



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:26 am GMT

PDB ID : 1VQK  
Title : The structure of CCDA-PHE-CAP-BIO bound to the a site of the ribosomal subunit of haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

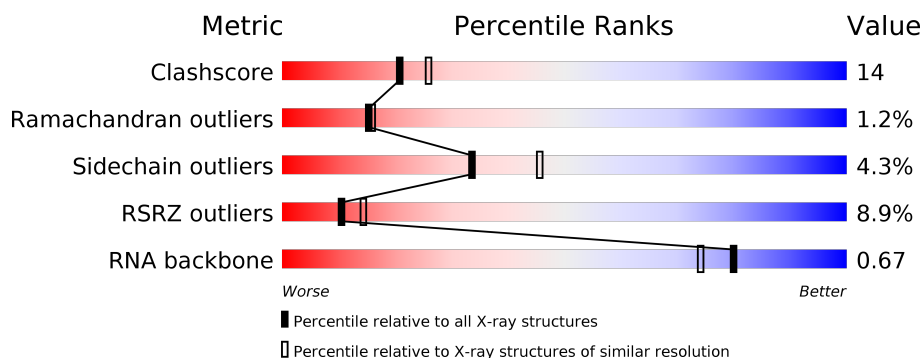
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)
RNA backbone	2435	1106 (2.80-1.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>3%</div> <div>65% 25% 6%</div> </div>
2	9	122	<div> <div>6%</div> <div>57% 34% 8%</div> </div>
3	4	5	<div> <div>20%</div> <div>40% 60%</div> </div>
4	A	240	<div> <div>8%</div> <div>63% 32%</div> </div>
5	B	338	<div> <div>4%</div> <div>59% 35% 6%</div> </div>
6	C	246	<div> <div>2%</div> <div>63% 32%</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	8001	-	-	-	X
33	MG	0	8008	-	-	-	X
33	MG	0	8012	-	-	-	X
33	MG	0	8013	-	-	-	X
33	MG	0	8017	-	-	-	X
33	MG	0	8020	-	-	-	X
33	MG	0	8027	-	-	-	X
33	MG	0	8038	-	-	-	X
33	MG	0	8057	-	-	-	X
33	MG	0	8080	-	-	-	X
33	MG	0	8084	-	-	-	X
33	MG	0	8097	-	-	-	X
33	MG	0	8107	-	-	-	X
34	K	0	9001	-	-	-	X
35	NA	0	9115	-	-	-	X
35	NA	0	9118	-	-	-	X
35	NA	0	9120	-	-	-	X
35	NA	0	9125	-	-	-	X
35	NA	0	9127	-	-	-	X
35	NA	0	9132	-	-	-	X
35	NA	0	9150	-	-	-	X
35	NA	0	9156	-	-	-	X
35	NA	0	9159	-	-	-	X
35	NA	0	9161	-	-	-	X
35	NA	0	9162	-	-	-	X
35	NA	0	9164	-	-	-	X
35	NA	0	9168	-	-	-	X
35	NA	0	9171	-	-	-	X
35	NA	0	9172	-	-	-	X
35	NA	0	9173	-	-	-	X
35	NA	0	9174	-	-	-	X
35	NA	0	9177	-	-	-	X
35	NA	0	9185	-	-	-	X
35	NA	9	9183	-	-	-	X
37	SR	0	9406	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	SR	0	9475	-	-	-	X
37	SR	0	9482	-	-	-	X
37	SR	0	9500	-	-	-	X
37	SR	0	9515	-	-	-	X
37	SR	B	9521	-	-	-	X

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99036 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	5	Total	C	N	O	P	0	0	0
			73	40	12	19	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	87	Total	Mg	0	0
			87	87		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	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	64	Total	Na	0	0
			64	64		
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	C	1	Total	Na	0	0
			1	1		
35	3	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	3	Total 3	Na 3	0	0
35	9	1	Total 1	Na 1	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	10	Total 10	Cl 10	0	0
36	J	3	Total 3	Cl 3	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	98	Total 98	Sr 98	0	0
37	1	2	Total 2	Sr 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	3	Total 3	Sr 3	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 CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5769	Total 5769	O 5769	0	0
39	9	140	Total 140	O 140	0	0
39	A	121	Total 121	O 121	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	B	144	Total 144	O 144	0	0
39	C	177	Total 177	O 177	0	0
39	D	48	Total 48	O 48	0	0
39	E	44	Total 44	O 44	0	0
39	F	27	Total 27	O 27	0	0
39	G	17	Total 17	O 17	0	0
39	H	69	Total 69	O 69	0	0
39	J	52	Total 52	O 52	0	0
39	K	57	Total 57	O 57	0	0
39	L	81	Total 81	O 81	0	0
39	M	130	Total 130	O 130	0	0
39	N	61	Total 61	O 61	0	0
39	O	40	Total 40	O 40	0	0
39	P	64	Total 64	O 64	0	0
39	Q	49	Total 49	O 49	0	0
39	R	82	Total 82	O 82	0	0
39	S	32	Total 32	O 32	0	0
39	T	37	Total 37	O 37	0	0
39	U	29	Total 29	O 29	0	0
39	V	14	Total 14	O 14	0	0
39	W	69	Total 69	O 69	0	0

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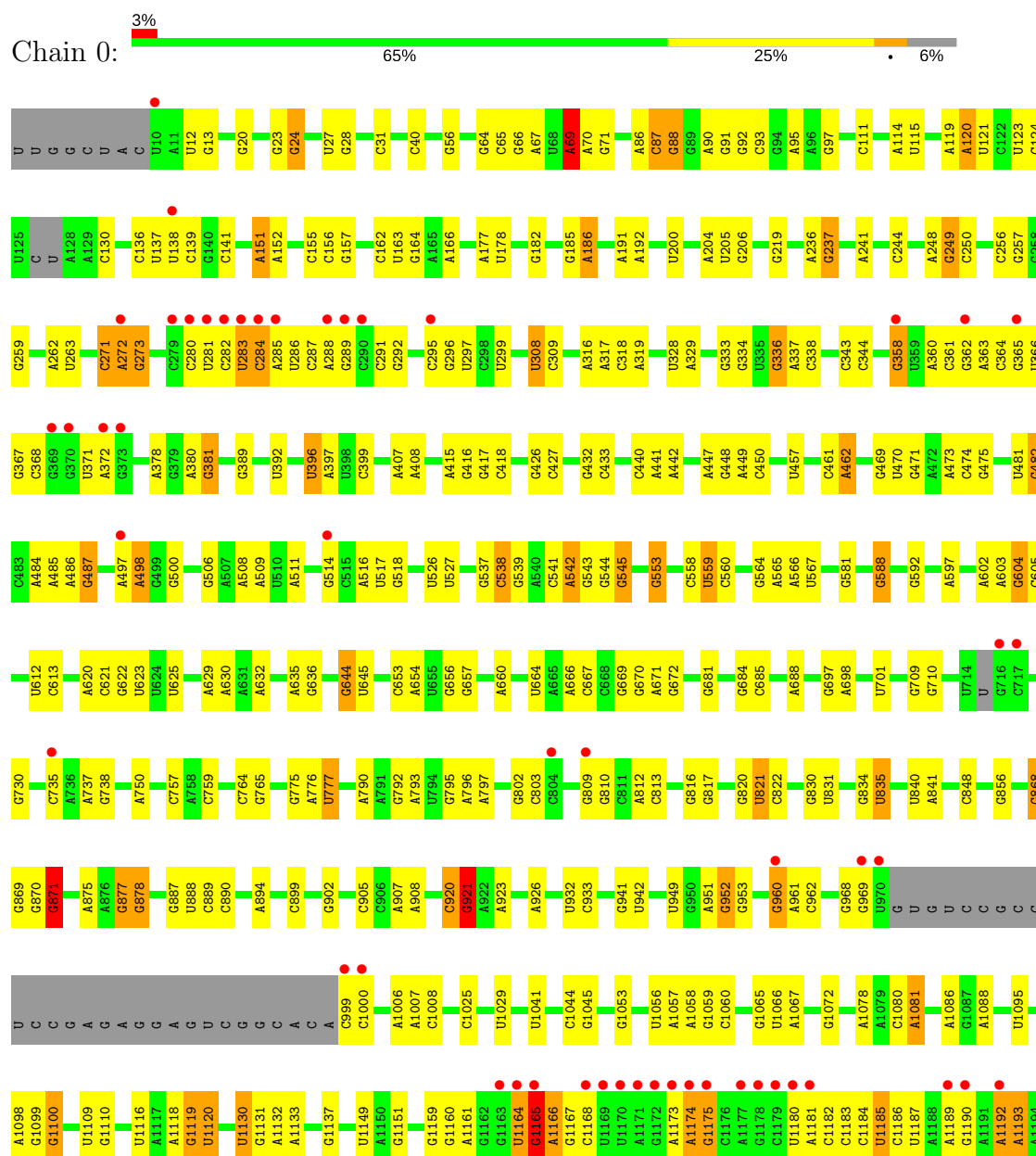
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	24	Total 24	O 24	0	0
39	Y	96	Total 96	O 96	0	0
39	Z	31	Total 31	O 31	0	0
39	1	50	Total 50	O 50	0	0
39	2	40	Total 40	O 40	0	0
39	3	67	Total 67	O 67	0	0
39	I	7	Total 7	O 7	0	0

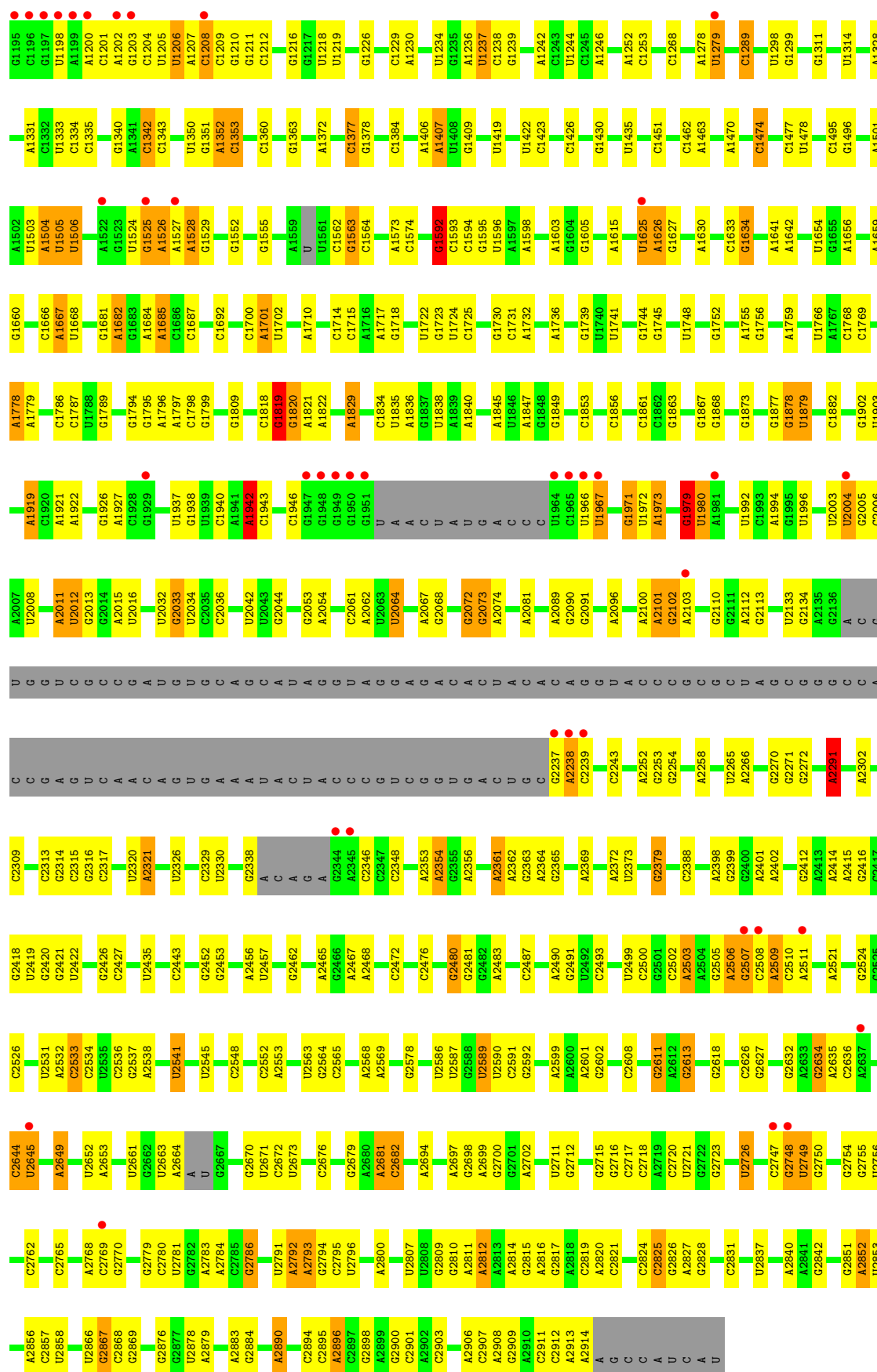
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

