



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 01:18 pm BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

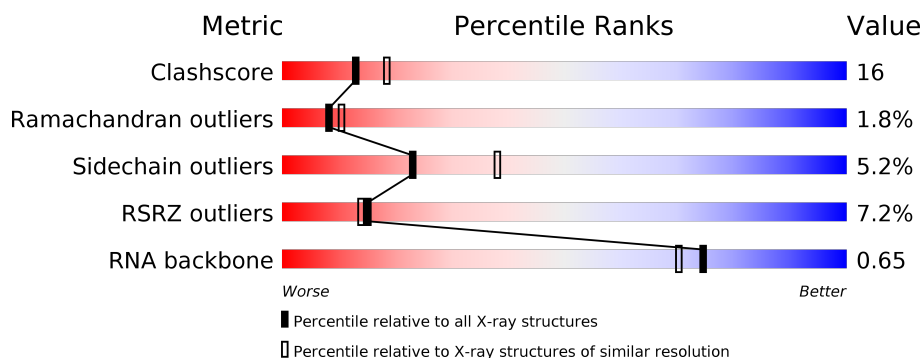
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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 on 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	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>30%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>34%</div> <div>11%</div> </div> </div>
3	4	5	<div> <div>80%</div> <div>20%</div> </div>
4	A	240	<div> <div>9%</div> <div> <div></div> <div>53%</div> <div>41%</div> <div>5%</div> </div> </div>
5	B	338	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>41%</div> <div>5%</div> </div> </div>
6	C	246	<div> <div>%</div> <div> <div></div> <div>62%</div> <div>33%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	

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Mol	Chain	Length	Quality of chain
32	I	162	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8024	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8108	-	-	-	X
35	NA	0	9102	-	-	-	X
35	NA	0	9132	-	-	-	X
35	NA	0	9172	-	-	-	X
35	NA	0	9184	-	-	-	X
37	SR	0	9482	-	-	-	X
37	SR	0	9601	-	-	-	X
37	SR	B	9521	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98979 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	62	Total	Na	0	0
			62	62		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	D	1	Total	Na	0	0
			1	1		
35	B	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	C	1	Total 1	Na 1	0	0
35	3	1	Total 1	Na 1	0	0
35	T	1	Total 1	Na 1	0	0
35	R	2	Total 2	Na 2	0	0
35	9	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

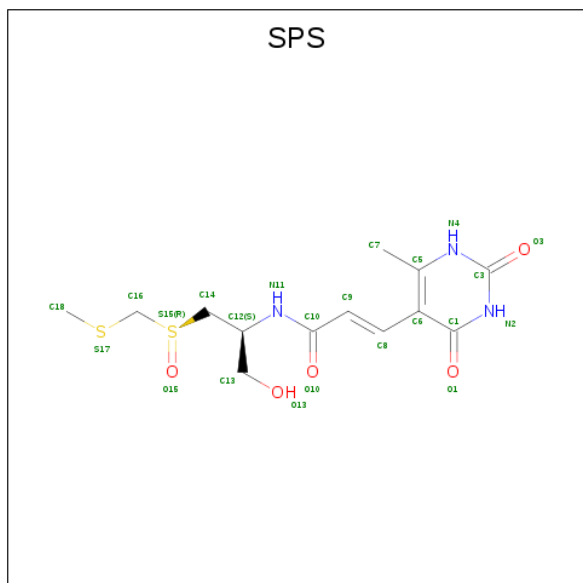
- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

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

- Molecule 38 is SPARSOMYCIN (three-letter code: SPS) (formula: C₁₃H₁₉N₃O₅S₂).



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

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 40 is water.

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

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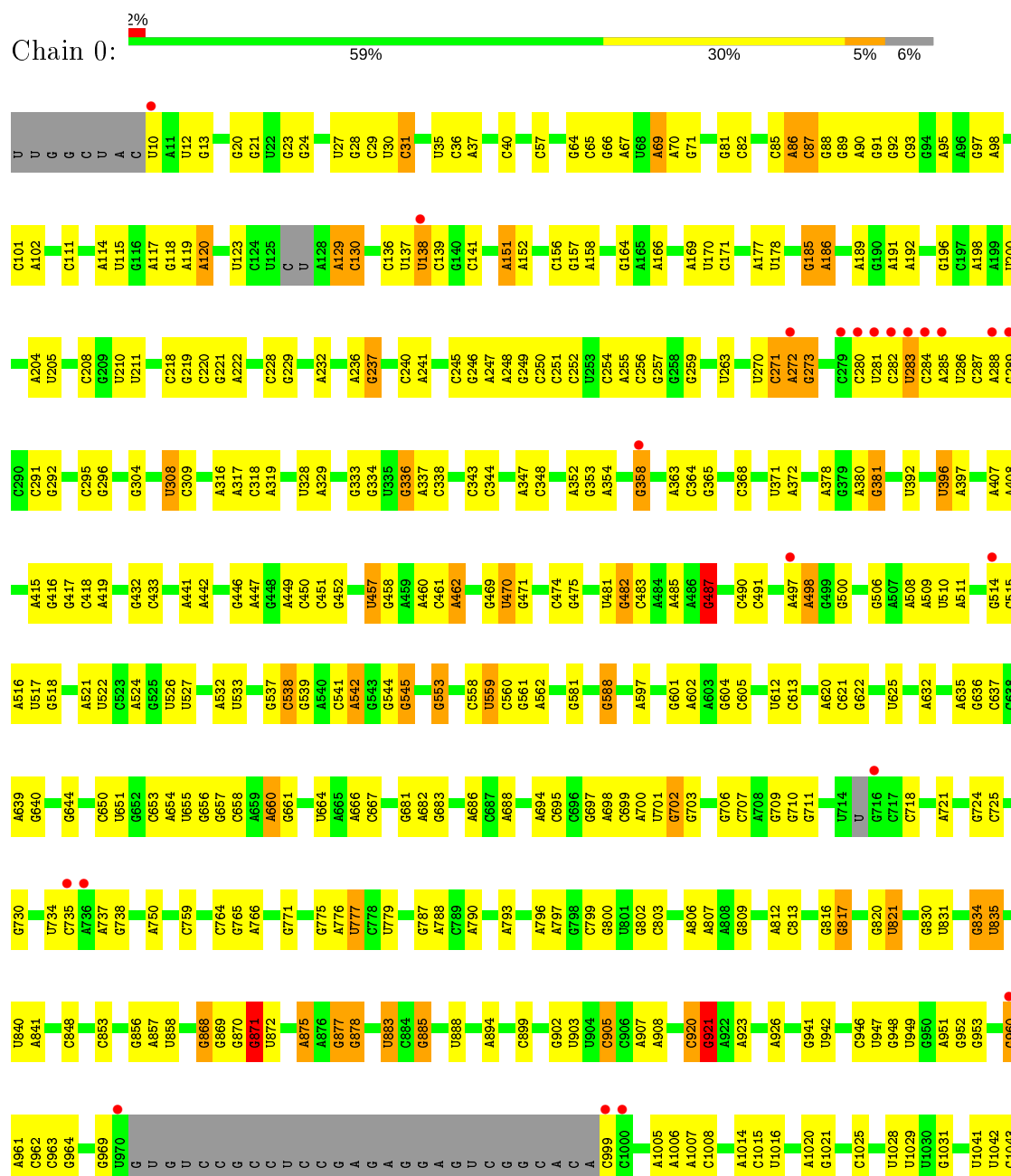
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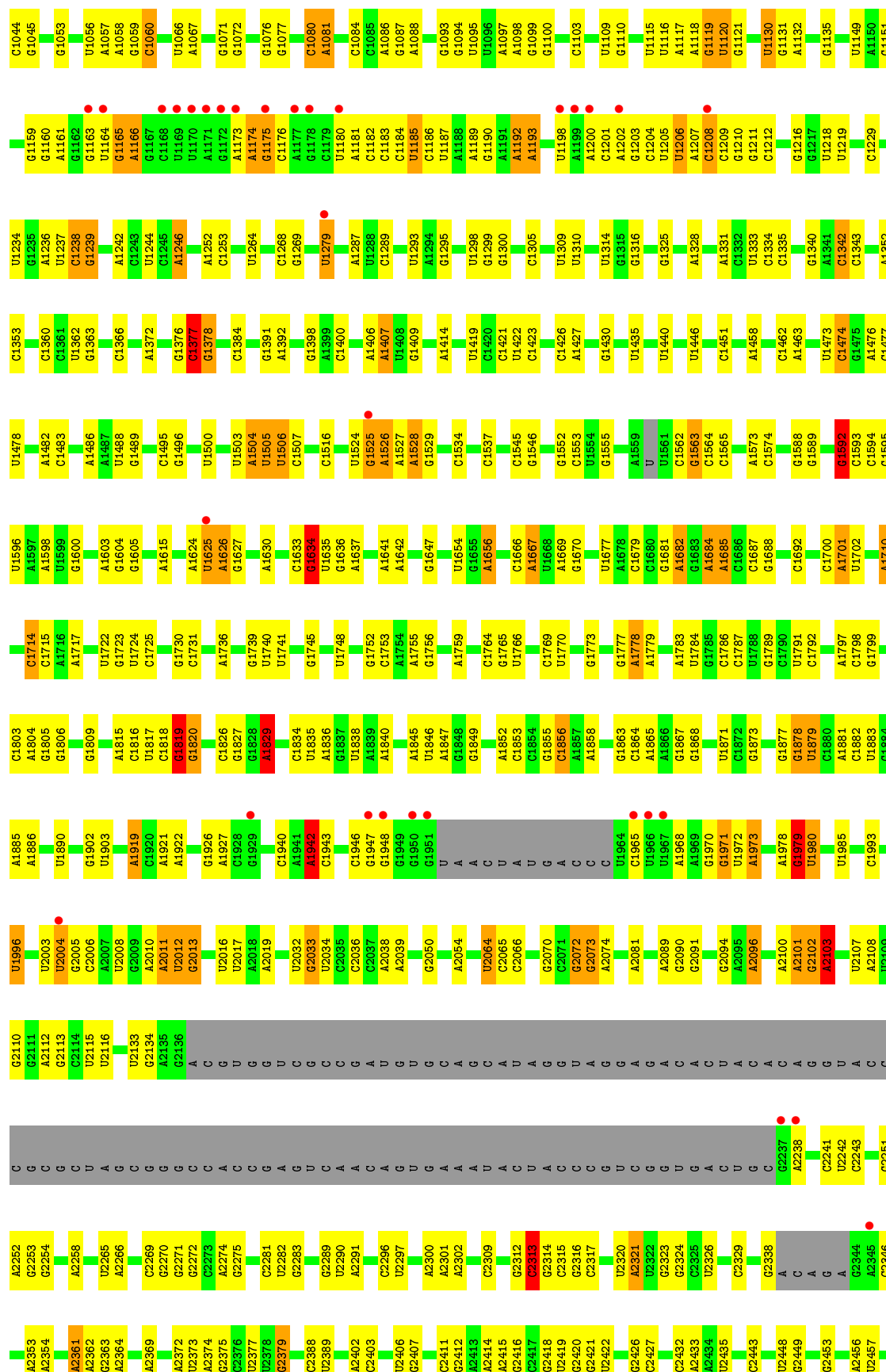
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	K	61	Total 61	O 61	0	0
40	L	93	Total 93	O 93	0	0
40	M	133	Total 133	O 133	0	0
40	N	66	Total 66	O 66	0	0
40	O	42	Total 42	O 42	0	0
40	P	68	Total 68	O 68	0	0
40	Q	53	Total 53	O 53	0	0
40	R	93	Total 93	O 93	0	0
40	S	35	Total 35	O 35	0	0
40	T	40	Total 40	O 40	0	0
40	U	28	Total 28	O 28	0	0
40	V	13	Total 13	O 13	0	0
40	W	70	Total 70	O 70	0	0
40	X	23	Total 23	O 23	0	0
40	Y	93	Total 93	O 93	0	0
40	Z	30	Total 30	O 30	0	0
40	1	60	Total 60	O 60	0	0
40	2	46	Total 46	O 46	0	0
40	3	70	Total 70	O 70	0	0
40	I	9	Total 9	O 9	0	0

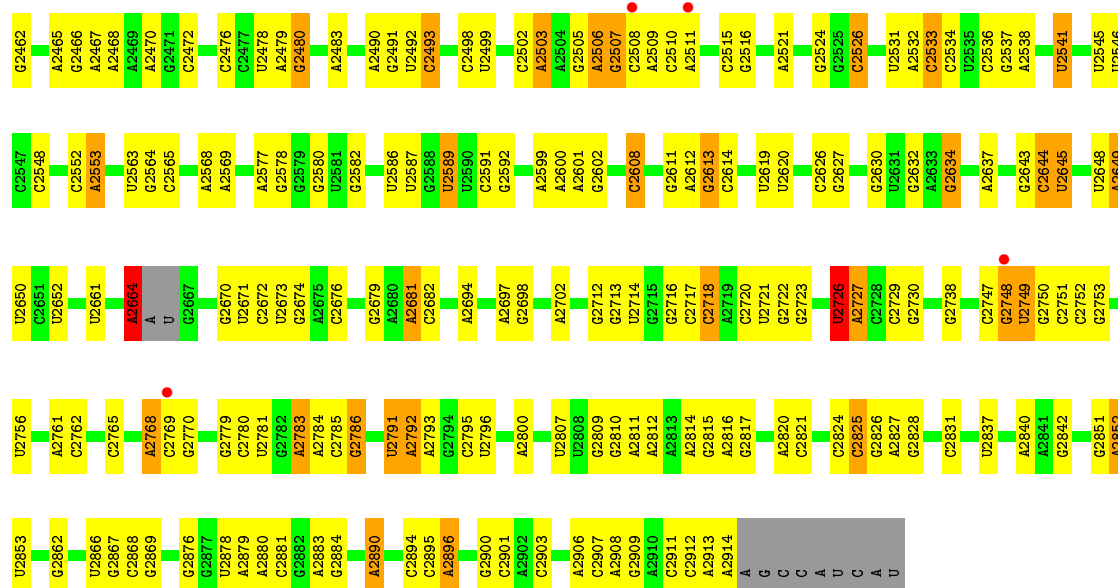
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal rna



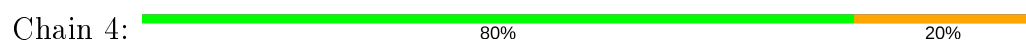




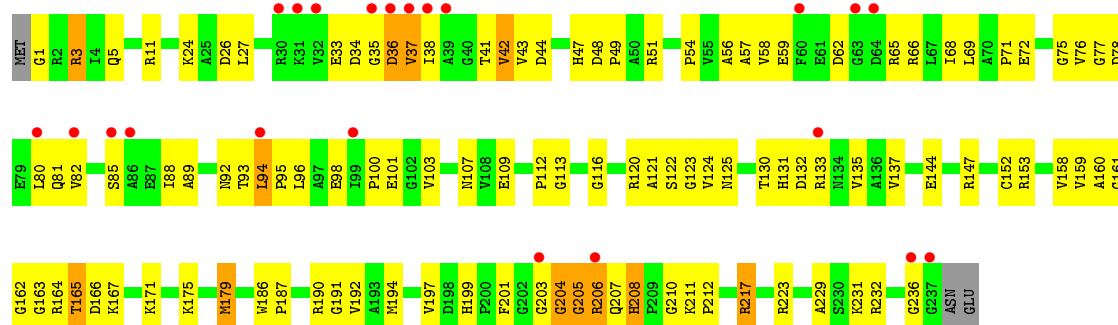
• Molecule 2: 5S ribosomal RNA



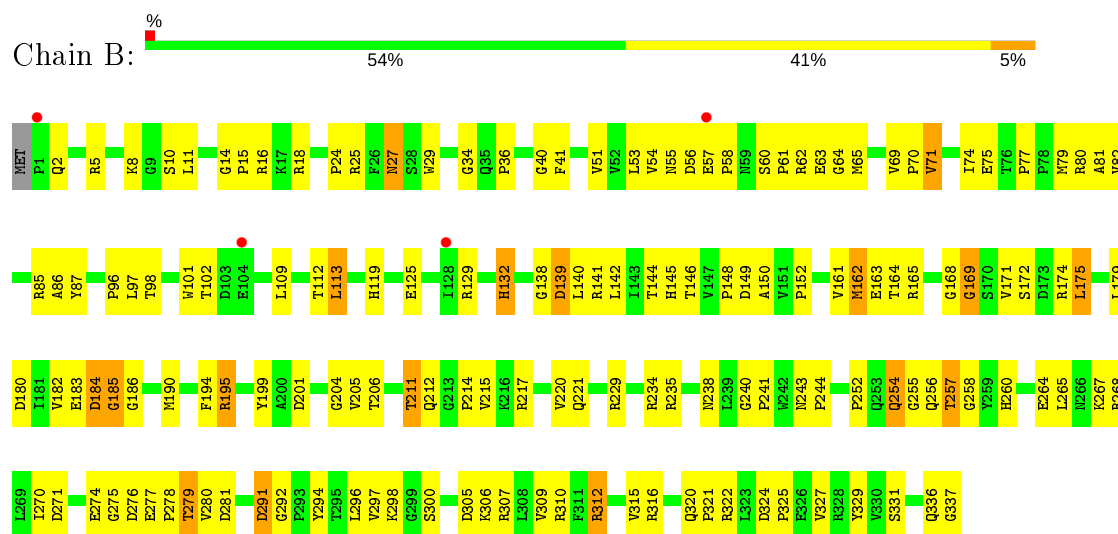
• Molecule 3: 5'-R(*CP*CP*AP*(PHE)*(ACA))-3'



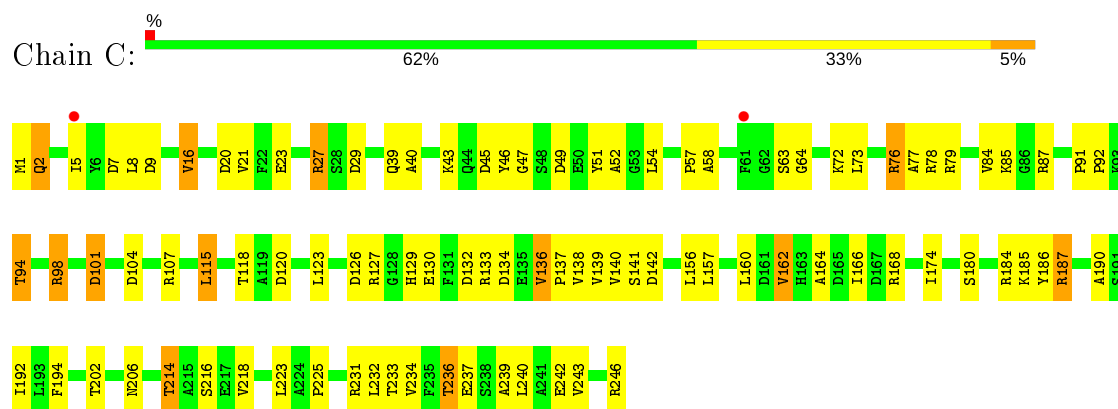
• Molecule 4: 50S ribosomal protein L2P



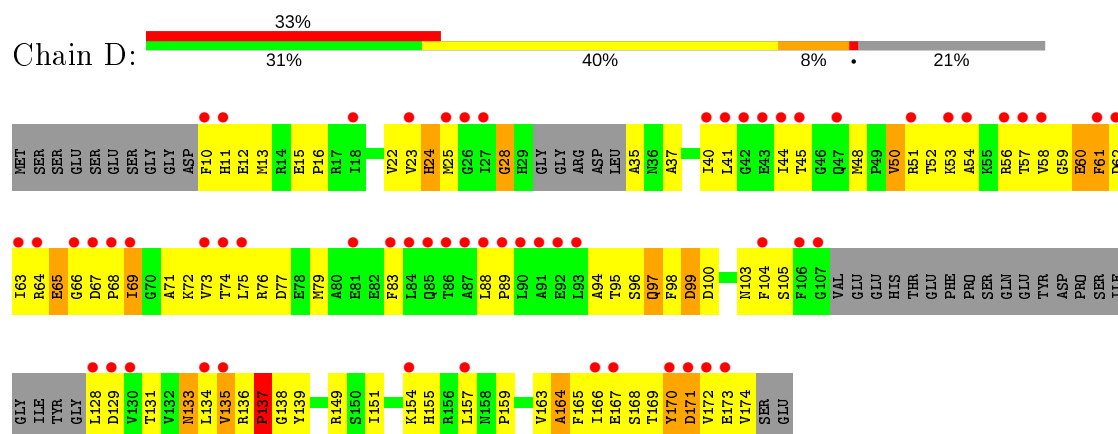
- Molecule 5: 50S ribosomal protein L3P



- Molecule 6: 50S ribosomal protein L4E

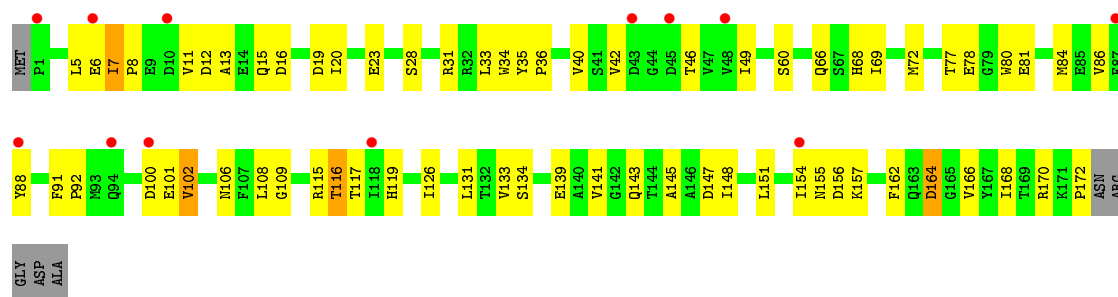


- Molecule 7: 50S ribosomal protein L5P

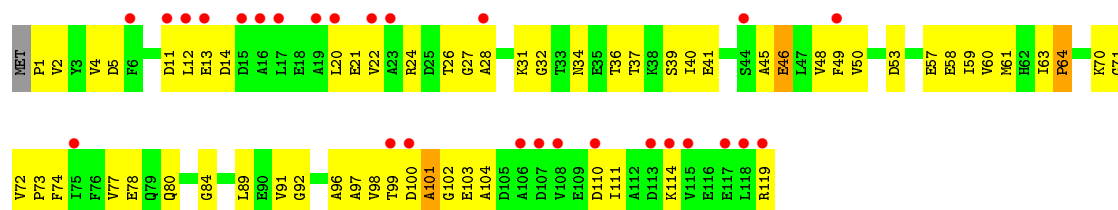


- Molecule 8: 50S ribosomal protein L6P

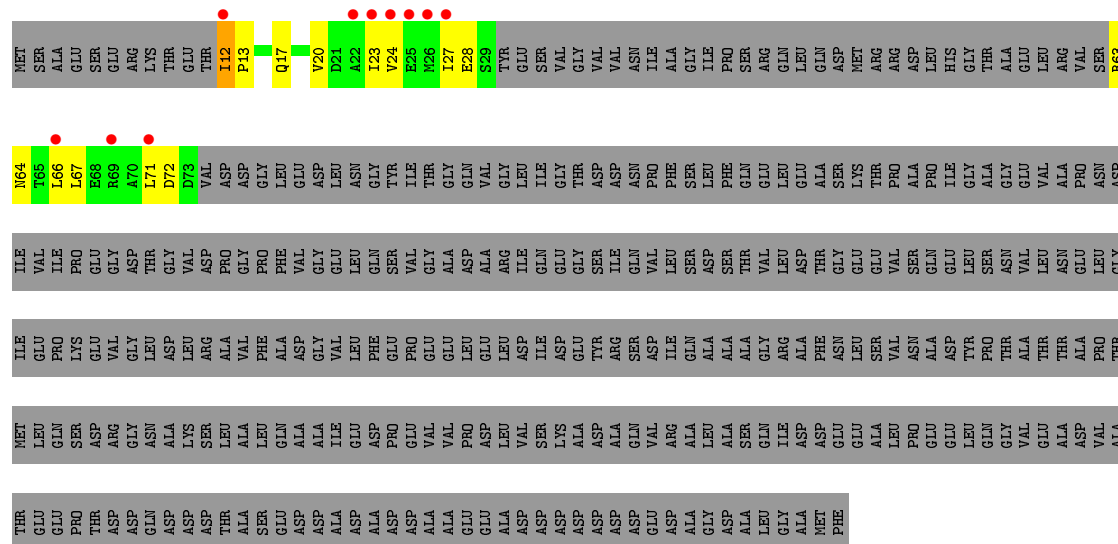




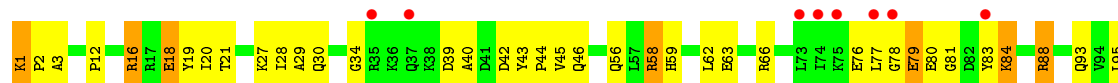
- Molecule 9: 50S ribosomal protein L7AE

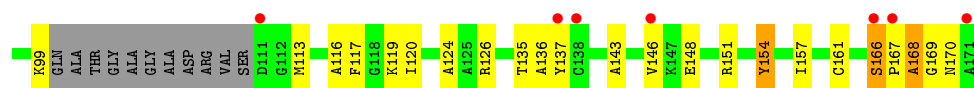


- Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

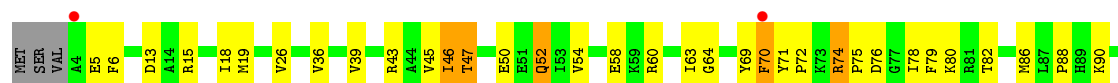


- Molecule 11: 50S RIBOSOMAL PROTEIN L10E

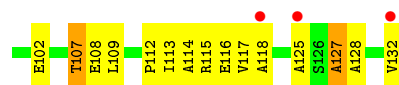
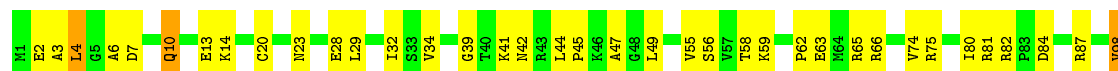




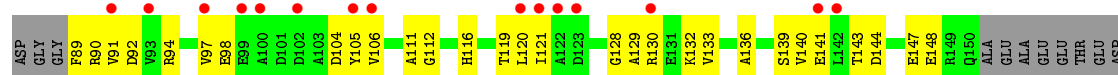
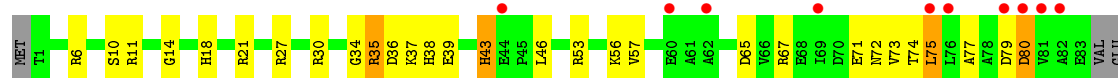
• Molecule 12: 50S ribosomal protein L13P



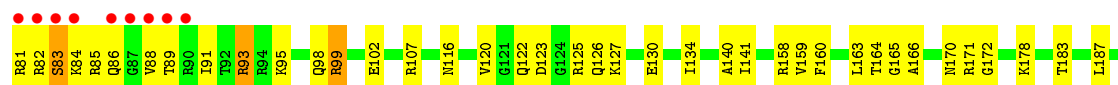
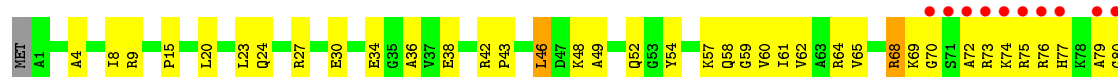
• Molecule 13: 50S ribosomal protein L14P



• Molecule 14: 50S ribosomal protein L15P

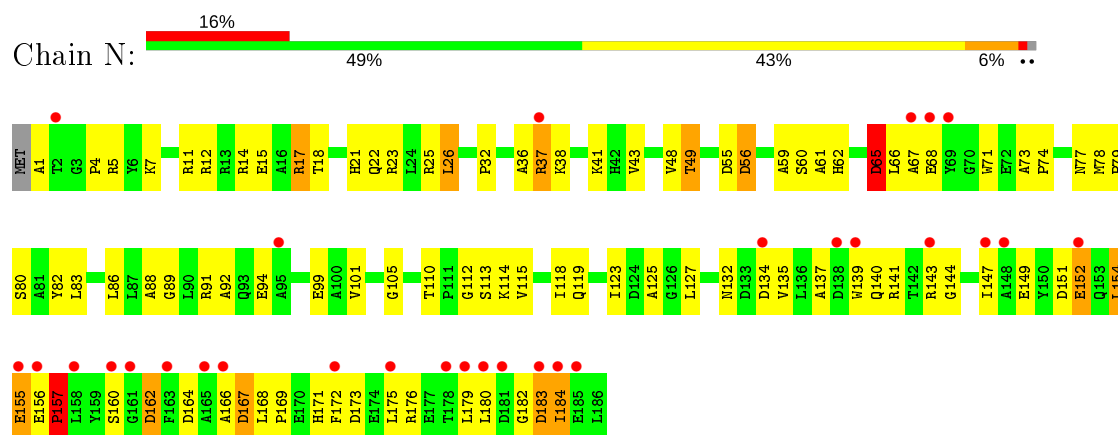


• Molecule 15: 50S Ribosomal Protein L15E

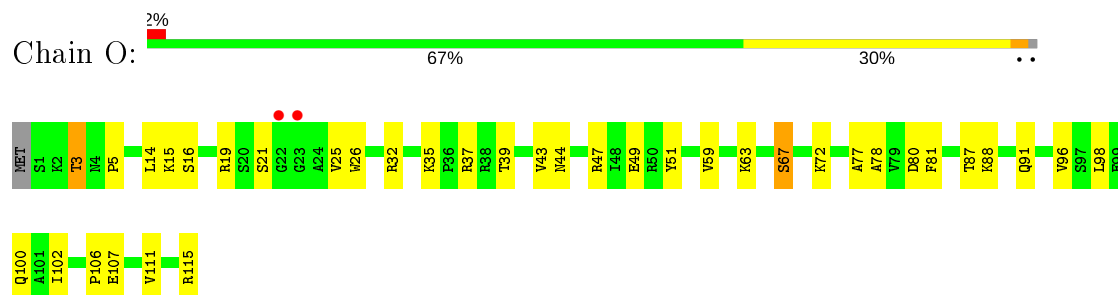


K193
A194

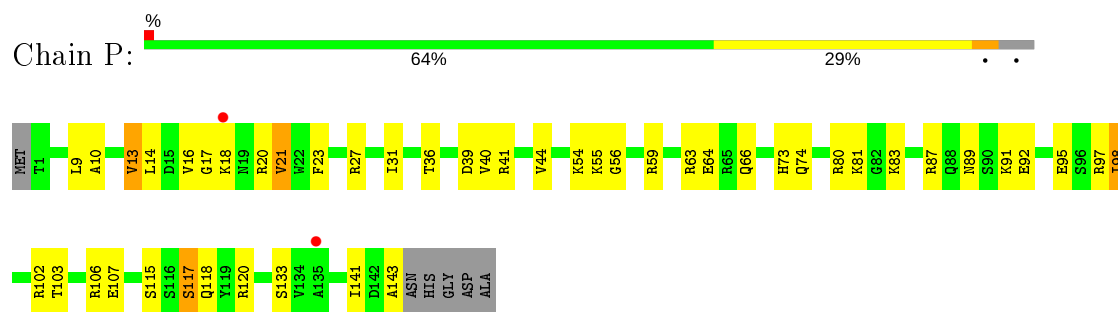
- Molecule 16: 50S ribosomal protein L18P



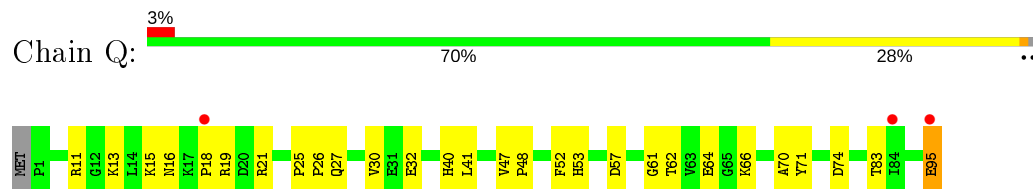
- Molecule 17: 50S ribosomal protein L18e



- Molecule 18: 50S ribosomal protein L19E

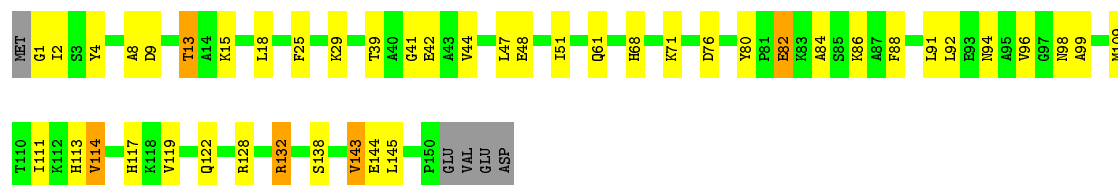


- Molecule 19: 50S ribosomal protein L21e

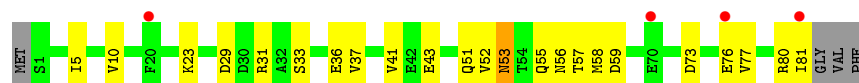


- Molecule 20: 50S ribosomal protein L22P

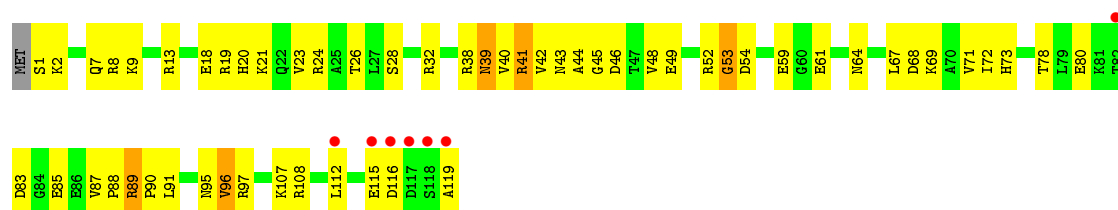




- Molecule 21: 50S ribosomal protein L23P



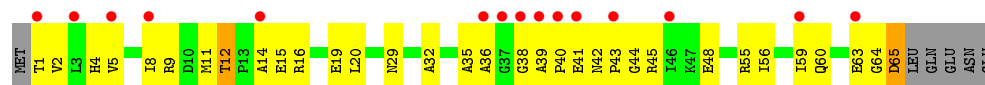
- Molecule 22: 50S ribosomal protein L24P



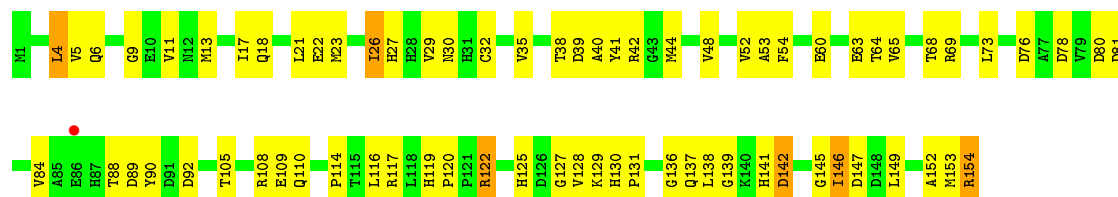
- Molecule 23: 50S ribosomal protein L24E



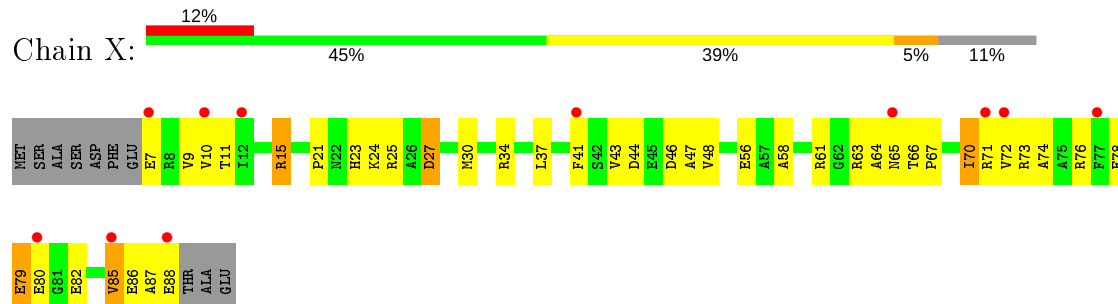
- Molecule 24: 50S ribosomal protein L29P



