



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:05 PM UTC

PDB ID : 3CPW / pdb_00003cpw
Title : The structure of the antibiotic LINEZOLID bound to the large ribosomal subunit of HALOARCUA MARISMORTUI
Authors : Ippolito, J.A.; Kanyo, Z.K.; Wang, D.; Franceschi, F.J.; Moore, P.B.; Steitz, T.A.; Duffy, E.M.
Deposited on : 2008-04-01
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

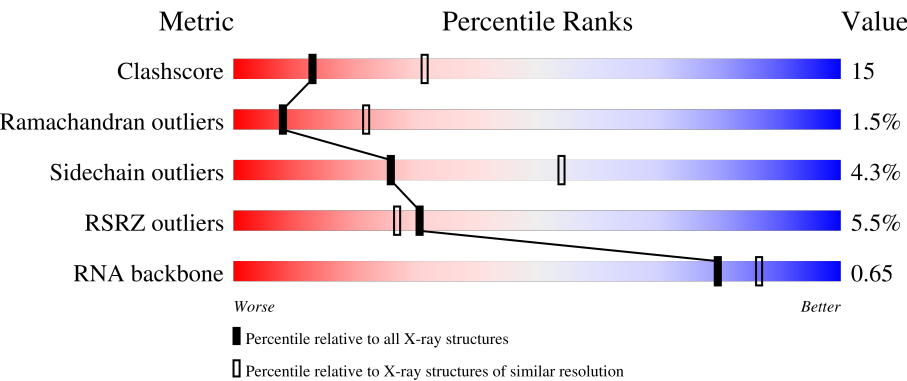
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	5% 54%34%5%6%
2	9	122	7% 47%40%11%
3	A	240	4% 59%32%8%
4	B	338	4% 59%36%5%

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	145	
12	J	132	
13	K	165	
14	L	196	
15	M	187	
16	N	116	
17	O	149	
18	P	96	
19	Q	155	
20	R	85	
21	S	120	
22	T	67	
23	U	71	
24	V	154	
25	W	92	
26	X	241	
27	Y	92	
28	Z	57	
29	1	50	

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Mol	Chain	Length	Quality of chain
30	2	92	
31	4	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8071	-	-	-	X
34	K	0	8401	-	-	-	X
35	NA	0	8544	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	0	8574	-	-	-	X
35	NA	0	8575	-	-	-	X
35	NA	9	8572	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98629 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
			59016	26346	10879	19046	2745			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	559	C	U	conflict	GB 3377779
0	560	C	U	conflict	GB 3377779
0	2099	A	G	engineered mutation	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 protein called 50S ribosomal protein L2P.

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

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

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

- Molecule 5 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

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

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

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

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

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

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

- Molecule 9 is a protein called 50S ribosomal protein L10E.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

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

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

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

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

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

- Molecule 16 is a protein called 50S ribosomal protein L18e.

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

- Molecule 17 is a protein called 50S ribosomal protein L19e.

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

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

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

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

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

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

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

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

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

- Molecule 22 is a protein called 50S ribosomal protein L24e.

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

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

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

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

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

- Molecule 25 is a protein called 50S ribosomal protein L31e.

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

- Molecule 26 is a protein called 50S ribosomal protein L32e.

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

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	72	Total	C	N	O	S			
			567	340	112	110	5	0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	46	Total	C	N	O	S			
			396	239	89	67	1	0	0	0

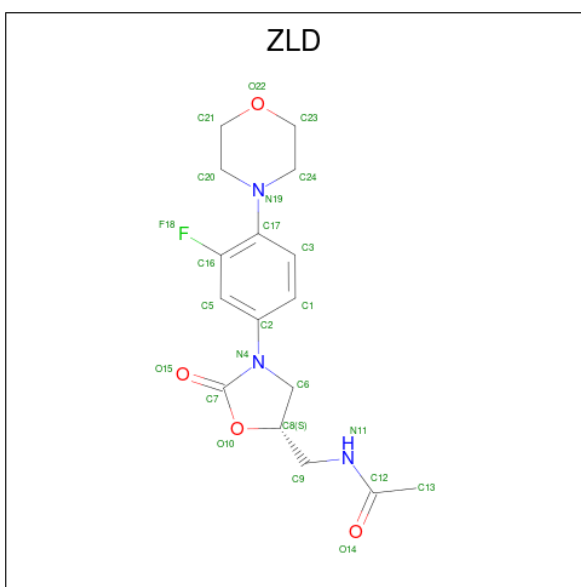
- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	92	Total	C	N	O	S			
			755	458	153	137	7	0	0	0

- Molecule 31 is a RNA chain called 5'-R(*CP*CP*AP*(PHE)*(ACA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	4	Total	C	N	O	P			
			70	37	12	19	2	0	0	0

- Molecule 32 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide (CCD ID: ZLD) (formula: C₁₆H₂₀FN₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	0	1	Total	C	F	N	O	0	0
			24	16	1	3	4		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	84	Total	Mg	0	0
			84	84		
33	9	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	B	1	Total	Mg	0	0
			1	1		
33	J	1	Total	Mg	0	0
			1	1		
33	S	1	Total	Mg	0	0
			1	1		
33	X	1	Total	Mg	0	0
			1	1		
33	1	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	64	Total Na 64 64	0	0
35	9	2	Total Na 2 2	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	I	1	Total Na 1 1	0	0
35	K	1	Total Na 1 1	0	0
35	L	1	Total Na 1 1	0	0
35	P	1	Total Na 1 1	0	0
35	Q	2	Total Na 2 2	0	0
35	R	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	9	Total Cl 9 9	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	I	3	Total Cl 3 3	0	0
36	J	1	Total Cl 1 1	0	0
36	K	1	Total Cl 1 1	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	Q	1	Total 1	Cl 1	0	0
36	X	1	Total 1	Cl 1	0	0
36	2	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	92	Total 92	Sr 92	0	0
37	9	3	Total 3	Sr 3	0	0
37	A	3	Total 3	Sr 3	0	0
37	B	2	Total 2	Sr 2	0	0
37	F	1	Total 1	Sr 1	0	0
37	H	1	Total 1	Sr 1	0	0
37	Q	1	Total 1	Sr 1	0	0
37	R	1	Total 1	Sr 1	0	0
37	S	1	Total 1	Sr 1	0	0
37	Z	2	Total 2	Sr 2	0	0
37	2	1	Total 1	Sr 1	0	0

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

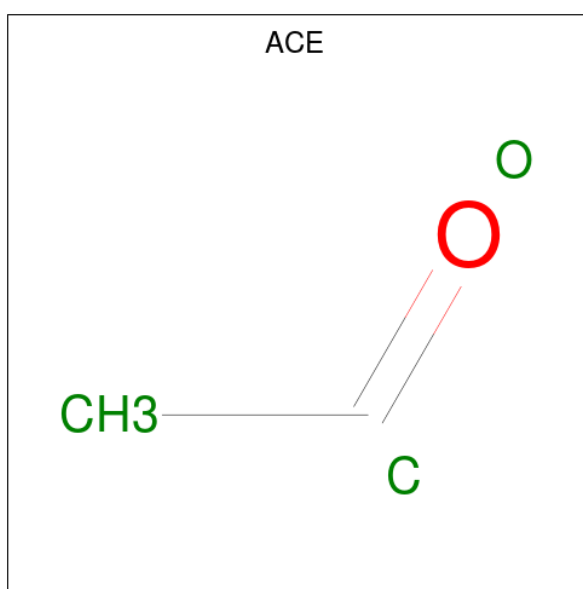
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	N	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	1	Total 1	Cd 1	0	0
38	Y	1	Total 1	Cd 1	0	0
38	Z	1	Total 1	Cd 1	0	0
38	2	1	Total 1	Cd 1	0	0

- Molecule 39 is ACETYL GROUP (CCD ID: ACE) (formula: C_2H_4O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	4	1	Total 3	C 2	O 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5757	Total 5757	O 5757	0	0
40	9	144	Total 144	O 144	0	0
40	A	129	Total 129	O 129	0	0
40	B	158	Total 158	O 158	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	C	183	Total 183	O 183	0	0
40	D	53	Total 53	O 53	0	0
40	E	50	Total 50	O 50	0	0
40	F	25	Total 25	O 25	0	0
40	G	22	Total 22	O 22	0	0
40	H	66	Total 66	O 66	0	0
40	I	57	Total 57	O 57	0	0
40	J	59	Total 59	O 59	0	0
40	K	84	Total 84	O 84	0	0
40	L	136	Total 136	O 136	0	0
40	M	66	Total 66	O 66	0	0
40	N	45	Total 45	O 45	0	0
40	O	70	Total 70	O 70	0	0
40	P	51	Total 51	O 51	0	0
40	Q	84	Total 84	O 84	0	0
40	R	38	Total 38	O 38	0	0
40	S	43	Total 43	O 43	0	0
40	T	28	Total 28	O 28	0	0
40	U	15	Total 15	O 15	0	0
40	V	75	Total 75	O 75	0	0
40	W	28	Total 28	O 28	0	0

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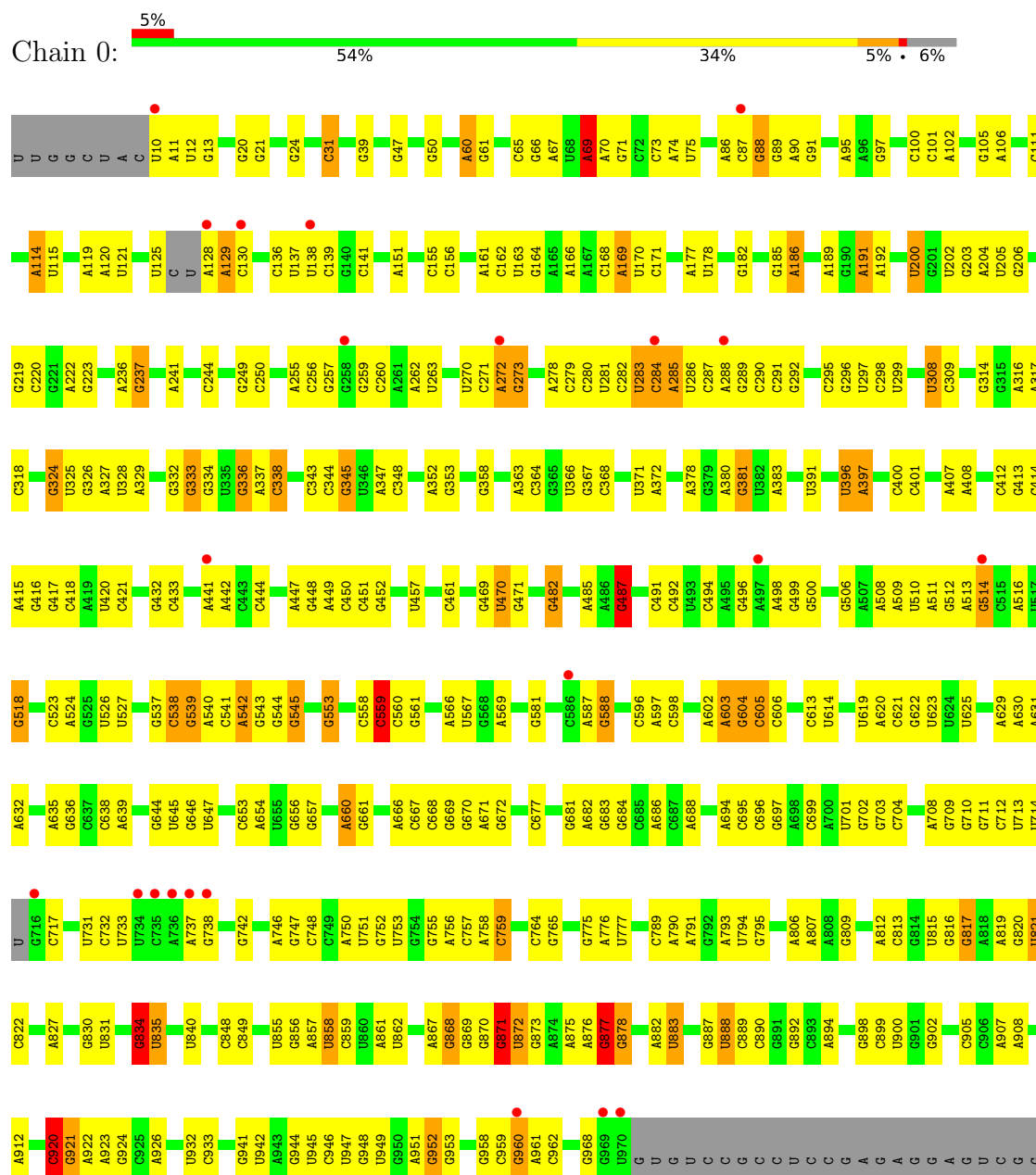
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	X	99	Total 99	O 99	0	0
40	Y	23	Total 23	O 23	0	0
40	Z	58	Total 58	O 58	0	0
40	1	40	Total 40	O 40	0	0
40	2	73	Total 73	O 73	0	0
40	4	3	Total 3	O 3	0	0

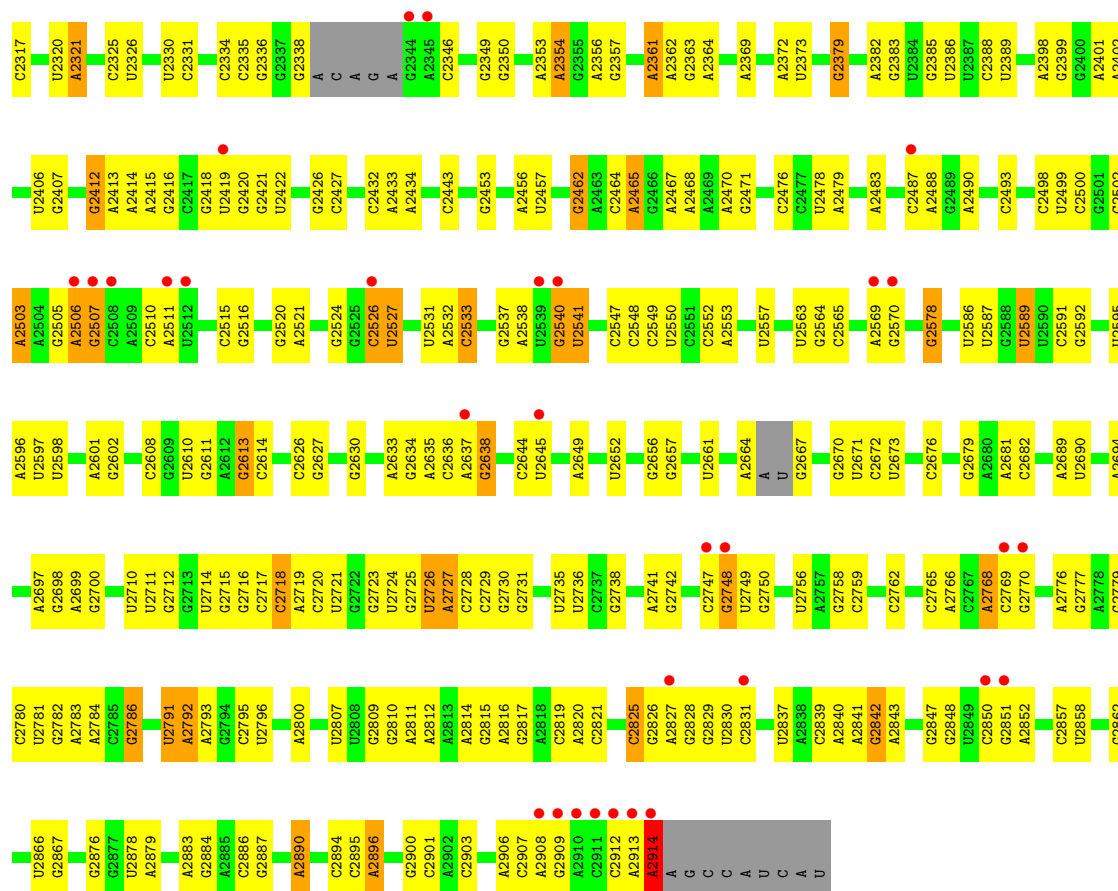
3 Residue-property plots

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.

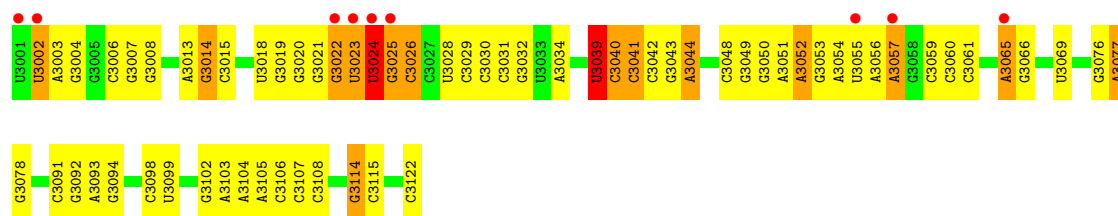
• Molecule 1: 23S RIBOSOMAL RNA



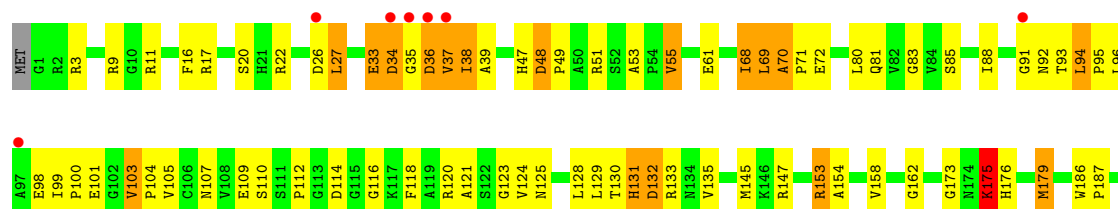




- Molecule 2: 5S RIBOSOMAL RNA

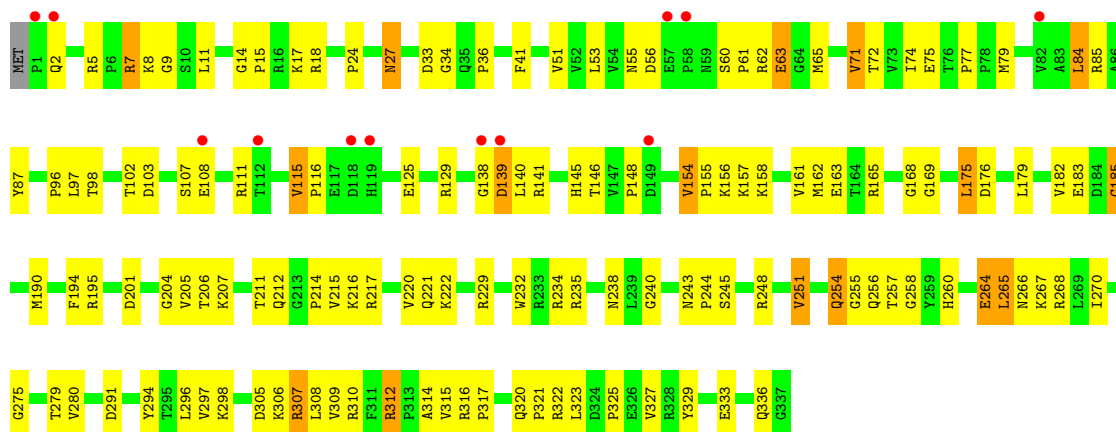


- Molecule 3: 50S ribosomal protein L2P

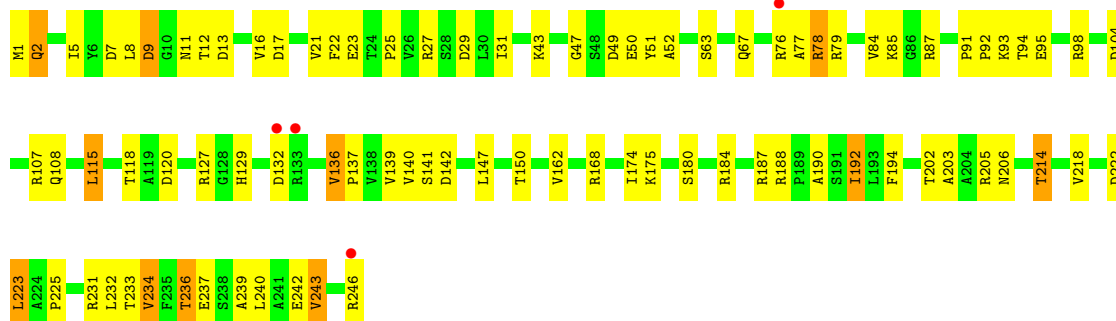




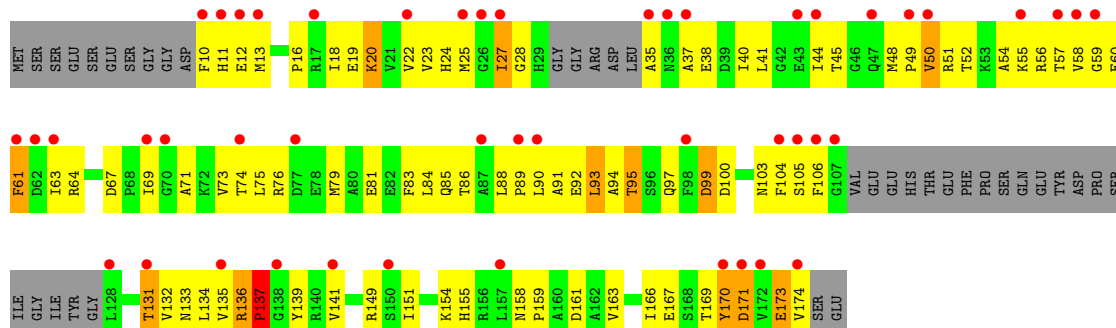
• Molecule 4: 50S ribosomal protein L3P



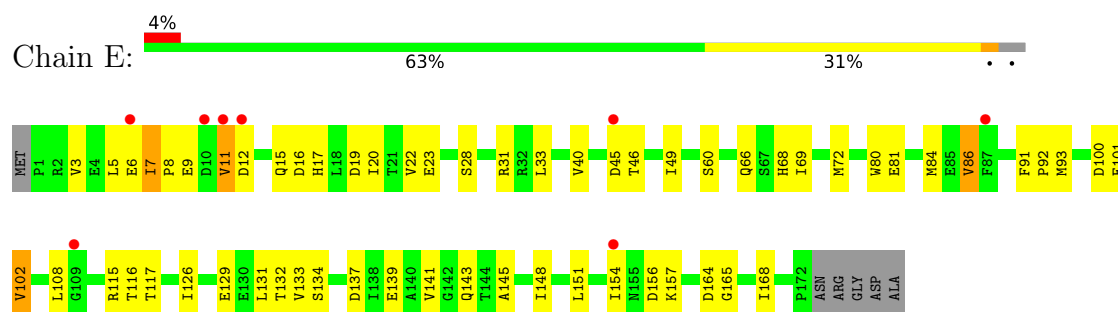
• Molecule 5: 50S ribosomal protein L4P



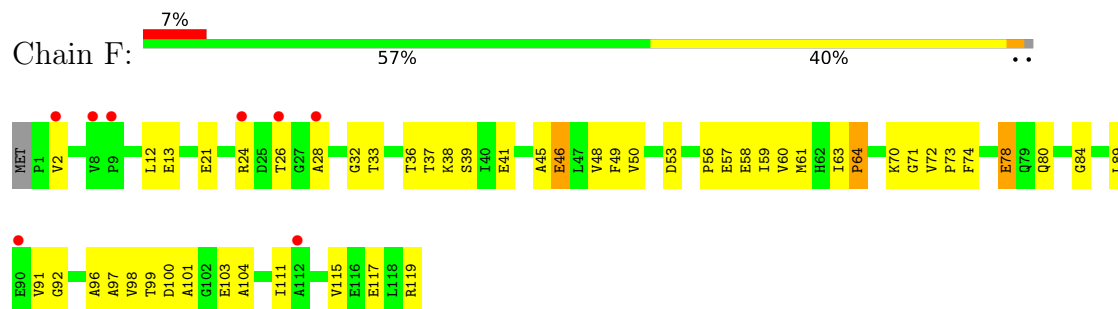
• Molecule 6: 50S ribosomal protein L5P



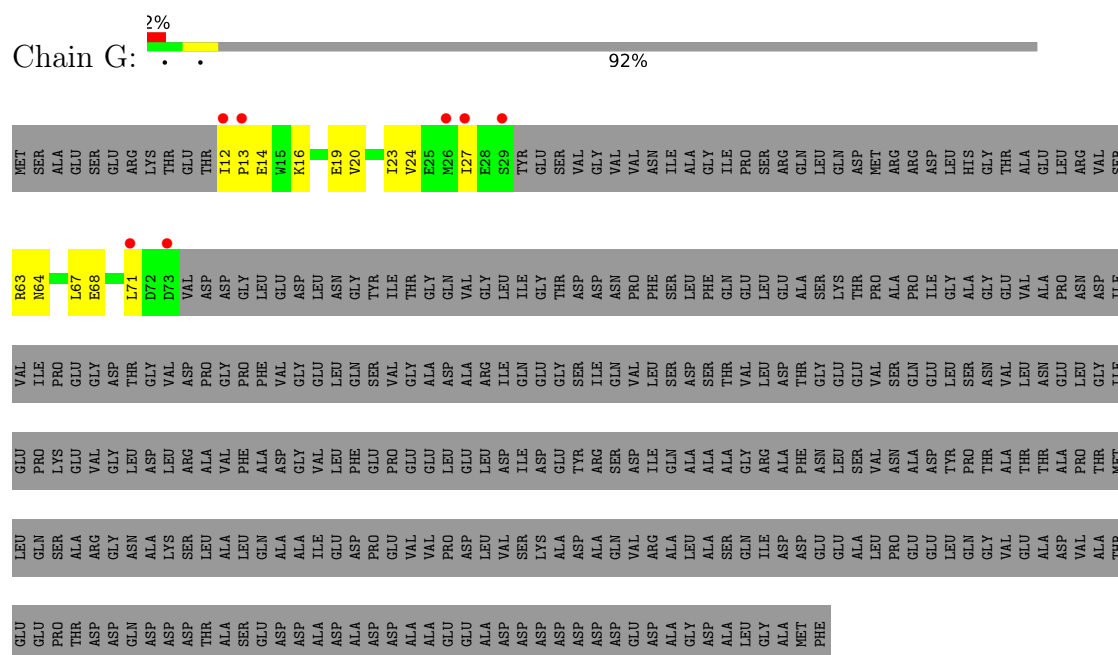
• Molecule 7: 50S ribosomal protein L6P



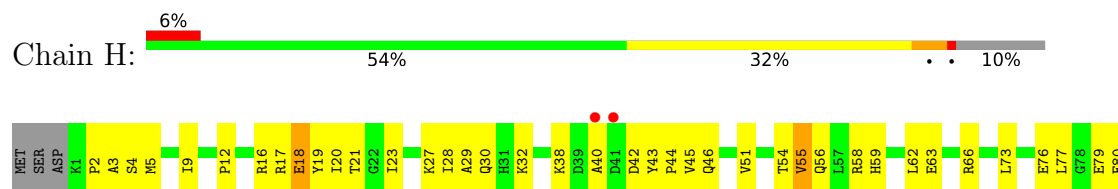
- Molecule 8: 50S ribosomal protein L7Ae

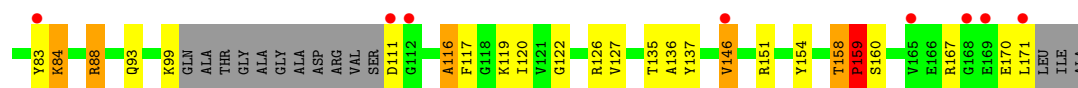


- Molecule 9: 50S ribosomal protein L10E



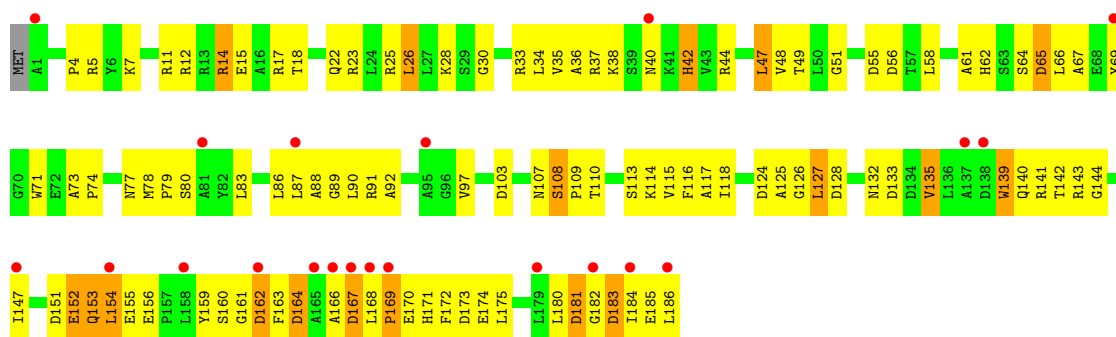
- Molecule 10: 50S ribosomal protein L10e



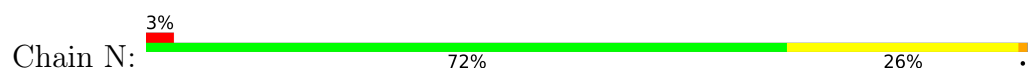


- Molecule 11: 50S ribosomal protein L13P

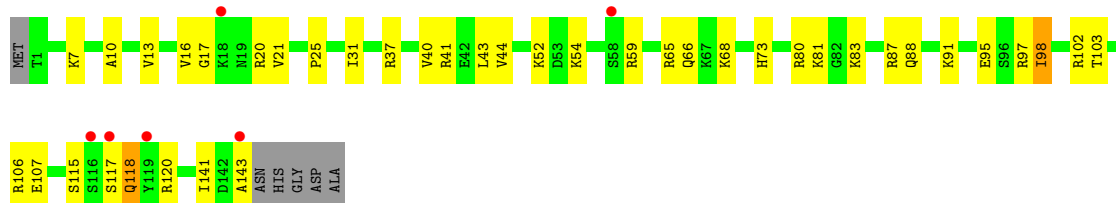




• Molecule 16: 50S ribosomal protein L18e



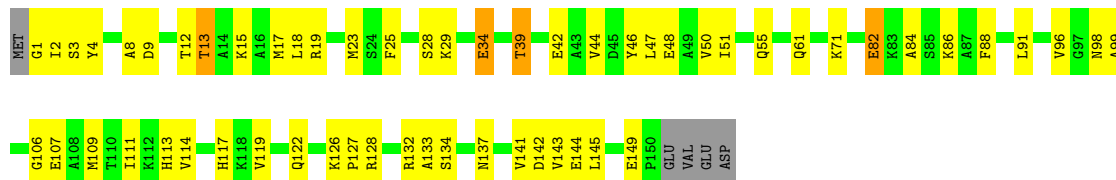
• Molecule 17: 50S ribosomal protein L19e



• Molecule 18: 50S ribosomal protein L21e



• Molecule 19: 50S ribosomal protein L22P



• Molecule 20: 50S ribosomal protein L23P





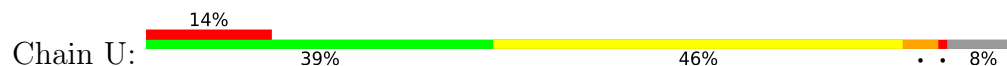
- Molecule 21: 50S ribosomal protein L24P



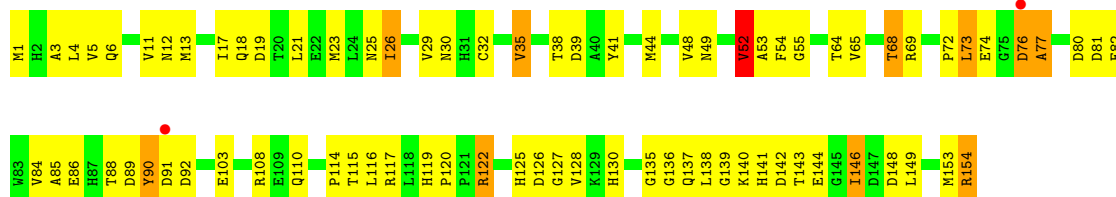
- Molecule 22: 50S ribosomal protein L24e



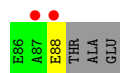
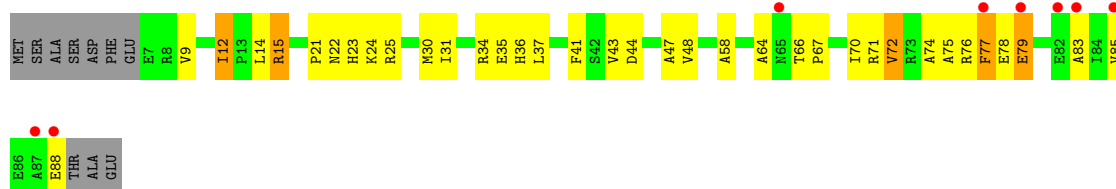
- Molecule 23: 50S ribosomal protein L29P



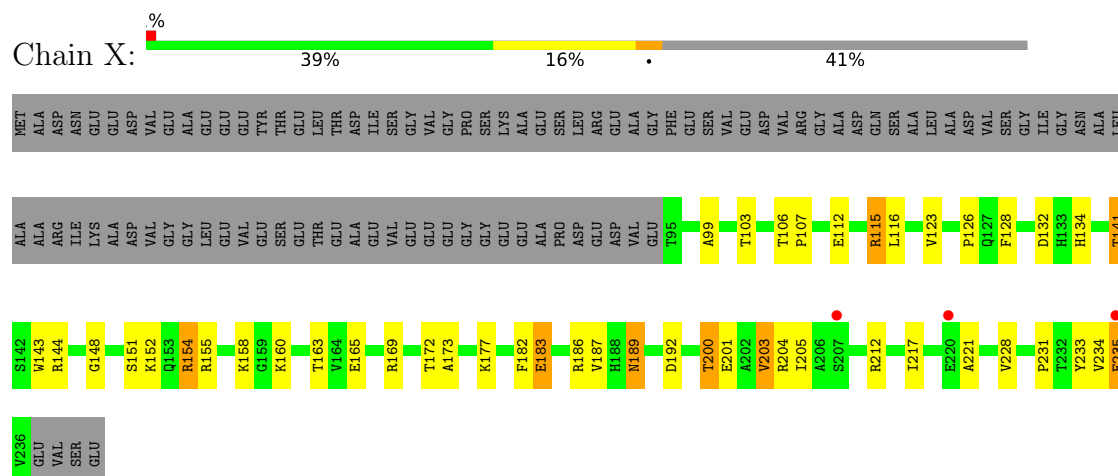
- Molecule 24: 50S ribosomal protein L30P



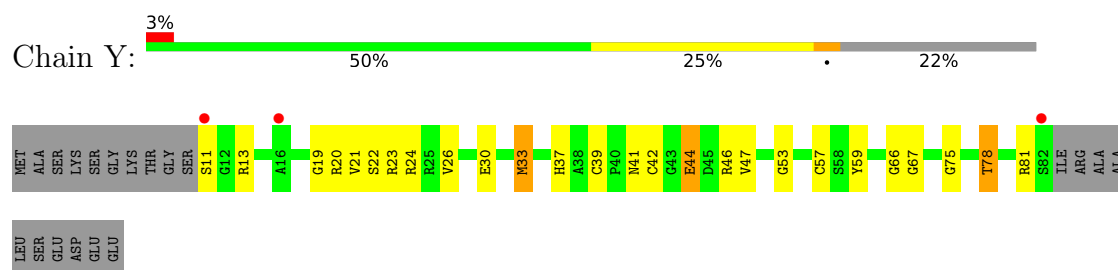
- Molecule 25: 50S ribosomal protein L31e



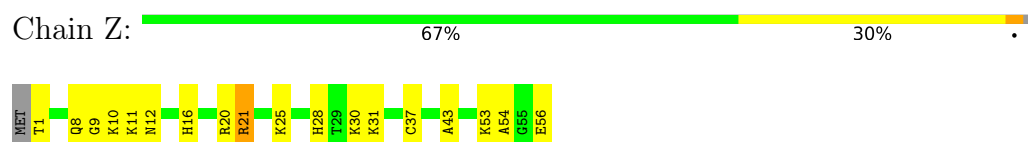
- Molecule 26: 50S ribosomal protein L32e