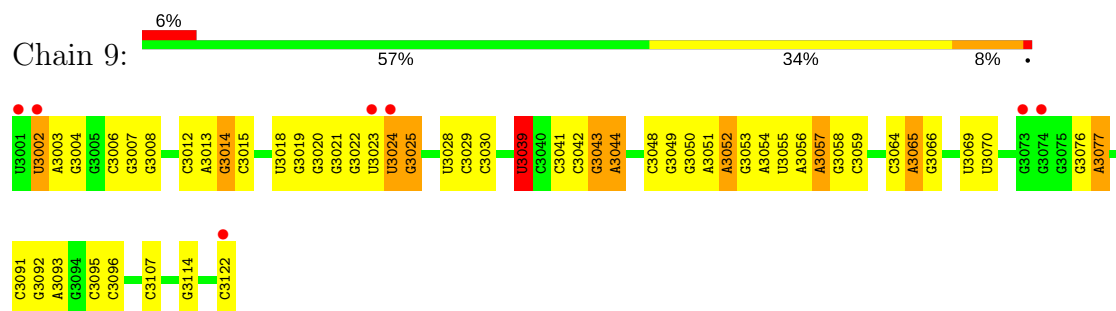
- Molecule 1: 23S ribosomal rna



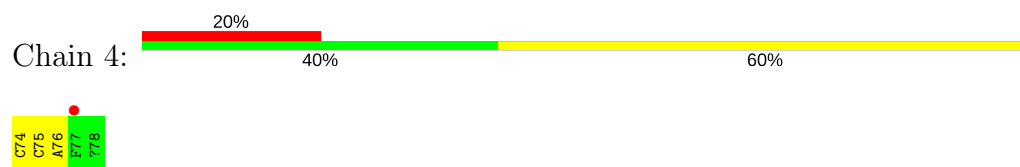




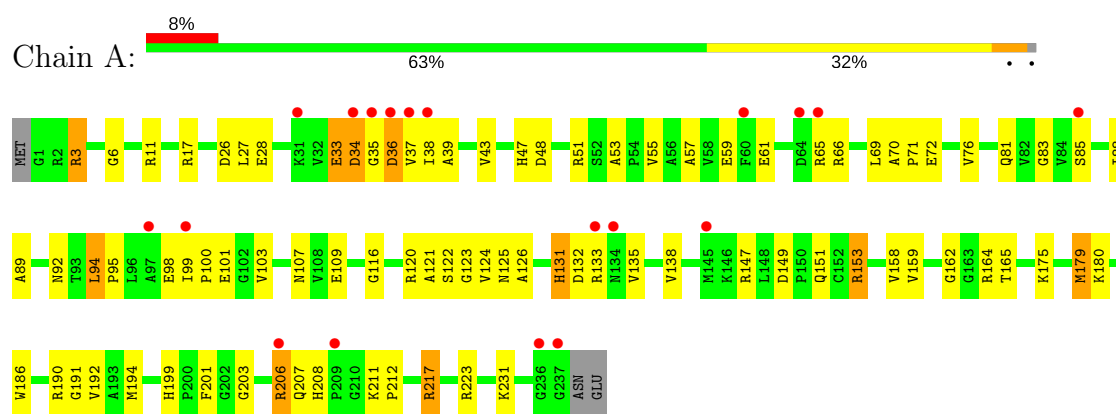
- Molecule 2: 5S ribosomal RNA



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



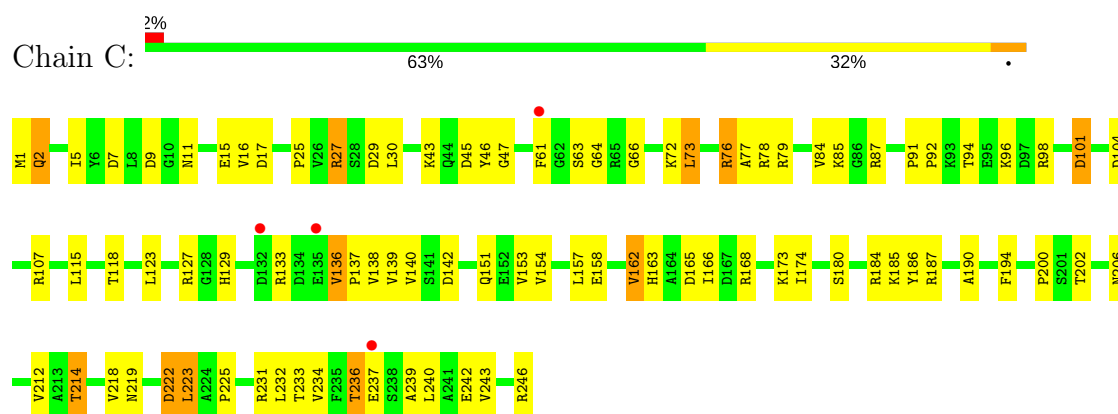
- Molecule 4: 50S ribosomal protein L2P



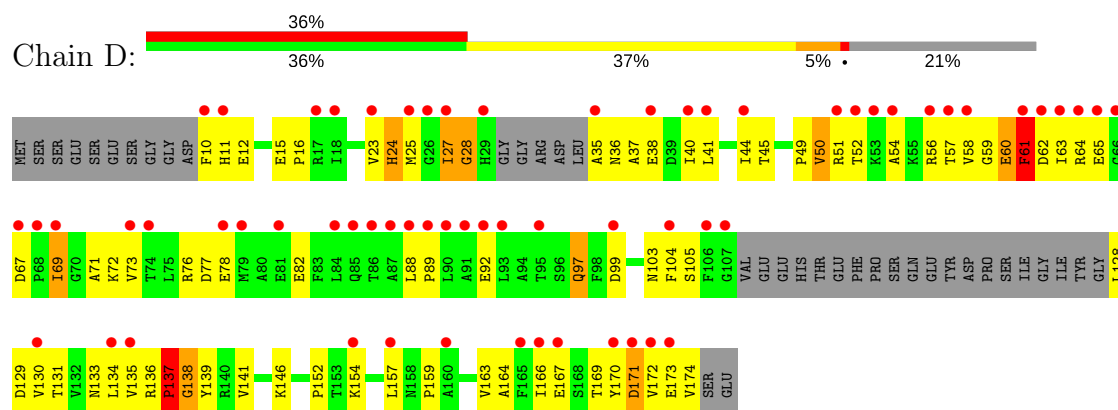
- Molecule 5: 50S ribosomal protein L3P



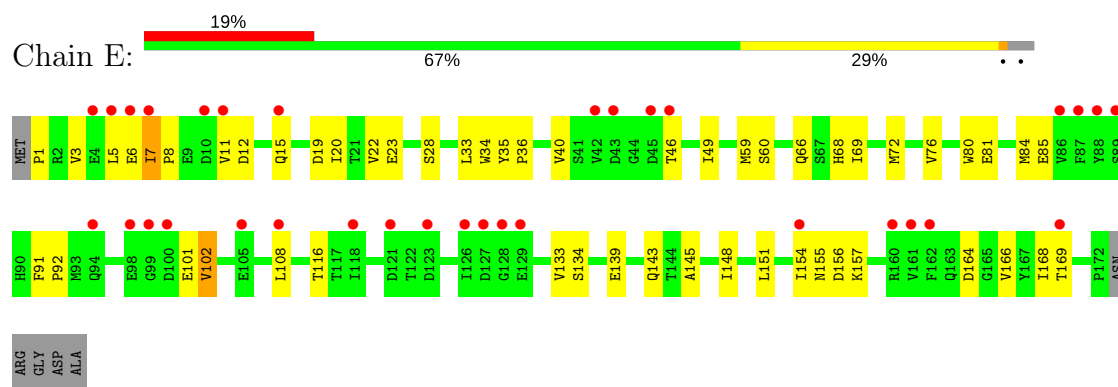
- Molecule 6: 50S ribosomal protein L4E



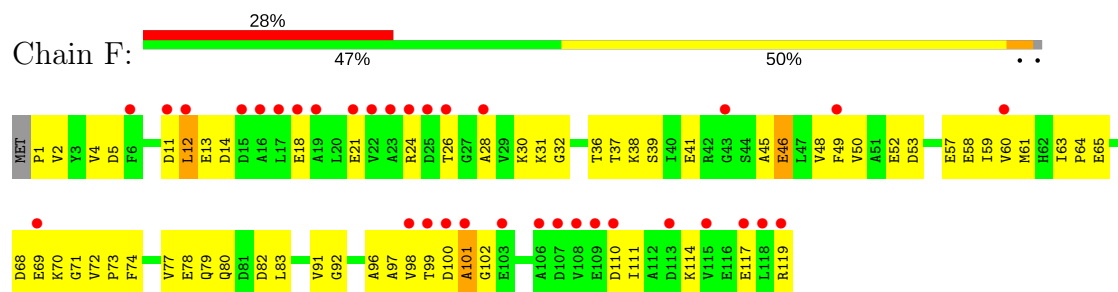
• Molecule 7: 50S ribosomal protein L5P



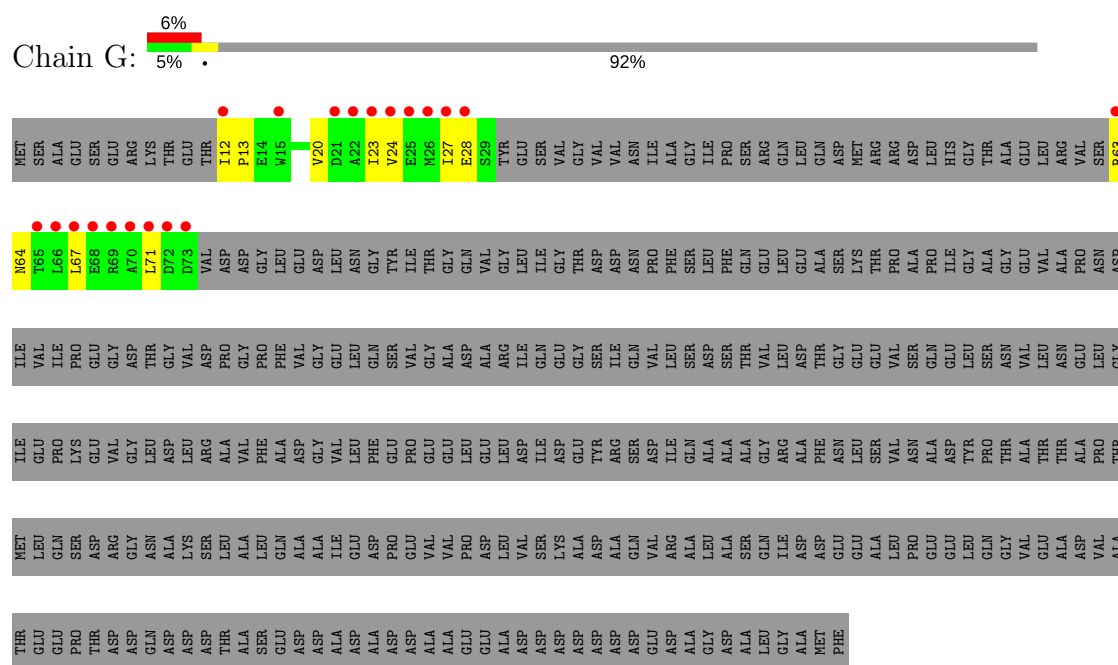
• Molecule 8: 50S ribosomal protein L6P



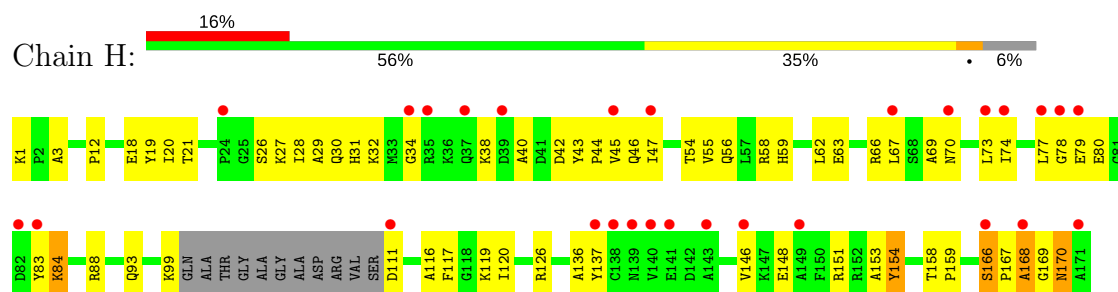
• Molecule 9: 50S ribosomal protein L7AE



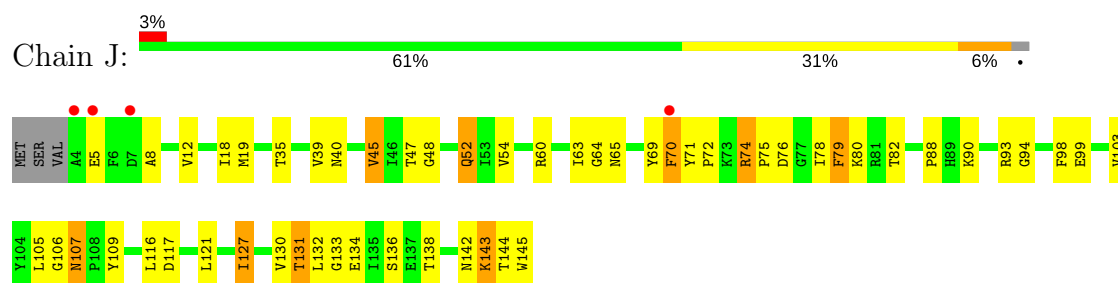
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



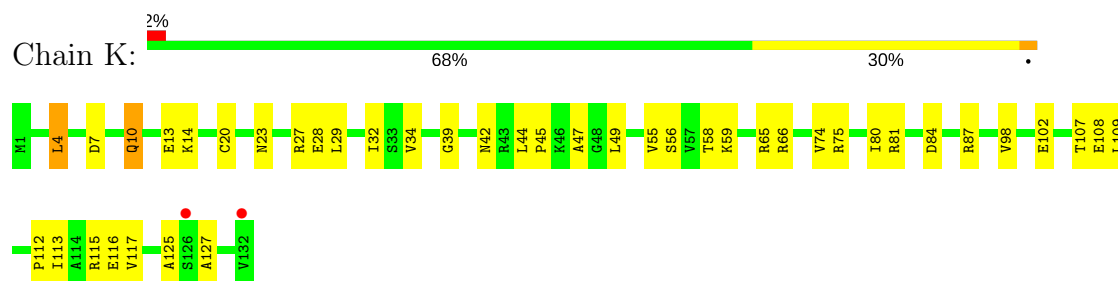
- Molecule 11: 50S RIBOSOMAL PROTEIN L10E



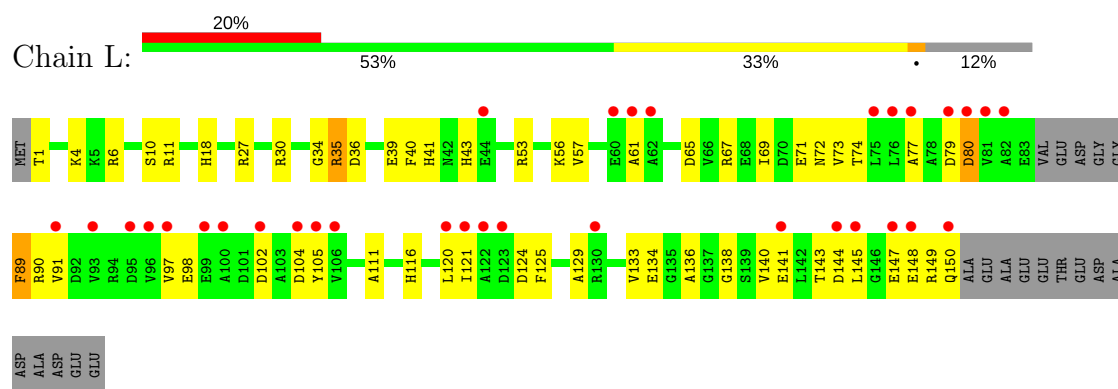
- Molecule 12: 50S ribosomal protein L13P



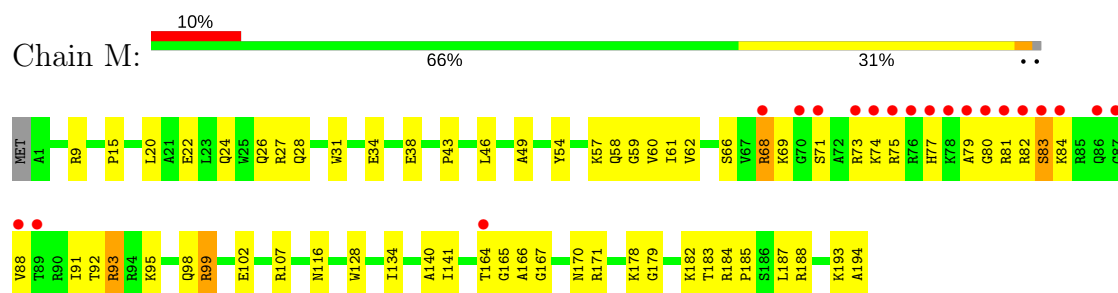
- Molecule 13: 50S ribosomal protein L14P