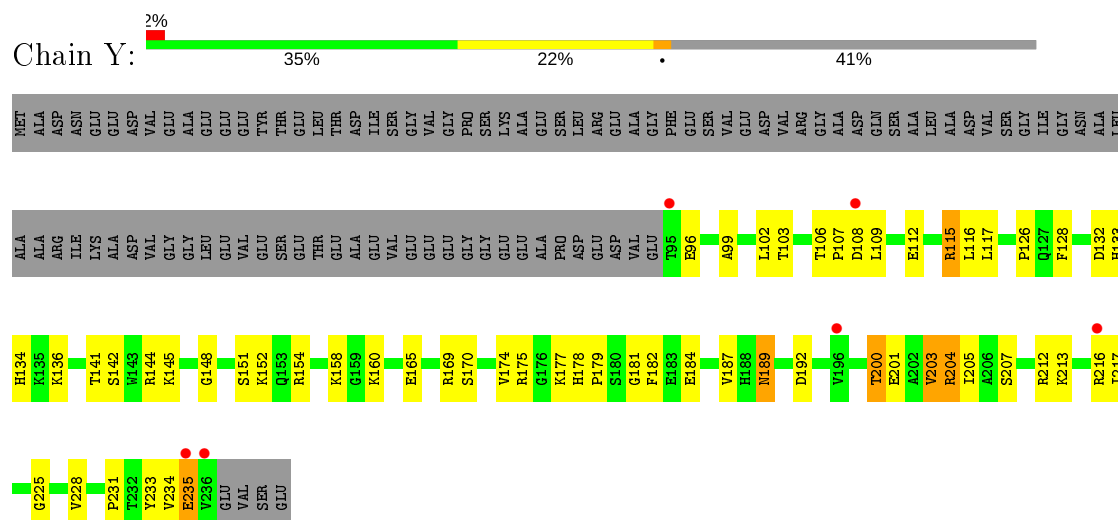
- Molecule 25: 50S ribosomal protein L30P



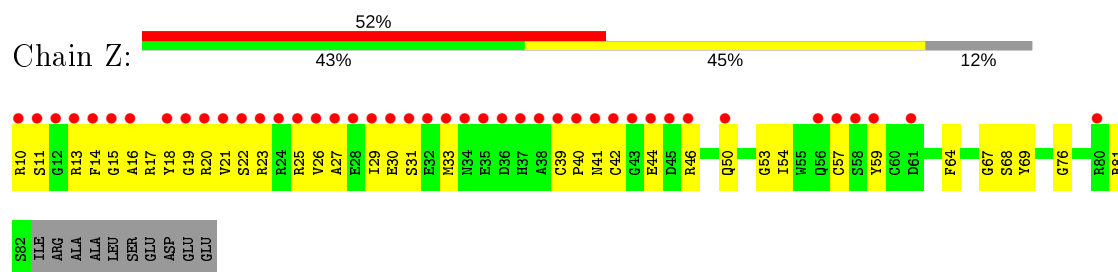
- Molecule 26: 50S ribosomal protein L31e



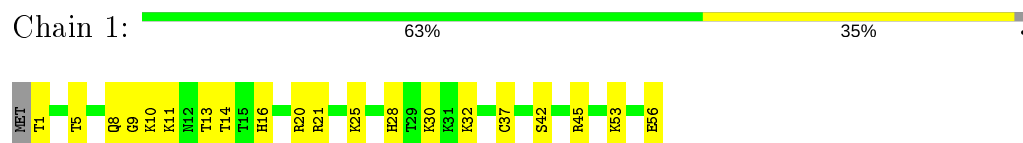
- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: 50S ribosomal protein L37Ae



- Molecule 29: 50S ribosomal protein L37e

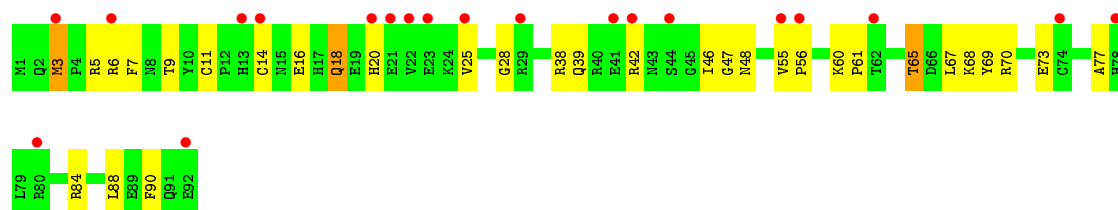


- Molecule 30: 50S ribosomal protein L39e

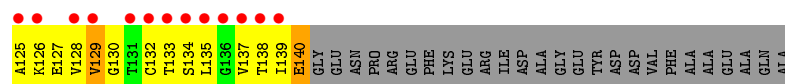
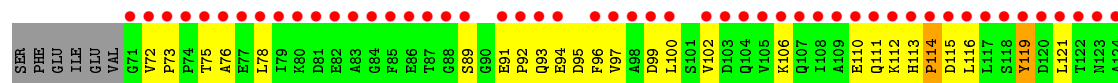
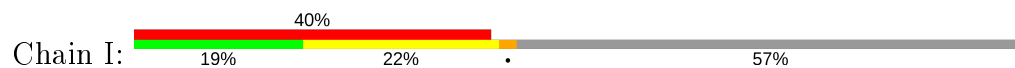




- Molecule 31: 50S ribosomal protein L44E



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.82Å 298.60Å 574.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.68 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.40) 89.6 (49.68-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.59 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.255 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	98979	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.42	0/65959	0.71	23/102870 (0.0%)
2	9	0.39	0/2905	0.73	1/4528 (0.0%)
3	4	0.50	0/76	0.74	0/112
4	A	0.34	0/1786	0.64	0/2408
5	B	0.36	0/2690	0.67	0/3652
6	C	0.39	0/1884	0.66	0/2551
7	D	0.34	0/1111	0.57	0/1498
8	E	0.37	0/1382	0.61	0/1880
9	F	0.36	0/901	0.57	0/1224
10	G	0.33	0/241	0.49	0/324
11	H	0.37	0/1287	0.66	0/1725
12	J	0.38	0/1136	0.64	0/1530
13	K	0.38	0/1001	0.68	0/1347
14	L	0.36	0/1130	0.66	0/1509
15	M	0.38	0/1584	0.61	0/2119
16	N	0.32	0/1474	0.63	0/1999
17	O	0.35	0/874	0.62	0/1181
18	P	0.36	0/1147	0.59	0/1528
19	Q	0.36	0/749	0.68	0/1005
20	R	0.37	0/1172	0.68	0/1578
21	S	0.37	0/648	0.60	0/875
22	T	0.34	0/958	0.63	0/1289
23	U	0.38	0/417	0.56	0/562
24	V	0.31	0/502	0.56	0/675
25	W	0.37	0/1219	0.64	0/1655
26	X	0.38	0/664	0.63	0/895
27	Y	0.39	0/1146	0.68	0/1536
28	Z	0.36	0/589	0.58	0/787
29	1	0.45	0/438	0.68	0/578
30	2	0.38	0/401	0.63	0/529
31	3	0.36	0/771	0.55	0/1024
32	I	0.32	0/526	0.55	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.40	0/98768	0.69	24/147689 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	44
2	9	0	1
All	All	1	45

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.83	131.13	109.50
1	0	871	G	C5'-C4'-O4'	-7.12	100.56	109.10
2	9	3039	U	N1-C1'-C2'	7.04	123.15	114.00
1	0	1979	G	C2'-C3'-O3'	6.99	124.88	113.70
1	0	883	U	N1-C1'-C2'	6.65	122.64	114.00
1	0	1504	A	C1'-O4'-C4'	-6.58	104.64	109.90
1	0	1942	A	C5'-C4'-C3'	6.44	126.30	116.00
1	0	1592	G	N9-C1'-C2'	6.42	122.34	114.00
1	0	1819	G	C5'-C4'-C3'	6.38	126.21	116.00
1	0	2313	C	C5'-C4'-O4'	6.37	116.74	109.10
1	0	1120	U	C5'-C4'-C3'	-6.14	106.18	116.00
1	0	1504	A	N9-C1'-C2'	5.87	121.63	114.00
1	0	841	A	C1'-O4'-C4'	-5.68	105.35	109.90
1	0	777	U	O4'-C1'-N1	5.54	112.63	108.20
1	0	921	G	N9-C1'-C2'	5.52	121.17	114.00
1	0	1615	A	C5'-C4'-C3'	5.48	124.77	116.00
1	0	1634	G	N9-C1'-C2'	5.47	121.12	114.00
1	0	2313	C	C5'-C4'-C3'	5.43	124.70	116.00
1	0	2726	U	N1-C1'-C2'	5.43	121.06	114.00
1	0	2664	A	N9-C1'-C2'	5.24	120.82	114.00
1	0	1819	G	C1'-O4'-C4'	-5.15	105.78	109.90
1	0	457	U	C1'-O4'-C4'	-5.10	105.82	109.90
1	0	2103	A	C5'-C4'-C3'	-5.06	107.91	116.00
1	0	2316	G	C5'-C4'-C3'	-5.03	107.96	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1080	C	Sidechain
1	0	1340	G	Sidechain
1	0	1376	G	Sidechain
1	0	1377	C	Sidechain
1	0	1430	G	Sidechain
1	0	1458	A	Sidechain
1	0	1592	G	Sidechain
1	0	1647	G	Sidechain
1	0	1714	C	Sidechain
1	0	1777	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1863	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1993	C	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2664	A	Sidechain
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	460	A	Sidechain
1	0	462	A	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	483	C	Sidechain

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Mol	Chain	Res	Type	Group
1	0	487	G	Sidechain
1	0	518	G	Sidechain
1	0	771	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
2	9	3065	A	Sidechain