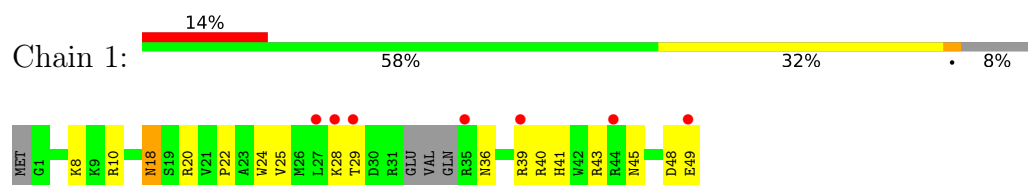
- Molecule 27: 50S ribosomal protein L37Ae



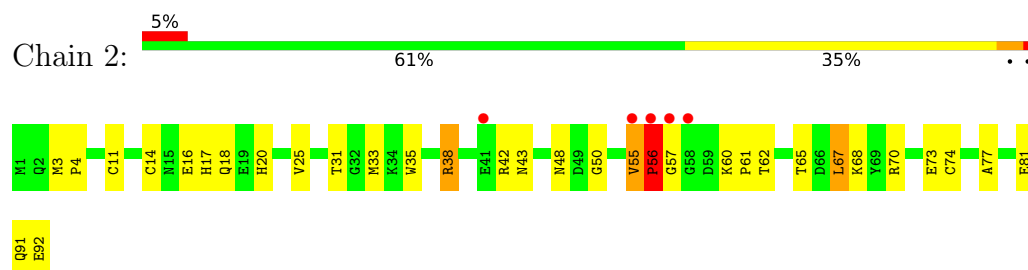
- Molecule 28: 50S ribosomal protein L37e



- Molecule 29: 50S ribosomal protein L39e



- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 5'-R(*CP*CP*AP*(PHE)*(ACA))-3'

Chain 4: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.73Å 298.58Å 575.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.70) 91.5 (40.00-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.69Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.191 , 0.230 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 71.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	98629	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 2.06% 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: ZLD, K, NA, MG, SR, ACE, CD, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.36	1/66075 (0.0%)	0.59	24/103050 (0.0%)
2	9	0.37	0/2905	0.66	4/4528 (0.1%)
3	A	0.46	0/1786	1.00	9/2408 (0.4%)
4	B	0.41	0/2690	0.99	10/3652 (0.3%)
5	C	0.46	0/1885	0.98	6/2552 (0.2%)
6	D	0.36	0/1111	0.95	8/1498 (0.5%)
7	E	0.38	0/1382	0.87	1/1880 (0.1%)
8	F	0.47	0/901	0.87	1/1224 (0.1%)
9	G	0.38	0/241	0.81	0/324
10	H	0.54	0/1302	1.00	8/1743 (0.5%)
11	I	0.41	0/1136	0.91	0/1530
12	J	0.39	0/1004	0.96	2/1351 (0.1%)
13	K	0.37	0/1130	0.98	5/1509 (0.3%)
14	L	0.58	1/1582 (0.1%)	0.95	4/2116 (0.2%)
15	M	0.36	0/1474	1.03	13/1999 (0.7%)
16	N	0.41	0/874	0.93	2/1181 (0.2%)
17	O	0.42	0/1147	0.90	1/1528 (0.1%)
18	P	0.41	0/749	1.04	6/1005 (0.6%)
19	Q	0.43	0/1172	0.96	5/1578 (0.3%)
20	R	0.36	0/648	0.89	3/875 (0.3%)
21	S	0.37	0/958	0.91	4/1289 (0.3%)
22	T	0.39	0/417	0.83	1/562 (0.2%)
23	U	0.36	0/502	0.93	3/675 (0.4%)
24	V	0.46	0/1219	0.96	4/1655 (0.2%)
25	W	0.42	0/664	0.92	3/895 (0.3%)
26	X	0.43	0/1146	0.96	4/1536 (0.3%)
27	Y	0.56	1/578 (0.2%)	1.01	1/773 (0.1%)
28	Z	0.46	0/438	0.96	2/578 (0.3%)
29	1	0.45	0/401	0.82	0/529
30	2	0.39	0/771	0.86	5/1024 (0.5%)
31	4	1.07	0/76	1.15	1/112 (0.9%)
All	All	0.39	3/98364 (0.0%)	0.71	140/147159 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	54
2	9	0	2
24	V	0	1
All	All	0	57

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	L	12	TRP	C-O	-6.94	1.14	1.24
27	Y	33	MET	SD-CE	5.73	1.93	1.79
1	0	559	C	C4-N4	-5.03	1.23	1.33

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	3024	U	C2'-C3'-O3'	12.46	128.19	109.50
1	0	1563	G	C2'-C3'-O3'	10.89	125.84	109.50
1	0	1979	G	C2'-C3'-O3'	10.51	125.27	109.50
6	D	136	ARG	CA-C-N	8.88	130.94	119.84
6	D	136	ARG	C-N-CA	8.88	130.94	119.84
2	9	3024	U	C4'-C3'-O3'	8.49	122.13	109.40
15	M	135	VAL	N-CA-C	-8.40	104.95	113.10
19	Q	141	VAL	N-CA-C	8.37	119.83	108.11
13	K	57	VAL	N-CA-C	-8.25	104.84	112.43
5	C	78	ARG	N-CA-C	7.88	119.62	108.74
4	B	323	LEU	N-CA-C	7.75	120.31	110.24
10	H	170	GLU	N-CA-C	-7.71	99.96	110.68
1	0	1559	A	C2'-C3'-O3'	7.57	125.05	113.70
15	M	169	PRO	N-CA-C	-7.41	104.27	114.27
18	P	47	VAL	CA-C-N	7.26	126.52	118.97
18	P	47	VAL	C-N-CA	7.26	126.52	118.97
6	D	100	ASP	N-CA-C	-7.06	104.67	113.28
25	W	22	ASN	N-CA-C	6.96	119.75	111.33
4	B	265	LEU	N-CA-C	6.88	119.83	110.55
19	Q	137	ASN	N-CA-C	6.85	120.60	110.46
26	X	143	TRP	N-CA-C	6.84	120.30	110.10
2	9	3039	U	N1-C1'-C2'	6.74	122.11	112.00
4	B	157	LYS	N-CA-C	-6.74	105.62	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	205	ARG	N-CA-C	6.72	119.47	111.33
14	L	89	THR	N-CA-C	6.65	118.61	111.36
1	0	871	G	C5'-C4'-O4'	-6.64	99.84	109.80
14	L	8	ILE	N-CA-C	-6.62	104.31	110.53
10	H	116	ALA	N-CA-C	6.62	120.61	112.54
1	0	2338	G	C2'-C3'-O3'	6.61	123.61	113.70
4	B	222	LYS	N-CA-C	-6.58	99.49	109.95
1	0	1592	G	N9-C1'-C2'	6.53	121.79	112.00
7	E	11	VAL	N-CA-C	6.52	119.31	109.20
15	M	117	ALA	N-CA-C	-6.50	104.12	111.14
10	H	88	ARG	N-CA-C	6.45	121.00	113.20
4	B	175	LEU	N-CA-C	-6.44	104.34	111.36
1	0	1120	U	C5'-C4'-C3'	-6.40	106.41	116.00
3	A	222	GLY	N-CA-C	-6.35	106.37	114.37
30	2	67	LEU	N-CA-C	6.33	119.32	109.52
15	M	133	ASP	N-CA-C	6.25	119.75	111.75
21	S	54	ASP	N-CA-C	-6.23	105.64	113.18
5	C	192	ILE	N-CA-C	6.21	118.06	109.80
1	0	2726	U	N1-C1'-C2'	6.20	121.30	112.00
13	K	145	LEU	N-CA-C	-6.14	104.58	111.28
24	V	143	THR	N-CA-C	-6.10	104.69	111.71
1	0	1942	A	C5'-C4'-C3'	6.06	125.08	116.00
23	U	42	ASN	CA-C-N	6.06	127.41	119.84
23	U	42	ASN	C-N-CA	6.06	127.41	119.84
17	O	118	GLN	N-CA-C	-6.04	104.25	111.69
4	B	154	VAL	CA-C-N	6.04	125.75	119.05
4	B	154	VAL	C-N-CA	6.04	125.75	119.05
14	L	123	ASP	N-CA-C	-5.98	100.86	109.29
19	Q	122	GLN	N-CA-C	-5.97	99.47	108.96
20	R	27	ALA	N-CA-C	-5.96	99.02	108.73
3	A	103	VAL	N-CA-C	5.94	114.36	107.89
30	2	43	ASN	N-CA-C	5.91	120.10	113.01
1	0	834	G	C2'-C3'-O3'	-5.88	104.89	113.70
1	0	1819	G	C5'-C4'-C3'	5.85	124.77	116.00
12	J	127	ALA	N-CA-C	-5.84	105.76	114.64
1	0	920	C	C2'-C3'-O3'	-5.83	104.95	113.70
1	0	206	G	C5'-C4'-C3'	-5.82	107.27	116.00
1	0	1504	A	N9-C1'-C2'	5.78	120.67	112.00
3	A	70	ALA	N-CA-C	5.77	116.92	109.65
22	T	50	GLU	N-CA-C	5.77	119.13	111.75
5	C	188	ARG	N-CA-C	5.76	114.94	108.25
4	B	161	VAL	N-CA-C	5.76	116.15	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	153	GLN	N-CA-C	-5.75	105.38	113.20
1	0	1450	C	C4'-C3'-O3'	5.70	121.55	113.00
1	0	2313	C	C5'-C4'-C3'	5.69	124.53	116.00
10	H	160	SER	N-CA-C	-5.68	102.88	110.55
1	0	2914	A	C2'-C3'-O3'	5.66	122.19	113.70
15	M	108	SER	CA-C-N	5.66	126.91	119.84
15	M	108	SER	C-N-CA	5.66	126.91	119.84
6	D	170	TYR	N-CA-C	5.65	119.65	111.56
14	L	13	LYS	N-CA-C	-5.62	105.30	111.82
19	Q	34	GLU	N-CA-C	5.60	117.47	111.36
20	R	57	THR	N-CA-C	5.59	117.91	110.53
12	J	8	VAL	N-CA-C	5.58	116.52	108.48
1	0	883	U	N1-C1'-C2'	5.58	120.36	112.00
18	P	49	ASN	N-CA-C	5.57	118.67	110.59
15	M	42	HIS	N-CA-C	5.56	117.87	109.41
10	H	158	THR	N-CA-C	5.56	122.09	109.81
3	A	38	ILE	N-CA-C	5.55	116.43	108.93
3	A	48	ASP	CA-C-N	5.54	125.37	119.28
3	A	48	ASP	C-N-CA	5.54	125.37	119.28
21	S	52	ARG	N-CA-C	5.53	122.59	110.80
10	H	159	PRO	N-CA-C	5.52	119.35	111.13
13	K	98	GLU	N-CA-C	-5.50	103.12	110.55
15	M	51	GLY	CA-C-N	5.50	125.32	119.28
15	M	51	GLY	C-N-CA	5.50	125.32	119.28
21	S	16	LEU	N-CA-C	5.49	117.70	111.11
4	B	115	VAL	CA-C-N	5.49	126.35	119.98
4	B	115	VAL	C-N-CA	5.49	126.35	119.98
26	X	221	ALA	N-CA-C	-5.47	104.85	112.45
25	W	12	ILE	N-CA-C	5.47	113.28	107.76
28	Z	21	ARG	N-CA-C	5.46	118.07	111.40
3	A	175	LYS	N-CA-C	-5.45	105.25	111.14
6	D	137	PRO	N-CA-C	5.41	123.61	112.47
15	M	30	GLY	N-CA-C	-5.41	107.78	115.30
19	Q	3	SER	N-CA-C	-5.40	100.86	109.23
26	X	183	GLU	N-CA-C	-5.39	100.52	109.46
16	N	23	GLY	N-CA-C	5.38	117.66	111.36
18	P	47	VAL	N-CA-C	5.35	112.43	107.56
1	0	1352	A	C4'-C3'-O3'	5.35	117.42	109.40
21	S	78	THR	N-CA-C	5.34	117.53	109.41
24	V	68	THR	N-CA-C	5.33	117.17	111.36
6	D	48	MET	N-CA-C	5.33	115.72	109.60
5	C	175	LYS	N-CA-C	5.31	117.57	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	V	52	VAL	N-CA-C	5.29	115.27	108.82
1	0	877	G	C2'-C3'-O3'	-5.26	105.80	113.70
6	D	151	ILE	CA-C-N	5.26	125.27	119.90
6	D	151	ILE	C-N-CA	5.26	125.27	119.90
31	4	76	A	C3'-C2'-C1'	5.26	106.77	101.50
1	0	69	A	C5'-C4'-O4'	-5.22	101.97	109.80
3	A	228	ILE	N-CA-C	5.22	115.98	108.93
15	M	14	ARG	N-CA-C	-5.22	105.48	111.07
1	0	1615	A	C5'-C4'-C3'	5.20	123.80	116.00
1	0	714	U	C2'-C3'-O3'	-5.20	101.71	109.50
2	9	3039	U	C4'-C3'-O3'	-5.18	105.23	113.00
13	K	42	ASN	N-CA-C	5.17	119.17	112.86
15	M	171	HIS	N-CA-C	-5.17	105.77	111.71
24	V	25	ASN	N-CA-C	5.16	119.16	112.86
27	Y	24	ARG	N-CA-C	-5.15	105.35	111.69
10	H	122	GLY	N-CA-C	5.15	118.06	110.80
16	N	82	SER	N-CA-C	-5.12	103.63	110.55
10	H	4	SER	N-CA-C	-5.12	106.13	112.38
1	0	2291	A	N9-C1'-C2'	5.12	119.67	112.00
8	F	104	ALA	N-CA-C	-5.12	106.86	114.64
28	Z	43	ALA	N-CA-C	-5.11	105.71	111.28
26	X	123	VAL	N-CA-C	5.11	115.34	110.53
23	U	64	GLY	N-CA-C	-5.10	108.02	115.72
3	A	118	PHE	N-CA-C	5.07	118.02	110.52
30	2	81	GLU	N-CA-C	-5.06	103.46	110.35
25	W	79	GLU	N-CA-C	5.05	119.07	113.01
30	2	55	VAL	CA-C-N	5.05	126.15	119.84
30	2	55	VAL	C-N-CA	5.05	126.15	119.84
5	C	9	ASP	N-CA-C	-5.05	107.16	113.72
20	R	59	ASP	N-CA-C	-5.01	106.59	113.30
18	P	24	SER	CA-C-N	5.01	125.54	120.38
18	P	24	SER	C-N-CA	5.01	125.54	120.38
13	K	12	THR	N-CA-C	5.00	119.37	113.16

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1327	G	Sidechain
1	0	1340	G	Sidechain