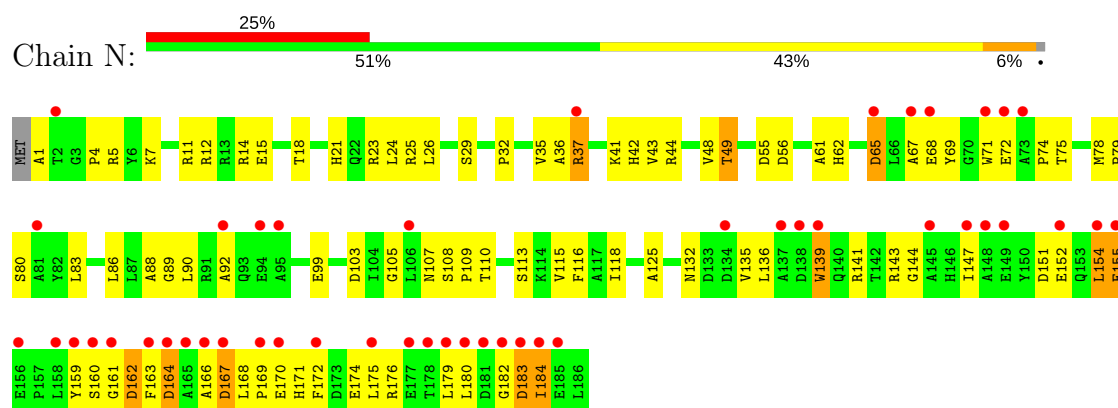
- Molecule 14: 50S ribosomal protein L15P



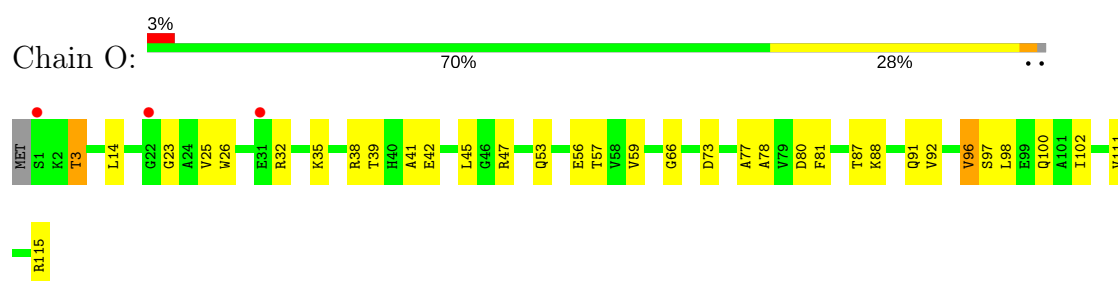
• Molecule 15: 50S Ribosomal Protein L15E



• Molecule 16: 50S ribosomal protein L18P

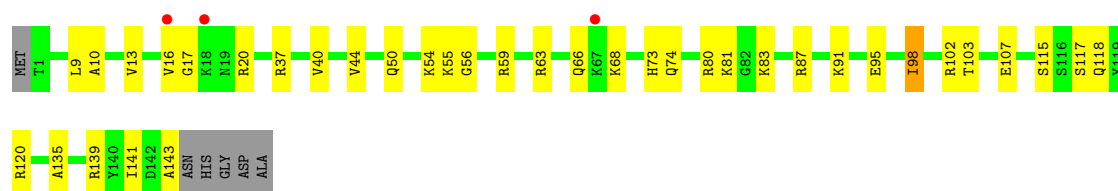


• Molecule 17: 50S ribosomal protein L18e

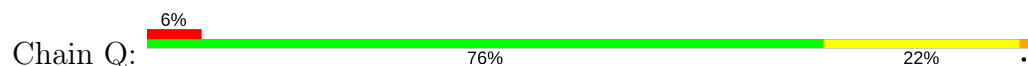


• Molecule 18: 50S ribosomal protein L19E





- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P



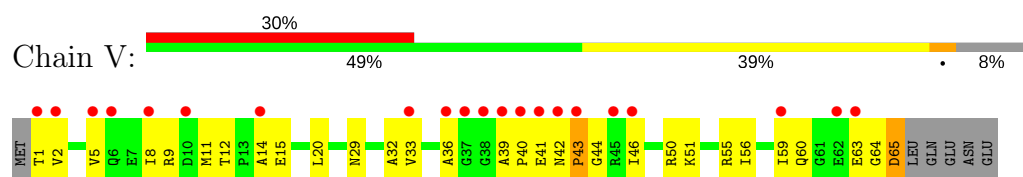
- Molecule 22: 50S ribosomal protein L24P



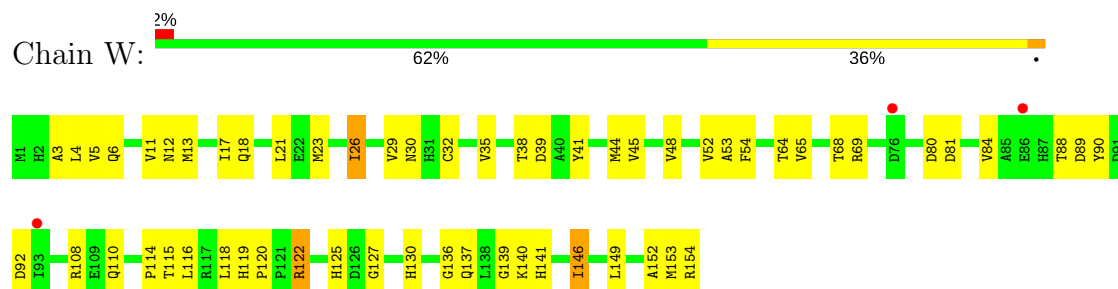
- Molecule 23: 50S ribosomal protein L24E



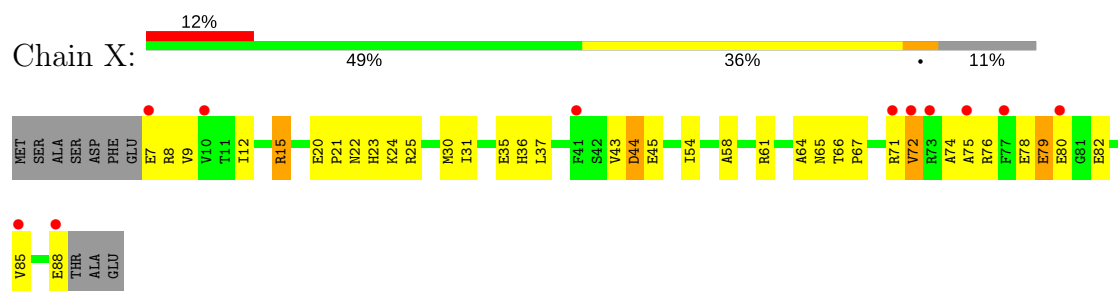
- Molecule 24: 50S ribosomal protein L29P



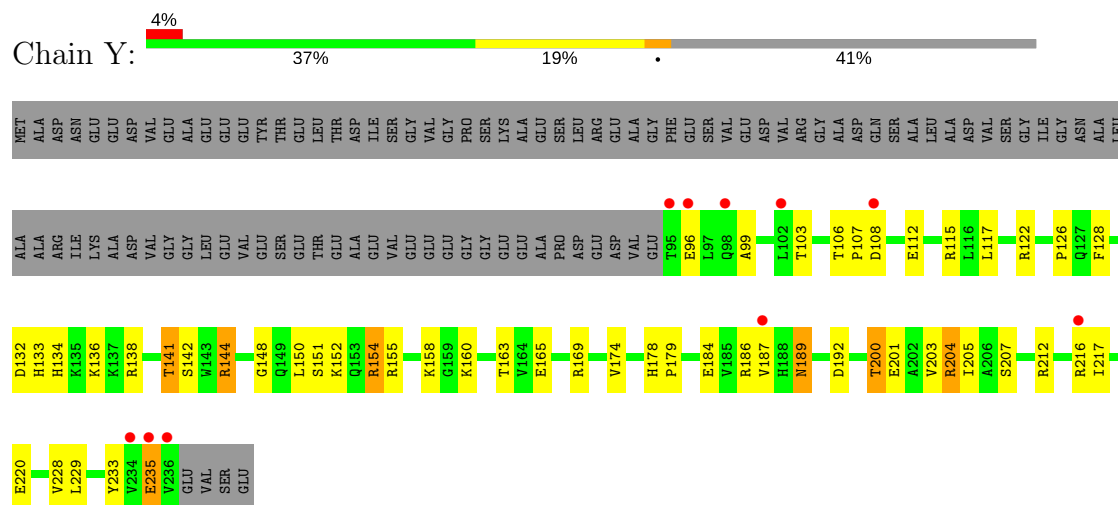
• Molecule 25: 50S ribosomal protein L30P



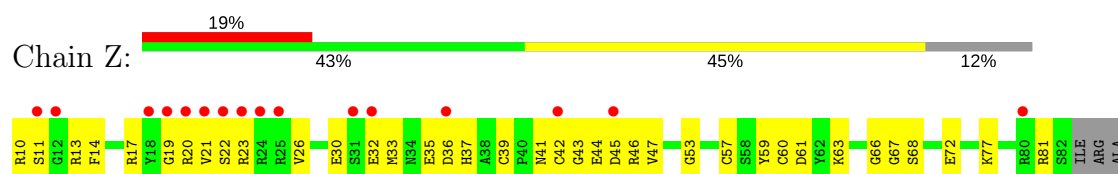
• Molecule 26: 50S ribosomal protein L31e



• Molecule 27: 50S ribosomal protein L32E



• Molecule 28: 50S ribosomal protein L37Ae







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.87Å 298.57Å 575.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.73 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.30) 89.6 (49.73-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.250 0.207 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 61.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99036	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, ACA, 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	0.37	0/65959	0.70	26/102870 (0.0%)
2	9	0.33	0/2905	0.71	1/4528 (0.0%)
3	4	0.52	0/75	0.73	0/110
4	A	0.34	0/1786	0.66	0/2408
5	B	0.33	0/2690	0.66	0/3652
6	C	0.38	0/1884	0.64	1/2551 (0.0%)
7	D	0.29	0/1111	0.54	0/1498
8	E	0.32	0/1382	0.57	0/1880
9	F	0.31	0/901	0.54	0/1224
10	G	0.27	0/241	0.47	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.35	0/1136	0.61	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.34	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.60	0/1999
17	O	0.33	0/874	0.59	1/1181 (0.1%)
18	P	0.34	0/1147	0.56	0/1528
19	Q	0.35	0/749	0.69	0/1005
20	R	0.35	0/1172	0.67	0/1578
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.31	0/958	0.63	0/1289
23	U	0.35	0/417	0.58	0/562
24	V	0.27	0/502	0.53	0/675
25	W	0.34	0/1219	0.60	0/1655
26	X	0.33	0/664	0.60	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.34	0/589	0.61	0/787
29	1	0.43	0/438	0.66	0/578
30	2	0.35	0/401	0.60	0/529
31	3	0.38	0/771	0.58	0/1024
32	I	0.28	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.36	0/98767	0.67	30/147687 (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	39
2	9	0	2
All	All	1	41

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.69	130.83	109.50
2	9	3039	U	N1-C1'-C2'	7.45	123.68	114.00
1	0	1942	A	C5'-C4'-C3'	7.27	127.63	116.00
1	0	1819	G	C5'-C4'-C3'	6.86	126.98	116.00
1	0	1592	G	N9-C1'-C2'	6.67	122.67	114.00
1	0	871	G	C5'-C4'-O4'	-6.63	101.14	109.10
1	0	1819	G	C1'-O4'-C4'	-6.35	104.82	109.90
1	0	1979	G	C2'-C3'-O3'	6.29	123.77	113.70
1	0	777	U	O4'-C1'-N1	6.26	113.21	108.20
1	0	2313	C	C5'-C4'-O4'	5.93	116.22	109.10
1	0	1504	A	C1'-O4'-C4'	-5.91	105.17	109.90
1	0	206	G	C5'-C4'-C3'	-5.84	106.66	116.00
1	0	1819	G	C4'-C3'-C2'	-5.79	96.81	102.60
1	0	1615	A	C5'-C4'-C3'	5.69	125.10	116.00
1	0	1352	A	OP1-P-O3'	5.62	117.57	105.20
1	0	2291	A	N9-C1'-C2'	5.46	121.11	114.00
1	0	2467	A	C1'-O4'-C4'	-5.43	105.56	109.90
1	0	841	A	C1'-O4'-C4'	-5.37	105.61	109.90
1	0	1504	A	N9-C1'-C2'	5.30	120.89	114.00
1	0	1942	A	C1'-O4'-C4'	-5.28	105.68	109.90
1	0	1352	A	C2'-C3'-O3'	5.26	122.12	113.70
1	0	1120	U	C5'-C4'-C3'	-5.23	107.63	116.00
1	0	2313	C	C5'-C4'-C3'	5.21	124.33	116.00
17	O	66	GLY	N-CA-C	5.19	126.08	113.10
21	S	27	ALA	N-CA-C	-5.19	96.99	111.00
6	C	73	LEU	CA-CB-CG	-5.12	103.52	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1165	G	C1'-O4'-C4'	-5.11	105.81	109.90
1	0	921	G	N9-C1'-C2'	5.07	120.58	114.00
1	0	389	G	C5'-C4'-C3'	-5.03	107.95	116.00
1	0	69	A	C5'-C4'-O4'	-5.01	103.09	109.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1078	A	Sidechain
1	0	1080	C	Sidechain
1	0	1340	G	Sidechain
1	0	1430	G	Sidechain
1	0	1718	G	Sidechain
1	0	1744	G	Sidechain
1	0	1794	G	Sidechain
1	0	1809	G	Sidechain
1	0	1819	G	Sidechain
1	0	182	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1861	C	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	2316	G	Sidechain
1	0	24	G	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2632	G	Sidechain
1	0	2793	A	Sidechain
1	0	2842	G	Sidechain
1	0	396	U	Sidechain

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Mol	Chain	Res	Type	Group
1	0	462	A	Sidechain
1	0	469	G	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	792	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	Sidechain
2	9	3065	A	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29813	722	0
2	9	2600	0	1326	50	0
3	4	73	0	44	2	0
4	A	1753	0	1766	101	0
5	B	2625	0	2532	145	0
6	C	1859	0	1816	106	0
7	D	1094	0	1085	79	0
8	E	1357	0	1266	45	0
9	F	890	0	843	57	0
10	G	240	0	231	11	0
11	H	1266	0	1268	68	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	53	0
14	L	1118	0	1076	61	0
15	M	1560	0	1568	63	0
16	N	1445	0	1401	97	0
17	O	865	0	873	40	0
18	P	1136	0	1123	35	0
19	Q	735	0	729	18	0
20	R	1149	0	1122	37	0
21	S	641	0	605	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	950	0	923	47	0
23	U	410	0	364	26	0
24	V	499	0	511	38	0
25	W	1196	0	1137	82	0
26	X	654	0	653	35	0
27	Y	1130	0	1133	57	0
28	Z	578	0	539	28	0
29	1	431	0	426	22	0
30	2	396	0	413	26	0
31	3	755	0	728	26	0
32	I	519	0	500	51	0
33	0	87	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	64	0	0	0	0
35	3	1	0	0	0	0
35	9	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5769	0	0	106	0
39	1	50	0	0	2	0
39	2	40	0	0	3	0
39	3	67	0	0	4	0
39	9	140	0	0	6	0
39	A	121	0	0	11	0
39	B	144	0	0	18	0
39	C	177	0	0	18	0
39	D	48	0	0	10	0
39	E	44	0	0	1	0
39	F	27	0	0	4	0
39	G	17	0	0	1	0
39	H	69	0	0	7	0
39	I	7	0	0	1	0
39	J	52	0	0	4	0
39	K	57	0	0	6	0
39	L	81	0	0	14	0
39	M	130	0	0	3	0
39	N	61	0	0	9	0
39	O	40	0	0	5	0
39	P	64	0	0	2	0
39	Q	49	0	0	5	0
39	R	82	0	0	3	0
39	S	32	0	0	1	0
39	T	37	0	0	3	0
39	U	29	0	0	3	0
39	V	14	0	0	2	0
39	W	69	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	X	24	0	0	6	0
39	Y	96	0	0	9	0
39	Z	31	0	0	2	0
All	All	99036	0	59943	2083	0