5.2 Too-close contacts [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	59021	0	29809	911	0
2	9	2600	0	1326	55	0
3	4	74	0	44	1	0
4	A	1753	0	1765	133	0
5	B	2625	0	2531	156	0
6	C	1859	0	1816	118	0
7	D	1094	0	1085	94	0
8	E	1357	0	1266	67	0
9	F	890	0	843	62	0
10	G	240	0	231	14	0
11	H	1266	0	1268	62	0
12	J	1120	0	1098	62	0
13	K	992	0	1031	60	0
14	L	1118	0	1076	65	0
15	M	1560	0	1567	91	0
16	N	1445	0	1401	96	0
17	O	865	0	873	46	0
18	P	1136	0	1123	44	0
19	Q	735	0	729	23	0
20	R	1149	0	1122	47	0
21	S	641	0	605	24	0
22	T	950	0	923	73	0
23	U	410	0	364	24	0
24	V	499	0	511	38	0
25	W	1196	0	1137	99	0
26	X	654	0	653	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	Y	1130	0	1133	67	0
28	Z	578	0	542	42	0
29	1	431	0	426	27	0
30	2	396	0	413	29	0
31	3	755	0	728	43	0
32	I	519	0	500	40	0
33	0	86	0	0	0	0
33	4	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	62	0	0	0	0
35	3	1	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	9	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	97	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	9	3	0	0	0	0
37	A	4	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	4	23	0	19	3	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5630	0	0	126	0
40	1	60	0	0	3	0
40	2	46	0	0	1	0
40	3	70	0	0	6	0
40	4	1	0	0	0	0
40	9	130	0	0	5	0
40	A	132	0	0	13	0
40	B	137	0	0	22	0
40	C	175	0	0	20	0
40	D	43	0	0	8	0
40	E	42	0	0	2	0
40	F	25	0	0	4	0
40	G	16	0	0	2	0
40	H	77	0	0	4	0
40	I	9	0	0	0	0
40	J	52	0	0	1	0
40	K	61	0	0	7	1
40	L	93	0	0	11	0
40	M	133	0	0	8	0
40	N	66	0	0	5	0
40	O	42	0	0	5	0
40	P	68	0	0	3	0
40	Q	53	0	0	2	0
40	R	93	0	0	5	0
40	S	35	0	0	2	0
40	T	40	0	0	4	0
40	U	28	0	0	2	0
40	V	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	W	70	0	0	4	0
40	X	23	0	0	3	0
40	Y	93	0	0	9	0
40	Z	30	0	0	5	0
All	All	98979	0	59958	2476	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (2476) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.29	1.15
1:O:1160:G:H5'	1:O:1161:A:H5'	1.27	1.13
15:M:68:ARG:HH21	15:M:73:ARG:HD3	1.12	1.13
6:C:236:THR:HG22	6:C:239:ALA:H	1.06	1.12
9:F:91:VAL:HG12	9:F:92:GLY:H	1.12	1.11
28:Z:46:ARG:HD3	28:Z:59:TYR:HB2	1.37	1.04
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.38	1.04
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.18	1.04
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.40	1.03
21:S:57:THR:HG22	21:S:59:ASP:H	1.23	1.03
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.23	1.02
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.42	1.01
13:K:107:THR:HG22	13:K:108:GLU:HG3	1.43	0.99
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.77	0.99
1:O:156:C:H5''	15:M:171:ARG:HD3	1.44	0.99
13:K:10:GLN:N	13:K:10:GLN:HE21	1.61	0.98
15:M:164:THR:HG22	15:M:166:ALA:H	1.27	0.98
1:O:1242:A:H5'	12:J:82:THR:HG23	1.47	0.97
13:K:10:GLN:H	13:K:10:GLN:NE2	1.63	0.96
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.29	0.95
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.29	0.95
1:O:871:G:C8	1:O:871:G:H5'	2.01	0.95
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.46	0.94
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.46	0.94
4:A:192:VAL:CG1	4:A:207:GLN:HB3	1.97	0.94
1:O:969:G:H1	1:O:999:C:H42	1.13	0.94
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.30	0.94
1:O:656:G:H5'	17:O:3:THR:HG22	1.49	0.93
2:9:3076:G:H3'	2:9:3077:A:H5''	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3056:A:H2'	2:9:3057:A:H5''	1.49	0.93
29:1:25:LYS:HD2	30:2:49:GLU:H	1.33	0.93
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.51	0.93
1:0:542:A:H5'	1:0:542:A:H8	1.34	0.93
16:N:113:SER:HB2	40:N:9358:HOH:O	1.70	0.91
18:P:115:SER:H	18:P:118:GLN:HE21	1.12	0.91
16:N:17:ARG:HB3	16:N:17:ARG:HH11	1.35	0.91
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.11	0.91
16:N:11:ARG:HG3	16:N:14:ARG:HH12	1.36	0.91
28:Z:39:CYS:SG	28:Z:57:CYS:HB2	2.11	0.91
1:0:2586:U:H3	1:0:2592:G:H22	1.14	0.90
5:B:86:ALA:HA	40:B:9573:HOH:O	1.70	0.90
1:0:21:G:H5'	20:R:2:ILE:HA	1.51	0.90
12:J:131:THR:HG22	12:J:134:GLU:H	1.34	0.90
16:N:144:GLY:O	16:N:147:ILE:HG22	1.71	0.89
1:0:1973:A:H5'	1:0:1973:A:H8	1.37	0.89
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.53	0.89
7:D:172:VAL:HG12	7:D:173:GLU:H	1.36	0.89
1:0:1593:C:OP1	18:P:117:SER:HB3	1.73	0.89
6:C:236:THR:HG22	6:C:239:ALA:N	1.87	0.88
5:B:238:ASN:HD22	5:B:240:GLY:H	1.16	0.88
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.51	0.88
4:A:33:GLU:CD	4:A:33:GLU:H	1.76	0.88
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.88	0.88
1:0:2717:C:C2'	1:0:2718:C:H5''	2.04	0.88
1:0:870:G:H2'	1:0:871:G:H5''	1.56	0.88
1:0:1603:A:H5'	1:0:1605:G:O4'	1.74	0.87
1:0:1835:U:H5	1:0:1840:A:N7	1.73	0.87
1:0:2717:C:H2'	1:0:2718:C:H5''	1.56	0.87
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.09	0.87
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.55	0.86
18:P:115:SER:OG	18:P:118:GLN:HG3	1.75	0.86
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.54	0.86
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.57	0.86
27:Y:174:VAL:HG13	27:Y:177:LYS:HD2	1.57	0.86
1:0:1474:C:H6	1:0:1474:C:H5'	1.39	0.86
1:0:2506:A:HO2'	1:0:2507:G:H8	0.86	0.86
15:M:68:ARG:HD3	15:M:68:ARG:O	1.76	0.85
6:C:78:ARG:HH11	6:C:78:ARG:HG3	1.39	0.85
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.58	0.85
15:M:68:ARG:NH2	15:M:73:ARG:HD3	1.89	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:46:GLU:OE1	9:F:100:ASP:HA	1.76	0.85
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.57	0.85
1:0:1160:G:C5'	1:0:1161:A:H5'	2.06	0.85
1:0:871:G:H8	1:0:871:G:H5'	1.38	0.85
5:B:179:LEU:O	5:B:183:GLU:HG2	1.77	0.85
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.60	0.84
1:0:545:G:H8	1:0:545:G:H5'	1.42	0.84
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.57	0.84
1:0:541:C:C2'	1:0:542:A:H5''	2.07	0.84
1:0:1701:A:H4'	1:0:1702:U:H5''	1.59	0.84
1:0:2524:G:H21	1:0:2526:C:H5	1.25	0.84
9:F:91:VAL:HG12	9:F:92:GLY:N	1.92	0.84
1:0:288:A:H61	1:0:364:C:H42	1.26	0.83
1:0:289:G:H22	1:0:363:A:H2	1.25	0.83
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.26	0.83
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.60	0.83
4:A:192:VAL:HG22	40:A:9669:HOH:O	1.78	0.83
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.61	0.83
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.59	0.83
1:0:2716:G:H5''	5:B:206:THR:HG21	1.61	0.83
1:0:2840:A:OP1	5:B:211:THR:HG23	1.77	0.83
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.14	0.83
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.44	0.83
6:C:236:THR:CG2	6:C:239:ALA:H	1.91	0.82
1:0:2506:A:O2'	1:0:2507:G:H8	1.63	0.82
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.62	0.82
18:P:9:LEU:O	18:P:13:VAL:HG12	1.78	0.82
1:0:1838:U:O2'	1:0:2644:C:H5'	1.80	0.82
6:C:5:ILE:HD11	6:C:16:VAL:HG22	1.60	0.81
7:D:25:MET:HE2	7:D:41:LEU:HG	1.62	0.81
24:V:1:THR:HG23	24:V:2:VAL:H	1.44	0.81
1:0:1116:U:O2'	1:0:1118:A:H2	1.63	0.81
1:0:1116:U:HO2'	1:0:1118:A:H2	0.81	0.81
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.62	0.81
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.63	0.81
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.46	0.80
7:D:57:THR:HG23	7:D:63:ILE:HA	1.64	0.80
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.61	0.80
1:0:541:C:H2'	1:0:542:A:H5''	1.64	0.80
22:T:115:GLU:HG3	22:T:116:ASP:H	1.44	0.80
25:W:88:THR:HB	40:W:6679:HOH:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:58:GLU:HA	9:F:61:MET:HE2	1.61	0.80
40:0:5723:HOH:O	13:K:39:GLY:HA2	1.82	0.80
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.46	0.80
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.45	0.80
1:0:2812:A:H2	1:0:2814:A:H62	1.24	0.80
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.16	0.80
25:W:125:HIS:HD2	25:W:127:GLY:H	1.25	0.80
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.62	0.79
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.81	0.79
22:T:115:GLU:HG3	22:T:116:ASP:N	1.97	0.79
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.83	0.79
1:0:1641:A:H2'	1:0:1642:A:H5'	1.64	0.79
20:R:39:THR:HB	20:R:42:GLU:HG3	1.64	0.79
1:0:553:G:P	27:Y:204:ARG:HH22	2.06	0.79
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.46	0.79
21:S:57:THR:HG22	21:S:59:ASP:N	1.95	0.79
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.65	0.79
1:0:1377:C:H6	1:0:1377:C:H5'	1.47	0.78
1:0:111:C:O2'	29:1:20:ARG:HG2	1.84	0.78
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.65	0.78
1:0:871:G:H8	1:0:871:G:C5'	1.96	0.78
14:L:73:VAL:HG23	14:L:74:THR:H	1.48	0.78
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.13	0.78
1:0:2005:G:H3'	1:0:2005:G:OP2	1.84	0.78
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.64	0.78
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.46	0.78
1:0:1184:C:H4'	32:I:126:LYS:HB3	1.63	0.78
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.49	0.78
1:0:1372:A:H3'	40:0:7554:HOH:O	1.84	0.78
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.65	0.78
15:M:79:ALA:HB3	15:M:81:ARG:NH1	1.99	0.78
18:P:91:LYS:O	18:P:95:GLU:HG3	1.84	0.78
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.66	0.77
1:0:1160:G:H5'	1:0:1161:A:C5'	2.10	0.77
29:1:25:LYS:HD2	30:2:49:GLU:N	1.98	0.77
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.66	0.77
1:0:1166:A:H61	1:0:1180:U:H3	1.33	0.77
4:A:194:MET:HE1	4:A:199:HIS:HB2	1.65	0.77
5:B:162:MET:CE	5:B:310:ARG:HD3	2.14	0.77
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.66	0.77
16:N:37:ARG:HG3	36:N:9307:CL:CL	2.22	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.67	0.77
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.49	0.77
1:O:1165:G:H1'	1:O:1174:A:H1'	1.64	0.77
32:I:102:VAL:O	32:I:106:LYS:HG3	1.85	0.77
12:J:74:ARG:NH1	12:J:76:ASP:HB2	1.99	0.77
1:O:2890:A:H1'	23:U:56:ARG:NH2	2.00	0.77
25:W:13:MET:HE1	25:W:18:GLN:HA	1.66	0.77
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.66	0.77
13:K:81:ARG:HD3	13:K:87:ARG:NH1	1.99	0.76
14:L:80:ASP:HB2	14:L:90:ARG:O	1.83	0.76
4:A:199:HIS:HD2	4:A:201:PHE:H	1.33	0.76
16:N:37:ARG:NH2	16:N:105:GLY:HA3	1.99	0.76
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.68	0.76
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.15	0.76
32:I:99:ASP:OD1	32:I:138:THR:HB	1.85	0.76
1:O:506:G:H22	1:O:509:A:C5'	1.98	0.76
5:B:74:ILE:HD13	5:B:309:VAL:HG21	1.68	0.76
1:O:560:C:H42	1:O:597:A:H61	1.33	0.76
1:O:962:C:H1'	16:N:5:ARG:NH1	2.00	0.76
17:O:32:ARG:NE	17:O:35:LYS:HD2	1.98	0.76
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.68	0.76
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.68	0.75
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.68	0.75
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.11	0.75
16:N:17:ARG:NH1	16:N:17:ARG:HB3	2.00	0.75
15:M:164:THR:HG22	15:M:166:ALA:N	2.00	0.75
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.67	0.75
20:R:99:ALA:HB1	20:R:109:MET:CE	2.16	0.75
4:A:167:LYS:HD2	28:Z:29:ILE:HG21	1.68	0.75
1:O:871:G:C8	1:O:871:G:C5'	2.70	0.75
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.67	0.75
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.86	0.75
1:O:1206:U:H6	1:O:1206:U:H5'	1.51	0.75
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.00	0.75
1:O:1118:A:H3'	1:O:1118:A:H8	1.52	0.74
6:C:242:GLU:HB2	40:C:9187:HOH:O	1.85	0.74
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.87	0.74
1:O:123:U:H5'	40:O:7067:HOH:O	1.86	0.74
1:O:506:G:H22	1:O:509:A:H5"	1.51	0.74
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.69	0.74
25:W:122:ARG:HG2	25:W:152:ALA:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:117:LEU:HD13	27:Y:174:VAL:HG11	1.69	0.74
30:2:18:ASN:HD21	30:2:40:ARG:H	1.34	0.74
1:0:21:G:C5'	20:R:2:ILE:HA	2.17	0.74
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.03	0.74
5:B:321:PRO:HA	40:B:9648:HOH:O	1.87	0.74
6:C:140:VAL:HB	40:C:9257:HOH:O	1.85	0.74
28:Z:19:GLY:O	28:Z:23:ARG:HG2	1.87	0.74
1:0:1700:C:H5''	1:0:1701:A:OP2	1.88	0.73
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.70	0.73
20:R:99:ALA:HB1	20:R:109:MET:HE3	1.70	0.73
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.88	0.73
1:0:1175:G:H1'	1:0:1193:A:H2'	1.69	0.73
16:N:132:ASN:O	16:N:135:VAL:HG12	1.88	0.73
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.53	0.73
1:0:93:C:H5''	24:V:1:THR:HB	1.69	0.73
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.87	0.73
1:0:381:G:H5''	40:0:4852:HOH:O	1.89	0.73
40:0:5949:HOH:O	10:G:12:ILE:HA	1.89	0.73
15:M:69:LYS:O	15:M:73:ARG:NH2	2.22	0.73
1:0:2346:C:O2'	7:D:52:THR:HG21	1.88	0.73
1:0:1118:A:H3'	1:0:1118:A:C8	2.23	0.72
28:Z:44:GLU:CG	28:Z:46:ARG:HD2	2.18	0.72
8:E:68:HIS:O	8:E:72:MET:HG3	1.90	0.72
15:M:24:GLN:NE2	15:M:27:ARG:HH11	1.86	0.72
1:0:2534:C:H1'	40:0:4052:HOH:O	1.89	0.72
1:0:481:U:H5''	40:0:6128:HOH:O	1.87	0.72
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.71	0.72
1:0:1666:C:H2'	1:0:1667:A:H5'	1.70	0.72
1:0:1919:A:H4'	40:0:5370:HOH:O	1.89	0.72
25:W:80:ASP:O	25:W:84:VAL:HG23	1.89	0.72
1:0:796:A:HO2'	28:Z:10:ARG:N	1.87	0.72
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.20	0.72
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.70	0.72
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.89	0.72
1:0:2468:A:H61	31:3:48:ASN:HD21	1.36	0.72
1:0:656:G:OP2	17:O:37:ARG:HD2	1.90	0.72
5:B:140:LEU:HA	40:B:9573:HOH:O	1.90	0.72
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.04	0.72
7:D:154:LYS:HD2	7:D:154:LYS:H	1.53	0.72
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.37	0.72
28:Z:13:ARG:HD3	40:Z:9214:HOH:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3029:C:H2'	2:9:3030:C:H5'	1.70	0.72
16:N:154:LEU:HG	16:N:155:GLU:H	1.53	0.72
1:0:1667:A:H8	1:0:1667:A:H5'	1.53	0.71
1:0:450:C:OP1	6:C:184:ARG:NH2	2.22	0.71
1:0:969:G:H1	1:0:999:C:N4	1.86	0.71
4:A:82:VAL:HG13	4:A:93:THR:HB	1.71	0.71
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.55	0.71
1:0:2578:G:H5'	1:0:2578:G:H8	1.55	0.71
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.19	0.71
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.73	0.71
2:9:3014:G:H8	2:9:3014:G:H5'	1.53	0.71
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.71	0.71
11:H:99:LYS:HD3	11:H:119:LYS:HD3	1.72	0.71
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.21	0.71
1:0:1474:C:C6	1:0:1474:C:H5'	2.23	0.71
1:0:541:C:H2'	1:0:542:A:C5'	2.21	0.71
1:0:544:G:H2'	1:0:545:G:H5''	1.72	0.71
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.19	0.71
21:S:73:ASP:OD1	21:S:76:GLU:HG3	1.90	0.71
40:0:7112:HOH:O	27:Y:165:GLU:HB3	1.90	0.71
17:O:32:ARG:HD3	17:O:32:ARG:O	1.89	0.71
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.91	0.71
40:0:9959:HOH:O	29:1:1:THR:HA	1.90	0.71
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.73	0.71
25:W:52:VAL:HG22	25:W:53:ALA:H	1.55	0.71
1:0:1687:C:O2	29:1:9:GLY:HA2	1.90	0.71
1:0:1748:U:H4'	40:0:7857:HOH:O	1.90	0.71
8:E:15:GLN:HG2	8:E:19:ASP:O	1.90	0.71
13:K:10:GLN:H	13:K:10:GLN:HE21	0.80	0.71
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.02	0.71
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.90	0.71
1:0:2851:G:C2'	1:0:2852:A:H5'	2.21	0.70
1:0:281:U:H2'	1:0:282:C:O4'	1.91	0.70
4:A:199:HIS:CD2	4:A:201:PHE:H	2.08	0.70
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.72	0.70
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.07	0.70
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.55	0.70
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.73	0.70
11:H:27:LYS:N	11:H:59:HIS:HD2	1.90	0.70
26:X:71:ARG:HD3	40:X:2171:HOH:O	1.91	0.70
1:0:1118:A:H8	1:0:1119:G:H5''	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1184:C:H1'	40:0:7803:HOH:O	1.91	0.70
1:0:656:G:C5'	17:O:3:THR:HG22	2.20	0.70
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.72	0.70
11:H:29:ALA:HB3	11:H:66:ARG:HH12	1.55	0.70
26:X:25:ARG:HD3	26:X:64:ALA:O	1.92	0.70
1:0:656:G:H5'	17:O:3:THR:CG2	2.21	0.70
6:C:139:VAL:HG13	40:C:9254:HOH:O	1.91	0.70
6:C:2:GLN:HB3	40:C:9190:HOH:O	1.90	0.70
18:P:115:SER:N	18:P:118:GLN:HE21	1.88	0.70
18:P:115:SER:H	18:P:118:GLN:NE2	1.89	0.70
31:3:38:ARG:HB3	31:3:42:ARG:NH1	2.04	0.69
4:A:121:ALA:O	4:A:124:VAL:HG22	1.91	0.69
5:B:238:ASN:HD22	5:B:240:GLY:N	1.89	0.69
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.40	0.69
1:0:542:A:H5'	1:0:542:A:C8	2.22	0.69
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.75	0.69
1:0:474:C:O3'	6:C:73:LEU:HD21	1.91	0.69
1:0:681:G:N3	1:0:681:G:H5'	2.07	0.69
4:A:211:LYS:CG	4:A:212:PRO:HD2	2.23	0.69
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.00	0.69
9:F:21:GLU:O	9:F:24:ARG:HG3	1.92	0.69
1:0:902:G:N7	14:L:18:HIS:HD2	1.91	0.69
7:D:172:VAL:HG12	7:D:173:GLU:N	2.07	0.69
1:0:1183:C:N4	1:0:1184:C:H41	1.90	0.69
1:0:1182:C:H1'	1:0:1192:A:H8	1.58	0.69
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.75	0.69
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.22	0.69
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.90	0.69
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.20	0.69
5:B:268:ARG:HH21	5:B:325:PRO:HG3	1.58	0.69
22:T:20:HIS:HB3	22:T:41:ARG:HD2	1.74	0.69
1:0:280:C:H2'	1:0:281:U:O4'	1.92	0.69
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.57	0.68
1:0:2073:G:H5''	40:0:4373:HOH:O	1.93	0.68
2:9:3056:A:C2'	2:9:3057:A:H5''	2.21	0.68
28:Z:29:ILE:O	28:Z:33:MET:HB2	1.93	0.68
1:0:2748:G:H5'	40:0:7878:HOH:O	1.92	0.68
4:A:51:ARG:HB2	40:A:9641:HOH:O	1.92	0.68
9:F:96:ALA:HA	40:F:3111:HOH:O	1.94	0.68
12:J:75:PRO:HD3	12:J:136:SER:OG	1.92	0.68
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.16	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.74	0.68
1:0:447:A:P	22:T:1:SER:HB2	2.34	0.68
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.23	0.68
1:0:2003:U:H4'	1:0:2004:U:C5	2.29	0.68
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.75	0.68
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.08	0.68
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.74	0.68
32:I:132:CYS:C	32:I:134:SER:H	1.97	0.68
13:K:32:ILE:HD11	13:K:56:SER:HB2	1.75	0.68
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.57	0.68
4:A:130:THR:HB	4:A:137:VAL:HB	1.75	0.68
1:0:657:G:OP1	6:C:27:ARG:NH2	2.26	0.68
11:H:30:GLN:H	11:H:66:ARG:NH1	1.92	0.68
27:Y:117:LEU:HD13	27:Y:174:VAL:CG1	2.25	0.68
27:Y:212:ARG:HD2	40:Y:9398:HOH:O	1.93	0.68
1:0:2491:G:H1'	40:0:7261:HOH:O	1.92	0.67
1:0:588:G:O6	25:W:154:ARG:NH1	2.28	0.67
6:C:132:ASP:HB3	40:C:9171:HOH:O	1.93	0.67
9:F:13:GLU:OE2	9:F:78:GLU:HG2	1.94	0.67
32:I:125:ALA:O	32:I:129:VAL:HG23	1.93	0.67
13:K:63:GLU:HB2	40:K:6344:HOH:O	1.93	0.67
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.28	0.67
1:0:2807:U:P	5:B:27:ASN:HD21	2.18	0.67
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.74	0.67
15:M:80:GLY:O	15:M:81:ARG:HD2	1.95	0.67
1:0:797:A:H5'	28:Z:10:ARG:N	2.08	0.67
1:0:1206:U:H2'	1:0:1207:A:O4'	1.93	0.67
5:B:195:ARG:NH1	5:B:324:ASP:OD1	2.28	0.67
2:9:3040:C:N4	7:D:53:LYS:HE3	2.10	0.67
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.05	0.67
1:0:282:C:O2'	1:0:283:U:H5'	1.93	0.67
25:W:5:VAL:HG22	25:W:32:CYS:HB2	1.77	0.67
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.29	0.66
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.77	0.66
23:U:47:ARG:HG3	40:U:4381:HOH:O	1.95	0.66
1:0:2533:C:H5'	1:0:2533:C:H6	1.59	0.66
1:0:316:A:N3	1:0:336:G:O2'	2.26	0.66
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.77	0.66
14:L:143:THR:HG22	14:L:144:ASP:N	2.10	0.66
1:0:1377:C:H5'	1:0:1377:C:C6	2.30	0.66
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:31:ARG:HH12	8:E:68:HIS:CD2	2.14	0.66
16:N:37:ARG:CZ	16:N:105:GLY:HA3	2.25	0.66
17:O:32:ARG:HH21	17:O:35:LYS:HZ2	1.40	0.66
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.25	0.66
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.78	0.66
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.25	0.66
1:O:95:A:H5''	1:O:97:G:O4'	1.96	0.66
1:O:2896:A:N3	1:O:2896:A:H2'	2.11	0.66
1:O:558:C:H2'	1:O:559:U:H5'	1.77	0.66
4:A:194:MET:CE	4:A:199:HIS:HB2	2.24	0.66
6:C:98:ARG:HH11	6:C:98:ARG:HG2	1.60	0.66
9:F:37:THR:O	9:F:41:GLU:HG3	1.95	0.66
11:H:27:LYS:H	11:H:59:HIS:HD2	1.44	0.66
1:O:2054:A:N3	20:R:128:ARG:NH2	2.44	0.66
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.78	0.66
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.10	0.66
5:B:275:GLY:O	5:B:291:ASP:HA	1.96	0.66
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.77	0.66
1:O:870:G:C2'	1:O:871:G:H5''	2.25	0.65
16:N:62:HIS:HB3	16:N:65:ASP:OD1	1.96	0.65
23:U:14:GLU:O	23:U:17:THR:HB	1.95	0.65
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.79	0.65
1:O:559:U:H5'	1:O:559:U:H6	1.60	0.65
1:O:2816:A:H2'	40:O:8334:HOH:O	1.96	0.65
4:A:135:VAL:HG21	4:A:147:ARG:NH1	2.11	0.65
8:E:31:ARG:NH1	8:E:68:HIS:CG	2.65	0.65
20:R:9:ASP:O	20:R:13:THR:HB	1.96	0.65
24:V:39:ALA:N	24:V:40:PRO:HD2	2.11	0.65
1:O:1476:A:O2'	1:O:1477:C:H5'	1.97	0.65
1:O:1701:A:H4'	1:O:1702:U:C5'	2.27	0.65
1:O:2505:G:O2'	1:O:2506:A:H5'	1.97	0.65
4:A:81:GLN:H	4:A:92:ASN:ND2	1.95	0.65
14:L:67:ARG:O	14:L:71:GLU:HG3	1.96	0.65
40:9:4707:HOH:O	16:N:147:ILE:HD12	1.95	0.65
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.61	0.65
28:Z:44:GLU:HG2	28:Z:46:ARG:HD2	1.79	0.65
1:O:1183:C:H2'	40:O:6686:HOH:O	1.97	0.65
1:O:220:C:H1'	40:O:6231:HOH:O	1.94	0.65
1:O:316:A:H5'	22:T:54:ASP:OD2	1.97	0.65
8:E:6:GLU:HA	8:E:46:THR:HG22	1.79	0.65
25:W:130:HIS:O	25:W:136:GLY:HA3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:4:LEU:HD22	25:W:52:VAL:CG2	2.26	0.65
1:0:1528:A:H2'	1:0:1529:G:O4'	1.97	0.65
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.61	0.65
1:0:1973:A:H5'	1:0:1973:A:C8	2.25	0.65
1:0:2426:G:H1'	40:0:6540:HOH:O	1.96	0.65
5:B:254:GLN:HG3	40:B:9533:HOH:O	1.97	0.65
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.78	0.65
1:0:1201:C:H2'	1:0:1202:A:H5'	1.79	0.64
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.26	0.64
13:K:81:ARG:HB2	13:K:87:ARG:NH1	2.13	0.64
1:0:1159:G:H21	1:0:1189:A:H8	1.46	0.64
1:0:1119:G:N2	1:0:1246:A:C2	2.56	0.64
1:0:1451:C:H5'	1:0:1505:U:C5	2.31	0.64
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.27	0.64
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.79	0.64
1:0:1205:U:H2'	1:0:1206:U:H5''	1.78	0.64
1:0:1299:G:O6	14:L:6:ARG:HD3	1.96	0.64
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.78	0.64
1:0:1165:G:H4'	1:0:1174:A:O2'	1.97	0.64
1:0:470:U:O2'	29:1:16:HIS:HD2	1.80	0.64
25:W:48:VAL:HG12	25:W:48:VAL:O	1.97	0.64
25:W:88:THR:HG22	25:W:89:ASP:N	2.12	0.64
1:0:1166:A:H1'	1:0:1192:A:C2	2.33	0.64
7:D:75:LEU:HD22	7:D:79:MET:HB3	1.80	0.64
1:0:282:C:H1'	1:0:368:C:N4	2.12	0.64
1:0:545:G:C8	1:0:545:G:H5'	2.30	0.64
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.44	0.64
16:N:119:GLN:O	16:N:123:ILE:HG13	1.97	0.64
1:0:962:C:H1'	16:N:5:ARG:HH12	1.62	0.64
1:0:1116:U:H3	1:0:1246:A:H62	1.46	0.64
6:C:162:VAL:HG13	6:C:192:ILE:HD11	1.79	0.64
6:C:236:THR:HA	40:C:9257:HOH:O	1.96	0.64
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.78	0.64
1:0:544:G:C2'	1:0:545:G:H5''	2.27	0.64
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.78	0.64
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.61	0.64
1:0:263:U:O4'	9:F:59:ILE:HD13	1.98	0.64
1:0:2908:A:H2'	1:0:2909:G:O4'	1.97	0.64
16:N:164:ASP:OD1	16:N:167:ASP:HA	1.98	0.64
6:C:236:THR:HG21	40:C:9180:HOH:O	1.98	0.63
11:H:169:GLY:C	11:H:170:ASN:HD22	2.00	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:16:ARG:NH2	24:V:63:GLU:HG3	2.13	0.63
30:2:18:ASN:ND2	30:2:40:ARG:H	1.96	0.63
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.80	0.63
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.28	0.63
1:0:1426:C:H2'	40:0:3189:HOH:O	1.97	0.63
1:0:1882:C:OP1	4:A:192:VAL:HG23	1.99	0.63
23:U:39:ASN:ND2	23:U:44:ARG:HH11	1.94	0.63
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.80	0.63
6:C:77:ALA:O	6:C:78:ARG:HG3	1.97	0.63
4:A:167:LYS:HB2	28:Z:29:ILE:HD13	1.80	0.63
1:0:1946:C:H2'	1:0:1971:G:C8	2.33	0.63
4:A:161:GLY:O	28:Z:68:SER:HB2	1.97	0.63
5:B:254:GLN:HG2	5:B:255:GLY:N	2.13	0.63
24:V:12:THR:HG23	24:V:14:ALA:H	1.64	0.63
31:3:3:MET:O	31:3:90:PHE:HA	1.98	0.63
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.13	0.63
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.99	0.63
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.14	0.63
25:W:5:VAL:O	25:W:52:VAL:HG23	1.98	0.63
1:0:1835:U:C5	1:0:1840:A:N7	2.63	0.63
1:0:1972:U:H2'	1:0:1973:A:H5''	1.81	0.63
1:0:949:U:H4'	19:Q:95:GLU:HA	1.81	0.63
5:B:51:VAL:HG23	5:B:329:TYR:O	1.99	0.63
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.64	0.63
7:D:22:VAL:HG22	7:D:74:THR:HG22	1.81	0.63
17:O:32:ARG:HH21	17:O:35:LYS:NZ	1.96	0.63
1:0:119:A:H2'	1:0:120:A:H5''	1.81	0.63
1:0:635:A:H2'	1:0:636:G:H5''	1.81	0.63
7:D:25:MET:SD	7:D:40:ILE:HD11	2.38	0.63
7:D:51:ARG:HH11	7:D:68:PRO:HB3	1.64	0.63
8:E:126:ILE:HB	8:E:131:LEU:HD23	1.80	0.63
15:M:83:SER:HB3	40:M:9378:HOH:O	1.99	0.63
26:X:71:ARG:HB3	26:X:88:GLU:OE1	1.99	0.63
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.99	0.62
11:H:166:SER:CB	11:H:167:PRO:CD	2.76	0.62
1:0:2073:G:OP2	1:0:2490:A:H5'	1.99	0.62
1:0:2644:C:O2'	1:0:2645:U:H5'	1.99	0.62
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.81	0.62
15:M:164:THR:HG22	15:M:165:GLY:N	2.13	0.62
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.34	0.62
28:Z:44:GLU:HG3	28:Z:46:ARG:HD2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2415:A:H2'	1:0:2416:G:H5'	1.80	0.62
9:F:46:GLU:O	9:F:73:PRO:HD2	1.99	0.62
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.13	0.62
1:0:1201:C:H5''	40:0:6676:HOH:O	1.97	0.62
4:A:48:ASP:HB3	40:A:9641:HOH:O	1.99	0.62
1:0:2820:A:OP1	5:B:98:THR:HG22	1.99	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.64	0.62
1:0:625:U:H5''	1:0:1044:C:N4	2.15	0.62
1:0:2827:A:H2'	1:0:2828:G:O4'	2.00	0.62
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.81	0.62
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.29	0.62
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.80	0.62
14:L:10:SER:O	14:L:11:ARG:HB3	1.99	0.62
25:W:119:HIS:HD2	25:W:120:PRO:O	1.81	0.62
1:0:797:A:C4'	28:Z:10:ARG:N	2.63	0.62
1:0:2670:G:O2'	1:0:2671:U:H5'	1.99	0.62
1:0:2718:C:H6	1:0:2718:C:H5'	1.64	0.62
4:A:179:MET:HA	4:A:179:MET:CE	2.30	0.62
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.15	0.62
21:S:37:VAL:O	21:S:41:VAL:HG23	1.99	0.62
1:0:156:C:H5''	15:M:171:ARG:CD	2.26	0.62
1:0:2291:A:C8	1:0:2309:C:H5'	2.34	0.62
4:A:179:MET:HG2	4:A:186:TRP:CB	2.30	0.62
27:Y:177:LYS:HD3	27:Y:181:GLY:O	1.99	0.62
1:0:2421:G:H1'	40:0:4250:HOH:O	1.98	0.62
6:C:107:ARG:NE	40:C:9263:HOH:O	2.29	0.62
11:H:154:TYR:HB2	40:H:9563:HOH:O	2.00	0.62
12:J:107:ASN:ND2	12:J:109:TYR:H	1.97	0.62
40:0:3751:HOH:O	15:M:9:ARG:HG3	1.99	0.62
25:W:84:VAL:HG12	40:W:6679:HOH:O	1.99	0.62
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.29	0.62
1:0:2064:U:H5'	1:0:2652:U:H4'	1.81	0.62
16:N:110:THR:HB	16:N:113:SER:OG	2.00	0.62
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.15	0.62
12:J:107:ASN:HD22	12:J:107:ASN:C	2.03	0.62
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.30	0.62
1:0:2508:C:H2'	40:0:7154:HOH:O	2.00	0.61
4:A:206:ARG:HD3	4:A:206:ARG:H	1.65	0.61
4:A:36:ASP:HB3	4:A:85:SER:HB2	1.83	0.61
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.11	0.61
1:0:558:C:H2'	1:0:559:U:C5'	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:48:LYS:O	15:M:52:GLN:HG3	1.99	0.61
16:N:17:ARG:HH11	16:N:17:ARG:CB	2.10	0.61
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.20	0.61
22:T:32:ARG:NH1	22:T:38:ARG:HH12	1.98	0.61
5:B:305:ASP:O	5:B:306:LYS:HB2	2.00	0.61
6:C:79:ARG:O	6:C:87:ARG:HG2	2.01	0.61
9:F:13:GLU:OE1	9:F:77:VAL:HG13	1.99	0.61
9:F:2:VAL:HG22	9:F:57:GLU:OE1	2.01	0.61
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.34	0.61
25:W:52:VAL:HG22	25:W:53:ALA:N	2.15	0.61
15:M:164:THR:CG2	15:M:165:GLY:N	2.64	0.61
1:O:2894:C:O2'	1:O:2895:C:H5'	1.99	0.61
1:O:447:A:OP2	22:T:1:SER:HB2	2.00	0.61
29:1:8:GLN:HE22	29:1:11:LYS:NZ	1.99	0.61
4:A:164:ARG:HA	28:Z:69:TYR:CE1	2.36	0.61
4:A:203:GLY:HA2	40:A:9581:HOH:O	2.01	0.61
4:A:232:ARG:NH2	4:A:236:GLY:O	2.31	0.61
7:D:170:TYR:O	7:D:171:ASP:HB3	1.99	0.61
1:O:2694:A:H4'	8:E:91:PHE:CE1	2.36	0.61
10:G:12:ILE:N	10:G:13:PRO:HD3	2.15	0.61
10:G:63:ARG:HB2	10:G:66:LEU:HG	1.82	0.61
14:L:35:ARG:HD3	14:L:35:ARG:C	2.21	0.61
15:M:70:GLY:HA3	15:M:73:ARG:HH22	1.66	0.61
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.00	0.61
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.30	0.61
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.83	0.61
22:T:49:GLU:HB3	22:T:59:GLU:CG	2.31	0.61