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Mol	Chain	Res	Type	Group
1	0	1376	G	Sidechain
1	0	1430	G	Sidechain
1	0	1458	A	Sidechain
1	0	1592	G	Sidechain
1	0	1682	A	Sidechain
1	0	1696	U	Sidechain
1	0	1741	U	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	182	G	Sidechain
1	0	1829	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1979	G	Sidechain
1	0	2102	G	Sidechain
1	0	2412	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2557	U	Sidechain
1	0	2630	G	Sidechain
1	0	2679	G	Sidechain
1	0	270	U	Sidechain
1	0	2714	U	Sidechain
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	324	G	Sidechain
1	0	332	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	482	G	Sidechain
1	0	487	G	Sidechain
1	0	50	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	742	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
1	0	900	U	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	Sidechain
24	V	90	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59016	0	29807	897	0
2	9	2600	0	1326	76	0
3	A	1753	0	1766	107	0
4	B	2625	0	2532	134	0
5	C	1860	0	1813	87	0
6	D	1094	0	1085	96	0
7	E	1357	0	1266	70	0
8	F	890	0	843	46	0
9	G	240	0	231	15	0
10	H	1282	0	1295	62	0
11	I	1120	0	1098	59	0
12	J	994	0	1027	50	0
13	K	1118	0	1076	50	0
14	L	1558	0	1573	60	0
15	M	1445	0	1401	117	0
16	N	865	0	873	28	0
17	O	1136	0	1123	41	0
18	P	735	0	728	19	0
19	Q	1149	0	1122	50	0
20	R	641	0	605	22	0
21	S	950	0	923	38	0
22	T	410	0	364	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	U	499	0	511	40	0
24	V	1196	0	1137	93	0
25	W	654	0	653	34	0
26	X	1130	0	1133	43	0
27	Y	567	0	526	18	0
28	Z	431	0	426	26	0
29	1	396	0	413	25	0
30	2	755	0	728	31	0
31	4	70	0	42	4	0
32	0	24	0	20	0	0
33	0	84	0	0	0	0
33	1	1	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	J	1	0	0	0	0
33	S	1	0	0	0	0
33	X	1	0	0	0	0
34	0	2	0	0	0	0
35	0	64	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	I	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	P	1	0	0	0	0
35	Q	2	0	0	0	0
35	R	1	0	0	0	0
36	0	9	0	0	0	0
36	2	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	I	3	0	0	1	0
36	J	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	1	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	Q	1	0	0	0	0
36	X	1	0	0	0	0
37	0	92	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	2	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	Q	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
37	Z	2	0	0	0	0
38	2	1	0	0	0	0
38	N	1	0	0	0	0
38	T	1	0	0	0	0
38	Y	1	0	0	0	0
38	Z	1	0	0	0	0
39	4	3	0	3	0	0
40	0	5757	0	0	72	0
40	1	40	0	0	1	0
40	2	73	0	0	5	0
40	4	3	0	0	0	0
40	9	144	0	0	5	0
40	A	129	0	0	10	0
40	B	158	0	0	12	0
40	C	183	0	0	12	0
40	D	53	0	0	4	0
40	E	50	0	0	4	0
40	F	25	0	0	2	0
40	G	22	0	0	2	0
40	H	66	0	0	6	0
40	I	57	0	0	3	0
40	J	59	0	0	4	0
40	K	84	0	0	9	0
40	L	136	0	0	5	0
40	M	66	0	0	10	0
40	N	45	0	0	3	0
40	O	70	0	0	1	0
40	P	51	0	0	2	0
40	Q	84	0	0	1	0
40	R	38	0	0	0	0
40	S	43	0	0	5	0
40	T	28	0	0	1	0
40	U	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	V	75	0	0	4	0
40	W	28	0	0	1	0
40	X	99	0	0	4	0
40	Y	23	0	0	2	0
40	Z	58	0	0	1	0
All	All	98629	0	59469	2247	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (2247) 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'	1.21	1.14
5:C:236:THR:HG22	5:C:239:ALA:H	1.07	1.11
19:Q:99:ALA:HB1	19:Q:109:MET:HE1	1.33	1.10
2:9:3023:U:H3'	2:9:3024:U:H5''	1.29	1.09
1:0:156:C:H5''	14:L:171:ARG:HD3	1.37	1.04
1:0:2637:A:H2'	31:4:74:C:H5''	1.35	1.04
2:9:3076:G:H3'	2:9:3077:A:H5''	1.38	1.03
21:S:71:VAL:HG11	21:S:90:PRO:HB3	1.34	1.03
25:W:37:LEU:HD13	25:W:85:VAL:HG21	1.38	1.02
2:9:3006:C:H5''	15:M:37:ARG:HH12	1.25	1.02
2:9:3006:C:H5''	15:M:37:ARG:NH1	1.74	1.02
23:U:12:THR:HG22	23:U:15:GLU:HG3	1.39	1.02
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.40	1.00
24:V:149:LEU:HG	24:V:153:MET:HE2	1.42	1.00
17:O:115:SER:H	17:O:118:GLN:HE21	1.06	1.00
6:D:25:MET:HE2	6:D:41:LEU:HG	1.40	1.00
12:J:29:LEU:HB3	12:J:55:VAL:HG11	1.43	1.00
24:V:88:THR:HG22	24:V:89:ASP:H	1.24	0.99
11:I:19:MET:HE3	11:I:132:LEU:HD11	1.41	0.98
14:L:107:ARG:HH11	14:L:107:ARG:HG3	1.25	0.98
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.45	0.98
4:B:162:MET:HE2	4:B:310:ARG:HD3	1.43	0.97
1:0:1242:A:H5'	11:I:82:THR:HG23	1.44	0.96
24:V:137:GLN:HE21	24:V:141:HIS:HE1	1.09	0.96
5:C:78:ARG:HH11	5:C:78:ARG:HG3	1.29	0.96
20:R:57:THR:HG22	20:R:59:ASP:H	1.26	0.96
1:0:870:G:H2'	1:0:871:G:H5''	1.45	0.95
12:J:10:GLN:H	12:J:10:GLN:NE2	1.62	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:144:GLY:O	15:M:147:ILE:HG22	1.65	0.94
12:J:10:GLN:HE21	12:J:10:GLN:N	1.65	0.94
1:0:871:G:C8	1:0:871:G:H5'	2.01	0.94
1:0:871:G:H5'	1:0:871:G:H8	1.31	0.94
2:9:3056:A:H2'	2:9:3057:A:H5''	1.50	0.93
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.83	0.93
1:0:2812:A:H2	1:0:2814:A:H62	1.16	0.92
24:V:4:LEU:HD22	24:V:52:VAL:HG21	1.51	0.92
8:F:58:GLU:HA	8:F:61:MET:HE2	1.53	0.91
15:M:47:LEU:HD11	15:M:127:LEU:HD21	1.52	0.91
24:V:122:ARG:HG2	24:V:122:ARG:HH11	1.35	0.91
3:A:153:ARG:HB2	3:A:153:ARG:HH11	1.33	0.91
10:H:27:LYS:H	10:H:59:HIS:HD2	1.19	0.90
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.53	0.90
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.51	0.90
4:B:162:MET:HE1	4:B:308:LEU:HD21	1.53	0.89
1:0:1166:A:H1'	1:0:1192:A:C2	2.08	0.89
15:M:113:SER:HB2	40:M:8860:HOH:O	1.72	0.89
1:0:1701:A:H4'	1:0:1702:U:H5''	1.53	0.88
14:L:99:ARG:HH21	14:L:170:ASN:HD22	1.18	0.88
19:Q:8:ALA:HB1	19:Q:13:THR:HG21	1.54	0.88
3:A:211:LYS:HB3	3:A:212:PRO:HD2	1.54	0.88
6:D:154:LYS:H	6:D:154:LYS:HD2	1.39	0.87
11:I:93:ARG:HB3	11:I:93:ARG:HH11	1.39	0.87
12:J:39:GLY:HA2	40:J:4183:HOH:O	1.72	0.87
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.55	0.87
1:0:542:A:H5'	1:0:542:A:H8	1.38	0.87
8:F:91:VAL:HG12	8:F:92:GLY:H	1.40	0.87
1:0:21:G:H5'	19:Q:2:ILE:HA	1.58	0.86
26:X:200:THR:HG22	26:X:201:GLU:HG3	1.54	0.86
30:2:70:ARG:HG2	30:2:77:ALA:HB2	1.58	0.86
4:B:238:ASN:HD22	4:B:240:GLY:H	1.24	0.86
15:M:83:LEU:HD13	15:M:175:LEU:HD23	1.56	0.86
5:C:236:THR:HG22	5:C:239:ALA:N	1.90	0.86
6:D:27:ILE:HG22	6:D:28:GLY:H	1.41	0.85
20:R:51:GLN:HE21	20:R:53:ASN:HD21	1.24	0.85
24:V:6:GLN:HB2	24:V:26:ILE:HD12	1.58	0.85
1:0:2506:A:O2'	1:0:2507:G:H8	1.60	0.85
12:J:74:VAL:HG13	12:J:113:ILE:HG23	1.56	0.85
1:0:2586:U:H3	1:0:2592:G:H22	1.23	0.85
5:C:104:ASP:HA	5:C:107:ARG:HH12	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.58	0.85
14:L:102:GLU:OE1	14:L:164:THR:HG21	1.77	0.84
24:V:88:THR:HG22	24:V:89:ASP:N	1.91	0.84
1:O:2717:C:C2'	1:O:2718:C:H5''	2.08	0.83
1:O:2840:A:OP1	4:B:211:THR:HG23	1.78	0.83
28:Z:25:LYS:HD2	29:1:49:GLU:H	1.42	0.83
1:O:1160:G:H5'	1:O:1161:A:C5'	2.06	0.83
10:H:167:ARG:HD2	40:H:8990:HOH:O	1.78	0.83
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.13	0.83
16:N:47:ARG:HG3	16:N:47:ARG:HH11	1.44	0.83
1:O:2637:A:H2'	31:4:74:C:C5'	2.09	0.82
22:T:20:MET:HE2	22:T:30:HIS:NE2	1.94	0.82
1:O:1603:A:H5'	1:O:1605:G:O4'	1.79	0.82
7:E:15:GLN:HG3	7:E:20:ILE:HG12	1.59	0.82
1:O:560:C:H42	1:O:597:A:H61	1.26	0.82
1:O:1835:U:H5	1:O:1840:A:N7	1.78	0.82
12:J:4:LEU:HD22	12:J:116:GLU:HB3	1.61	0.82
6:D:20:LYS:HA	6:D:75:LEU:O	1.80	0.82
1:O:541:C:C2'	1:O:542:A:H5''	2.10	0.82
23:U:1:THR:HG23	23:U:2:VAL:H	1.45	0.82
1:O:289:G:H22	1:O:363:A:H2	1.28	0.81
11:I:74:ARG:HB3	11:I:74:ARG:HH11	1.45	0.81
24:V:88:THR:HB	40:V:6679:HOH:O	1.81	0.81
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.63	0.81
2:9:3023:U:C3'	2:9:3024:U:H5''	2.11	0.80
1:O:1119:G:N2	1:O:1246:A:C2	2.50	0.80
24:V:88:THR:HG23	24:V:110:GLN:NE2	1.95	0.80
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.11	0.80
2:9:3025:G:H3'	2:9:3026:C:C5'	2.12	0.80
6:D:105:SER:HB2	6:D:131:THR:HG23	1.63	0.80
1:O:2694:A:H4'	7:E:91:PHE:HE1	1.47	0.80
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.64	0.80
15:M:38:LYS:HE2	15:M:107:ASN:ND2	1.96	0.80
1:O:541:C:H2'	1:O:542:A:H5''	1.64	0.79
1:O:1160:G:C5'	1:O:1161:A:H5'	2.07	0.79
1:O:2506:A:HO2'	1:O:2507:G:H8	0.80	0.79
3:A:179:MET:HA	3:A:179:MET:HE3	1.64	0.79
1:O:870:G:C2'	1:O:871:G:H5''	2.10	0.79
1:O:962:C:H1'	15:M:5:ARG:NH1	1.96	0.79
19:Q:17:MET:HE1	19:Q:19:ARG:NH2	1.97	0.79
12:J:74:VAL:HG11	12:J:113:ILE:HG12	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2054:A:N3	19:Q:128:ARG:NH2	2.30	0.79
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.65	0.79
1:0:288:A:H61	1:0:364:C:H42	1.31	0.79
24:V:88:THR:HG23	24:V:110:GLN:HE21	1.47	0.79
21:S:9:LYS:HE3	21:S:13:ARG:NH1	1.98	0.78
26:X:187:VAL:HG23	26:X:192:ASP:HB2	1.63	0.78
15:M:87:LEU:HD12	15:M:186:LEU:HD21	1.66	0.78
24:V:137:GLN:HE21	24:V:141:HIS:CE1	1.99	0.78
16:N:32:ARG:O	16:N:32:ARG:HD3	1.82	0.78
14:L:107:ARG:HG3	14:L:107:ARG:NH1	1.98	0.78
28:Z:21:ARG:HD2	28:Z:37:CYS:SG	2.24	0.78
29:1:41:HIS:H	29:1:45:ASN:HD22	1.28	0.78
2:9:3023:U:H3'	2:9:3024:U:C5'	2.13	0.78
2:9:3051:A:H5'	15:M:160:SER:HB3	1.64	0.78
10:H:45:VAL:HA	10:H:167:ARG:O	1.83	0.77
25:W:15:ARG:HB3	25:W:15:ARG:HH11	1.49	0.77
24:V:21:LEU:HD21	24:V:48:VAL:HG11	1.65	0.77
1:0:2717:C:O2'	1:0:2718:C:H5''	1.84	0.77
12:J:10:GLN:H	12:J:10:GLN:HE21	0.82	0.77
20:R:57:THR:HG22	20:R:59:ASP:N	1.98	0.77
14:L:134:ILE:HG23	14:L:141:ILE:HD13	1.65	0.77
3:A:191:GLY:HA2	3:A:194:MET:CE	2.13	0.77
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.66	0.77
11:I:19:MET:HE2	11:I:79:PHE:HA	1.67	0.77
3:A:199:HIS:HD2	3:A:201:PHE:H	1.33	0.77
24:V:5:VAL:HG11	24:V:153:MET:HE1	1.66	0.77
1:0:21:G:C5'	19:Q:2:ILE:HA	2.15	0.76
1:0:1474:C:H6	1:0:1474:C:H5'	1.50	0.76
3:A:35:GLY:O	3:A:36:ASP:HB3	1.85	0.76
25:W:30:MET:HE1	25:W:58:ALA:HB3	1.66	0.76
24:V:84:VAL:HG12	40:V:6679:HOH:O	1.85	0.76
1:0:1116:U:H3	1:0:1246:A:H62	1.32	0.76
9:G:12:ILE:N	9:G:13:PRO:HD3	2.00	0.76
2:9:3024:U:O2'	2:9:3025:G:H4'	1.85	0.76
2:9:3025:G:H3'	2:9:3026:C:H5'	1.66	0.76
1:0:1209:C:H2'	1:0:1210:G:H8	1.50	0.76
30:2:25:VAL:HG22	30:2:68:LYS:HG3	1.67	0.76
17:O:115:SER:OG	17:O:118:GLN:HG3	1.86	0.76
1:0:2676:C:H4'	11:I:70:PHE:CE1	2.20	0.75
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.22	0.75
2:9:3092:G:H2'	2:9:3093:A:C8	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.67	0.75
1:O:2780:C:H1'	7:E:143:GLN:HE21	1.51	0.75
19:Q:9:ASP:O	19:Q:13:THR:HB	1.87	0.75
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.67	0.75
1:O:544:G:H2'	1:O:545:G:H5''	1.69	0.74
1:O:545:G:H5'	1:O:545:G:H8	1.52	0.74
3:A:153:ARG:HH11	3:A:153:ARG:CB	2.00	0.74
7:E:6:GLU:HA	7:E:46:THR:HG22	1.70	0.74
11:I:45:VAL:HG23	11:I:130:VAL:O	1.87	0.74
12:J:32:ILE:HD11	12:J:56:SER:HB3	1.68	0.74
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.70	0.74
4:B:62:ARG:HA	4:B:65:MET:HE3	1.67	0.74
12:J:14:LYS:HB2	12:J:45:PRO:HG2	1.68	0.74
1:O:506:G:H22	1:O:509:A:C5'	2.00	0.74
1:O:1751:G:H2'	1:O:1752:G:H5''	1.69	0.74
1:O:1165:G:H4'	1:O:1174:A:O2'	1.88	0.73
1:O:871:G:H8	1:O:871:G:C5'	2.02	0.73
1:O:2890:A:H1'	22:T:56:ARG:NH2	2.03	0.73
3:A:200:PRO:HG2	3:A:225:VAL:HG21	1.70	0.73
1:O:2420:G:O2'	1:O:2421:G:H5'	1.87	0.73
8:F:91:VAL:HG12	8:F:92:GLY:N	2.02	0.73
24:V:21:LEU:HD22	24:V:26:ILE:CD1	2.19	0.73
23:U:39:ALA:N	23:U:40:PRO:HD2	2.03	0.73
10:H:21:THR:O	10:H:120:ILE:HD12	1.89	0.73
19:Q:18:LEU:HD12	19:Q:143:VAL:HG11	1.70	0.73
1:O:284:C:H4'	1:O:285:A:O5'	1.89	0.72
15:M:48:VAL:CG1	15:M:55:ASP:HB3	2.19	0.72
29:1:18:ASN:HD21	29:1:40:ARG:H	1.34	0.72
24:V:80:ASP:O	24:V:84:VAL:HG23	1.88	0.72
10:H:27:LYS:N	10:H:59:HIS:HD2	1.86	0.72
15:M:38:LYS:HE2	15:M:107:ASN:HD21	1.54	0.72
1:O:657:G:OP1	5:C:27:ARG:NH2	2.21	0.72
2:9:3039:U:H1'	2:9:3044:A:H61	1.53	0.72
24:V:21:LEU:HD22	24:V:26:ILE:HD11	1.72	0.72
2:9:3006:C:C5'	15:M:37:ARG:HH12	2.01	0.72
1:O:2505:G:O2'	1:O:2506:A:H5'	1.90	0.72
2:9:3029:C:H2'	2:9:3030:C:H5'	1.71	0.72
1:O:2716:G:H5''	4:B:206:THR:HG21	1.71	0.72
13:K:143:THR:HG22	13:K:144:ASP:N	2.05	0.72
15:M:49:THR:HG22	15:M:56:ASP:HB2	1.72	0.72
1:O:877:G:H5'	1:O:878:G:OP1	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:91:LYS:O	17:O:95:GLU:HG3	1.90	0.72
1:O:2831:C:O3'	19:Q:71:LYS:HE2	1.90	0.71
3:A:153:ARG:HB2	3:A:153:ARG:NH1	2.05	0.71
1:O:1164:U:H4'	1:O:1165:G:OP1	1.89	0.71
1:O:1182:C:H1'	1:O:1192:A:H8	1.56	0.71
4:B:275:GLY:O	4:B:291:ASP:HA	1.90	0.71
15:M:80:SER:HB2	40:M:8837:HOH:O	1.90	0.71
15:M:183:ASP:OD2	15:M:186:LEU:HD12	1.88	0.71
23:U:8:ILE:HA	23:U:11:MET:HE3	1.71	0.71
4:B:162:MET:HE2	4:B:310:ARG:CD	2.19	0.71
1:O:282:C:H1'	1:O:368:C:N4	2.05	0.71
1:O:1116:U:HO2'	1:O:1118:A:H2	1.36	0.71
1:O:2717:C:H2'	1:O:2718:C:H5''	1.73	0.71
24:V:68:THR:HG23	24:V:69:ARG:HG2	1.73	0.71
1:O:1666:C:H2'	1:O:1667:A:H5'	1.73	0.71
1:O:1819:G:H2'	1:O:1820:G:H4'	1.72	0.71
2:9:3056:A:C2'	2:9:3057:A:H5''	2.21	0.71
10:H:56:GLN:NE2	10:H:126:ARG:HE	1.89	0.71
21:S:49:GLU:OE2	21:S:97:ARG:HD2	1.90	0.71
24:V:88:THR:CG2	24:V:89:ASP:H	1.99	0.71
25:W:72:VAL:HG22	25:W:85:VAL:HG12	1.72	0.70
30:2:62:THR:HB	40:2:8981:HOH:O	1.90	0.70
1:O:1244:U:OP1	11:I:18:ILE:HD13	1.91	0.70
4:B:179:LEU:O	4:B:183:GLU:HG2	1.90	0.70
17:O:115:SER:H	17:O:118:GLN:NE2	1.85	0.70
1:O:371:U:H2'	1:O:372:A:H8	1.55	0.70
1:O:1119:G:H2'	11:I:52:GLN:NE2	2.05	0.70
1:O:2468:A:H61	30:2:48:ASN:HD21	1.40	0.70
6:D:54:ALA:CB	6:D:69:ILE:HD12	2.21	0.70
1:O:541:C:H2'	1:O:542:A:C5'	2.21	0.70
1:O:1641:A:H2'	1:O:1642:A:H5'	1.73	0.70
1:O:1701:A:H4'	1:O:1702:U:C5'	2.20	0.70
10:H:20:ILE:HG23	10:H:120:ILE:HD11	1.73	0.70
23:U:55:ARG:O	23:U:59:ILE:HG12	1.91	0.70
1:O:2827:A:H2'	1:O:2828:G:O4'	1.91	0.70
1:O:2769:C:H2'	1:O:2770:G:O4'	1.92	0.70
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.72	0.70
5:C:104:ASP:HA	5:C:107:ARG:NH1	2.06	0.70
13:K:67:ARG:O	13:K:71:GLU:HG3	1.92	0.69
1:O:1189:A:H1'	1:O:1209:C:O4'	1.92	0.69
27:Y:11:SER:HB3	27:Y:23:ARG:HB2	1.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.57	0.69
2:9:3006:C:C5'	15:M:37:ARG:NH1	2.53	0.69
5:C:76:ARG:HG2	5:C:78:ARG:NH1	2.07	0.69
11:I:74:ARG:O	11:I:78:ILE:HG12	1.92	0.69
3:A:33:GLU:O	3:A:34:ASP:HB2	1.92	0.69
24:V:137:GLN:NE2	24:V:141:HIS:HE1	1.87	0.69
1:0:470:U:O2'	28:Z:16:HIS:HD2	1.76	0.69
1:0:506:G:H22	1:0:509:A:H5'	1.56	0.69
1:0:1116:U:O2'	1:0:1118:A:H2	1.76	0.69
1:0:2851:G:O2'	1:0:2852:A:H5'	1.92	0.69
3:A:199:HIS:CD2	3:A:201:PHE:H	2.09	0.69
13:K:90:ARG:NH2	13:K:121:ILE:HD11	2.08	0.69
17:O:80:ARG:HG2	17:O:87:ARG:CZ	2.22	0.69
24:V:125:HIS:CD2	24:V:127:GLY:H	2.11	0.69
24:V:141:HIS:HB2	24:V:146:ILE:HG12	1.75	0.69
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.93	0.69
19:Q:18:LEU:HB2	19:Q:143:VAL:HG12	1.73	0.69
23:U:12:THR:HG22	23:U:15:GLU:CG	2.18	0.69
24:V:125:HIS:HD2	24:V:127:GLY:H	1.39	0.69
1:0:1209:C:H2'	1:0:1210:G:C8	2.28	0.69
1:0:2502:C:C2'	1:0:2503:A:H5'	2.23	0.69
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.28	0.69
19:Q:25:PHE:CE2	19:Q:29:LYS:HE2	2.28	0.68
12:J:81:ARG:HB2	12:J:87:ARG:NH1	2.09	0.68
2:9:3023:U:H4'	2:9:3024:U:OP2	1.93	0.68
12:J:81:ARG:HB2	12:J:87:ARG:HH11	1.57	0.68
14:L:80:GLY:O	14:L:81:ARG:HD2	1.94	0.68
26:X:187:VAL:HG23	26:X:192:ASP:CB	2.23	0.68
1:0:2005:G:H3'	1:0:2005:G:OP2	1.94	0.68
19:Q:106:GLY:HA2	19:Q:109:MET:HE3	1.76	0.68
25:W:78:GLU:HG2	25:W:79:GLU:H	1.59	0.68
24:V:6:GLN:HB2	24:V:26:ILE:CD1	2.23	0.68
30:2:65:THR:HG23	30:2:67:LEU:HG	1.74	0.68
1:0:2346:C:O2'	6:D:52:THR:HG21	1.93	0.68
1:0:2908:A:H2'	1:0:2909:G:O4'	1.92	0.68
7:E:154:ILE:HD11	7:E:157:LYS:HB2	1.76	0.68
25:W:71:ARG:HB3	25:W:88:GLU:OE1	1.93	0.68
5:C:236:THR:CG2	5:C:239:ALA:H	1.96	0.68
1:0:544:G:C2'	1:0:545:G:H5''	2.23	0.67
2:9:3006:C:OP1	15:M:37:ARG:NH1	2.27	0.67
4:B:258:GLY:H	4:B:260:HIS:CE1	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:68:HIS:O	7:E:72:MET:HG3	1.95	0.67
26:X:154:ARG:HH12	26:X:155:ARG:HG3	1.59	0.67
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.02	0.67
6:D:86:THR:O	6:D:90:LEU:HG	1.94	0.67
6:D:99:ASP:HB2	6:D:103:ASN:HB2	1.74	0.67
1:O:432:G:O2'	1:O:433:C:H5'	1.95	0.67
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.24	0.67
17:O:59:ARG:NH2	17:O:66:GLN:HE22	1.91	0.67
24:V:122:ARG:NH2	24:V:154:ARG:OXT	2.27	0.67
1:O:1116:U:O2'	1:O:1118:A:C2	2.48	0.67
3:A:101:GLU:OE2	3:A:131:HIS:HB2	1.95	0.67
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.25	0.67
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.76	0.67
17:O:10:ALA:HA	17:O:13:VAL:HG12	1.76	0.67
6:D:25:MET:HE3	6:D:37:ALA:HB1	1.76	0.67
1:O:20:G:H21	19:Q:117:HIS:HD2	1.42	0.67
14:L:24:GLN:NE2	14:L:27:ARG:HH11	1.92	0.67
1:O:450:C:OP1	5:C:184:ARG:NH2	2.26	0.67
1:O:1450:C:H4'	1:O:1451:C:OP2	1.95	0.67
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.77	0.67
5:C:1:MET:HG2	5:C:2:GLN:H	1.60	0.67
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.77	0.67
6:D:170:TYR:O	6:D:171:ASP:HB3	1.95	0.67
10:H:167:ARG:CD	40:H:8990:HOH:O	2.38	0.67
21:S:41:ARG:HG2	21:S:41:ARG:HH11	1.60	0.67
28:Z:25:LYS:HD2	29:1:49:GLU:N	2.10	0.67
1:O:1118:A:H8	1:O:1118:A:H3'	1.60	0.66
6:D:19:GLU:O	6:D:20:LYS:HG2	1.95	0.66
24:V:21:LEU:HD21	24:V:48:VAL:CG1	2.25	0.66
4:B:53:LEU:HD11	4:B:327:VAL:HG22	1.75	0.66
22:T:17:THR:HG22	22:T:18:GLY:N	2.10	0.66
2:9:3020:G:O2'	2:9:3021:G:H5'	1.95	0.66
6:D:25:MET:CE	6:D:37:ALA:HB1	2.25	0.66
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.76	0.66
10:H:29:ALA:HB3	10:H:66:ARG:HH12	1.60	0.66
1:O:1377:C:H5'	1:O:1377:C:H6	1.60	0.66
10:H:58:ARG:HH11	10:H:58:ARG:HG3	1.60	0.66
21:S:9:LYS:HE3	21:S:13:ARG:HH11	1.57	0.66
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.76	0.66
15:M:61:ALA:HB3	15:M:88:ALA:HB2	1.77	0.66
26:X:189:ASN:HA	26:X:217:ILE:HD11	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:27:ARG:HG3	5:C:29:ASP:OD1	1.94	0.66
23:U:20:LEU:HD22	23:U:60:GLN:HE22	1.60	0.66
24:V:13:MET:HE2	24:V:18:GLN:HA	1.78	0.66
24:V:122:ARG:HH11	24:V:122:ARG:CG	2.07	0.66
27:Y:30:GLU:HA	27:Y:33:MET:HE3	1.78	0.66
15:M:164:ASP:CG	15:M:167:ASP:HA	2.19	0.66
21:S:61:GLU:HG3	40:S:3851:HOH:O	1.95	0.66
15:M:71:TRP:CE3	15:M:175:LEU:HD22	2.31	0.66
8:F:37:THR:O	8:F:41:GLU:HG3	1.95	0.66
1:O:2547:C:OP2	4:B:5:ARG:NH1	2.29	0.65
3:A:36:ASP:HA	3:A:83:GLY:HA3	1.78	0.65
21:S:47:THR:HB	21:S:100:ASP:HB3	1.78	0.65
12:J:49:LEU:HD12	12:J:80:ILE:HG21	1.79	0.65
20:R:51:GLN:NE2	20:R:53:ASN:HD21	1.94	0.65
8:F:58:GLU:OE1	14:L:27:ARG:NH2	2.28	0.65
11:I:107:ASN:ND2	11:I:109:TYR:H	1.94	0.65
12:J:34:VAL:HG22	12:J:47:ALA:HB2	1.79	0.65
1:O:1201:C:H5''	40:O:6599:HOH:O	1.96	0.65
1:O:2526:C:O2'	1:O:2527:U:H5'	1.97	0.65
2:9:3039:U:H1'	2:9:3044:A:N6	2.10	0.65
20:R:10:VAL:HG11	23:U:36:ALA:HA	1.76	0.65
1:O:2414:A:H2'	1:O:2415:A:C8	2.32	0.65
1:O:559:C:H6	1:O:559:C:H5'	1.62	0.65
6:D:95:THR:C	6:D:97:GLN:H	2.05	0.65
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.78	0.65
15:M:155:GLU:O	15:M:156:GLU:HG3	1.97	0.65
25:W:66:THR:HG23	25:W:67:PRO:HD2	1.77	0.65
6:D:64:ARG:HG2	6:D:67:ASP:HB3	1.78	0.65
15:M:152:GLU:C	15:M:154:LEU:H	2.03	0.65
5:C:162:VAL:HG12	5:C:192:ILE:HD11	1.76	0.65
6:D:57:THR:HG23	6:D:63:ILE:HG22	1.79	0.65
2:9:3025:G:C3'	2:9:3026:C:H5'	2.27	0.65
1:O:1462:C:H2'	1:O:1463:A:C8	2.32	0.64
1:O:2502:C:H2'	1:O:2503:A:H5'	1.79	0.64
3:A:131:HIS:O	3:A:132:ASP:HB2	1.95	0.64
4:B:62:ARG:HA	4:B:65:MET:CE	2.26	0.64
11:I:74:ARG:HH11	11:I:74:ARG:CB	2.10	0.64
21:S:9:LYS:CE	21:S:13:ARG:NH1	2.59	0.64
23:U:56:ILE:O	23:U:60:GLN:HG3	1.96	0.64
8:F:58:GLU:CD	14:L:27:ARG:HH22	2.04	0.64
22:T:39:ASN:ND2	22:T:44:ARG:HH11	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:74:ALA:HB2	25:W:85:VAL:HG13	1.79	0.64
1:0:281:U:H2'	1:0:282:C:O4'	1.97	0.64
1:0:289:G:N2	1:0:363:A:H2	1.93	0.64
1:0:558:C:O2'	1:0:559:C:H5''	1.96	0.64
24:V:13:MET:HE3	24:V:17:ILE:HG22	1.77	0.64
27:Y:11:SER:CB	27:Y:23:ARG:HB2	2.27	0.64
28:Z:10:LYS:HG3	40:Z:8984:HOH:O	1.97	0.64
1:0:1234:U:N3	4:B:244:PRO:HB3	2.12	0.64
10:H:46:GLN:HE21	10:H:137:TYR:HE2	1.43	0.64
21:S:32:ARG:NH1	21:S:38:ARG:HH12	1.96	0.64
8:F:2:VAL:HG22	8:F:57:GLU:OE1	1.97	0.64
14:L:164:THR:HG22	14:L:167:GLY:H	1.63	0.64
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.79	0.64
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.78	0.64
27:Y:53:GLY:HA2	27:Y:67:GLY:O	1.98	0.64
1:0:1878:G:O2'	1:0:1879:U:C6	2.51	0.64
1:0:1942:A:H3'	40:0:7683:HOH:O	1.98	0.64
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.79	0.64
1:0:775:G:OP1	28:Z:16:HIS:HE1	1.81	0.64
1:0:1118:A:H3'	1:0:1118:A:C8	2.33	0.64
1:0:1170:U:O2'	1:0:1172:G:N7	2.29	0.64
8:F:96:ALA:HA	40:F:3111:HOH:O	1.96	0.64
24:V:13:MET:HE2	24:V:18:GLN:CA	2.29	0.64
1:0:1118:A:H8	1:0:1119:G:H5''	1.64	0.63
1:0:2878:U:H2'	1:0:2879:A:O4'	1.99	0.63
11:I:45:VAL:HG21	11:I:129:PHE:CD1	2.33	0.63
15:M:169:PRO:O	15:M:172:PHE:HB3	1.97	0.63
10:H:27:LYS:H	10:H:59:HIS:CD2	2.08	0.63
21:S:71:VAL:HG11	21:S:90:PRO:CB	2.21	0.63
26:X:154:ARG:NH1	26:X:155:ARG:HG3	2.13	0.63
1:0:2426:G:H1'	40:0:6457:HOH:O	1.96	0.63
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.32	0.63
4:B:238:ASN:HD22	4:B:240:GLY:N	1.96	0.63
15:M:7:LYS:HE3	18:P:21:ARG:O	1.99	0.63
1:0:371:U:H2'	1:0:372:A:C8	2.32	0.63
1:0:2064:U:H5'	1:0:2652:U:H4'	1.81	0.63
7:E:31:ARG:HH12	7:E:68:HIS:CD2	2.16	0.63
1:0:1766:U:O2	1:0:1778:A:H5'	1.99	0.63
7:E:133:VAL:HG12	7:E:141:VAL:HG13	1.81	0.63
9:G:12:ILE:O	9:G:12:ILE:HG22	1.99	0.63
1:0:1183:C:N4	1:0:1184:C:H41	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:140:LEU:HA	40:B:9055:HOH:O	1.98	0.63
6:D:69:ILE:HG22	6:D:69:ILE:O	1.98	0.63
17:O:59:ARG:HH22	17:O:66:GLN:HE22	1.46	0.63
1:O:2533:C:H5'	1:O:2533:C:H6	1.64	0.63
3:A:121:ALA:O	3:A:124:VAL:HG22	1.99	0.63
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.29	0.63
6:D:44:ILE:HG12	6:D:83:PHE:HE1	1.63	0.63
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.34	0.63
15:M:62:HIS:HB3	15:M:65:ASP:OD1	1.99	0.63
24:V:4:LEU:HD23	24:V:54:PHE:HB3	1.79	0.63
1:O:542:A:H5'	1:O:542:A:C8	2.28	0.62
7:E:93:MET:HE1	7:E:165:GLY:N	2.14	0.62
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.29	0.62
11:I:74:ARG:NH1	11:I:76:ASP:HB2	2.13	0.62
16:N:39:THR:O	16:N:115:ARG:NH2	2.33	0.62
1:O:1080:C:H4'	1:O:1081:A:OP1	1.97	0.62
1:O:1206:U:H5'	1:O:1206:U:H6	1.62	0.62
1:O:1333:U:H2'	1:O:1334:C:C6	2.34	0.62
11:I:107:ASN:HD22	11:I:107:ASN:C	2.06	0.62
12:J:74:VAL:CG1	12:J:113:ILE:HG12	2.29	0.62
1:O:285:A:H2'	1:O:286:U:O4'	1.99	0.62
12:J:29:LEU:HB3	12:J:55:VAL:CG1	2.26	0.62
1:O:282:C:O2'	1:O:283:U:H5'	1.99	0.62
1:O:603:A:H5''	1:O:604:G:OP1	1.99	0.62
4:B:51:VAL:HG23	4:B:329:TYR:O	2.00	0.62
5:C:246:ARG:HB3	5:C:246:ARG:NH1	2.14	0.62
8:F:117:GLU:C	8:F:119:ARG:H	2.07	0.62
1:O:121:U:OP2	29:1:10:ARG:NH2	2.32	0.62
5:C:104:ASP:O	5:C:108:GLN:HG3	1.99	0.62
7:E:23:GLU:HG2	7:E:28:SER:HB3	1.82	0.62
23:U:39:ALA:C	23:U:41:GLU:H	2.08	0.62
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.65	0.62
6:D:38:GLU:HB3	6:D:49:PRO:HG2	1.80	0.62
13:K:73:VAL:HG23	13:K:74:THR:H	1.64	0.62
1:O:119:A:H2'	1:O:120:A:H5''	1.80	0.62
1:O:2676:C:H4'	11:I:70:PHE:HE1	1.63	0.62
7:E:11:VAL:HG12	7:E:12:ASP:N	2.14	0.62
12:J:115:ARG:HG3	12:J:116:GLU:N	2.14	0.62
15:M:139:TRP:CE3	15:M:139:TRP:HA	2.35	0.62
21:S:69:LYS:O	21:S:71:VAL:HG23	2.00	0.62
1:O:2346:C:H6	1:O:2346:C:O5'	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.80	0.62
15:M:11:ARG:O	15:M:15:GLU:HG3	2.00	0.62
19:Q:99:ALA:CB	19:Q:109:MET:HE1	2.20	0.62
24:V:21:LEU:HD13	24:V:26:ILE:HD11	1.82	0.62
1:0:1189:A:H1'	1:0:1209:C:C1'	2.30	0.61
1:0:1191:A:H3'	1:0:1192:A:H5''	1.81	0.61
1:0:1299:G:O6	13:K:6:ARG:HD3	2.00	0.61
3:A:135:VAL:HG21	3:A:147:ARG:NH1	2.15	0.61
1:0:1165:G:H1'	1:0:1174:A:H1'	1.82	0.61
19:Q:44:VAL:O	19:Q:48:GLU:HG3	2.00	0.61
30:2:73:GLU:HB3	40:2:8990:HOH:O	2.00	0.61
1:0:1189:A:H3'	40:0:8098:HOH:O	2.01	0.61
3:A:109:GLU:HG2	3:A:116:GLY:N	2.14	0.61
15:M:49:THR:CG2	15:M:56:ASP:HB2	2.31	0.61
1:0:1730:G:H5'	1:0:1731:C:C5	2.36	0.61
3:A:51:ARG:NH1	3:A:120:ARG:O	2.34	0.61
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.14	0.61
1:0:2768:A:H2'	1:0:2769:C:O4'	2.01	0.61
19:Q:39:THR:HG23	19:Q:107:GLU:O	1.99	0.61
25:W:37:LEU:CD1	25:W:85:VAL:HG21	2.22	0.61
11:I:75:PRO:HG2	11:I:105:LEU:HD21	1.83	0.61
19:Q:18:LEU:HB2	19:Q:143:VAL:CG1	2.30	0.61
29:1:22:PRO:HG2	29:1:25:VAL:HG23	1.81	0.61
1:0:2851:G:C2'	1:0:2852:A:H5'	2.30	0.61
6:D:44:ILE:HG23	6:D:45:THR:HG23	1.83	0.61
1:0:1328:A:OP1	26:X:169:ARG:HD2	2.00	0.61
1:0:1701:A:H5''	1:0:1702:U:H3'	1.83	0.61
3:A:125:ASN:CB	3:A:158:VAL:HG12	2.31	0.61
14:L:57:LYS:HE2	14:L:140:ALA:O	2.01	0.61
4:B:248:ARG:O	4:B:251:VAL:HG13	2.01	0.61
19:Q:18:LEU:HG	19:Q:91:LEU:HD13	1.83	0.61
30:2:70:ARG:HB3	40:2:9001:HOH:O	2.00	0.61
1:0:338:C:H4'	5:C:174:ILE:HD11	1.82	0.61
1:0:1714:C:O2'	1:0:1715:C:H5'	2.01	0.61
4:B:321:PRO:HA	40:B:9136:HOH:O	2.01	0.61
6:D:41:LEU:HA	6:D:44:ILE:HG22	1.82	0.61
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.30	0.60
5:C:76:ARG:HG2	5:C:78:ARG:HH12	1.65	0.60
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.81	0.60
24:V:13:MET:CE	24:V:17:ILE:HG22	2.31	0.60
1:0:2862:G:H4'	4:B:336:GLN:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3114:G:O6	15:M:11:ARG:HD3	2.00	0.60
24:V:4:LEU:HD22	24:V:52:VAL:CG2	2.27	0.60
1:0:1441:G:O2'	1:0:1442:A:H5'	2.01	0.60
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.30	0.60
1:0:1477:C:O2'	1:0:1478:U:H5'	2.01	0.60
1:0:1926:G:H2'	1:0:1927:A:C8	2.36	0.60
5:C:118:THR:HG22	5:C:137:PRO:HB3	1.83	0.60
5:C:139:VAL:HG13	40:C:8656:HOH:O	2.02	0.60
9:G:64:ASN:O	9:G:68:GLU:HG3	2.01	0.60
1:0:155:C:OP2	14:L:188:ARG:HD3	2.00	0.60
1:0:871:G:C8	1:0:871:G:C5'	2.78	0.60
2:9:3023:U:H6	2:9:3023:U:H5''	1.67	0.60
6:D:25:MET:HE1	6:D:40:ILE:HD11	1.84	0.60
1:0:1120:U:H5'	1:0:1121:G:OP2	2.02	0.60
1:0:1667:A:H5'	1:0:1667:A:H8	1.67	0.60
15:M:110:THR:HB	15:M:113:SER:OG	2.02	0.60
18:P:53:HIS:ND1	18:P:55:ARG:HB2	2.16	0.60
3:A:69:LEU:HD21	3:A:120:ARG:HB3	1.83	0.60
5:C:246:ARG:HB3	5:C:246:ARG:HH11	1.67	0.60
27:Y:37:HIS:HB2	27:Y:47:VAL:HB	1.84	0.60
1:0:1878:G:O2'	1:0:1879:U:P	2.60	0.59
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.84	0.59
12:J:28:GLU:HB3	12:J:59:LYS:HB2	1.84	0.59
12:J:55:VAL:HG12	12:J:56:SER:N	2.15	0.59
27:Y:19:GLY:O	27:Y:23:ARG:HG2	2.02	0.59
1:0:645:U:OP2	13:K:4:LYS:HE2	2.02	0.59
10:H:30:GLN:H	10:H:66:ARG:NH1	1.99	0.59
1:0:2779:G:H21	7:E:143:GLN:NE2	2.00	0.59
4:B:62:ARG:CA	4:B:65:MET:HE3	2.33	0.59
15:M:114:LYS:O	15:M:118:ILE:HG13	2.02	0.59
19:Q:23:MET:HE3	19:Q:28:SER:OG	2.03	0.59
29:1:18:ASN:ND2	29:1:40:ARG:H	2.00	0.59
1:0:1973:A:H5'	1:0:1973:A:H8	1.67	0.59
4:B:108:GLU:HB3	4:B:111:ARG:HD2	1.85	0.59
5:C:16:VAL:HG12	5:C:17:ASP:N	2.17	0.59
5:C:233:THR:HG22	5:C:234:VAL:N	2.17	0.59
27:Y:22:SER:O	27:Y:26:VAL:HG23	2.03	0.59
4:B:297:VAL:HB	40:B:9084:HOH:O	2.03	0.59
1:0:111:C:O2'	28:Z:20:ARG:HG2	2.03	0.59
1:0:2676:C:H4'	11:I:70:PHE:CD1	2.37	0.59
26:X:126:PRO:HG2	26:X:128:PHE:CE1	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1:22:PRO:HG2	29:1:25:VAL:CG2	2.32	0.59
4:B:307:ARG:HH11	4:B:307:ARG:CG	2.15	0.59
8:F:46:GLU:OE1	8:F:100:ASP:HA	2.03	0.59
23:U:39:ALA:N	23:U:40:PRO:CD	2.65	0.59
24:V:81:ASP:OD1	24:V:92:ASP:HB2	2.03	0.59
25:W:25:ARG:HD3	25:W:64:ALA:O	2.02	0.59
5:C:236:THR:H	5:C:239:ALA:HB3	1.68	0.59
9:G:23:ILE:O	9:G:27:ILE:HG13	2.03	0.59
1:O:259:G:H21	14:L:58:GLN:NE2	2.00	0.59
15:M:47:LEU:HD13	15:M:97:VAL:HG11	1.83	0.59
30:2:60:LYS:HG3	30:2:61:PRO:HD2	1.83	0.59
4:B:72:THR:HB	40:B:9084:HOH:O	2.03	0.58
7:E:7:ILE:HD11	7:E:11:VAL:C	2.28	0.58
10:H:56:GLN:HE21	10:H:126:ARG:HE	1.47	0.58
1:O:2478:U:O2'	1:O:2479:A:H5'	2.03	0.58
6:D:158:ASN:HB2	6:D:161:ASP:OD2	2.03	0.58
7:E:84:MET:HE2	7:E:133:VAL:CG2	2.33	0.58
14:L:134:ILE:CG2	14:L:141:ILE:HD13	2.31	0.58
23:U:1:THR:HG23	23:U:2:VAL:N	2.17	0.58
1:O:558:C:H2'	1:O:559:C:H5'	1.85	0.58
1:O:902:G:N7	13:K:18:HIS:HD2	2.01	0.58
1:O:926:A:H5'	13:K:39:GLU:OE2	2.04	0.58
4:B:329:TYR:CE2	22:T:15:PRO:HG2	2.37	0.58
9:G:12:ILE:N	9:G:13:PRO:CD	2.65	0.58
25:W:9:VAL:HG22	25:W:88:GLU:OE2	2.04	0.58
1:O:156:C:H5''	14:L:171:ARG:CD	2.24	0.58
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.85	0.58
6:D:64:ARG:CG	6:D:67:ASP:HB3	2.34	0.58
19:Q:18:LEU:HD12	19:Q:143:VAL:CG1	2.34	0.58
20:R:8:PRO:HD2	23:U:32:ALA:HA	1.85	0.58
24:V:130:HIS:O	24:V:136:GLY:HA3	2.03	0.58
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.36	0.58
12:J:34:VAL:CG2	12:J:47:ALA:HB2	2.34	0.58
1:O:656:G:OP2	16:N:37:ARG:HD2	2.03	0.58
1:O:962:C:H1'	15:M:5:ARG:HH12	1.69	0.58
1:O:1236:A:H2'	1:O:1237:U:O4'	2.04	0.58
4:B:24:PRO:HG3	4:B:204:GLY:HA2	1.86	0.58
8:F:36:THR:HG23	8:F:97:ALA:HB2	1.86	0.58
8:F:46:GLU:O	8:F:73:PRO:HD2	2.04	0.58
1:O:1175:G:H1'	1:O:1193:A:H2'	1.86	0.58
1:O:1594:C:OP2	17:O:120:ARG:HD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1755:A:H2'	1:0:1756:G:O4'	2.03	0.58
6:D:64:ARG:CD	6:D:67:ASP:HB3	2.32	0.58
6:D:97:GLN:HG2	6:D:97:GLN:O	2.04	0.58
12:J:82:ARG:NH2	12:J:115:ARG:HG2	2.18	0.58
15:M:89:GLY:O	15:M:92:ALA:HB3	2.03	0.58
17:O:98:ILE:HD12	17:O:102:ARG:NE	2.19	0.58
1:0:396:U:O2'	1:0:418:C:H4'	2.04	0.58
1:0:21:G:H5''	19:Q:1:GLY:O	2.04	0.58
1:0:280:C:H2'	1:0:281:U:O4'	2.04	0.58
1:0:338:C:H4'	5:C:174:ILE:CD1	2.34	0.58
1:0:512:G:O3'	1:0:513:A:H8	1.87	0.58
2:9:3004:G:H21	15:M:44:ARG:NH1	2.01	0.58
3:A:88:ILE:HD13	3:A:100:PRO:CD	2.33	0.58
4:B:305:ASP:O	4:B:306:LYS:HB2	2.04	0.58
6:D:11:HIS:C	6:D:13:MET:H	2.11	0.58
6:D:95:THR:O	6:D:97:GLN:N	2.31	0.58
11:I:107:ASN:HD22	11:I:109:TYR:H	1.49	0.58
1:0:949:U:O2'	18:P:40:HIS:HE1	1.87	0.58
1:0:2265:U:H2'	1:0:2266:A:C8	2.38	0.58
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.69	0.58
1:0:2670:G:O2'	1:0:2671:U:H5'	2.04	0.58
1:0:2768:A:O2'	1:0:2769:C:H5'	2.04	0.58
4:B:265:LEU:HD21	4:B:316:ARG:HD3	1.86	0.58
14:L:164:THR:CG2	14:L:165:GLY:N	2.66	0.58
20:R:29:ASP:OD1	20:R:31:ARG:NH1	2.37	0.58
1:0:272:A:H5'	1:0:273:G:OP2	2.04	0.57
1:0:960:G:N3	1:0:960:G:H2'	2.19	0.57
2:9:3014:G:H5'	2:9:3014:G:H8	1.68	0.57
2:9:3029:C:C2'	2:9:3030:C:H5'	2.34	0.57
13:K:143:THR:HG22	13:K:144:ASP:H	1.68	0.57
1:0:1342:C:O2'	1:0:1343:C:H5'	2.04	0.57
10:H:76:GLU:C	10:H:77:LEU:HD23	2.29	0.57
14:L:60:VAL:C	14:L:61:ILE:HD12	2.30	0.57
24:V:52:VAL:HG22	24:V:53:ALA:H	1.69	0.57
24:V:65:VAL:HA	24:V:68:THR:HG22	1.86	0.57
1:0:1185:U:H2'	1:0:1186:C:C6	2.38	0.57
4:B:254:GLN:HG2	4:B:255:GLY:N	2.17	0.57
7:E:15:GLN:HG2	7:E:19:ASP:O	2.04	0.57
14:L:164:THR:HG22	14:L:166:ALA:N	2.20	0.57
25:W:9:VAL:HG13	25:W:88:GLU:OE2	2.04	0.57
1:0:1878:G:O2'	1:0:1879:U:H6	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3054:A:O2'	2:9:3055:U:H5'	2.04	0.57
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.85	0.57
4:B:221:GLN:HE22	12:J:42:ASN:HD22	1.53	0.57
11:I:107:ASN:HD21	11:I:109:TYR:HB2	1.68	0.57
14:L:34:GLU:HB3	14:L:38:GLU:HG3	1.86	0.57
17:O:103:THR:HA	17:O:106:ARG:NH1	2.19	0.57
1:0:2587:U:H2'	1:0:2589:U:H5''	1.87	0.57
2:9:3076:G:C3'	2:9:3077:A:H5''	2.25	0.57
15:M:139:TRP:HA	15:M:139:TRP:HE3	1.69	0.57
16:N:87:THR:O	16:N:91:GLN:HG3	2.05	0.57
17:O:40:VAL:O	17:O:44:VAL:HG23	2.05	0.57
1:0:613:C:H2'	1:0:614:U:H6	1.70	0.57
4:B:258:GLY:H	4:B:260:HIS:HE1	1.53	0.57
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.86	0.57
1:0:506:G:H22	1:0:509:A:H5''	1.69	0.57
1:0:2637:A:C2'	31:4:74:C:H5''	2.21	0.57
4:B:5:ARG:HD2	4:B:8:LYS:NZ	2.19	0.57
1:0:282:C:H1'	1:0:368:C:H42	1.69	0.57
1:0:291:C:H2'	1:0:292:G:O4'	2.05	0.57
1:0:2816:A:H5''	1:0:2817:G:H5'	1.87	0.57
3:A:33:GLU:H	3:A:33:GLU:CD	2.10	0.57
15:M:154:LEU:HG	15:M:155:GLU:H	1.70	0.57
1:0:1130:U:H2'	1:0:1131:G:O4'	2.04	0.57
1:0:2721:U:H4'	12:J:87:ARG:HG3	1.86	0.57
3:A:128:LEU:HD21	3:A:131:HIS:HE1	1.69	0.57
4:B:85:ARG:NH1	40:B:9113:HOH:O	2.37	0.57
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.87	0.57
5:C:107:ARG:NH1	5:C:107:ARG:HB3	2.20	0.57
3:A:36:ASP:OD2	3:A:85:SER:HB2	2.05	0.57
3:A:192:VAL:HB	40:A:9066:HOH:O	2.04	0.57
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.69	0.57
7:E:81:GLU:HG2	7:E:134:SER:CB	2.35	0.57
19:Q:111:ILE:HG23	19:Q:145:LEU:HD11	1.87	0.57
1:0:1563:G:O2'	1:0:1564:C:OP2	2.19	0.56
1:0:2515:C:H2'	1:0:2516:G:O4'	2.05	0.56
4:B:212:GLN:OE1	4:B:216:LYS:HD3	2.05	0.56
4:B:268:ARG:NH2	4:B:325:PRO:HG3	2.19	0.56
5:C:115:LEU:O	5:C:118:THR:HB	2.05	0.56
1:0:1669:A:H2'	1:0:1670:G:C8	2.40	0.56
12:J:109:LEU:HD13	12:J:113:ILE:HD11	1.87	0.56
1:0:1118:A:H62	1:0:1244:U:H3	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:56:ASP:OD1	4:B:322:ARG:HB3	2.04	0.56
6:D:136:ARG:HD2	6:D:155:HIS:O	2.05	0.56
7:E:69:ILE:HA	7:E:72:MET:CE	2.35	0.56
15:M:36:ALA:HB1	15:M:118:ILE:HD12	1.86	0.56
22:T:14:GLU:O	22:T:17:THR:HB	2.05	0.56
23:U:64:GLY:O	23:U:65:ASP:HB2	2.03	0.56
26:X:187:VAL:CG2	26:X:192:ASP:HB2	2.35	0.56
1:O:500:G:H21	19:Q:98:ASN:HD21	1.52	0.56
1:O:2812:A:C2	1:O:2814:A:N6	2.67	0.56
5:C:77:ALA:O	5:C:78:ARG:HG3	2.04	0.56
6:D:23:VAL:HG22	6:D:73:VAL:HB	1.87	0.56
6:D:50:VAL:O	6:D:71:ALA:HA	2.04	0.56
10:H:63:GLU:HA	40:H:9029:HOH:O	2.04	0.56
15:M:69:TYR:HE2	15:M:183:ASP:OD2	1.89	0.56
18:P:25:PRO:HB2	40:P:4350:HOH:O	2.05	0.56
24:V:13:MET:HE3	24:V:17:ILE:CG2	2.35	0.56
1:O:2251:G:H2'	1:O:2252:A:C8	2.40	0.56
6:D:27:ILE:HG22	6:D:28:GLY:N	2.16	0.56
15:M:154:LEU:O	15:M:155:GLU:HB3	2.05	0.56
15:M:184:ILE:HG22	15:M:185:GLU:N	2.19	0.56
17:O:115:SER:N	17:O:118:GLN:HE21	1.89	0.56
1:O:308:U:H5'	21:S:97:ARG:NH2	2.20	0.56
1:O:794:U:H3	1:O:819:A:H61	1.53	0.56
1:O:1666:C:C2'	1:O:1667:A:H5'	2.36	0.56
1:O:2506:A:O2'	1:O:2507:G:O5'	2.23	0.56
14:L:107:ARG:NH1	14:L:107:ARG:CG	2.69	0.56
1:O:168:C:O2'	1:O:169:A:H5'	2.06	0.56
1:O:482:G:H4'	1:O:508:A:N1	2.21	0.56
1:O:1641:A:C2'	1:O:1642:A:H5'	2.35	0.56
1:O:1787:C:OP1	17:O:68:LYS:HE2	2.06	0.56
4:B:265:LEU:CD2	4:B:316:ARG:HD3	2.35	0.56
22:T:17:THR:CG2	22:T:18:GLY:N	2.69	0.56
27:Y:21:VAL:HG12	40:Y:8711:HOH:O	2.06	0.56
1:O:2507:G:H2'	1:O:2510:C:H42	1.71	0.56
1:O:2698:G:H2'	1:O:2699:A:C8	2.41	0.56
1:O:2791:U:H1'	1:O:2792:A:H5''	1.88	0.56
5:C:118:THR:O	5:C:136:VAL:HG13	2.06	0.56
13:K:125:PHE:CE1	13:K:140:VAL:HG13	2.41	0.56
15:M:71:TRP:HE3	15:M:175:LEU:HD22	1.70	0.56
25:W:76:ARG:HH11	25:W:76:ARG:HG3	1.68	0.56
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:175:LEU:O	4:B:175:LEU:HD23	2.05	0.56
8:F:48:VAL:HG12	8:F:97:ALA:HB2	1.88	0.56
14:L:99:ARG:NH2	14:L:170:ASN:HD22	1.97	0.56
15:M:12:ARG:HD3	15:M:18:THR:OG1	2.05	0.56
17:O:10:ALA:HA	17:O:13:VAL:CG1	2.34	0.56
24:V:29:VAL:O	24:V:30:ASN:HB2	2.06	0.56
1:O:88:G:N7	29:1:28:LYS:HD2	2.20	0.56
2:9:3041:C:O4'	6:D:50:VAL:HG23	2.06	0.56
3:A:107:ASN:OD1	3:A:120:ARG:HD2	2.06	0.56
3:A:179:MET:HG2	3:A:186:TRP:CB	2.36	0.56