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

All (2083) 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	1.14
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.29	1.10
6:C:236:THR:HG22	6:C:239:ALA:H	1.19	1.07
1:O:656:G:H5'	17:O:3:THR:HG22	1.38	1.05
1:O:1160:G:H5'	1:O:1161:A:H5'	1.40	1.04
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.72	1.03
2:9:3076:G:H3'	2:9:3077:A:H5''	1.41	1.02
9:F:91:VAL:HG12	9:F:92:GLY:H	1.25	1.00
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.42	0.99
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.38	0.99
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.45	0.98
6:C:127:ARG:NH2	6:C:225:PRO:HG2	1.78	0.97
18:P:115:SER:H	18:P:118:GLN:HE21	1.12	0.96
1:O:156:C:H5''	15:M:171:ARG:HD3	1.47	0.95
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.32	0.94
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.68	0.94
12:J:93:ARG:HH11	12:J:93:ARG:HB3	1.29	0.93
7:D:57:THR:HG23	7:D:63:ILE:HA	1.51	0.93
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.15	0.93
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.51	0.93
5:B:307:ARG:HH11	5:B:307:ARG:HG3	1.34	0.92
21:S:57:THR:HG22	21:S:59:ASP:H	1.34	0.92
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.50	0.92
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.91
2:9:3056:A:H2'	2:9:3057:A:H5''	1.52	0.89
1:O:2506:A:HO2'	1:O:2507:G:H8	0.92	0.89
8:E:20:ILE:HD11	8:E:40:VAL:HG11	1.54	0.89
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.53	0.89
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.21	0.89
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2717:C:H2'	1:0:2718:C:H5''	1.54	0.89
8:E:36:PRO:HD3	12:J:127:ILE:HD12	1.53	0.88
13:K:10:GLN:H	13:K:10:GLN:HE21	0.89	0.88
1:0:1593:C:OP1	18:P:117:SER:HB3	1.74	0.88
8:E:15:GLN:HG3	8:E:20:ILE:HG12	1.56	0.88
13:K:10:GLN:N	13:K:10:GLN:HE21	1.71	0.88
1:0:542:A:H5'	1:0:542:A:H8	1.40	0.87
6:C:104:ASP:HA	6:C:107:ARG:HH12	1.37	0.87
1:0:2717:C:C2'	1:0:2718:C:H5''	2.04	0.87
13:K:10:GLN:H	13:K:10:GLN:NE2	1.73	0.87
4:A:81:GLN:HB2	4:A:92:ASN:ND2	1.89	0.87
5:B:238:ASN:HD22	5:B:240:GLY:H	1.17	0.87
1:0:1603:A:H5'	1:0:1605:G:O4'	1.74	0.87
6:C:1:MET:HG2	6:C:2:GLN:H	1.40	0.87
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.57	0.87
1:0:1242:A:H5'	12:J:82:THR:HG23	1.55	0.86
1:0:1372:A:H3'	39:0:7681:HOH:O	1.75	0.86
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.57	0.86
1:0:288:A:H61	1:0:364:C:H42	1.21	0.86
5:B:162:MET:HE2	5:B:310:ARG:HD3	1.57	0.86
25:W:122:ARG:HH11	25:W:122:ARG:HG2	1.40	0.86
16:N:144:GLY:O	16:N:147:ILE:HG22	1.76	0.86
6:C:115:LEU:HD13	6:C:223:LEU:HD21	1.58	0.85
1:0:2812:A:H2	1:0:2814:A:H62	1.21	0.85
7:D:25:MET:HE2	7:D:41:LEU:HG	1.58	0.84
1:0:1835:U:H5	1:0:1840:A:N7	1.75	0.84
7:D:58:VAL:HB	7:D:62:ASP:HB3	1.58	0.84
7:D:28:GLY:HA2	7:D:69:ILE:HG23	1.59	0.84
1:0:2541:U:H3	1:0:2618:G:H1	1.24	0.84
18:P:115:SER:OG	18:P:118:GLN:HG3	1.77	0.83
1:0:2073:G:H5''	39:0:4410:HOH:O	1.77	0.83
1:0:289:G:H22	1:0:363:A:H2	1.22	0.83
25:W:122:ARG:NH2	25:W:154:ARG:HG2	1.93	0.83
27:Y:235:GLU:H	27:Y:235:GLU:CD	1.80	0.83
2:9:3039:U:H1'	2:9:3044:A:H61	1.43	0.83
15:M:164:THR:HG22	15:M:166:ALA:H	1.43	0.83
16:N:113:SER:HB2	39:N:9356:HOH:O	1.77	0.83
1:0:2840:A:OP1	5:B:211:THR:HG23	1.78	0.82
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.26	0.82
6:C:5:ILE:HD11	6:C:16:VAL:HG23	1.61	0.82
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:V:1:THR:HG23	24:V:2:VAL:H	1.44	0.82
25:W:88:THR:HB	39:W:6679:HOH:O	1.80	0.82
4:A:206:ARG:HD3	4:A:206:ARG:H	1.44	0.81
1:0:560:C:H42	1:0:597:A:H61	1.25	0.81
39:0:5402:HOH:O	12:J:47:THR:HB	1.80	0.81
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.62	0.81
1:0:2506:A:O2'	1:0:2507:G:H8	1.62	0.81
1:0:1116:U:HO2'	1:0:1118:A:H2	0.82	0.81
4:A:192:VAL:HB	39:A:9578:HOH:O	1.79	0.81
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.95	0.81
4:A:211:LYS:HG2	4:A:212:PRO:HD2	1.60	0.81
5:B:162:MET:CE	5:B:310:ARG:HD3	2.09	0.81
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.60	0.81
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.11	0.80
1:0:1377:C:H6	1:0:1377:C:H5'	1.44	0.80
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.63	0.80
1:0:1041:U:H5'	39:L:9489:HOH:O	1.80	0.80
4:A:192:VAL:HG22	39:A:9618:HOH:O	1.81	0.80
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.64	0.80
25:W:125:HIS:HD2	25:W:127:GLY:H	1.30	0.80
1:0:1474:C:H6	1:0:1474:C:H5'	1.46	0.79
31:3:65:THR:HG22	31:3:67:LEU:HG	1.64	0.79
25:W:13:MET:HE1	25:W:18:GLN:HA	1.63	0.79
5:B:36:PRO:HA	5:B:168:GLY:HA3	1.64	0.79
1:0:1116:U:O2'	1:0:1118:A:H2	1.64	0.79
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.65	0.79
1:0:2005:G:H3'	1:0:2005:G:OP2	1.83	0.78
6:C:5:ILE:HD11	6:C:16:VAL:CG2	2.14	0.78
1:0:1165:G:H4'	1:0:1174:A:O2'	1.84	0.78
7:D:25:MET:HE1	7:D:37:ALA:HB1	1.66	0.78
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.13	0.78
30:2:41:HIS:H	30:2:45:ASN:HD22	1.32	0.78
5:B:58:PRO:HA	5:B:63:GLU:OE1	1.83	0.78
1:0:2054:A:N3	20:R:128:ARG:NH2	2.32	0.78
1:0:381:G:H5''	39:M:9376:HOH:O	1.85	0.78
18:P:115:SER:H	18:P:118:GLN:NE2	1.82	0.78
6:C:236:THR:HG22	6:C:239:ALA:N	1.97	0.77
9:F:91:VAL:HG12	9:F:92:GLY:N	1.99	0.77
18:P:115:SER:N	18:P:118:GLN:HE21	1.82	0.77
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.66	0.77
1:0:1701:A:H4'	1:0:1702:U:H5''	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1205:U:H2'	1:0:1206:U:H5''	1.67	0.77
1:0:2635:A:O2'	1:0:2636:C:H5'	1.85	0.76
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.50	0.76
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.66	0.76
1:0:1166:A:H61	1:0:1180:U:H3	1.31	0.76
5:B:53:LEU:HD11	5:B:327:VAL:HG22	1.65	0.76
25:W:21:LEU:CD2	25:W:48:VAL:HG11	2.13	0.76
20:R:25:PHE:CE2	20:R:29:LYS:HE2	2.20	0.76
1:0:545:G:H8	1:0:545:G:H5'	1.49	0.76
1:0:962:C:H1'	16:N:5:ARG:NH1	2.00	0.76
32:I:132:CYS:HB3	32:I:137:VAL:HB	1.68	0.76
1:0:559:U:H5'	1:0:559:U:H6	1.51	0.76
7:D:135:VAL:HG21	7:D:139:TYR:CD1	2.20	0.76
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.68	0.76
16:N:37:ARG:HG3	36:N:9307:CL:CL	2.23	0.76
1:0:2534:C:H1'	39:0:4089:HOH:O	1.86	0.75
13:K:107:THR:HG22	13:K:108:GLU:HG3	1.68	0.75
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.86	0.75
1:0:1119:G:N2	1:0:1246:A:C2	2.53	0.75
1:0:1206:U:H6	1:0:1206:U:H5'	1.51	0.75
1:0:871:G:H8	1:0:871:G:H5''	1.49	0.75
1:0:1175:G:H1'	1:0:1193:A:H2'	1.67	0.75
4:A:199:HIS:HD2	4:A:201:PHE:H	1.33	0.75
4:A:191:GLY:HA2	4:A:194:MET:CE	2.17	0.75
4:A:33:GLU:CD	4:A:33:GLU:H	1.89	0.75
6:C:236:THR:CG2	6:C:239:ALA:H	1.99	0.75
1:0:544:G:H2'	1:0:545:G:H5''	1.69	0.75
4:A:153:ARG:HH11	4:A:153:ARG:HB2	1.52	0.75
39:0:6067:HOH:O	5:B:298:LYS:HG2	1.86	0.75
8:E:15:GLN:HG2	8:E:19:ASP:O	1.85	0.75
1:0:871:G:C8	1:0:871:G:C5'	2.69	0.75
5:B:179:LEU:O	5:B:183:GLU:HG2	1.86	0.74
16:N:110:THR:HB	16:N:113:SER:OG	1.87	0.74
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.69	0.74
32:I:99:ASP:OD1	32:I:138:THR:HB	1.88	0.74
9:F:96:ALA:HA	39:F:3111:HOH:O	1.88	0.74
13:K:32:ILE:HD11	13:K:56:SER:HB2	1.69	0.74
14:L:73:VAL:HG23	14:L:74:THR:H	1.52	0.74
27:Y:154:ARG:HH12	27:Y:155:ARG:HG3	1.53	0.74
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.85	0.74
1:0:1973:A:H5'	1:0:1973:A:H8	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:871:G:H8	1:0:871:G:C5'	2.01	0.74
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.51	0.74
1:0:1159:G:H21	1:0:1189:A:H8	1.36	0.73
25:W:88:THR:HG23	25:W:110:GLN:NE2	2.02	0.73
9:F:46:GLU:OE1	9:F:100:ASP:HA	1.89	0.73
1:0:656:G:C5'	17:O:3:THR:HG22	2.17	0.73
1:0:1667:A:H8	1:0:1667:A:H5'	1.54	0.73
11:H:27:LYS:H	11:H:59:HIS:HD2	1.35	0.73
6:C:107:ARG:NH1	6:C:107:ARG:HB3	2.03	0.73
1:0:2491:G:H1'	39:O:7375:HOH:O	1.88	0.73
1:0:656:G:H5'	17:O:3:THR:CG2	2.17	0.73
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.70	0.73
1:0:2851:G:C2'	1:0:2852:A:H5'	2.18	0.73
1:0:506:G:H22	1:0:509:A:C5'	2.02	0.73
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.70	0.73
1:0:1299:G:O6	14:L:6:ARG:HD3	1.89	0.72
16:N:80:SER:HB2	39:N:9335:HOH:O	1.89	0.72
21:S:57:THR:HG22	21:S:59:ASP:N	2.02	0.72
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.70	0.72
1:0:2749:U:H5'	39:O:8471:HOH:O	1.89	0.72
7:D:58:VAL:HG12	7:D:60:GLU:HG2	1.71	0.72
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.70	0.72
1:0:1160:G:C5'	1:0:1161:A:H5'	2.15	0.72
1:0:481:U:H5''	39:O:6188:HOH:O	1.89	0.72
4:A:192:VAL:HG12	4:A:207:GLN:HB3	1.71	0.72
1:0:1118:A:H3'	1:0:1118:A:H8	1.55	0.72
7:D:23:VAL:HG22	7:D:73:VAL:HB	1.70	0.72
1:0:1116:U:O2'	1:0:1118:A:C2	2.41	0.72
5:B:141:ARG:HD2	5:B:163:GLU:OE2	1.90	0.72
2:9:3014:G:H8	2:9:3014:G:H5'	1.55	0.71
4:A:94:LEU:HD12	4:A:98:GLU:HB2	1.71	0.71
27:Y:165:GLU:HB3	39:Y:9394:HOH:O	1.90	0.71
1:0:541:C:H2'	1:0:542:A:H5''	1.72	0.71
11:H:30:GLN:H	11:H:66:ARG:NH1	1.87	0.71
25:W:137:GLN:HE21	25:W:141:HIS:CE1	2.04	0.71
4:A:35:GLY:O	4:A:36:ASP:HB3	1.89	0.71
10:G:12:ILE:N	10:G:13:PRO:HD3	2.06	0.71
1:0:1700:C:H5''	1:0:1701:A:OP2	1.91	0.71
1:0:506:G:H22	1:0:509:A:H5''	1.54	0.71
32:I:110:GLU:HA	32:I:113:HIS:CE1	2.25	0.71
9:F:50:VAL:HG13	9:F:60:VAL:HG11	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.05	0.71
1:0:541:C:C2'	1:0:542:A:H5''	2.20	0.71
4:A:191:GLY:HA2	4:A:194:MET:HE2	1.71	0.71
9:F:13:GLU:OE2	9:F:78:GLU:HG2	1.90	0.71