31:3:55:VAL:HG22	40:3:9444:HOH:O	2.00	0.61
8:E:31:ARG:HH12	8:E:68:HIS:CG	2.19	0.60
11:H:170:ASN:N	11:H:170:ASN:HD22	1.99	0.60
22:T:48:VAL:HG13	22:T:97:ARG:O	2.01	0.60
1:O:2420:G:O2'	1:O:2421:G:H5'	2.00	0.60
1:O:343:C:O2'	1:O:344:C:H5'	2.00	0.60
2:9:3014:G:C8	2:9:3014:G:H5'	2.36	0.60
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.82	0.60
5:B:56:ASP:OD1	5:B:322:ARG:HB3	2.02	0.60
11:H:157:ILE:HD11	11:H:161:CYS:SG	2.41	0.60
32:I:113:HIS:N	32:I:114:PRO:HD2	2.15	0.60
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.82	0.60
1:O:1773:G:C8	28:Z:16:ALA:HA	2.36	0.60
1:O:1189:A:O2'	1:O:1208:C:H2'	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:164:ASP:CG	16:N:167:ASP:HA	2.21	0.60
21:S:33:SER:O	21:S:37:VAL:HG23	2.01	0.60
25:W:4:LEU:CD2	25:W:54:PHE:HB3	2.28	0.60
4:A:75:GLY:HA2	28:Z:64:PHE:HA	1.83	0.60
1:0:2524:G:N2	1:0:2526:C:H5	1.97	0.60
1:0:371:U:H2'	1:0:372:A:H8	1.66	0.60
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.00	0.60
5:B:125:GLU:O	5:B:129:ARG:HG3	2.00	0.60
14:L:133:VAL:HA	40:L:9477:HOH:O	2.00	0.60
27:Y:117:LEU:CD1	27:Y:174:VAL:HG11	2.32	0.60
1:0:1666:C:O2'	1:0:1667:A:H5''	2.02	0.60
5:B:138:GLY:O	5:B:139:ASP:O	2.20	0.60
24:V:1:THR:HG23	24:V:2:VAL:N	2.16	0.60
1:0:396:U:O2'	1:0:418:C:H4'	2.01	0.60
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.83	0.60
18:P:14:LEU:O	18:P:16:VAL:HG23	2.01	0.60
1:0:289:G:N2	1:0:363:A:H2	1.96	0.60
14:L:136:ALA:HB3	40:L:9477:HOH:O	2.02	0.60
18:P:97:ARG:HD2	40:P:163:HOH:O	2.02	0.60
32:I:134:SER:O	32:I:135:LEU:HD23	2.00	0.60
12:J:45:VAL:HG23	12:J:130:VAL:O	2.01	0.60
2:9:3039:U:HO2'	2:9:3042:C:H5	1.50	0.60
23:U:5:GLU:HG2	23:U:10:GLY:O	2.02	0.60
1:0:899:C:H5'	40:0:3768:HOH:O	2.00	0.60
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.67	0.60
27:Y:144:ARG:NE	40:Y:9410:HOH:O	2.34	0.60
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.84	0.60
1:0:2003:U:H4'	1:0:2004:U:H5	1.67	0.59
1:0:2541:U:H5'	1:0:2541:U:H6	1.65	0.59
31:3:70:ARG:HB3	40:3:9506:HOH:O	2.02	0.59
25:W:108:ARG:HH21	25:W:114:PRO:HG2	1.66	0.59
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.84	0.59
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.17	0.59
15:M:60:VAL:C	15:M:61:ILE:HD12	2.21	0.59
13:K:82:ARG:NH2	13:K:115:ARG:HG2	2.17	0.59
14:L:148:GLU:HB2	40:L:9496:HOH:O	2.00	0.59
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.84	0.59
27:Y:187:VAL:HG23	27:Y:192:ASP:HB2	1.82	0.59
1:0:1681:G:H5''	1:0:1682:A:H5'	1.83	0.59
4:A:179:MET:HG2	4:A:186:TRP:HB2	1.83	0.59
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:99:ASP:O	32:I:100:LEU:HD23	2.02	0.59
16:N:80:SER:HB2	40:N:9339:HOH:O	2.01	0.59
1:0:1060:C:H6	1:0:1060:C:H5'	1.68	0.59
1:0:1118:A:C8	1:0:1119:G:H5''	2.37	0.59
1:0:1333:U:H2'	1:0:1334:C:C6	2.38	0.59
4:A:41:THR:HG23	4:A:77:GLY:O	2.03	0.59
7:D:41:LEU:HA	7:D:44:ILE:CG2	2.31	0.59
16:N:49:THR:HG22	16:N:56:ASP:CB	2.32	0.59
5:B:217:ARG:HG3	5:B:257:THR:CG2	2.32	0.59
22:T:48:VAL:CG1	22:T:96:VAL:HG22	2.32	0.59
23:U:52:THR:HG22	23:U:54:THR:N	2.17	0.59
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.03	0.59
1:0:2101:A:H2'	6:C:63:SER:OG	2.01	0.59
15:M:68:ARG:HH21	15:M:73:ARG:CD	2.02	0.59
25:W:13:MET:HE2	25:W:17:ILE:HG22	1.85	0.59
25:W:13:MET:CE	25:W:17:ILE:HG22	2.32	0.59
1:0:1595:G:O2'	1:0:1596:U:H5'	2.02	0.59
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.38	0.59
5:B:175:LEU:O	5:B:175:LEU:HD23	2.03	0.59
11:H:63:GLU:HA	40:H:9551:HOH:O	2.02	0.59
40:9:5071:HOH:O	16:N:23:ARG:HD3	2.01	0.59
25:W:142:ASP:HB3	25:W:145:GLY:H	1.68	0.59
19:Q:25:PRO:HB2	40:Q:4350:HOH:O	2.03	0.59
20:R:82:GLU:O	20:R:86:LYS:HG3	2.03	0.59
1:0:1878:G:H1'	40:0:6567:HOH:O	2.02	0.58
1:0:2032:U:H2'	1:0:2033:G:C5'	2.33	0.58
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.43	0.58
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.67	0.58
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.32	0.58
17:O:14:LEU:HG	17:O:102:ILE:HD11	1.84	0.58
21:S:77:VAL:O	21:S:80:ARG:HG2	2.03	0.58
2:9:3039:U:H3'	2:9:3040:C:H5''	1.85	0.58
4:A:33:GLU:CD	4:A:33:GLU:N	2.51	0.58
6:C:1:MET:HG2	6:C:2:GLN:H	1.67	0.58
13:K:75:ARG:HD3	13:K:112:PRO:O	2.02	0.58
1:0:1555:G:H4'	1:0:1630:A:H2	1.69	0.58
1:0:558:C:O2'	1:0:559:U:H5''	2.02	0.58
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.03	0.58
4:A:122:SER:O	4:A:124:VAL:HG13	2.02	0.58
32:I:92:PRO:C	32:I:94:GLU:H	2.07	0.58
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:57:THR:CG2	21:S:59:ASP:HB2	2.33	0.58
22:T:89:ARG:HG3	22:T:89:ARG:O	2.03	0.58
1:0:2563:U:H2'	1:0:2565:C:O5'	2.03	0.58
1:0:2643:G:H5''	40:0:4473:HOH:O	2.03	0.58
7:D:50:VAL:O	7:D:71:ALA:HA	2.03	0.58
18:P:55:LYS:HG2	18:P:56:GLY:N	2.17	0.58
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.84	0.58
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.58
24:V:38:GLY:C	24:V:40:PRO:HD2	2.24	0.58
1:0:1666:C:H2'	1:0:1667:A:C5'	2.33	0.58
1:0:2749:U:H5'	40:0:8329:HOH:O	2.03	0.58
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.87	0.58
5:B:140:LEU:HD23	40:B:9573:HOH:O	2.03	0.58
5:B:214:PRO:HD2	40:B:9524:HOH:O	2.02	0.58
15:M:24:GLN:HE22	15:M:27:ARG:HH11	1.52	0.58
18:P:89:ASN:HB3	18:P:92:GLU:HB2	1.84	0.58
24:V:5:VAL:HG23	40:V:2271:HOH:O	2.03	0.58
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.37	0.58
1:0:87:C:H2'	30:2:28:LYS:O	2.03	0.58
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.31	0.58
12:J:26:VAL:HG13	12:J:36:VAL:HG11	1.85	0.58
14:L:143:THR:HG22	14:L:144:ASP:H	1.69	0.58
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.51	0.58
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.67	0.58
6:C:233:THR:HG22	6:C:234:VAL:H	1.69	0.58
9:F:34:ASN:HA	15:M:4:ALA:HB2	1.86	0.58
24:V:39:ALA:C	24:V:41:GLU:H	2.06	0.58
1:0:1384:C:H5'	26:X:30:MET:HG2	1.84	0.58
29:1:8:GLN:HE22	29:1:11:LYS:HZ2	1.50	0.58
30:2:41:HIS:H	30:2:45:ASN:HD22	1.50	0.58
8:E:11:VAL:HG12	8:E:12:ASP:N	2.18	0.58
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.86	0.58
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.39	0.58
1:0:1053:G:OP1	11:H:12:PRO:HG3	2.04	0.58
1:0:151:A:H2'	1:0:152:A:O4'	2.04	0.58
1:0:1714:C:O2'	1:0:1715:C:H5'	2.03	0.58
1:0:1819:G:H2'	1:0:1820:G:H4'	1.85	0.58
1:0:200:U:H2'	40:0:4002:HOH:O	2.04	0.58
1:0:2769:C:C2'	1:0:2770:G:H5'	2.34	0.58
1:0:877:G:H5'	1:0:878:G:OP1	2.03	0.58
4:A:94:LEU:N	4:A:94:LEU:HD23	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:0:6006:HOH:O	5:B:298:LYS:HG2	2.03	0.58
8:E:116:THR:CG2	8:E:151:LEU:HD22	2.30	0.58
40:0:6143:HOH:O	28:Z:17:ARG:HD3	2.04	0.58
1:0:380:A:OP2	15:M:9:ARG:HD2	2.03	0.58
1:0:120:A:H5'	29:1:20:ARG:HH21	1.69	0.58
31:3:70:ARG:NH1	31:3:77:ALA:HB2	2.18	0.58
11:H:58:ARG:HG3	11:H:58:ARG:NH1	2.19	0.58
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.84	0.58
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.04	0.58
22:T:71:VAL:HG13	22:T:91:LEU:O	2.03	0.58
23:U:52:THR:CG2	23:U:54:THR:HB	2.34	0.58
26:X:43:VAL:HG12	26:X:44:ASP:N	2.19	0.58
1:0:236:A:H8	1:0:236:A:OP1	1.87	0.57
5:B:75:GLU:C	5:B:77:PRO:HD3	2.23	0.57
9:F:48:VAL:HG23	9:F:74:PHE:HB3	1.86	0.57
32:I:112:LYS:C	32:I:114:PRO:HD2	2.24	0.57
1:0:263:U:O2	15:M:42:ARG:HD2	2.04	0.57
16:N:169:PRO:O	16:N:172:PHE:HB3	2.03	0.57
1:0:920:C:H4'	1:0:921:G:C2	2.39	0.57
40:0:4766:HOH:O	30:2:38:LYS:HE3	2.04	0.57
4:A:43:VAL:HG21	4:A:59:GLU:HG3	1.86	0.57
1:0:1205:U:H2'	1:0:1206:U:C5'	2.35	0.57
1:0:1209:C:H2'	1:0:1210:G:H8	1.69	0.57
1:0:775:G:OP1	29:1:16:HIS:HE1	1.87	0.57
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.86	0.57
5:B:102:THR:HG23	5:B:182:VAL:HG12	1.85	0.57
11:H:56:GLN:NE2	11:H:93:GLN:HG2	2.19	0.57
22:T:38:ARG:NH1	40:T:6217:HOH:O	2.37	0.57
1:0:1778:A:H2'	1:0:1779:A:H5'	1.86	0.57
1:0:2103:A:H5'	40:0:4975:HOH:O	2.04	0.57
1:0:2851:G:O2'	1:0:2852:A:H5'	2.04	0.57
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.35	0.57
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.86	0.57
1:0:2320:U:H4'	1:0:2321:A:O4'	2.04	0.57
1:0:485:A:HO2'	1:0:487:G:H8	1.52	0.57
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.86	0.57
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.86	0.57
20:R:44:VAL:O	20:R:48:GLU:HG3	2.03	0.57
22:T:28:SER:O	22:T:32:ARG:HG3	2.03	0.57
22:T:71:VAL:HG12	22:T:72:ILE:N	2.19	0.57
1:0:12:U:H2'	1:0:13:G:H5'	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:25:VAL:HG13	31:3:68:LYS:HE3	1.87	0.57
4:A:165:THR:HG22	40:A:9656:HOH:O	2.04	0.57
8:E:23:GLU:HG2	8:E:28:SER:CB	2.35	0.57
9:F:57:GLU:HB2	15:M:23:LEU:HD11	1.85	0.57
17:O:15:LYS:HD3	17:O:19:ARG:NH2	2.20	0.57
22:T:26:THR:HA	22:T:39:ASN:HB3	1.86	0.57
1:0:204:A:H2'	1:0:205:U:H5'	1.86	0.57
1:0:2851:G:H2'	1:0:2852:A:H5'	1.86	0.57
4:A:109:GLU:HG2	4:A:116:GLY:N	2.20	0.57
11:H:166:SER:HB3	11:H:167:PRO:CD	2.33	0.57
18:P:16:VAL:HG12	18:P:17:GLY:N	2.19	0.57
22:T:48:VAL:HG11	22:T:96:VAL:HG13	1.87	0.57
26:X:78:GLU:HG2	26:X:79:GLU:OE2	2.05	0.57
40:O:7894:HOH:O	31:3:60:LYS:HG3	2.04	0.57
31:3:65:THR:HG22	31:3:67:LEU:HG	1.86	0.57
7:D:51:ARG:NH1	7:D:68:PRO:HB3	2.19	0.57
9:F:58:GLU:HG3	9:F:61:MET:HE1	1.87	0.57
12:J:74:ARG:CB	12:J:74:ARG:HH11	2.17	0.57
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.07	0.57
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.45	0.57
1:0:1165:G:O3'	1:0:1174:A:H4'	2.04	0.57
1:0:1187:U:O2'	1:0:1189:A:H2	1.88	0.57
7:D:138:GLY:N	40:D:7597:HOH:O	2.38	0.57
15:M:77:HIS:HD2	15:M:79:ALA:O	1.88	0.57
16:N:49:THR:HG22	16:N:56:ASP:HB3	1.87	0.57
1:0:946:C:H2'	1:0:947:U:C6	2.38	0.57
11:H:45:VAL:HA	11:H:167:PRO:O	2.05	0.57
15:M:58:GLN:HG3	40:M:9410:HOH:O	2.05	0.57
2:9:3011:A:P	19:Q:19:ARG:HH21	2.28	0.57
1:0:816:G:OP1	18:P:91:LYS:HE2	2.04	0.56
6:C:1:MET:HG2	6:C:2:GLN:N	2.20	0.56
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.40	0.56
16:N:162:ASP:HA	40:N:9333:HOH:O	2.03	0.56
17:O:59:VAL:HG23	17:O:111:VAL:CG2	2.35	0.56
1:0:2415:A:N3	16:N:26:LEU:HD13	2.20	0.56
1:0:2878:U:H2'	1:0:2879:A:O4'	2.05	0.56
5:B:199:TYR:CE2	5:B:268:ARG:HB2	2.40	0.56
12:J:74:ARG:O	12:J:78:ILE:HG12	2.05	0.56
1:0:709:G:O2'	17:O:25:VAL:HG12	2.05	0.56
4:A:88:ILE:HG22	4:A:88:ILE:O	2.03	0.56
5:B:85:ARG:NH1	40:B:9628:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:37:ALA:O	7:D:40:ILE:HG12	2.06	0.56
25:W:38:THR:HG22	25:W:39:ASP:N	2.19	0.56
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.87	0.56
1:0:1066:U:H2'	1:0:1067:A:C8	2.41	0.56
1:0:1116:U:O2'	1:0:1118:A:C2	2.45	0.56
1:0:1641:A:C2'	1:0:1642:A:H5'	2.34	0.56
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.40	0.56
10:G:24:VAL:O	10:G:28:GLU:HB2	2.04	0.56
24:V:42:ASN:O	24:V:44:GLY:N	2.38	0.56
1:0:2432:C:O2'	1:0:2433:A:H5'	2.06	0.56
1:0:2812:A:N7	40:0:7853:HOH:O	2.33	0.56
1:0:364:C:H2'	1:0:365:G:O4'	2.05	0.56
1:0:506:G:H22	1:0:509:A:H5'	1.71	0.56
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.36	0.56
2:9:3029:C:O3'	7:D:138:GLY:HA2	2.06	0.56
1:0:2531:U:O2'	1:0:2532:A:H5'	2.05	0.56
1:0:737:A:H2'	1:0:738:G:O4'	2.06	0.56
1:0:853:C:H3'	40:0:5080:HOH:O	2.04	0.56
7:D:173:GLU:HG3	7:D:174:VAL:N	2.21	0.56
7:D:57:THR:HA	40:D:5146:HOH:O	2.05	0.56
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.27	0.56
1:0:1766:U:O2	1:0:1778:A:H5'	2.06	0.56
1:0:432:G:O2'	1:0:433:C:H5'	2.06	0.56
2:9:3013:A:O2'	2:9:3014:G:H5''	2.05	0.56
2:9:3042:C:H5'	2:9:3043:G:OP2	2.06	0.56
4:A:69:LEU:HB3	40:A:9612:HOH:O	2.05	0.56
1:0:338:C:H4'	6:C:174:ILE:CD1	2.36	0.56
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.88	0.56
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.88	0.56
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.36	0.56
13:K:115:ARG:HG3	13:K:116:GLU:N	2.21	0.56
22:T:48:VAL:O	22:T:59:GLU:HA	2.06	0.56
1:0:1603:A:H5''	1:0:1604:G:H3'	1.87	0.56
1:0:2072:G:C6	1:0:2533:C:H1'	2.41	0.56
1:0:2480:G:H3'	40:0:4723:HOH:O	2.06	0.56
1:0:2502:C:C2'	1:0:2503:A:H5'	2.35	0.56
1:0:241:A:C2	1:0:378:A:H4'	2.41	0.56
1:0:482:G:H4'	1:0:508:A:N1	2.21	0.56
1:0:500:G:H21	20:R:98:ASN:HD21	1.53	0.56
1:0:558:C:C2'	1:0:559:U:H5''	2.36	0.56
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:20:ARG:HG3	30:2:21:VAL:N	2.21	0.56
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.86	0.56
30:2:48:ASP:O	30:2:49:GLU:HB2	2.06	0.56
6:C:233:THR:HG22	6:C:234:VAL:N	2.20	0.56
27:Y:200:THR:CG2	27:Y:201:GLU:HG3	2.35	0.56
1:0:2645:U:OP2	1:0:2645:U:C6	2.59	0.55
10:G:64:ASN:N	10:G:64:ASN:HD22	2.02	0.55
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.06	0.55
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.41	0.55
1:0:2649:A:C8	1:0:2649:A:H5'	2.41	0.55
1:0:2649:A:H5'	1:0:2649:A:H8	1.71	0.55
1:0:272:A:H5'	1:0:273:G:OP2	2.06	0.55
1:0:288:A:H2'	1:0:289:G:C8	2.40	0.55
1:0:797:A:H4'	28:Z:10:ARG:N	2.21	0.55
4:A:43:VAL:O	4:A:44:ASP:HB2	2.07	0.55
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.26	0.55
1:0:271:C:H41	1:0:378:A:H2	1.54	0.55
32:I:106:LYS:O	32:I:110:GLU:HG3	2.06	0.55
13:K:23:ASN:HD21	13:K:107:THR:HB	1.71	0.55
20:R:29:LYS:NZ	40:R:9451:HOH:O	2.39	0.55
23:U:17:THR:HG22	23:U:18:GLY:N	2.21	0.55
1:0:1972:U:C2'	1:0:1973:A:H5''	2.36	0.55
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.89	0.55
6:C:184:ARG:HB3	40:C:9172:HOH:O	2.07	0.55
17:O:96:VAL:CG1	17:O:100:GLN:HB2	2.37	0.55
27:Y:106:THR:HG22	27:Y:107:PRO:O	2.07	0.55
1:0:2419:U:H5''	1:0:2420:G:H5'	1.89	0.55
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.71	0.55
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.71	0.55
1:0:138:U:H5''	1:0:139:C:OP2	2.06	0.55
1:0:2515:C:H2'	1:0:2516:G:O4'	2.06	0.55
32:I:129:VAL:O	32:I:129:VAL:HG12	2.07	0.55
12:J:131:THR:HG22	12:J:134:GLU:N	2.15	0.55
21:S:53:ASN:N	21:S:53:ASN:HD22	2.05	0.55
1:0:1736:A:H1'	40:0:7921:HOH:O	2.06	0.55
1:0:21:G:H5''	20:R:1:GLY:O	2.07	0.55
9:F:31:LYS:HE3	40:F:2623:HOH:O	2.06	0.55
4:A:167:LYS:CB	28:Z:29:ILE:HD13	2.36	0.55
1:0:1189:A:H1'	1:0:1209:C:H1'	1.89	0.55
1:0:291:C:H2'	1:0:292:G:O4'	2.06	0.55
1:0:952:G:N3	1:0:2302:A:H2'	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:11:ASP:O	9:F:14:ASP:HB2	2.07	0.55
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.37	0.55
11:H:116:ALA:O	11:H:117:PHE:C	2.46	0.55
1:0:1724:U:H5''	40:0:4281:HOH:O	2.06	0.55
1:0:1886:A:H4'	40:Z:9206:HOH:O	2.07	0.55
2:9:3002:U:OP2	2:9:3003:A:H5'	2.07	0.55
2:9:3051:A:H5'	16:N:160:SER:HB3	1.89	0.55
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.36	0.55
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.36	0.55
1:0:20:G:H21	20:R:117:HIS:HD2	1.53	0.55
1:0:2421:G:H2'	40:0:4620:HOH:O	2.06	0.54
1:0:485:A:N3	1:0:487:G:H5''	2.21	0.54
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.42	0.54
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.37	0.54
8:E:126:ILE:HB	8:E:131:LEU:CD2	2.37	0.54
1:0:1786:C:OP1	18:P:74:GLN:HG2	2.06	0.54
1:0:2102:G:H5''	1:0:2538:A:C2	2.42	0.54
8:E:81:GLU:HG2	8:E:134:SER:HB3	1.88	0.54
1:0:475:G:OP1	6:C:73:LEU:HD22	2.07	0.54
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.89	0.54
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.37	0.54
12:J:107:ASN:HD22	12:J:109:TYR:H	1.53	0.54
1:0:1086:A:C6	25:W:11:VAL:HG11	2.42	0.54
1:0:1926:G:H2'	1:0:1927:A:C8	2.42	0.54
1:0:2032:U:C2'	1:0:2033:G:H5''	2.38	0.54
1:0:2748:G:H2'	40:0:7878:HOH:O	2.06	0.54
30:2:20:ARG:HG3	30:2:21:VAL:H	1.72	0.54
4:A:65:ARG:C	4:A:66:ARG:HG3	2.28	0.54
5:B:40:GLY:HA3	40:B:9639:HOH:O	2.08	0.54
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.37	0.54
1:0:709:G:O2'	17:O:25:VAL:CG1	2.55	0.54
26:X:72:VAL:CG2	26:X:85:VAL:HG12	2.33	0.54
1:0:1132:A:N6	1:0:1229:C:H2'	2.23	0.54
1:0:834:G:H4'	1:0:835:U:OP2	2.07	0.54
1:0:951:A:C2'	1:0:952:G:H5'	2.38	0.54
5:B:97:LEU:O	5:B:98:THR:HG23	2.07	0.54
6:C:76:ARG:CG	6:C:76:ARG:HH11	2.21	0.54
11:H:79:GLU:C	11:H:80:GLU:HG3	2.26	0.54
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.42	0.54
1:0:497:A:H2'	1:0:498:A:C5'	2.38	0.54
4:A:36:ASP:O	4:A:38:ILE:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:297:VAL:HB	40:B:9599:HOH:O	2.08	0.54
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.38	0.54
16:N:154:LEU:CG	16:N:155:GLU:H	2.19	0.54
22:T:41:ARG:HH11	22:T:41:ARG:CG	2.07	0.54
1:0:1626:A:H2'	1:0:1627:G:O4'	2.08	0.54
1:0:415:A:O2'	1:0:416:G:H5'	2.08	0.54
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.08	0.54
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.17	0.54
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.90	0.54
6:C:214:THR:HG22	6:C:216:SER:H	1.72	0.54
32:I:113:HIS:N	32:I:114:PRO:CD	2.70	0.54
1:0:1119:G:N2	1:0:1246:A:N1	2.56	0.54
1:0:1829:A:H61	28:Z:18:TYR:H	1.56	0.54
1:0:1838:U:H1'	1:0:2644:C:O4'	2.08	0.54
1:0:2326:U:H4'	1:0:2412:G:C4'	2.38	0.54
1:0:2717:C:O2'	1:0:2718:C:H5''	2.06	0.54
1:0:69:A:H5'	1:0:69:A:C8	2.42	0.54
40:0:5195:HOH:O	21:S:23:LYS:HE2	2.07	0.54
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.56	0.54
24:V:20:LEU:HD22	24:V:60:GLN:NE2	2.18	0.54
1:0:1525:G:H5'	1:0:1526:A:OP2	2.08	0.54
1:0:2717:C:H2'	1:0:2718:C:C5'	2.35	0.54
11:H:76:GLU:C	11:H:77:LEU:HD23	2.28	0.54
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.43	0.54
17:O:39:THR:O	17:O:115:ARG:NH2	2.41	0.54
1:0:2862:G:H4'	5:B:336:GLN:O	2.07	0.54
31:3:38:ARG:CB	31:3:42:ARG:HH12	2.11	0.54
2:9:3076:G:C3'	2:9:3077:A:H5''	2.31	0.54
7:D:59:GLY:O	7:D:61:PHE:N	2.39	0.54
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.43	0.54
15:M:89:THR:O	15:M:89:THR:HG22	2.08	0.54
25:W:13:MET:CE	25:W:18:GLN:HA	2.36	0.54
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.89	0.54
1:0:1667:A:C8	1:0:1667:A:H5'	2.40	0.53
4:A:36:ASP:C	4:A:38:ILE:H	2.12	0.53
9:F:40:ILE:HD11	9:F:48:VAL:HG11	1.89	0.53
17:O:78:ALA:C	17:O:98:LEU:HD13	2.28	0.53
1:0:1181:A:N1	1:0:1192:A:O2'	2.40	0.53
1:0:1834:C:H2'	1:0:1840:A:N6	2.23	0.53
1:0:441:A:H1'	1:0:442:A:N7	2.23	0.53
7:D:167:GLU:C	7:D:169:THR:H	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.90	0.53
11:H:21:THR:O	11:H:120:ILE:HD12	2.07	0.53
1:O:1086:A:OP1	25:W:9:GLY:N	2.40	0.53
1:O:1677:U:OP2	30:2:8:LYS:NZ	2.41	0.53
2:9:3092:G:H2'	2:9:3093:A:C8	2.44	0.53
1:O:1943:C:H4'	4:A:211:LYS:O	2.09	0.53
1:O:1654:U:H2'	4:A:47:HIS:HD2	1.72	0.53
4:A:81:GLN:HB2	4:A:92:ASN:ND2	2.24	0.53
7:D:44:ILE:HG12	7:D:83:PHE:HE1	1.73	0.53
17:O:88:LYS:HD3	40:O:7061:HOH:O	2.08	0.53
19:Q:62:THR:O	19:Q:64:GLU:HG2	2.08	0.53
26:X:72:VAL:HG22	26:X:85:VAL:CG1	2.34	0.53
1:O:2795:C:O2'	1:O:2796:U:H5'	2.09	0.53
2:9:3020:G:O2'	2:9:3021:G:H5'	2.08	0.53
2:9:3052:A:H2'	2:9:3053:G:O4'	2.08	0.53
5:B:185:GLY:HA2	40:B:9627:HOH:O	2.08	0.53
2:9:3029:C:C2'	2:9:3030:C:H5'	2.38	0.53
5:B:10:SER:O	5:B:16:ARG:NH1	2.40	0.53
5:B:139:ASP:HB2	5:B:165:ARG:HE	1.73	0.53
5:B:321:PRO:HG3	40:B:9594:HOH:O	2.08	0.53
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.91	0.53
12:J:131:THR:HB	12:J:134:GLU:OE1	2.09	0.53
6:C:27:ARG:HD2	17:O:5:PRO:HD2	1.89	0.53
28:Z:11:SER:O	28:Z:14:PHE:HB2	2.08	0.53
1:O:2502:C:H2'	1:O:2503:A:H5'	1.91	0.53
29:1:10:LYS:HG3	40:1:9489:HOH:O	2.07	0.53
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.91	0.53
13:K:49:LEU:CD1	13:K:80:ILE:HD13	2.37	0.53
25:W:139:GLY:O	25:W:141:HIS:HD2	1.90	0.53
28:Z:50:GLN:HB2	28:Z:54:ILE:HG22	1.91	0.53
1:O:1202:A:H2'	1:O:1203:G:O4'	2.09	0.53
1:O:1205:U:C2'	1:O:1206:U:H5''	2.37	0.53
1:O:1295:G:H5''	14:L:14:GLY:O	2.09	0.53
1:O:622:G:P	27:Y:148:GLY:HA3	2.48	0.53
1:O:706:G:N2	1:O:707:C:N4	2.57	0.53
6:C:218:VAL:HG12	40:C:9232:HOH:O	2.08	0.53
20:R:114:VAL:HA	20:R:144:GLU:O	2.08	0.53
22:T:48:VAL:HG12	22:T:49:GLU:N	2.24	0.53
25:W:88:THR:HG22	25:W:89:ASP:H	1.72	0.53
1:O:816:G:C6	1:O:817:G:N1	2.77	0.53
29:1:25:LYS:O	29:1:25:LYS:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:162:MET:HE3	5:B:310:ARG:HD3	1.90	0.53
14:L:36:ASP:HB2	40:L:9434:HOH:O	2.08	0.53
22:T:41:ARG:NH1	22:T:42:VAL:O	2.42	0.53
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.41	0.53
1:O:1845:A:OP2	4:A:190:ARG:NH1	2.42	0.53
1:O:185:G:O3'	1:O:186:A:H4'	2.09	0.53
1:O:2414:A:H2'	1:O:2415:A:C8	2.44	0.53
1:O:553:G:P	27:Y:204:ARG:NH2	2.81	0.53
2:9:3014:G:H2'	2:9:3015:C:H5'	1.91	0.53
4:A:217:ARG:CG	4:A:217:ARG:HH11	2.21	0.53
1:O:1654:U:H2'	4:A:47:HIS:CD2	2.44	0.53
14:L:104:ASP:HB2	40:L:9464:HOH:O	2.09	0.53
25:W:4:LEU:HD23	25:W:54:PHE:CB	2.35	0.53
4:A:96:LEU:O	4:A:131:HIS:HE1	1.92	0.53
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.91	0.53
6:C:180:SER:HB2	40:C:9252:HOH:O	2.08	0.53
7:D:172:VAL:CG1	7:D:173:GLU:H	2.14	0.53
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.90	0.53
9:F:27:GLY:HA3	9:F:101:ALA:O	2.09	0.53
17:O:87:THR:O	17:O:91:GLN:HG3	2.09	0.53
25:W:78:ASP:HB2	40:W:6694:HOH:O	2.09	0.53
1:O:2587:OMU:H6	1:O:2587:OMU:O5'	2.09	0.52
1:O:2720:C:O2	13:K:87:ARG:NH2	2.42	0.52
24:V:12:THR:HB	24:V:15:GLU:OE2	2.09	0.52
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.90	0.52
1:O:204:A:C2'	1:O:205:U:H5'	2.38	0.52
1:O:2533:C:C6	1:O:2533:C:H5'	2.43	0.52
1:O:2896:A:H5''	40:X:5399:HOH:O	2.08	0.52
1:O:949:U:C4'	19:Q:95:GLU:HA	2.39	0.52
4:A:35:GLY:O	4:A:36:ASP:CB	2.56	0.52
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.74	0.52
5:B:145:HIS:HD2	5:B:146:THR:O	1.91	0.52
6:C:118:THR:O	6:C:136:VAL:HG13	2.09	0.52
6:C:236:THR:H	6:C:239:ALA:HB3	1.73	0.52
11:H:39:ASP:HB2	11:H:42:ASP:OD2	2.08	0.52
14:L:144:ASP:HA	14:L:147:GLU:OE1	2.10	0.52
20:R:99:ALA:CB	20:R:109:MET:HE3	2.38	0.52
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.44	0.52
1:O:1482:A:O2'	1:O:1483:C:H5'	2.09	0.52
1:O:2324:G:N2	1:O:2377:U:H1'	2.24	0.52
5:B:190:MET:CE	5:B:194:PHE:CD1	2.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:130:VAL:HG12	12:J:131:THR:H	1.74	0.52
15:M:158:ARG:HB2	15:M:163:LEU:HB2	1.89	0.52
1:0:1118:A:C8	1:0:1118:A:C3'	2.87	0.52
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.09	0.52
15:M:83:SER:HB2	31:3:47:GLY:CA	2.39	0.52
2:9:3044:A:O4'	7:D:76:ARG:NE	2.42	0.52
12:J:76:ASP:HA	40:J:5907:HOH:O	2.09	0.52
1:0:2296:C:H2'	1:0:2297:U:H6	1.73	0.52
1:0:2883:A:H2'	1:0:2884:G:O4'	2.10	0.52
2:9:3023:U:O2'	2:9:3024:U:H4'	2.10	0.52
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.91	0.52
22:T:48:VAL:HG12	22:T:96:VAL:HG22	1.92	0.52
1:0:1189:A:H1'	1:0:1209:C:C1'	2.40	0.52
1:0:338:C:H5''	40:C:9229:HOH:O	2.10	0.52
1:0:40:C:H4'	40:0:7388:HOH:O	2.08	0.52
40:0:7894:HOH:O	31:3:61:PRO:HG2	2.09	0.52
13:K:118:ALA:CA	13:K:125:ALA:HB2	2.35	0.52
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.21	0.52
1:0:2786:G:H2'	40:0:7552:HOH:O	2.10	0.52
1:0:2812:A:C2	1:0:2814:A:N6	2.69	0.52
2:9:3107:C:H5	40:9:3167:HOH:O	1.92	0.52
5:B:53:LEU:HD21	5:B:270:ILE:HD12	1.92	0.52
15:M:68:ARG:HE	15:M:73:ARG:NE	2.08	0.52
15:M:70:GLY:HA3	15:M:73:ARG:NH2	2.25	0.52
16:N:154:LEU:O	16:N:155:GLU:CB	2.58	0.52
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.92	0.52
25:W:65:VAL:HA	25:W:68:THR:HG22	1.91	0.52
1:0:1333:U:H2'	1:0:1334:C:H6	1.74	0.52
1:0:1943:C:O4'	4:A:212:PRO:HA	2.08	0.52
1:0:558:C:C2'	1:0:559:U:C5'	2.88	0.52
5:B:58:PRO:HA	5:B:63:GLU:CD	2.31	0.52
21:S:52:VAL:C	21:S:53:ASN:HD22	2.12	0.52
1:0:1476:A:O2'	1:0:1868:G:H5'	2.10	0.52
1:0:2840:A:OP1	5:B:211:THR:CG2	2.54	0.52
2:9:3008:G:H4'	19:Q:27:GLN:NE2	2.25	0.52
6:C:136:VAL:HG22	6:C:137:PRO:HA	1.92	0.52
7:D:128:LEU:HB2	40:D:6007:HOH:O	2.08	0.52
2:9:3041:C:H4'	7:D:48:MET:HB3	1.92	0.52
9:F:84:GLY:O	9:F:89:LEU:HB2	2.10	0.52
14:L:35:ARG:HH12	14:L:43:HIS:CD2	2.28	0.52
15:M:57:LYS:HE2	15:M:140:ALA:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:516:A:H5'	40:0:6128:HOH:O	2.10	0.52
6:C:194:PHE:HA	6:C:234:VAL:HG13	1.92	0.52
8:E:133:VAL:HG12	8:E:141:VAL:HG13	1.92	0.52
13:K:14:LYS:HG3	13:K:32:ILE:O	2.09	0.52
1:0:2825:C:H4'	1:0:2826:G:O5'	2.10	0.51
1:0:706:G:N2	1:0:707:C:H41	2.08	0.51
1:0:92:G:H4'	24:V:44:GLY:HA3	1.92	0.51
40:0:7793:HOH:O	5:B:211:THR:HG21	2.08	0.51
5:B:62:ARG:HA	5:B:65:MET:CE	2.40	0.51
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.10	0.51
14:L:11:ARG:NH2	14:L:18:HIS:CG	2.78	0.51
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.10	0.51
27:Y:115:ARG:HH11	27:Y:115:ARG:HB3	1.75	0.51
27:Y:144:ARG:NH1	40:Y:9374:HOH:O	2.38	0.51
1:0:1057:A:H1'	1:0:2492:U:O2'	2.10	0.51
1:0:2578:G:C8	1:0:2578:G:H5'	2.42	0.51
6:C:133:ARG:HG2	6:C:134:ASP:N	2.25	0.51
1:0:475:G:OP1	6:C:73:LEU:CD2	2.58	0.51
15:M:81:ARG:HG2	15:M:85:ARG:O	2.09	0.51
18:P:40:VAL:O	18:P:44:VAL:HG23	2.10	0.51
22:T:48:VAL:HG11	22:T:96:VAL:CG1	2.38	0.51
25:W:105:THR:HA	25:W:109:GLU:OE1	2.10	0.51
1:0:1878:G:O2'	1:0:1879:U:C6	2.61	0.51
1:0:447:A:OP1	22:T:2:LYS:HG2	2.11	0.51
31:3:70:ARG:NH1	31:3:77:ALA:CB	2.73	0.51
6:C:156:LEU:O	6:C:160:LEU:HG	2.11	0.51
18:P:89:ASN:HB3	18:P:92:GLU:CB	2.40	0.51
23:U:17:THR:CG2	23:U:18:GLY:N	2.73	0.51
1:0:1342:C:C2'	1:0:1343:C:H5'	2.40	0.51
1:0:236:A:H4'	1:0:237:G:H5'	1.92	0.51
1:0:451:C:O2'	1:0:452:G:H5'	2.09	0.51
4:A:223:ARG:NH1	40:A:9549:HOH:O	2.41	0.51
7:D:25:MET:CE	7:D:41:LEU:HG	2.38	0.51
1:0:1186:C:H5''	32:I:119:TYR:CE1	2.45	0.51
15:M:120:VAL:HG11	15:M:130:GLU:HG3	1.91	0.51
26:X:41:PHE:O	26:X:43:VAL:HG23	2.11	0.51
27:Y:174:VAL:CG1	27:Y:177:LYS:HD2	2.35	0.51
1:0:1679:C:H5'	40:0:9927:HOH:O	2.11	0.51
6:C:84:VAL:HG12	6:C:85:LYS:HG2	1.93	0.51
8:E:131:LEU:HD12	8:E:166:VAL:HG11	1.92	0.51
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.10	0.51
12:J:130:VAL:HG12	12:J:131:THR:N	2.26	0.51
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.24	0.51
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.93	0.51
27:Y:151:SER:HB3	27:Y:154:ARG:CB	2.38	0.51
1:0:157:G:H4'	15:M:95:LYS:HE2	1.92	0.51
1:0:1745:G:H22	1:0:2033:G:H5'	1.76	0.51
1:0:2779:G:H21	8:E:143:GLN:NE2	2.09	0.51
1:0:304:G:H1'	1:0:347:A:N6	2.25	0.51
40:0:5465:HOH:O	6:C:202:THR:HB	2.10	0.51
8:E:81:GLU:O	8:E:172:PRO:HD3	2.11	0.51
1:0:164:G:H4'	14:L:30:ARG:HD3	1.93	0.51
40:9:1361:HOH:O	16:N:41:LYS:HE3	2.10	0.51
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.93	0.51
1:0:1098:A:O3'	25:W:129:LYS:HE2	2.10	0.51
1:0:21:G:H4'	20:R:2:ILE:HG22	1.92	0.51
1:0:2769:C:H2'	1:0:2770:G:H5'	1.92	0.51
7:D:51:ARG:HD3	40:D:7636:HOH:O	2.11	0.51
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.34	0.51
12:J:50:GLU:O	12:J:54:VAL:HG23	2.10	0.51
40:0:7883:HOH:O	15:M:91:ILE:HG23	2.11	0.51
25:W:149:LEU:HG	25:W:153:MET:CE	2.40	0.51
27:Y:170:SER:OG	27:Y:175:ARG:HG3	2.10	0.51
1:0:117:A:H2'	1:0:118:G:O4'	2.11	0.51
29:1:13:THR:HG22	29:1:14:THR:N	2.26	0.51
31:3:56:PRO:HA	40:3:9483:HOH:O	2.11	0.51
31:3:65:THR:CG2	31:3:88:LEU:HD22	2.41	0.51
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.76	0.51
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.46	0.51
26:X:15:ARG:HB3	26:X:15:ARG:NH1	2.25	0.51
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.46	0.51
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.45	0.51
1:0:317:A:H5''	22:T:52:ARG:HD2	1.93	0.51
1:0:776:A:OP1	29:1:28:HIS:HE1	1.94	0.51
29:1:45:ARG:NH2	40:1:9484:HOH:O	2.28	0.51
40:0:3716:HOH:O	31:3:46:ILE:HG12	2.11	0.51
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.93	0.51
11:H:143:ALA:O	11:H:146:VAL:HG12	2.11	0.51
20:R:4:TYR:CE1	20:R:15:LYS:HD3	2.46	0.51
1:0:1234:U:N3	5:B:244:PRO:HB3	2.26	0.51
1:0:1118:A:H62	1:0:1244:U:H3	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2011:A:H5'	1:0:2013:G:H1'	1.93	0.51
1:0:2032:U:H2'	1:0:2033:G:H5''	1.91	0.51
1:0:249:G:O2'	1:0:250:C:H5'	2.11	0.51
1:0:949:U:O2'	19:Q:40:HIS:HE1	1.94	0.51
30:2:36:ASN:HB3	30:2:39:ARG:HG3	1.93	0.51
7:D:159:PRO:O	7:D:163:VAL:HG23	2.11	0.51
11:H:170:ASN:N	11:H:170:ASN:ND2	2.59	0.51
13:K:81:ARG:HD3	13:K:87:ARG:CZ	2.41	0.51
14:L:75:LEU:N	14:L:75:LEU:HD23	2.26	0.51
24:V:12:THR:HG23	24:V:14:ALA:N	2.26	0.51
25:W:4:LEU:CD2	25:W:52:VAL:HG21	2.36	0.51
1:0:2070:G:H2'	1:0:2072:G:OP1	2.10	0.50
1:0:2432:C:H2'	1:0:2433:A:H8	1.76	0.50
1:0:407:A:H2'	1:0:408:A:C8	2.46	0.50
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.40	0.50
2:9:3049:G:O2'	2:9:3050:G:H5'	2.12	0.50
5:B:171:VAL:HG23	5:B:172:SER:N	2.26	0.50
1:0:721:A:H4'	17:O:51:TYR:CD1	2.46	0.50
24:V:64:GLY:O	24:V:65:ASP:HB2	2.09	0.50
1:0:1803:C:H2'	1:0:1804:A:C8	2.47	0.50
1:0:2054:A:C2	20:R:128:ARG:NH2	2.79	0.50
1:0:812:A:H1'	40:0:4503:HOH:O	2.12	0.50
5:B:150:ALA:O	5:B:152:PRO:HD3	2.11	0.50
5:B:51:VAL:HG22	5:B:53:LEU:CD1	2.41	0.50
6:C:234:VAL:HG13	6:C:234:VAL:O	2.11	0.50
32:I:128:VAL:C	32:I:130:GLY:H	2.15	0.50
16:N:36:ALA:HB1	16:N:118:ILE:HD12	1.92	0.50
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.41	0.50
1:0:1180:U:H1'	40:0:3801:HOH:O	2.12	0.50
1:0:1203:G:O2'	1:0:1204:C:H5'	2.11	0.50
1:0:1268:C:O2'	1:0:1269:G:H5'	2.11	0.50
1:0:1902:G:H2'	1:0:1903:U:O4'	2.11	0.50
1:0:2895:C:H4'	40:X:4132:HOH:O	2.11	0.50
15:M:83:SER:HB2	31:3:47:GLY:HA3	1.93	0.50
5:B:140:LEU:HD13	5:B:175:LEU:HA	1.91	0.50
12:J:6:PHE:HB3	12:J:109:TYR:OH	2.11	0.50
1:0:1500:U:P	18:P:41:ARG:HH22	2.34	0.50
1:0:2612:A:H4'	40:0:4231:HOH:O	2.10	0.50
1:0:2769:C:H2'	1:0:2770:G:C5'	2.41	0.50
1:0:2769:C:O2'	1:0:2770:G:H5'	2.12	0.50
1:0:2661:U:H3	1:0:2812:A:H62	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:132:CYS:C	32:I:134:SER:N	2.63	0.50