20:R:51:GLN:HE21	20:R:53:ASN:ND2	2.00	0.56
21:S:71:VAL:CG1	21:S:90:PRO:HB3	2.24	0.56
24:V:21:LEU:HB3	24:V:26:ILE:HG12	1.87	0.56
1:O:588:G:O6	24:V:154:ARG:NH1	2.39	0.55
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.87	0.55
8:F:60:VAL:O	8:F:60:VAL:HG12	2.06	0.55
11:I:75:PRO:HD3	11:I:136:SER:OG	2.06	0.55
1:O:1205:U:C2'	1:O:1206:U:H5''	2.36	0.55
1:O:2106:C:H5'	1:O:2284:G:H21	1.70	0.55
1:O:2807:U:P	4:B:27:ASN:HD21	2.28	0.55
6:D:37:ALA:O	6:D:40:ILE:HG12	2.06	0.55
10:H:99:LYS:HD3	10:H:119:LYS:HD3	1.88	0.55
11:I:75:PRO:HG2	11:I:105:LEU:CD2	2.35	0.55
15:M:87:LEU:CD1	15:M:186:LEU:HD21	2.34	0.55
1:O:380:A:OP2	14:L:9:ARG:HD2	2.05	0.55
40:O:7890:HOH:O	30:2:60:LYS:HG3	2.07	0.55
5:C:1:MET:HG2	5:C:2:GLN:N	2.20	0.55
7:E:84:MET:HE1	7:E:148:ILE:HD12	1.88	0.55
1:O:449:A:N7	5:C:43:LYS:HG2	2.22	0.55
1:O:1150:A:C2	9:G:20:VAL:HG21	2.41	0.55
1:O:1528:A:H2'	1:O:1529:G:O4'	2.07	0.55
6:D:94:ALA:HB3	6:D:174:VAL:HA	1.88	0.55
13:K:53:ARG:NH2	13:K:57:VAL:HG12	2.22	0.55
25:W:15:ARG:HB3	25:W:15:ARG:NH1	2.19	0.55
1:O:1666:C:O2'	1:O:1667:A:H5''	2.06	0.55
7:E:84:MET:HE1	7:E:148:ILE:CD1	2.37	0.55
14:L:71:SER:O	14:L:73:ARG:NH1	2.36	0.55
1:O:545:G:H5'	1:O:545:G:C8	2.39	0.55
1:O:621:C:H5'	26:X:132:ASP:OD2	2.06	0.55
1:O:1057:A:H2'	1:O:1058:A:C8	2.41	0.55
1:O:1132:A:N6	1:O:1229:C:H2'	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1462:C:H2'	1:0:1463:A:H8	1.71	0.55
1:0:2320:U:H4'	1:0:2321:A:O4'	2.07	0.55
2:9:3041:C:C6	6:D:50:VAL:HG21	2.42	0.55
28:Z:25:LYS:CD	29:1:49:GLU:H	2.16	0.55
1:0:968:G:H1'	10:H:32:LYS:HD2	1.89	0.55
1:0:1167:G:O2'	1:0:1168:C:H5'	2.06	0.55
1:0:1667:A:H2'	1:0:1668:U:C6	2.41	0.55
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.88	0.55
15:M:170:GLU:O	15:M:174:GLU:HG3	2.07	0.55
23:U:12:THR:CG2	23:U:15:GLU:HG3	2.26	0.55
24:V:4:LEU:O	24:V:32:CYS:HA	2.06	0.55
1:0:2769:C:O2'	1:0:2770:G:H5'	2.07	0.55
4:B:87:TYR:HD1	40:B:9055:HOH:O	1.90	0.55
19:Q:119:VAL:O	19:Q:119:VAL:HG12	2.05	0.55
24:V:6:GLN:CB	24:V:26:ILE:HD12	2.34	0.55
3:A:211:LYS:HB3	3:A:212:PRO:CD	2.31	0.55
1:0:470:U:O2'	28:Z:16:HIS:CD2	2.60	0.55
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.72	0.55
5:C:233:THR:HG22	5:C:234:VAL:H	1.71	0.55
7:E:31:ARG:NH1	7:E:68:HIS:CG	2.75	0.55
13:K:120:LEU:HD12	13:K:133:VAL:HG21	1.89	0.55
14:L:120:VAL:HG11	14:L:130:GLU:HG3	1.87	0.55
1:0:263:U:O4'	8:F:59:ILE:HD13	2.06	0.54
1:0:1853:C:OP1	3:A:231:LYS:HG3	2.08	0.54
3:A:53:ALA:HB3	40:A:9078:HOH:O	2.05	0.54
4:B:96:PRO:HG3	40:B:9113:HOH:O	2.06	0.54
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.36	0.54
23:U:8:ILE:HG21	23:U:59:ILE:HG13	1.88	0.54
23:U:44:GLY:O	23:U:48:GLU:HG2	2.06	0.54
1:0:1717:A:H5''	17:O:54:LYS:HB2	1.87	0.54
1:0:2291:A:C8	1:0:2309:C:H5'	2.41	0.54
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.42	0.54
17:O:103:THR:O	17:O:107:GLU:HG3	2.07	0.54
21:S:71:VAL:HG12	21:S:72:ILE:N	2.22	0.54
1:0:2073:G:OP2	1:0:2490:A:H5'	2.07	0.54
21:S:32:ARG:NH1	21:S:38:ARG:NH1	2.55	0.54
26:X:189:ASN:HD22	26:X:189:ASN:C	2.14	0.54
1:0:1182:C:H1'	1:0:1192:A:C8	2.40	0.54
1:0:2314:G:C2'	1:0:2315:C:H5'	2.37	0.54
3:A:96:LEU:HD22	3:A:128:LEU:HD13	1.90	0.54
6:D:23:VAL:HG23	6:D:23:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:99:ASP:CB	6:D:103:ASN:HB2	2.37	0.54
15:M:159:TYR:HB3	15:M:162:ASP:HB2	1.90	0.54
1:0:553:G:P	26:X:204:ARG:HH22	2.31	0.54
1:0:625:U:H5''	1:0:1044:C:N4	2.23	0.54
1:0:1283:G:O2'	1:0:1284:G:H5'	2.06	0.54
40:0:9823:HOH:O	28:Z:1:THR:HA	2.08	0.54
7:E:69:ILE:HA	7:E:72:MET:HE3	1.90	0.54
8:F:91:VAL:CG1	8:F:92:GLY:H	2.17	0.54
11:I:93:ARG:HH11	11:I:93:ARG:CB	2.17	0.54
15:M:64:SER:C	15:M:66:LEU:H	2.16	0.54
21:S:26:THR:HA	21:S:39:ASN:HB3	1.89	0.54
1:0:1119:G:H22	1:0:1246:A:H2	1.47	0.54
1:0:2715:G:N2	4:B:264:GLU:OE1	2.40	0.54
40:0:5224:HOH:O	11:I:47:THR:HB	2.07	0.54
1:0:1687:C:O2	28:Z:9:GLY:HA2	2.08	0.54
1:0:2894:C:O2'	1:0:2895:C:H5'	2.07	0.54
1:0:2896:A:N3	1:0:2896:A:H2'	2.23	0.54
2:9:3044:A:O4'	6:D:76:ARG:NE	2.40	0.54
9:G:16:LYS:O	9:G:20:VAL:HG23	2.07	0.54
13:K:143:THR:CG2	13:K:144:ASP:N	2.70	0.54
15:M:47:LEU:HD12	15:M:92:ALA:HB1	1.90	0.54
1:0:2637:A:C8	31:4:74:C:H3'	2.43	0.54
1:0:2718:C:H6	1:0:2718:C:H5'	1.73	0.54
1:0:558:C:C2'	1:0:559:C:H5''	2.38	0.54
1:0:681:G:N3	1:0:681:G:H5'	2.23	0.54
1:0:2432:C:O2'	1:0:2433:A:H5'	2.08	0.54
4:B:14:GLY:HA2	4:B:15:PRO:C	2.33	0.54
1:0:69:A:H5'	1:0:69:A:C8	2.43	0.54
1:0:420:U:H2'	1:0:421:C:C6	2.42	0.54
1:0:2102:G:H5''	1:0:2538:A:C2	2.43	0.54
1:0:2563:U:H2'	1:0:2565:C:O5'	2.08	0.54
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.89	0.54
1:0:1053:G:OP1	10:H:12:PRO:HG3	2.07	0.53
1:0:1946:C:H2'	1:0:1971:G:C8	2.43	0.53
1:0:2638:G:H5'	40:0:8342:HOH:O	2.09	0.53
4:B:17:LYS:O	4:B:260:HIS:HD2	1.91	0.53
24:V:122:ARG:CG	24:V:122:ARG:NH1	2.70	0.53
1:0:21:G:H4'	19:Q:2:ILE:HG22	1.89	0.53
1:0:1118:A:C8	1:0:1119:G:H5''	2.42	0.53
1:0:2456:A:H2'	1:0:2457:U:C6	2.43	0.53
1:0:2487:C:H2'	1:0:2488:A:O4'	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:H2'	1:0:2718:C:C5'	2.38	0.53
2:9:3069:U:OP1	15:M:4:PRO:HG3	2.08	0.53
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.08	0.53
10:H:54:THR:O	10:H:55:VAL:HG13	2.07	0.53
11:I:130:VAL:HG12	11:I:131:THR:N	2.23	0.53
1:0:65:C:O2'	1:0:66:G:H5'	2.08	0.53
1:0:1733:A:H4'	4:B:212:GLN:HA	1.88	0.53
2:9:3048:C:H4'	15:M:141:ARG:HH21	1.73	0.53
14:L:98:GLN:O	14:L:102:GLU:HG3	2.07	0.53
25:W:43:VAL:HG12	25:W:44:ASP:N	2.23	0.53
26:X:152:LYS:HB3	26:X:160:LYS:HG3	1.90	0.53
1:0:136:C:H2'	1:0:137:U:O4'	2.08	0.53
1:0:281:U:O2'	1:0:282:C:H5'	2.08	0.53
2:9:3092:G:H2'	2:9:3093:A:H8	1.72	0.53
8:F:13:GLU:OE2	8:F:78:GLU:HG2	2.09	0.53
15:M:11:ARG:HG3	15:M:14:ARG:NH1	2.23	0.53
24:V:19:ASP:O	24:V:23:MET:HG3	2.09	0.53
1:0:244:C:OP2	8:F:38:LYS:HE3	2.09	0.53
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.91	0.53
16:N:14:LEU:CD2	16:N:102:ILE:HD11	2.39	0.53
19:Q:96:VAL:HG13	19:Q:106:GLY:HA3	1.90	0.53
1:0:60:A:O2'	1:0:61:G:H5'	2.09	0.53
1:0:558:C:H2'	1:0:559:C:C5'	2.39	0.53
1:0:2094:G:H4'	4:B:245:SER:HB3	1.91	0.53
25:W:31:ILE:O	25:W:35:GLU:HG3	2.08	0.53
26:X:235:GLU:H	26:X:235:GLU:CD	2.17	0.53
1:0:514:G:O5'	1:0:514:G:H8	1.92	0.53
1:0:560:C:H2'	1:0:561:G:H8	1.72	0.53
1:0:920:C:H4'	1:0:921:G:C2	2.44	0.53
4:B:139:ASP:CB	4:B:165:ARG:HE	2.21	0.53
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.89	0.53
20:R:57:THR:CG2	20:R:58:MET:N	2.72	0.53
1:0:256:C:H2'	1:0:257:G:O4'	2.09	0.53
1:0:299:U:H5'	40:0:7672:HOH:O	2.08	0.53
1:0:316:A:H5'	21:S:54:ASP:OD2	2.08	0.53
1:0:821:U:H2'	1:0:822:C:H6	1.73	0.53
1:0:1159:G:H21	1:0:1189:A:H8	1.57	0.53
6:D:11:HIS:O	6:D:12:GLU:HB3	2.09	0.53
8:F:99:THR:HG23	8:F:99:THR:O	2.08	0.53
13:K:97:VAL:HG12	13:K:98:GLU:O	2.09	0.53
24:V:139:GLY:O	24:V:141:HIS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1684:A:H1'	29:1:43:ARG:HH22	1.74	0.53
1:0:2270:G:H4'	3:A:223:ARG:NH1	2.24	0.53
1:0:2866:U:H4'	1:0:2867:G:H5'	1.90	0.53
22:T:9:CYS:HA	22:T:52:THR:HG23	1.91	0.53
23:U:20:LEU:HD11	23:U:53:ILE:HG23	1.91	0.53
1:0:2081:A:H4'	11:I:69:TYR:CE1	2.44	0.53
1:0:2363:G:O3'	18:P:11:ARG:NH1	2.42	0.53
2:9:3008:G:O6	15:M:11:ARG:NH1	2.42	0.53
10:H:16:ARG:HH21	10:H:18:GLU:CD	2.16	0.53
15:M:182:GLY:O	15:M:183:ASP:O	2.27	0.53
1:0:1972:U:H2'	1:0:1973:A:H5'	1.90	0.52
1:0:2912:C:O2'	1:0:2913:A:H5'	2.09	0.52
5:C:180:SER:HB2	40:C:8654:HOH:O	2.09	0.52
6:D:99:ASP:HA	40:D:5675:HOH:O	2.09	0.52
7:E:145:ALA:HB1	7:E:168:ILE:CD1	2.38	0.52
10:H:29:ALA:C	10:H:30:GLN:HG3	2.34	0.52
23:U:49:LEU:O	23:U:53:ILE:HG13	2.09	0.52
24:V:38:THR:HG22	24:V:39:ASP:N	2.24	0.52
26:X:106:THR:HG23	26:X:107:PRO:HD2	1.89	0.52
26:X:165:GLU:HB3	40:X:8895:HOH:O	2.09	0.52
1:0:288:A:H2'	1:0:289:G:C8	2.44	0.52
1:0:1289:C:O2'	1:0:1290:G:H5'	2.09	0.52
1:0:1477:C:H5'	1:0:1868:G:C5'	2.38	0.52
1:0:2356:A:H2'	1:0:2357:G:O4'	2.09	0.52
1:0:2499:U:H2'	1:0:2500:C:H6	1.74	0.52
1:0:2569:A:H2'	1:0:2570:G:O5'	2.08	0.52
4:B:215:VAL:HB	4:B:234:ARG:HH12	1.73	0.52
5:C:132:ASP:HB3	40:C:8571:HOH:O	2.09	0.52
6:D:23:VAL:CG2	6:D:73:VAL:HB	2.39	0.52
2:9:3023:U:H5''	2:9:3023:U:C6	2.44	0.52
2:9:3091:C:H2'	2:9:3092:G:O4'	2.09	0.52
3:A:88:ILE:O	3:A:88:ILE:HG22	2.09	0.52
4:B:280:VAL:HG13	4:B:333:GLU:O	2.10	0.52
10:H:58:ARG:HG3	10:H:58:ARG:NH1	2.23	0.52
1:0:702:G:O2'	1:0:703:G:H5'	2.10	0.52
1:0:876:A:H2'	1:0:876:A:N3	2.24	0.52
1:0:1474:C:H5'	1:0:1474:C:C6	2.37	0.52
1:0:1926:G:H2'	1:0:1927:A:H8	1.74	0.52
1:0:2330:U:H4'	1:0:2331:C:OP1	2.10	0.52
1:0:2361:A:H2'	1:0:2362:A:C8	2.44	0.52
4:B:138:GLY:O	4:B:139:ASP:O	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:5:ILE:CD1	5:C:16:VAL:HG23	2.34	0.52
11:I:6:PHE:HB3	11:I:109:TYR:OH	2.10	0.52
13:K:57:VAL:HG12	13:K:57:VAL:O	2.08	0.52
21:S:24:ARG:HH21	21:S:39:ASN:HD22	1.58	0.52
22:T:46:ALA:HB1	22:T:52:THR:HG21	1.90	0.52
1:0:812:A:H2'	1:0:813:C:C6	2.44	0.52
2:9:3107:C:H2'	2:9:3108:C:C6	2.44	0.52
9:G:67:LEU:O	9:G:71:LEU:HG	2.09	0.52
1:0:635:A:H2'	1:0:636:G:H5''	1.92	0.52
1:0:1595:G:O2'	1:0:1596:U:H5'	2.09	0.52
1:0:1838:U:O2'	1:0:2644:C:H5'	2.09	0.52
1:0:2241:C:O2'	1:0:2242:U:H5'	2.09	0.52
1:0:2531:U:O2'	1:0:2532:A:H5'	2.08	0.52
1:0:2591:C:H2'	1:0:2592:G:O4'	2.10	0.52
19:Q:114:VAL:HA	19:Q:144:GLU:O	2.10	0.52
1:0:538:C:H5''	1:0:539:G:C8	2.45	0.52
1:0:1155:G:H2'	1:0:1156:C:C6	2.45	0.52
1:0:1298:U:H2'	1:0:1299:G:C8	2.44	0.52
1:0:1384:C:H5'	25:W:30:MET:HG2	1.91	0.52
1:0:1494:A:O2'	1:0:1505:U:O2	2.23	0.52
4:B:125:GLU:O	4:B:129:ARG:HG3	2.09	0.52
10:H:56:GLN:HE22	10:H:93:GLN:HG2	1.73	0.52
17:O:115:SER:HG	17:O:118:GLN:HG3	1.74	0.52
25:W:76:ARG:O	25:W:77:PHE:HB3	2.10	0.52
1:0:746:A:H4'	1:0:747:G:H5'	1.91	0.52
1:0:1181:A:H2'	1:0:1182:C:O4'	2.09	0.52
15:M:164:ASP:OD2	15:M:167:ASP:HA	2.09	0.52
26:X:212:ARG:HD2	40:X:8902:HOH:O	2.09	0.52
30:2:42:ARG:HG3	30:2:42:ARG:HH11	1.74	0.52
1:0:1098:A:H2'	1:0:1099:G:O4'	2.10	0.52
1:0:1333:U:H2'	1:0:1334:C:H6	1.73	0.52
1:0:1681:G:H5''	1:0:1682:A:H5'	1.92	0.52
1:0:2265:U:H2'	1:0:2266:A:H8	1.74	0.52
1:0:2781:U:C2'	1:0:2782:G:H5'	2.39	0.52
3:A:210:GLY:HA3	40:A:9058:HOH:O	2.09	0.52
16:N:44:ASN:CG	16:N:67:SER:HB2	2.34	0.52
27:Y:13:ARG:NH1	40:Y:8717:HOH:O	2.43	0.52
29:1:39:ARG:HG2	40:1:3143:HOH:O	2.10	0.52
1:0:381:G:H5''	40:L:8869:HOH:O	2.09	0.52
1:0:391:U:OP2	14:L:84:LYS:NZ	2.41	0.52
1:0:894:A:C2	5:C:87:ARG:NH2	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1164:U:H3	1:0:1192:A:H2	1.58	0.52
1:0:2072:G:C6	1:0:2533:C:H1'	2.45	0.52
1:0:2795:C:O2'	1:0:2796:U:H5'	2.10	0.52
15:M:180:LEU:O	15:M:181:ASP:HB3	2.10	0.52
17:O:7:LYS:HD2	17:O:21:VAL:CG2	2.40	0.52
19:Q:39:THR:HB	19:Q:42:GLU:HG3	1.91	0.52
26:X:154:ARG:HH12	26:X:155:ARG:CG	2.22	0.52
1:0:138:U:H5''	1:0:139:C:OP2	2.11	0.51
1:0:328:U:O4'	5:C:202:THR:HG22	2.10	0.51
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.42	0.51
1:0:1423:C:O2'	1:0:1424:A:H5'	2.10	0.51
2:9:3049:G:O2'	2:9:3050:G:H5'	2.11	0.51
3:A:51:ARG:HB2	40:A:9078:HOH:O	2.09	0.51
3:A:55:VAL:HG22	3:A:68:ILE:O	2.10	0.51
15:M:34:LEU:HA	15:M:47:LEU:HD23	1.93	0.51
1:0:241:A:C2	1:0:378:A:H4'	2.45	0.51
3:A:36:ASP:HB2	3:A:85:SER:H	1.74	0.51
3:A:48:ASP:HB3	40:A:9078:HOH:O	2.08	0.51
4:B:175:LEU:HD23	4:B:175:LEU:C	2.36	0.51
5:C:25:PRO:HG2	40:C:8525:HOH:O	2.10	0.51
16:N:14:LEU:HD23	16:N:102:ILE:HD11	1.93	0.51
1:0:1751:G:C2'	1:0:1752:G:H5''	2.40	0.51
16:N:96:VAL:HG13	16:N:100:GLN:HB2	1.93	0.51
25:W:78:GLU:HG2	25:W:79:GLU:N	2.23	0.51
29:1:48:ASP:O	29:1:49:GLU:HB2	2.11	0.51
1:0:2644:C:O2'	1:0:2645:U:H5'	2.10	0.51
1:0:2886:C:O2'	1:0:2887:G:H5'	2.10	0.51
2:9:3059:C:H2'	2:9:3060:C:C6	2.45	0.51
4:B:55:ASN:HB3	4:B:63:GLU:HA	1.91	0.51
4:B:71:VAL:HG11	4:B:296:LEU:HD22	1.93	0.51
4:B:215:VAL:HB	4:B:234:ARG:NH1	2.25	0.51
6:D:10:PHE:CG	6:D:11:HIS:N	2.78	0.51
6:D:95:THR:C	6:D:97:GLN:N	2.68	0.51
21:S:41:ARG:HG2	21:S:41:ARG:NH1	2.25	0.51
1:0:1118:A:C8	1:0:1118:A:C3'	2.93	0.51
1:0:1158:G:O2'	1:0:1159:G:H5'	2.11	0.51
1:0:1406:A:H4'	1:0:1407:A:H5''	1.92	0.51
1:0:1636:G:O2'	1:0:1637:A:H5'	2.10	0.51
1:0:2667:G:H1'	1:0:2914:A:N3	2.25	0.51
15:M:78:MET:HB2	15:M:79:PRO:HD3	1.93	0.51
1:0:793:A:H5''	17:O:83:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2721:U:OP1	22:T:17:THR:HG23	2.10	0.51
1:0:2820:A:H2'	1:0:2821:C:C6	2.44	0.51
5:C:236:THR:O	5:C:237:GLU:C	2.53	0.51
15:M:5:ARG:HG3	18:P:18:PRO:HB3	1.91	0.51
26:X:112:GLU:CD	26:X:115:ARG:NH1	2.69	0.51
1:0:138:U:OP2	1:0:139:C:H5	1.94	0.51
1:0:2470:A:H5''	40:0:3679:HOH:O	2.10	0.51
1:0:2735:U:H2'	1:0:2736:U:C6	2.46	0.51
5:C:140:VAL:HB	40:C:8659:HOH:O	2.10	0.51
10:H:76:GLU:O	10:H:77:LEU:HD23	2.11	0.51
10:H:116:ALA:O	10:H:117:PHE:C	2.54	0.51
13:K:101:ASP:C	13:K:103:ALA:H	2.17	0.51
17:O:16:VAL:HG13	17:O:20:ARG:CZ	2.41	0.51
23:U:11:MET:HB3	23:U:15:GLU:HB2	1.93	0.51
24:V:54:PHE:CZ	24:V:140:LYS:HB2	2.46	0.51
1:0:1730:G:C5'	1:0:1731:C:C6	2.94	0.51
1:0:2443:C:O3'	13:K:56:LYS:HE3	2.11	0.51
2:9:3039:U:H3'	2:9:3040:C:H5''	1.93	0.51
4:B:307:ARG:HG3	4:B:307:ARG:NH1	2.26	0.51
24:V:126:ASP:HB3	24:V:135:GLY:O	2.11	0.51
26:X:177:LYS:HE3	26:X:183:GLU:OE2	2.11	0.51
1:0:830:G:H2'	1:0:831:U:C6	2.46	0.51
1:0:1881:A:OP1	3:A:199:HIS:HE1	1.94	0.51
5:C:218:VAL:N	40:C:8631:HOH:O	2.43	0.51
8:F:117:GLU:C	8:F:119:ARG:N	2.69	0.51
12:J:125:ALA:C	12:J:127:ALA:H	2.19	0.51
14:L:114:VAL:HG23	36:L:8818:CL:CL	2.48	0.51
15:M:115:VAL:HG22	40:M:8860:HOH:O	2.11	0.51
18:P:53:HIS:CE1	18:P:55:ARG:HB2	2.46	0.51
24:V:119:HIS:HD2	24:V:120:PRO:O	1.94	0.51
30:2:14:CYS:HB3	30:2:16:GLU:HG2	1.93	0.51
1:0:352:A:H2'	1:0:353:G:C8	2.46	0.51
1:0:603:A:H4'	1:0:604:G:O5'	2.11	0.51
1:0:1921:A:O2'	1:0:1922:A:H5'	2.12	0.51
1:0:1947:G:H2'	1:0:1948:G:H8	1.76	0.51
4:B:75:GLU:C	4:B:77:PRO:HD3	2.36	0.51
4:B:162:MET:CE	4:B:308:LEU:HD21	2.34	0.51
6:D:91:ALA:HB2	6:D:106:PHE:CD2	2.45	0.51
10:H:59:HIS:HA	10:H:62:LEU:HD23	1.92	0.51
20:R:10:VAL:HG11	23:U:36:ALA:CA	2.41	0.51
1:0:1730:G:H5'	1:0:1731:C:C6	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2900:G:H2'	1:0:2901:C:O4'	2.11	0.50
2:9:3002:U:OP2	2:9:3002:U:H4'	2.11	0.50
6:D:67:ASP:O	6:D:69:ILE:HG13	2.11	0.50
7:E:11:VAL:HG11	7:E:22:VAL:HG13	1.92	0.50
10:H:79:GLU:C	10:H:80:GLU:HG3	2.35	0.50
11:I:131:THR:HG22	11:I:133:GLY:N	2.27	0.50
15:M:73:ALA:HB2	15:M:163:PHE:CZ	2.46	0.50
18:P:86:VAL:HG11	18:P:91:LEU:HD21	1.92	0.50
30:2:65:THR:CG2	30:2:67:LEU:HG	2.42	0.50
1:0:262:A:OP2	8:F:91:VAL:HG11	2.11	0.50
1:0:2413:A:N7	15:M:109:PRO:HB3	2.27	0.50
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.93	0.50
15:M:67:ALA:HA	15:M:71:TRP:HB3	1.93	0.50
30:2:48:ASN:ND2	30:2:50:GLY:H	2.10	0.50
1:0:1942:A:H5'	3:A:233:THR:HB	1.94	0.50
5:C:118:THR:CG2	5:C:137:PRO:HB3	2.41	0.50
6:D:57:THR:HG23	6:D:63:ILE:CB	2.42	0.50
25:W:15:ARG:HH11	25:W:15:ARG:CB	2.21	0.50
25:W:21:PRO:HG2	25:W:24:LYS:HD3	1.92	0.50
27:Y:26:VAL:O	27:Y:30:GLU:HG3	2.10	0.50
1:0:1894:C:N4	1:0:1939:U:H2'	2.27	0.50
1:0:2334:C:O2'	1:0:2335:C:H5'	2.12	0.50
1:0:2611:G:H5'	1:0:2613:G:C8	2.46	0.50
1:0:2720:C:O2	12:J:87:ARG:NH2	2.44	0.50
5:C:93:LYS:O	5:C:98:ARG:NH2	2.41	0.50
7:E:31:ARG:HH12	7:E:68:HIS:CG	2.28	0.50
15:M:184:ILE:HG22	15:M:185:GLU:HG3	1.93	0.50
29:1:36:ASN:HB3	29:1:39:ARG:HG3	1.93	0.50
1:0:1768:C:H2'	1:0:1769:C:O4'	2.12	0.50
1:0:2089:A:O2'	1:0:2090:G:H5'	2.11	0.50
2:9:3013:A:O2'	2:9:3014:G:H5''	2.11	0.50
7:E:15:GLN:NE2	7:E:40:VAL:O	2.43	0.50
8:F:48:VAL:HG23	8:F:74:PHE:HB3	1.93	0.50
12:J:34:VAL:HB	40:J:7169:HOH:O	2.11	0.50
15:M:159:TYR:HE2	15:M:163:PHE:HE2	1.59	0.50
1:0:101:C:H2'	1:0:102:A:H8	1.76	0.50
1:0:1730:G:C5'	1:0:1731:C:H6	2.24	0.50
1:0:1741:U:O2'	1:0:2723:G:H4'	2.10	0.50
1:0:2780:C:H1'	7:E:143:GLN:NE2	2.24	0.50
4:B:24:PRO:HG2	4:B:204:GLY:HA2	1.92	0.50
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:20:ILE:HG23	10:H:120:ILE:CD1	2.41	0.50
15:M:161:GLY:O	15:M:162:ASP:C	2.54	0.50
23:U:64:GLY:O	23:U:65:ASP:CB	2.59	0.50
1:0:204:A:C2'	1:0:205:U:H5'	2.41	0.50
1:0:1501:A:OP2	17:O:37:ARG:HD2	2.12	0.50
40:O:5897:HOH:O	4:B:298:LYS:HD3	2.11	0.50
2:9:3028:U:H2'	2:9:3029:C:C6	2.47	0.50
3:A:109:GLU:HG2	3:A:116:GLY:H	1.76	0.50
4:B:125:GLU:OE2	4:B:129:ARG:NH1	2.45	0.50
4:B:205:VAL:O	4:B:307:ARG:NE	2.45	0.50
6:D:154:LYS:HD2	6:D:154:LYS:N	2.17	0.50
10:H:83:TYR:CD1	10:H:83:TYR:C	2.90	0.50
12:J:45:PRO:HB2	40:J:7169:HOH:O	2.11	0.50
19:Q:34:GLU:HG2	19:Q:46:TYR:OH	2.12	0.50
1:0:289:G:O2'	1:0:290:C:H5'	2.12	0.50
1:0:945:U:H2'	1:0:946:C:H6	1.76	0.50
1:0:1250:C:O2'	1:0:1251:C:H5'	2.11	0.50
1:0:2364:A:H5''	18:P:15:LYS:HD3	1.92	0.50
8:F:21:GLU:O	8:F:24:ARG:HG3	2.11	0.50
23:U:12:THR:HG23	23:U:14:ALA:H	1.77	0.50
25:W:78:GLU:CG	25:W:79:GLU:H	2.24	0.50
1:0:12:U:H2'	1:0:13:G:H5'	1.93	0.50
1:0:960:G:H4'	40:O:7764:HOH:O	2.11	0.50
1:0:1269:G:H2'	1:0:1270:U:C6	2.47	0.50
1:0:1419:U:H2'	1:0:1685:A:C2	2.47	0.50
1:0:2672:C:O2'	1:0:2673:U:H5'	2.12	0.50
10:H:154:TYR:CD1	10:H:154:TYR:C	2.90	0.50
17:O:13:VAL:HG21	17:O:41:ARG:HG2	1.94	0.50
19:Q:39:THR:HG22	19:Q:42:GLU:H	1.77	0.50
24:V:90:TYR:N	24:V:90:TYR:CD1	2.79	0.50
1:0:316:A:N3	1:0:336:G:O2'	2.40	0.49
1:0:412:C:O2'	1:0:413:G:H5'	2.12	0.49
1:0:447:A:O2'	1:0:448:G:H5'	2.12	0.49
1:0:951:A:C2'	1:0:952:G:H5'	2.42	0.49
1:0:1165:G:OP1	1:0:1165:G:H3'	2.12	0.49
1:0:1535:G:H2'	1:0:1536:C:C6	2.47	0.49
1:0:1701:A:H5'	40:O:6649:HOH:O	2.11	0.49
10:H:40:ALA:HB1	10:H:137:TYR:CE2	2.47	0.49
12:J:58:THR:HG22	12:J:59:LYS:HG3	1.93	0.49
12:J:62:PRO:HG3	12:J:65:ARG:HH21	1.76	0.49
13:K:10:SER:O	13:K:11:ARG:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:105:G:O2'	1:0:106:A:H5'	2.12	0.49
2:9:3003:A:N6	2:9:3022:G:H1'	2.27	0.49
5:C:168:ARG:NH2	5:C:190:ALA:O	2.45	0.49
6:D:75:LEU:HD22	6:D:79:MET:HB3	1.94	0.49
6:D:99:ASP:CB	6:D:103:ASN:H	2.24	0.49
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.42	0.49
12:J:75:ARG:HE	12:J:94:ALA:HB3	1.77	0.49
15:M:151:ASP:O	15:M:154:LEU:HB2	2.11	0.49
21:S:9:LYS:NZ	21:S:13:ARG:NH1	2.60	0.49
25:W:9:VAL:HG13	25:W:88:GLU:CD	2.37	0.49
1:0:629:A:H2'	1:0:630:A:O4'	2.13	0.49
1:0:2540:G:O2'	1:0:2541:U:H5''	2.12	0.49
7:E:84:MET:HE2	7:E:133:VAL:HG23	1.93	0.49
10:H:3:ALA:HA	10:H:58:ARG:NH1	2.27	0.49
13:K:143:THR:CG2	13:K:144:ASP:H	2.25	0.49
20:R:11:THR:H	20:R:14:ALA:HB3	1.77	0.49
1:0:709:G:O2'	16:N:25:VAL:HG12	2.12	0.49
1:0:1211:G:O2'	1:0:1212:C:H5'	2.13	0.49
1:0:1218:U:H2'	1:0:1219:U:C6	2.47	0.49
1:0:1342:C:C2'	1:0:1343:C:H5'	2.42	0.49
1:0:2090:G:H2'	1:0:2091:G:C8	2.47	0.49
1:0:2635:A:O2'	1:0:2636:C:H5'	2.12	0.49
6:D:41:LEU:HA	6:D:44:ILE:CG2	2.41	0.49
9:G:20:VAL:O	9:G:24:VAL:HG23	2.12	0.49
19:Q:106:GLY:HA2	19:Q:109:MET:CE	2.40	0.49
1:0:1778:A:H2'	1:0:1779:A:H5'	1.93	0.49
1:0:2520:G:O2'	1:0:2521:A:H5'	2.12	0.49
1:0:2570:G:H5''	40:0:5298:HOH:O	2.13	0.49
6:D:58:VAL:HG12	6:D:59:GLY:N	2.27	0.49
7:E:92:PRO:HB2	40:E:4917:HOH:O	2.12	0.49
11:I:19:MET:HE3	11:I:132:LEU:CD1	2.30	0.49
1:0:861:A:H4'	1:0:1697:G:H4'	1.94	0.49
40:9:9094:HOH:O	15:M:23:ARG:HD3	2.12	0.49
5:C:1:MET:HG2	5:C:2:GLN:NE2	2.27	0.49
13:K:121:ILE:HG12	13:K:141:GLU:HB2	1.94	0.49
14:L:24:GLN:O	14:L:28:GLN:HG3	2.12	0.49
27:Y:57:CYS:SG	27:Y:59:TYR:HB3	2.52	0.49
1:0:441:A:H1'	1:0:442:A:N7	2.28	0.49
1:0:945:U:H2'	1:0:946:C:C6	2.46	0.49
1:0:2499:U:H2'	1:0:2500:C:C6	2.47	0.49
2:9:3106:C:O2'	2:9:3107:C:H5'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:84:LEU:HD13	4:B:84:LEU:O	2.12	0.49
12:J:30:LYS:O	12:J:55:VAL:HG13	2.13	0.49
20:R:33:SER:O	20:R:37:VAL:HG23	2.13	0.49
27:Y:39:CYS:O	27:Y:42:CYS:O	2.31	0.49
1:O:1007:A:H2'	10:H:19:TYR:CZ	2.48	0.49
1:O:1044:C:H5''	40:O:9518:HOH:O	2.12	0.49
1:O:1181:A:O2'	1:O:1182:C:H5'	2.13	0.49
1:O:1482:A:O2'	1:O:1483:C:H5'	2.13	0.49
40:O:6650:HOH:O	26:X:158:LYS:HD3	2.12	0.49
2:9:3052:A:O2'	2:9:3053:G:H5'	2.13	0.49
6:D:173:GLU:HG3	6:D:174:VAL:N	2.27	0.49
14:L:30:GLU:O	14:L:34:GLU:HG3	2.12	0.49
20:R:57:THR:HG22	20:R:58:MET:N	2.26	0.49
1:O:344:C:H2'	1:O:345:G:O4'	2.13	0.49
1:O:887:G:H2'	1:O:888:U:C6	2.47	0.49
1:O:1205:U:H2'	1:O:1206:U:H5''	1.94	0.49
1:O:1268:C:O2'	1:O:1269:G:H5'	2.12	0.49
1:O:1268:C:H2'	1:O:1269:G:H8	1.78	0.49
1:O:1527:A:H1'	1:O:1528:A:C8	2.47	0.49
7:E:100:ASP:HB2	40:E:2789:HOH:O	2.13	0.49
9:G:63:ARG:O	9:G:67:LEU:HG	2.12	0.49
24:V:149:LEU:CG	24:V:153:MET:HE2	2.29	0.49
1:O:2815:G:N7	11:I:80:LYS:NZ	2.58	0.49
2:9:3018:U:H2'	2:9:3019:G:H8	1.78	0.49
14:L:164:THR:HG22	14:L:166:ALA:H	1.78	0.49
19:Q:113:HIS:HE1	19:Q:144:GLU:CD	2.21	0.49
1:O:101:C:H2'	1:O:102:A:C8	2.48	0.48
1:O:596:C:H2'	1:O:597:A:C8	2.47	0.48
1:O:1654:U:H2'	3:A:47:HIS:CD2	2.47	0.48
1:O:1913:C:H2'	1:O:1914:C:H6	1.78	0.48
1:O:2101:A:H2'	5:C:63:SER:OG	2.13	0.48
6:D:154:LYS:H	6:D:154:LYS:CD	2.14	0.48
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.94	0.48
13:K:118:LEU:HB2	40:K:8878:HOH:O	2.13	0.48
16:N:80:ASP:OD1	16:N:81:PHE:N	2.46	0.48
26:X:186:ARG:HH11	26:X:186:ARG:HG2	1.78	0.48
1:O:558:C:C2'	1:O:559:C:C5'	2.92	0.48
1:O:1086:A:C6	24:V:11:VAL:HG11	2.48	0.48
1:O:2781:U:H2'	1:O:2782:G:H5'	1.95	0.48
40:O:9995:HOH:O	17:O:81:LYS:HG2	2.12	0.48
3:A:93:THR:C	3:A:94:LEU:HD23	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:194:PHE:CD2	5:C:234:VAL:HG11	2.47	0.48
10:H:38:LYS:HE2	10:H:42:ASP:HB2	1.95	0.48
1:0:185:G:H4'	1:0:186:A:H4'	1.94	0.48
1:0:1187:U:O2'	1:0:1189:A:H2	1.96	0.48
6:D:81:GLU:O	6:D:85:GLN:HG3	2.13	0.48
7:E:11:VAL:HG12	7:E:12:ASP:H	1.77	0.48
15:M:116:PHE:N	40:M:8860:HOH:O	2.46	0.48
24:V:76:ASP:O	24:V:77:ALA:C	2.56	0.48
1:0:95:A:H5''	1:0:97:G:O4'	2.14	0.48
1:0:249:G:O2'	1:0:250:C:H5'	2.13	0.48
1:0:366:U:H2'	1:0:367:G:O4'	2.12	0.48
1:0:1252:A:H2'	1:0:1253:C:O4'	2.12	0.48
1:0:1913:C:H2'	1:0:1914:C:C6	2.48	0.48
1:0:2895:C:H4'	40:W:4132:HOH:O	2.13	0.48
1:0:2427:C:OP2	30:2:84:ARG:HD2	2.12	0.48
1:0:2699:A:H2'	1:0:2700:G:O4'	2.12	0.48
1:0:2781:U:H1'	7:E:139:GLU:OE2	2.13	0.48
5:C:246:ARG:NE	40:C:8631:HOH:O	2.38	0.48
8:F:48:VAL:HG12	8:F:97:ALA:CB	2.43	0.48
10:H:17:ARG:HD3	10:H:23:ILE:HD12	1.96	0.48
10:H:46:GLN:NE2	10:H:137:TYR:HE2	2.09	0.48
11:I:47:THR:HG22	11:I:48:GLY:N	2.29	0.48
15:M:164:ASP:OD1	15:M:167:ASP:HA	2.13	0.48
18:P:64:GLU:HG3	18:P:74:ASP:OD2	2.13	0.48
26:X:112:GLU:OE1	26:X:112:GLU:HA	2.13	0.48
1:0:236:A:H4'	1:0:237:G:H5'	1.96	0.48
1:0:290:C:O2'	1:0:291:C:H5'	2.13	0.48
1:0:858:U:H2'	1:0:859:C:C6	2.48	0.48
1:0:1241:G:N3	11:I:86:MET:HE2	2.27	0.48
1:0:2712:G:H5'	40:J:4183:HOH:O	2.14	0.48
5:C:194:PHE:HA	5:C:234:VAL:HG13	1.95	0.48
6:D:173:GLU:O	6:D:174:VAL:C	2.56	0.48
14:L:164:THR:HG23	14:L:165:GLY:N	2.28	0.48
16:N:47:ARG:HG3	16:N:47:ARG:NH1	2.16	0.48
16:N:105:ASN:HD21	16:N:109:SER:H	1.62	0.48
17:O:97:ARG:HD2	40:O:163:HOH:O	2.13	0.48
18:P:30:VAL:O	18:P:30:VAL:HG12	2.13	0.48
1:0:189:A:OP1	14:L:171:ARG:NH2	2.46	0.48
1:0:776:A:OP1	28:Z:28:HIS:HE1	1.97	0.48
1:0:1096:U:O2'	1:0:1097:A:H5'	2.13	0.48
1:0:1173:A:H4'	1:0:1174:A:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1500:U:P	17:O:41:ARG:HH22	2.37	0.48
1:O:2271:G:H5'	40:A:9045:HOH:O	2.14	0.48
2:9:3060:C:O2'	2:9:3061:C:H5'	2.13	0.48
4:B:190:MET:HE2	4:B:194:PHE:HD1	1.72	0.48
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.38	0.48
5:C:214:THR:HG21	40:C:8610:HOH:O	2.13	0.48
8:F:32:GLY:N	40:F:3111:HOH:O	2.46	0.48
9:G:19:GLU:O	9:G:23:ILE:HG13	2.14	0.48
26:X:189:ASN:ND2	26:X:192:ASP:H	2.12	0.48
1:O:960:G:N3	1:O:960:G:C2'	2.77	0.48
1:O:1335:C:H2'	1:O:1336:U:C6	2.48	0.48
1:O:1835:U:C5	1:O:1840:A:N7	2.69	0.48
1:O:2401:A:H2'	1:O:2402:A:C8	2.48	0.48
2:9:3107:C:H2'	2:9:3108:C:H6	1.76	0.48
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.79	0.48
5:C:242:GLU:HG3	40:C:8589:HOH:O	2.14	0.48
8:F:58:GLU:HG3	8:F:61:MET:HE2	1.94	0.48
10:H:73:LEU:HD21	10:H:146:VAL:HA	1.95	0.48
1:O:2837:U:H1'	4:B:307:ARG:HH12	1.78	0.48
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.78	0.48
5:C:162:VAL:CG1	5:C:192:ILE:HD11	2.43	0.48
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.44	0.48
6:D:103:ASN:ND2	6:D:134:LEU:H	2.12	0.48
15:M:154:LEU:O	15:M:155:GLU:CB	2.62	0.48
21:S:71:VAL:CG1	21:S:72:ILE:N	2.76	0.48
24:V:115:THR:HG23	40:V:5420:HOH:O	2.13	0.48
1:O:415:A:O2'	1:O:416:G:H5'	2.14	0.48
1:O:541:C:O2'	1:O:542:A:H5''	2.14	0.48
1:O:1236:A:C8	11:I:63:ILE:HD11	2.49	0.48
1:O:1298:U:H2'	1:O:1299:G:H8	1.79	0.48
1:O:1819:G:H2'	1:O:1820:G:C4'	2.40	0.48
1:O:2503:A:P	10:H:151:ARG:HH22	2.37	0.48
1:O:2595:U:H2'	1:O:2596:A:C8	2.48	0.48
8:F:60:VAL:O	8:F:60:VAL:CG1	2.61	0.48
13:K:129:ALA:O	13:K:133:VAL:HG23	2.14	0.48
16:N:99:GLU:HG3	40:N:6044:HOH:O	2.13	0.48
28:Z:56:GLU:HG2	28:Z:56:GLU:OXT	2.14	0.48
1:O:894:A:N1	5:C:87:ARG:NH2	2.61	0.47
1:O:1021:G:O2'	1:O:1022:A:H5'	2.14	0.47
1:O:1878:G:O2'	1:O:1879:U:OP2	2.32	0.47
4:B:7:ARG:HD3	4:B:9:GLY:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:55:LYS:O	6:D:56:ARG:HB2	2.13	0.47
9:G:12:ILE:HG13	40:G:6833:HOH:O	2.13	0.47
11:I:131:THR:HG22	11:I:134:GLU:H	1.78	0.47
15:M:86:LEU:HD12	15:M:125:ALA:HB2	1.96	0.47
18:P:32:GLU:HA	18:P:71:TYR:OH	2.14	0.47
19:Q:84:ALA:O	19:Q:88:PHE:HD1	1.97	0.47
20:R:38:ALA:O	20:R:42:GLU:HG3	2.14	0.47
1:0:542:A:H2'	1:0:543:G:O4'	2.14	0.47
1:0:1066:U:H2'	1:0:1067:A:C8	2.49	0.47
1:0:1362:U:H2'	1:0:1363:G:C8	2.50	0.47
1:0:2349:G:O2'	1:0:2350:G:H5'	2.13	0.47
1:0:2498:C:O2'	1:0:2499:U:H5'	2.14	0.47
1:0:2569:A:C2'	1:0:2570:G:O5'	2.62	0.47
3:A:217:ARG:HH11	3:A:217:ARG:CG	2.27	0.47
6:D:57:THR:HG23	6:D:63:ILE:CG2	2.42	0.47
6:D:59:GLY:O	6:D:61:PHE:N	2.39	0.47
8:F:58:GLU:CA	8:F:61:MET:HE2	2.34	0.47
11:I:76:ASP:HA	40:I:5907:HOH:O	2.13	0.47
12:J:118:ALA:C	12:J:120:ARG:H	2.22	0.47
13:K:149:ARG:O	13:K:150:GLN:HB2	2.14	0.47
23:U:58:THR:O	23:U:62:GLU:HG3	2.14	0.47
30:2:11:CYS:HB2	30:2:20:HIS:CE1	2.48	0.47
1:0:946:C:H2'	1:0:947:U:C6	2.49	0.47
1:0:1042:U:O2'	1:0:1043:C:H5'	2.14	0.47
1:0:2379:G:N3	1:0:2418:G:H2'	2.28	0.47
5:C:142:ASP:OD1	5:C:236:THR:HG23	2.13	0.47
10:H:2:PRO:HD2	10:H:5:MET:SD	2.54	0.47
13:K:134:GLU:HG3	40:K:8861:HOH:O	2.13	0.47
30:2:17:HIS:O	30:2:18:GLN:HG3	2.14	0.47
1:0:222:A:H2'	1:0:223:G:O4'	2.13	0.47
1:0:622:G:O2'	1:0:623:U:H5'	2.14	0.47
1:0:1871:U:O4'	1:0:1873:G:C8	2.67	0.47
10:H:30:GLN:H	10:H:66:ARG:HH11	1.61	0.47
15:M:152:GLU:C	15:M:154:LEU:N	2.71	0.47
19:Q:119:VAL:O	19:Q:119:VAL:CG1	2.61	0.47
1:0:200:U:H2'	40:0:3874:HOH:O	2.15	0.47
1:0:1592:G:O2'	1:0:1593:C:O4'	2.31	0.47
1:0:1789:G:O6	17:O:73:HIS:HE1	1.97	0.47
14:L:72:ALA:HB2	14:L:93:ARG:HG2	1.97	0.47
1:0:286:U:H2'	1:0:287:C:C6	2.50	0.47
1:0:889:C:H2'	1:0:890:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1131:G:C6	1:0:1230:A:C4	3.03	0.47
1:0:1189:A:H1'	1:0:1209:C:H1'	1.94	0.47
1:0:1249:U:H2'	1:0:1250:C:C6	2.49	0.47
1:0:1328:A:C8	26:X:169:ARG:HD3	2.48	0.47
40:0:7221:HOH:O	14:L:178:LYS:HB2	2.15	0.47
2:9:3049:G:H2'	2:9:3050:G:O4'	2.14	0.47
7:E:108:LEU:HD11	7:E:164:ASP:HB2	1.97	0.47
10:H:158:THR:HB	10:H:159:PRO:HD3	1.97	0.47
19:Q:25:PHE:CE2	19:Q:29:LYS:CE	2.97	0.47
21:S:96:VAL:HG13	21:S:97:ARG:N	2.30	0.47
1:0:653:C:H2'	1:0:654:A:C8	2.49	0.47
1:0:856:G:H2'	40:0:5807:HOH:O	2.13	0.47
1:0:962:C:H5'	40:0:7312:HOH:O	2.15	0.47
1:0:1515:A:H2'	1:0:1516:C:C6	2.50	0.47
1:0:1562:C:H42	1:0:2738:G:H1	1.62	0.47
1:0:1574:C:H2'	1:0:1575:C:C6	2.50	0.47
1:0:2252:A:H2'	1:0:2253:G:O4'	2.14	0.47
1:0:2257:G:H4'	1:0:2259:C:C2	2.50	0.47
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.96	0.47
11:I:45:VAL:HG22	11:I:46:ILE:N	2.29	0.47
23:U:39:ALA:O	23:U:41:GLU:N	2.48	0.47
24:V:3:ALA:O	24:V:54:PHE:HA	2.14	0.47
24:V:65:VAL:HG12	24:V:116:LEU:HD13	1.95	0.47
1:0:947:U:H2'	1:0:948:G:C8	2.50	0.47
1:0:1500:U:OP2	17:O:41:ARG:NH2	2.48	0.47
3:A:94:LEU:HD23	3:A:94:LEU:N	2.29	0.47
4:B:53:LEU:CD1	4:B:327:VAL:HG22	2.43	0.47
6:D:94:ALA:HB3	6:D:174:VAL:CA	2.45	0.47
12:J:28:GLU:OE2	12:J:58:THR:HG21	2.14	0.47
14:L:120:VAL:CG1	14:L:130:GLU:HG3	2.43	0.47
15:M:61:ALA:CB	15:M:88:ALA:HB2	2.43	0.47
15:M:71:TRP:N	40:M:8840:HOH:O	2.48	0.47
17:O:31:ILE:HG12	17:O:43:LEU:HD13	1.96	0.47
24:V:144:GLU:O	24:V:148:ASP:OD2	2.33	0.47
1:0:69:A:H5'	1:0:69:A:H8	1.80	0.47
1:0:907:A:H2'	1:0:908:A:C8	2.50	0.47
1:0:1309:U:O2'	1:0:1310:U:H5'	2.15	0.47
1:0:1753:C:O2	4:B:229:ARG:NH2	2.46	0.47
1:0:2626:C:H2'	1:0:2627:G:C8	2.50	0.47
40:0:9568:HOH:O	4:B:214:PRO:HD2	2.15	0.47
5:C:13:ASP:OD1	5:C:13:ASP:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:93:MET:HE1	7:E:165:GLY:CA	2.45	0.47
19:Q:114:VAL:HG13	19:Q:114:VAL:O	2.15	0.47
1:0:1001:U:O2'	1:0:1002:G:H5'	2.15	0.47
1:0:1361:C:H2'	1:0:1362:U:C6	2.50	0.47
1:0:1659:A:H2'	1:0:1660:G:O4'	2.15	0.47
2:9:3014:G:H5'	2:9:3014:G:C8	2.50	0.47
11:I:99:GLU:HA	40:I:7377:HOH:O	2.15	0.47
15:M:49:THR:CG2	15:M:58:LEU:HD11	2.45	0.47
16:N:96:VAL:CG1	16:N:100:GLN:HB2	2.44	0.47
16:N:98:LEU:O	16:N:102:ILE:HG13	2.14	0.47
19:Q:132:ARG:HG2	19:Q:133:ALA:N	2.29	0.47
1:0:407:A:O2'	1:0:408:A:H5'	2.14	0.46
1:0:2300:A:H4'	1:0:2301:A:O5'	2.15	0.46
2:9:3006:C:H4'	15:M:35:VAL:HG11	1.97	0.46
5:C:16:VAL:HG12	5:C:17:ASP:H	1.78	0.46
6:D:167:GLU:C	6:D:169:THR:H	2.23	0.46
21:S:18:GLU:O	21:S:21:LYS:HG2	2.14	0.46
29:1:25:VAL:O	29:1:29:THR:HG23	2.15	0.46
1:0:31:C:H4'	40:S:7242:HOH:O	2.14	0.46
1:0:220:C:C2	13:K:48:LYS:HE2	2.50	0.46
1:0:666:A:H2'	1:0:667:C:O4'	2.15	0.46
1:0:907:A:H2'	1:0:908:A:H8	1.79	0.46
1:0:1189:A:O2'	1:0:1208:C:H2'	2.14	0.46
1:0:1741:U:H5'	1:0:1742:A:OP1	2.14	0.46
1:0:1826:C:O2'	1:0:1827:G:H5'	2.15	0.46
1:0:1942:A:O2'	1:0:1943:C:H5'	2.15	0.46
1:0:2087:C:O2'	1:0:2088:C:H5'	2.15	0.46
1:0:2388:C:O2'	1:0:2389:U:H5'	2.15	0.46
1:0:2697:A:H2'	1:0:2698:G:O4'	2.15	0.46
1:0:2906:A:H5'	1:0:2907:C:O4'	2.16	0.46
11:I:19:MET:HE1	11:I:78:ILE:HG22	1.96	0.46
15:M:37:ARG:NE	40:M:8835:HOH:O	2.48	0.46
26:X:234:VAL:HG12	26:X:235:GLU:N	2.30	0.46
28:Z:28:HIS:CE1	28:Z:31:LYS:HE2	2.49	0.46
28:Z:28:HIS:CD2	28:Z:31:LYS:HG3	2.50	0.46
1:0:162:C:H2'	1:0:163:U:H5'	1.97	0.46
1:0:1168:C:H2'	1:0:1169:U:O4'	2.16	0.46
1:0:1421:C:O2'	1:0:1422:U:H5'	2.15	0.46
1:0:2419:U:H5''	1:0:2420:G:H5'	1.96	0.46
12:J:62:PRO:HG3	12:J:65:ARG:NH2	2.30	0.46
14:L:9:ARG:HG3	40:L:8846:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:33:SER:OG	20:R:36:GLU:HG3	2.14	0.46
21:S:19:ARG:HD3	21:S:67:LEU:O	2.14	0.46
24:V:48:VAL:O	24:V:48:VAL:HG12	2.15	0.46
25:W:9:VAL:HG13	25:W:88:GLU:OE1	2.15	0.46
1:0:907:A:H4'	1:0:1328:A:C2	2.51	0.46
1:0:1304:U:H2'	1:0:1305:C:C6	2.51	0.46
1:0:1477:C:C5'	1:0:1868:G:H5''	2.45	0.46
1:0:2689:A:H2'	1:0:2690:U:H5'	1.98	0.46
7:E:81:GLU:HA	7:E:133:VAL:O	2.15	0.46
17:O:10:ALA:CA	17:O:13:VAL:HG12	2.43	0.46
19:Q:50:VAL:HA	19:Q:55:GLN:O	2.16	0.46
21:S:9:LYS:HB2	40:S:7242:HOH:O	2.15	0.46
26:X:107:PRO:HB3	26:X:182:PHE:CD2	2.51	0.46
1:0:1819:G:H2'	1:0:1820:G:C5'	2.45	0.46
1:0:1925:G:O2'	1:0:1926:G:H5'	2.15	0.46
1:0:2826:G:C6	1:0:2913:A:N6	2.84	0.46
10:H:56:GLN:NE2	10:H:93:GLN:HG2	2.30	0.46
19:Q:25:PHE:CZ	19:Q:29:LYS:HE2	2.50	0.46
26:X:141:THR:HG23	40:X:8889:HOH:O	2.15	0.46
30:2:91:GLN:O	30:2:92:GLU:HB2	2.15	0.46
1:0:1739:G:O2'	1:0:1740:U:H5'	2.15	0.46
1:0:1840:A:H4'	1:0:1841:C:O5'	2.15	0.46
1:0:2112:A:H2'	1:0:2113:G:C8	2.50	0.46
1:0:2453:G:H4'	13:K:50:GLY:C	2.40	0.46
40:O:5085:HOH:O	27:Y:13:ARG:HD3	2.16	0.46
2:9:3023:U:C3'	2:9:3024:U:C5'	2.84	0.46
6:D:136:ARG:HB2	6:D:137:PRO:HD2	1.96	0.46
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.16	0.46
15:M:37:ARG:HH11	15:M:37:ARG:HG3	1.80	0.46
16:N:44:ASN:OD1	16:N:67:SER:HB2	2.16	0.46
24:V:73:LEU:O	24:V:74:GLU:HG3	2.16	0.46
28:Z:28:HIS:CD2	28:Z:30:LYS:HB2	2.50	0.46
28:Z:28:HIS:HD2	28:Z:31:LYS:H	1.63	0.46
1:0:171:C:OP2	14:L:84:LYS:HG3	2.16	0.46
1:0:343:C:O2'	1:0:344:C:H5'	2.16	0.46
1:0:396:U:O2'	1:0:397:A:P	2.73	0.46
1:0:602:A:O2'	1:0:605:C:H4'	2.16	0.46
1:0:1909:A:H2'	1:0:1910:A:C8	2.51	0.46
1:0:2256:G:O2'	1:0:2257:G:H5'	2.16	0.46
1:0:2830:U:O2'	1:0:2831:C:H5'	2.15	0.46
1:0:2847:G:O2'	1:0:2848:G:H5'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3102:G:O2'	2:9:3103:A:H5'	2.15	0.46
3:A:36:ASP:CA	3:A:83:GLY:HA3	2.44	0.46
11:I:15:ARG:NH1	11:I:43:ARG:NH1	2.63	0.46
16:N:42:GLU:HB2	40:N:2176:HOH:O	2.16	0.46
20:R:81:ILE:HG22	23:U:29:ASN:OD1	2.16	0.46
24:V:21:LEU:HB3	24:V:26:ILE:CG1	2.46	0.46
1:0:622:G:P	26:X:148:GLY:HA3	2.56	0.46
1:0:820:G:H5'	1:0:821:U:H5'	1.97	0.46
1:0:1087:G:H4'	1:0:1088:A:OP1	2.16	0.46
1:0:2044:G:OP1	25:W:23:HIS:HE1	1.99	0.46
1:0:2251:G:H2'	1:0:2252:A:H8	1.79	0.46
1:0:2815:G:OP2	11:I:99:GLU:HG2	2.15	0.46
3:A:217:ARG:HG3	40:A:9008:HOH:O	2.15	0.46
13:K:73:VAL:HG23	13:K:74:THR:N	2.29	0.46
14:L:66:SER:HB3	14:L:128:TRP:CD1	2.51	0.46
23:U:45:ARG:C	23:U:47:LYS:N	2.71	0.46
25:W:43:VAL:CG1	25:W:44:ASP:N	2.78	0.46
1:0:39:G:N2	1:0:444:C:C2	2.84	0.46
1:0:526:U:H2'	1:0:527:U:C6	2.51	0.46
1:0:613:C:H2'	1:0:614:U:C6	2.51	0.46
1:0:1056:U:H2'	1:0:1057:A:O4'	2.15	0.46
1:0:1544:U:H2'	1:0:1545:C:H6	1.81	0.46
1:0:1783:A:O2'	1:0:1784:U:H5'	2.16	0.46
1:0:2842:G:C2'	1:0:2843:A:H5'	2.46	0.46
6:D:10:PHE:CD1	6:D:11:HIS:N	2.84	0.46
7:E:7:ILE:HG22	7:E:45:ASP:O	2.16	0.46
7:E:154:ILE:HG13	7:E:156:ASP:OD1	2.16	0.46
11:I:56:LYS:HE2	11:I:60:ARG:NH2	2.31	0.46
11:I:103:VAL:HG12	40:I:5907:HOH:O	2.16	0.46
15:M:73:ALA:HB1	15:M:74:PRO:CD	2.46	0.46
1:0:834:G:H3'	1:0:835:U:H4'	1.97	0.46
1:0:2115:U:H2'	1:0:2116:U:C6	2.50	0.46
2:9:3104:A:O2'	2:9:3105:A:H5'	2.16	0.46
40:9:9090:HOH:O	24:V:13:MET:HA	2.14	0.46
3:A:36:ASP:CB	3:A:85:SER:H	2.29	0.46
6:D:27:ILE:HB	40:D:5858:HOH:O	2.16	0.46
12:J:101:ASN:O	12:J:102:GLU:HB2	2.16	0.46
13:K:133:VAL:HG13	40:K:8878:HOH:O	2.16	0.46
21:S:111:ARG:HB3	21:S:119:ALA:HB2	1.98	0.46
23:U:5:VAL:HG11	23:U:9:ARG:NH1	2.31	0.46
23:U:8:ILE:CG2	23:U:59:ILE:HG13	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:42:CYS:SG	27:Y:44:GLU:HB2	2.56	0.46
29:1:20:ARG:HG3	29:1:39:ARG:HH21	1.81	0.46
1:0:876:A:N3	1:0:876:A:C2'	2.80	0.45
1:0:958:G:O2'	1:0:959:C:H5'	2.15	0.45
1:0:2362:A:H2'	1:0:2363:G:C8	2.52	0.45
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.43	0.45
12:J:55:VAL:CG1	12:J:56:SER:N	2.78	0.45
14:L:184:ARG:HG3	14:L:185:PRO:HA	1.98	0.45
22:T:14:GLU:OE1	22:T:15:PRO:HD2	2.16	0.45
22:T:52:THR:HG22	22:T:54:THR:N	2.31	0.45
1:0:283:U:H5''	1:0:284:C:P	2.56	0.45
1:0:559:C:H2'	1:0:560:C:O4'	2.17	0.45
1:0:1115:U:O2'	1:0:1116:U:H5'	2.16	0.45
1:0:1780:G:O2'	1:0:1781:G:H5'	2.16	0.45
1:0:1942:A:H5'	3:A:233:THR:CB	2.46	0.45
1:0:2296:C:H2'	1:0:2297:U:H6	1.81	0.45
1:0:2385:G:H2'	1:0:2386:U:C6	2.51	0.45
6:D:27:ILE:HD11	6:D:37:ALA:CB	2.46	0.45
6:D:38:GLU:OE2	6:D:51:ARG:CZ	2.64	0.45
15:M:22:GLN:HG2	15:M:26:LEU:HD22	1.97	0.45
15:M:33:ARG:NH1	15:M:103:ASP:OD2	2.47	0.45
16:N:26:TRP:CE3	16:N:26:TRP:HA	2.51	0.45
21:S:43:ASN:C	21:S:45:GLY:H	2.24	0.45