20:R:99:ALA:HB1	20:R:109:MET:CE	2.19	0.71
14:L:80:ASP:HB2	14:L:90:ARG:O	1.91	0.71
23:U:17:THR:HG22	23:U:18:GLY:N	2.06	0.71
1:0:1166:A:H1'	1:0:1192:A:C2	2.26	0.70
9:F:53:ASP:OD1	9:F:80:GLN:HB2	1.91	0.70
12:J:45:VAL:HG11	12:J:121:LEU:HD22	1.73	0.70
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.90	0.70
1:0:2716:G:H5''	5:B:206:THR:HG21	1.73	0.70
2:9:3039:U:H1'	2:9:3044:A:N6	2.06	0.70
5:B:268:ARG:NH2	5:B:325:PRO:HG3	2.06	0.70
1:0:2765:C:H4'	39:0:6067:HOH:O	1.92	0.70
18:P:91:LYS:O	18:P:95:GLU:HG3	1.91	0.70
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.21	0.70
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.72	0.70
1:0:2042:U:H1'	39:0:7798:HOH:O	1.90	0.70
1:0:2586:U:H3	1:0:2592:G:H22	1.39	0.70
1:0:949:U:H4'	19:Q:95:GLU:HA	1.72	0.70
4:A:48:ASP:HB3	39:A:9587:HOH:O	1.91	0.70
7:D:23:VAL:HG21	7:D:45:THR:HG21	1.73	0.70
16:N:12:ARG:HD3	16:N:18:THR:OG1	1.92	0.70
1:0:1838:U:O2'	1:0:2644:C:H5'	1.91	0.70
1:0:1979:G:H2'	39:0:3890:HOH:O	1.90	0.70
4:A:192:VAL:CG1	4:A:207:GLN:HB3	2.22	0.70
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.72	0.70
1:0:1878:G:H1'	39:0:6649:HOH:O	1.90	0.70
1:0:796:A:HO2'	28:Z:10:ARG:N	1.89	0.70
1:0:470:U:O2'	29:1:16:HIS:HD2	1.75	0.70
6:C:2:GLN:HB3	39:C:9191:HOH:O	1.90	0.70
6:C:194:PHE:CD2	6:C:234:VAL:HG11	2.26	0.70
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.73	0.70
15:M:69:LYS:O	15:M:73:ARG:NH2	2.25	0.70
1:0:1183:C:N4	1:0:1184:C:H41	1.90	0.70
1:0:2073:G:OP2	1:0:2490:A:H5'	1.92	0.70
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.74	0.70
28:Z:22:SER:O	28:Z:26:VAL:HG23	1.92	0.70
39:0:7927:HOH:O	5:B:211:THR:HG21	1.92	0.69
8:E:20:ILE:CD1	8:E:40:VAL:HG11	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:141:THR:HG23	39:Y:9389:HOH:O	1.92	0.69
1:0:1118:A:C8	1:0:1118:A:H3'	2.27	0.69
1:0:1206:U:H2'	1:0:1207:A:O4'	1.92	0.69
24:V:39:ALA:N	24:V:40:PRO:HD2	2.08	0.69
5:B:307:ARG:NH1	5:B:307:ARG:HG3	2.02	0.69
6:C:104:ASP:HA	6:C:107:ARG:NH1	2.07	0.69
14:L:148:GLU:HB2	39:L:9485:HOH:O	1.91	0.69
25:W:125:HIS:CD2	25:W:127:GLY:H	2.11	0.69
2:9:3029:C:O3'	7:D:138:GLY:HA2	1.92	0.69
39:0:8484:HOH:O	5:B:2:GLN:HG3	1.91	0.69
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.23	0.69
1:0:280:C:H2'	1:0:281:U:O4'	1.93	0.69
4:A:51:ARG:HB2	39:A:9587:HOH:O	1.90	0.69
6:C:1:MET:HG2	6:C:2:GLN:N	2.08	0.69
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.23	0.69
1:0:282:C:H1'	1:0:368:C:N4	2.07	0.69
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.75	0.69
1:0:2578:G:H5'	1:0:2578:G:H8	1.57	0.69
2:9:3056:A:C2'	2:9:3057:A:H5''	2.23	0.69
5:B:5:ARG:NH1	5:B:8:LYS:HE2	2.08	0.69
8:E:35:TYR:HA	12:J:127:ILE:HD12	1.75	0.69
18:P:9:LEU:O	18:P:13:VAL:HG12	1.93	0.69
1:0:1666:C:H2'	1:0:1667:A:H5'	1.75	0.68
1:0:2468:A:H61	31:3:48:ASN:HD21	1.38	0.68
5:B:201:ASP:HB2	5:B:312:ARG:HD2	1.75	0.68
22:T:9:LYS:HE3	22:T:13:ARG:CZ	2.22	0.68
1:0:2533:C:H5'	1:0:2533:C:H6	1.57	0.68
29:1:18:LYS:HB2	30:2:49:GLU:HG2	1.76	0.68
9:F:37:THR:O	9:F:41:GLU:HG3	1.94	0.68
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.94	0.68
1:0:1160:G:H5'	1:0:1161:A:C5'	2.19	0.68
5:B:140:LEU:HA	39:B:9576:HOH:O	1.91	0.68
5:B:190:MET:HE2	5:B:194:PHE:HD1	1.57	0.68
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.94	0.68
17:O:32:ARG:HD3	17:O:32:ARG:O	1.93	0.68
1:0:541:C:H2'	1:0:542:A:C5'	2.23	0.68
1:0:2890:A:H1'	23:U:56:ARG:NH2	2.08	0.68
1:0:93:C:H5''	24:V:1:THR:HB	1.76	0.68
5:B:125:GLU:O	5:B:129:ARG:HG3	1.94	0.68
11:H:166:SER:HB3	11:H:167:PRO:HD3	1.74	0.68
1:0:111:C:O2'	29:1:20:ARG:HG2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:81:GLN:HB2	4:A:92:ASN:HD21	1.57	0.68
20:R:39:THR:HB	20:R:42:GLU:HG3	1.74	0.68
25:W:88:THR:HG22	25:W:89:ASP:N	2.09	0.67
4:A:95:PRO:HG2	4:A:98:GLU:HG2	1.75	0.67
9:F:63:ILE:HB	9:F:64:PRO:HD3	1.75	0.67
17:O:32:ARG:NE	17:O:35:LYS:HD2	2.08	0.67
1:O:1474:C:C6	1:O:1474:C:H5'	2.28	0.67
1:O:281:U:H2'	1:O:282:C:O4'	1.94	0.67
6:C:78:ARG:HG3	6:C:78:ARG:HH11	1.59	0.67
32:I:89:SER:HB2	32:I:95:ASP:HB2	1.76	0.67
27:Y:144:ARG:CZ	39:Y:9412:HOH:O	2.42	0.67
1:O:2346:C:O2'	7:D:52:THR:HG21	1.94	0.67
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.08	0.67
6:C:27:ARG:HG3	6:C:29:ASP:OD1	1.95	0.67
8:E:116:THR:HG22	8:E:151:LEU:HD22	1.77	0.67
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.77	0.67
14:L:143:THR:HG22	14:L:144:ASP:N	2.09	0.67
1:O:1209:C:H2'	1:O:1210:G:H8	1.60	0.67
32:I:102:VAL:HG12	32:I:106:LYS:HE3	1.76	0.67
1:O:1184:C:H4'	32:I:126:LYS:HB3	1.77	0.67
9:F:2:VAL:HG22	9:F:57:GLU:OE1	1.95	0.66
1:O:553:G:P	27:Y:204:ARG:HH22	2.18	0.66
11:H:166:SER:CB	11:H:167:PRO:CD	2.73	0.66
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.76	0.66
1:O:1189:A:H3'	39:O:8231:HOH:O	1.95	0.66
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.94	0.66
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.25	0.66
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.76	0.66
5:B:102:THR:HG23	5:B:182:VAL:HG12	1.78	0.66
4:A:69:LEU:HD23	4:A:107:ASN:HB2	1.76	0.66
5:B:275:GLY:O	5:B:291:ASP:HA	1.95	0.66
24:V:12:THR:HG22	24:V:15:GLU:CG	2.24	0.66
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.25	0.66
25:W:80:ASP:O	25:W:84:VAL:HG23	1.94	0.66
1:O:2779:G:H21	8:E:143:GLN:NE2	1.94	0.66
1:O:380:A:OP2	15:M:9:ARG:HD2	1.96	0.66
1:O:657:G:OP1	6:C:27:ARG:NH2	2.26	0.66
29:1:25:LYS:HD2	30:2:49:GLU:N	2.11	0.66
5:B:102:THR:HG21	5:B:182:VAL:O	1.96	0.66
1:O:797:A:C4'	28:Z:10:ARG:N	2.59	0.66
1:O:544:G:C2'	1:O:545:G:H5''	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3013:A:O2'	2:9:3014:G:H5''	1.95	0.66
8:E:68:HIS:O	8:E:72:MET:HG3	1.94	0.66
15:M:80:GLY:O	15:M:81:ARG:HD2	1.95	0.66
4:A:100:PRO:HG2	4:A:103:VAL:HG21	1.77	0.65
5:B:8:LYS:HG3	5:B:220:VAL:HG12	1.78	0.65
11:H:170:ASN:N	11:H:170:ASN:HD22	1.95	0.65
1:0:871:G:C8	1:0:871:G:H5'	2.30	0.65
1:0:338:C:H4'	6:C:174:ILE:CD1	2.26	0.65
7:D:154:LYS:HD2	7:D:154:LYS:H	1.61	0.65
11:H:3:ALA:HA	11:H:58:ARG:NH1	2.10	0.65
1:0:2363:G:O2'	19:Q:11:ARG:HG3	1.97	0.65
11:H:46:GLN:HE21	11:H:137:TYR:HE2	1.45	0.65
14:L:91:VAL:HG13	14:L:120:LEU:HD23	1.78	0.65
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	1.96	0.65
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.11	0.65
7:D:65:GLU:HA	39:D:6752:HOH:O	1.97	0.65
12:J:93:ARG:NH1	12:J:93:ARG:HB3	2.08	0.65
15:M:183:THR:HG22	15:M:194:ALA:HB1	1.78	0.65
4:A:125:ASN:HB3	4:A:158:VAL:HG12	1.78	0.65
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.97	0.65
16:N:164:ASP:CG	16:N:167:ASP:HA	2.15	0.65
1:0:709:G:O2'	17:O:25:VAL:HG12	1.96	0.65
12:J:19:MET:CE	12:J:132:LEU:HD11	2.26	0.65
1:0:1426:C:H2'	39:O:3209:HOH:O	1.96	0.65
1:0:1641:A:H2'	1:0:1642:A:H5'	1.78	0.65
9:F:58:GLU:OE1	15:M:27:ARG:NH2	2.25	0.65
11:H:56:GLN:HE21	11:H:126:ARG:HE	1.43	0.65
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.26	0.65
1:0:447:A:P	22:T:1:SER:HB2	2.37	0.65
29:1:25:LYS:HD2	30:2:49:GLU:H	1.60	0.65
5:B:51:VAL:CG2	5:B:327:VAL:HG13	2.26	0.65
9:F:77:VAL:HG21	9:F:83:LEU:HD13	1.77	0.65
22:T:26:THR:HA	22:T:39:ASN:HB3	1.79	0.65
4:A:199:HIS:CD2	4:A:201:PHE:H	2.13	0.64
4:A:66:ARG:HH11	4:A:66:ARG:HB2	1.62	0.64
15:M:107:ARG:NH1	15:M:107:ARG:HG3	2.11	0.64
21:S:51:GLN:NE2	21:S:53:ASN:HD21	1.94	0.64
1:0:1184:C:H1'	39:O:7937:HOH:O	1.95	0.64
7:D:159:PRO:O	7:D:163:VAL:HG23	1.96	0.64
23:U:47:ARG:HG3	39:U:4381:HOH:O	1.97	0.64
24:V:56:ILE:O	24:V:60:GLN:HG3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1201:C:H2'	1:0:1202:A:H5'	1.79	0.64
1:0:2718:C:H6	1:0:2718:C:H5'	1.63	0.64
1:0:2661:U:H3	1:0:2812:A:H62	1.44	0.64
23:U:52:THR:HG22	23:U:54:THR:N	2.13	0.64
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.79	0.64
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.27	0.64
1:0:1205:U:H2'	1:0:1206:U:C5'	2.27	0.64
1:0:2420:G:O2'	1:0:2421:G:H5'	1.97	0.64
1:0:2780:C:H1'	8:E:143:GLN:HE21	1.62	0.64
32:I:105:VAL:HG11	32:I:129:VAL:HG22	1.80	0.64
15:M:187:LEU:CD2	15:M:194:ALA:HB3	2.27	0.64
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.19	0.64
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.33	0.64
28:Z:17:ARG:HD3	39:Z:9219:HOH:O	1.97	0.64
5:B:62:ARG:HA	5:B:65:MET:CE	2.28	0.64
1:0:962:C:H1'	16:N:5:ARG:HH12	1.63	0.64
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.44	0.64
22:T:38:ARG:NH1	39:T:6217:HOH:O	2.31	0.64
22:T:71:VAL:HG12	22:T:72:ILE:N	2.13	0.64
25:W:48:VAL:HG12	25:W:48:VAL:O	1.98	0.64
26:X:25:ARG:HD3	26:X:64:ALA:O	1.98	0.64
1:0:1205:U:C2'	1:0:1206:U:H5''	2.27	0.64
8:E:8:PRO:HB2	8:E:11:VAL:HG23	1.80	0.64
25:W:13:MET:CE	25:W:17:ILE:HG22	2.28	0.64
1:0:1119:G:H22	1:0:1246:A:H2	1.40	0.63
11:H:20:ILE:HG23	11:H:120:ILE:HD11	1.80	0.63
11:H:56:GLN:NE2	11:H:126:ARG:HE	1.96	0.63
1:0:2507:G:H2'	1:0:2510:C:H42	1.62	0.63
1:0:1666:C:O2'	1:0:1667:A:H5''	1.98	0.63
1:0:2896:A:N3	1:0:2896:A:H2'	2.14	0.63
6:C:129:HIS:CE1	6:C:231:ARG:HA	2.34	0.63
6:C:139:VAL:HG13	39:C:9254:HOH:O	1.98	0.63
9:F:12:LEU:HD21	9:F:111:ILE:HG23	1.79	0.63
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.26	0.63
16:N:132:ASN:O	16:N:135:VAL:HG12	1.97	0.63
15:M:164:THR:HG22	15:M:166:ALA:N	2.11	0.63
1:0:1687:C:O2	29:I:9:GLY:HA2	1.99	0.63
1:0:2748:G:H2'	39:O:8049:HOH:O	1.99	0.63
32:I:125:ALA:O	32:I:129:VAL:HG23	1.99	0.63
1:0:1168:C:H5''	32:I:87:THR:HG23	1.81	0.63
16:N:23:ARG:HH11	16:N:23:ARG:HG2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:59:HIS:HA	11:H:62:LEU:HD23	1.79	0.63