14:L:143:THR:O	14:L:147:GLU:HG3	2.11	0.50
16:N:115:VAL:HG22	40:N:9358:HOH:O	2.11	0.50
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.92	0.50
1:O:1972:U:H2'	1:O:1973:A:C5'	2.41	0.50
1:O:2089:A:O2'	1:O:2090:G:H5'	2.11	0.50
1:O:497:A:H2'	1:O:498:A:H5'	1.94	0.50
4:A:210:GLY:N	40:A:9621:HOH:O	2.44	0.50
7:D:99:ASP:HB2	7:D:103:ASN:HB2	1.93	0.50
7:D:103:ASN:ND2	7:D:133:ASN:HD22	2.09	0.50
15:M:76:ARG:HA	40:M:9329:HOH:O	2.11	0.50
27:Y:145:LYS:HE2	40:Y:9404:HOH:O	2.11	0.50
1:O:1298:U:H2'	1:O:1299:G:C8	2.45	0.50
1:O:1942:A:H3'	40:O:7693:HOH:O	2.12	0.50
6:C:236:THR:HG22	6:C:239:ALA:CB	2.42	0.50
8:E:5:LEU:HD21	8:E:66:GLN:HG3	1.93	0.50
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.47	0.50
1:O:1198:U:H2'	1:O:1200:A:OP2	2.11	0.50
1:O:1666:C:C2'	1:O:1667:A:C5'	2.90	0.50
9:F:99:THR:O	9:F:100:ASP:HB2	2.10	0.50
25:W:122:ARG:NH2	40:W:5817:HOH:O	2.40	0.50
26:X:34:ARG:NH1	26:X:48:VAL:O	2.45	0.50
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.94	0.50
6:C:57:PRO:HG2	6:C:73:LEU:HD13	1.94	0.50
11:H:30:GLN:H	11:H:66:ARG:HH11	1.60	0.50
25:W:128:VAL:O	25:W:138:LEU:HD11	2.12	0.50
1:O:812:A:H2'	1:O:813:C:C6	2.46	0.50
4:A:36:ASP:CB	4:A:85:SER:HB2	2.41	0.50
5:B:132:HIS:NE2	5:B:171:VAL:HG23	2.27	0.50
5:B:41:PHE:CG	5:B:79:MET:HE2	2.47	0.50
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.41	0.50
22:T:23:VAL:HG23	22:T:41:ARG:HG3	1.93	0.50
26:X:7:GLU:HA	26:X:74:ALA:O	2.12	0.50
27:Y:189:ASN:CA	27:Y:217:ILE:HD11	2.38	0.50
1:O:2472:C:O2'	1:O:2634:G:H4'	2.12	0.49
1:O:2748:G:H4'	1:O:2749:U:C5'	2.41	0.49
1:O:834:G:H3'	1:O:835:U:H4'	1.94	0.49
1:O:1853:C:OP1	4:A:231:LYS:HG3	2.12	0.49
1:O:475:G:C5'	6:C:73:LEU:HD23	2.43	0.49
1:O:797:A:C5'	28:Z:10:ARG:N	2.73	0.49
1:O:255:A:H2'	1:O:256:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:799:C:O2'	1:0:800:G:H5'	2.12	0.49
1:0:1486:A:C5	30:2:2:LYS:HG3	2.46	0.49
2:9:3049:G:C2'	2:9:3050:G:H5'	2.42	0.49
8:E:154:ILE:HD11	8:E:157:LYS:HE2	1.94	0.49
8:E:20:ILE:HD12	8:E:33:LEU:CD1	2.41	0.49
1:0:1180:U:O2'	32:I:92:PRO:HD2	2.13	0.49
1:0:1845:A:O2'	1:0:1846:U:H5'	2.12	0.49
1:0:1878:G:O2'	1:0:1879:U:OP2	2.29	0.49
1:0:2050:G:H5''	20:R:80:TYR:O	2.13	0.49
1:0:2072:G:H3'	1:0:2073:G:C5'	2.42	0.49
1:0:2265:U:H2'	1:0:2266:A:C8	2.47	0.49
1:0:248:A:H5'	1:0:249:G:OP2	2.13	0.49
1:0:1881:A:OP1	4:A:199:HIS:HE1	1.95	0.49
5:B:276:ASP:O	5:B:279:THR:HG22	2.12	0.49
7:D:10:PHE:CG	7:D:11:HIS:N	2.81	0.49
32:I:138:THR:HG22	32:I:139:ILE:N	2.27	0.49
26:X:61:ARG:HB2	26:X:65:ASN:HB2	1.94	0.49
1:0:905:C:OP1	27:Y:144:ARG:NH1	2.45	0.49
1:0:1826:C:O2'	1:0:1827:G:H5'	2.12	0.49
1:0:2326:U:H4'	1:0:2412:G:H4'	1.95	0.49
31:3:69:TYR:O	31:3:77:ALA:HA	2.13	0.49
5:B:144:THR:HG21	40:B:9618:HOH:O	2.12	0.49
9:F:5:ASP:O	9:F:119:ARG:NH1	2.45	0.49
12:J:131:THR:HG23	12:J:133:GLY:H	1.78	0.49
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.94	0.49
17:O:14:LEU:CG	17:O:102:ILE:HD11	2.42	0.49
1:0:1077:G:H2'	1:0:1080:C:H42	1.76	0.49
1:0:1940:C:H4'	40:0:7693:HOH:O	2.11	0.49
1:0:2016:U:H2'	1:0:2017:U:O4'	2.13	0.49
1:0:259:G:H21	15:M:58:GLN:NE2	2.10	0.49
1:0:816:G:H5'	1:0:1598:A:H4'	1.94	0.49
5:B:101:TRP:HB2	5:B:119:HIS:CD2	2.47	0.49
5:B:254:GLN:HG2	5:B:255:GLY:H	1.77	0.49
5:B:277:GLU:N	5:B:278:PRO:HD2	2.27	0.49
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.95	0.49
14:L:27:ARG:HH21	14:L:30:ARG:HG2	1.77	0.49
14:L:74:THR:OG1	14:L:75:LEU:HD23	2.13	0.49
23:U:47:ARG:HG2	23:U:54:THR:CG2	2.42	0.49
28:Z:42:CYS:SG	28:Z:44:GLU:HB2	2.53	0.49
1:0:218:C:P	31:3:39:GLN:HE21	2.34	0.49
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.12	0.49
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	2.13	0.49
1:0:1264:U:P	25:W:117:ARG:HH22	2.35	0.49
28:Z:15:GLY:HA3	40:Z:9229:HOH:O	2.12	0.49
1:0:1474:C:H6	1:0:1474:C:C5'	2.18	0.49
1:0:2101:A:H5'	6:C:63:SER:HB3	1.95	0.49
1:0:2112:A:H2'	1:0:2113:G:C8	2.48	0.49
1:0:2372:A:H2'	1:0:2373:U:C6	2.48	0.49
1:0:2374:A:H2'	1:0:2375:G:C8	2.48	0.49
1:0:380:A:H2'	40:M:9440:HOH:O	2.12	0.49
2:9:3052:A:O2'	2:9:3053:G:H5'	2.12	0.49
5:B:77:PRO:HG3	40:B:9571:HOH:O	2.12	0.49
7:D:25:MET:CE	7:D:40:ILE:HD11	2.43	0.49
7:D:62:ASP:HA	40:D:4233:HOH:O	2.12	0.49
8:E:166:VAL:HG12	40:E:3134:HOH:O	2.13	0.49
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.77	0.49
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.43	0.49
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.76	0.49
1:0:2036:C:O4'	13:K:44:LEU:HG	2.13	0.49
18:P:103:THR:O	18:P:107:GLU:HG3	2.13	0.49
1:0:120:A:H2'	1:0:120:A:N3	2.28	0.49
1:0:653:C:H2'	1:0:654:A:C8	2.47	0.49
1:0:1688:G:O2'	29:1:5:THR:HG23	2.13	0.49
11:H:88:ARG:NH1	11:H:135:THR:OG1	2.45	0.49
21:S:57:THR:HG22	21:S:59:ASP:HB2	1.95	0.49
1:0:317:A:OP1	22:T:52:ARG:O	2.31	0.49
22:T:78:THR:HB	22:T:87:VAL:O	2.13	0.49
1:0:1314:U:H2'	40:0:6340:HOH:O	2.13	0.49
1:0:1476:A:H1'	1:0:1867:G:O2'	2.12	0.49
1:0:2133:U:H4'	1:0:2134:G:H5'	1.93	0.49
1:0:2281:C:C2'	1:0:2282:U:H5'	2.42	0.49
1:0:2415:A:C2'	1:0:2416:G:H5'	2.43	0.49
1:0:2912:C:H2'	1:0:2913:A:O4'	2.12	0.49
1:0:946:C:H2'	1:0:947:U:H6	1.78	0.49
31:3:7:PHE:CE1	31:3:9:THR:HB	2.48	0.49
5:B:102:THR:HG21	5:B:182:VAL:O	2.13	0.49
7:D:23:VAL:O	7:D:23:VAL:HG23	2.12	0.49
8:E:119:HIS:HE1	8:E:147:ASP:OD2	1.95	0.49
8:E:84:MET:HB2	8:E:131:LEU:HB2	1.94	0.49
14:L:119:THR:HG23	14:L:139:SER:OG	2.12	0.49
16:N:67:ALA:HA	16:N:71:TRP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:48:VAL:HG11	22:T:96:VAL:HG22	1.95	0.49
1:0:1204:C:H2'	1:0:1205:U:O4'	2.12	0.49
1:0:2824:C:O3'	1:0:2825:C:H6	1.96	0.49
2:9:3114:G:O6	16:N:11:ARG:HD3	2.12	0.49
4:A:191:GLY:HA2	4:A:194:MET:CE	2.42	0.49
6:C:20:ASP:O	6:C:23:GLU:HB2	2.12	0.49
6:C:45:ASP:OD2	6:C:98:ARG:HD2	2.13	0.49
9:F:110:ASP:O	9:F:114:LYS:HG3	2.12	0.49
9:F:57:GLU:O	9:F:61:MET:HG3	2.13	0.49
20:R:132:ARG:NH2	40:R:9500:HOH:O	2.46	0.49
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.13	0.49
25:W:38:THR:O	25:W:42:ARG:HB2	2.12	0.49
1:0:1166:A:H1'	1:0:1192:A:N3	2.27	0.48
1:0:1878:G:O2'	1:0:1879:U:P	2.71	0.48
1:0:371:U:H2'	1:0:372:A:C8	2.46	0.48
2:9:3092:G:H2'	2:9:3093:A:H8	1.78	0.48
5:B:254:GLN:NE2	40:B:9585:HOH:O	2.46	0.48
14:L:129:ALA:O	14:L:133:VAL:HG23	2.13	0.48
15:M:72:ALA:HB2	15:M:93:ARG:HG2	1.94	0.48
17:O:25:VAL:HG23	17:O:26:TRP:H	1.78	0.48
1:0:1174:A:C6	1:0:1201:C:H4'	2.48	0.48
1:0:1218:U:H2'	1:0:1219:U:C6	2.49	0.48
1:0:2748:G:H4'	1:0:2749:U:H5'	1.94	0.48
2:9:3064:C:C2'	2:9:3065:A:H5'	2.42	0.48
5:B:51:VAL:HG23	5:B:327:VAL:HG13	1.94	0.48
5:B:96:PRO:HG3	40:B:9628:HOH:O	2.13	0.48
6:C:237:GLU:HB2	40:C:9238:HOH:O	2.13	0.48
11:H:167:PRO:O	11:H:168:ALA:HB2	2.12	0.48
15:M:107:ARG:NH1	40:M:9380:HOH:O	2.46	0.48
1:0:1149:U:H5''	1:0:1151:G:O4'	2.13	0.48
1:0:1741:U:H3'	40:0:3343:HOH:O	2.12	0.48
2:9:3008:G:O6	16:N:11:ARG:NH1	2.44	0.48
2:9:3108:C:O2'	2:9:3109:G:H5'	2.12	0.48
40:0:7400:HOH:O	15:M:68:ARG:HB2	2.13	0.48
22:T:48:VAL:HG13	22:T:97:ARG:C	2.33	0.48
27:Y:144:ARG:CZ	40:Y:9410:HOH:O	2.59	0.48
1:0:1185:U:H5'	40:0:7803:HOH:O	2.13	0.48
1:0:1600:G:H8	1:0:1600:G:OP2	1.96	0.48
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.39	0.48
1:0:2809:G:H2'	1:0:2810:G:O4'	2.13	0.48
1:0:319:A:H4'	1:0:338:C:C5	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:951:A:O2'	1:0:952:G:H5'	2.13	0.48
4:A:69:LEU:O	4:A:71:PRO:HD3	2.13	0.48
10:G:20:VAL:O	10:G:24:VAL:HG23	2.13	0.48
11:H:95:LEU:HD11	11:H:124:ALA:HB2	1.95	0.48
1:0:1242:A:C5'	12:J:82:THR:HG23	2.31	0.48
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.78	0.48
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.43	0.48
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.67	0.48
27:Y:144:ARG:NH2	40:Y:9410:HOH:O	2.47	0.48
1:0:1187:U:H2'	1:0:1189:A:OP2	2.12	0.48
1:0:1741:U:O2'	1:0:2723:G:H4'	2.14	0.48
5:B:305:ASP:O	5:B:306:LYS:CB	2.60	0.48
9:F:60:VAL:HG12	9:F:60:VAL:O	2.14	0.48
15:M:48:LYS:HE3	15:M:52:GLN:NE2	2.28	0.48
21:S:57:THR:HG21	21:S:59:ASP:HB2	1.96	0.48
22:T:69:LYS:O	22:T:71:VAL:HG23	2.14	0.48
1:0:1422:U:H2'	1:0:1423:C:C6	2.49	0.48
1:0:368:C:H1'	40:0:5722:HOH:O	2.12	0.48
5:B:81:ALA:O	5:B:186:GLY:HA3	2.13	0.48
7:D:134:LEU:CD1	7:D:166:ILE:HD11	2.40	0.48
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.96	0.48
14:L:34:GLY:HA3	14:L:38:HIS:CE1	2.49	0.48
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.12	0.48
18:P:55:LYS:CG	18:P:56:GLY:N	2.76	0.48
23:U:47:ARG:HG2	23:U:54:THR:HG21	1.95	0.48
24:V:55:ARG:O	24:V:59:ILE:HG12	2.14	0.48
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.96	0.48
25:W:64:THR:O	25:W:68:THR:HG22	2.13	0.48
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.40	0.48
1:0:1058:A:H2'	1:0:1060:C:H5''	1.95	0.48
1:0:1947:G:H2'	1:0:1948:G:C8	2.47	0.48
1:0:1947:G:H2'	1:0:1948:G:H8	1.78	0.48
1:0:2289:G:O2'	1:0:2290:U:H5'	2.14	0.48
31:3:6:ARG:HA	31:3:20:HIS:O	2.13	0.48
2:9:3064:C:H2'	2:9:3065:A:H5'	1.95	0.48
1:0:894:A:C2	6:C:87:ARG:NH2	2.81	0.48
7:D:12:GLU:O	7:D:15:GLU:HG2	2.13	0.48
7:D:103:ASN:HD21	7:D:133:ASN:HD22	1.59	0.48
7:D:60:GLU:O	7:D:60:GLU:HG3	2.14	0.48
8:E:7:ILE:HD11	8:E:11:VAL:C	2.33	0.48
12:J:19:MET:CE	12:J:132:LEU:HD11	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3051:A:H5'	16:N:160:SER:CB	2.43	0.48
18:P:36:THR:O	18:P:39:ASP:HB2	2.13	0.48
20:R:84:ALA:O	20:R:88:PHE:HD1	1.97	0.48
22:T:48:VAL:HG11	22:T:96:VAL:CG2	2.44	0.48
25:W:5:VAL:O	25:W:52:VAL:CG2	2.62	0.48
1:0:1435:U:H5'	40:0:3189:HOH:O	2.13	0.48
1:0:2591:C:H2'	1:0:2592:G:O4'	2.14	0.48
1:0:2676:C:H4'	12:J:70:PHE:HD1	1.74	0.48
1:0:524:A:H5''	20:R:29:LYS:HD3	1.96	0.48
31:3:67:LEU:HD21	31:3:88:LEU:CD2	2.43	0.48
5:B:24:PRO:HG3	5:B:204:GLY:HA2	1.95	0.48
5:B:81:ALA:HB1	5:B:142:LEU:HD13	1.94	0.48
6:C:49:ASP:HB3	6:C:52:ALA:HB2	1.94	0.48
9:F:102:GLY:O	9:F:103:GLU:HB2	2.13	0.48
14:L:53:ARG:NH2	14:L:57:VAL:CG1	2.77	0.48
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.12	0.48
27:Y:178:HIS:CD2	27:Y:179:PRO:HD2	2.49	0.48
1:0:2411:C:H4'	40:0:5466:HOH:O	2.12	0.48
1:0:247:A:H2'	40:0:4470:HOH:O	2.13	0.48
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.95	0.48
5:B:16:ARG:NH1	40:B:9610:HOH:O	2.46	0.48
5:B:41:PHE:CB	5:B:190:MET:HE3	2.44	0.48
7:D:10:PHE:CD1	7:D:11:HIS:N	2.82	0.48
15:M:68:ARG:CD	15:M:68:ARG:O	2.56	0.48
1:0:1189:A:H3'	40:0:8033:HOH:O	2.13	0.48
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.45	0.48
1:0:2868:C:H2'	1:0:2869:G:O4'	2.14	0.48
1:0:329:A:OP2	6:C:206:ASN:HB2	2.14	0.48
38:4:9701:SPS:O1	38:4:9701:SPS:H91	2.14	0.48
8:E:81:GLU:HG2	8:E:134:SER:CB	2.42	0.48
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.96	0.48
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.49	0.48
18:P:141:ILE:C	18:P:143:ALA:H	2.16	0.48
24:V:12:THR:HG22	24:V:15:GLU:H	1.78	0.48
1:0:2498:C:O2'	1:0:2499:U:H5'	2.13	0.47
1:0:1787:C:H4'	1:0:2883:A:O4'	2.14	0.47
1:0:802:G:H2'	1:0:803:C:C6	2.49	0.47
4:A:207:GLN:O	4:A:208:HIS:HB3	2.14	0.47
5:B:80:ARG:HB2	5:B:145:HIS:CE1	2.49	0.47
1:0:328:U:O2	6:C:202:THR:HG21	2.15	0.47
25:W:4:LEU:O	25:W:32:CYS:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:61:ARG:HG3	26:X:61:ARG:HH11	1.79	0.47
1:0:907:A:H4'	1:0:1328:A:C2	2.49	0.47
1:0:2506:A:O2'	1:0:2507:G:P	2.72	0.47
1:0:285:A:H2'	1:0:286:U:O4'	2.14	0.47
1:0:462:A:H2'	40:0:5402:HOH:O	2.14	0.47
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.49	0.47
13:K:74:VAL:HG11	13:K:113:ILE:CG1	2.37	0.47
24:V:44:GLY:O	24:V:48:GLU:HG2	2.13	0.47
25:W:48:VAL:CG1	25:W:48:VAL:O	2.62	0.47
28:Z:59:TYR:HA	40:Z:9233:HOH:O	2.14	0.47
1:0:960:G:H2'	1:0:960:G:N3	2.29	0.47
6:C:218:VAL:N	40:C:9232:HOH:O	2.47	0.47
7:D:40:ILE:HG13	7:D:41:LEU:N	2.29	0.47
11:H:16:ARG:HH21	11:H:18:GLU:CD	2.17	0.47
11:H:78:GLY:C	11:H:80:GLU:H	2.18	0.47
32:I:75:THR:HA	32:I:112:LYS:HZ3	1.80	0.47
12:J:45:VAL:HG22	12:J:46:ILE:N	2.29	0.47
14:L:6:ARG:NH2	40:L:9445:HOH:O	2.47	0.47
14:L:72:ASN:HB2	40:L:9486:HOH:O	2.14	0.47
14:L:73:VAL:HG23	14:L:74:THR:N	2.22	0.47
22:T:19:ARG:HD3	22:T:67:LEU:O	2.14	0.47
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.45	0.47
1:0:2090:G:H2'	1:0:2091:G:C8	2.48	0.47
1:0:2824:C:H5''	1:0:2825:C:H5'	1.97	0.47
1:0:655:U:O2'	17:O:3:THR:HB	2.13	0.47
2:9:3014:G:C2'	2:9:3015:C:H5'	2.45	0.47
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.15	0.47
4:A:123:GLY:HA2	4:A:159:VAL:O	2.14	0.47
4:A:112:PRO:HD3	4:A:152:CYS:SG	2.55	0.47
6:C:54:LEU:HD23	6:C:79:ARG:HG3	1.96	0.47
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.47	0.47
24:V:64:GLY:O	24:V:65:ASP:CB	2.62	0.47
1:0:1120:U:H5'	1:0:1121:G:OP2	2.14	0.47
1:0:137:U:H2'	1:0:139:C:C5	2.49	0.47
1:0:2032:U:H2'	1:0:2033:G:H5'	1.95	0.47
1:0:2906:A:H5'	1:0:2907:C:O4'	2.15	0.47
1:0:57:C:H42	1:0:89:G:H1	1.61	0.47
16:N:112:GLY:HA2	16:N:137:ALA:N	2.29	0.47
17:O:77:ALA:HA	17:O:96:VAL:O	2.15	0.47
24:V:4:HIS:O	24:V:8:ILE:HG13	2.13	0.47
1:0:1015:C:H2'	1:0:1016:U:H6	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1309:U:O2'	1:0:1310:U:H5'	2.15	0.47
1:0:1477:C:H5'	1:0:1868:G:C5'	2.43	0.47
1:0:2784:A:H1'	8:E:60:SER:OG	2.15	0.47
1:0:2866:U:H4'	1:0:2867:G:H5'	1.95	0.47
1:0:541:C:O2'	1:0:542:A:H5''	2.14	0.47
1:0:883:U:H2'	1:0:883:U:O2	2.14	0.47
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.50	0.47
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.48	0.47
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.12	0.47
5:B:215:VAL:HA	5:B:220:VAL:HG22	1.97	0.47
6:C:123:LEU:O	6:C:126:ASP:N	2.47	0.47
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.80	0.47
13:K:125:ALA:O	13:K:127:ALA:N	2.44	0.47
20:R:68:HIS:CD2	20:R:76:ASP:HB2	2.49	0.47
22:T:41:ARG:NH1	22:T:41:ARG:CG	2.71	0.47
1:0:2019:A:H5'	40:0:5068:HOH:O	2.15	0.47
1:0:256:C:H2'	1:0:257:G:O4'	2.14	0.47
1:0:2580:G:N3	1:0:2600:A:H2	2.13	0.47
1:0:65:C:O2'	1:0:66:G:H5'	2.15	0.47
6:C:76:ARG:NH1	6:C:76:ARG:CG	2.78	0.47
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.38	0.47
1:0:1163:G:H5'	32:I:115:ASP:O	2.15	0.47
13:K:49:LEU:HD12	13:K:80:ILE:HG21	1.95	0.47
17:O:21:SER:OG	17:O:106:PRO:HB2	2.14	0.47
25:W:38:THR:HG22	25:W:40:ALA:H	1.79	0.47
27:Y:216:ARG:HD2	40:Y:9367:HOH:O	2.14	0.47
1:0:1020:A:H2'	1:0:1021:G:C8	2.49	0.47
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.74	0.47
1:0:1174:A:C5	1:0:1201:C:H4'	2.50	0.47
1:0:517:U:H1'	40:0:7913:HOH:O	2.14	0.47
30:2:14:LEU:HD13	30:2:47:THR:CG2	2.45	0.47
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.80	0.47
6:C:84:VAL:O	6:C:85:LYS:HB2	2.15	0.47
7:D:64:ARG:HB3	7:D:67:ASP:OD2	2.15	0.47
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.96	0.47
12:J:64:GLY:HA3	36:J:9321:CL:CL	2.51	0.47
14:L:57:VAL:O	14:L:57:VAL:HG12	2.15	0.47
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.45	0.47
18:P:64:GLU:HG2	40:P:168:HOH:O	2.15	0.47
1:0:2253:G:O2'	1:0:2254:G:H5'	2.15	0.47
1:0:2312:G:H2'	1:0:2313:C:H5'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2619:UR3:H2'	1:0:2620:U:C6	2.49	0.47
1:0:559:U:H5'	1:0:559:U:C6	2.45	0.47
4:A:43:VAL:HG12	4:A:43:VAL:O	2.14	0.47
5:B:87:TYR:O	5:B:138:GLY:N	2.33	0.47
6:C:168:ARG:NH2	6:C:190:ALA:O	2.47	0.47
8:E:102:VAL:HG11	8:E:148:ILE:HD11	1.96	0.47
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.79	0.47
15:M:98:GLN:O	15:M:102:GLU:HG3	2.15	0.47
40:0:7136:HOH:O	19:Q:13:LYS:HE2	2.14	0.47
1:0:2032:U:O2'	1:0:2033:G:H5''	2.14	0.47
1:0:2478:U:O2'	1:0:2479:A:H5'	2.15	0.47
1:0:333:G:O2'	1:0:334:G:H5'	2.15	0.47
1:0:407:A:H8	40:0:4990:HOH:O	1.96	0.47
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.79	0.47
7:D:88:LEU:HB2	7:D:89:PRO:HD3	1.97	0.47
9:F:11:ASP:HA	9:F:14:ASP:OD2	2.14	0.47
12:J:54:VAL:O	12:J:58:GLU:HG3	2.15	0.47
1:0:1753:C:O2	5:B:229:ARG:NH2	2.48	0.47
1:0:2269:C:H2'	1:0:2270:G:O4'	2.15	0.47
1:0:2679:G:H2'	1:0:2681:A:OP2	2.14	0.47
4:A:81:GLN:N	4:A:92:ASN:ND2	2.62	0.47
5:B:264:GLU:HG2	5:B:267:LYS:CE	2.45	0.47
5:B:274:GLU:HA	5:B:292:GLY:O	2.14	0.47
5:B:307:ARG:HG3	5:B:307:ARG:NH1	2.21	0.47
6:C:45:ASP:OD2	6:C:98:ARG:CD	2.63	0.47
8:E:101:GLU:HB3	8:E:117:THR:HA	1.97	0.47
8:E:11:VAL:CG1	8:E:12:ASP:N	2.78	0.47
9:F:1:PRO:H3	9:F:4:VAL:HG23	1.79	0.47
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.45	0.47
4:A:109:GLU:HG2	4:A:116:GLY:H	1.80	0.46
6:C:140:VAL:HG12	6:C:141:SER:N	2.29	0.46
7:D:151:ILE:HG23	7:D:155:HIS:HB3	1.97	0.46
7:D:95:THR:OG1	7:D:174:VAL:HG22	2.15	0.46
8:E:80:TRP:O	8:E:134:SER:HA	2.15	0.46
10:G:12:ILE:HD12	40:G:692:HOH:O	2.16	0.46
18:P:27:ARG:O	18:P:31:ILE:HG13	2.15	0.46
23:U:45:GLU:HB2	23:U:48:ASN:HD22	1.78	0.46
24:V:11:MET:HB3	24:V:15:GLU:HB2	1.96	0.46
1:0:1965:C:H6	1:0:1965:C:O5'	1.98	0.46
1:0:35:U:O2'	1:0:36:C:H5'	2.16	0.46
1:0:40:C:H6	1:0:40:C:O5'	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:848:C:H5'	40:0:7630:HOH:O	2.16	0.46
5:B:241:PRO:HD2	40:B:9646:HOH:O	2.15	0.46
6:C:21:VAL:C	6:C:23:GLU:H	2.19	0.46
8:E:100:ASP:HB2	40:E:2789:HOH:O	2.16	0.46
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.44	0.46
40:0:3801:HOH:O	32:I:92:PRO:HD3	2.14	0.46
13:K:114:ALA:HA	13:K:132:VAL:O	2.15	0.46
15:M:122:GLN:OE1	15:M:127:LYS:HE2	2.15	0.46
1:0:793:A:H5''	18:P:83:LYS:HG2	1.97	0.46
1:0:817:G:OP2	18:P:91:LYS:HE3	2.16	0.46
20:R:122:GLN:HB3	20:R:138:SER:HB2	1.96	0.46
20:R:39:THR:HB	20:R:42:GLU:CG	2.40	0.46
1:0:1183:C:H5	1:0:1192:A:OP1	1.97	0.46
1:0:1406:A:H4'	1:0:1407:A:H5''	1.95	0.46
1:0:660:A:H4'	1:0:661:G:O5'	2.15	0.46
6:C:98:ARG:NH1	6:C:98:ARG:HG2	2.29	0.46
7:D:24:HIS:HB2	7:D:72:LYS:HB3	1.98	0.46
9:F:20:LEU:HB2	9:F:49:PHE:CZ	2.50	0.46
10:G:12:ILE:N	10:G:13:PRO:CD	2.78	0.46
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.17	0.46
16:N:140:GLN:HA	16:N:143:ARG:HD3	1.97	0.46
22:T:32:ARG:HH12	22:T:38:ARG:HH12	1.62	0.46
22:T:83:ASP:OD1	22:T:85:GLU:HB3	2.15	0.46
23:U:9:CYS:HA	23:U:52:THR:HG23	1.96	0.46
24:V:32:ALA:O	24:V:35:ALA:HB3	2.16	0.46
25:W:73:LEU:HA	25:W:73:LEU:HD12	1.82	0.46
1:0:1044:C:H5''	40:0:9647:HOH:O	2.14	0.46
1:0:1236:A:C8	12:J:63:ILE:HD11	2.50	0.46
1:0:1636:G:O2'	1:0:1637:A:H5'	2.15	0.46
1:0:2613:G:O2'	1:0:2614:C:H5'	2.15	0.46
1:0:710:G:O2'	1:0:711:G:H5'	2.15	0.46
1:0:87:C:C2	30:2:30:ASP:OD2	2.68	0.46
1:0:1363:G:OP1	6:C:76:ARG:NH2	2.47	0.46
8:E:106:ASN:ND2	8:E:109:GLY:HA2	2.31	0.46
10:G:64:ASN:N	10:G:64:ASN:ND2	2.63	0.46
15:M:172:GLY:HA2	40:M:9321:HOH:O	2.15	0.46
1:0:171:C:OP2	15:M:84:LYS:HG3	2.16	0.46
15:M:99:ARG:HH21	15:M:170:ASN:ND2	2.10	0.46
16:N:89:GLY:O	16:N:92:ALA:HB3	2.15	0.46
25:W:88:THR:CG2	25:W:89:ASP:N	2.78	0.46
26:X:27:ASP:OD2	26:X:27:ASP:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1562:C:N4	40:0:6331:HOH:O	2.47	0.46
1:0:2453:G:H5''	40:L:9440:HOH:O	2.15	0.46
1:0:81:G:N3	1:0:98:A:C2	2.84	0.46
4:A:206:ARG:N	4:A:206:ARG:HD3	2.30	0.46
32:I:139:ILE:HG22	32:I:140:GLU:N	2.29	0.46
1:0:392:U:H5''	15:M:193:LYS:HB3	1.96	0.46
1:0:500:G:O2'	20:R:94:ASN:ND2	2.49	0.46
40:0:3152:HOH:O	25:W:119:HIS:HE1	1.99	0.46
26:X:86:GLU:HG3	26:X:87:ALA:O	2.16	0.46
1:0:1067:A:H5'	40:0:4882:HOH:O	2.15	0.46
1:0:1071:G:H4'	27:Y:154:ARG:NH2	2.31	0.46
1:0:1103:C:O2	12:J:86:MET:HG2	2.16	0.46
1:0:129:A:H4'	1:0:130:C:OP1	2.16	0.46
1:0:1462:C:H2'	1:0:1463:A:C8	2.51	0.46
1:0:1759:A:N3	1:0:1818:C:H2'	2.31	0.46
1:0:2748:G:OP1	1:0:2749:U:H5''	2.16	0.46
31:3:11:CYS:HB2	31:3:20:HIS:HE1	1.77	0.46
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.96	0.46
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.15	0.46
15:M:30:GLU:O	15:M:34:GLU:HG3	2.15	0.46
16:N:59:ALA:O	16:N:60:SER:HB3	2.16	0.46
1:0:136:C:H2'	1:0:137:U:O4'	2.15	0.46
1:0:2432:C:H2'	1:0:2433:A:C8	2.50	0.46
1:0:2443:C:H1'	14:L:56:LYS:HE3	1.98	0.46
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.15	0.46
5:B:337:GLY:N	40:B:9542:HOH:O	2.49	0.46
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.98	0.46
9:F:91:VAL:CG1	9:F:92:GLY:H	1.97	0.46
32:I:132:CYS:O	32:I:134:SER:N	2.49	0.46
12:J:88:PRO:O	12:J:94:GLY:HA3	2.16	0.46
13:K:62:PRO:HA	13:K:65:ARG:HH21	1.80	0.46
20:R:119:VAL:O	20:R:119:VAL:CG1	2.63	0.46
21:S:81:ILE:HG22	24:V:29:ASN:OD1	2.15	0.46
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.15	0.46
1:0:1200:A:H3'	40:0:6230:HOH:O	2.15	0.46
1:0:1159:G:H1	1:0:1208:C:H42	1.64	0.46
1:0:189:A:OP1	15:M:171:ARG:NH2	2.48	0.46
1:0:1849:G:H1'	1:0:2011:A:N1	2.31	0.46
1:0:2300:A:H4'	1:0:2301:A:O5'	2.16	0.46
1:0:2448:U:O2'	1:0:2449:G:H5'	2.16	0.46
1:0:289:G:N1	1:0:363:A:C2	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:601:G:O2'	1:0:602:A:H5'	2.16	0.46
4:A:217:ARG:NH1	4:A:217:ARG:CG	2.78	0.46
1:0:870:G:OP2	4:A:3:ARG:HD3	2.15	0.46
9:F:70:LYS:C	9:F:72:VAL:H	2.19	0.46
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.97	0.46
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.51	0.46
1:0:1056:U:H2'	1:0:1057:A:O4'	2.15	0.46
1:0:10:U:O4	1:0:532:A:OP2	2.33	0.46
1:0:1634:G:H2'	1:0:1635:U:C6	2.51	0.46
1:0:1755:A:H2'	1:0:1756:G:O4'	2.16	0.46
1:0:1829:A:C8	1:0:1885:A:C8	3.04	0.46
1:0:2064:U:H5'	1:0:2652:U:O3'	2.16	0.46
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.16	0.46
1:0:328:U:O4'	6:C:202:THR:HG22	2.15	0.46
1:0:820:G:C5	4:A:171:LYS:HB2	2.50	0.46
5:B:139:ASP:CB	5:B:165:ARG:HE	2.29	0.46
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.15	0.46
40:0:9643:HOH:O	14:L:30:ARG:HD2	2.14	0.46
16:N:167:ASP:C	16:N:168:LEU:HG	2.36	0.46
16:N:36:ALA:O	16:N:37:ARG:HD2	2.15	0.46
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.51	0.46
20:R:47:LEU:O	20:R:51:ILE:HG13	2.15	0.46
1:0:2866:U:C4	23:U:50:GLU:HB3	2.51	0.46
24:V:1:THR:CG2	24:V:2:VAL:H	2.13	0.46
1:0:1130:U:H2'	1:0:1131:G:O4'	2.15	0.46
1:0:1504:A:H5'	40:0:4945:HOH:O	2.15	0.46
1:0:1789:G:O6	18:P:73:HIS:HE1	1.99	0.46
30:2:5:LYS:O	30:2:9:LYS:HG3	2.15	0.46
31:3:55:VAL:HG23	40:3:9457:HOH:O	2.15	0.46
31:3:73:GLU:HB2	40:3:9462:HOH:O	2.15	0.46
4:A:94:LEU:HD12	4:A:98:GLU:HB2	1.98	0.46
5:B:41:PHE:HB3	5:B:190:MET:CE	2.46	0.46
6:C:236:THR:O	6:C:237:GLU:C	2.54	0.46
11:H:79:GLU:O	11:H:80:GLU:HG3	2.16	0.46
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.97	0.46
27:Y:203:VAL:HG12	27:Y:228:VAL:HG22	1.97	0.46
1:0:1182:C:C1'	1:0:1192:A:H8	2.28	0.45
1:0:1299:G:N7	14:L:6:ARG:NH1	2.64	0.45
1:0:292:G:H2'	1:0:358:G:N2	2.32	0.45
2:9:3042:C:O2	7:D:76:ARG:NH1	2.49	0.45
5:B:53:LEU:CD1	5:B:327:VAL:HG22	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:136:ARG:HB3	7:D:137:PRO:HD2	1.97	0.45
7:D:170:TYR:O	7:D:171:ASP:CB	2.64	0.45
13:K:4:LEU:CD2	13:K:116:GLU:HB3	2.44	0.45
15:M:125:ARG:HE	15:M:126:GLN:HE21	1.64	0.45
15:M:64:ARG:HD2	40:M:9388:HOH:O	2.16	0.45
1:0:1042:U:O2'	1:0:1043:C:H5'	2.16	0.45
1:0:1819:G:H2'	1:0:1820:G:C5'	2.46	0.45
1:0:2769:C:H2'	1:0:2770:G:O4'	2.16	0.45
1:0:920:C:H5''	1:0:921:G:O5'	2.16	0.45
1:0:920:C:H4'	1:0:921:G:N2	2.31	0.45
30:2:14:LEU:HD13	30:2:47:THR:HG21	1.98	0.45
31:3:20:HIS:HA	31:3:70:ARG:O	2.16	0.45
1:0:875:A:C2	4:A:194:MET:SD	3.09	0.45
7:D:154:LYS:H	7:D:154:LYS:CD	2.27	0.45
11:H:18:GLU:HG3	11:H:19:TYR:CE1	2.51	0.45
14:L:35:ARG:NH1	14:L:43:HIS:CD2	2.83	0.45
14:L:77:ALA:C	14:L:79:ASP:H	2.19	0.45
25:W:38:THR:CG2	25:W:39:ASP:N	2.78	0.45
38:4:9701:SPS:H81	38:4:9701:SPS:H71	1.84	0.45
4:A:81:GLN:CB	4:A:92:ASN:ND2	2.79	0.45
5:B:294:TYR:C	5:B:294:TYR:CD1	2.89	0.45
6:C:51:TYR:CE2	29:1:53:LYS:HB3	2.51	0.45
6:C:7:ASP:O	6:C:9:ASP:N	2.49	0.45
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.97	0.45
17:O:49:GLU:OE1	17:O:72:LYS:HG3	2.16	0.45
1:0:97:G:N1	22:T:107:LYS:HD2	2.31	0.45
1:0:1427:A:H61	1:0:1440:U:H1'	1.81	0.45
1:0:1574:C:H6	1:0:1574:C:O5'	1.99	0.45
1:0:2672:C:O2'	1:0:2673:U:H5'	2.17	0.45
1:0:2852:A:H5''	40:0:5736:HOH:O	2.16	0.45
1:0:561:G:O2'	1:0:562:A:H5'	2.16	0.45
31:3:5:ARG:HG3	31:3:6:ARG:HG3	1.99	0.45
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.17	0.45
1:0:2283:G:C6	11:H:113:MET:HB3	2.52	0.45
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.76	0.45
14:L:97:VAL:HG12	14:L:98:GLU:O	2.16	0.45
22:T:73:HIS:HD2	22:T:88:PRO:HG3	1.81	0.45
26:X:70:ILE:O	26:X:70:ILE:HG23	2.17	0.45
28:Z:14:PHE:HE1	28:Z:26:VAL:HG21	1.81	0.45
1:0:1701:A:H5''	1:0:1702:U:H3'	1.98	0.45
1:0:2716:G:H5''	5:B:206:THR:CG2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:352:A:H2'	1:0:353:G:C8	2.51	0.45
1:0:541:C:H2'	1:0:542:A:H5'	1.99	0.45
2:9:3029:C:H2'	2:9:3030:C:C5'	2.43	0.45
1:0:2716:G:C5'	5:B:206:THR:HG21	2.42	0.45
6:C:46:TYR:HE2	6:C:98:ARG:HH12	1.55	0.45
12:J:13:ASP:OD1	12:J:15:ARG:HB3	2.17	0.45
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.46	0.45
17:O:32:ARG:HB2	40:O:4656:HOH:O	2.16	0.45
18:P:59:ARG:HH22	18:P:66:GLN:NE2	2.04	0.45
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.79	0.45
25:W:149:LEU:HG	25:W:153:MET:HE2	1.98	0.45
25:W:29:VAL:O	25:W:30:ASN:HB2	2.16	0.45
1:0:1400:C:H4'	26:X:56:GLU:HG2	1.98	0.45
1:0:1342:C:O2'	1:0:1343:C:H5'	2.17	0.45
30:2:41:HIS:HB3	30:2:44:ARG:HB2	1.98	0.45
5:B:58:PRO:HA	5:B:63:GLU:OE2	2.16	0.45
8:E:145:ALA:HB1	8:E:168:ILE:HD11	1.98	0.45
8:E:154:ILE:CD1	8:E:157:LYS:HE2	2.47	0.45
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.98	0.45
11:H:83:TYR:C	11:H:83:TYR:CD1	2.90	0.45
19:Q:64:GLU:HG3	19:Q:74:ASP:CG	2.36	0.45
23:U:52:THR:HG22	23:U:54:THR:HB	1.98	0.45
1:0:2435:U:H1'	40:O:5923:HOH:O	2.17	0.45
1:0:2880:A:H2'	1:0:2881:C:H5'	1.99	0.45
1:0:666:A:H2'	1:0:667:C:O4'	2.17	0.45
4:A:113:GLY:HA2	4:A:153:ARG:NH2	2.31	0.45
4:A:88:ILE:HD13	4:A:100:PRO:CD	2.44	0.45
40:O:3526:HOH:O	6:C:78:ARG:HD3	2.16	0.45
7:D:105:SER:HB2	7:D:131:THR:HG23	1.98	0.45
16:N:166:ALA:O	16:N:167:ASP:O	2.35	0.45
17:O:81:PHE:N	17:O:81:PHE:CD1	2.85	0.45
20:R:92:LEU:HD23	20:R:145:LEU:HD21	1.97	0.45
40:C:9175:HOH:O	22:T:2:LYS:HE2	2.16	0.45
1:0:1495:C:H2'	1:0:1496:G:C8	2.52	0.45
1:0:1871:U:O4'	1:0:1873:G:C8	2.70	0.45
1:0:2608:C:H3'	40:O:8217:HOH:O	2.16	0.45
1:0:2672:C:P	5:B:25:ARG:NH1	2.90	0.45
1:0:37:A:C2	1:0:446:G:C2	3.05	0.45
4:A:217:ARG:HH11	4:A:217:ARG:HG3	1.82	0.45
4:A:35:GLY:O	4:A:36:ASP:HB2	2.15	0.45
7:D:170:TYR:CD1	7:D:170:TYR:N	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:56:GLN:NE2	11:H:126:ARG:HE	2.14	0.45
14:L:104:ASP:O	14:L:105:TYR:HB3	2.17	0.45
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.99	0.45
40:0:3136:HOH:O	18:P:81:LYS:HG2	2.17	0.45
1:0:1160:G:HO2'	1:0:1190:G:H8	1.62	0.45
1:0:1421:C:O2'	1:0:1422:U:H5'	2.17	0.45
1:0:2785:C:H4'	1:0:2786:G:OP2	2.17	0.45
1:0:541:C:C2'	1:0:542:A:C5'	2.83	0.45
1:0:764:C:H2'	1:0:765:G:O4'	2.17	0.45
1:0:907:A:H2'	1:0:908:A:C8	2.52	0.45
29:1:28:HIS:HD2	29:1:30:LYS:H	1.64	0.45
4:A:54:PRO:HG2	4:A:160:ALA:HB3	1.99	0.45
5:B:41:PHE:HA	5:B:79:MET:HE1	1.97	0.45
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.99	0.45
16:N:168:LEU:HA	16:N:169:PRO:HD3	1.84	0.45
17:O:26:TRP:HA	17:O:26:TRP:HE3	1.81	0.45
26:X:23:HIS:O	26:X:63:ARG:HD3	2.16	0.45
40:0:6724:HOH:O	27:Y:158:LYS:HD3	2.16	0.45
1:0:1014:A:H2'	1:0:1015:C:H5'	1.98	0.45
1:0:1086:A:N6	25:W:11:VAL:HG11	2.32	0.45
1:0:2323:G:H5'	40:0:7402:HOH:O	2.17	0.45
1:0:432:G:H2'	1:0:433:C:H6	1.82	0.45
1:0:806:A:H2'	1:0:807:A:O4'	2.17	0.45
4:A:192:VAL:HB	40:A:9627:HOH:O	2.17	0.45
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.47	0.45
5:B:205:VAL:O	5:B:307:ARG:NE	2.49	0.45
1:0:1119:G:H8	12:J:52:GLN:HE22	1.65	0.45
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.54	0.45
16:N:175:LEU:O	16:N:179:LEU:HG	2.17	0.45
40:9:466:HOH:O	19:Q:25:PRO:HB3	2.17	0.45
40:0:5790:HOH:O	25:W:119:HIS:CG	2.70	0.45
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.52	0.44
1:0:1185:U:H2'	1:0:1186:C:C6	2.51	0.44
1:0:1218:U:H2'	1:0:1219:U:H6	1.80	0.44
1:0:1819:G:H2'	1:0:1820:G:C4'	2.47	0.44
1:0:1942:A:H2'	1:0:1943:C:H6	1.81	0.44
1:0:661:G:C5	1:0:686:A:C2	3.05	0.44
1:0:734:U:H1'	1:0:737:A:N6	2.32	0.44
1:0:877:G:C2	1:0:885:G:O4'	2.70	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.80	0.44
31:3:14:CYS:HB3	31:3:16:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:81:GLN:HG3	4:A:92:ASN:HD21	1.83	0.44
5:B:54:VAL:O	5:B:55:ASN:C	2.55	0.44
7:D:96:SER:C	7:D:98:PHE:H	2.20	0.44
9:F:101:ALA:HA	40:F:5413:HOH:O	2.17	0.44
32:I:113:HIS:CE1	32:I:121:LEU:HD22	2.48	0.44
14:L:128:GLY:O	14:L:132:LYS:HG3	2.16	0.44
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.48	0.44
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.47	0.44
23:U:49:LEU:HG	40:U:3805:HOH:O	2.16	0.44
40:O:5790:HOH:O	25:W:122:ARG:NH2	2.51	0.44
1:O:1093:G:H2'	1:O:1094:G:O4'	2.18	0.44
1:O:750:A:O3'	6:C:101:ASP:HB2	2.17	0.44
40:O:5905:HOH:O	4:A:164:ARG:CZ	2.65	0.44
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.82	0.44
13:K:74:VAL:HG12	13:K:74:VAL:O	2.15	0.44
15:M:61:ILE:N	15:M:61:ILE:HD12	2.32	0.44
16:N:154:LEU:O	16:N:155:GLU:HB2	2.16	0.44
23:U:52:THR:HG21	23:U:54:THR:HB	1.99	0.44
25:W:131:PRO:O	25:W:136:GLY:N	2.46	0.44
27:Y:152:LYS:HB3	27:Y:160:LYS:HG3	2.00	0.44
1:O:1180:U:H2'	1:O:1181:A:C8	2.52	0.44
1:O:1331:A:OP2	27:Y:142:SER:OG	2.28	0.44
1:O:1419:U:H2'	1:O:1685:A:C2	2.52	0.44
29:1:28:HIS:O	29:1:32:LYS:N	2.44	0.44
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.82	0.44