29:1:36:ASN:O	29:1:39:ARG:HG3	2.16	0.45
1:0:695:C:H2'	1:0:696:C:C6	2.51	0.45
1:0:1406:A:H4'	1:0:1407:A:C5'	2.46	0.45
4:B:243:ASN:HA	4:B:244:PRO:C	2.40	0.45
7:E:80:TRP:O	7:E:134:SER:HA	2.16	0.45
15:M:47:LEU:CD1	15:M:97:VAL:HG11	2.45	0.45
15:M:132:ASN:O	15:M:135:VAL:HG12	2.16	0.45
29:1:10:ARG:HH11	29:1:49:GLU:CD	2.24	0.45
1:0:326:G:O2'	1:0:327:A:H5'	2.16	0.45
1:0:512:G:O3'	1:0:513:A:C8	2.68	0.45
1:0:1080:C:O5'	1:0:1080:C:H6	1.99	0.45
1:0:1525:G:H5'	1:0:1526:A:OP2	2.16	0.45
3:A:20:SER:C	3:A:22:ARG:H	2.24	0.45
3:A:88:ILE:CD1	3:A:100:PRO:HD3	2.40	0.45
3:A:95:PRO:HA	3:A:153:ARG:HA	1.98	0.45
5:C:27:ARG:O	5:C:31:ILE:HG13	2.17	0.45
11:I:54:VAL:O	11:I:58:GLU:HG3	2.15	0.45
24:V:55:GLY:CA	24:V:146:ILE:HG13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:108:ARG:HE	24:V:114:PRO:HG3	1.82	0.45
1:0:1377:C:H5'	1:0:1377:C:C6	2.47	0.45
1:0:1799:G:H21	17:O:88:GLN:HE22	1.65	0.45
1:0:2578:G:H5'	1:0:2578:G:H8	1.81	0.45
1:0:2717:C:OP1	4:B:207:LYS:HG3	2.15	0.45
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.47	0.45
5:C:21:VAL:C	5:C:23:GLU:H	2.24	0.45
8:F:70:LYS:C	8:F:72:VAL:H	2.25	0.45
14:L:66:SER:HB3	14:L:128:TRP:NE1	2.31	0.45
15:M:37:ARG:HD3	15:M:37:ARG:HA	1.78	0.45
19:Q:111:ILE:HG23	19:Q:145:LEU:CD1	2.46	0.45
1:0:120:A:H2'	1:0:120:A:N3	2.32	0.45
1:0:710:G:O2'	1:0:711:G:H5'	2.15	0.45
1:0:899:C:H5'	40:0:3638:HOH:O	2.17	0.45
1:0:920:C:H5''	1:0:921:G:O5'	2.17	0.45
1:0:1314:U:H2'	40:0:6245:HOH:O	2.17	0.45
1:0:1398:G:O4'	17:O:25:PRO:HG3	2.17	0.45
1:0:1706:G:OP1	17:O:65:ARG:HD2	2.16	0.45
1:0:1902:G:H2'	1:0:1903:U:O4'	2.16	0.45
1:0:2032:U:H2'	1:0:2033:G:H5'	1.98	0.45
1:0:2121:G:O2'	1:0:2122:C:H5'	2.17	0.45
1:0:2769:C:C2'	1:0:2770:G:H5'	2.45	0.45
1:0:2809:G:H2'	1:0:2810:G:O4'	2.17	0.45
3:A:39:ALA:O	3:A:61:GLU:HG3	2.16	0.45
3:A:186:TRP:CG	3:A:187:PRO:HA	2.52	0.45
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.28	0.45
5:C:140:VAL:HG12	5:C:141:SER:N	2.31	0.45
7:E:16:ASP:O	7:E:17:HIS:HB2	2.16	0.45
7:E:101:GLU:OE2	7:E:115:ARG:HD3	2.16	0.45
8:F:28:ALA:HB3	8:F:99:THR:O	2.17	0.45
26:X:189:ASN:HD22	26:X:192:ASP:H	1.64	0.45
26:X:203:VAL:CG1	26:X:228:VAL:HG22	2.46	0.45
1:0:128:A:O2'	1:0:129:A:H5'	2.17	0.45
1:0:708:A:H2'	1:0:709:G:O4'	2.17	0.45
1:0:1679:C:O2'	1:0:1685:A:N1	2.46	0.45
1:0:2011:A:H4'	1:0:2012:U:O5'	2.17	0.45
1:0:2065:C:O2'	1:0:2066:C:H5'	2.17	0.45
1:0:2415:A:H2'	1:0:2416:G:H5'	1.98	0.45
1:0:2521:A:OP2	10:H:3:ALA:HB3	2.17	0.45
10:H:66:ARG:HD3	40:H:9029:HOH:O	2.17	0.45
14:L:115:LEU:HD13	14:L:116:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:67:ALA:C	15:M:69:TYR:H	2.23	0.45
18:P:86:VAL:HG13	18:P:91:LEU:HD11	1.97	0.45
21:S:53:GLY:HA3	40:S:6384:HOH:O	2.17	0.45
26:X:99:ALA:HB2	26:X:233:TYR:CZ	2.52	0.45
1:0:333:G:O2'	1:0:334:G:H5'	2.17	0.45
1:0:696:C:O2'	1:0:697:G:H5'	2.16	0.45
1:0:750:A:H2'	1:0:751:U:C6	2.51	0.45
1:0:1119:G:N2	1:0:1246:A:N1	2.64	0.45
1:0:1641:A:H2'	1:0:1642:A:C5'	2.44	0.45
1:0:1850:U:H2'	1:0:1851:G:H8	1.81	0.45
4:B:145:HIS:HD2	4:B:146:THR:O	1.99	0.45
6:D:10:PHE:CE1	6:D:11:HIS:HB3	2.52	0.45
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.99	0.45
10:H:136:ALA:HB3	10:H:146:VAL:HG21	1.97	0.45
16:N:26:TRP:HA	16:N:26:TRP:HE3	1.81	0.45
24:V:21:LEU:CD2	24:V:48:VAL:HG11	2.39	0.45
25:W:75:ALA:O	25:W:83:ALA:HA	2.17	0.45
1:0:485:A:N3	1:0:487:G:H5''	2.31	0.45
1:0:790:A:H2'	1:0:791:A:O4'	2.17	0.45
1:0:2839:C:H2'	1:0:2840:A:H5''	1.99	0.45
40:0:6495:HOH:O	29:1:20:ARG:HB3	2.17	0.45
2:9:3014:G:O2'	2:9:3015:C:H5'	2.16	0.45
4:B:268:ARG:HH21	4:B:325:PRO:HG3	1.82	0.45
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.47	0.45
13:K:24:ALA:HB2	13:K:30:ARG:HD2	1.99	0.45
15:M:4:PRO:HD2	40:M:8859:HOH:O	2.16	0.45
24:V:48:VAL:CG1	24:V:48:VAL:O	2.65	0.45
1:0:396:U:H1'	40:0:7960:HOH:O	2.17	0.45
1:0:400:C:O2'	1:0:401:C:H5'	2.16	0.45
1:0:407:A:H2'	1:0:408:A:C8	2.51	0.45
1:0:912:A:C4	1:0:1294:A:C2	3.04	0.45
1:0:1192:A:O2'	1:0:1193:A:OP1	2.35	0.45
1:0:1836:A:H1'	28:Z:1:THR:O	2.17	0.45
1:0:2825:C:H4'	1:0:2826:G:O5'	2.17	0.45
2:9:3028:U:H5''	15:M:40:ASN:ND2	2.32	0.45
2:9:3114:G:H2'	2:9:3115:C:C6	2.52	0.45
3:A:34:ASP:OD1	3:A:35:GLY:N	2.49	0.45
5:C:8:LEU:HD13	5:C:147:LEU:HD21	1.98	0.45
5:C:51:TYR:CE2	28:Z:53:LYS:HB3	2.52	0.45
5:C:162:VAL:HG13	5:C:232:LEU:HD21	2.00	0.45
6:D:41:LEU:CA	6:D:44:ILE:HG22	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:94:ALA:O	6:D:95:THR:O	2.34	0.45
21:S:73:HIS:CD2	21:S:88:PRO:HG3	2.52	0.45
24:V:72:PRO:HG2	24:V:77:ALA:HB3	1.98	0.45
1:0:278:A:H2'	1:0:279:C:O4'	2.17	0.44
1:0:499:G:O2'	1:0:500:G:H5'	2.17	0.44
1:0:764:C:C2'	1:0:765:G:H5'	2.46	0.44
1:0:1759:A:N3	1:0:1818:C:H2'	2.31	0.44
1:0:1803:C:H2'	1:0:1804:A:C8	2.52	0.44
1:0:2314:G:H2'	1:0:2315:C:H5'	1.99	0.44
1:0:2416:G:O2'	15:M:25:ARG:HG2	2.17	0.44
1:0:2776:A:H2'	1:0:2777:G:O4'	2.16	0.44
2:9:3049:G:H5''	40:M:8847:HOH:O	2.16	0.44
6:D:35:ALA:C	6:D:37:ALA:N	2.73	0.44
6:D:170:TYR:CD1	6:D:170:TYR:N	2.85	0.44
15:M:42:HIS:CG	15:M:62:HIS:HE1	2.35	0.44
25:W:34:ARG:NH1	25:W:48:VAL:O	2.47	0.44
1:0:661:G:C5	1:0:686:A:C2	3.06	0.44
1:0:737:A:H2'	1:0:738:G:O4'	2.17	0.44
1:0:1372:A:H3'	40:0:7526:HOH:O	2.18	0.44
3:A:17:ARG:HD2	40:A:9018:HOH:O	2.17	0.44
3:A:194:MET:HE3	3:A:199:HIS:CB	2.47	0.44
4:B:140:LEU:HD13	4:B:175:LEU:HA	1.98	0.44
14:L:47:ASP:CG	14:L:48:LYS:N	2.75	0.44
17:O:16:VAL:HG12	17:O:17:GLY:N	2.32	0.44
19:Q:4:TYR:CZ	19:Q:15:LYS:HB3	2.52	0.44
19:Q:61:GLN:CD	40:Q:8945:HOH:O	2.59	0.44
24:V:21:LEU:HD22	24:V:26:ILE:HD13	1.96	0.44
24:V:41:TYR:HA	24:V:44:MET:HE3	1.99	0.44
24:V:149:LEU:HG	24:V:153:MET:CE	2.31	0.44
25:W:41:PHE:O	25:W:43:VAL:HG23	2.17	0.44
30:2:3:MET:O	30:2:90:PHE:HA	2.16	0.44
1:0:137:U:OP1	1:0:259:G:O2'	2.34	0.44
1:0:447:A:OP1	21:S:2:LYS:HG2	2.17	0.44
1:0:2274:A:O2'	1:0:2275:G:H5'	2.17	0.44
1:0:2828:G:O2'	1:0:2829:G:H5'	2.17	0.44
40:0:5354:HOH:O	10:H:58:ARG:HG3	2.17	0.44
4:B:258:GLY:N	4:B:260:HIS:CE1	2.81	0.44
6:D:19:GLU:O	6:D:133:ASN:HB3	2.18	0.44
6:D:104:PHE:CE2	6:D:166:ILE:CD1	3.00	0.44
8:F:84:GLY:O	8:F:89:LEU:HB2	2.17	0.44
10:H:28:ILE:HA	10:H:63:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:46:GLN:HB3	10:H:167:ARG:H	1.83	0.44
13:K:145:LEU:C	13:K:147:GLU:H	2.26	0.44
15:M:48:VAL:HG11	15:M:55:ASP:HB3	1.98	0.44
24:V:35:VAL:HG23	24:V:41:TYR:CD2	2.52	0.44
24:V:64:THR:O	24:V:68:THR:HG22	2.17	0.44
24:V:110:GLN:NE2	24:V:110:GLN:HA	2.32	0.44
1:0:541:C:H2'	1:0:542:A:H5'	1.99	0.44
1:0:758:A:H2'	1:0:759:C:O4'	2.17	0.44
1:0:932:U:H2'	1:0:933:C:C6	2.53	0.44
1:0:1213:C:O2'	1:0:1214:G:H5'	2.18	0.44
1:0:1657:A:H2'	1:0:1658:A:C8	2.53	0.44
1:0:1790:C:H2'	1:0:1791:U:H6	1.82	0.44
1:0:1994:A:P	12:J:66:ARG:HH22	2.41	0.44
1:0:2524:G:H21	1:0:2526:C:N4	2.15	0.44
1:0:2883:A:H2'	1:0:2884:G:O4'	2.18	0.44
5:C:21:VAL:HG13	40:C:8603:HOH:O	2.17	0.44
5:C:79:ARG:O	5:C:87:ARG:HG2	2.16	0.44
5:C:120:ASP:C	5:C:120:ASP:OD1	2.60	0.44
7:E:101:GLU:HB2	7:E:116:THR:O	2.17	0.44
26:X:107:PRO:HB3	26:X:182:PHE:CE2	2.53	0.44
1:0:1321:A:H2'	1:0:1322:G:C8	2.53	0.44
1:0:1544:U:H2'	1:0:1545:C:C6	2.53	0.44
1:0:1616:A:H2'	1:0:1618:G:C8	2.53	0.44
7:E:108:LEU:HB3	40:E:1306:HOH:O	2.16	0.44
10:H:43:TYR:HA	10:H:44:PRO:HD3	1.80	0.44
13:K:145:LEU:O	13:K:145:LEU:HD23	2.18	0.44
25:W:12:ILE:HD12	25:W:36:HIS:ND1	2.32	0.44
1:0:523:C:H2'	1:0:524:A:C8	2.53	0.44
1:0:883:U:H5'	40:0:3248:HOH:O	2.17	0.44
1:0:952:G:N3	1:0:2302:A:H2'	2.32	0.44
1:0:1139:U:H2'	1:0:1140:C:C6	2.52	0.44
1:0:1192:A:H3'	1:0:1193:A:H5'	1.99	0.44
1:0:1422:U:H2'	1:0:1423:C:C6	2.53	0.44
1:0:1849:G:H1'	1:0:2011:A:N1	2.33	0.44
1:0:2100:A:H5'	40:0:7723:HOH:O	2.17	0.44
1:0:2842:G:H2'	1:0:2843:A:H5'	2.00	0.44
1:0:2857:C:H2'	1:0:2858:U:C6	2.53	0.44
3:A:72:GLU:HG3	27:Y:66:GLY:HA2	1.99	0.44
8:F:49:PHE:HE1	8:F:98:VAL:HG23	1.83	0.44
11:I:13:ASP:OD1	11:I:15:ARG:HB3	2.17	0.44
15:M:140:GLN:HA	15:M:143:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:32:ARG:HH12	21:S:38:ARG:HH12	1.63	0.44
24:V:26:ILE:O	24:V:26:ILE:HG13	2.18	0.44
26:X:126:PRO:HG2	26:X:128:PHE:CZ	2.51	0.44
30:2:35:TRP:HA	30:2:38:ARG:NH1	2.32	0.44
1:0:538:C:OP2	26:X:134:HIS:HE1	2.01	0.44
1:0:1284:G:O2'	1:0:1285:U:H5'	2.17	0.44
1:0:1476:A:O2'	1:0:1477:C:H5'	2.17	0.44
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.48	0.44
10:H:28:ILE:HG23	40:H:9029:HOH:O	2.17	0.44
14:L:64:ARG:HD2	40:L:8886:HOH:O	2.17	0.44
22:T:31:PHE:CG	22:T:37:GLU:HG2	2.52	0.44
1:0:204:A:H2'	1:0:205:U:H5'	2.00	0.44
1:0:605:C:H2'	1:0:606:C:C6	2.53	0.44
1:0:926:A:O2'	13:K:41:HIS:HD2	2.00	0.44
1:0:1278:A:H4'	1:0:1279:U:C4	2.53	0.44
1:0:1667:A:H2'	1:0:1668:U:H6	1.82	0.44
1:0:2730:G:O2'	1:0:2731:G:H5'	2.18	0.44
2:9:3103:A:O2'	2:9:3104:A:H5'	2.18	0.44
6:D:159:PRO:O	6:D:163:VAL:HG23	2.17	0.44
11:I:90:LYS:HB2	36:I:8802:CL:CL	2.55	0.44
15:M:91:ARG:HG3	15:M:186:LEU:HD23	2.00	0.44
21:S:71:VAL:HG13	21:S:91:LEU:O	2.18	0.44
23:U:39:ALA:C	23:U:41:GLU:N	2.75	0.44
1:0:821:U:H2'	1:0:822:C:C6	2.53	0.44
1:0:1016:U:O2'	1:0:2303:A:N7	2.46	0.44
1:0:1199:A:H2'	1:0:1200:A:C8	2.52	0.44
1:0:1855:G:H4'	1:0:1856:C:O5'	2.18	0.44
1:0:2462:G:O6	30:2:61:PRO:HG3	2.18	0.44
2:9:3023:U:H6	2:9:3023:U:C5'	2.30	0.44
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.52	0.44
5:C:7:ASP:OD1	5:C:11:ASN:N	2.48	0.44
5:C:127:ARG:HG2	5:C:127:ARG:HH11	1.83	0.44
5:C:237:GLU:HB2	40:C:8637:HOH:O	2.18	0.44
14:L:24:GLN:HE21	14:L:27:ARG:HH11	1.64	0.44
15:M:77:ASN:OD1	15:M:79:PRO:HD2	2.18	0.44
23:U:42:ASN:HB3	40:U:7247:HOH:O	2.18	0.44
1:0:295:C:O2'	1:0:296:G:H5'	2.17	0.43
1:0:1380:U:H5'	40:0:9699:HOH:O	2.17	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.53	0.43
1:0:2443:C:H5'	13:K:57:VAL:HG21	1.99	0.43
2:9:3057:A:C8	6:D:141:VAL:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:57:GLU:HB2	14:L:23:LEU:HD11	2.00	0.43
15:M:154:LEU:HG	15:M:155:GLU:N	2.32	0.43
20:R:42:GLU:HG2	20:R:49:VAL:HG23	1.99	0.43
1:0:949:U:H4'	18:P:95:GLU:HA	2.00	0.43
1:0:1044:C:H3'	1:0:1045:G:H5''	2.00	0.43
1:0:1180:U:H2'	1:0:1181:A:O4'	2.18	0.43
1:0:1943:C:O4'	3:A:212:PRO:HA	2.18	0.43
1:0:2032:U:H2'	1:0:2033:G:C5'	2.47	0.43
1:0:2254:G:O2'	1:0:2255:A:H5'	2.18	0.43
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.43
3:A:36:ASP:O	3:A:38:ILE:N	2.51	0.43
4:B:129:ARG:NH2	4:B:176:ASP:OD1	2.50	0.43
4:B:266:ASN:OD1	4:B:317:PRO:HA	2.17	0.43
4:B:305:ASP:O	4:B:306:LYS:CB	2.64	0.43
5:C:78:ARG:NH1	5:C:78:ARG:CG	2.72	0.43
1:0:709:G:O2'	16:N:25:VAL:CG1	2.66	0.43
1:0:1609:C:H2'	1:0:1610:G:C8	2.54	0.43
3:A:110:SER:N	3:A:114:ASP:OD2	2.49	0.43
3:A:132:ASP:OD1	3:A:133:ARG:N	2.49	0.43
4:B:102:THR:HG21	4:B:182:VAL:O	2.17	0.43
4:B:232:TRP:HD1	4:B:235:ARG:HD2	1.82	0.43
6:D:104:PHE:CE2	6:D:166:ILE:HD13	2.52	0.43
12:J:81:ARG:HD3	12:J:87:ARG:NH1	2.32	0.43
13:K:77:ALA:C	13:K:79:ASP:H	2.26	0.43
19:Q:128:ARG:HB2	19:Q:132:ARG:O	2.19	0.43
1:0:848:C:H2'	1:0:849:C:C6	2.53	0.43
1:0:848:C:H5'	40:0:7610:HOH:O	2.19	0.43
1:0:1119:G:N2	1:0:1246:A:H2	2.09	0.43
1:0:1682:A:H2'	40:0:3244:HOH:O	2.19	0.43
1:0:2004:U:H4'	40:0:5688:HOH:O	2.17	0.43
1:0:2133:U:H4'	1:0:2134:G:H5'	1.99	0.43
1:0:2610:U:H4'	40:0:4172:HOH:O	2.18	0.43
4:B:5:ARG:HD2	4:B:8:LYS:HZ3	1.83	0.43
4:B:60:SER:HA	4:B:61:PRO:HD3	1.87	0.43
11:I:46:ILE:HD11	11:I:53:ILE:HG23	2.00	0.43
11:I:74:ARG:HH12	11:I:76:ASP:HB2	1.79	0.43
13:K:144:ASP:O	13:K:147:GLU:HB2	2.19	0.43
15:M:166:ALA:O	15:M:167:ASP:O	2.35	0.43
17:O:141:ILE:C	17:O:143:ALA:H	2.25	0.43
24:V:11:VAL:O	24:V:12:ASN:HB2	2.17	0.43
1:0:90:A:H2'	1:0:91:G:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:202:U:O2'	1:0:203:G:H5'	2.18	0.43
1:0:830:G:O2'	1:0:831:U:H5'	2.18	0.43
1:0:1268:C:O2'	26:X:169:ARG:HB2	2.18	0.43
1:0:2656:G:O2'	1:0:2657:G:H5'	2.18	0.43
40:0:4762:HOH:O	3:A:212:PRO:HB2	2.19	0.43
40:0:6722:HOH:O	3:A:205:GLY:HA3	2.19	0.43
2:9:3007:G:H5'	40:9:9094:HOH:O	2.18	0.43
2:9:3007:G:H4'	15:M:55:ASP:OD2	2.18	0.43
2:9:3034:A:H1'	15:M:153:GLN:HE22	1.84	0.43
10:H:51:VAL:HG21	10:H:127:VAL:HG11	1.99	0.43
20:R:29:ASP:OD1	20:R:31:ARG:HG3	2.19	0.43
23:U:38:GLY:C	23:U:40:PRO:HD2	2.44	0.43
24:V:122:ARG:NH2	40:V:4276:HOH:O	2.48	0.43
26:X:187:VAL:HG12	26:X:205:ILE:HA	2.01	0.43
27:Y:75:GLY:O	27:Y:78:THR:HB	2.18	0.43
28:Z:25:LYS:O	28:Z:25:LYS:HG2	2.19	0.43
1:0:569:A:H5''	1:0:587:A:N1	2.34	0.43
1:0:712:C:O2'	1:0:713:U:H2'	2.19	0.43
1:0:747:G:H2'	1:0:748:C:C6	2.54	0.43
1:0:816:G:C6	1:0:817:G:N1	2.87	0.43
1:0:1183:C:N4	1:0:1184:C:N4	2.64	0.43
1:0:1444:G:O2'	1:0:1502:A:N1	2.45	0.43
1:0:1669:A:H2'	1:0:1670:G:H8	1.82	0.43
1:0:1677:U:OP2	29:1:8:LYS:NZ	2.49	0.43
1:0:1816:C:H2'	1:0:1817:U:O4'	2.19	0.43
1:0:1850:U:H2'	1:0:1851:G:C8	2.52	0.43
40:0:4589:HOH:O	5:C:76:ARG:HD3	2.18	0.43
4:B:60:SER:C	4:B:62:ARG:H	2.27	0.43
18:P:66:LYS:HB2	18:P:70:ALA:O	2.19	0.43
1:0:24:G:N2	1:0:518:G:H1'	2.33	0.43
1:0:451:C:O2'	1:0:452:G:H5'	2.18	0.43
1:0:1470:A:OP1	14:L:93:ARG:HD2	2.18	0.43
1:0:2515:C:O2'	1:0:2516:G:H5'	2.19	0.43
1:0:2597:U:H2'	1:0:2598:U:H5'	1.99	0.43
1:0:2727:A:H2'	1:0:2728:C:H5'	2.00	0.43
1:0:2896:A:H5''	40:0:6464:HOH:O	2.18	0.43
3:A:26:ASP:OD1	3:A:26:ASP:O	2.36	0.43
5:C:49:ASP:HB3	5:C:52:ALA:HB2	2.01	0.43
12:J:98:VAL:HG22	12:J:102:GLU:C	2.44	0.43
15:M:5:ARG:HG3	18:P:18:PRO:CB	2.48	0.43
29:1:48:ASP:O	29:1:49:GLU:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:73:GLU:HB2	40:2:8957:HOH:O	2.18	0.43
1:0:806:A:H2'	1:0:807:A:O4'	2.19	0.43
1:0:858:U:H2'	1:0:859:C:H6	1.84	0.43
1:0:1945:G:O2'	1:0:1946:C:H5'	2.19	0.43
1:0:2326:U:H4'	1:0:2412:G:H4'	2.00	0.43
1:0:2385:G:H2'	1:0:2386:U:H6	1.83	0.43
1:0:2786:G:H2'	40:0:7524:HOH:O	2.17	0.43
40:0:7789:HOH:O	4:B:211:THR:HG21	2.18	0.43
3:A:103:VAL:O	3:A:105:VAL:HG23	2.18	0.43
4:B:7:ARG:CG	4:B:7:ARG:NH1	2.82	0.43
22:T:13:ILE:HG12	22:T:32:CYS:HB3	2.00	0.43
22:T:52:THR:CG2	22:T:54:THR:HB	2.49	0.43
30:2:65:THR:HB	30:2:83:TRP:H	1.84	0.43
1:0:125:U:H2'	40:0:4182:HOH:O	2.18	0.43
1:0:177:A:H2'	1:0:178:U:O4'	2.18	0.43
1:0:539:G:H2'	1:0:540:A:C8	2.54	0.43
1:0:1142:C:O2'	1:0:1143:G:H5'	2.19	0.43
1:0:1362:U:H2'	1:0:1363:G:H8	1.83	0.43
1:0:1834:C:H2'	1:0:1840:A:N6	2.34	0.43
4:B:115:VAL:HA	4:B:116:PRO:HD3	1.78	0.43
4:B:258:GLY:HA2	40:B:9029:HOH:O	2.18	0.43
4:B:307:ARG:CG	4:B:307:ARG:NH1	2.80	0.43
6:D:11:HIS:C	6:D:13:MET:N	2.75	0.43
6:D:58:VAL:CG1	6:D:59:GLY:N	2.82	0.43
15:M:124:ASP:C	15:M:126:GLY:N	2.75	0.43
16:N:29:VAL:O	16:N:33:LEU:HG	2.19	0.43
28:Z:25:LYS:HD2	29:1:48:ASP:HA	2.01	0.43
1:0:283:U:H5''	1:0:284:C:OP2	2.19	0.43
1:0:553:G:H5'	40:0:3929:HOH:O	2.19	0.43
1:0:1280:A:OP1	1:0:1280:A:H3'	2.18	0.43
1:0:1503:U:H2'	1:0:1504:A:O4'	2.18	0.43
1:0:1609:C:H2'	1:0:1610:G:H8	1.84	0.43
1:0:1829:A:C2'	1:0:1830:C:H5'	2.48	0.43
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.43
3:A:69:LEU:C	3:A:69:LEU:HD12	2.44	0.43
3:A:80:LEU:HD22	3:A:91:GLY:O	2.19	0.43
4:B:138:GLY:O	4:B:139:ASP:C	2.62	0.43
4:B:146:THR:C	4:B:148:PRO:HD3	2.44	0.43
4:B:215:VAL:HA	4:B:220:VAL:HG22	2.01	0.43
6:D:49:PRO:HG3	40:D:5828:HOH:O	2.17	0.43
7:E:86:VAL:CG1	7:E:129:GLU:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:101:GLU:CB	7:E:117:THR:HA	2.49	0.43
11:I:93:ARG:HB3	11:I:93:ARG:NH1	2.20	0.43
30:2:74:CYS:N	40:2:8990:HOH:O	2.52	0.43
1:0:491:C:O2'	1:0:492:C:H5'	2.19	0.42
1:0:947:U:H2'	1:0:948:G:H8	1.83	0.42
1:0:1512:G:O2'	1:0:1513:C:H5'	2.19	0.42
1:0:1947:G:H2'	1:0:1948:G:C8	2.53	0.42
1:0:2507:G:H2'	1:0:2510:C:N4	2.33	0.42
1:0:2781:U:O2'	1:0:2782:G:H5'	2.19	0.42
3:A:39:ALA:HB3	3:A:61:GLU:OE2	2.19	0.42
4:B:154:VAL:HA	4:B:155:PRO:HD3	1.87	0.42
6:D:81:GLU:C	6:D:83:PHE:N	2.77	0.42
7:E:11:VAL:HG13	7:E:23:GLU:O	2.19	0.42
7:E:20:ILE:CD1	7:E:33:LEU:HD12	2.49	0.42
8:F:33:THR:HG21	8:F:59:ILE:O	2.19	0.42
13:K:133:VAL:HB	40:K:8861:HOH:O	2.18	0.42
15:M:141:ARG:HB3	40:M:8868:HOH:O	2.19	0.42
15:M:164:ASP:OD1	15:M:164:ASP:C	2.62	0.42
16:N:26:TRP:HB2	40:N:3062:HOH:O	2.19	0.42
18:P:3:SER:HB3	40:P:5998:HOH:O	2.19	0.42
28:Z:53:LYS:HD3	28:Z:53:LYS:HA	1.85	0.42
1:0:1234:U:C4	4:B:244:PRO:HB3	2.54	0.42
1:0:1399:A:H2'	1:0:1400:C:C6	2.55	0.42
1:0:1419:U:H5'	1:0:1420:C:OP2	2.19	0.42
1:0:1679:C:H5'	40:0:9791:HOH:O	2.19	0.42
1:0:1909:A:N1	1:0:2128:G:H1'	2.34	0.42
1:0:2382:A:O2'	1:0:2383:G:H5'	2.20	0.42
3:A:36:ASP:CB	3:A:83:GLY:HA3	2.49	0.42
7:E:7:ILE:HA	7:E:8:PRO:HD3	1.92	0.42
7:E:11:VAL:CG1	7:E:22:VAL:HG13	2.49	0.42
10:H:38:LYS:HE2	10:H:42:ASP:CB	2.50	0.42
11:I:131:THR:HB	11:I:134:GLU:HG3	2.01	0.42
15:M:25:ARG:HA	15:M:28:LYS:HG3	2.00	0.42
15:M:163:PHE:O	15:M:164:ASP:O	2.37	0.42
19:Q:12:THR:HG22	19:Q:149:GLU:OE1	2.19	0.42
19:Q:82:GLU:O	19:Q:86:LYS:HG3	2.19	0.42
1:0:414:C:H5'	40:0:3106:HOH:O	2.19	0.42
1:0:541:C:C2'	1:0:542:A:C5'	2.85	0.42
1:0:694:A:H2'	1:0:695:C:H5'	2.00	0.42
1:0:789:C:H1'	1:0:827:A:C2	2.53	0.42
1:0:2004:U:H2'	1:0:2004:U:O2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2784:A:H1'	7:E:60:SER:OG	2.18	0.42
2:9:3025:G:C2'	2:9:3026:C:H5'	2.49	0.42
3:A:9:ARG:HG2	3:A:16:PHE:CD2	2.55	0.42
3:A:192:VAL:HG13	40:A:9032:HOH:O	2.19	0.42
15:M:86:LEU:O	15:M:90:LEU:HG	2.20	0.42
24:V:82:GLU:O	24:V:86:GLU:HG3	2.20	0.42
24:V:88:THR:CG2	24:V:90:TYR:HD1	2.31	0.42
26:X:151:SER:HB3	26:X:154:ARG:HB3	2.02	0.42
1:0:255:A:H2'	1:0:256:C:C6	2.54	0.42
1:0:383:A:H4'	40:0:5709:HOH:O	2.19	0.42
1:0:494:C:H2'	1:0:496:G:OP2	2.19	0.42
1:0:669:G:O2'	1:0:670:G:H5'	2.20	0.42
1:0:703:G:O2'	1:0:704:C:H5'	2.19	0.42
1:0:757:C:OP1	13:K:27:ARG:HD2	2.19	0.42
1:0:872:U:O2'	1:0:873:G:H5'	2.19	0.42
1:0:1819:G:H5'	40:0:6189:HOH:O	2.18	0.42
1:0:2716:G:C5'	4:B:206:THR:HG21	2.45	0.42
3:A:173:GLY:O	3:A:176:HIS:HB3	2.19	0.42
4:B:27:ASN:HD22	4:B:27:ASN:H	1.66	0.42
6:D:18:ILE:HD13	6:D:84:LEU:HD12	2.02	0.42
16:N:15:LYS:HD3	16:N:19:ARG:NH2	2.34	0.42
22:T:20:MET:CG	22:T:28:THR:HG23	2.49	0.42
22:T:34:SER:HA	22:T:37:GLU:OE1	2.20	0.42
25:W:70:ILE:HG23	25:W:70:ILE:O	2.19	0.42
26:X:99:ALA:HB2	26:X:233:TYR:CE2	2.54	0.42
30:2:18:GLN:OE1	30:2:73:GLU:HB3	2.20	0.42
1:0:191:A:C4	1:0:237:G:N7	2.88	0.42
1:0:631:A:C6	1:0:2074:A:H5'	2.55	0.42
1:0:1039:G:H2'	1:0:1040:A:O4'	2.20	0.42
1:0:1257:C:O2'	1:0:1258:G:H5'	2.20	0.42
1:0:1565:C:H2'	1:0:1566:C:H6	1.83	0.42
1:0:2758:G:H2'	1:0:2759:C:C6	2.55	0.42
2:9:3002:U:OP2	2:9:3003:A:H5'	2.20	0.42
3:A:129:LEU:CD1	3:A:145:MET:HE1	2.50	0.42
3:A:130:THR:HG22	3:A:131:HIS:O	2.19	0.42
4:B:279:THR:CG2	4:B:280:VAL:N	2.83	0.42
6:D:99:ASP:HB3	6:D:103:ASN:H	1.83	0.42
7:E:9:GLU:HA	40:E:5240:HOH:O	2.19	0.42
7:E:11:VAL:CG1	7:E:12:ASP:N	2.82	0.42
10:H:38:LYS:O	10:H:84:LYS:HE2	2.20	0.42
13:K:34:GLY:HA3	13:K:38:HIS:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:108:SER:HA	15:M:109:PRO:HD3	1.75	0.42
15:M:184:ILE:HG22	15:M:185:GLU:H	1.84	0.42
23:U:12:THR:OG1	23:U:13:PRO:HD2	2.19	0.42
1:O:100:C:O2	21:S:17:HIS:HB3	2.19	0.42
1:O:317:A:H5''	21:S:52:ARG:HD2	2.02	0.42
1:O:347:A:O2'	1:O:348:C:H5'	2.19	0.42
1:O:1537:C:H1'	40:O:6946:HOH:O	2.19	0.42
1:O:1730:G:H5''	1:O:1731:C:H6	1.85	0.42
2:9:3093:A:C5	2:9:3094:G:H1'	2.55	0.42
3:A:20:SER:C	3:A:22:ARG:N	2.75	0.42
3:A:27:LEU:HD21	3:A:55:VAL:HG21	2.01	0.42
4:B:294:TYR:HE2	40:B:9129:HOH:O	2.03	0.42
5:C:7:ASP:OD2	5:C:9:ASP:HB2	2.19	0.42
7:E:20:ILE:HD12	7:E:33:LEU:HD12	2.01	0.42
8:F:56:PRO:HG2	14:L:43:PRO:O	2.19	0.42
13:K:145:LEU:O	13:K:148:GLU:HG3	2.20	0.42
1:O:272:A:H3'	40:O:7862:HOH:O	2.19	0.42
1:O:560:C:H2'	1:O:561:G:C8	2.54	0.42
1:O:646:G:H2'	1:O:647:U:C6	2.55	0.42
1:O:682:A:H2'	1:O:683:G:O4'	2.19	0.42
1:O:1552:G:H2'	1:O:1553:C:C6	2.55	0.42
1:O:1644:C:O2'	1:O:1645:U:H5'	2.20	0.42
40:O:7810:HOH:O	14:L:55:LYS:HE2	2.19	0.42
40:9:9105:HOH:O	15:M:115:VAL:HG13	2.18	0.42
7:E:132:THR:HG23	7:E:132:THR:O	2.19	0.42
16:N:81:PHE:N	16:N:81:PHE:CD1	2.87	0.42
20:R:30:ASP:HA	20:R:62:LYS:HE3	2.01	0.42
24:V:108:ARG:HE	24:V:114:PRO:CG	2.32	0.42
1:O:308:U:H5'	21:S:97:ARG:HH21	1.83	0.42
1:O:514:G:H5'	40:O:7435:HOH:O	2.20	0.42
1:O:683:G:O2'	1:O:684:G:H5'	2.20	0.42
1:O:1205:U:H2'	1:O:1206:U:C5'	2.50	0.42
1:O:1516:C:H2'	1:O:1517:U:C6	2.55	0.42
1:O:1555:G:H4'	1:O:1630:A:H2	1.84	0.42
1:O:1666:C:C2'	1:O:1667:A:C5'	2.97	0.42
1:O:1979:G:H2'	40:O:3730:HOH:O	2.20	0.42
1:O:2433:A:H2'	1:O:2434:A:C8	2.54	0.42
2:9:3039:U:O2'	2:9:3042:C:C5	2.72	0.42
6:D:92:GLU:O	6:D:93:LEU:O	2.37	0.42
10:H:167:ARG:CG	40:H:8990:HOH:O	2.67	0.42
11:I:42:GLU:O	11:I:131:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:99:ASP:OD1	12:J:101:ASN:N	2.52	0.42
12:J:118:ALA:C	12:J:120:ARG:N	2.78	0.42
13:K:148:GLU:HA	40:K:8877:HOH:O	2.19	0.42
16:N:21:SER:HB2	16:N:106:PRO:O	2.20	0.42
24:V:13:MET:HE2	24:V:18:GLN:N	2.34	0.42
24:V:65:VAL:CG1	24:V:116:LEU:HD13	2.49	0.42
25:W:14:LEU:HD12	25:W:67:PRO:O	2.19	0.42
1:0:74:A:H2'	1:0:75:U:C6	2.54	0.42
1:0:86:A:C2	29:1:25:VAL:HG13	2.55	0.42
1:0:259:G:O2'	1:0:260:C:H5'	2.20	0.42
1:0:710:G:H5'	16:N:25:VAL:HG13	2.02	0.42
1:0:922:A:N7	1:0:2281:C:H5'	2.35	0.42
1:0:1244:U:H4'	1:0:1246:A:O4'	2.20	0.42
1:0:1847:A:OP1	3:A:175:LYS:HG3	2.19	0.42
4:B:185:GLY:HA2	40:B:9112:HOH:O	2.19	0.42
5:C:127:ARG:HG2	5:C:127:ARG:NH1	2.34	0.42
8:F:61:MET:HB3	14:L:19:GLN:OE1	2.19	0.42
10:H:88:ARG:NH1	10:H:135:THR:OG1	2.51	0.42
12:J:118:ALA:O	12:J:120:ARG:N	2.53	0.42
13:K:79:ASP:HB3	40:K:8862:HOH:O	2.20	0.42
14:L:61:ILE:HD12	14:L:61:ILE:N	2.35	0.42
22:T:37:GLU:HB3	40:T:408:HOH:O	2.19	0.42
24:V:52:VAL:HG13	24:V:53:ALA:N	2.34	0.42
26:X:116:LEU:HD12	26:X:173:ALA:HB3	2.01	0.42
26:X:144:ARG:NE	40:X:8914:HOH:O	2.53	0.42
29:1:36:ASN:HB3	29:1:39:ARG:NE	2.34	0.42
1:0:329:A:OP2	5:C:206:ASN:HB2	2.19	0.42
1:0:660:A:H4'	1:0:661:G:O5'	2.20	0.42
1:0:696:C:HO2'	1:0:697:G:H5'	1.84	0.42
1:0:764:C:O2'	1:0:765:G:H5'	2.19	0.42
1:0:815:U:O2'	1:0:1598:A:H4'	2.19	0.42
1:0:1724:U:H5''	40:0:4151:HOH:O	2.19	0.42
1:0:1829:A:H5''	40:0:3517:HOH:O	2.19	0.42
1:0:1845:A:O2'	1:0:1846:U:H5'	2.19	0.42
1:0:2464:C:H5''	1:0:2465:A:OP1	2.19	0.42
4:B:87:TYR:OH	4:B:163:GLU:OE2	2.37	0.42
5:C:95:GLU:H	5:C:95:GLU:CD	2.23	0.42
15:M:58:LEU:HD12	15:M:58:LEU:N	2.35	0.42
18:P:75:ILE:CD1	18:P:84:ILE:HD11	2.50	0.42
24:V:119:HIS:CD2	24:V:120:PRO:HD2	2.55	0.42
24:V:128:VAL:O	24:V:138:LEU:HD11	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:314:G:N2	1:0:316:A:H3'	2.34	0.41
1:0:677:C:H4'	5:C:246:ARG:NH2	2.35	0.41
1:0:752:G:H2'	1:0:753:U:O4'	2.20	0.41
1:0:1171:A:H2'	1:0:1172:G:H5'	2.02	0.41
1:0:1299:G:N2	40:0:5073:HOH:O	2.52	0.41
1:0:1400:C:O2'	1:0:1401:G:H5'	2.20	0.41
1:0:2064:U:H5'	1:0:2652:U:O3'	2.20	0.41
1:0:2281:C:C2'	1:0:2282:U:H5'	2.49	0.41
4:B:158:LYS:HB2	40:B:9036:HOH:O	2.19	0.41
4:B:254:GLN:HG2	4:B:255:GLY:H	1.85	0.41
8:F:26:THR:HG21	8:F:103:GLU:HG3	2.01	0.41
12:J:22:ASP:O	12:J:110:LYS:HE3	2.20	0.41
17:O:115:SER:C	17:O:117:SER:N	2.77	0.41
24:V:85:ALA:HB2	24:V:91:ASP:O	2.19	0.41
1:0:47:G:N3	1:0:114:A:C2	2.89	0.41
1:0:566:A:H2'	1:0:567:U:O4'	2.20	0.41
1:0:764:C:H2'	1:0:765:G:O4'	2.20	0.41
1:0:941:G:C5	1:0:942:U:C4	3.09	0.41
1:0:1393:A:H2'	1:0:1394:C:C6	2.55	0.41
1:0:1407:A:O2'	1:0:1408:U:H3'	2.20	0.41
1:0:2661:U:H3	1:0:2812:A:H62	1.68	0.41
1:0:2890:A:C4	22:T:56:ARG:CZ	3.03	0.41
4:B:217:ARG:HG3	4:B:257:THR:CG2	2.51	0.41
7:E:84:MET:HG2	7:E:168:ILE:HA	2.01	0.41
14:L:46:LEU:HD22	14:L:50:ARG:HG3	2.02	0.41
15:M:73:ALA:HB1	15:M:74:PRO:HD2	2.01	0.41
17:O:115:SER:C	17:O:117:SER:H	2.28	0.41
19:Q:47:LEU:O	19:Q:51:ILE:HG13	2.20	0.41
23:U:43:PRO:O	23:U:46:ILE:HG22	2.19	0.41
26:X:106:THR:CG2	26:X:107:PRO:HD2	2.51	0.41
30:2:70:ARG:HG2	30:2:70:ARG:NH1	2.35	0.41
1:0:638:C:H2'	1:0:639:A:C8	2.55	0.41
1:0:1171:A:C2'	1:0:1172:G:H5'	2.51	0.41
1:0:1184:C:H1'	40:0:7798:HOH:O	2.19	0.41
1:0:1311:G:C2	1:0:1312:G:C8	3.09	0.41
1:0:1367:A:H2'	1:0:1368:U:O4'	2.20	0.41
2:9:3098:C:O2'	2:9:3099:U:H5'	2.20	0.41
3:A:128:LEU:HG	40:A:9046:HOH:O	2.19	0.41
6:D:84:LEU:C	6:D:86:THR:H	2.29	0.41
7:E:23:GLU:HG2	7:E:28:SER:CB	2.49	0.41
14:L:159:VAL:HG13	14:L:160:PHE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:164:THR:HB	40:L:8819:HOH:O	2.20	0.41
15:M:143:ARG:HH12	15:M:173:ASP:CG	2.26	0.41
17:O:80:ARG:HG2	17:O:87:ARG:NH2	2.34	0.41
23:U:29:ASN:O	23:U:33:VAL:HG23	2.20	0.41
24:V:65:VAL:HA	24:V:68:THR:CG2	2.49	0.41
24:V:139:GLY:O	24:V:141:HIS:CD2	2.71	0.41
27:Y:46:ARG:HD2	27:Y:59:TYR:HB2	2.03	0.41
1:O:170:U:H2'	1:O:171:C:H5'	2.01	0.41
1:O:559:C:N4	1:O:598:C:H42	2.19	0.41
1:O:1173:A:H2'	40:O:4746:HOH:O	2.20	0.41
1:O:1245:C:O5'	1:O:1245:C:H6	2.03	0.41
1:O:1565:C:O4'	1:O:2738:G:H1'	2.20	0.41
1:O:1845:A:OP2	3:A:190:ARG:NH1	2.54	0.41
1:O:1966:U:H2'	1:O:1967:U:C6	2.54	0.41
40:O:4960:HOH:O	5:C:50:GLU:HG2	2.19	0.41
3:A:103:VAL:HA	3:A:104:PRO:HD3	1.94	0.41
9:G:14:GLU:HB3	40:G:4173:HOH:O	2.20	0.41
10:H:54:THR:O	10:H:55:VAL:CG1	2.67	0.41
12:J:14:LYS:HG3	12:J:32:ILE:O	2.20	0.41
13:K:117:GLU:HA	40:K:8855:HOH:O	2.20	0.41
14:L:69:LYS:O	14:L:73:ARG:NH2	2.42	0.41
22:T:52:THR:HG22	22:T:54:THR:HB	2.02	0.41
1:O:297:U:H2'	1:O:298:C:C6	2.56	0.41
1:O:755:G:O2'	1:O:756:A:H5'	2.21	0.41
1:O:1051:C:H2'	1:O:1052:G:O4'	2.21	0.41
1:O:1453:G:H2'	1:O:1454:U:O4'	2.20	0.41
1:O:1520:G:H2'	1:O:1521:C:C6	2.55	0.41
1:O:2032:U:O2'	1:O:2033:G:H5''	2.20	0.41
1:O:2266:A:H2'	1:O:2267:G:C8	2.56	0.41
1:O:2335:C:H2'	1:O:2336:G:H8	1.85	0.41
40:O:7365:HOH:O	3:A:211:LYS:HG2	2.20	0.41
40:O:7890:HOH:O	30:2:61:PRO:HG2	2.21	0.41
13:K:105:TYR:CD1	13:K:105:TYR:C	2.98	0.41
15:M:91:ARG:HG3	15:M:186:LEU:CD2	2.50	0.41
17:O:16:VAL:HG12	17:O:20:ARG:HB2	2.02	0.41
20:R:73:ASP:OD1	20:R:76:GLU:HG3	2.20	0.41
1:O:88:G:N3	29:1:24:TRP:HB2	2.36	0.41
1:O:324:G:O2'	1:O:325:U:H5'	2.21	0.41
1:O:1119:G:H2'	11:I:52:GLN:HE22	1.83	0.41
1:O:1335:C:H2'	1:O:1336:U:H6	1.84	0.41
1:O:1588:G:C6	1:O:1589:G:N1	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1705:C:H2'	1:0:1706:G:O4'	2.20	0.41
1:0:1804:A:H2'	1:0:1805:G:C8	2.55	0.41
1:0:2103:A:N7	1:0:2538:A:N6	2.68	0.41
1:0:2406:U:O2'	1:0:2407:G:H5'	2.20	0.41
1:0:2689:A:C2'	1:0:2690:U:H5'	2.50	0.41
1:0:2729:C:O2'	1:0:2730:G:H5'	2.20	0.41
1:0:2765:C:H2'	1:0:2766:A:C8	2.56	0.41
1:0:2819:C:O4'	4:B:96:PRO:HB2	2.20	0.41
3:A:36:ASP:O	3:A:37:VAL:C	2.63	0.41
3:A:48:ASP:HA	3:A:49:PRO:HD3	1.91	0.41
3:A:194:MET:HE3	3:A:199:HIS:HB2	2.03	0.41
5:C:84:VAL:O	5:C:85:LYS:HB2	2.21	0.41
6:D:93:LEU:HG	40:D:3862:HOH:O	2.20	0.41
8:F:59:ILE:HD11	40:L:8924:HOH:O	2.21	0.41
10:H:9:ILE:HD12	10:H:54:THR:HG22	2.03	0.41
14:L:49:ALA:C	14:L:54:TYR:HB3	2.45	0.41
21:S:49:GLU:HB3	21:S:59:GLU:CG	2.50	0.41
22:T:33:SER:O	22:T:37:GLU:HG3	2.20	0.41
30:2:3:MET:HG3	30:2:4:PRO:HD2	2.03	0.41
1:0:73:C:O2'	1:0:74:A:H5'	2.21	0.41
1:0:671:A:O2'	1:0:672:G:H2'	2.21	0.41
1:0:1119:G:H8	11:I:52:GLN:NE2	2.18	0.41
1:0:1138:G:H2'	1:0:1139:U:O4'	2.21	0.41
1:0:1279:U:O2	1:0:1279:U:H2'	2.19	0.41
1:0:2502:C:O3'	10:H:151:ARG:NH2	2.54	0.41
1:0:2783:A:H2'	1:0:2784:A:C8	2.55	0.41
1:0:2842:G:H2'	1:0:2843:A:C5'	2.50	0.41
7:E:102:VAL:HG11	7:E:148:ILE:HD11	2.03	0.41
23:U:1:THR:C	23:U:3:LEU:N	2.77	0.41
1:0:396:U:OP2	30:2:38:ARG:NH1	2.54	0.41
1:0:944:G:C8	24:V:23:MET:HE1	2.56	0.41
1:0:1557:G:O2'	1:0:1558:C:H5'	2.21	0.41
1:0:2502:C:H2'	1:0:2503:A:C5'	2.49	0.41
1:0:2502:C:O2'	1:0:2503:A:H5'	2.21	0.41
1:0:2741:A:H2'	1:0:2742:G:O4'	2.21	0.41
1:0:2756:U:O2	1:0:2896:A:H2	2.03	0.41
1:0:2837:U:H2'	40:0:7186:HOH:O	2.20	0.41
40:0:4806:HOH:O	3:A:11:ARG:NE	2.53	0.41
2:9:3020:G:H3'	40:9:9055:HOH:O	2.20	0.41
2:9:3031:C:O2'	2:9:3032:G:H5'	2.20	0.41
5:C:21:VAL:HG23	5:C:22:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:35:ALA:C	6:D:37:ALA:H	2.28	0.41
14:L:59:GLY:HA3	14:L:141:ILE:HD12	2.02	0.41
15:M:67:ALA:C	15:M:69:TYR:N	2.78	0.41
17:O:16:VAL:HG13	17:O:20:ARG:NH1	2.35	0.41
23:U:1:THR:CG2	23:U:2:VAL:N	2.82	0.41
25:W:43:VAL:CG1	25:W:47:ALA:HB3	2.51	0.41
30:2:31:THR:HB	30:2:33:MET:HE3	2.02	0.41
1:0:161:A:H2'	1:0:162:C:C6	2.55	0.41
1:0:862:U:H5'	40:0:7614:HOH:O	2.21	0.41
1:0:1062:U:O2'	1:0:2307:A:N3	2.53	0.41
1:0:1110:G:O2'	1:0:1111:U:H5'	2.20	0.41
1:0:1123:A:C2	1:0:1129:C:H4'	2.56	0.41
1:0:1165:G:O2'	1:0:1166:A:OP1	2.36	0.41
1:0:1246:A:O2'	1:0:1247:A:H3'	2.21	0.41
1:0:1477:C:H2'	1:0:1478:U:C6	2.56	0.41
1:0:1634:G:H2'	1:0:1635:U:C6	2.56	0.41
1:0:1787:C:H4'	1:0:2883:A:O4'	2.21	0.41
1:0:1856:C:H5'	1:0:1858:A:O4'	2.21	0.41
1:0:2055:A:H5'	19:Q:134:SER:HB2	2.03	0.41
1:0:2471:G:N3	1:0:2633:A:H2	2.18	0.41
40:0:7341:HOH:O	18:P:9:GLY:HA2	2.21	0.41
7:E:69:ILE:HA	7:E:72:MET:HE2	2.02	0.41
11:I:45:VAL:CG2	11:I:129:PHE:HD1	2.33	0.41
11:I:54:VAL:HG11	11:I:138:THR:HG21	2.03	0.41
13:K:121:ILE:HA	13:K:141:GLU:O	2.21	0.41
13:K:148:GLU:HB2	40:K:8894:HOH:O	2.20	0.41
15:M:79:PRO:HG3	15:M:142:THR:O	2.21	0.41
17:O:59:ARG:HH22	17:O:66:GLN:NE2	2.15	0.41
23:U:42:ASN:O	23:U:44:GLY:N	2.54	0.41
28:Z:8:GLN:HE22	28:Z:11:LYS:NZ	2.18	0.41
1:0:855:U:H4'	1:0:856:G:O4'	2.20	0.41
1:0:1596:U:H2'	1:0:1598:A:OP2	2.21	0.41
1:0:1666:C:O2'	1:0:1667:A:C5'	2.69	0.41
1:0:1730:G:H5'	1:0:1731:C:H5	1.85	0.41
1:0:2724:U:H2'	1:0:2725:G:O4'	2.21	0.41
40:0:4806:HOH:O	3:A:11:ARG:CZ	2.68	0.41
40:0:5005:HOH:O	16:N:39:THR:HB	2.20	0.41
4:B:53:LEU:HD21	4:B:270:ILE:HD12	2.03	0.41
10:H:154:TYR:C	10:H:154:TYR:HD1	2.29	0.41
11:I:77:GLY:O	11:I:78:ILE:C	2.62	0.41
11:I:107:ASN:ND2	11:I:107:ASN:C	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:72:ASN:HB2	40:K:8886:HOH:O	2.20	0.41
14:L:82:ARG:O	14:L:83:SER:C	2.62	0.41
15:M:38:LYS:HB2	15:M:38:LYS:HE3	1.78	0.41
23:U:5:VAL:CG1	23:U:9:ARG:NH1	2.84	0.41
28:Z:28:HIS:CD2	28:Z:31:LYS:H	2.39	0.41
1:0:921:G:H4'	1:0:924:G:N1	2.36	0.40
1:0:926:A:O2'	13:K:41:HIS:CD2	2.75	0.40
1:0:1267:C:O2'	1:0:1268:C:H5'	2.21	0.40
1:0:1513:C:O2'	1:0:1514:C:H5'	2.21	0.40
1:0:1592:G:H2'	1:0:1593:C:C6	2.55	0.40
1:0:1823:G:O2'	1:0:1824:C:H5'	2.21	0.40
1:0:2710:U:H2'	1:0:2711:U:C6	2.56	0.40
40:0:3338:HOH:O	11:I:46:ILE:HA	2.22	0.40
4:B:62:ARG:CB	4:B:65:MET:HE3	2.51	0.40
11:I:63:ILE:HG22	11:I:64:GLY:N	2.36	0.40
11:I:88:PRO:O	11:I:94:GLY:HA3	2.21	0.40
13:K:66:VAL:HG23	13:K:67:ARG:N	2.36	0.40
13:K:124:ASP:OD1	13:K:149:ARG:NH2	2.54	0.40
19:Q:119:VAL:HG21	19:Q:142:ASP:CG	2.46	0.40
21:S:41:ARG:NH1	21:S:42:VAL:O	2.53	0.40
1:0:88:G:H2'	1:0:89:G:C8	2.56	0.40
1:0:164:G:O3'	13:K:30:ARG:HB2	2.20	0.40
1:0:289:G:N1	1:0:363:A:C2	2.86	0.40
1:0:524:A:H5''	19:Q:29:LYS:HD3	2.04	0.40
1:0:731:U:H2'	1:0:732:C:C6	2.56	0.40
1:0:732:C:O2'	1:0:733:U:H5'	2.21	0.40
1:0:1041:U:H4'	1:0:1295:G:H5'	2.04	0.40
1:0:2325:C:H2'	1:0:2326:U:C6	2.57	0.40
1:0:2335:C:H2'	1:0:2336:G:C8	2.57	0.40
1:0:2791:U:H4'	1:0:2792:A:OP1	2.19	0.40
5:C:150:THR:HA	5:C:203:ALA:O	2.21	0.40
6:D:104:PHE:CE2	6:D:132:VAL:HB	2.55	0.40
7:E:108:LEU:CD1	7:E:164:ASP:HB2	2.51	0.40
8:F:111:ILE:O	8:F:115:VAL:HG23	2.21	0.40
10:H:3:ALA:HB2	10:H:58:ARG:HH12	1.87	0.40
22:T:9:CYS:CA	22:T:52:THR:HG23	2.51	0.40
24:V:73:LEU:HD12	24:V:73:LEU:HA	1.95	0.40
1:0:204:A:O2'	1:0:205:U:H5'	2.22	0.40
1:0:668:C:H2'	1:0:669:G:H8	1.86	0.40
1:0:892:G:H5''	28:Z:54:ALA:HB2	2.04	0.40
1:0:1287:A:O4'	24:V:117:ARG:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1800:G:H2'	1:0:1801:A:H8	1.86	0.40
1:0:2088:C:H1'	1:0:2841:A:N1	2.36	0.40
1:0:2284:G:H1'	40:0:3028:HOH:O	2.21	0.40
1:0:2526:C:C6	1:0:2526:C:H5'	2.56	0.40
1:0:2549:C:H2'	1:0:2550:U:O4'	2.22	0.40
2:9:3078:G:N2	2:9:3102:G:H2'	2.36	0.40
3:A:36:ASP:HB2	3:A:83:GLY:HA3	2.04	0.40
4:B:7:ARG:HH11	4:B:7:ARG:CG	2.24	0.40
5:C:12:THR:HB	40:C:8650:HOH:O	2.22	0.40
7:E:84:MET:HE3	7:E:131:LEU:HD13	2.02	0.40
7:E:93:MET:HE1	7:E:165:GLY:H	1.85	0.40
10:H:20:ILE:CG2	10:H:120:ILE:CD1	2.99	0.40
12:J:117:VAL:O	12:J:117:VAL:HG12	2.22	0.40
14:L:133:LEU:O	14:L:134:ILE:HD13	2.22	0.40
15:M:147:ILE:HD12	40:M:8847:HOH:O	2.21	0.40
20:R:10:VAL:CG1	23:U:36:ALA:HA	2.48	0.40
21:S:45:GLY:C	40:S:3851:HOH:O	2.64	0.40
25:W:23:HIS:CD2	25:W:24:LYS:HG3	2.56	0.40
30:2:55:VAL:HB	30:2:56:PRO:HD2	2.02	0.40
1:0:1154:A:H2'	1:0:1155:G:C8	2.56	0.40
1:0:1415:G:H5'	28:Z:12:ASN:O	2.21	0.40
1:0:1418:U:C4	20:R:58:MET:HE2	2.57	0.40
1:0:2398:A:H2'	1:0:2399:G:O4'	2.21	0.40
1:0:2748:G:H1'	40:0:8331:HOH:O	2.19	0.40
2:9:3053:G:O2'	2:9:3054:A:H5'	2.21	0.40
4:B:79:MET:HE1	40:B:9104:HOH:O	2.21	0.40
12:J:101:ASN:O	12:J:102:GLU:CB	2.70	0.40
14:L:134:ILE:O	14:L:136:PRO:HD3	2.21	0.40
15:M:168:LEU:HA	15:M:169:PRO:HD3	1.88	0.40
19:Q:126:LYS:HA	19:Q:127:PRO:HD3	1.93	0.40
27:Y:21:VAL:O	27:Y:22:SER:C	2.64	0.40
30:2:55:VAL:O	30:2:56:PRO:C	2.65	0.40
1:0:920:C:H4'	1:0:921:G:N2	2.36	0.40
1:0:1218:U:H2'	1:0:1219:U:H6	1.87	0.40
1:0:1614:G:H2'	40:0:5017:HOH:O	2.20	0.40
1:0:1920:C:O2'	1:0:1921:A:H5'	2.21	0.40
1:0:2613:G:O2'	1:0:2614:C:H5'	2.22	0.40
1:0:2783:A:H3'	40:0:5613:HOH:O	2.21	0.40
3:A:35:GLY:O	3:A:36:ASP:CB	2.63	0.40
6:D:54:ALA:HB3	6:D:69:ILE:HD12	2.01	0.40
12:J:14:LYS:CB	12:J:45:PRO:HG2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:66:ARG:HG2	12:J:66:ARG:HH11	1.86	0.40
12:J:114:ALA:HB3	12:J:117:VAL:HG23	2.03	0.40
24:V:1:MET:HB2	24:V:103:GLU:HG2	2.03	0.40
24:V:88:THR:HG22	24:V:90:TYR:HD1	1.86	0.40
26:X:187:VAL:HB	26:X:203:VAL:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	210 (89%)	19 (8%)	6 (3%)	4	11
4	B	335/338 (99%)	311 (93%)	18 (5%)	6 (2%)	6	18
5	C	244/246 (99%)	227 (93%)	17 (7%)	0	100	100
6	D	134/177 (76%)	99 (74%)	25 (19%)	10 (8%)	1	1
7	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
8	F	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	4	11
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/177 (88%)	140 (90%)	15 (10%)	1 (1%)	21	44
11	I	140/145 (97%)	128 (91%)	8 (6%)	4 (3%)	3	9
12	J	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	16	37
13	K	141/165 (86%)	120 (85%)	20 (14%)	1 (1%)	18	41
14	L	192/196 (98%)	179 (93%)	12 (6%)	1 (0%)	24	48
15	M	184/187 (98%)	162 (88%)	15 (8%)	7 (4%)	2	5
16	N	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
17	O	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
18	P	93/96 (97%)	87 (94%)	4 (4%)	2 (2%)	5	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Q	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
20	R	79/85 (93%)	77 (98%)	1 (1%)	1 (1%)	9	25
21	S	117/120 (98%)	108 (92%)	7 (6%)	2 (2%)	7	19
22	T	51/67 (76%)	47 (92%)	4 (8%)	0	100	100
23	U	63/71 (89%)	57 (90%)	4 (6%)	2 (3%)	3	7
24	V	152/154 (99%)	145 (95%)	5 (3%)	2 (1%)	9	25
25	W	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	9	25
26	X	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
27	Y	70/92 (76%)	61 (87%)	6 (9%)	3 (4%)	2	4
28	Z	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
29	1	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
30	2	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	5	14
All	All	3636/4286 (85%)	3345 (92%)	236 (6%)	55 (2%)	8	22