1:O:1182:C:H1'	1:O:1192:A:H8	1.63	0.63
1:O:1563:G:H4'	39:O:4808:HOH:O	1.98	0.63
14:L:40:PHE:HB3	39:L:9458:HOH:O	1.99	0.63
27:Y:144:ARG:HH11	27:Y:144:ARG:HG3	1.63	0.63
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.29	0.63
4:A:88:ILE:HD13	4:A:100:PRO:HD3	1.81	0.63
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.62	0.63
1:O:1766:U:O2	1:O:1778:A:H5'	1.99	0.63
5:B:254:GLN:HG2	5:B:255:GLY:N	2.13	0.63
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.80	0.63
5:B:102:THR:CG2	5:B:182:VAL:HG12	2.29	0.62
16:N:164:ASP:OD1	16:N:167:ASP:HA	1.99	0.62
1:O:1377:C:H5'	1:O:1377:C:C6	2.30	0.62
7:D:138:GLY:N	39:D:7597:HOH:O	2.32	0.62
15:M:79:ALA:HB3	15:M:81:ARG:NH1	2.14	0.62
6:C:236:THR:HG21	39:C:9180:HOH:O	1.98	0.62
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.29	0.62
1:O:2878:U:H2'	1:O:2879:A:O4'	1.99	0.62
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.82	0.62
11:H:27:LYS:N	11:H:59:HIS:HD2	1.98	0.62
24:V:56:ILE:HG22	24:V:60:GLN:HE21	1.63	0.62
5:B:212:GLN:HB2	5:B:257:THR:CG2	2.26	0.62
1:O:1116:U:H3	1:O:1246:A:H62	1.47	0.62
5:B:18:ARG:HG3	5:B:256:GLN:HG3	1.80	0.62
7:D:58:VAL:CG1	7:D:60:GLU:HG2	2.29	0.62
12:J:74:ARG:NH1	12:J:105:LEU:HD11	2.14	0.62
11:H:154:TYR:HB2	39:H:9555:HOH:O	1.99	0.62
11:H:166:SER:CB	11:H:167:PRO:HD3	2.30	0.62
7:D:170:TYR:O	7:D:171:ASP:HB3	1.99	0.62
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.63	0.62
2:9:3020:G:O2'	2:9:3021:G:H5'	1.99	0.62
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.48	0.61
27:Y:144:ARG:HH11	27:Y:144:ARG:CG	2.11	0.61
1:O:282:C:O2'	1:O:283:U:H5'	2.00	0.61
5:B:215:VAL:HB	5:B:234:ARG:HH12	1.65	0.61
32:I:92:PRO:C	32:I:94:GLU:H	2.02	0.61
16:N:143:ARG:HH21	16:N:169:PRO:HB2	1.65	0.61
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.82	0.61
24:V:43:PRO:O	24:V:46:ILE:HG22	2.00	0.61
1:O:396:U:O2'	1:O:418:C:H4'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:121:ALA:O	4:A:124:VAL:HG22	2.01	0.61
9:F:50:VAL:CG1	9:F:60:VAL:HG11	2.29	0.61
1:O:902:G:N7	14:L:18:HIS:HD2	1.98	0.61
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.81	0.61
1:O:2502:C:H2'	1:O:2503:A:H5'	1.82	0.61
32:I:110:GLU:HA	32:I:113:HIS:NE2	2.16	0.61
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.15	0.61
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.31	0.61
22:T:115:GLU:HG3	22:T:116:ASP:N	2.16	0.61
23:U:17:THR:CG2	23:U:18:GLY:N	2.64	0.61
24:V:64:GLY:O	24:V:65:ASP:HB2	2.00	0.61
25:W:84:VAL:HG12	39:W:6679:HOH:O	2.00	0.61
1:O:1118:A:H62	1:O:1244:U:H3	1.47	0.61
1:O:156:C:H5''	15:M:171:ARG:CD	2.27	0.61
1:O:1701:A:H4'	1:O:1702:U:C5'	2.31	0.61
11:H:3:ALA:HA	11:H:58:ARG:HH12	1.65	0.61
32:I:102:VAL:O	32:I:106:LYS:HG3	2.00	0.61
24:V:39:ALA:C	24:V:41:GLU:H	2.03	0.61
25:W:52:VAL:HG22	25:W:53:ALA:H	1.64	0.61
6:C:107:ARG:NE	39:C:9264:HOH:O	2.31	0.61
14:L:133:VAL:HA	39:L:9470:HOH:O	2.01	0.61
1:O:164:G:H4'	14:L:30:ARG:HD3	1.82	0.61
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.24	0.61
1:O:2769:C:H2'	1:O:2770:G:O4'	1.99	0.60
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.64	0.60
22:T:48:VAL:HG22	22:T:96:VAL:HG22	1.82	0.60
1:O:2064:U:H5'	1:O:2652:U:H4'	1.82	0.60
5:B:5:ARG:HH11	5:B:8:LYS:HE2	1.65	0.60
25:W:130:HIS:O	25:W:136:GLY:HA3	2.01	0.60
1:O:1528:A:H2'	1:O:1529:G:O4'	2.02	0.60
1:O:2851:G:H2'	1:O:2852:A:H5'	1.82	0.60
1:O:621:C:H5'	27:Y:132:ASP:OD2	2.02	0.60
5:B:71:VAL:HG11	5:B:296:LEU:HD22	1.82	0.60
6:C:16:VAL:HG12	6:C:17:ASP:H	1.65	0.60
32:I:138:THR:HG22	32:I:139:ILE:H	1.65	0.60
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.83	0.60
16:N:110:THR:HB	16:N:113:SER:HG	1.64	0.60
29:1:10:LYS:HG3	39:1:9488:HOH:O	2.00	0.60
6:C:118:THR:O	6:C:136:VAL:HG13	2.00	0.60
27:Y:189:ASN:HD22	27:Y:189:ASN:C	2.04	0.60
6:C:236:THR:HA	39:C:9257:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:681:G:N3	1:0:681:G:H5'	2.17	0.60
4:A:125:ASN:CB	4:A:158:VAL:HG12	2.31	0.60
5:B:16:ARG:NH1	39:B:9615:HOH:O	2.33	0.60
7:D:25:MET:SD	7:D:40:ILE:HD11	2.42	0.60
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.65	0.60
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.66	0.60
1:0:1201:C:H5''	39:0:6761:HOH:O	2.02	0.60
2:9:3029:C:H2'	2:9:3030:C:H5'	1.83	0.60
12:J:131:THR:HG22	12:J:134:GLU:H	1.65	0.60
1:0:2748:G:H5'	39:0:8049:HOH:O	2.00	0.60
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.84	0.60
11:H:166:SER:HB2	11:H:167:PRO:CD	2.32	0.60
12:J:93:ARG:HH11	12:J:93:ARG:CB	2.07	0.60
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.84	0.60
27:Y:187:VAL:HG12	27:Y:205:ILE:HA	1.83	0.60
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.02	0.60
2:9:3014:G:C8	2:9:3014:G:H5'	2.35	0.60
18:P:40:VAL:O	18:P:44:VAL:HG23	2.01	0.60
1:0:1555:G:H4'	1:0:1630:A:H2	1.67	0.60
1:0:2291:A:C8	1:0:2309:C:H5'	2.37	0.60
1:0:960:G:H4'	39:0:7904:HOH:O	2.00	0.60
32:I:134:SER:O	32:I:135:LEU:HD23	2.02	0.60
1:0:2502:C:C2'	1:0:2503:A:H5'	2.32	0.59
1:0:272:A:H5'	1:0:273:G:OP2	2.02	0.59
1:0:380:A:H2'	39:0:7718:HOH:O	2.01	0.59
6:C:140:VAL:HB	39:C:9257:HOH:O	2.01	0.59
17:O:32:ARG:HH21	17:O:35:LYS:HZ1	1.50	0.59
1:0:263:U:O4'	9:F:59:ILE:HD13	2.02	0.59
32:I:78:LEU:HD12	32:I:112:LYS:NZ	2.16	0.59
12:J:74:ARG:O	12:J:78:ILE:HG12	2.02	0.59
14:L:35:ARG:HB2	14:L:35:ARG:HH11	1.67	0.59
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.37	0.59
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.84	0.59
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.83	0.59
5:B:297:VAL:HB	39:B:9604:HOH:O	2.01	0.59
5:B:85:ARG:NH1	39:B:9633:HOH:O	2.35	0.59
9:F:91:VAL:CG1	9:F:92:GLY:H	2.08	0.59
17:O:42:GLU:HB2	39:O:2176:HOH:O	2.02	0.59
1:0:834:G:H4'	1:0:835:U:OP2	2.03	0.59
15:M:77:HIS:HD2	15:M:79:ALA:O	1.85	0.59
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:542:A:H5'	1:0:542:A:C8	2.28	0.59
5:B:96:PRO:HG3	39:B:9633:HOH:O	2.00	0.59
7:D:136:ARG:HH12	7:D:157:LEU:HA	1.65	0.59
14:L:73:VAL:HG23	14:L:74:THR:N	2.17	0.59
16:N:176:ARG:HG3	16:N:180:LEU:HD13	1.84	0.59
1:0:2100:A:H4'	6:C:64:GLY:O	2.02	0.59
16:N:154:LEU:O	16:N:155:GLU:HB3	2.03	0.59
24:V:1:THR:HG23	24:V:2:VAL:N	2.16	0.59
1:0:2003:U:H4'	1:0:2004:U:H5	1.68	0.59
1:0:2795:C:O2'	1:0:2796:U:H5'	2.03	0.59
32:I:113:HIS:N	32:I:114:PRO:HD2	2.18	0.59
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.33	0.59
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.68	0.59
1:0:516:A:H5'	39:0:6188:HOH:O	2.03	0.59
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.33	0.59
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.59
1:0:870:G:H2'	1:0:871:G:H5''	1.85	0.59
39:0:9698:HOH:O	5:B:214:PRO:HD2	2.03	0.59
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.84	0.59
1:0:1328:A:OP1	27:Y:169:ARG:HD2	2.02	0.59
1:0:1819:G:H2'	1:0:1820:G:H4'	1.84	0.59
1:0:2851:G:O2'	1:0:2852:A:H5'	2.03	0.59
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.38	0.59
14:L:35:ARG:HB2	14:L:35:ARG:NH1	2.18	0.59
21:S:51:GLN:HE21	21:S:53:ASN:ND2	1.95	0.59
23:U:14:GLU:OE1	23:U:15:PRO:HD2	2.03	0.59
39:0:9972:HOH:O	29:1:1:THR:HA	2.03	0.58
5:B:88:GLU:HB3	5:B:97:LEU:HD12	1.84	0.58
9:F:46:GLU:O	9:F:73:PRO:HD2	2.03	0.58
13:K:23:ASN:HD21	13:K:107:THR:HB	1.68	0.58
9:F:58:GLU:CD	15:M:27:ARG:HH22	2.05	0.58
1:0:2505:G:O2'	1:0:2506:A:H5'	2.04	0.58
4:A:33:GLU:O	4:A:34:ASP:HB2	2.03	0.58
16:N:69:TYR:HE2	16:N:184:ILE:HG13	1.67	0.58
1:0:545:G:C8	1:0:545:G:H5'	2.35	0.58
7:D:59:GLY:O	7:D:61:PHE:N	2.36	0.58
17:O:53:GLN:HG2	17:O:56:GLU:OE1	2.03	0.58
15:M:68:ARG:NH2	15:M:73:ARG:HD3	2.18	0.58
39:0:3154:HOH:O	18:P:81:LYS:HG2	2.03	0.58
1:0:20:G:H21	20:R:117:HIS:HD2	1.48	0.58
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.19	0.58
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.39	0.58
1:0:289:G:N2	1:0:363:A:H2	1.96	0.58
1:0:877:G:H5'	1:0:878:G:OP1	2.03	0.58
1:0:969:G:H1	1:0:999:C:H42	1.49	0.58
11:H:63:GLU:HA	39:H:9544:HOH:O	2.03	0.58
14:L:143:THR:HG22	14:L:144:ASP:H	1.68	0.58
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.32	0.58
1:0:2426:G:H1'	39:0:6621:HOH:O	2.03	0.58
1:0:625:U:H5'	39:0:3784:HOH:O	2.04	0.58
4:A:57:ALA:HB1	4:A:65:ARG:HE	1.69	0.58
11:H:111:ASP:HA	39:H:9510:HOH:O	2.02	0.58
1:0:2081:A:H4'	12:J:69:TYR:CE1	2.39	0.58
16:N:169:PRO:O	16:N:172:PHE:HB3	2.03	0.58
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.33	0.58
1:0:2726:U:O2'	26:X:22:ASN:ND2	2.37	0.58
1:0:558:C:C2'	1:0:559:U:H5''	2.34	0.58
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.03	0.58
5:B:238:ASN:ND2	5:B:240:GLY:H	1.95	0.58
6:C:236:THR:H	6:C:239:ALA:HB3	1.68	0.58
8:E:20:ILE:HD12	8:E:33:LEU:HD12	1.86	0.58
10:G:20:VAL:O	10:G:24:VAL:HG23	2.03	0.58
20:R:96:VAL:HG13	20:R:106:GLY:HA3	1.86	0.58
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.04	0.58
14:L:104:ASP:HB2	39:L:9460:HOH:O	2.03	0.58
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.85	0.58
1:0:1352:A:O2'	1:0:1353:C:OP1	2.20	0.58
5:B:238:ASN:HD22	5:B:240:GLY:N	1.95	0.58
1:0:1181:A:H5'	32:I:94:GLU:OE2	2.04	0.58
1:0:1384:C:H5'	26:X:30:MET:HG2	1.85	0.57
4:A:26:ASP:O	4:A:28:GLU:N	2.36	0.57
5:B:221:GLN:HE22	13:K:42:ASN:HD22	1.51	0.57
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.04	0.57
1:0:447:A:OP2	22:T:1:SER:HB2	2.04	0.57
1:0:558:C:O2'	1:0:559:U:H5''	2.04	0.57
17:O:57:THR:O	17:O:111:VAL:HG23	2.03	0.57
22:T:49:GLU:OE2	22:T:97:ARG:HD2	2.04	0.57
