95	0.08	42,42,42,42	0
33	MG	0	8034	1/1	0.95	0.07	38,38,38,38	0
33	MG	0	8006	1/1	0.95	0.06	37,37,37,37	0
33	MG	0	8060	1/1	0.95	0.10	46,46,46,46	0
33	MG	4	8118	1/1	0.95	0.05	41,41,41,41	0
33	MG	A	8065	1/1	0.95	0.07	45,45,45,45	0
33	MG	A	8066	1/1	0.96	0.06	66,66,66,66	0
33	MG	0	8007	1/1	0.96	0.06	27,27,27,27	0
33	MG	0	8020	1/1	0.96	0.05	31,31,31,31	0
35	NA	0	9128	1/1	0.96	0.09	43,43,43,43	0
33	MG	0	8112	1/1	0.96	0.08	39,39,39,39	0
33	MG	0	8004	1/1	0.96	0.05	34,34,34,34	0
33	MG	2	8076	1/1	0.96	0.07	55,55,55,55	0
35	NA	J	9146	1/1	0.96	0.04	42,42,42,42	0
33	MG	0	8036	1/1	0.96	0.06	35,35,35,35	0
33	MG	0	8071	1/1	0.96	0.10	66,66,66,66	0
33	MG	0	8010	1/1	0.96	0.05	28,28,28,28	0
33	MG	0	8089	1/1	0.96	0.06	56,56,56,56	0
33	MG	0	8024	1/1	0.96	0.07	39,39,39,39	0
36	CL	R	9306	1/1	0.96	0.08	57,57,57,57	0
33	MG	0	8012	1/1	0.96	0.04	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8104	1/1	0.96	0.07	55,55,55,55	0
33	MG	0	8080	1/1	0.96	0.07	41,41,41,41	0
33	MG	0	8061	1/1	0.96	0.05	37,37,37,37	0
37	CD	Z	9203	1/1	0.96	0.05	67,67,67,67	0
37	CD	1	9202	1/1	0.96	0.06	62,62,62,62	0
33	MG	0	8048	1/1	0.97	0.05	56,56,56,56	0
33	MG	0	8038	1/1	0.97	0.04	32,32,32,32	0
33	MG	0	8067	1/1	0.97	0.08	49,49,49,49	0
33	MG	K	8069	1/1	0.97	0.04	52,52,52,52	0
33	MG	0	8003	1/1	0.97	0.04	31,31,31,31	0
35	NA	M	9147	1/1	0.97	0.03	25,25,25,25	0
33	MG	0	8027	1/1	0.97	0.04	37,37,37,37	0
33	MG	0	8030	1/1	0.97	0.07	35,35,35,35	0
33	MG	0	8022	1/1	0.97	0.05	35,35,35,35	0
36	CL	M	9318	1/1	0.97	0.07	47,47,47,47	0
33	MG	0	8001	1/1	0.97	0.05	35,35,35,35	0
33	MG	0	8035	1/1	0.97	0.06	49,49,49,49	0
35	NA	0	9130	1/1	0.97	0.08	45,45,45,45	0
36	CL	0	9305	1/1	0.97	0.07	55,55,55,55	0
33	MG	0	8079	1/1	0.97	0.05	29,29,29,29	0
35	NA	0	9154	1/1	0.97	0.06	33,33,33,33	0
33	MG	0	8018	1/1	0.97	0.06	42,42,42,42	0
36	CL	0	9314	1/1	0.97	0.10	49,49,49,49	0
33	MG	0	8002	1/1	0.97	0.05	39,39,39,39	0
33	MG	0	8033	1/1	0.98	0.05	38,38,38,38	0
33	MG	0	8005	1/1	0.98	0.07	36,36,36,36	0
33	MG	0	8107	1/1	0.98	0.07	53,53,53,53	0
33	MG	0	8014	1/1	0.98	0.08	43,43,43,43	0
33	MG	0	8008	1/1	0.98	0.04	37,37,37,37	0
33	MG	0	8028	1/1	0.98	0.05	41,41,41,41	0
33	MG	0	8016	1/1	0.98	0.14	50,50,50,50	0
33	MG	0	8031	1/1	0.98	0.06	30,30,30,30	0
33	MG	0	8062	1/1	0.98	0.04	51,51,51,51	0
33	MG	0	8040	1/1	0.98	0.05	56,56,56,56	0
33	MG	0	8011	1/1	0.98	0.09	20,20,20,20	0
35	NA	0	9132	1/1	0.98	0.03	34,34,34,34	0
33	MG	0	8074	1/1	0.99	0.03	37,37,37,37	0
33	MG	0	8083	1/1	0.99	0.03	42,42,42,42	0
33	MG	0	8019	1/1	0.99	0.08	35,35,35,35	0
33	MG	0	8054	1/1	0.99	0.03	29,29,29,29	0
33	MG	0	8029	1/1	0.99	0.03	36,36,36,36	0
33	MG	0	8017	1/1	0.99	0.08	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8013	1/1	0.99	0.03	33,33,33,33	0
37	CD	3	9204	1/1	0.99	0.03	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.