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	LEU
4	B	139	ASP
6	D	93	LEU
6	D	95	THR
6	D	137	PRO
6	D	173	GLU
8	F	101	ALA
13	K	80	ASP
15	M	154	LEU
15	M	164	ASP
15	M	183	ASP
27	Y	81	ARG
30	2	56	PRO
3	A	34	ASP
4	B	34	GLY
4	B	169	GLY
6	D	20	LYS
6	D	171	ASP
11	I	143	LYS
15	M	162	ASP
15	M	167	ASP

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Mol	Chain	Res	Type
23	U	43	PRO
24	V	77	ALA
3	A	132	ASP
4	B	185	GLY
11	I	7	ASP
12	J	119	GLN
15	M	65	ASP
15	M	181	ASP
21	S	44	ALA
21	S	53	GLY
25	W	77	PHE
27	Y	20	ARG
30	2	57	GLY
6	D	16	PRO
6	D	61	PHE
11	I	5	GLU
20	R	30	ASP
27	Y	41	ASN
3	A	37	VAL
4	B	2	GLN
4	B	107	SER
6	D	60	GLU
11	I	65	ASN
14	L	83	SER
18	P	78	GLY
18	P	18	PRO
24	V	49	ASN
3	A	112	PRO
6	D	27	ILE
23	U	40	PRO
8	F	64	PRO
8	F	71	GLY
10	H	55	VAL
3	A	211	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	167 (93%)	12 (7%)	15	36
4	B	282/283 (100%)	266 (94%)	16 (6%)	18	43
5	C	193/193 (100%)	179 (93%)	14 (7%)	13	32
6	D	117/148 (79%)	111 (95%)	6 (5%)	21	48
7	E	152/156 (97%)	149 (98%)	3 (2%)	48	76
8	F	93/94 (99%)	90 (97%)	3 (3%)	34	64
9	G	27/282 (10%)	27 (100%)	0	100	100
10	H	134/145 (92%)	128 (96%)	6 (4%)	24	52
11	I	118/121 (98%)	110 (93%)	8 (7%)	14	35
12	J	106/106 (100%)	102 (96%)	4 (4%)	29	58
13	K	113/127 (89%)	109 (96%)	4 (4%)	32	61
14	L	158/160 (99%)	154 (98%)	4 (2%)	42	71
15	M	149/150 (99%)	142 (95%)	7 (5%)	23	51
16	N	93/94 (99%)	91 (98%)	2 (2%)	45	74
17	O	113/117 (97%)	111 (98%)	2 (2%)	51	78
18	P	79/80 (99%)	75 (95%)	4 (5%)	21	48
19	Q	117/122 (96%)	114 (97%)	3 (3%)	40	70
20	R	71/74 (96%)	70 (99%)	1 (1%)	59	82
21	S	105/106 (99%)	102 (97%)	3 (3%)	37	67
22	T	44/53 (83%)	44 (100%)	0	100	100
23	U	51/57 (90%)	50 (98%)	1 (2%)	48	76
24	V	130/130 (100%)	121 (93%)	9 (7%)	14	34
25	W	66/74 (89%)	64 (97%)	2 (3%)	36	66
26	X	120/196 (61%)	109 (91%)	11 (9%)	8	22
27	Y	59/74 (80%)	57 (97%)	2 (3%)	32	62
28	Z	46/47 (98%)	46 (100%)	0	100	100
29	1	42/46 (91%)	41 (98%)	1 (2%)	43	72
30	2	79/79 (100%)	77 (98%)	2 (2%)	42	71
All	All	3036/3496 (87%)	2906 (96%)	130 (4%)	26	54