4:A:217:ARG:HG2	4:A:229:ALA:HB2	1.99	0.44
5:B:62:ARG:HA	5:B:65:MET:HE2	1.99	0.44
6:C:72:LYS:HE3	40:C:9107:HOH:O	2.17	0.44
7:D:22:VAL:HA	7:D:73:VAL:O	2.17	0.44
8:E:34:TRP:O	12:J:127:ILE:HD11	2.16	0.44
11:H:46:GLN:HG3	11:H:137:TYR:CD2	2.52	0.44
16:N:11:ARG:O	16:N:15:GLU:HG3	2.17	0.44
40:O:5254:HOH:O	16:N:21:HIS:HD2	2.00	0.44
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.32	0.44
1:O:963:C:H2'	1:O:964:G:C8	2.53	0.44
4:A:36:ASP:HB2	4:A:85:SER:H	1.81	0.44
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.47	0.44
8:E:13:ALA:O	8:E:42:VAL:HG11	2.18	0.44
9:F:28:ALA:CB	9:F:99:THR:HG23	2.47	0.44
1:O:2521:A:OP2	11:H:3:ALA:HB3	2.17	0.44
15:M:74:LYS:HG2	15:M:75:ARG:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:51:GLN:NE2	21:S:53:ASN:HD21	2.16	0.44
25:W:92:ASP:OD1	25:W:92:ASP:N	2.51	0.44
1:0:1098:A:H2'	1:0:1099:G:O4'	2.17	0.44
1:0:2470:A:H5''	40:0:3808:HOH:O	2.16	0.44
1:0:251:C:H2'	1:0:252:C:H6	1.82	0.44
29:1:10:LYS:N	40:1:9489:HOH:O	2.48	0.44
4:A:163:GLY:HA2	4:A:166:ASP:OD2	2.17	0.44
4:A:81:GLN:H	4:A:92:ASN:CG	2.20	0.44
5:B:109:LEU:HD11	5:B:113:LEU:HD11	1.99	0.44
6:C:54:LEU:O	29:1:53:LYS:HE3	2.17	0.44
7:D:76:ARG:O	7:D:77:ASP:HB2	2.18	0.44
14:L:143:THR:CG2	14:L:144:ASP:N	2.79	0.44
17:O:25:VAL:HG23	17:O:26:TRP:N	2.33	0.44
20:R:144:GLU:HB3	40:R:9460:HOH:O	2.17	0.44
1:0:308:U:H5'	22:T:97:ARG:NH2	2.33	0.44
1:0:1298:U:H2'	1:0:1299:G:H8	1.83	0.44
1:0:2241:C:O2'	1:0:2242:U:H5'	2.18	0.44
1:0:245:C:H2'	1:0:246:G:H5'	2.00	0.44
1:0:625:U:H5''	1:0:1044:C:H41	1.81	0.44
1:0:694:A:H2'	1:0:695:C:H5'	1.99	0.44
31:3:65:THR:HG23	31:3:88:LEU:HD22	1.99	0.44
2:9:3059:C:H2'	2:9:3060:C:C6	2.53	0.44
5:B:277:GLU:N	5:B:278:PRO:CD	2.81	0.44
5:B:320:GLN:HE21	5:B:321:PRO:CD	2.31	0.44
6:C:138:VAL:O	6:C:234:VAL:HA	2.17	0.44
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.53	0.44
11:H:1:LYS:HA	11:H:2:PRO:HD3	1.84	0.44
14:L:89:PHE:CD1	14:L:89:PHE:N	2.86	0.44
15:M:125:ARG:HE	15:M:126:GLN:NE2	2.16	0.44
16:N:43:VAL:CG1	16:N:118:ILE:HD11	2.47	0.44
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.99	0.44
17:O:26:TRP:N	40:O:3062:HOH:O	2.51	0.44
17:O:44:ASN:OD1	17:O:67:SER:HB2	2.17	0.44
22:T:18:GLU:O	22:T:21:LYS:HG2	2.17	0.44
25:W:65:VAL:CG1	25:W:116:LEU:HD13	2.47	0.44
1:0:1180:U:H2'	1:0:1181:A:O4'	2.18	0.44
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.47	0.44
1:0:1942:A:H2'	1:0:1943:C:C6	2.53	0.44
1:0:2100:A:H4'	6:C:64:GLY:O	2.18	0.44
1:0:1486:A:C4	30:2:2:LYS:HG3	2.53	0.44
4:A:48:ASP:HA	4:A:49:PRO:HD3	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:102:THR:HB	40:B:9627:HOH:O	2.17	0.44
5:B:60:SER:HA	5:B:61:PRO:HD3	1.86	0.44
6:C:130:GLU:O	6:C:164:ALA:HB3	2.18	0.44
9:F:58:GLU:HB3	15:M:8:ILE:HG23	1.99	0.44
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.99	0.44
13:K:98:VAL:HG11	13:K:102:GLU:HA	2.00	0.44
13:K:2:GLU:O	13:K:3:ALA:C	2.56	0.44
1:0:392:U:C5'	15:M:193:LYS:HB3	2.48	0.44
15:M:46:LEU:HG	40:M:9422:HOH:O	2.18	0.44
15:M:73:ARG:N	15:M:73:ARG:HD2	2.33	0.44
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.17	0.44
22:T:71:VAL:CG1	22:T:72:ILE:N	2.80	0.44
22:T:80:GLU:HG2	40:T:2885:HOH:O	2.17	0.44
24:V:39:ALA:O	24:V:41:GLU:N	2.44	0.44
1:0:1025:C:H5'	25:W:23:MET:O	2.17	0.44
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.18	0.44
27:Y:109:LEU:HA	40:Y:9369:HOH:O	2.18	0.44
27:Y:96:GLU:O	27:Y:235:GLU:HA	2.18	0.44
1:0:1883:U:H5'	1:0:2012:U:OP2	2.17	0.44
1:0:820:G:H5'	1:0:821:U:H5'	1.98	0.44
30:2:19:SER:HB3	40:2:4479:HOH:O	2.18	0.44
4:A:43:VAL:HG21	4:A:59:GLU:CG	2.47	0.44
5:B:168:GLY:O	5:B:169:GLY:O	2.36	0.44
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.44
5:B:214:PRO:C	5:B:220:VAL:HG22	2.38	0.44
5:B:221:GLN:HE22	13:K:42:ASN:ND2	2.14	0.44
7:D:75:LEU:HD13	7:D:79:MET:O	2.18	0.44
11:H:66:ARG:HD3	40:H:9551:HOH:O	2.18	0.44
1:0:1739:G:O2'	1:0:1740:U:H5'	2.18	0.44
1:0:177:A:H2'	1:0:178:U:O4'	2.18	0.44
1:0:2505:G:C2'	1:0:2506:A:H5'	2.48	0.44
1:0:2911:C:O2'	1:0:2912:C:H5'	2.18	0.44
1:0:36:C:C2	1:0:447:A:C2	3.06	0.44
31:3:67:LEU:HD21	31:3:88:LEU:HD23	2.00	0.44
2:9:3031:C:H2'	2:9:3032:G:O4'	2.18	0.44
2:9:3091:C:H2'	2:9:3092:G:O4'	2.17	0.44
5:B:260:HIS:HE1	40:B:9581:HOH:O	2.00	0.44
7:D:25:MET:HE1	7:D:37:ALA:CB	2.36	0.44
8:E:101:GLU:OE2	8:E:115:ARG:HD3	2.18	0.44
8:E:116:THR:HG22	8:E:151:LEU:CD2	2.38	0.44
40:0:7267:HOH:O	15:M:178:LYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:63:LYS:HA	17:O:80:ASP:O	2.18	0.44
23:U:20:MET:HG3	23:U:30:HIS:CD2	2.53	0.44
26:X:43:VAL:HG12	26:X:47:ALA:HB3	2.00	0.44
1:O:254:C:O2	1:O:254:C:H2'	2.17	0.43
2:9:3095:C:O2'	2:9:3096:C:H5'	2.18	0.43
4:A:171:LYS:NZ	40:A:9557:HOH:O	2.51	0.43
4:A:41:THR:O	4:A:43:VAL:HG23	2.18	0.43
5:B:55:ASN:HB3	5:B:64:GLY:H	1.83	0.43
13:K:87:ARG:NH1	40:K:4066:HOH:O	2.51	0.43
14:L:35:ARG:CB	14:L:35:ARG:HH11	2.15	0.43
15:M:120:VAL:CG1	15:M:130:GLU:HG3	2.47	0.43
15:M:159:VAL:HG13	15:M:160:PHE:N	2.33	0.43
16:N:137:ALA:HB1	16:N:141:ARG:HD3	2.00	0.43
21:S:57:THR:CG2	21:S:58:MET:N	2.81	0.43
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.43	0.43
1:O:1015:C:H2'	1:O:1016:U:C6	2.53	0.43
1:O:1362:U:H2'	1:O:1363:G:C8	2.53	0.43
1:O:1503:U:H2'	1:O:1504:A:O4'	2.19	0.43
1:O:1516:C:H42	1:O:1670:G:H1	1.65	0.43
1:O:2673:U:C4	1:O:2674:G:C6	3.06	0.43
1:O:2768:A:O2'	1:O:2769:C:H5'	2.17	0.43
4:A:206:ARG:CD	4:A:206:ARG:H	2.29	0.43
5:B:113:LEU:HD21	5:B:161:VAL:HG21	2.00	0.43
14:L:21:ARG:N	40:L:9428:HOH:O	2.50	0.43
16:N:11:ARG:HA	16:N:14:ARG:CZ	2.48	0.43
16:N:77:ASN:O	16:N:80:SER:HB3	2.18	0.43
1:O:101:C:H2'	1:O:102:A:C8	2.53	0.43
1:O:1166:A:N6	1:O:1180:U:H3	2.08	0.43
1:O:1391:G:H2'	1:O:1392:A:H5'	2.01	0.43
1:O:1527:A:H1'	1:O:1528:A:C8	2.54	0.43
1:O:790:A:H1'	1:O:1710:A:O2'	2.18	0.43
1:O:2453:G:H5'	40:O:5219:HOH:O	2.18	0.43
1:O:288:A:H2'	1:O:289:G:H8	1.83	0.43
1:O:407:A:O2'	1:O:408:A:H5'	2.18	0.43
1:O:766:A:H5'	40:O:5178:HOH:O	2.18	0.43
4:A:42:VAL:O	4:A:76:VAL:HG13	2.17	0.43
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.80	0.43
14:L:53:ARG:HH22	14:L:57:VAL:HG12	1.79	0.43
16:N:61:ALA:HA	16:N:91:ARG:NH1	2.34	0.43
22:T:1:SER:O	22:T:7:GLN:NE2	2.51	0.43
1:O:1025:C:OP1	25:W:108:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1669:A:H2'	1:0:1670:G:C8	2.54	0.43
1:0:2406:U:O2'	1:0:2407:G:H5'	2.19	0.43
1:0:2726:U:O2	1:0:2749:U:O5'	2.37	0.43
1:0:289:G:H1	1:0:363:A:H2	1.56	0.43
1:0:347:A:H2'	1:0:348:C:O4'	2.19	0.43
1:0:449:A:N7	6:C:43:LYS:HG2	2.33	0.43
5:B:258:GLY:O	5:B:260:HIS:CD2	2.71	0.43
6:C:157:LEU:CD1	6:C:166:ILE:HD11	2.48	0.43
8:E:77:THR:OG1	8:E:78:GLU:N	2.49	0.43
8:E:88:TYR:CE1	8:E:92:PRO:HA	2.53	0.43
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.99	0.43
32:I:119:TYR:N	32:I:119:TYR:CD1	2.85	0.43
13:K:66:ARG:HD3	40:K:2777:HOH:O	2.18	0.43
1:0:926:A:H5'	14:L:39:GLU:OE2	2.18	0.43
21:S:56:ASN:O	30:2:8:LYS:NZ	2.46	0.43
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.52	0.43
24:V:64:GLY:O	24:V:65:ASP:OD1	2.36	0.43
1:0:1211:G:H2'	1:0:1212:C:C6	2.53	0.43
1:0:1377:C:C5'	1:0:1377:C:H6	2.25	0.43
1:0:2644:C:H6	40:0:7480:HOH:O	2.02	0.43
1:0:2712:G:H5'	40:0:5723:HOH:O	2.19	0.43
1:0:2900:G:H2'	1:0:2901:C:O4'	2.17	0.43
1:0:941:G:C5	1:0:942:U:C4	3.07	0.43
1:0:1414:A:P	30:2:1:GLY:HA2	2.58	0.43
4:A:95:PRO:HA	4:A:153:ARG:HA	2.01	0.43
40:0:5197:HOH:O	5:B:300:SER:HB3	2.18	0.43
6:C:120:ASP:C	6:C:120:ASP:OD1	2.56	0.43
6:C:40:ALA:O	6:C:43:LYS:HB2	2.18	0.43
9:F:91:VAL:CG1	9:F:92:GLY:N	2.65	0.43
12:J:142:ASN:O	12:J:144:THR:N	2.52	0.43
16:N:82:TYR:OH	16:N:176:ARG:NH1	2.52	0.43
21:S:43:GLU:HB3	40:S:9501:HOH:O	2.18	0.43
40:0:6140:HOH:O	22:T:68:ASP:HB2	2.18	0.43
25:W:139:GLY:O	25:W:141:HIS:CD2	2.69	0.43
25:W:60:GLU:O	25:W:63:GLU:HB2	2.18	0.43
26:X:15:ARG:CB	26:X:15:ARG:HH11	2.32	0.43
1:0:1335:C:OP2	27:Y:207:SER:HB3	2.18	0.43
1:0:1625:U:H4'	40:0:5193:HOH:O	2.18	0.43
1:0:1717:A:H5''	18:P:54:LYS:HB2	2.01	0.43
1:0:2765:C:H4'	40:0:6006:HOH:O	2.18	0.43
1:0:85:C:H3'	1:0:86:A:H2'	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3007:G:H4'	16:N:55:ASP:OD2	2.19	0.43
5:B:14:GLY:HA2	5:B:15:PRO:C	2.39	0.43
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.33	0.43
27:Y:234:VAL:HG12	27:Y:235:GLU:N	2.33	0.43
1:0:1135:G:H5'	40:0:6389:HOH:O	2.18	0.43
1:0:1427:A:H61	1:0:1440:U:C1'	2.32	0.43
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.19	0.43
1:0:2506:A:O2'	1:0:2507:G:C8	2.48	0.43
1:0:2634:G:OP2	4:A:204:GLY:N	2.48	0.43
1:0:2713:G:O2'	1:0:2714:U:H5'	2.19	0.43
1:0:353:G:O2'	1:0:354:A:H5'	2.18	0.43
1:0:271:C:N4	1:0:378:A:H2	2.17	0.43
40:0:4941:HOH:O	4:A:11:ARG:CZ	2.65	0.43
5:B:41:PHE:HA	5:B:79:MET:CE	2.49	0.43
6:C:162:VAL:HG13	6:C:192:ILE:CD1	2.48	0.43
6:C:57:PRO:HG2	6:C:73:LEU:CD1	2.49	0.43
7:D:151:ILE:CG2	7:D:155:HIS:HB3	2.49	0.43
7:D:12:GLU:HA	7:D:15:GLU:OE1	2.19	0.43
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.18	0.43
9:F:32:GLY:N	40:F:3111:HOH:O	2.51	0.43
10:G:12:ILE:HG22	10:G:17:GLN:HE21	1.83	0.43
15:M:102:GLU:CD	15:M:164:THR:HG21	2.38	0.43
16:N:32:PRO:HD2	16:N:99:GLU:O	2.19	0.43
17:O:49:GLU:O	17:O:72:LYS:HE3	2.19	0.43
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.84	0.43
20:R:113:HIS:HE1	20:R:144:GLU:CD	2.22	0.43
1:0:1209:C:H2'	1:0:1210:G:C8	2.53	0.43
1:0:1279:U:O2	1:0:1279:U:H2'	2.18	0.43
1:0:1926:G:H2'	1:0:1927:A:H8	1.82	0.43
1:0:208:C:C2	1:0:232:A:C2	3.07	0.43
1:0:2361:A:H2'	1:0:2362:A:C8	2.53	0.43
1:0:2524:G:N2	1:0:2526:C:H41	2.17	0.43
1:0:2577:A:H5'	40:0:8161:HOH:O	2.19	0.43
2:9:3001:U:O3'	2:9:3003:A:H5''	2.19	0.43
1:0:1014:A:H5''	2:9:3101:G:O2'	2.19	0.43
4:A:88:ILE:CD1	4:A:100:PRO:HD3	2.46	0.43
4:A:179:MET:HA	4:A:179:MET:HE2	2.00	0.43
4:A:204:GLY:O	4:A:205:GLY:C	2.57	0.43
4:A:37:VAL:HG22	40:A:9631:HOH:O	2.19	0.43
5:B:278:PRO:HD3	5:B:294:TYR:CE2	2.54	0.43
1:0:2545:U:OP2	5:B:2:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:69:VAL:HA	5:B:70:PRO:HD3	1.84	0.43
8:E:162:PHE:CD1	8:E:162:PHE:N	2.86	0.43
11:H:77:LEU:HD12	11:H:83:TYR:HD2	1.83	0.43
13:K:6:ALA:HB1	13:K:81:ARG:O	2.19	0.43
21:S:81:ILE:HG23	40:S:9492:HOH:O	2.18	0.43
22:T:53:GLY:HA3	40:T:6384:HOH:O	2.18	0.43
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.19	0.43
1:O:170:U:H2'	1:O:171:C:H5'	2.01	0.43
1:O:1985:U:C2	1:O:1996:U:O4'	2.72	0.43
1:O:82:C:OP1	22:T:67:LEU:HB2	2.19	0.43
6:C:133:ARG:HG2	6:C:134:ASP:H	1.83	0.43
1:O:1310:U:OP2	6:C:168:ARG:NH1	2.51	0.43
13:K:10:GLN:N	13:K:10:GLN:NE2	2.42	0.43
13:K:13:GLU:OE1	13:K:44:LEU:HD12	2.19	0.43
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.49	0.43
18:P:63:ARG:NH2	40:P:194:HOH:O	2.49	0.43
1:O:1446:U:H2'	21:S:55:GLN:NE2	2.34	0.43
24:V:56:ILE:O	24:V:60:GLN:HG3	2.19	0.43
28:Z:33:MET:HG3	28:Z:69:TYR:O	2.18	0.43
1:O:1211:G:O2'	1:O:1212:C:H5'	2.19	0.43
1:O:1238:C:H5'	1:O:1239:G:OP2	2.18	0.43
1:O:2011:A:H5'	1:O:2013:G:C1'	2.48	0.43
1:O:2722:G:H4'	40:K:5029:HOH:O	2.18	0.43
1:O:2783:A:H3'	40:O:5734:HOH:O	2.19	0.43
1:O:1473:U:C1'	29:1:42:SER:HB3	2.49	0.43
31:3:55:VAL:HB	31:3:56:PRO:HD2	2.00	0.43
2:9:3059:C:O5'	2:9:3059:C:H6	2.01	0.43
1:O:2780:C:C1'	8:E:143:GLN:HE21	2.28	0.43
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.54	0.43
16:N:26:LEU:HD12	16:N:101:VAL:CG1	2.48	0.43
16:N:151:ASP:OD1	16:N:166:ALA:HA	2.19	0.43
1:O:2415:A:C2	16:N:25:ARG:HB3	2.54	0.43
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.33	0.43
1:O:2402:A:O2'	1:O:2403:C:H5'	2.19	0.42
1:O:2506:A:O2'	1:O:2507:G:O5'	2.37	0.42
30:2:48:ASP:O	30:2:49:GLU:CB	2.67	0.42
6:C:187:ARG:NH2	40:C:9173:HOH:O	2.52	0.42
11:H:18:GLU:H	11:H:18:GLU:HG2	1.58	0.42
12:J:107:ASN:C	12:J:107:ASN:ND2	2.71	0.42
14:L:121:ILE:HG12	14:L:141:GLU:HB2	2.01	0.42
16:N:149:GLU:HA	16:N:152:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:64:ASN:HB3	22:T:73:HIS:HB2	2.00	0.42
1:0:1081:A:H5''	40:0:3720:HOH:O	2.18	0.42
1:0:2251:G:H2'	1:0:2252:A:C8	2.54	0.42
1:0:2274:A:O2'	1:0:2275:G:H5'	2.19	0.42
1:0:2456:A:H2'	1:0:2457:U:C6	2.54	0.42
1:0:1815:A:H4'	1:0:2751:C:O4'	2.18	0.42
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.83	0.42
4:A:1:GLY:HA2	4:A:197:VAL:HG23	2.01	0.42
5:B:214:PRO:HB2	5:B:220:VAL:HG21	2.00	0.42
5:B:41:PHE:CD1	5:B:79:MET:CE	3.01	0.42
7:D:164:ALA:O	7:D:165:PHE:C	2.57	0.42
8:E:102:VAL:HG11	8:E:148:ILE:CD1	2.48	0.42
8:E:81:GLU:HA	8:E:133:VAL:O	2.19	0.42
9:F:99:THR:HG23	9:F:99:THR:O	2.19	0.42
1:0:2353:A:O2'	16:N:7:LYS:HB3	2.18	0.42
1:0:1537:C:H1'	40:0:7007:HOH:O	2.18	0.42
1:0:1855:G:H4'	1:0:1856:C:O5'	2.19	0.42
1:0:2296:C:H2'	1:0:2297:U:C6	2.53	0.42
1:0:2817:G:P	40:0:8334:HOH:O	2.77	0.42
1:0:553:G:OP2	27:Y:204:ARG:NH2	2.51	0.42
4:A:89:ALA:HB3	40:A:9662:HOH:O	2.18	0.42
5:B:29:TRP:CZ3	5:B:164:THR:HG23	2.55	0.42
8:E:15:GLN:NE2	8:E:40:VAL:O	2.51	0.42
11:H:46:GLN:HG3	11:H:137:TYR:CE2	2.54	0.42
11:H:27:LYS:H	11:H:59:HIS:CD2	2.31	0.42
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.48	0.42
14:L:94:ARG:HG2	14:L:106:VAL:HG21	2.00	0.42
15:M:77:HIS:CE1	15:M:86:GLN:HG2	2.53	0.42
16:N:182:GLY:O	16:N:183:ASP:C	2.57	0.42
20:R:39:THR:HG22	20:R:41:GLY:N	2.34	0.42
25:W:125:HIS:HB2	25:W:137:GLN:OE1	2.19	0.42
1:0:1305:C:H5'	40:0:3410:HOH:O	2.18	0.42
1:0:1666:C:C2'	1:0:1667:A:H5''	2.49	0.42
1:0:2346:C:O5'	1:0:2346:C:H6	2.02	0.42
1:0:2729:C:O2'	1:0:2730:G:H5'	2.20	0.42
1:0:2727:A:C6	1:0:2756:U:C2	3.07	0.42
1:0:2837:U:H2'	40:0:7233:HOH:O	2.20	0.42
1:0:639:A:C6	1:0:640:G:C6	3.08	0.42
1:0:64:G:H2'	1:0:65:C:O4'	2.20	0.42
7:D:173:GLU:HG3	7:D:174:VAL:H	1.83	0.42
7:D:66:GLY:O	7:D:67:ASP:HB3	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:170:ARG:HE	8:E:170:ARG:HB2	1.60	0.42
14:L:35:ARG:NE	14:L:46:LEU:HD21	2.34	0.42
16:N:179:LEU:HD23	16:N:184:ILE:HD12	2.01	0.42
19:Q:61:GLY:HA2	40:Q:6286:HOH:O	2.19	0.42
22:T:73:HIS:CD2	22:T:88:PRO:CG	3.03	0.42
25:W:122:ARG:NH1	25:W:152:ALA:O	2.52	0.42
26:X:74:ALA:CB	26:X:85:VAL:HG13	2.46	0.42
1:0:1184:C:O2'	1:0:1185:U:OP2	2.30	0.42
1:0:1545:C:H2'	1:0:1546:G:O4'	2.20	0.42
1:0:1890:U:H4'	1:0:2010:A:C6	2.55	0.42
1:0:2112:A:H2'	1:0:2113:G:H8	1.84	0.42
1:0:240:C:OP2	1:0:270:U:H5	2.02	0.42
1:0:2816:A:H5''	1:0:2817:G:H5'	2.02	0.42
1:0:664:U:O4	1:0:681:G:H5''	2.19	0.42
31:3:70:ARG:HH11	31:3:77:ALA:HB2	1.82	0.42
4:A:27:LEU:HD13	4:A:69:LEU:HA	2.00	0.42
5:B:139:ASP:HB2	5:B:165:ARG:NE	2.35	0.42
6:C:123:LEU:HD23	6:C:123:LEU:HA	1.84	0.42
12:J:132:LEU:HA	12:J:132:LEU:HD23	1.88	0.42
12:J:78:ILE:HG21	12:J:132:LEU:HD21	2.01	0.42
14:L:144:ASP:O	14:L:147:GLU:HB2	2.20	0.42
1:0:1805:G:O2'	1:0:1806:G:H5'	2.20	0.42
1:0:2697:A:H2'	1:0:2698:G:O4'	2.19	0.42
1:0:612:U:H2'	1:0:613:C:C6	2.55	0.42
1:0:779:U:H5'	1:0:1836:A:C2	2.55	0.42
4:A:203:GLY:CA	40:A:9581:HOH:O	2.63	0.42
4:A:56:ALA:O	4:A:68:ILE:HG22	2.19	0.42
4:A:58:VAL:HG21	4:A:80:LEU:HD12	2.02	0.42
1:0:2548:C:OP2	5:B:5:ARG:NH2	2.52	0.42
5:B:71:VAL:HG11	5:B:296:LEU:HD22	2.01	0.42
7:D:94:ALA:HA	7:D:174:VAL:O	2.19	0.42
16:N:171:HIS:CE1	40:N:9364:HOH:O	2.71	0.42
16:N:183:ASP:O	16:N:184:ILE:C	2.58	0.42
16:N:66:LEU:HG	16:N:175:LEU:HD21	2.01	0.42
1:0:2388:C:H5'	19:Q:83:THR:O	2.20	0.42
25:W:125:HIS:CD2	25:W:127:GLY:H	2.17	0.42
1:0:1076:G:C2	1:0:1084:C:C2	3.08	0.42
1:0:1477:C:H2'	1:0:1478:U:O4'	2.20	0.42
1:0:1864:C:H2'	1:0:1865:A:O4'	2.19	0.42
1:0:23:G:C6	1:0:24:G:N1	2.88	0.42
1:0:490:C:O2'	1:0:491:C:H5'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:3:ARG:HG2	4:A:3:ARG:H	1.55	0.42
40:0:4008:HOH:O	4:A:5:GLN:HB2	2.18	0.42
12:J:15:ARG:NH1	12:J:43:ARG:NH1	2.68	0.42
24:V:19:GLU:OE1	24:V:19:GLU:HA	2.19	0.42
25:W:65:VAL:HA	25:W:68:THR:CG2	2.49	0.42
1:0:130:C:H5'	40:0:5715:HOH:O	2.19	0.42
1:0:1588:G:C6	1:0:1589:G:N1	2.88	0.42
1:0:1816:C:H2'	1:0:1817:U:O4'	2.20	0.42
1:0:1829:A:H61	28:Z:18:TYR:N	2.18	0.42
1:0:2094:G:O6	1:0:2649:A:H2	2.03	0.42
1:0:2568:A:H5''	1:0:2702:A:O2'	2.19	0.42
1:0:255:A:H2'	1:0:256:C:H6	1.81	0.42
1:0:2718:C:H5'	1:0:2718:C:C6	2.50	0.42
1:0:2748:G:H8	40:0:7878:HOH:O	2.03	0.42
1:0:682:A:H2'	1:0:683:G:O4'	2.18	0.42
40:0:7512:HOH:O	29:1:1:THR:HB	2.19	0.42
3:4:76:A:H8	38:4:9701:SPS:H81	1.84	0.42
4:A:109:GLU:CD	4:A:153:ARG:NH1	2.73	0.42
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.54	0.42
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.48	0.42
9:F:20:LEU:O	9:F:20:LEU:HD12	2.20	0.42
9:F:21:GLU:HG2	9:F:24:ARG:HH21	1.84	0.42
1:0:1180:U:HO2'	32:I:92:PRO:HD2	1.84	0.42
40:0:5358:HOH:O	12:J:47:THR:HB	2.19	0.42
14:L:89:PHE:N	40:L:9474:HOH:O	2.52	0.42
19:Q:47:VAL:HA	19:Q:48:PRO:HD3	1.83	0.42
1:0:553:G:O4'	1:0:1325:G:H5'	2.20	0.42
1:0:196:G:H1'	1:0:198:A:N7	2.35	0.42
1:0:2379:G:N3	1:0:2418:G:H2'	2.34	0.42
1:0:2507:G:H2'	1:0:2510:C:H42	1.85	0.42
1:0:29:C:C2'	1:0:30:U:H5'	2.49	0.42
1:0:506:G:N2	1:0:509:A:H5''	2.27	0.42
11:H:34:GLY:HA3	11:H:84:LYS:HA	2.02	0.42
1:0:2582:G:O3'	13:K:41:LYS:HA	2.20	0.42
15:M:36:ALA:O	15:M:65:VAL:HA	2.19	0.42
15:M:82:ARG:O	15:M:83:SER:C	2.57	0.42
16:N:86:LEU:HD21	16:N:180:LEU:HD12	2.02	0.42
17:O:14:LEU:HD23	17:O:102:ILE:HD11	2.00	0.42
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.26	0.42
28:Z:29:ILE:HA	40:Z:9225:HOH:O	2.19	0.42
28:Z:39:CYS:HA	28:Z:40:PRO:HD3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1979:G:O2'	1:0:1980:U:OP1	2.36	0.42
1:0:2107:U:O2'	1:0:2108:A:H5'	2.20	0.42
1:0:2363:G:O3'	19:Q:11:ARG:NH1	2.52	0.42
1:0:2748:G:C5'	40:0:7878:HOH:O	2.61	0.42
1:0:31:C:OP2	22:T:8:ARG:NH1	2.52	0.42
1:0:697:G:H4'	1:0:730:G:O3'	2.19	0.42
1:0:963:C:O2	1:0:1005:A:N1	2.53	0.42
1:0:396:U:C2	31:3:38:ARG:NH1	2.87	0.42
5:B:41:PHE:HB3	5:B:190:MET:HE3	2.01	0.42
5:B:243:ASN:HA	5:B:244:PRO:C	2.39	0.42
14:L:130:ARG:O	14:L:133:VAL:N	2.53	0.42
22:T:61:GLU:HG3	40:T:3851:HOH:O	2.19	0.42
23:U:52:THR:HG22	23:U:54:THR:H	1.84	0.42
25:W:13:MET:HE3	25:W:17:ILE:HG22	2.02	0.42
27:Y:107:PRO:HD3	27:Y:182:PHE:CE1	2.55	0.42
27:Y:133:HIS:HD2	40:Y:9381:HOH:O	2.01	0.42
1:0:1293:U:H5'	27:Y:154:ARG:HH21	1.85	0.42
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.52	0.42
1:0:228:C:H2'	1:0:229:G:H5'	2.02	0.41
1:0:526:U:H2'	1:0:527:U:C6	2.55	0.41
1:0:93:C:H5''	24:V:1:THR:CB	2.42	0.41
1:0:1845:A:O3'	4:A:187:PRO:HB2	2.20	0.41
5:B:309:VAL:HG12	40:B:9644:HOH:O	2.20	0.41
5:B:62:ARG:HA	5:B:65:MET:HE3	2.02	0.41
6:C:107:ARG:HH11	6:C:107:ARG:HB3	1.84	0.41
8:E:7:ILE:HG13	8:E:8:PRO:HD2	2.01	0.41
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.55	0.41
16:N:156:GLU:O	16:N:157:PRO:C	2.59	0.41
17:O:98:LEU:O	17:O:102:ILE:HG13	2.20	0.41
18:P:18:LYS:O	18:P:21:VAL:HG13	2.20	0.41
4:A:72:GLU:CD	28:Z:76:GLY:HA3	2.40	0.41
1:0:1552:G:C6	1:0:1553:C:C4	3.08	0.41
1:0:2038:A:O2'	1:0:2039:A:H5'	2.19	0.41
1:0:2115:U:H2'	1:0:2116:U:C6	2.54	0.41
1:0:650:C:O2'	1:0:651:U:H5'	2.20	0.41
1:0:907:A:H2'	1:0:908:A:H8	1.85	0.41
5:B:145:HIS:CD2	5:B:146:THR:O	2.73	0.41
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.55	0.41
7:D:58:VAL:CB	7:D:62:ASP:HB3	2.47	0.41
7:D:28:GLY:CA	7:D:69:ILE:HG23	2.42	0.41
13:K:115:ARG:HG3	13:K:116:GLU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:103:THR:HA	18:P:106:ARG:NH2	2.35	0.41
25:W:122:ARG:NH1	25:W:122:ARG:HG2	2.31	0.41
1:0:1097:A:H5'	25:W:125:HIS:CE1	2.55	0.41
27:Y:213:LYS:HE3	27:Y:213:LYS:HB2	1.87	0.41
1:0:1398:G:H5'	18:P:23:PHE:O	2.19	0.41
1:0:1565:C:O4'	1:0:2738:G:H1'	2.20	0.41
1:0:2032:U:C2'	1:0:2033:G:C5'	2.95	0.41
1:0:2820:A:H2'	1:0:2821:C:C6	2.54	0.41
1:0:282:C:O2'	1:0:283:U:C5'	2.67	0.41
1:0:2908:A:C2'	1:0:2909:G:H5'	2.50	0.41
30:2:11:LEU:HA	30:2:11:LEU:HD23	1.88	0.41
2:9:3005:G:OP1	16:N:17:ARG:NH2	2.53	0.41
4:A:194:MET:CE	4:A:199:HIS:CB	2.96	0.41
4:A:33:GLU:O	4:A:34:ASP:HB2	2.20	0.41
5:B:183:GLU:O	5:B:184:ASP:C	2.59	0.41
9:F:34:ASN:O	9:F:37:THR:HB	2.20	0.41
11:H:28:ILE:HG23	40:H:9551:HOH:O	2.19	0.41
17:O:106:PRO:HG2	17:O:107:GLU:OE2	2.20	0.41
17:O:59:VAL:CG2	17:O:111:VAL:CG2	2.98	0.41
20:R:61:GLN:CD	40:R:9451:HOH:O	2.58	0.41
25:W:122:ARG:NH2	25:W:154:ARG:HG2	2.35	0.41
1:0:1028:U:H5'	1:0:1031:G:O4'	2.20	0.41
1:0:1175:G:H2'	1:0:1176:C:O4'	2.20	0.41
1:0:1878:G:O2'	1:0:1879:U:H6	2.01	0.41
1:0:221:G:H2'	1:0:222:A:C8	2.55	0.41
1:0:2568:A:H2'	1:0:2569:A:O4'	2.21	0.41
1:0:787:G:O2'	1:0:788:A:H5'	2.20	0.41
1:0:2435:U:OP1	31:3:28:GLY:HA3	2.21	0.41
2:9:3001:U:H5'	2:9:3121:C:O2	2.20	0.41
4:A:132:ASP:OD1	4:A:133:ARG:N	2.38	0.41
40:0:3398:HOH:O	5:B:252:PRO:HD3	2.20	0.41
6:C:104:ASP:OD1	6:C:107:ARG:NH1	2.52	0.41
8:E:84:MET:CE	8:E:148:ILE:HD12	2.50	0.41
11:H:154:TYR:CD1	11:H:154:TYR:C	2.93	0.41
11:H:59:HIS:HA	11:H:62:LEU:HD23	2.02	0.41
17:O:37:ARG:HG3	40:O:3002:HOH:O	2.20	0.41
20:R:15:LYS:HE3	40:R:9492:HOH:O	2.20	0.41
28:Z:25:ARG:HB3	28:Z:29:ILE:CD1	2.51	0.41
1:0:522:U:O2'	1:0:1366:C:H5'	2.21	0.41
1:0:1406:A:H4'	1:0:1407:A:C5'	2.51	0.41
1:0:1488:U:H4'	1:0:1489:G:OP1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1507:C:H4'	40:0:4154:HOH:O	2.20	0.41
1:0:1783:A:O2'	1:0:1784:U:H5'	2.20	0.41
1:0:1856:C:H5'	1:0:1858:A:O4'	2.21	0.41
1:0:2096:A:H3'	1:0:2096:A:N3	2.35	0.41
1:0:27:U:H2'	1:0:28:G:O4'	2.20	0.41
1:0:295:C:H2'	1:0:296:G:O4'	2.21	0.41
30:2:19:SER:O	30:2:36:ASN:ND2	2.53	0.41
2:9:3018:U:H2'	2:9:3019:G:H8	1.86	0.41
1:0:2091:G:O3'	5:B:235:ARG:HD3	2.19	0.41
5:B:294:TYR:HE2	40:B:9641:HOH:O	2.02	0.41
6:C:115:LEU:HA	6:C:115:LEU:HD12	1.77	0.41
7:D:99:ASP:CB	7:D:103:ASN:H	2.33	0.41
7:D:65:GLU:HA	40:D:6752:HOH:O	2.20	0.41
7:D:71:ALA:HB2	40:D:7636:HOH:O	2.20	0.41
40:0:7171:HOH:O	16:N:4:PRO:HD2	2.20	0.41
22:T:43:ASN:C	22:T:45:GLY:H	2.24	0.41
25:W:41:TYR:CD2	25:W:44:MET:HE3	2.56	0.41
1:0:157:G:C6	1:0:158:A:N7	2.89	0.41
1:0:1634:G:H2'	1:0:1635:U:H6	1.85	0.41
1:0:1921:A:O2'	1:0:1922:A:H5'	2.21	0.41
1:0:2553:A:H2'	1:0:2553:A:N3	2.35	0.41
1:0:702:G:O2'	1:0:703:G:H5'	2.21	0.41
1:0:90:A:H2'	1:0:91:G:O4'	2.21	0.41
31:3:73:GLU:HG2	40:3:9493:HOH:O	2.19	0.41
6:C:246:ARG:NH1	40:C:9177:HOH:O	2.49	0.41
6:C:57:PRO:O	6:C:58:ALA:C	2.58	0.41
9:F:26:THR:CG2	9:F:102:GLY:HA3	2.51	0.41
9:F:60:VAL:CG1	9:F:60:VAL:O	2.69	0.41
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.35	0.41
25:W:88:THR:CG2	25:W:89:ASP:H	2.33	0.41
1:0:1041:U:H2'	1:0:1042:U:H5'	2.02	0.41
1:0:1182:C:H1'	1:0:1192:A:C8	2.47	0.41
1:0:1202:A:C2'	1:0:1203:G:H5'	2.51	0.41
1:0:2815:G:N7	12:J:80:LYS:NZ	2.68	0.41
1:0:441:A:C2	1:0:442:A:N6	2.89	0.41
1:0:521:A:H2'	1:0:522:U:H5'	2.02	0.41
1:0:830:G:O2'	1:0:831:U:H5'	2.21	0.41
29:1:56:GLU:HG2	29:1:56:GLU:OXT	2.20	0.41
4:A:65:ARG:HH11	4:A:65:ARG:HG2	1.85	0.41
6:C:78:ARG:CG	6:C:78:ARG:NH1	2.79	0.41
13:K:80:ILE:HG23	40:K:7064:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:122:GLN:HB2	15:M:126:GLN:O	2.20	0.41
40:O:4062:HOH:O	18:P:133:SER:HA	2.20	0.41
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.20	0.41
21:S:33:SER:OG	21:S:36:GLU:HG3	2.20	0.41
40:O:7765:HOH:O	22:T:9:LYS:HB2	2.19	0.41
26:X:10:VAL:HG12	26:X:11:THR:N	2.36	0.41
27:Y:187:VAL:CG1	27:Y:205:ILE:HA	2.51	0.41
1:O:1252:A:H2'	1:O:1253:C:O4'	2.21	0.41
1:O:1463:A:O5'	1:O:1463:A:H8	2.03	0.41
1:O:2314:G:C2'	1:O:2315:C:H5'	2.51	0.41
1:O:2532:A:H2	40:O:7900:HOH:O	2.03	0.41
1:O:363:A:H1'	40:O:5783:HOH:O	2.21	0.41
6:C:98:ARG:HH11	6:C:98:ARG:CG	2.29	0.41
7:D:166:ILE:HB	40:D:6326:HOH:O	2.20	0.41
10:G:63:ARG:N	40:G:2569:HOH:O	2.53	0.41
15:M:43:PRO:HG3	15:M:62:VAL:HG21	2.02	0.41
16:N:22:GLN:O	16:N:26:LEU:HD22	2.21	0.41
22:T:18:GLU:O	22:T:21:LYS:HE2	2.20	0.41
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.21	0.41
28:Z:27:ALA:O	28:Z:31:SER:HB2	2.20	0.41
1:O:1119:G:H22	1:O:1246:A:H2	1.48	0.41
1:O:1764:C:H2'	1:O:1765:G:O4'	2.21	0.41
1:O:2546:U:H4'	40:O:6621:HOH:O	2.20	0.41
1:O:2752:C:O2'	1:O:2753:G:H5'	2.20	0.41
1:O:2908:A:H2'	1:O:2909:G:C4'	2.51	0.41
1:O:560:C:C2	1:O:561:G:C8	3.09	0.41
1:O:724:G:O2'	1:O:725:C:H5'	2.21	0.41
4:A:93:THR:C	4:A:94:LEU:HD23	2.40	0.41
8:E:108:LEU:CD1	8:E:164:ASP:HB2	2.51	0.41
8:E:31:ARG:HH11	8:E:68:HIS:HB3	1.85	0.41
11:H:29:ALA:CB	11:H:66:ARG:HH12	2.28	0.41
13:K:114:ALA:HB3	13:K:117:VAL:HG23	2.02	0.41
13:K:113:ILE:HD12	13:K:128:ALA:HB2	2.02	0.41
14:L:92:ASP:HA	14:L:121:ILE:HB	2.03	0.41
18:P:16:VAL:HG12	18:P:17:GLY:H	1.83	0.41
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.55	0.41
1:O:1314:U:H5''	1:O:1316:G:O4'	2.20	0.41
1:O:1406:A:H5'	1:O:1407:A:C8	2.56	0.41
1:O:1477:C:O2'	1:O:1478:U:H5'	2.21	0.41
1:O:1506:U:H5'	1:O:1506:U:H6	1.86	0.41
1:O:2065:C:O2'	1:O:2066:C:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2089:A:C2'	1:0:2090:G:H5'	2.51	0.41
1:0:2362:A:H2'	1:0:2363:G:C8	2.56	0.41
1:0:2582:G:H4'	40:K:4440:HOH:O	2.20	0.41
1:0:2626:C:H2'	1:0:2627:G:C8	2.56	0.41
1:0:481:U:H4'	1:0:515:C:H2'	2.03	0.41
7:D:23:VAL:HG21	7:D:45:THR:CG2	2.50	0.41
32:I:114:PRO:HG2	32:I:115:ASP:H	1.86	0.41
14:L:67:ARG:HB2	14:L:112:GLY:HA3	2.03	0.41
1:0:700:A:C2	14:L:71:GLU:HG2	2.56	0.41
15:M:49:ALA:C	15:M:54:TYR:HB3	2.41	0.41
1:0:2364:A:H5''	19:Q:15:LYS:HD3	2.03	0.41
22:T:43:ASN:HD22	22:T:108:ARG:NH2	2.19	0.41
5:B:331:SER:OG	23:U:14:GLU:OE2	2.26	0.41
23:U:38:ASN:O	23:U:42:LEU:HG	2.21	0.41
1:0:1119:G:H8	12:J:52:GLN:NE2	2.18	0.41
1:0:1534:C:O2'	1:0:1656:A:OP1	2.34	0.41
1:0:2493:C:H2'	1:0:2493:C:O2	2.20	0.41
1:0:657:G:H2'	1:0:658:C:O4'	2.21	0.41
32:I:72:VAL:HG11	32:I:111:GLN:O	2.21	0.41
1:0:903:U:O4	14:L:18:HIS:HB2	2.21	0.41
15:M:164:THR:CG2	15:M:165:GLY:H	2.33	0.41
20:R:96:VAL:O	20:R:99:ALA:HB3	2.19	0.41
1:0:1095:U:O2	25:W:120:PRO:HG2	2.20	0.40
1:0:1791:U:O2'	1:0:1792:C:H5'	2.21	0.40
1:0:419:A:H1'	1:0:1921:A:C2	2.56	0.40
1:0:286:U:H2'	1:0:287:C:C6	2.56	0.40
1:0:637:C:OP1	27:Y:136:LYS:NZ	2.42	0.40
30:2:23:ALA:O	30:2:26:MET:HG2	2.21	0.40
6:C:107:ARG:CB	6:C:107:ARG:HH11	2.33	0.40
6:C:157:LEU:HD22	6:C:162:VAL:CG1	2.51	0.40
7:D:103:ASN:OD1	7:D:133:ASN:ND2	2.54	0.40
13:K:62:PRO:HA	13:K:65:ARG:HE	1.86	0.40
14:L:140:VAL:HB	40:L:9454:HOH:O	2.20	0.40
15:M:163:LEU:N	15:M:163:LEU:HD23	2.36	0.40
20:R:98:ASN:N	20:R:98:ASN:HD22	2.18	0.40
25:W:146:ILE:HA	25:W:146:ILE:HD13	1.85	0.40
1:0:1151:G:OP1	10:G:63:ARG:NH1	2.55	0.40
1:0:1173:A:H4'	1:0:1174:A:C8	2.56	0.40
1:0:1377:C:O2'	1:0:1378:G:H5''	2.22	0.40
1:0:1592:G:O2'	1:0:1593:C:O4'	2.25	0.40
1:0:2389:U:H4'	19:Q:53:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:790:A:H8	40:0:6549:HOH:O	2.04	0.40
1:0:95:A:O5'	1:0:97:G:H5'	2.21	0.40
2:9:3056:A:C3'	2:9:3057:A:H5''	2.51	0.40
15:M:123:ASP:OD1	15:M:123:ASP:C	2.59	0.40
15:M:34:GLU:HB3	15:M:38:GLU:HG3	2.02	0.40
16:N:114:LYS:O	16:N:118:ILE:HG13	2.21	0.40
16:N:91:ARG:O	16:N:94:GLU:HB2	2.22	0.40
17:O:47:ARG:NH1	40:O:4564:HOH:O	2.54	0.40
21:S:5:ILE:HD11	21:S:41:VAL:HG22	2.04	0.40
22:T:21:LYS:HA	22:T:24:ARG:HG3	2.03	0.40
1:0:1115:U:O2'	1:0:1116:U:H5'	2.21	0.40
1:0:119:A:H2'	1:0:120:A:C5'	2.50	0.40
1:0:1299:G:H5'	40:0:4616:HOH:O	2.20	0.40
1:0:210:U:H2'	1:0:211:U:C6	2.56	0.40
1:0:2791:U:H1'	1:0:2792:A:H5''	2.03	0.40
1:0:533:U:C5	1:0:2812:A:C2	3.09	0.40
1:0:711:G:C2	1:0:718:C:C2	3.09	0.40
1:0:947:U:O2'	1:0:948:G:H5'	2.21	0.40
29:1:53:LYS:HA	29:1:53:LYS:HD3	1.92	0.40
5:B:205:VAL:HB	5:B:307:ARG:HD3	2.03	0.40
5:B:280:VAL:HG12	5:B:281:ASP:N	2.36	0.40
6:C:118:THR:HG23	40:C:9106:HOH:O	2.21	0.40
6:C:94:THR:HB	40:C:9162:HOH:O	2.20	0.40
9:F:26:THR:HG21	9:F:102:GLY:C	2.41	0.40
9:F:22:VAL:HG23	9:F:104:ALA:HB2	2.02	0.40
32:I:132:CYS:O	32:I:135:LEU:N	2.53	0.40
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.54	0.40
28:Z:39:CYS:O	28:Z:42:CYS:O	2.39	0.40
1:0:1071:G:H4'	27:Y:154:ARG:HH22	1.86	0.40
1:0:1165:G:H21	1:0:1173:A:C5'	2.34	0.40
1:0:1342:C:H2'	1:0:1343:C:H5'	2.04	0.40
1:0:1573:A:N7	1:0:1574:C:C2	2.90	0.40
1:0:1592:G:H2'	1:0:1593:C:C6	2.56	0.40
1:0:1624:A:H4'	1:0:1625:U:H5'	2.02	0.40
1:0:1803:C:H2'	1:0:1804:A:H8	1.86	0.40
2:9:3088:G:OP1	25:W:130:HIS:NE2	2.39	0.40
1:0:1852:A:H5''	4:A:232:ARG:O	2.22	0.40
7:D:13:MET:HA	7:D:137:PRO:HG2	2.02	0.40
1:0:2466:G:OP2	14:L:37:LYS:HE2	2.22	0.40
15:M:59:GLY:C	15:M:141:ILE:HD11	2.40	0.40
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:40:VAL:HG22	22:T:41:ARG:N	2.35	0.40
40:K:7438:HOH:O	23:U:20:MET:HE1	2.20	0.40
1:0:1117:A:C2	1:0:1244:U:C2	3.09	0.40
1:0:1603:A:H5'	1:0:1605:G:C4'	2.51	0.40
1:0:1769:C:O2'	1:0:1770:U:H5'	2.22	0.40
1:0:1797:A:H2'	1:0:1799:G:O5'	2.21	0.40
1:0:2565:C:H4'	40:0:5357:HOH:O	2.22	0.40
1:0:2896:A:C2'	1:0:2896:A:N3	2.81	0.40
1:0:820:G:O2'	1:0:856:G:H4'	2.21	0.40
1:0:951:A:H2'	1:0:952:G:H5'	2.03	0.40
4:A:81:GLN:CG	4:A:92:ASN:HD21	2.34	0.40
5:B:146:THR:C	5:B:148:PRO:HD3	2.41	0.40
5:B:270:ILE:O	5:B:271:ASP:HB2	2.22	0.40
5:B:57:GLU:OE1	5:B:60:SER:HB2	2.21	0.40
6:C:39:GLN:O	6:C:43:LYS:HD3	2.22	0.40
1:0:475:G:H5'	6:C:73:LEU:HD23	2.04	0.40
7:D:35:ALA:C	7:D:37:ALA:H	2.23	0.40
1:0:2346:C:O3'	7:D:52:THR:CG2	2.70	0.40
32:I:91:GLU:HB2	32:I:95:ASP:OD2	2.21	0.40
13:K:66:ARG:HH11	13:K:66:ARG:HG2	1.86	0.40
15:M:77:HIS:HB2	15:M:81:ARG:HD3	2.03	0.40
15:M:82:ARG:O	15:M:84:LYS:N	2.55	0.40
7:D:149:ARG:HH12	16:N:15:GLU:HA	1.86	0.40
16:N:74:PRO:HB2	16:N:77:ASN:ND2	2.37	0.40
19:Q:41:LEU:HB3	19:Q:52:PHE:CZ	2.56	0.40
25:W:146:ILE:HG22	25:W:147:ASP:N	2.36	0.40
27:Y:102:LEU:HD11	27:Y:225:GLY:HA2	2.04	0.40
27:Y:112:GLU:O	27:Y:116:LEU:HG	2.21	0.40