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.69	0.57
24:V:55:ARG:O	24:V:59:ILE:HG12	2.04	0.57
39:0:9983:HOH:O	4:A:180:LYS:HG2	2.04	0.57
5:B:190:MET:HE2	5:B:194:PHE:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:195:ARG:HG2	5:B:323:LEU:HD22	1.86	0.57
32:I:78:LEU:HD12	32:I:112:LYS:HZ2	1.68	0.57
16:N:170:GLU:O	16:N:174:GLU:HG3	2.04	0.57
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.86	0.57
26:X:31:ILE:O	26:X:35:GLU:HG3	2.05	0.57
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.37	0.57
1:O:1552:G:N2	1:O:1634:G:H1'	2.19	0.57
1:O:2726:U:O2	1:O:2749:U:O5'	2.22	0.57
5:B:185:GLY:HA2	39:B:9632:HOH:O	2.04	0.57
7:D:172:VAL:HG12	7:D:173:GLU:N	2.18	0.57
9:F:21:GLU:O	9:F:24:ARG:HG3	2.05	0.57
14:L:67:ARG:O	14:L:71:GLU:HG3	2.04	0.57
27:Y:203:VAL:CG1	27:Y:228:VAL:HG22	2.35	0.57
1:O:1066:U:H2'	1:O:1067:A:C8	2.40	0.57
1:O:2421:G:H1'	39:O:4289:HOH:O	2.03	0.57
1:O:558:C:H2'	1:O:559:U:C5'	2.34	0.57
31:3:3:MET:HB2	31:3:88:LEU:HD11	1.85	0.57
31:3:62:THR:HB	39:3:9482:HOH:O	2.04	0.57
1:O:1943:C:H4'	4:A:211:LYS:O	2.05	0.57
6:C:236:THR:HG22	6:C:239:ALA:CB	2.34	0.57
14:L:136:ALA:HB3	39:L:9470:HOH:O	2.03	0.57
1:O:1189:A:O2'	1:O:1208:C:H2'	2.04	0.57
1:O:538:C:OP2	27:Y:134:HIS:HE1	1.88	0.57
2:9:3069:U:OP1	16:N:4:PRO:HG3	2.05	0.57
15:M:164:THR:CG2	15:M:165:GLY:N	2.68	0.57
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.70	0.57
1:O:308:U:H5'	22:T:97:ARG:NH2	2.19	0.57
1:O:1218:U:H2'	1:O:1219:U:C6	2.40	0.57
1:O:871:G:C8	1:O:871:G:H5''	2.34	0.57
10:G:12:ILE:N	10:G:13:PRO:CD	2.68	0.57
14:L:36:ASP:HB2	39:L:9433:HOH:O	2.05	0.57
1:O:256:C:H2'	1:O:257:G:O4'	2.05	0.57
12:J:39:VAL:HG13	12:J:106:GLY:O	2.05	0.57
7:D:146:LYS:NZ	16:N:107:ASN:HD21	2.02	0.57
39:9:4707:HOH:O	16:N:147:ILE:HD12	2.05	0.57
17:O:39:THR:O	17:O:115:ARG:NH2	2.37	0.57
1:O:138:U:H5''	1:O:139:C:OP2	2.04	0.56
1:O:2270:G:H4'	4:A:223:ARG:HH12	1.70	0.56
4:A:107:ASN:OD1	4:A:120:ARG:HD2	2.04	0.56
4:A:33:GLU:CD	4:A:33:GLU:N	2.57	0.56
6:C:214:THR:HG23	39:C:9242:HOH:O	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:244:C:OP2	9:F:38:LYS:HE3	2.05	0.56
9:F:39:SER:HB3	9:F:45:ALA:HB2	1.85	0.56
18:P:16:VAL:HG12	18:P:17:GLY:N	2.20	0.56
21:S:77:VAL:O	21:S:80:ARG:HG2	2.05	0.56
2:9:3002:U:OP2	2:9:3003:A:H5'	2.06	0.56
7:D:54:ALA:HB2	7:D:69:ILE:HD12	1.87	0.56
8:E:34:TRP:O	12:J:127:ILE:HD11	2.05	0.56
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.85	0.56
1:0:1634:G:H3'	39:0:4478:HOH:O	2.05	0.56
1:0:2563:U:H2'	1:0:2565:C:O5'	2.05	0.56
6:C:194:PHE:HA	6:C:234:VAL:HG13	1.86	0.56
13:K:55:VAL:HG12	13:K:56:SER:N	2.19	0.56
15:M:182:LYS:O	15:M:194:ALA:HB2	2.06	0.56
1:0:775:G:OP1	29:1:16:HIS:HE1	1.89	0.56
5:B:145:HIS:HD2	5:B:146:THR:O	1.89	0.56
15:M:60:VAL:C	15:M:61:ILE:HD12	2.25	0.56
9:F:1:PRO:H3	9:F:4:VAL:HG23	1.71	0.56
11:H:148:GLU:HA	11:H:148:GLU:OE1	2.05	0.56
11:H:56:GLN:HE22	11:H:93:GLN:HG2	1.70	0.56
25:W:65:VAL:HA	25:W:68:THR:HG22	1.87	0.56
1:0:2064:U:H5'	1:0:2652:U:O3'	2.05	0.56
5:B:51:VAL:HG23	5:B:329:TYR:O	2.06	0.56
2:9:3014:G:O2'	16:N:1:ALA:HB2	2.05	0.56
25:W:88:THR:HG22	25:W:89:ASP:H	1.69	0.56
1:0:151:A:H2'	1:0:152:A:O4'	2.05	0.56
1:0:2032:U:H2'	1:0:2033:G:C5'	2.35	0.56
1:0:432:G:O2'	1:0:433:C:H5'	2.06	0.56
23:U:5:GLU:HG2	23:U:10:GLY:O	2.05	0.56
5:B:264:GLU:OE2	5:B:302:PRO:HD3	2.05	0.56
6:C:154:VAL:O	6:C:158:GLU:HG3	2.06	0.56
11:H:38:LYS:HE2	11:H:42:ASP:HB2	1.88	0.56
1:0:185:G:H4'	1:0:186:A:H4'	1.87	0.56
12:J:107:ASN:HD22	12:J:109:TYR:H	1.53	0.56
22:T:49:GLU:CB	22:T:59:GLU:HG2	2.34	0.56
25:W:4:LEU:HD11	25:W:45:VAL:HG12	1.87	0.56
26:X:25:ARG:HG2	39:X:5356:HOH:O	2.06	0.56
1:0:1118:A:H8	1:0:1119:G:H5''	1.71	0.56
1:0:1187:U:O2'	1:0:1189:A:H2	1.89	0.56
1:0:316:A:H5'	22:T:54:ASP:OD2	2.03	0.56
7:D:54:ALA:CB	7:D:69:ILE:HD12	2.35	0.56
1:0:2694:A:H4'	8:E:91:PHE:HE1	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:24:VAL:O	10:G:28:GLU:HB2	2.05	0.56
32:I:138:THR:HG22	32:I:139:ILE:N	2.20	0.56
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.35	0.56
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.03	0.56
1:O:558:C:H2'	1:O:559:U:H5'	1.88	0.56
6:C:162:VAL:HG22	6:C:232:LEU:HD21	1.88	0.56
39:O:9738:HOH:O	15:M:82:ARG:HD2	2.06	0.56
39:9:1361:HOH:O	16:N:41:LYS:HE3	2.05	0.56
4:A:135:VAL:HG11	4:A:147:ARG:NH1	2.21	0.55
10:G:67:LEU:O	10:G:71:LEU:HG	2.05	0.55
12:J:107:ASN:ND2	12:J:109:TYR:H	2.04	0.55
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.88	0.55
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.88	0.55
1:O:1736:A:H1'	39:O:8143:HOH:O	2.07	0.55
2:9:3076:G:C3'	2:9:3077:A:H5''	2.27	0.55
5:B:53:LEU:CD1	5:B:327:VAL:HG22	2.36	0.55
9:F:58:GLU:HA	9:F:61:MET:HE2	1.88	0.55
26:X:61:ARG:HB2	26:X:65:ASN:HB2	1.87	0.55
1:O:1926:G:H2'	1:O:1927:A:C8	2.41	0.55
4:A:36:ASP:OD2	4:A:85:SER:HB2	2.06	0.55
30:2:49:GLU:HB2	39:2:131:HOH:O	2.06	0.55
4:A:89:ALA:HB3	39:A:9608:HOH:O	2.05	0.55
9:F:48:VAL:HG23	9:F:74:PHE:CB	2.36	0.55
1:O:1778:A:H2'	1:O:1779:A:H5'	1.88	0.55
1:O:2456:A:H2'	1:O:2457:U:C6	2.42	0.55
1:O:291:C:H2'	1:O:292:G:O4'	2.06	0.55
5:B:305:ASP:O	5:B:306:LYS:HB2	2.07	0.55
13:K:4:LEU:CD2	13:K:116:GLU:HB3	2.35	0.55
1:O:475:G:H5'	6:C:73:LEU:HD23	1.87	0.55
15:M:71:SER:HB2	15:M:92:THR:HG22	1.89	0.55
5:B:329:TYR:CE2	23:U:15:PRO:HG2	2.41	0.55
4:A:123:GLY:HA3	4:A:162:GLY:HA2	1.87	0.55
10:G:12:ILE:HD12	39:G:692:HOH:O	2.06	0.55
12:J:75:PRO:HD3	12:J:136:SER:OG	2.05	0.55
14:L:57:VAL:HG12	14:L:57:VAL:O	2.07	0.55
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.21	0.55
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.88	0.55
1:O:1789:G:O6	18:P:73:HIS:HE1	1.89	0.55
1:O:1973:A:H5'	1:O:1973:A:C8	2.39	0.55
1:O:960:G:H2'	1:O:960:G:N3	2.21	0.55
6:C:246:ARG:NH1	6:C:246:ARG:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.88	0.55
27:Y:154:ARG:HH12	27:Y:155:ARG:CG	2.17	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.21	0.55
1:0:441:A:H1'	1:0:442:A:N7	2.21	0.55
4:A:194:MET:HE1	4:A:199:HIS:HB2	1.88	0.55
8:E:20:ILE:CD1	8:E:33:LEU:HD12	2.37	0.55
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.37	0.55
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.05	0.55
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.05	0.55
39:O:8105:HOH:O	31:3:60:LYS:HG3	2.06	0.55
2:9:3051:A:H5'	16:N:160:SER:HB3	1.89	0.55
4:A:191:GLY:HA2	4:A:194:MET:HE3	1.89	0.55
7:D:135:VAL:HG22	7:D:136:ARG:H	1.72	0.55
1:0:1882:C:OP1	4:A:192:VAL:HG23	2.07	0.54
5:B:307:ARG:HB3	39:B:9650:HOH:O	2.06	0.54
1:0:1183:C:H2'	39:O:6772:HOH:O	2.07	0.54
5:B:258:GLY:H	5:B:260:HIS:CE1	2.25	0.54
15:M:68:ARG:HD3	15:M:68:ARG:O	2.08	0.54
1:0:2769:C:O2'	1:0:2770:G:H5'	2.07	0.54
1:0:2827:A:H2'	1:0:2828:G:O4'	2.06	0.54
1:0:2866:U:H4'	1:0:2867:G:H5'	1.89	0.54
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.72	0.54
9:F:60:VAL:HG12	9:F:60:VAL:O	2.06	0.54
16:N:11:ARG:O	16:N:15:GLU:HG3	2.07	0.54
2:9:3051:A:H5'	16:N:160:SER:CB	2.37	0.54
22:T:78:THR:HB	22:T:87:VAL:O	2.08	0.54
1:0:1189:A:H1'	1:0:1209:C:O4'	2.07	0.54
7:D:24:HIS:HB2	7:D:72:LYS:CB	2.37	0.54
32:I:139:ILE:HG22	32:I:140:GLU:N	2.23	0.54
16:N:115:VAL:HG22	39:N:9356:HOH:O	2.07	0.54
1:0:2591:C:H2'	1:0:2592:G:O4'	2.07	0.54
12:J:107:ASN:HD22	12:J:107:ASN:C	2.11	0.54
1:0:2533:C:C6	1:0:2533:C:H5'	2.42	0.54
4:A:153:ARG:CB	4:A:153:ARG:HH11	2.21	0.54
11:H:21:THR:O	11:H:120:ILE:HD12	2.08	0.54
16:N:154:LEU:HG	16:N:155:GLU:H	1.71	0.54
1:0:1626:A:H2'	1:0:1627:G:O4'	2.08	0.54
1:0:1681:G:H5''	1:0:1682:A:H5'	1.89	0.54
1:0:1878:G:O2'	1:0:1879:U:OP2	2.25	0.54
1:0:797:A:H4'	28:Z:10:ARG:N	2.22	0.54
5:B:40:GLY:HA3	39:B:9645:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:72:THR:HB	39:B:9604:HOH:O	2.07	0.54
1:O:474:C:O3'	6:C:73:LEU:HD21	2.07	0.54
23:U:14:GLU:O	23:U:17:THR:HB	2.08	0.54
26:X:43:VAL:HG12	26:X:44:ASP:N	2.23	0.54
1:O:1350:U:H2'	1:O:1351:G:O4'	2.07	0.54
1:O:1666:C:H2'	1:O:1667:A:C5'	2.36	0.54
1:O:2670:G:O2'	1:O:2671:U:H5'	2.08	0.54
1:O:2717:C:O2'	1:O:2718:C:H5''	2.07	0.54
1:O:2769:C:C2'	1:O:2770:G:H5'	2.38	0.54
7:D:50:VAL:O	7:D:71:ALA:HA	2.07	0.54
28:Z:72:GLU:OE1	28:Z:77:LYS:HE2	2.07	0.54
1:O:1209:C:H2'	1:O:1210:G:C8	2.42	0.54
4:A:190:ARG:NH2	4:A:207:GLN:OE1	2.40	0.54
11:H:46:GLN:NE2	11:H:137:TYR:HE2	2.05	0.54
1:O:1595:G:O2'	1:O:1596:U:H5'	2.08	0.54
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.88	0.54
5:B:254:GLN:HG3	39:B:9530:HOH:O	2.08	0.54
5:B:62:ARG:HA	5:B:65:MET:HE2	1.90	0.54
12:J:8:ALA:HA	12:J:35:THR:HG22	1.90	0.54
17:O:59:VAL:HG23	17:O:111:VAL:CG2	2.37	0.54
22:T:12:ARG:NH1	39:T:3035:HOH:O	2.40	0.54
25:W:4:LEU:O	25:W:32:CYS:HA	2.08	0.54
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.42	0.54
1:O:1406:A:H4'	1:O:1407:A:H5''	1.90	0.53
1:O:1625:U:H4'	39:O:5232:HOH:O	2.08	0.53
1:O:2817:G:P	39:O:8476:HOH:O	2.66	0.53
5:B:17:LYS:O	5:B:260:HIS:HD2	1.91	0.53
5:B:56:ASP:OD1	5:B:322:ARG:HB3	2.08	0.53
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.89	0.53
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.90	0.53
1:O:949:U:O2'	19:Q:40:HIS:HE1	1.91	0.53
1:O:1594:C:OP2	18:P:120:ARG:HD2	2.08	0.53
23:U:49:LEU:HG	39:U:3805:HOH:O	2.07	0.53
1:O:2265:U:H2'	1:O:2266:A:C8	2.43	0.53
5:B:195:ARG:HD2	5:B:324:ASP:OD1	2.07	0.53
6:C:107:ARG:HH11	6:C:107:ARG:HB3	1.71	0.53
39:O:7381:HOH:O	15:M:178:LYS:HB2	2.07	0.53
1:O:2645:U:OP2	1:O:2645:U:C6	2.61	0.53
1:O:2894:C:O2'	1:O:2895:C:H5'	2.08	0.53
31:3:3:MET:O	31:3:90:PHE:HA	2.09	0.53