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	3	ARG
3	A	33	GLU
3	A	36	ASP
3	A	55	VAL
3	A	68	ILE
3	A	69	LEU
3	A	94	LEU
3	A	131	HIS
3	A	153	ARG
3	A	175	LYS
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	33	ASP
4	B	63	GLU
4	B	71	VAL
4	B	84	LEU
4	B	97	LEU
4	B	98	THR
4	B	103	ASP
4	B	195	ARG
4	B	251	VAL
4	B	254	GLN
4	B	264	GLU
4	B	307	ARG
4	B	312	ARG
5	C	2	GLN
5	C	67	GLN
5	C	91	PRO
5	C	94	THR
5	C	115	LEU
5	C	136	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	240	LEU
5	C	243	VAL
6	D	24	HIS

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Mol	Chain	Res	Type
6	D	50	VAL
6	D	99	ASP
6	D	131	THR
6	D	137	PRO
6	D	149	ARG
7	E	7	ILE
7	E	86	VAL
7	E	102	VAL
8	F	12	LEU
8	F	46	GLU
8	F	78	GLU
10	H	18	GLU
10	H	84	LYS
10	H	111	ASP
10	H	146	VAL
10	H	159	PRO
10	H	171	LEU
11	I	39	VAL
11	I	46	ILE
11	I	74	ARG
11	I	76	ASP
11	I	93	ARG
11	I	125	SER
11	I	127	ILE
11	I	131	THR
12	J	4	LEU
12	J	7	ASP
12	J	10	GLN
12	J	98	VAL
13	K	30	ARG
13	K	35	ARG
13	K	117	GLU
13	K	140	VAL
14	L	46	LEU
14	L	93	ARG
14	L	107	ARG
14	L	164	THR
15	M	17	ARG
15	M	26	LEU
15	M	47	LEU
15	M	127	LEU
15	M	128	ASP

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Mol	Chain	Res	Type
15	M	139	TRP
15	M	152	GLU
16	N	3	THR
16	N	98	LEU
17	O	52	LYS
17	O	98	ILE
18	P	11	ARG
18	P	16	ASN
18	P	18	PRO
18	P	95	GLU
19	Q	13	THR
19	Q	39	THR
19	Q	82	GLU
20	R	10	VAL
21	S	39	ASN
21	S	48	VAL
21	S	96	VAL
23	U	43	PRO
24	V	26	ILE
24	V	35	VAL
24	V	52	VAL
24	V	73	LEU
24	V	76	ASP
24	V	122	ARG
24	V	142	ASP
24	V	146	ILE
24	V	154	ARG
25	W	15	ARG
25	W	72	VAL
26	X	103	THR
26	X	115	ARG
26	X	141	THR
26	X	154	ARG
26	X	163	THR
26	X	172	THR
26	X	189	ASN
26	X	200	THR
26	X	203	VAL
26	X	231	PRO
26	X	235	GLU
27	Y	44	GLU
27	Y	78	THR

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Mol	Chain	Res	Type
29	1	18	ASN
30	2	38	ARG
30	2	56	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	7	GLN
3	A	92	ASN
3	A	199	HIS
4	B	27	ASN
4	B	55	ASN
4	B	145	HIS
4	B	230	GLN
4	B	238	ASN
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	129	HIS
5	C	163	HIS
5	C	178	GLN
6	D	47	GLN
6	D	103	ASN
6	D	133	ASN
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
8	F	79	GLN
8	F	80	GLN
9	G	64	ASN
10	H	37	GLN
10	H	56	GLN
10	H	59	HIS
10	H	70	ASN
11	I	25	GLN
11	I	107	ASN
12	J	10	GLN
12	J	42	ASN
13	K	18	HIS
13	K	41	HIS

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Mol	Chain	Res	Type
13	K	42	ASN
13	K	58	GLN
13	K	116	HIS
14	L	24	GLN
14	L	26	GLN
14	L	58	GLN
14	L	77	HIS
14	L	126	GLN
14	L	170	ASN
15	M	22	GLN
15	M	107	ASN
15	M	153	GLN
17	O	50	GLN
17	O	66	GLN
17	O	73	HIS
17	O	88	GLN
17	O	118	GLN
18	P	40	HIS
19	Q	22	GLN
19	Q	61	GLN
19	Q	98	ASN
19	Q	102	GLN
19	Q	113	HIS
19	Q	117	HIS
19	Q	140	GLN
20	R	9	HIS
20	R	51	GLN
20	R	53	ASN
20	R	55	GLN
21	S	39	ASN
21	S	73	HIS
22	T	39	ASN
22	T	48	ASN
23	U	60	GLN
24	V	6	GLN
24	V	27	HIS
24	V	59	GLN
24	V	110	GLN
24	V	119	HIS
24	V	125	HIS
24	V	141	HIS
25	W	23	HIS

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Mol	Chain	Res	Type
26	X	133	HIS
26	X	134	HIS
26	X	149	GLN
26	X	153	GLN
26	X	189	ASN
28	Z	8	GLN
28	Z	16	HIS
28	Z	28	HIS
29	1	16	ASN
29	1	18	ASN
29	1	37	HIS
29	1	41	HIS
29	1	45	ASN
30	2	2	GLN
30	2	13	HIS
30	2	30	GLN
30	2	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	245 (8%)	29 (1%)
2	9	121/122 (99%)	17 (14%)	2 (1%)
31	4	2/4 (50%)	1 (50%)	0
All	All	2869/3048 (94%)	263 (9%)	31 (1%)

All (263) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	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	130	C

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Mol	Chain	Res	Type
1	0	141	C
1	0	151	A
1	0	166	A
1	0	169	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	U
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	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	457	U
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	516	A
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	C
1	0	581	G

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Mol	Chain	Res	Type
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	701	U
1	0	717	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	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	882	A
1	0	898	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	1129	C
1	0	1130	U
1	0	1161	A
1	0	1162	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1171	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1287	A
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1407	A
1	0	1409	G
1	0	1451	C
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1563	G
1	0	1564	C
1	0	1580	A

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Mol	Chain	Res	Type
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1974	G
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2034	U
1	0	2064	U
1	0	2072	G

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Mol	Chain	Res	Type
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	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	2379	G
1	0	2422	U
1	0	2462	G
1	0	2476	C
1	0	2483	A
1	0	2507	G
1	0	2511	A
1	0	2526	C
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2540	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2578	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2638	G
1	0	2649	A
1	0	2664	A

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Mol	Chain	Res	Type
1	0	2681	A
1	0	2682	C
1	0	2718	C
1	0	2719	A
1	0	2726	U
1	0	2727	A
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2850	C
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	3026	C
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C
31	4	76	A

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	10	U
1	0	69	A
1	0	129	A
1	0	284	C
1	0	338	C
1	0	603	A
1	0	604	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	898	G
1	0	1080	C
1	0	1164	U
1	0	1232	A
1	0	1237	U
1	0	1352	A
1	0	1450	C
1	0	1563	G
1	0	1684	A
1	0	1856	C
1	0	1979	G
1	0	2011	A
1	0	2467	A
1	0	2526	C
1	0	2718	C
1	0	2726	U
1	0	2791	U
2	9	3024	U
2	9	3065	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 306 ligands modelled in this entry, 304 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	ZLD	0	9500	-	26,26,26	3.18	13 (50%)	36,36,36	3.24	15 (41%)
39	ACE	4	78	31	1,2,2	1.09	0	0,1,1	-	-

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
32	ZLD	0	9500	-	-	0/13/33/33	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	ZLD	C3-C1	6.80	1.49	1.38
32	0	9500	ZLD	C3-C17	6.72	1.50	1.39
32	0	9500	ZLD	C17-C16	5.60	1.51	1.40
32	0	9500	ZLD	C1-C2	5.32	1.49	1.39
32	0	9500	ZLD	C24-C23	4.80	1.68	1.50
32	0	9500	ZLD	C20-N19	4.36	1.54	1.46
32	0	9500	ZLD	C5-C16	3.81	1.44	1.37
32	0	9500	ZLD	C20-C21	2.86	1.61	1.50
32	0	9500	ZLD	C9-C8	2.74	1.55	1.51
32	0	9500	ZLD	O15-C7	2.60	1.25	1.21
32	0	9500	ZLD	C2-N4	2.57	1.48	1.43
32	0	9500	ZLD	O10-C8	-2.19	1.43	1.46
32	0	9500	ZLD	O10-C7	2.18	1.38	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9500	ZLD	C6-C8-C9	9.38	124.01	113.38
32	0	9500	ZLD	C2-N4-C7	7.57	133.92	125.98
32	0	9500	ZLD	C6-N4-C7	-7.53	105.60	111.17
32	0	9500	ZLD	O15-C7-N4	-5.32	123.88	128.80
32	0	9500	ZLD	O10-C7-N4	5.03	114.16	109.92
32	0	9500	ZLD	C23-C24-N19	4.19	117.86	109.93
32	0	9500	ZLD	O22-C21-C20	3.57	119.47	111.77
32	0	9500	ZLD	F18-C16-C17	3.31	121.53	118.37
32	0	9500	ZLD	C3-C17-C16	-3.21	110.98	117.31
32	0	9500	ZLD	F18-C16-C5	-3.08	112.47	118.64
32	0	9500	ZLD	C5-C16-C17	2.95	125.96	123.35
32	0	9500	ZLD	C8-C6-N4	2.83	104.52	101.85
32	0	9500	ZLD	C16-C17-N19	2.71	123.58	120.42
32	0	9500	ZLD	C8-O10-C7	-2.62	108.01	110.10
32	0	9500	ZLD	C1-C3-C17	2.58	124.27	119.10

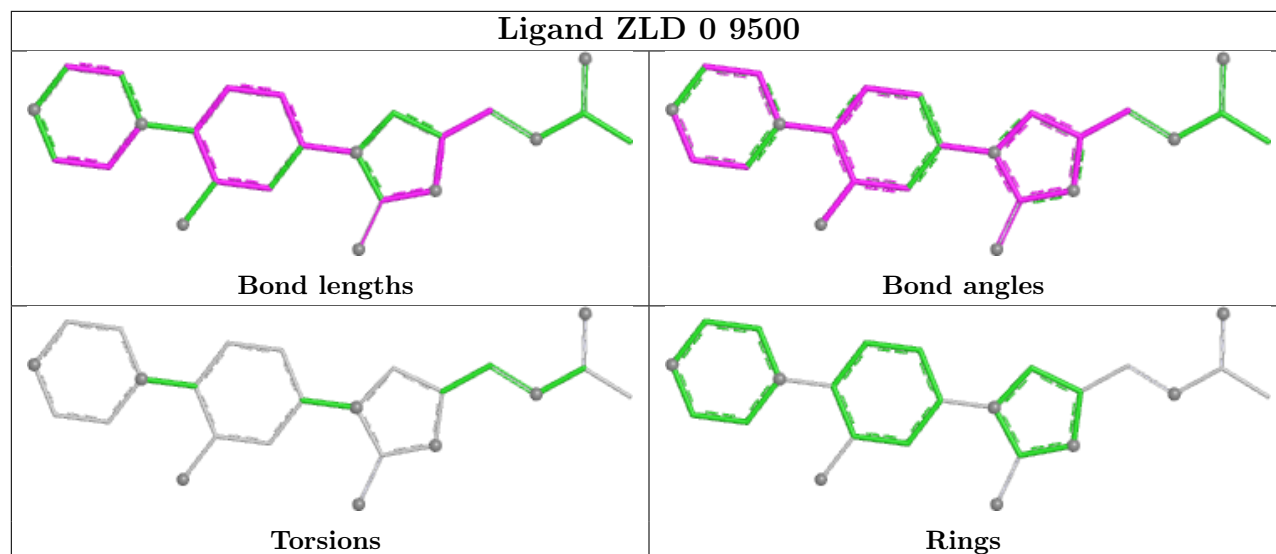
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	2754/2922 (94%)	-0.09	138 (5%) 34 30	29, 53, 97, 144	0
2	9	122/122 (100%)	0.82	9 (7%) 20 18	45, 75, 98, 149	0
3	A	237/240 (98%)	0.25	10 (4%) 40 37	34, 58, 90, 107	0
4	B	337/338 (99%)	0.26	12 (3%) 46 42	35, 60, 86, 96	0
5	C	246/246 (100%)	0.10	4 (1%) 70 68	28, 53, 75, 86	0
6	D	140/177 (79%)	1.70	47 (33%) 1 1	67, 101, 122, 127	0
7	E	172/178 (96%)	0.59	8 (4%) 36 33	48, 74, 93, 98	0
8	F	119/120 (99%)	0.76	8 (6%) 24 21	57, 78, 99, 108	0
9	G	29/348 (8%)	1.48	7 (24%) 2 1	79, 99, 105, 109	0
10	H	160/177 (90%)	0.70	10 (6%) 26 23	41, 55, 80, 88	0
11	I	142/145 (97%)	0.23	3 (2%) 63 61	43, 56, 75, 94	0
12	J	132/132 (100%)	0.12	2 (1%) 72 70	40, 54, 78, 90	0
13	K	145/165 (87%)	0.71	18 (12%) 8 7	34, 73, 107, 120	0
14	L	194/196 (98%)	0.12	5 (2%) 57 54	33, 42, 65, 70	0
15	M	186/187 (99%)	0.91	21 (11%) 10 8	52, 72, 110, 120	0
16	N	115/116 (99%)	0.31	3 (2%) 57 54	45, 62, 77, 82	0
17	O	143/149 (95%)	0.38	6 (4%) 40 37	46, 59, 71, 82	0
18	P	95/96 (98%)	0.18	2 (2%) 63 61	46, 55, 72, 84	0
19	Q	150/155 (96%)	-0.22	0 100 100	37, 51, 70, 76	0
20	R	81/85 (95%)	0.29	2 (2%) 58 55	50, 65, 85, 90	0
21	S	119/120 (99%)	0.50	5 (4%) 40 37	47, 61, 87, 108	0
22	T	53/67 (79%)	0.41	0 100 100	47, 59, 78, 86	0
23	U	65/71 (91%)	0.99	10 (15%) 5 4	59, 79, 115, 121	0
24	V	154/154 (100%)	0.29	2 (1%) 75 73	43, 58, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	82/92 (89%)	0.60	8 (9%) 13 11	48, 64, 88, 106	0
26	X	142/241 (58%)	0.07	3 (2%) 63 61	32, 49, 71, 91	0
27	Y	72/92 (78%)	0.76	3 (4%) 40 37	43, 59, 70, 76	0
28	Z	56/57 (98%)	-0.27	0 100 100	33, 40, 46, 57	0
29	1	46/50 (92%)	0.81	7 (15%) 5 4	41, 62, 87, 99	0
30	2	92/92 (100%)	0.32	5 (5%) 31 27	47, 64, 77, 86	0
31	4	4/4 (100%)	2.52	2 (50%) 0 0	78, 83, 85, 88	0
All	All	6584/7334 (89%)	0.22	360 (5%) 30 27	28, 57, 98, 149	0

All (360) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	9	3001	U	7.9
4	B	1	PRO	7.0
1	0	1161	A	7.0
1	0	737	A	6.7
6	D	107	GLY	6.5
2	9	3002	U	6.4
2	9	3024	U	6.4
1	0	10	U	6.3
15	M	186	LEU	6.2
1	0	736	A	6.2
15	M	166	ALA	6.0
25	W	65	ASN	5.8
23	U	1	THR	5.7
3	A	37	VAL	5.5
21	S	119	ALA	5.5
10	H	171	LEU	5.5
1	0	1190	G	5.4
1	0	1162	G	5.3
1	0	735	C	5.1
29	1	28	LYS	5.1
6	D	10	PHE	5.0
1	0	2748	G	5.0
15	M	184	ILE	4.9
1	0	1175	G	4.7
6	D	35	ALA	4.7
10	H	168	GLY	4.7
13	K	81	VAL	4.7
29	1	49	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	0	2645	U	4.6
1	0	1181	A	4.6
1	0	1160	G	4.6
1	0	1197	G	4.6
31	4	77	PHE	4.6
6	D	26	GLY	4.5
25	W	88	GLU	4.5
1	0	1208	C	4.5
1	0	2912	C	4.5
21	S	117	ASP	4.5
1	0	1207	A	4.5
25	W	85	VAL	4.4
2	9	3025	G	4.4
15	M	154	LEU	4.4
6	D	135	VAL	4.4
1	0	1192	A	4.3
25	W	82	GLU	4.3
7	E	10	ASP	4.2
1	0	1202	A	4.2
1	0	1195	G	4.2
15	M	95	ALA	4.1
15	M	167	ASP	4.1
1	0	1191	A	4.1
1	0	1947	G	4.1
1	0	1186	C	4.1
1	0	514	G	4.0
1	0	2911	C	4.0
1	0	734	U	4.0
1	0	1206	U	4.0
1	0	1176	C	3.9
1	0	1525	G	3.9
1	0	1172	G	3.9
6	D	27	ILE	3.9
15	M	165	ALA	3.9
11	I	70	PHE	3.9
1	0	1159	G	3.8
1	0	1200	A	3.8
1	0	2769	C	3.8
23	U	40	PRO	3.8
25	W	87	ALA	3.8
1	0	2637	A	3.7
15	M	162	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
15	M	158	LEU	3.7
1	0	1199	A	3.7
13	K	77	ALA	3.7
1	0	2344	G	3.7
4	B	57	GLU	3.7
1	0	1205	U	3.7
1	0	87	C	3.7
1	0	138	U	3.6
1	0	1948	G	3.6
6	D	17	ARG	3.6
23	U	39	ALA	3.6
6	D	174	VAL	3.6
1	0	738	G	3.6
14	L	74	LYS	3.6
6	D	69	ILE	3.6
7	E	154	ILE	3.6
9	G	12	ILE	3.6
6	D	62	ASP	3.6
1	0	1163	G	3.6
27	Y	82	SER	3.6
1	0	1164	U	3.5
2	9	3023	U	3.5
6	D	37	ALA	3.5
15	M	168	LEU	3.5
1	0	1185	U	3.5
1	0	2511	A	3.5
1	0	1196	C	3.5
29	1	44	ARG	3.5
1	0	2909	G	3.5
6	D	50	VAL	3.5
6	D	157	LEU	3.4
6	D	63	ILE	3.4
10	H	40	ALA	3.4
1	0	1203	G	3.4
3	A	36	ASP	3.4
6	D	44	ILE	3.4
1	0	2569	A	3.4
6	D	131	THR	3.4
6	D	55	LYS	3.3
1	0	1169	U	3.3
1	0	2747	C	3.3
6	D	105	SER	3.3