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

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	208 (88%)	20 (8%)	7 (3%)	4	3
5	B	335/338 (99%)	296 (88%)	32 (10%)	7 (2%)	7	8
6	C	244/246 (99%)	221 (91%)	22 (9%)	1 (0%)	34	48
7	D	134/177 (76%)	104 (78%)	19 (14%)	11 (8%)	1	0
8	E	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
9	F	117/120 (98%)	102 (87%)	12 (10%)	3 (3%)	5	5
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	136 (87%)	15 (10%)	5 (3%)	4	3
12	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	11	15
13	K	130/132 (98%)	118 (91%)	11 (8%)	1 (1%)	19	29
14	L	141/165 (86%)	115 (82%)	25 (18%)	1 (1%)	22	32
15	M	192/195 (98%)	179 (93%)	11 (6%)	2 (1%)	15	23
16	N	184/187 (98%)	158 (86%)	17 (9%)	9 (5%)	2	1
17	O	113/116 (97%)	105 (93%)	8 (7%)	0	100	100
18	P	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
19	Q	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	14	20
20	R	148/155 (96%)	137 (93%)	10 (7%)	1 (1%)	22	32
21	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
22	T	117/120 (98%)	110 (94%)	4 (3%)	3 (3%)	5	5
23	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
24	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	9	13
25	W	152/154 (99%)	145 (95%)	7 (5%)	0	100	100
26	X	80/92 (87%)	71 (89%)	8 (10%)	1 (1%)	12	17
27	Y	140/241 (58%)	135 (96%)	5 (4%)	0	100	100
28	Z	71/83 (86%)	58 (82%)	9 (13%)	4 (6%)	2	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
30	2	42/50 (84%)	39 (93%)	2 (5%)	1 (2%)	6	6
31	3	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
32	I	68/162 (42%)	52 (76%)	12 (18%)	4 (6%)	1	0
All	All	3705/4431 (84%)	3338 (90%)	302 (8%)	65 (2%)	8	10

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	36	ASP
4	A	37	VAL
5	B	139	ASP
5	B	169	GLY
7	D	164	ALA
9	F	101	ALA
11	H	166	SER
11	H	168	ALA
14	L	80	ASP
16	N	154	LEU
16	N	167	ASP
16	N	184	ILE
28	Z	20	ARG
28	Z	81	ARG
4	A	205	GLY
5	B	34	GLY
5	B	279	THR
5	B	291	ASP
6	C	8	LEU
7	D	16	PRO
7	D	56	ARG
7	D	60	GLU
7	D	65	GLU
7	D	97	GLN
7	D	137	PRO
13	K	127	ALA
16	N	155	GLU
16	N	183	ASP
24	V	43	PRO
32	I	76	ALA
32	I	129	VAL
5	B	184	ASP

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Mol	Chain	Res	Type
7	D	168	SER
7	D	171	ASP
11	H	16	ARG
12	J	5	GLU
15	M	83	SER
26	X	70	ILE
32	I	133	THR
4	A	24	LYS
5	B	185	GLY
9	F	64	PRO
11	H	79	GLU
12	J	143	LYS
16	N	157	PRO
16	N	162	ASP
22	T	46	ASP
22	T	53	GLY
28	Z	41	ASN
16	N	65	ASP
16	N	68	GLU
22	T	44	ALA
30	2	37	HIS
32	I	114	PRO
4	A	208	HIS
4	A	42	VAL
7	D	69	ILE
11	H	81	GLY
7	D	28	GLY
15	M	88	VAL
28	Z	21	VAL
9	F	71	GLY
4	A	204	GLY
19	Q	18	PRO
20	R	114	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/182 (98%)	169 (94%)	10 (6%)	21	34
5	B	282/283 (100%)	266 (94%)	16 (6%)	20	33
6	C	193/193 (100%)	176 (91%)	17 (9%)	10	15
7	D	117/148 (79%)	108 (92%)	9 (8%)	13	20
8	E	152/156 (97%)	144 (95%)	8 (5%)	22	37
9	F	93/94 (99%)	92 (99%)	1 (1%)	73	87
10	G	27/283 (10%)	25 (93%)	2 (7%)	13	22
11	H	132/138 (96%)	126 (96%)	6 (4%)	27	44
12	J	118/121 (98%)	106 (90%)	12 (10%)	7	10
13	K	106/106 (100%)	99 (93%)	7 (7%)	16	26
14	L	113/127 (89%)	110 (97%)	3 (3%)	44	65
15	M	158/159 (99%)	153 (97%)	5 (3%)	39	59
16	N	149/150 (99%)	138 (93%)	11 (7%)	13	22
17	O	93/94 (99%)	89 (96%)	4 (4%)	29	46
18	P	113/117 (97%)	109 (96%)	4 (4%)	36	55
19	Q	79/80 (99%)	76 (96%)	3 (4%)	33	51
20	R	117/122 (96%)	113 (97%)	4 (3%)	37	56
21	S	71/74 (96%)	70 (99%)	1 (1%)	67	82
22	T	105/106 (99%)	101 (96%)	4 (4%)	33	51
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	48 (94%)	3 (6%)	19	32
25	W	130/130 (100%)	122 (94%)	8 (6%)	18	29
26	X	66/74 (89%)	59 (89%)	7 (11%)	6	9
27	Y	120/196 (61%)	111 (92%)	9 (8%)	13	21
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	40 (95%)	2 (5%)	25	41
31	3	79/79 (100%)	76 (96%)	3 (4%)	33	51
32	I	58/130 (45%)	56 (97%)	2 (3%)	37	56
All	All	3093/3612 (86%)	2932 (95%)	161 (5%)	23	38

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

Mol	Chain	Res	Type
4	A	3	ARG
4	A	26	ASP
4	A	62	ASP
4	A	78	ASP
4	A	94	LEU
4	A	144	GLU
4	A	165	THR
4	A	179	MET
4	A	206	ARG
4	A	217	ARG
5	B	11	LEU
5	B	27	ASN
5	B	71	VAL
5	B	82	VAL
5	B	112	THR
5	B	113	LEU
5	B	132	HIS
5	B	149	ASP
5	B	162	MET
5	B	175	LEU
5	B	180	ASP
5	B	195	ARG
5	B	211	THR
5	B	254	GLN
5	B	257	THR
5	B	312	ARG
6	C	2	GLN
6	C	16	VAL
6	C	27	ARG
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	98	ARG
6	C	101	ASP
6	C	115	LEU
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	223	LEU
6	C	236	THR
6	C	240	LEU
6	C	243	VAL

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Mol	Chain	Res	Type
7	D	24	HIS
7	D	50	VAL
7	D	61	PHE
7	D	99	ASP
7	D	100	ASP
7	D	133	ASN
7	D	135	VAL
7	D	137	PRO
7	D	170	TYR
8	E	7	ILE
8	E	16	ASP
8	E	86	VAL
8	E	102	VAL
8	E	116	THR
8	E	155	ASN
8	E	156	ASP
8	E	164	ASP
9	F	46	GLU
10	G	12	ILE
10	G	72	ASP
11	H	1	LYS
11	H	18	GLU
11	H	58	ARG
11	H	84	LYS
11	H	88	ARG
11	H	154	TYR
12	J	39	VAL
12	J	46	ILE
12	J	47	THR
12	J	52	GLN
12	J	70	PHE
12	J	74	ARG
12	J	79	PHE
12	J	93	ARG
12	J	107	ASN
12	J	127	ILE
12	J	131	THR
12	J	132	LEU
13	K	4	LEU
13	K	7	ASP
13	K	10	GLN
13	K	55	VAL

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Mol	Chain	Res	Type
13	K	84	ASP
13	K	98	VAL
13	K	107	THR
14	L	35	ARG
14	L	43	HIS
14	L	75	LEU
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
16	N	17	ARG
16	N	26	LEU
16	N	37	ARG
16	N	38	LYS
16	N	49	THR
16	N	56	ASP
16	N	65	ASP
16	N	127	LEU
16	N	134	ASP
16	N	152	GLU
16	N	157	PRO
17	O	3	THR
17	O	16	SER
17	O	43	VAL
17	O	67	SER
18	P	13	VAL
18	P	21	VAL
18	P	98	ILE
18	P	117	SER
19	Q	16	ASN
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	82	GLU
20	R	132	ARG
20	R	143	VAL
21	S	53	ASN
22	T	39	ASN
22	T	41	ARG
22	T	89	ARG
22	T	96	VAL

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Mol	Chain	Res	Type
24	V	12	THR
24	V	45	ARG
24	V	65	ASP
25	W	4	LEU
25	W	26	ILE
25	W	35	VAL
25	W	76	ASP
25	W	122	ARG
25	W	142	ASP
25	W	146	ILE
25	W	154	ARG
26	X	15	ARG
26	X	27	ASP
26	X	46	ASP
26	X	79	GLU
26	X	80	GLU
26	X	82	GLU
26	X	85	VAL
27	Y	103	THR
27	Y	115	ARG
27	Y	141	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	204	ARG
27	Y	231	PRO
27	Y	235	GLU
30	2	16	ASN
30	2	18	ASN
31	3	3	MET
31	3	18	GLN
31	3	65	THR
32	I	119	TYR
32	I	140	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
4	A	47	HIS
4	A	92	ASN
4	A	199	HIS

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Mol	Chain	Res	Type
5	B	2	GLN
5	B	27	ASN
5	B	145	HIS
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	11	ASN
6	C	39	GLN
6	C	129	HIS
7	D	47	GLN
7	D	103	ASN
7	D	133	ASN
8	E	106	ASN
8	E	119	HIS
8	E	143	GLN
10	G	17	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	70	ASN
11	H	170	ASN
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	43	HIS
15	M	24	GLN
15	M	58	GLN
15	M	77	HIS
15	M	126	GLN
15	M	137	ASN
15	M	143	ASN
15	M	170	ASN
16	N	93	GLN
16	N	107	ASN

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Mol	Chain	Res	Type
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	88	GLN
18	P	89	ASN
18	P	118	GLN
19	Q	16	ASN
19	Q	40	HIS
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
21	S	21	GLN
21	S	53	ASN
21	S	55	GLN
22	T	39	ASN
22	T	43	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	2	HIS
25	W	27	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
27	Y	133	HIS
27	Y	134	HIS
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS
30	2	16	ASN
30	2	18	ASN
30	2	41	HIS
30	2	45	ASN
31	3	2	GLN
31	3	30	GLN
31	3	48	ASN

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Mol	Chain	Res	Type
31	3	78	HIS
32	I	113	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	249 (9%)	33 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
3	4	2/5 (40%)	1 (50%)	0
All	All	2868/3049 (94%)	268 (9%)	34 (1%)

All (268) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	120	A
1	0	130	C
1	0	138	U
1	0	141	C
1	0	151	A
1	0	166	A
1	0	185	G
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C

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Mol	Chain	Res	Type
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	487	G
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	605	C
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	702	G
1	0	735	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U

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Mol	Chain	Res	Type
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	885	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C

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Mol	Chain	Res	Type
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1287	A
1	0	1289	C
1	0	1300	G
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1526	A
1	0	1528	A
1	0	1564	C
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1710	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C
1	0	1752	G

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Mol	Chain	Res	Type
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1968	A
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2004	U
1	0	2006	C
1	0	2008	U
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2329	C
1	0	2354	A

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Mol	Chain	Res	Type
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2611	G
1	0	2613	G
1	0	2634	G
1	0	2637	A
1	0	2644	C
1	0	2645	U
1	0	2648	U
1	0	2649	A
1	0	2650	U
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2727	A
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2783	A

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Mol	Chain	Res	Type
1	0	2786	G
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2825	C
1	0	2852	A
1	0	2853	U
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3039	U
2	9	3040	C
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C
3	4	76	A

All (34) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	87	C
1	0	129	A
1	0	169	A
1	0	604	G
1	0	644	G
1	0	699	C

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	0	2621	1	17,21,22	1.63	3 (17%)	20,30,33	5.47	4 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	0	2588	1	18,26,27	1.08	2 (11%)	20,38,41	2.60	5 (25%)
3	ACA	4	78	3	3,3,8	0.52	0	2,2,8	0.72	0
1	UR3	0	2619	1	14,22,23	0.86	0	15,32,35	0.59	0
1	OMU	0	2587	1	14,22,23	1.08	1 (7%)	14,31,34	1.20	1 (7%)
1	1MA	0	628	1,35	15,25,26	0.81	1 (6%)	15,37,40	1.41	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
3	ACA	4	78	3	-	0/0/1/6	-
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2
1	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.80	1.48	1.52
1	0	2588	OMG	C6-N1	3.54	1.39	1.33
1	0	2621	PSU	C4-N3	3.27	1.38	1.33
1	0	2587	OMU	C4-N3	3.06	1.38	1.33
1	0	2621	PSU	C2-N1	2.65	1.43	1.38
1	0	628	1MA	C2-N3	2.07	1.34	1.30
1	0	2588	OMG	C8-N7	-2.02	1.31	1.34

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.37	114.62	128.43
1	0	2621	PSU	C4-N3-C2	14.45	127.34	115.14
1	0	2588	OMG	C5-C6-N1	-8.68	111.56	123.43
1	0	2621	PSU	C5-C4-N3	-8.38	114.56	125.36
1	0	2588	OMG	C6-N1-C2	5.86	125.25	115.93
1	0	628	1MA	C2-N3-C4	-4.60	110.83	116.58
1	0	2587	OMU	C5-C4-N3	-3.92	114.68	123.31
1	0	2588	OMG	C2-N3-C4	-2.97	111.97	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-N1-C2	2.58	119.61	115.36
1	0	2588	OMG	N3-C2-N1	-2.55	123.83	127.22
1	0	2588	OMG	C6-C5-C4	-2.00	118.88	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 313 ligands modelled in this entry, 312 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
38	SPS	4	9701	33	20,23,23	1.61	4 (20%)	18,30,30	2.78	4 (22%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	9701	SPS	C1-C6	3.67	1.53	1.43
38	4	9701	SPS	C5-N4	3.11	1.39	1.34
38	4	9701	SPS	C9-C10	-3.01	1.41	1.48
38	4	9701	SPS	C1-N2	2.61	1.37	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	9701	SPS	C6-C1-N2	-8.17	118.70	124.40
38	4	9701	SPS	C1-N2-C3	7.16	121.19	115.14
38	4	9701	SPS	C6-C5-N4	-2.37	119.42	122.12
38	4	9701	SPS	O15-S15-C16	2.10	108.97	106.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

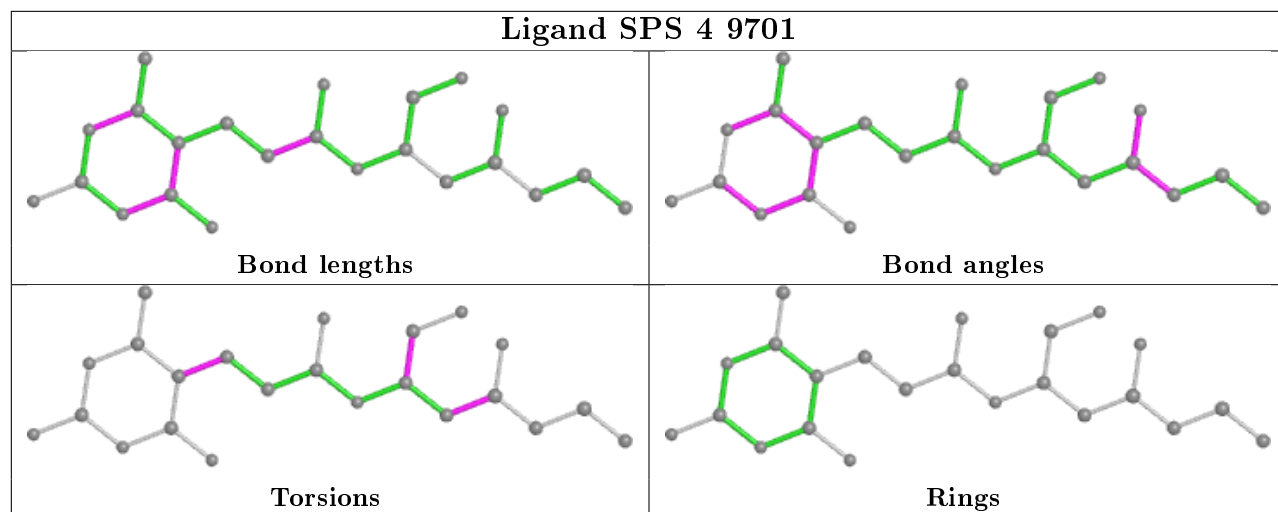
Mol	Chain	Res	Type	Atoms
38	4	9701	SPS	C5-C6-C8-C9
38	4	9701	SPS	N11-C12-C13-O13
38	4	9701	SPS	C14-C12-C13-O13
38	4	9701	SPS	C12-C14-S15-O15
38	4	9701	SPS	C12-C14-S15-C16

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	4	9701	SPS	3	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.61	58 (2%) 63 61	19, 43, 80, 130	0
2	9	122/122 (100%)	-0.36	5 (4%) 37 36	35, 59, 79, 129	0
3	4	4/5 (80%)	0.22	0 100 100	44, 46, 51, 57	0
4	A	237/240 (98%)	0.51	22 (9%) 8 8	28, 51, 79, 92	0
5	B	337/338 (99%)	0.03	4 (1%) 79 77	25, 46, 66, 77	0
6	C	246/246 (100%)	-0.06	2 (0%) 86 84	24, 43, 61, 72	0
7	D	140/177 (79%)	1.90	59 (42%) 0 0	53, 76, 103, 111	0
8	E	172/178 (96%)	0.43	12 (6%) 16 15	37, 55, 69, 73	0
9	F	119/120 (99%)	1.04	27 (22%) 0 0	45, 64, 88, 91	0
10	G	29/348 (8%)	2.24	10 (34%) 0 0	60, 77, 82, 85	0
11	H	160/171 (93%)	0.43	15 (9%) 8 7	39, 54, 80, 84	0
12	J	142/145 (97%)	-0.08	2 (1%) 75 73	32, 43, 59, 75	0
13	K	132/132 (100%)	-0.18	3 (2%) 60 58	30, 42, 59, 67	0
14	L	145/165 (87%)	0.70	25 (17%) 1 1	26, 60, 92, 101	0
15	M	194/195 (99%)	0.61	19 (9%) 7 7	31, 42, 80, 85	0
16	N	186/187 (99%)	0.86	30 (16%) 1 1	43, 58, 93, 98	0
17	O	115/116 (99%)	-0.09	2 (1%) 70 68	36, 49, 61, 67	0
18	P	143/149 (95%)	0.08	2 (1%) 75 73	35, 47, 58, 66	0
19	Q	95/96 (98%)	0.11	3 (3%) 47 46	39, 46, 59, 65	0
20	R	150/155 (96%)	-0.16	0 100 100	27, 39, 56, 67	0
21	S	81/85 (95%)	0.28	4 (4%) 29 28	39, 52, 69, 84	0
22	T	119/120 (99%)	0.42	7 (5%) 22 21	35, 50, 72, 96	0
23	U	53/66 (80%)	0.43	4 (7%) 14 13	39, 50, 66, 72	0
24	V	65/71 (91%)	1.51	15 (23%) 0 0	47, 65, 94, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.10	1 (0%) 89 88	31, 44, 58, 68	0
26	X	82/92 (89%)	0.56	11 (13%) 3 2	37, 49, 69, 85	0
27	Y	142/241 (58%)	0.17	6 (4%) 36 35	24, 41, 57, 76	0
28	Z	73/83 (87%)	3.82	43 (58%) 0 0	63, 85, 94, 98	0
29	1	56/57 (98%)	-0.35	0 100 100	25, 31, 38, 47	0
30	2	46/50 (92%)	0.44	4 (8%) 10 9	32, 51, 65, 70	0
31	3	92/92 (100%)	1.37	20 (21%) 0 0	48, 65, 72, 81	0
32	I	70/162 (43%)	5.16	64 (91%) 0 0	92, 106, 120, 121	0
All	All	6650/7480 (88%)	0.05	479 (7%) 15 14	19, 47, 85, 130	0

All (479) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	16.4
24	V	1	THR	13.7
28	Z	11	SER	13.1
28	Z	22	SER	12.7
32	I	133	THR	12.5
7	D	63	ILE	11.5
28	Z	45	ASP	11.1
28	Z	21	VAL	11.0
16	N	166	ALA	10.8
28	Z	20	ARG	10.3
32	I	79	ILE	10.2
24	V	40	PRO	10.1
15	M	70	GLY	9.9
32	I	118	SER	9.8
28	Z	12	GLY	9.5
7	D	57	THR	9.3
7	D	90	LEU	9.2
32	I	77	GLU	9.1
28	Z	14	PHE	9.0
32	I	76	ALA	9.0
32	I	116	LEU	8.9
32	I	75	THR	8.8
28	Z	29	ILE	8.8
28	Z	33	MET	8.7
28	Z	31	SER	8.5
28	Z	18	TYR	8.1

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Mol	Chain	Res	Type	RSRZ
28	Z	34	ASN	8.0
32	I	132	CYS	8.0
32	I	121	LEU	7.9
28	Z	15	GLY	7.8
32	I	81	ASP	7.6
24	V	39	ALA	7.6
24	V	38	GLY	7.6
28	Z	16	ALA	7.5
28	Z	32	GLU	7.4
32	I	137	VAL	7.4
28	Z	19	GLY	7.3
28	Z	23	ARG	7.2
32	I	104	GLN	7.2
32	I	108	ILE	7.2
2	9	3001	U	7.2
32	I	96	PHE	7.1
28	Z	26	VAL	7.1
32	I	74	PRO	7.1
32	I	107	GLN	7.0
22	T	119	ALA	6.9
32	I	117	LEU	6.9
32	I	85	PHE	6.8
15	M	80	GLY	6.7
32	I	105	VAL	6.7
32	I	87	THR	6.7
32	I	113	HIS	6.6
32	I	102	VAL	6.6
10	G	23	ILE	6.5
32	I	109	ALA	6.4
26	X	88	GLU	6.4
28	Z	24	ARG	6.4
15	M	79	ALA	6.4
4	A	237	GLY	6.3
32	I	129	VAL	6.2
28	Z	41	ASN	6.2
4	A	37	VAL	6.1
32	I	111	GLN	6.1
10	G	26	MET	6.1
28	Z	40	PRO	6.0
15	M	74	LYS	5.8
15	M	72	ALA	5.8
32	I	125	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
31	3	20	HIS	5.8
15	M	89	THR	5.7
24	V	37	GLY	5.7
15	M	86	GLN	5.6
7	D	44	ILE	5.5
30	2	49	GLU	5.5
10	G	27	ILE	5.5
32	I	93	GLN	5.4
16	N	165	ALA	5.4
32	I	138	THR	5.3
21	S	81	ILE	5.3
32	I	86	GLU	5.3
28	Z	46	ARG	5.2
15	M	87	GLY	5.2
32	I	136	GLY	5.2
32	I	114	PRO	5.2
15	M	71	SER	5.2
1	0	1951	G	5.0
32	I	78	LEU	5.0
22	T	118	SER	5.0
32	I	83	ALA	5.0
32	I	134	SER	5.0
15	M	76	ARG	5.0
31	3	62	THR	5.0
1	0	1199	A	4.9
15	M	81	ARG	4.9
2	9	3024	U	4.9
7	D	61	PHE	4.9
16	N	175	LEU	4.9
32	I	119	TYR	4.9
28	Z	25	ARG	4.9
31	3	56	PRO	4.8
32	I	122	THR	4.8
32	I	91	GLU	4.8
32	I	89	SER	4.8
1	0	1169	U	4.8
14	L	81	VAL	4.8
32	I	97	VAL	4.7
28	Z	27	ALA	4.7
23	U	47	ARG	4.7
15	M	84	LYS	4.7
28	Z	30	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	0	735	C	4.6
32	I	126	LYS	4.6
28	Z	44	GLU	4.6
7	D	69	ILE	4.6
1	0	282	C	4.5
2	9	3002	U	4.5
28	Z	58	SER	4.5
15	M	75	ARG	4.5
1	0	1172	G	4.4
4	A	36	ASP	4.4
15	M	88	VAL	4.3
7	D	91	ALA	4.3
2	9	3023	U	4.3
14	L	106	VAL	4.3
1	0	970	U	4.2
28	Z	37	HIS	4.2
7	D	170	TYR	4.2
7	D	10	PHE	4.2
7	D	88	LEU	4.2
28	Z	10	ARG	4.2
24	V	41	GLU	4.2
7	D	26	GLY	4.2
32	I	98	ALA	4.2
7	D	128	LEU	4.1
32	I	80	LYS	4.1
22	T	117	ASP	4.1
1	0	2004	U	4.1
28	Z	39	CYS	4.1
28	Z	42	CYS	4.1
4	A	31	LYS	4.1
9	F	119	ARG	4.0
4	A	85	SER	4.0
28	Z	13	ARG	4.0
7	D	11	HIS	4.0
32	I	123	ASN	4.0
7	D	73	VAL	4.0
4	A	82	VAL	4.0
15	M	83	SER	3.9
7	D	134	LEU	3.9
16	N	68	GLU	3.9
7	D	62	ASP	3.9
7	D	130	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
32	I	72	VAL	3.9
4	A	38	ILE	3.9
7	D	18	ILE	3.9
15	M	73	ARG	3.9
14	L	80	ASP	3.8
16	N	163	PHE	3.8
28	Z	38	ALA	3.8
32	I	88	GLY	3.8
32	I	103	ASP	3.8
27	Y	235	GLU	3.8
7	D	64	ARG	3.8
1	0	1965	C	3.8
7	D	41	LEU	3.8
15	M	82	ARG	3.8
22	T	116	ASP	3.8
7	D	104	PHE	3.7
7	D	27	ILE	3.7
1	0	1948	G	3.7
9	F	117	GLU	3.7
1	0	514	G	3.7
4	A	32	VAL	3.7
14	L	93	VAL	3.7
1	0	10	U	3.7
1	0	1177	A	3.6
7	D	93	LEU	3.6
7	D	166	ILE	3.6
16	N	160	SER	3.6
10	G	71	LEU	3.6
16	N	2	THR	3.6
1	0	2238	A	3.6
14	L	105	TYR	3.6
8	E	87	PHE	3.5
7	D	106	PHE	3.5
28	Z	36	ASP	3.5
7	D	25	MET	3.5
16	N	178	THR	3.5
10	G	22	ALA	3.5
30	2	35	ARG	3.5
31	3	6	ARG	3.5
9	F	106	ALA	3.5
1	0	1173	A	3.4
1	0	1168	C	3.4

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Mol	Chain	Res	Type	RSRZ
16	N	179	LEU	3.4
7	D	87	ALA	3.4
27	Y	216	ARG	3.4
32	I	106	LYS	3.4
26	X	80	GLU	3.4
6	C	61	PHE	3.4
1	0	272	A	3.4
7	D	172	VAL	3.4
1	0	1202	A	3.3
9	F	16	ALA	3.3
4	A	64	ASP	3.3
8	E	100	ASP	3.3
1	0	1163	G	3.3
1	0	1170	U	3.3
1	0	1200	A	3.3
1	0	497	A	3.3
9	F	19	ALA	3.3
16	N	172	PHE	3.3
1	0	2237	G	3.3
31	3	29	ARG	3.3
31	3	22	VAL	3.3
1	0	280	C	3.2
28	Z	56	GLN	3.2
14	L	91	VAL	3.2
26	X	85	VAL	3.2
27	Y	95	THR	3.2
31	3	41	GLU	3.2
4	A	133	ARG	3.2
16	N	95	ALA	3.2
4	A	60	PHE	3.2
28	Z	35	GLU	3.2
11	H	138	CYS	3.2
1	0	1966	U	3.2
28	Z	28	GLU	3.2
14	L	100	ALA	3.2
26	X	77	PHE	3.2
2	9	3122	C	3.1
4	A	99	ILE	3.1
16	N	147	ILE	3.1
7	D	66	GLY	3.1
1	0	285	A	3.1
14	L	76	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
16	N	184	ILE	3.1
1	0	1525	G	3.1
10	G	24	VAL	3.1
1	0	288	A	3.1
9	F	118	LEU	3.1
7	D	68	PRO	3.1
32	I	82	GLU	3.1
31	3	92	GLU	3.0
10	G	12	ILE	3.0
9	F	17	LEU	3.0
16	N	158	LEU	3.0
32	I	135	LEU	3.0
32	I	115	ASP	3.0
11	H	74	ILE	3.0
16	N	155	GLU	3.0
9	F	115	VAL	3.0
22	T	115	GLU	3.0
15	M	90	ARG	3.0
8	E	10	ASP	3.0
24	V	36	ALA	3.0
9	F	22	VAL	3.0
28	Z	43	GLY	3.0
7	D	40	ILE	3.0
7	D	86	THR	3.0
16	N	180	LEU	3.0
1	0	284	C	2.9
11	H	171	ALA	2.9
1	0	2508	C	2.9
26	X	71	ARG	2.9
7	D	154	LYS	2.9
7	D	92	GLU	2.9
26	X	10	VAL	2.9
7	D	53	LYS	2.9
1	0	1198	U	2.9
25	W	86	GLU	2.9
32	I	94	GLU	2.9
8	E	45	ASP	2.9
9	F	99	THR	2.9
7	D	51	ARG	2.8
1	0	2748	G	2.8
15	M	77	HIS	2.8
31	3	23	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
17	O	22	GLY	2.8
11	H	146	VAL	2.8
1	0	1950	G	2.8
1	0	1967	U	2.8
14	L	130	ARG	2.8
19	Q	95	GLU	2.8
9	F	110	ASP	2.8
28	Z	61	ASP	2.8
10	G	66	LEU	2.8
10	G	69	ARG	2.8
1	0	1625	U	2.8
16	N	134	ASP	2.8
9	F	49	PHE	2.8
7	D	75	LEU	2.8
13	K	118	ALA	2.8
7	D	67	ASP	2.8
8	E	43	ASP	2.8
28	Z	50	GLN	2.7
32	I	124	ALA	2.7
12	J	4	ALA	2.7
9	F	12	LEU	2.7
16	N	183	ASP	2.7
13	K	132	VAL	2.7
5	B	57	GLU	2.7
28	Z	57	CYS	2.7
7	D	84	LEU	2.7
31	3	13	HIS	2.7
1	0	736	A	2.7
31	3	78	HIS	2.7
11	H	78	GLY	2.7
7	D	45	THR	2.7
7	D	89	PRO	2.7
12	J	70	PHE	2.6
9	F	107	ASP	2.6
7	D	56	ARG	2.6
9	F	114	LYS	2.6
16	N	139	TRP	2.6
11	H	77	LEU	2.6
5	B	128	ILE	2.6
1	0	279	C	2.6
16	N	161	GLY	2.6
7	D	157	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
32	I	99	ASP	2.6
24	V	8	ILE	2.6
7	D	43	GLU	2.6
21	S	70	GLU	2.6
4	A	203	GLY	2.6
7	D	23	VAL	2.6
26	X	7	GLU	2.6
32	I	110	GLU	2.6
1	0	1279	U	2.6
28	Z	80	ARG	2.6
21	S	20	PHE	2.5
24	V	59	ILE	2.5
7	D	167	GLU	2.5
16	N	152	GLU	2.5
9	F	15	ASP	2.5
16	N	185	GLU	2.5
14	L	99	GLU	2.5
11	H	111	ASP	2.5
14	L	97	VAL	2.5
1	0	1947	G	2.5
31	3	3	MET	2.5
14	L	60	GLU	2.5
4	A	39	ALA	2.5
5	B	1	PRO	2.5
8	E	48	VAL	2.5
31	3	25	VAL	2.5
1	0	2769	C	2.5
7	D	81	GLU	2.5
16	N	37	ARG	2.5
26	X	41	PHE	2.5
9	F	100	ASP	2.5
14	L	62	ALA	2.5
31	3	74	CYS	2.5
23	U	54	THR	2.5
4	A	30	ARG	2.5
16	N	143	ARG	2.5
9	F	6	PHE	2.5
4	A	35	GLY	2.5
7	D	85	GLN	2.4
27	Y	236	VAL	2.4
23	U	53	ASP	2.4
1	0	999	C	2.4

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Mol	Chain	Res	Type	RSRZ
8	E	6	GLU	2.4
4	A	86	ALA	2.4
32	I	120	ASP	2.4
32	I	84	GLY	2.4
14	L	120	LEU	2.4
24	V	5	VAL	2.4
24	V	46	ILE	2.4
26	X	65	ASN	2.4
8	E	154	ILE	2.4
31	3	14	CYS	2.4
31	3	21	GLU	2.4
9	F	28	ALA	2.4
23	U	55	ALA	2.4
31	3	80	ARG	2.4
8	E	88	TYR	2.4
7	D	47	GLN	2.4
7	D	74	THR	2.4
1	0	138	U	2.3
13	K	125	ALA	2.3
7	D	42	GLY	2.3
1	0	1178	G	2.3
9	F	108	VAL	2.3
27	Y	108	ASP	2.3
1	0	1171	A	2.3
11	H	137	TYR	2.3
8	E	118	ILE	2.3
9	F	75	ILE	2.3
7	D	54	ALA	2.3
11	H	35	ARG	2.3
9	F	44	SER	2.3
24	V	3	LEU	2.3
7	D	173	GLU	2.3
7	D	107	GLY	2.3
16	N	148	ALA	2.3
7	D	135	VAL	2.3
27	Y	196	VAL	2.3
32	I	112	LYS	2.3
11	H	73	LEU	2.3
10	G	25	GLU	2.2
4	A	94	LEU	2.2
14	L	102	ASP	2.2
1	0	716	G	2.2

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Mol	Chain	Res	Type	RSRZ
1	0	960	G	2.2
26	X	12	ILE	2.2
11	H	75	LYS	2.2
30	2	39	ARG	2.2
14	L	142	LEU	2.2
8	E	1	PRO	2.2
4	A	236	GLY	2.2
16	N	181	ASP	2.2
7	D	58	VAL	2.2
1	0	281	U	2.2
1	0	2345	A	2.2
1	0	1175	G	2.2
1	0	1929	G	2.2
11	H	83	TYR	2.2
16	N	69	TYR	2.2
11	H	37	GLN	2.2
14	L	44	GLU	2.2
7	D	171	ASP	2.2
24	V	43	PRO	2.2
1	0	1164	U	2.2
1	0	1000	C	2.2
14	L	141	GLU	2.2
32	I	131	THR	2.2
14	L	79	ASP	2.2
32	I	73	PRO	2.2
32	I	92	PRO	2.2
11	H	166	SER	2.2
31	3	44	SER	2.2
24	V	14	ALA	2.2
14	L	121	ILE	2.2
32	I	139	ILE	2.2
11	H	167	PRO	2.2
31	3	42	ARG	2.2
16	N	67	ALA	2.1
30	2	30	ASP	2.1
18	P	135	ALA	2.1
32	I	128	VAL	2.1
7	D	83	PHE	2.1
4	A	80	LEU	2.1
14	L	75	LEU	2.1
1	0	2511	A	2.1
24	V	63	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
22	T	112	LEU	2.1
1	0	289	G	2.1
4	A	206	ARG	2.1
16	N	138	ASP	2.1
22	T	82	THR	2.1
14	L	122	ALA	2.1
1	0	1180	U	2.1
16	N	156	GLU	2.1
26	X	72	VAL	2.1
31	3	55	VAL	2.1
19	Q	84	ILE	2.1
32	I	100	LEU	2.1
7	D	129	ASP	2.1
9	F	113	ASP	2.1
14	L	123	ASP	2.1
6	C	5	ILE	2.1
17	O	23	GLY	2.1
9	F	23	ALA	2.0
14	L	82	ALA	2.0
19	Q	18	PRO	2.0
9	F	13	GLU	2.0
1	0	283	U	2.0
1	0	1208	C	2.0
5	B	104	GLU	2.0
8	E	94	GLN	2.0
9	F	20	LEU	2.0
1	0	358	G	2.0
4	A	63	GLY	2.0
14	L	69	ILE	2.0
28	Z	59	TYR	2.0
9	F	11	ASP	2.0
21	S	76	GLU	2.0
18	P	18	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACA	4	78	4/9	0.88	0.22	52,52,52,52	0
1	OMG	0	2588	24/25	0.97	0.12	31,32,34,36	0
1	PSU	0	2621	20/21	0.98	0.14	32,35,39,40	0
1	UR3	0	2619	21/22	0.98	0.14	30,33,37,40	0
1	OMU	0	2587	21/22	0.98	0.12	31,34,36,38	0
1	1MA	0	628	23/24	0.98	0.14	27,30,32,32	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	B	9521	1/1	0.32	0.53	196,196,196,196	0
35	NA	0	9122	1/1	0.33	0.35	75,75,75,75	0
35	NA	0	9184	1/1	0.40	1.39	87,87,87,87	0
35	NA	0	9172	1/1	0.43	0.71	76,76,76,76	0
37	SR	0	9484	1/1	0.45	0.14	148,148,148,148	0
33	MG	0	8047	1/1	0.47	0.83	92,92,92,92	0
33	MG	0	8102	1/1	0.47	0.20	94,94,94,94	0
37	SR	0	9501	1/1	0.57	0.25	193,193,193,193	0
35	NA	S	9112	1/1	0.58	0.21	71,71,71,71	0
33	MG	0	8108	1/1	0.58	0.41	88,88,88,88	0
37	SR	0	9590	1/1	0.59	0.12	131,131,131,131	0
33	MG	B	8055	1/1	0.60	0.21	85,85,85,85	0
37	SR	A	9537	1/1	0.60	0.11	159,159,159,159	0
37	SR	0	9601	1/1	0.62	0.93	196,196,196,196	0
33	MG	0	8050	1/1	0.62	0.26	91,91,91,91	0
33	MG	0	8113	1/1	0.64	0.21	78,78,78,78	0
37	SR	9	9588	1/1	0.68	0.14	132,132,132,132	0
35	NA	0	9129	1/1	0.69	0.24	74,74,74,74	0
35	NA	0	9132	1/1	0.71	0.55	77,77,77,77	0
37	SR	0	9547	1/1	0.71	0.30	175,175,175,175	0
37	SR	0	9482	1/1	0.75	0.47	175,175,175,175	0
34	K	0	9002	1/1	0.75	0.28	91,91,91,91	0
37	SR	0	9468	1/1	0.76	0.09	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	9102	1/1	0.77	0.45	68,68,68,68	0
33	MG	0	8024	1/1	0.77	0.65	87,87,87,87	0
35	NA	0	9171	1/1	0.77	0.15	67,67,67,67	0
33	MG	0	8101	1/1	0.77	0.16	68,68,68,68	0
33	MG	0	8075	1/1	0.80	0.11	49,49,49,49	0
33	MG	0	8045	1/1	0.80	0.24	73,73,73,73	0
33	MG	0	8040	1/1	0.81	0.31	73,73,73,73	0
33	MG	0	8090	1/1	0.81	0.32	67,67,67,67	0
35	NA	0	9174	1/1	0.81	0.61	67,67,67,67	0
33	MG	0	8093	1/1	0.82	0.11	45,45,45,45	0
37	SR	0	9490	1/1	0.82	0.11	129,129,129,129	0
39	CD	O	9205	1/1	0.83	0.41	196,196,196,196	0
35	NA	0	9185	1/1	0.83	0.64	53,53,53,53	0
33	MG	0	8057	1/1	0.84	0.24	64,64,64,64	0
33	MG	0	8115	1/1	0.84	0.12	58,58,58,58	0
33	MG	0	8104	1/1	0.84	0.21	58,58,58,58	0
35	NA	B	9161	1/1	0.84	0.52	73,73,73,73	0
35	NA	0	9181	1/1	0.84	0.18	58,58,58,58	0
35	NA	0	9177	1/1	0.84	0.54	76,76,76,76	0
35	NA	3	9169	1/1	0.84	0.34	84,84,84,84	0
33	MG	0	8083	1/1	0.85	0.18	51,51,51,51	0
33	MG	0	8103	1/1	0.85	0.18	53,53,53,53	0
33	MG	0	8060	1/1	0.85	0.21	88,88,88,88	0
35	NA	0	9164	1/1	0.85	0.51	56,56,56,56	0
33	MG	0	8097	1/1	0.85	0.26	65,65,65,65	0
33	MG	0	8088	1/1	0.85	0.10	42,42,42,42	0
35	NA	0	9182	1/1	0.86	0.19	68,68,68,68	0
33	MG	0	8107	1/1	0.86	0.19	61,61,61,61	0
33	MG	0	8094	1/1	0.86	0.26	65,65,65,65	0
33	MG	0	8052	1/1	0.86	0.27	75,75,75,75	0
33	MG	0	8014	1/1	0.87	0.36	74,74,74,74	0
37	SR	0	9505	1/1	0.87	0.10	117,117,117,117	0
35	NA	0	9107	1/1	0.87	0.34	52,52,52,52	0
37	SR	0	9425	1/1	0.87	0.14	151,151,151,151	0
35	NA	0	9179	1/1	0.87	0.79	94,94,94,94	0
33	MG	0	8099	1/1	0.87	0.29	77,77,77,77	0
35	NA	0	9126	1/1	0.87	0.11	49,49,49,49	0
35	NA	0	9125	1/1	0.87	0.66	93,93,93,93	0
35	NA	9	9152	1/1	0.87	0.29	59,59,59,59	0
37	SR	0	9581	1/1	0.87	0.04	105,105,105,105	0
35	NA	0	9101	1/1	0.87	0.15	41,41,41,41	0
35	NA	0	9150	1/1	0.88	0.22	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	9154	1/1	0.88	0.30	54,54,54,54	0
35	NA	0	9159	1/1	0.88	0.46	56,56,56,56	0
35	NA	0	9175	1/1	0.88	0.18	42,42,42,42	0
35	NA	0	9127	1/1	0.88	0.35	75,75,75,75	0
33	MG	0	8092	1/1	0.88	0.52	68,68,68,68	0
35	NA	0	9155	1/1	0.88	0.25	65,65,65,65	0
35	NA	0	9139	1/1	0.89	0.15	61,61,61,61	0
33	MG	0	8089	1/1	0.89	0.20	54,54,54,54	0
33	MG	0	8076	1/1	0.89	0.20	57,57,57,57	0
35	NA	0	9163	1/1	0.89	0.19	72,72,72,72	0
33	MG	0	8046	1/1	0.89	0.16	37,37,37,37	0
37	SR	9	9503	1/1	0.89	0.06	105,105,105,105	0
35	NA	9	9183	1/1	0.89	0.18	84,84,84,84	0
33	MG	0	8065	1/1	0.89	0.31	92,92,92,92	0
37	SR	0	9570	1/1	0.90	0.11	117,117,117,117	0
35	NA	0	9149	1/1	0.90	0.10	46,46,46,46	0
37	SR	0	9465	1/1	0.90	0.12	105,105,105,105	0
33	MG	0	8041	1/1	0.90	0.12	52,52,52,52	0
37	SR	0	9508	1/1	0.90	0.12	87,87,87,87	0
37	SR	0	9506	1/1	0.90	0.05	108,108,108,108	0
33	MG	0	8054	1/1	0.90	0.11	61,61,61,61	0
35	NA	0	9110	1/1	0.90	0.22	39,39,39,39	0
33	MG	0	8022	1/1	0.90	0.51	67,67,67,67	0
35	NA	J	9146	1/1	0.91	0.12	58,58,58,58	0
35	NA	0	9167	1/1	0.91	0.14	59,59,59,59	0
35	NA	0	9141	1/1	0.91	0.09	64,64,64,64	0
33	MG	0	8112	1/1	0.91	0.08	44,44,44,44	0
33	MG	0	8051	1/1	0.91	0.21	24,24,24,24	0
35	NA	0	9157	1/1	0.91	0.18	35,35,35,35	0
33	MG	0	8085	1/1	0.91	0.35	69,69,69,69	0
35	NA	0	9173	1/1	0.91	0.19	57,57,57,57	0
35	NA	0	9113	1/1	0.91	0.17	67,67,67,67	0
35	NA	0	9168	1/1	0.91	0.21	74,74,74,74	0
34	K	0	9001	1/1	0.92	0.32	101,101,101,101	0
33	MG	0	8068	1/1	0.92	0.10	36,36,36,36	0
33	MG	0	8098	1/1	0.92	0.09	40,40,40,40	0
37	SR	0	9585	1/1	0.92	0.11	91,91,91,91	0
35	NA	0	9134	1/1	0.92	0.06	38,38,38,38	0
37	SR	0	9539	1/1	0.92	0.35	173,173,173,173	0
35	NA	0	9111	1/1	0.92	0.11	46,46,46,46	0
35	NA	0	9114	1/1	0.92	0.21	56,56,56,56	0
33	MG	0	8061	1/1	0.92	0.11	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	9124	1/1	0.92	0.21	52,52,52,52	0
39	CD	Z	9203	1/1	0.92	0.10	155,155,155,155	0
35	NA	0	9140	1/1	0.92	0.41	65,65,65,65	0
37	SR	0	9532	1/1	0.92	0.09	114,114,114,114	0
37	SR	0	9517	1/1	0.93	0.07	94,94,94,94	0
33	MG	A	8066	1/1	0.93	0.18	57,57,57,57	0
36	CL	3	9304	1/1	0.93	0.06	74,74,74,74	0
35	NA	0	9158	1/1	0.93	0.33	46,46,46,46	0
33	MG	0	8019	1/1	0.93	0.08	52,52,52,52	0
37	SR	0	9529	1/1	0.93	0.16	123,123,123,123	0
37	SR	H	9486	1/1	0.93	0.14	121,121,121,121	0
35	NA	0	9135	1/1	0.93	0.19	42,42,42,42	0
37	SR	0	9459	1/1	0.93	0.07	93,93,93,93	0
33	MG	9	8095	1/1	0.93	0.26	46,46,46,46	0
35	NA	0	9116	1/1	0.93	0.16	51,51,51,51	0
37	SR	0	9500	1/1	0.93	1.21	196,196,196,196	0
35	NA	0	9120	1/1	0.93	0.17	59,59,59,59	0
33	MG	0	8036	1/1	0.93	0.07	47,47,47,47	0
37	SR	0	9566	1/1	0.93	0.07	97,97,97,97	0
33	MG	Y	8109	1/1	0.93	0.13	39,39,39,39	0
37	SR	0	9530	1/1	0.93	0.16	107,107,107,107	0
33	MG	0	8043	1/1	0.93	0.07	56,56,56,56	0
33	MG	0	8082	1/1	0.93	0.36	80,80,80,80	0
37	SR	0	9483	1/1	0.94	0.10	77,77,77,77	0
33	MG	0	8059	1/1	0.94	0.20	46,46,46,46	0
35	NA	0	9128	1/1	0.94	0.22	40,40,40,40	0
33	MG	0	8116	1/1	0.94	0.07	69,69,69,69	0
35	NA	0	9166	1/1	0.94	0.17	76,76,76,76	0
33	MG	0	8106	1/1	0.94	0.04	39,39,39,39	0
36	CL	0	9317	1/1	0.94	0.13	58,58,58,58	0
36	CL	M	9318	1/1	0.94	0.21	40,40,40,40	0
33	MG	0	8063	1/1	0.94	0.16	74,74,74,74	0
37	SR	F	9595	1/1	0.94	0.16	92,92,92,92	0
36	CL	0	9316	1/1	0.94	0.25	74,74,74,74	0
33	MG	0	8117	1/1	0.94	0.15	40,40,40,40	0
33	MG	0	8042	1/1	0.94	0.07	50,50,50,50	0
35	NA	0	9115	1/1	0.94	0.23	42,42,42,42	0
33	MG	0	8114	1/1	0.94	0.21	74,74,74,74	0
35	NA	D	9151	1/1	0.94	0.19	60,60,60,60	0
38	SPS	4	9701	23/23	0.94	0.17	39,45,57,60	0
36	CL	L	9310	1/1	0.94	0.16	51,51,51,51	0
33	MG	0	8072	1/1	0.94	0.15	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8058	1/1	0.94	0.28	34,34,34,34	0
33	MG	0	8096	1/1	0.94	0.07	37,37,37,37	0
33	MG	0	8030	1/1	0.95	0.09	38,38,38,38	0
37	SR	0	9568	1/1	0.95	0.04	86,86,86,86	0
36	CL	Y	9320	1/1	0.95	0.11	42,42,42,42	0
33	MG	0	8032	1/1	0.95	0.07	34,34,34,34	0
37	SR	0	9515	1/1	0.95	0.09	109,109,109,109	0
33	MG	0	8084	1/1	0.95	0.56	107,107,107,107	0
33	MG	0	8021	1/1	0.95	0.20	49,49,49,49	0
35	NA	0	9170	1/1	0.95	0.27	92,92,92,92	0
33	MG	0	8110	1/1	0.95	0.25	40,40,40,40	0
36	CL	R	9306	1/1	0.95	0.11	45,45,45,45	0
37	SR	0	9489	1/1	0.95	0.09	101,101,101,101	0
35	NA	0	9131	1/1	0.95	0.15	51,51,51,51	0
33	MG	0	8091	1/1	0.95	0.08	55,55,55,55	0
37	SR	A	9497	1/1	0.95	0.09	99,99,99,99	0
36	CL	A	9309	1/1	0.95	0.18	70,70,70,70	0
36	CL	B	9319	1/1	0.95	0.20	54,54,54,54	0
35	NA	T	9143	1/1	0.95	0.08	37,37,37,37	0
35	NA	0	9106	1/1	0.95	0.32	39,39,39,39	0
33	MG	0	8026	1/1	0.95	0.18	25,25,25,25	0
37	SR	0	9522	1/1	0.95	0.07	100,100,100,100	0
35	NA	0	9156	1/1	0.96	0.38	57,57,57,57	0
35	NA	0	9165	1/1	0.96	0.32	37,37,37,37	0
35	NA	0	9178	1/1	0.96	0.52	44,44,44,44	0
33	MG	0	8039	1/1	0.96	0.09	45,45,45,45	0
33	MG	T	8073	1/1	0.96	0.11	34,34,34,34	0
35	NA	0	9117	1/1	0.96	0.11	31,31,31,31	0
35	NA	0	9136	1/1	0.96	0.16	32,32,32,32	0
37	SR	0	9441	1/1	0.96	0.08	64,64,64,64	0
37	SR	0	9560	1/1	0.96	0.09	94,94,94,94	0
37	SR	0	9446	1/1	0.96	0.07	93,93,93,93	0
35	NA	0	9162	1/1	0.96	0.14	43,43,43,43	0
36	CL	J	9301	1/1	0.96	0.07	50,50,50,50	0
37	SR	0	9626	1/1	0.96	0.27	146,146,146,146	0
37	SR	A	9436	1/1	0.96	0.06	87,87,87,87	0
37	SR	0	9467	1/1	0.96	0.11	73,73,73,73	0
33	MG	0	8037	1/1	0.96	0.08	42,42,42,42	0
33	MG	0	8025	1/1	0.96	0.30	19,19,19,19	0
37	SR	9	9481	1/1	0.96	0.08	86,86,86,86	0
33	MG	0	8005	1/1	0.96	0.06	31,31,31,31	0
37	SR	0	9452	1/1	0.96	0.16	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CL	N	9307	1/1	0.96	0.19	60,60,60,60	0
37	SR	0	9477	1/1	0.97	0.12	79,79,79,79	0
37	SR	0	9426	1/1	0.97	0.08	72,72,72,72	0
37	SR	0	9480	1/1	0.97	0.05	83,83,83,83	0
37	SR	0	9454	1/1	0.97	0.14	79,79,79,79	0
33	MG	0	8020	1/1	0.97	0.19	37,37,37,37	0
37	SR	0	9629	1/1	0.97	0.09	73,73,73,73	0
37	SR	0	9545	1/1	0.97	0.08	84,84,84,84	0
35	NA	0	9130	1/1	0.97	0.13	41,41,41,41	0
36	CL	0	9313	1/1	0.97	0.08	51,51,51,51	0
35	NA	R	9186	1/1	0.97	0.15	75,75,75,75	0
33	MG	4	8118	1/1	0.97	0.22	29,29,29,29	0
33	MG	0	8080	1/1	0.97	0.18	46,46,46,46	0
36	CL	0	9322	1/1	0.97	0.21	53,53,53,53	0
33	MG	0	8002	1/1	0.97	0.12	33,33,33,33	0
35	NA	0	9123	1/1	0.97	0.12	50,50,50,50	0
35	NA	0	9118	1/1	0.97	0.20	43,43,43,43	0
35	NA	C	9104	1/1	0.97	0.17	26,26,26,26	0
37	SR	0	9464	1/1	0.97	0.07	80,80,80,80	0
37	SR	0	9504	1/1	0.97	0.10	92,92,92,92	0
37	SR	0	9433	1/1	0.97	0.17	74,74,74,74	0
37	SR	0	9461	1/1	0.97	0.04	86,86,86,86	0
37	SR	0	9478	1/1	0.97	0.08	72,72,72,72	0
35	NA	R	9137	1/1	0.97	0.10	23,23,23,23	0
35	NA	M	9147	1/1	0.97	0.15	33,33,33,33	0
35	NA	0	9138	1/1	0.97	0.11	56,56,56,56	0
37	SR	0	9534	1/1	0.97	0.12	113,113,113,113	0
36	CL	0	9303	1/1	0.97	0.14	47,47,47,47	0
35	NA	Q	9148	1/1	0.97	0.10	48,48,48,48	0
33	MG	0	8070	1/1	0.97	0.15	26,26,26,26	0
35	NA	0	9105	1/1	0.97	0.06	36,36,36,36	0
36	CL	0	9315	1/1	0.97	0.13	58,58,58,58	0
33	MG	B	8056	1/1	0.97	0.22	46,46,46,46	0
36	CL	0	9311	1/1	0.97	0.14	66,66,66,66	0
33	MG	0	8028	1/1	0.98	0.12	31,31,31,31	0
33	MG	0	8067	1/1	0.98	0.14	35,35,35,35	0
33	MG	0	8004	1/1	0.98	0.09	24,24,24,24	0
33	MG	0	8015	1/1	0.98	0.09	29,29,29,29	0
33	MG	0	8031	1/1	0.98	0.09	48,48,48,48	0
35	NA	0	9108	1/1	0.98	0.10	31,31,31,31	0
36	CL	0	9314	1/1	0.98	0.17	52,52,52,52	0
37	SR	0	9438	1/1	0.98	0.11	66,66,66,66	0

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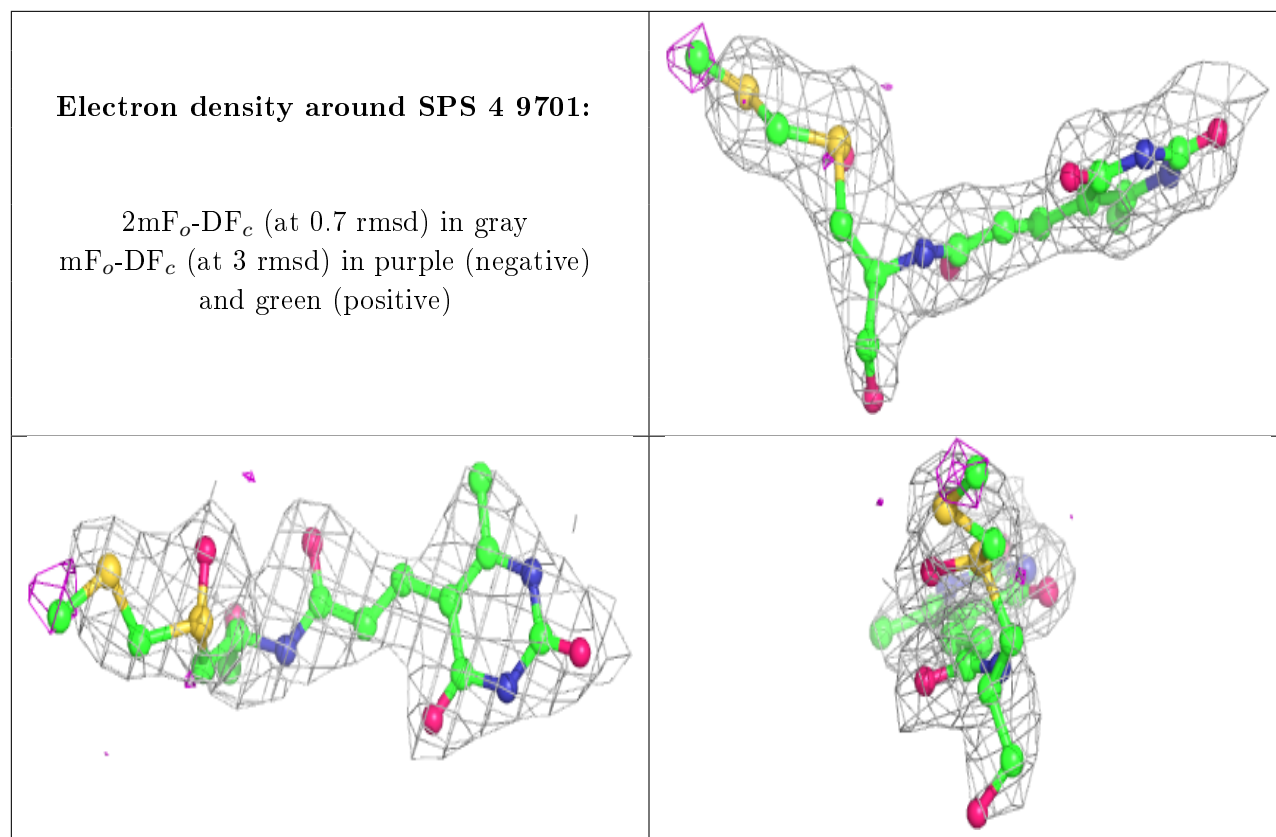
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	9422	1/1	0.98	0.13	57,57,57,57	0
33	MG	0	8038	1/1	0.98	0.24	16,16,16,16	0
37	SR	0	9445	1/1	0.98	0.12	62,62,62,62	0
37	SR	0	9432	1/1	0.98	0.16	65,65,65,65	0
33	MG	0	8009	1/1	0.98	0.08	31,31,31,31	0
33	MG	K	8069	1/1	0.98	0.18	20,20,20,20	0
36	CL	J	9302	1/1	0.98	0.06	54,54,54,54	0
33	MG	0	8079	1/1	0.98	0.11	29,29,29,29	0
37	SR	0	9444	1/1	0.98	0.12	52,52,52,52	0
37	SR	S	9470	1/1	0.98	0.16	98,98,98,98	0
35	NA	0	9160	1/1	0.98	0.17	45,45,45,45	0
37	SR	0	9466	1/1	0.98	0.05	95,95,95,95	0
37	SR	0	9405	1/1	0.98	0.04	81,81,81,81	0
36	CL	O	9308	1/1	0.98	0.14	56,56,56,56	0
37	SR	0	9488	1/1	0.98	0.15	80,80,80,80	0
37	SR	0	9473	1/1	0.98	0.06	77,77,77,77	0
36	CL	J	9321	1/1	0.98	0.14	65,65,65,65	0
37	SR	0	9495	1/1	0.98	0.12	90,90,90,90	0
37	SR	0	9509	1/1	0.98	0.14	86,86,86,86	0
37	SR	A	9437	1/1	0.98	0.11	70,70,70,70	0
37	SR	0	9421	1/1	0.98	0.12	68,68,68,68	0
37	SR	0	9427	1/1	0.98	0.15	55,55,55,55	0
33	MG	0	8012	1/1	0.98	0.25	26,26,26,26	0
33	MG	0	8001	1/1	0.98	0.23	17,17,17,17	0
33	MG	0	8029	1/1	0.98	0.26	22,22,22,22	0
37	SR	0	9430	1/1	0.99	0.17	48,48,48,48	0
37	SR	0	9451	1/1	0.99	0.19	57,57,57,57	0
37	SR	0	9498	1/1	0.99	0.07	65,65,65,65	0
37	SR	0	9424	1/1	0.99	0.21	49,49,49,49	0
36	CL	K	9312	1/1	0.99	0.10	45,45,45,45	0
37	SR	0	9449	1/1	0.99	0.11	61,61,61,61	0
37	SR	0	9462	1/1	0.99	0.15	67,67,67,67	0
37	SR	0	9469	1/1	0.99	0.07	88,88,88,88	0
37	SR	0	9411	1/1	0.99	0.20	49,49,49,49	0
37	SR	0	9435	1/1	0.99	0.10	71,71,71,71	0
37	SR	0	9413	1/1	0.99	0.17	50,50,50,50	0
37	SR	1	9419	1/1	0.99	0.18	47,47,47,47	0
37	SR	1	9460	1/1	0.99	0.14	52,52,52,52	0
33	MG	0	8044	1/1	0.99	0.06	35,35,35,35	0
37	SR	0	9414	1/1	0.99	0.15	56,56,56,56	0
37	SR	0	9428	1/1	0.99	0.12	51,51,51,51	0
33	MG	0	8008	1/1	0.99	0.18	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	9408	1/1	0.99	0.22	48,48,48,48	0
37	SR	0	9410	1/1	0.99	0.20	46,46,46,46	0
37	SR	0	9447	1/1	0.99	0.14	62,62,62,62	0
37	SR	0	9434	1/1	0.99	0.17	61,61,61,61	0
39	CD	1	9202	1/1	0.99	0.08	58,58,58,58	0
37	SR	0	9456	1/1	0.99	0.13	69,69,69,69	0
37	SR	3	9439	1/1	0.99	0.03	79,79,79,79	0
37	SR	0	9448	1/1	0.99	0.10	64,64,64,64	0
37	SR	0	9407	1/1	0.99	0.20	50,50,50,50	0
33	MG	0	8074	1/1	0.99	0.20	15,15,15,15	0
37	SR	0	9455	1/1	0.99	0.10	66,66,66,66	0
37	SR	0	9450	1/1	0.99	0.08	63,63,63,63	0
37	SR	0	9431	1/1	0.99	0.16	57,57,57,57	0
37	SR	0	9440	1/1	0.99	0.08	60,60,60,60	0
37	SR	0	9417	1/1	0.99	0.14	58,58,58,58	0
39	CD	U	9201	1/1	0.99	0.11	61,61,61,61	0
37	SR	0	9474	1/1	0.99	0.11	68,68,68,68	0
36	CL	0	9305	1/1	0.99	0.08	58,58,58,58	0
37	SR	0	9416	1/1	0.99	0.15	48,48,48,48	0
37	SR	0	9442	1/1	0.99	0.15	63,63,63,63	0
33	MG	0	8027	1/1	0.99	0.24	31,31,31,31	0
33	MG	0	8017	1/1	0.99	0.14	18,18,18,18	0
37	SR	0	9453	1/1	0.99	0.11	76,76,76,76	0
37	SR	0	9443	1/1	0.99	0.13	62,62,62,62	0
37	SR	0	9412	1/1	0.99	0.15	51,51,51,51	0
37	SR	0	9420	1/1	0.99	0.17	74,74,74,74	0
37	SR	0	9457	1/1	0.99	0.14	50,50,50,50	0
39	CD	3	9204	1/1	0.99	0.02	70,70,70,70	0
33	MG	0	8003	1/1	0.99	0.13	24,24,24,24	0
37	SR	0	9429	1/1	0.99	0.15	67,67,67,67	0
37	SR	0	9475	1/1	0.99	0.09	80,80,80,80	0
37	SR	R	9418	1/1	0.99	0.17	58,58,58,58	0
33	MG	0	8013	1/1	0.99	0.40	10,10,10,10	0
37	SR	B	9458	1/1	0.99	0.13	66,66,66,66	0
37	SR	L	9409	1/1	0.99	0.14	46,46,46,46	0
37	SR	0	9415	1/1	1.00	0.16	57,57,57,57	0
37	SR	0	9406	1/1	1.00	0.22	45,45,45,45	0
37	SR	0	9423	1/1	1.00	0.12	56,56,56,56	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.