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Mol	Chain	Res	Type	RSRZ
13	K	146	GLY	3.3
1	0	1171	A	3.3
1	0	2913	A	3.3
6	D	57	THR	3.3
1	0	1966	U	3.3
1	0	2831	C	3.3
1	0	497	A	3.3
1	0	1193	A	3.3
1	0	1170	U	3.3
7	E	45	ASP	3.3
1	0	1184	C	3.2
7	E	12	ASP	3.2
1	0	1967	U	3.2
6	D	12	GLU	3.2
23	U	2	VAL	3.2
1	0	288	A	3.2
1	0	1173	A	3.2
1	0	1177	A	3.2
1	0	2345	A	3.2
1	0	1524	U	3.2
1	0	1000	C	3.1
1	0	2910	A	3.1
30	2	41	GLU	3.1
1	0	1964	U	3.1
1	0	1929	G	3.1
21	S	118	SER	3.1
1	0	2512	U	3.1
1	0	1157	C	3.1
1	0	1183	C	3.1
1	0	2914	A	3.0
6	D	36	ASN	3.0
11	I	4	ALA	3.0
6	D	22	VAL	3.0
2	9	3065	A	3.0
6	D	171	ASP	3.0
4	B	108	GLU	3.0
1	0	1156	C	3.0
3	A	203	GLY	3.0
1	0	2507	G	3.0
1	0	2851	G	3.0
15	M	179	LEU	2.9
12	J	119	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	0	1194	A	2.9
21	S	36	GLY	2.9
23	U	43	PRO	2.9
27	Y	11	SER	2.9
1	0	272	A	2.9
1	0	1168	C	2.9
1	0	1965	C	2.9
15	M	1	ALA	2.9
15	M	81	ALA	2.9
15	M	137	ALA	2.9
20	R	1	SER	2.8
3	A	35	GLY	2.8
1	0	1180	U	2.8
4	B	2	GLN	2.8
6	D	170	TYR	2.8
15	M	69	TYR	2.8
4	B	119	HIS	2.8
6	D	106	PHE	2.8
13	K	148	GLU	2.8
1	0	1204	C	2.8
3	A	211	LYS	2.7
3	A	91	GLY	2.7
5	C	132	ASP	2.7
6	D	141	VAL	2.7
13	K	91	VAL	2.7
18	P	18	PRO	2.7
1	0	1165	G	2.7
1	0	1523	G	2.7
2	9	3022	G	2.7
9	G	71	LEU	2.7
6	D	11	HIS	2.7
6	D	59	GLY	2.7
27	Y	16	ALA	2.7
1	0	2487	C	2.7
1	0	1950	G	2.7
8	F	90	GLU	2.7
10	H	83	TYR	2.7
1	0	2770	G	2.6
6	D	47	GLN	2.6
1	0	1981	A	2.6
6	D	90	LEU	2.6
29	1	27	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	0	1179	C	2.6
30	2	55	VAL	2.6
23	U	65	ASP	2.6
13	K	99	GLU	2.6
14	L	87	GLY	2.6
1	0	1182	C	2.6
1	0	1213	C	2.6
10	H	112	GLY	2.6
1	0	969	G	2.6
4	B	58	PRO	2.6
1	0	1700	C	2.6
5	C	133	ARG	2.6
6	D	58	VAL	2.6
1	0	1167	G	2.5
10	H	111	ASP	2.5
9	G	27	ILE	2.5
1	0	2908	A	2.5
13	K	75	LEU	2.5
3	A	205	GLY	2.5
1	0	2539	U	2.5
1	0	1951	G	2.5
20	R	12	GLU	2.5
14	L	194	GLY	2.5
11	I	47	THR	2.5
23	U	46	ILE	2.5
7	E	11	VAL	2.5
3	A	97	ALA	2.5
6	D	13	MET	2.5
1	0	1187	U	2.5
1	0	1198	U	2.5
1	0	2004	U	2.5
4	B	138	GLY	2.5
13	K	150	GLN	2.5
8	F	28	ALA	2.5
29	1	39	ARG	2.4
1	0	2241	C	2.4
13	K	57	VAL	2.4
13	K	82	ALA	2.4
17	O	143	ALA	2.4
29	1	29	THR	2.4
4	B	118	ASP	2.4
13	K	83	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
26	X	235	GLU	2.4
1	0	2570	G	2.4
9	G	26	MET	2.4
30	2	56	PRO	2.4
8	F	8	VAL	2.4
10	H	165	VAL	2.4
5	C	76	ARG	2.4
23	U	42	ASN	2.4
1	0	1155	G	2.4
1	0	1153	C	2.4
1	0	2419	U	2.4
1	0	2508	C	2.4
17	O	58	SER	2.4
17	O	117	SER	2.4
4	B	149	ASP	2.4
9	G	73	ASP	2.4
6	D	128	LEU	2.3
10	H	169	GLU	2.3
3	A	34	ASP	2.3
24	V	76	ASP	2.3
6	D	49	PRO	2.3
15	M	169	PRO	2.3
13	K	89	PHE	2.3
10	H	41	ASP	2.3
1	0	258	G	2.3
1	0	2526	C	2.3
13	K	130	ARG	2.3
6	D	172	VAL	2.3
7	E	87	PHE	2.3
15	M	87	LEU	2.3
25	W	83	ALA	2.3
18	P	84	ILE	2.3
1	0	1561	U	2.3
1	0	586	C	2.3
1	0	1201	C	2.3
31	4	74	C	2.3
26	X	220	GLU	2.3
4	B	139	ASP	2.3
5	C	246	ARG	2.3
9	G	13	PRO	2.3
1	0	2827	A	2.3
6	D	104	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
4	B	112	THR	2.2
13	K	60	GLU	2.2
1	0	284	C	2.2
1	0	999	C	2.2
1	0	2850	C	2.2
1	0	960	G	2.2
1	0	1178	G	2.2
13	K	80	ASP	2.2
15	M	138	ASP	2.2
1	0	1174	A	2.2
1	0	2506	A	2.2
6	D	98	PHE	2.2
6	D	87	ALA	2.2
6	D	89	PRO	2.2
6	D	150	SER	2.2
1	0	1563	G	2.2
16	N	22	GLY	2.2
17	O	116	SER	2.2
1	0	441	A	2.2
6	D	74	THR	2.2
8	F	26	THR	2.2
1	0	970	U	2.2
8	F	24	ARG	2.2
8	F	2	VAL	2.2
10	H	146	VAL	2.2
6	D	61	PHE	2.2
23	U	36	ALA	2.2
1	0	1529	G	2.2
1	0	1970	G	2.2
1	0	2005	G	2.2
1	0	2540	G	2.2
1	0	1625	U	2.2
21	S	107	LYS	2.2
15	M	182	GLY	2.2
13	K	104	ASP	2.2
9	G	29	SER	2.2
25	W	77	PHE	2.2
8	F	112	ALA	2.1
16	N	31	GLU	2.1
12	J	27	ARG	2.1
1	0	1604	G	2.1
1	0	2237	G	2.1

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Mol	Chain	Res	Type	RSRZ
1	0	1166	A	2.1
6	D	70	GLY	2.1
30	2	57	GLY	2.1
16	N	24	ALA	2.1
13	K	55	GLN	2.1
1	0	2256	G	2.1
4	B	82	VAL	2.1
7	E	6	GLU	2.1
14	L	75	ARG	2.1
23	U	16	ARG	2.1
17	O	18	LYS	2.1
6	D	25	MET	2.1
29	1	35	ARG	2.1
1	0	128	A	2.1
1	0	1188	A	2.1
1	0	1701	A	2.1
8	F	9	PRO	2.1
30	2	58	GLY	2.1
15	M	147	ILE	2.1
17	O	119	TYR	2.1
6	D	77	ASP	2.0
24	V	91	ASP	2.0
6	D	43	GLU	2.0
14	L	22	GLU	2.0
1	0	716	G	2.0
1	0	1189	A	2.0
7	E	109	GLY	2.0
3	A	26	ASP	2.0
25	W	79	GLU	2.0
26	X	207	SER	2.0
1	0	130	C	2.0
13	K	145	LEU	2.0
1	0	1488	U	2.0
2	9	3055	U	2.0
6	D	138	GLY	2.0
15	M	40	ASN	2.0
1	0	2103	A	2.0
2	9	3057	A	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	9	8543	1/1	0.44	0.21	116,116,116,116	0
35	NA	0	8525	1/1	0.51	0.31	92,92,92,92	0
35	NA	0	8571	1/1	0.54	0.41	103,103,103,103	0
33	MG	0	8035	1/1	0.57	0.26	80,80,80,80	0
33	MG	0	8071	1/1	0.59	0.48	84,84,84,84	0
33	MG	0	8038	1/1	0.59	0.17	88,88,88,88	0
35	NA	R	8510	1/1	0.60	0.26	127,127,127,127	0
34	K	0	8401	1/1	0.66	0.47	129,129,129,129	0
35	NA	9	8572	1/1	0.67	0.46	99,99,99,99	0
35	NA	0	8561	1/1	0.71	0.73	122,122,122,122	0
33	MG	0	8073	1/1	0.73	0.30	105,105,105,105	0
37	SR	0	9006	1/1	0.73	0.34	150,150,150,150	0
33	MG	0	8030	1/1	0.74	0.33	99,99,99,99	0
33	MG	0	8085	1/1	0.74	0.23	105,105,105,105	0
35	NA	0	8544	1/1	0.75	0.50	86,86,86,86	0
33	MG	0	8040	1/1	0.76	0.23	97,97,97,97	0
33	MG	0	8063	1/1	0.77	0.27	94,94,94,94	0
35	NA	0	8518	1/1	0.77	0.30	107,107,107,107	0
35	NA	0	8555	1/1	0.78	0.67	75,75,75,75	0
35	NA	0	8573	1/1	0.78	0.15	92,92,92,92	0
37	SR	0	8979	1/1	0.78	0.16	150,150,150,150	0
35	NA	0	8562	1/1	0.78	0.53	78,78,78,78	0
33	MG	0	8066	1/1	0.79	0.32	103,103,103,103	0
35	NA	0	8574	1/1	0.79	0.41	66,66,66,66	0
35	NA	0	8575	1/1	0.79	0.47	104,104,104,104	0
35	NA	0	8548	1/1	0.79	0.28	59,59,59,59	0
35	NA	0	8559	1/1	0.80	0.47	85,85,85,85	0
36	CL	B	8819	1/1	0.82	0.29	72,72,72,72	0
35	NA	0	8564	1/1	0.82	0.13	74,74,74,74	0
33	MG	9	8074	1/1	0.82	0.33	64,64,64,64	0
33	MG	0	8047	1/1	0.83	0.20	98,98,98,98	0
35	NA	0	8507	1/1	0.84	0.14	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8523	1/1	0.84	0.20	51,51,51,51	0
35	NA	0	8536	1/1	0.85	0.12	71,71,71,71	0
33	MG	0	8044	1/1	0.85	0.14	79,79,79,79	0
35	NA	0	8522	1/1	0.85	0.42	77,77,77,77	0
32	ZLD	0	9500	24/24	0.85	0.23	69,77,79,80	0
35	NA	0	8508	1/1	0.85	0.17	55,55,55,55	0
35	NA	0	8529	1/1	0.85	0.20	46,46,46,46	0
35	NA	0	8512	1/1	0.86	0.36	72,72,72,72	0
37	SR	0	8971	1/1	0.86	0.11	150,150,150,150	0
33	MG	0	8010	1/1	0.86	0.20	70,70,70,70	0
37	SR	0	8996	1/1	0.86	0.27	150,150,150,150	0
33	MG	0	8087	1/1	0.86	0.21	61,61,61,61	0
35	NA	0	8549	1/1	0.87	0.33	75,75,75,75	0
35	NA	0	8565	1/1	0.87	0.20	66,66,66,66	0
37	SR	9	9003	1/1	0.87	0.15	150,150,150,150	0
38	CD	N	8705	1/1	0.87	0.27	150,150,150,150	0
35	NA	0	8558	1/1	0.88	0.15	63,63,63,63	0
33	MG	0	8007	1/1	0.88	0.10	53,53,53,53	0
35	NA	0	8516	1/1	0.88	0.41	52,52,52,52	0
37	SR	0	8994	1/1	0.88	0.53	150,150,150,150	0
35	NA	0	8550	1/1	0.88	0.28	66,66,66,66	0
35	NA	0	8502	1/1	0.88	0.34	75,75,75,75	0
35	NA	0	8556	1/1	0.88	0.27	66,66,66,66	0
37	SR	B	8987	1/1	0.88	0.39	150,150,150,150	0
35	NA	0	8570	1/1	0.88	0.09	57,57,57,57	0
33	MG	0	8081	1/1	0.89	0.19	82,82,82,82	0
33	MG	0	8017	1/1	0.89	0.20	121,121,121,121	0
33	MG	0	8039	1/1	0.89	0.11	68,68,68,68	0
35	NA	0	8542	1/1	0.89	0.30	68,68,68,68	0
35	NA	0	8511	1/1	0.89	0.24	71,71,71,71	0
37	SR	0	8976	1/1	0.89	0.09	139,139,139,139	0
33	MG	0	8092	1/1	0.89	0.08	72,72,72,72	0
35	NA	0	8567	1/1	0.89	0.30	83,83,83,83	0
33	MG	0	8029	1/1	0.89	0.14	100,100,100,100	0
37	SR	0	9001	1/1	0.89	0.10	150,150,150,150	0
33	MG	B	8042	1/1	0.89	0.09	85,85,85,85	0
37	SR	0	9007	1/1	0.89	0.51	150,150,150,150	0
35	NA	0	8551	1/1	0.89	0.14	46,46,46,46	0
33	MG	S	8057	1/1	0.89	0.23	55,55,55,55	0
33	MG	0	8076	1/1	0.89	0.14	68,68,68,68	0
37	SR	0	8982	1/1	0.90	0.24	144,144,144,144	0
35	NA	0	8517	1/1	0.90	0.13	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	8995	1/1	0.90	0.13	107,107,107,107	0
35	NA	0	8535	1/1	0.90	0.28	79,79,79,79	0
33	MG	0	8043	1/1	0.90	0.15	72,72,72,72	0
37	SR	0	8944	1/1	0.90	0.18	135,135,135,135	0
33	MG	0	8036	1/1	0.90	0.17	58,58,58,58	0
37	SR	0	8975	1/1	0.90	0.14	133,133,133,133	0
33	MG	0	8069	1/1	0.90	0.16	78,78,78,78	0
33	MG	0	8033	1/1	0.90	0.07	58,58,58,58	0
35	NA	0	8514	1/1	0.91	0.15	51,51,51,51	0
33	MG	0	8016	1/1	0.91	0.17	94,94,94,94	0
33	MG	0	8037	1/1	0.91	0.21	102,102,102,102	0
36	CL	0	8813	1/1	0.91	0.09	59,59,59,59	0
35	NA	0	8569	1/1	0.91	0.15	61,61,61,61	0
35	NA	0	8541	1/1	0.91	0.09	62,62,62,62	0
33	MG	A	8051	1/1	0.91	0.10	71,71,71,71	0
33	MG	0	8001	1/1	0.91	0.18	31,31,31,31	0
33	MG	0	8065	1/1	0.91	0.37	100,100,100,100	0
33	MG	1	8060	1/1	0.91	0.06	58,58,58,58	0
37	SR	0	8989	1/1	0.92	0.12	150,150,150,150	0
35	NA	0	8545	1/1	0.92	0.30	57,57,57,57	0
33	MG	0	8002	1/1	0.92	0.19	82,82,82,82	0
37	SR	0	8959	1/1	0.92	0.09	150,150,150,150	0
35	NA	I	8538	1/1	0.92	0.07	51,51,51,51	0
37	SR	0	9002	1/1	0.92	0.11	125,125,125,125	0
37	SR	0	9004	1/1	0.92	0.11	150,150,150,150	0
35	NA	L	8539	1/1	0.92	0.10	43,43,43,43	0
35	NA	Q	8533	1/1	0.92	0.17	68,68,68,68	0
33	MG	0	8090	1/1	0.92	0.08	83,83,83,83	0
37	SR	0	8981	1/1	0.92	0.11	150,150,150,150	0
35	NA	0	8509	1/1	0.92	0.23	83,83,83,83	0
39	ACE	4	78	3/3	0.92	0.26	79,79,80,81	0
37	SR	0	8960	1/1	0.93	0.10	116,116,116,116	0
33	MG	0	8048	1/1	0.93	0.06	64,64,64,64	0
33	MG	0	8049	1/1	0.93	0.08	85,85,85,85	0
35	NA	0	8553	1/1	0.93	0.18	63,63,63,63	0
35	NA	0	8554	1/1	0.93	0.10	63,63,63,63	0
35	NA	0	8530	1/1	0.93	0.12	56,56,56,56	0
35	NA	0	8534	1/1	0.93	0.07	61,61,61,61	0
37	SR	0	8983	1/1	0.93	0.10	150,150,150,150	0
37	SR	0	8986	1/1	0.93	0.09	131,131,131,131	0
35	NA	0	8557	1/1	0.93	0.22	67,67,67,67	0
37	SR	0	8990	1/1	0.93	0.10	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	C	8503	1/1	0.93	0.07	34,34,34,34	0
33	MG	0	8053	1/1	0.93	0.23	64,64,64,64	0
33	MG	0	8078	1/1	0.93	0.14	64,64,64,64	0
35	NA	P	8540	1/1	0.93	0.10	73,73,73,73	0
35	NA	0	8501	1/1	0.93	0.10	46,46,46,46	0
33	MG	0	8056	1/1	0.93	0.14	83,83,83,83	0
35	NA	0	8505	1/1	0.93	0.13	51,51,51,51	0
35	NA	0	8520	1/1	0.93	0.24	61,61,61,61	0
36	CL	I	8802	1/1	0.93	0.10	71,71,71,71	0
33	MG	A	8050	1/1	0.93	0.12	93,93,93,93	0
37	SR	0	8951	1/1	0.93	0.14	113,113,113,113	0
33	MG	0	8082	1/1	0.93	0.12	78,78,78,78	0
37	SR	0	8985	1/1	0.94	0.25	116,116,116,116	0
35	NA	0	8506	1/1	0.94	0.14	66,66,66,66	0
33	MG	0	8024	1/1	0.94	0.14	81,81,81,81	0
37	SR	0	8943	1/1	0.94	0.11	110,110,110,110	0
37	SR	0	8991	1/1	0.94	0.11	150,150,150,150	0
33	MG	0	8089	1/1	0.94	0.08	49,49,49,49	0
33	MG	0	8077	1/1	0.94	0.08	47,47,47,47	0
33	MG	0	8068	1/1	0.94	0.15	86,86,86,86	0
37	SR	0	8997	1/1	0.94	0.09	142,142,142,142	0
35	NA	0	8546	1/1	0.94	0.20	77,77,77,77	0
37	SR	0	8966	1/1	0.94	0.08	98,98,98,98	0
35	NA	0	8526	1/1	0.94	0.11	50,50,50,50	0
35	NA	0	8563	1/1	0.94	0.30	69,69,69,69	0
35	NA	0	8528	1/1	0.94	0.10	57,57,57,57	0
33	MG	0	8019	1/1	0.94	0.12	37,37,37,37	0
37	SR	A	8977	1/1	0.94	0.12	99,99,99,99	0
33	MG	0	8046	1/1	0.94	0.09	65,65,65,65	0
35	NA	0	8504	1/1	0.94	0.10	42,42,42,42	0
33	MG	0	8052	1/1	0.94	0.14	49,49,49,49	0
36	CL	I	8821	1/1	0.95	0.10	67,67,67,67	0
36	CL	M	8807	1/1	0.95	0.07	71,71,71,71	0
36	CL	2	8804	1/1	0.95	0.16	88,88,88,88	0
37	SR	0	8908	1/1	0.95	0.09	90,90,90,90	0
37	SR	0	8939	1/1	0.95	0.08	100,100,100,100	0
33	MG	0	8059	1/1	0.95	0.05	56,56,56,56	0
33	MG	0	8020	1/1	0.95	0.15	52,52,52,52	0
35	NA	Q	8532	1/1	0.95	0.12	49,49,49,49	0
37	SR	0	8993	1/1	0.95	0.10	139,139,139,139	0
37	SR	0	8955	1/1	0.95	0.09	122,122,122,122	0
37	SR	0	8956	1/1	0.95	0.07	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	SR	0	8957	1/1	0.95	0.08	120,120,120,120	0
37	SR	0	8958	1/1	0.95	0.06	96,96,96,96	0
37	SR	0	8998	1/1	0.95	0.13	133,133,133,133	0
35	NA	0	8566	1/1	0.95	0.26	54,54,54,54	0
33	MG	0	8064	1/1	0.95	0.06	69,69,69,69	0
37	SR	0	8964	1/1	0.95	0.10	101,101,101,101	0
36	CL	0	8805	1/1	0.95	0.10	65,65,65,65	0
36	CL	0	8811	1/1	0.95	0.12	83,83,83,83	0
37	SR	9	8980	1/1	0.95	0.07	137,137,137,137	0
37	SR	0	8973	1/1	0.95	0.08	101,101,101,101	0
37	SR	0	8974	1/1	0.95	0.12	134,134,134,134	0
33	MG	0	8045	1/1	0.95	0.15	71,71,71,71	0
33	MG	0	8031	1/1	0.95	0.06	57,57,57,57	0
35	NA	0	8519	1/1	0.95	0.10	49,49,49,49	0
35	NA	0	8547	1/1	0.96	0.16	75,75,75,75	0
33	MG	0	8067	1/1	0.96	0.06	58,58,58,58	0
37	SR	0	8984	1/1	0.96	0.06	109,109,109,109	0
37	SR	0	8946	1/1	0.96	0.07	99,99,99,99	0
37	SR	0	8947	1/1	0.96	0.13	109,109,109,109	0
37	SR	0	8988	1/1	0.96	0.09	125,125,125,125	0
37	SR	0	8948	1/1	0.96	0.08	102,102,102,102	0
35	NA	B	8552	1/1	0.96	0.19	59,59,59,59	0
36	CL	0	8815	1/1	0.96	0.15	61,61,61,61	0
36	CL	0	8816	1/1	0.96	0.12	77,77,77,77	0
36	CL	A	8809	1/1	0.96	0.08	65,65,65,65	0
35	NA	0	8537	1/1	0.96	0.05	43,43,43,43	0
34	K	0	8402	1/1	0.96	0.07	70,70,70,70	0
35	NA	0	8560	1/1	0.96	0.23	88,88,88,88	0
35	NA	0	8513	1/1	0.96	0.09	50,50,50,50	0
37	SR	0	8965	1/1	0.96	0.09	108,108,108,108	0
33	MG	0	8032	1/1	0.96	0.07	56,56,56,56	0
37	SR	0	8967	1/1	0.96	0.11	113,113,113,113	0
37	SR	0	8969	1/1	0.96	0.24	127,127,127,127	0
33	MG	0	8080	1/1	0.96	0.09	78,78,78,78	0
37	SR	0	8915	1/1	0.96	0.07	93,93,93,93	0
37	SR	0	8919	1/1	0.96	0.08	131,131,131,131	0
37	SR	0	8924	1/1	0.96	0.15	112,112,112,112	0
37	SR	B	8950	1/1	0.96	0.06	106,106,106,106	0
37	SR	0	8931	1/1	0.96	0.11	94,94,94,94	0
37	SR	F	9005	1/1	0.96	0.12	116,116,116,116	0
37	SR	R	8961	1/1	0.96	0.08	122,122,122,122	0
37	SR	0	8938	1/1	0.96	0.15	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8062	1/1	0.96	0.14	61,61,61,61	0
33	MG	0	8070	1/1	0.97	0.04	62,62,62,62	0
36	CL	0	8803	1/1	0.97	0.12	61,61,61,61	0
33	MG	0	8091	1/1	0.97	0.06	54,54,54,54	0
37	SR	0	8918	1/1	0.97	0.09	59,59,59,59	0
37	SR	0	8992	1/1	0.97	0.12	115,115,115,115	0
37	SR	0	8962	1/1	0.97	0.06	108,108,108,108	0
37	SR	0	8963	1/1	0.97	0.08	83,83,83,83	0
35	NA	0	8521	1/1	0.97	0.15	110,110,110,110	0
37	SR	0	8920	1/1	0.97	0.06	96,96,96,96	0
33	MG	0	8008	1/1	0.97	0.06	34,34,34,34	0
33	MG	0	8006	1/1	0.97	0.18	27,27,27,27	0
37	SR	0	8999	1/1	0.97	0.06	88,88,88,88	0
37	SR	0	8933	1/1	0.97	0.08	103,103,103,103	0
37	SR	0	8970	1/1	0.97	0.08	80,80,80,80	0
37	SR	0	8937	1/1	0.97	0.09	80,80,80,80	0
35	NA	0	8524	1/1	0.97	0.09	56,56,56,56	0
36	CL	0	8817	1/1	0.97	0.05	56,56,56,56	0
37	SR	9	8968	1/1	0.97	0.08	132,132,132,132	0
33	MG	0	8083	1/1	0.97	0.05	55,55,55,55	0
33	MG	0	8022	1/1	0.97	0.13	46,46,46,46	0
37	SR	A	8929	1/1	0.97	0.10	103,103,103,103	0
36	CL	I	8801	1/1	0.97	0.12	61,61,61,61	0
33	MG	0	8018	1/1	0.97	0.21	44,44,44,44	0
33	MG	0	8027	1/1	0.97	0.07	53,53,53,53	0
37	SR	0	8949	1/1	0.97	0.06	80,80,80,80	0
36	CL	K	8810	1/1	0.97	0.09	55,55,55,55	0
33	MG	X	8086	1/1	0.97	0.09	51,51,51,51	0
36	CL	X	8820	1/1	0.97	0.04	49,49,49,49	0
37	SR	0	8945	1/1	0.98	0.07	92,92,92,92	0
33	MG	0	8072	1/1	0.98	0.04	47,47,47,47	0
36	CL	L	8818	1/1	0.98	0.04	48,48,48,48	0
33	MG	0	8093	1/1	0.98	0.03	41,41,41,41	0
36	CL	N	8808	1/1	0.98	0.06	76,76,76,76	0
36	CL	Q	8806	1/1	0.98	0.05	49,49,49,49	0
37	SR	0	8953	1/1	0.98	0.07	96,96,96,96	0
37	SR	0	8954	1/1	0.98	0.07	94,94,94,94	0
33	MG	0	8011	1/1	0.98	0.04	33,33,33,33	0
35	NA	0	8515	1/1	0.98	0.05	34,34,34,34	0
37	SR	0	8901	1/1	0.98	0.09	75,75,75,75	0
37	SR	0	8907	1/1	0.98	0.05	63,63,63,63	0
35	NA	0	8527	1/1	0.98	0.06	51,51,51,51	0

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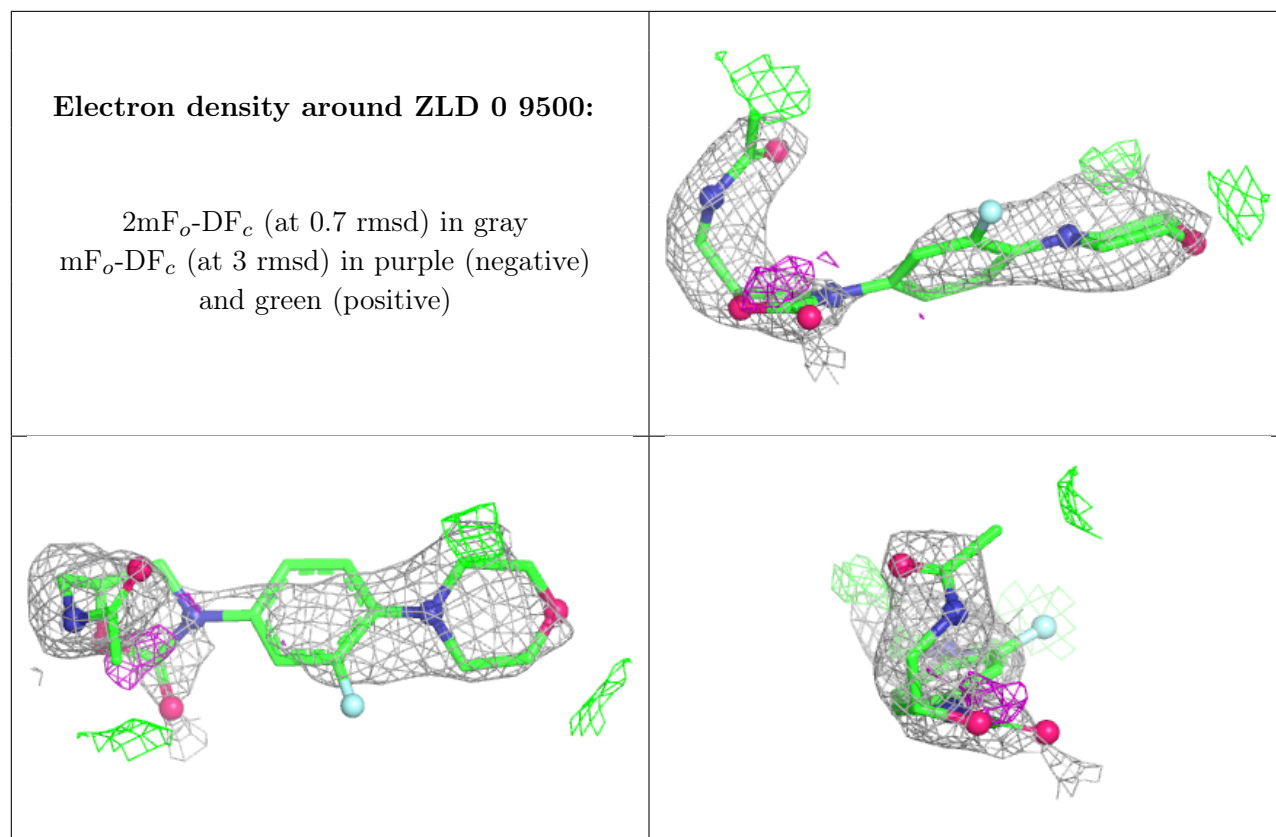
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	8910	1/1	0.98	0.06	59,59,59,59	0
33	MG	0	8075	1/1	0.98	0.04	50,50,50,50	0
37	SR	0	9000	1/1	0.98	0.05	111,111,111,111	0
36	CL	0	8814	1/1	0.98	0.11	57,57,57,57	0
33	MG	0	8084	1/1	0.98	0.12	66,66,66,66	0
33	MG	0	8026	1/1	0.98	0.03	61,61,61,61	0
37	SR	0	8921	1/1	0.98	0.10	70,70,70,70	0
37	SR	0	8923	1/1	0.98	0.05	83,83,83,83	0
37	SR	0	9008	1/1	0.98	0.07	91,91,91,91	0
35	NA	0	8531	1/1	0.98	0.03	41,41,41,41	0
37	SR	0	8926	1/1	0.98	0.09	82,82,82,82	0
37	SR	0	8927	1/1	0.98	0.09	90,90,90,90	0
37	SR	0	8928	1/1	0.98	0.08	91,91,91,91	0
37	SR	A	8930	1/1	0.98	0.10	81,81,81,81	0
36	CL	0	8822	1/1	0.98	0.23	69,69,69,69	0
33	MG	0	8055	1/1	0.98	0.11	40,40,40,40	0
35	NA	K	8568	1/1	0.98	0.09	57,57,57,57	0
33	MG	0	8034	1/1	0.98	0.04	44,44,44,44	0
37	SR	H	8972	1/1	0.98	0.16	148,148,148,148	0
33	MG	0	8079	1/1	0.98	0.06	72,72,72,72	0
37	SR	S	8911	1/1	0.98	0.06	72,72,72,72	0
37	SR	Z	8952	1/1	0.98	0.04	71,71,71,71	0
33	MG	0	8015	1/1	0.98	0.05	62,62,62,62	0
36	CL	J	8812	1/1	0.98	0.10	54,54,54,54	0
37	SR	0	8914	1/1	0.99	0.11	84,84,84,84	0
37	SR	0	8940	1/1	0.99	0.04	77,77,77,77	0
37	SR	0	8942	1/1	0.99	0.05	89,89,89,89	0
33	MG	0	8003	1/1	0.99	0.03	35,35,35,35	0
37	SR	0	8916	1/1	0.99	0.06	85,85,85,85	0
37	SR	0	8917	1/1	0.99	0.09	81,81,81,81	0
33	MG	0	8088	1/1	0.99	0.07	57,57,57,57	0
33	MG	0	8023	1/1	0.99	0.02	39,39,39,39	0
37	SR	0	8978	1/1	0.99	0.03	85,85,85,85	0
33	MG	0	8012	1/1	0.99	0.03	30,30,30,30	0
33	MG	0	8025	1/1	0.99	0.06	43,43,43,43	0
37	SR	0	8922	1/1	0.99	0.04	77,77,77,77	0
33	MG	0	8041	1/1	0.99	0.04	44,44,44,44	0
37	SR	0	8902	1/1	0.99	0.10	49,49,49,49	0
37	SR	0	8925	1/1	0.99	0.13	79,79,79,79	0
37	SR	0	8904	1/1	0.99	0.06	52,52,52,52	0
37	SR	0	8905	1/1	0.99	0.13	59,59,59,59	0
37	SR	0	8906	1/1	0.99	0.08	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8009	1/1	0.99	0.16	23,23,23,23	0
33	MG	0	8004	1/1	0.99	0.05	36,36,36,36	0
37	SR	Q	8912	1/1	0.99	0.07	75,75,75,75	0
37	SR	0	8934	1/1	0.99	0.07	90,90,90,90	0
37	SR	0	8935	1/1	0.99	0.07	80,80,80,80	0
37	SR	Z	8913	1/1	0.99	0.04	52,52,52,52	0
37	SR	0	8936	1/1	0.99	0.05	70,70,70,70	0
37	SR	2	8932	1/1	0.99	0.03	76,76,76,76	0
37	SR	0	8909	1/1	0.99	0.07	74,74,74,74	0
38	CD	Z	8702	1/1	0.99	0.03	67,67,67,67	0
38	CD	2	8704	1/1	0.99	0.02	65,65,65,65	0
33	MG	0	8021	1/1	0.99	0.03	38,38,38,38	0
33	MG	0	8058	1/1	1.00	0.11	28,28,28,28	0
33	MG	0	8014	1/1	1.00	0.03	37,37,37,37	0
37	SR	0	8941	1/1	1.00	0.07	81,81,81,81	0
33	MG	J	8054	1/1	1.00	0.04	37,37,37,37	0
33	MG	0	8061	1/1	1.00	0.06	36,36,36,36	0
38	CD	T	8701	1/1	1.00	0.01	64,64,64,64	0
38	CD	Y	8703	1/1	1.00	0.02	59,59,59,59	0
33	MG	0	8005	1/1	1.00	0.02	39,39,39,39	0
37	SR	0	8903	1/1	1.00	0.07	59,59,59,59	0
33	MG	0	8028	1/1	1.00	0.09	29,29,29,29	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.