5:B:51:VAL:HG23	5:B:327:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:78:ARG:HG3	6:C:78:ARG:NH1	2.21	0.53
1:O:2694:A:H4'	8:E:91:PHE:CE1	2.44	0.53
30:2:18:ASN:ND2	30:2:40:ARG:H	2.06	0.53
7:D:172:VAL:HG12	7:D:173:GLU:H	1.74	0.53
7:D:92:GLU:HB2	39:D:3862:HOH:O	2.07	0.53
12:J:47:THR:HG22	12:J:48:GLY:N	2.23	0.53
24:V:42:ASN:HB3	39:V:7247:HOH:O	2.08	0.53
1:O:1419:U:H2'	1:O:1685:A:C2	2.43	0.53
31:3:65:THR:HG23	31:3:88:LEU:HD22	1.91	0.53
5:B:51:VAL:HG22	5:B:53:LEU:HD13	1.90	0.53
6:C:25:PRO:HG2	39:C:9126:HOH:O	2.08	0.53
1:O:1168:C:H5''	32:I:87:THR:CG2	2.38	0.53
27:Y:187:VAL:HG23	27:Y:192:ASP:CB	2.38	0.53
1:O:2456:A:H2'	1:O:2457:U:H6	1.73	0.53
1:O:2676:C:H6	1:O:2676:C:H5''	1.73	0.53
5:B:86:ALA:HA	39:B:9576:HOH:O	2.09	0.53
11:H:136:ALA:HB3	11:H:146:VAL:HG21	1.90	0.53
26:X:7:GLU:HA	26:X:74:ALA:O	2.09	0.53
1:O:951:A:C2'	1:O:952:G:H5'	2.38	0.53
4:A:203:GLY:HA2	39:A:9531:HOH:O	2.08	0.53
5:B:18:ARG:HE	5:B:256:GLN:NE2	2.06	0.53
12:J:103:VAL:HG12	39:J:5907:HOH:O	2.09	0.53
1:O:2320:U:H4'	1:O:2321:A:O4'	2.08	0.53
1:O:2912:C:H2'	1:O:2913:A:O4'	2.09	0.53
5:B:51:VAL:HG21	5:B:327:VAL:HG13	1.90	0.53
6:C:233:THR:HG22	6:C:234:VAL:N	2.23	0.53
14:L:80:ASP:CB	14:L:90:ARG:HB3	2.38	0.53
1:O:1501:A:OP2	18:P:37:ARG:HD2	2.08	0.53
22:T:89:ARG:HG3	22:T:89:ARG:O	2.09	0.53
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.08	0.53
1:O:1724:U:H5''	39:O:4320:HOH:O	2.08	0.53
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.48	0.53
5:B:141:ARG:HG2	5:B:165:ARG:HA	1.90	0.53
5:B:62:ARG:HA	5:B:65:MET:HE3	1.90	0.53
6:C:246:ARG:NH1	39:C:9176:HOH:O	2.40	0.53
11:H:45:VAL:HA	11:H:167:PRO:O	2.09	0.53
13:K:55:VAL:CG1	13:K:56:SER:N	2.72	0.53
18:P:103:THR:O	18:P:107:GLU:HG3	2.08	0.53
23:U:4:ARG:HH11	23:U:4:ARG:HG2	1.74	0.53
1:O:2419:U:H5''	1:O:2420:G:H5'	1.91	0.52
5:B:321:PRO:HA	39:B:9655:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:2548:C:OP2	5:B:5:ARG:NH2	2.41	0.52
24:V:56:ILE:HG22	24:V:60:GLN:NE2	2.24	0.52
1:O:564:G:H1'	39:O:6837:HOH:O	2.09	0.52
9:F:50:VAL:HG21	9:F:63:ILE:HG21	1.91	0.52
15:M:107:ARG:NH1	39:M:9383:HOH:O	2.42	0.52
1:O:248:A:H5'	1:O:249:G:OP2	2.10	0.52
6:C:47:GLY:HA2	6:C:92:PRO:HB2	1.90	0.52
10:G:64:ASN:N	10:G:64:ASN:HD22	2.05	0.52
32:I:93:GLN:HA	32:I:96:PHE:HE2	1.74	0.52
22:T:41:ARG:NH1	22:T:41:ARG:HG2	2.22	0.52
1:O:2508:C:H2'	39:O:7264:HOH:O	2.09	0.52
4:A:69:LEU:HD23	4:A:107:ASN:CB	2.40	0.52
7:D:136:ARG:HB3	7:D:137:PRO:HD2	1.90	0.52
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.09	0.52
20:R:18:LEU:HB2	20:R:143:VAL:HG13	1.91	0.52
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.70	0.52
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.33	0.52
1:O:121:U:OP2	30:2:10:ARG:NH2	2.38	0.52
1:O:848:C:H5'	39:O:7760:HOH:O	2.10	0.52
4:A:109:GLU:HG2	4:A:116:GLY:N	2.25	0.52
6:C:127:ARG:CZ	6:C:225:PRO:HG2	2.39	0.52
9:F:48:VAL:HG12	9:F:97:ALA:HB2	1.91	0.52
32:I:129:VAL:O	32:I:129:VAL:HG12	2.10	0.52
14:L:145:LEU:O	14:L:148:GLU:HG3	2.08	0.52
17:O:59:VAL:CG2	17:O:111:VAL:HG21	2.39	0.52
1:O:119:A:H2'	1:O:120:A:H5''	1.92	0.52
1:O:1234:U:N3	5:B:244:PRO:HB3	2.25	0.52
1:O:2541:U:O2	1:O:2618:G:N2	2.43	0.52
1:O:2816:A:H2'	39:O:8476:HOH:O	2.10	0.52
4:A:88:ILE:HG22	4:A:88:ILE:O	2.09	0.52
32:I:106:LYS:O	32:I:110:GLU:HG3	2.09	0.52
14:L:97:VAL:HG12	14:L:98:GLU:O	2.09	0.52
16:N:154:LEU:O	16:N:155:GLU:CB	2.58	0.52
16:N:162:ASP:HA	39:N:9331:HOH:O	2.10	0.52
1:O:1462:C:H2'	1:O:1463:A:C8	2.45	0.52
1:O:1527:A:H1'	1:O:1528:A:C8	2.45	0.52
4:A:179:MET:HA	4:A:179:MET:CE	2.39	0.52
14:L:91:VAL:CG1	14:L:120:LEU:HD23	2.39	0.52
22:T:69:LYS:O	22:T:71:VAL:HG23	2.10	0.52
1:O:1218:U:H2'	1:O:1219:U:H6	1.74	0.52
1:O:2896:A:H5''	39:X:5399:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:737:A:H2'	1:0:738:G:O4'	2.09	0.52
4:A:94:LEU:HB2	4:A:95:PRO:HD2	1.90	0.52
5:B:41:PHE:CD1	5:B:79:MET:HE2	2.45	0.52
12:J:80:LYS:NZ	39:J:7377:HOH:O	2.42	0.52
15:M:98:GLN:O	15:M:102:GLU:HG3	2.10	0.52
15:M:164:THR:HG22	15:M:165:GLY:N	2.23	0.52
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.08	0.52
21:S:33:SER:OG	21:S:36:GLU:HG3	2.10	0.52
24:V:8:ILE:HG21	24:V:59:ILE:HG13	1.91	0.52
25:W:38:THR:HG22	25:W:39:ASP:N	2.24	0.52
1:0:1211:G:O2'	1:0:1212:C:H5'	2.10	0.52
5:B:41:PHE:CD2	5:B:190:MET:HE3	2.45	0.52
1:0:2101:A:H2'	6:C:63:SER:OG	2.10	0.52
8:E:23:GLU:HG2	8:E:28:SER:HB3	1.91	0.52
1:0:1946:C:H2'	1:0:1971:G:C8	2.45	0.52
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.91	0.52
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.25	0.52
16:N:152:GLU:C	16:N:154:LEU:H	2.13	0.52
16:N:42:HIS:CE1	16:N:75:THR:HG1	2.28	0.52
17:O:97:SER:OG	17:O:100:GLN:HG3	2.10	0.52
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.92	0.52
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.10	0.52
1:0:1741:U:H3'	39:0:3369:HOH:O	2.09	0.51
15:M:99:ARG:NH2	15:M:170:ASN:HD22	2.00	0.51
6:C:163:HIS:HD2	39:C:9243:HOH:O	1.92	0.51
6:C:142:ASP:OD1	6:C:237:GLU:HB3	2.10	0.51
15:M:24:GLN:O	15:M:28:GLN:HG3	2.11	0.51
16:N:18:THR:HG21	39:N:9346:HOH:O	2.08	0.51
16:N:49:THR:HG22	16:N:56:ASP:CB	2.40	0.51
20:R:44:VAL:O	20:R:48:GLU:HG3	2.10	0.51
1:0:1477:C:H5'	1:0:1868:G:C5'	2.40	0.51
1:0:1835:U:C5	1:0:1840:A:N7	2.67	0.51
7:D:57:THR:HG23	7:D:63:ILE:CA	2.31	0.51
9:F:48:VAL:HG23	9:F:74:PHE:HB3	1.92	0.51
12:J:90:LYS:HB2	36:J:9302:CL:CL	2.46	0.51
15:M:15:PRO:HA	15:M:20:LEU:HD23	1.92	0.51
15:M:79:ALA:HB3	15:M:81:ARG:HH12	1.72	0.51
1:0:284:C:H4'	1:0:285:A:H8	1.74	0.51
1:0:776:A:OP1	29:1:28:HIS:HE1	1.92	0.51
4:A:36:ASP:O	4:A:38:ILE:N	2.42	0.51
7:D:23:VAL:CG2	7:D:73:VAL:HB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:110:GLN:HE21	25:W:110:GLN:HA	1.76	0.51
1:O:2032:U:H2'	1:O:2033:G:H5''	1.92	0.51
1:O:407:A:H5'	39:O:6556:HOH:O	2.10	0.51
39:O:8484:HOH:O	5:B:2:GLN:CG	2.53	0.51
6:C:115:LEU:O	6:C:118:THR:HB	2.10	0.51
1:O:1363:G:OP1	6:C:76:ARG:NH2	2.43	0.51
12:J:39:VAL:HG11	12:J:107:ASN:CG	2.30	0.51
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.92	0.51
6:C:118:THR:HG22	6:C:137:PRO:HB3	1.92	0.51
18:P:55:LYS:HG2	18:P:56:GLY:N	2.25	0.51
20:R:18:LEU:HG	20:R:91:LEU:HD13	1.92	0.51
1:O:2883:A:H2'	1:O:2884:G:O4'	2.11	0.51
5:B:62:ARG:HG2	5:B:65:MET:HE3	1.92	0.51
14:L:120:LEU:HD12	14:L:133:VAL:HG21	1.92	0.51
14:L:90:ARG:NH2	14:L:121:ILE:HD11	2.25	0.51
20:R:29:LYS:NZ	39:R:9449:HOH:O	2.44	0.51
1:O:1067:A:H5'	39:O:4922:HOH:O	2.10	0.51
1:O:1919:A:H4'	39:O:5416:HOH:O	2.10	0.51
1:O:2270:G:H4'	4:A:223:ARG:NH1	2.25	0.51
1:O:2443:C:H5'	14:L:57:VAL:HG21	1.93	0.51
1:O:2626:C:H2'	1:O:2627:G:C8	2.46	0.51
1:O:2717:C:H2'	1:O:2718:C:C5'	2.35	0.51
4:A:36:ASP:C	4:A:38:ILE:H	2.14	0.51
9:F:49:PHE:HE1	9:F:98:VAL:HG23	1.76	0.51
11:H:54:THR:O	11:H:55:VAL:HG13	2.11	0.51
16:N:86:LEU:HD21	16:N:180:LEU:HD12	1.92	0.51
1:O:1278:A:H4'	1:O:1279:U:C4	2.46	0.51
1:O:1966:U:H2'	1:O:1967:U:H2'	1.93	0.51
1:O:2524:G:H21	1:O:2526:C:N4	2.08	0.51
1:O:2711:U:H1'	39:O:4035:HOH:O	2.09	0.51
1:O:559:U:H2'	1:O:560:C:O4'	2.11	0.51
1:O:69:A:H5'	1:O:69:A:C8	2.45	0.51
8:E:11:VAL:HG12	8:E:12:ASP:N	2.26	0.51
19:Q:3:SER:HB3	39:Q:5998:HOH:O	2.11	0.51
22:T:40:VAL:HG22	22:T:41:ARG:N	2.26	0.51
1:O:1333:U:H2'	1:O:1334:C:C6	2.46	0.51
6:C:142:ASP:CG	6:C:237:GLU:HB3	2.31	0.51
9:F:58:GLU:HA	9:F:61:MET:HG3	1.93	0.51
13:K:7:ASP:OD2	13:K:81:ARG:NH2	2.44	0.51
1:O:2821:C:H4'	5:B:116:PRO:HG3	1.92	0.50
1:O:1853:C:OP1	4:A:231:LYS:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:41:PHE:CG	5:B:79:MET:HE2	2.46	0.50
8:E:7:ILE:HD11	8:E:11:VAL:C	2.32	0.50
12:J:54:VAL:HG11	12:J:138:THR:HG21	1.93	0.50
12:J:99:GLU:HA	39:J:7377:HOH:O	2.09	0.50
21:S:57:THR:CG2	21:S:58:MET:N	2.74	0.50
1:O:1165:G:H1'	1:O:1174:A:H1'	1.94	0.50
1:O:90:A:H2'	1:O:91:G:O4'	2.11	0.50
2:9:3008:G:O6	16:N:11:ARG:NH1	2.39	0.50
5:B:175:LEU:O	5:B:175:LEU:HD23	2.11	0.50
1:O:1363:G:P	6:C:76:ARG:HH22	2.35	0.50
9:F:26:THR:HG21	9:F:102:GLY:C	2.32	0.50
11:H:116:ALA:O	11:H:117:PHE:C	2.50	0.50
32:I:72:VAL:CG1	32:I:73:PRO:HD2	2.41	0.50
15:M:167:GLY:O	15:M:171:ARG:HG3	2.11	0.50
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.26	0.50
26:X:78:GLU:HG2	26:X:79:GLU:OE2	2.11	0.50
26:X:7:GLU:HA	26:X:75:ALA:HA	1.92	0.50
1:O:1198:U:H2'	1:O:1200:A:OP2	2.11	0.50
6:C:16:VAL:HG12	6:C:17:ASP:N	2.25	0.50
7:D:104:PHE:CE2	7:D:166:ILE:HD13	2.46	0.50
1:O:1120:U:H5''	1:O:1120:U:C6	2.46	0.50
1:O:926:A:O2'	14:L:41:HIS:HD2	1.94	0.50
31:3:35:TRP:HB2	39:3:9488:HOH:O	2.09	0.50
1:O:475:G:C5'	6:C:73:LEU:HD23	2.42	0.50
11:H:58:ARG:HG3	11:H:58:ARG:HH11	1.75	0.50
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.92	0.50
1:O:1118:A:C8	1:O:1118:A:C3'	2.89	0.50
1:O:2812:A:C2	1:O:2814:A:N6	2.68	0.50
1:O:362:G:H2'	1:O:363:A:C8	2.46	0.50
1:O:474:C:O3'	6:C:73:LEU:CD2	2.60	0.50
1:O:485:A:N3	1:O:487:G:H5''	2.26	0.50
5:B:310:ARG:HD2	39:B:9588:HOH:O	2.10	0.50
7:D:51:ARG:HD3	39:D:7636:HOH:O	2.11	0.50
23:U:9:CYS:O	23:U:52:THR:HG23	2.10	0.50
1:O:1592:G:O2'	1:O:1593:C:O4'	2.29	0.50
6:C:162:VAL:CG2	6:C:232:LEU:HD21	2.42	0.50
32:I:100:LEU:O	32:I:139:ILE:HG23	2.11	0.50
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.77	0.50
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.11	0.50
28:Z:42:CYS:SG	28:Z:43:GLY:N	2.85	0.50
1:O:1119:G:H8	12:J:52:GLN:NE2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1167:G:H2'	1:0:1168:C:O4'	2.11	0.50
1:0:1252:A:H2'	1:0:1253:C:O4'	2.12	0.50
1:0:1979:G:O2'	1:0:1980:U:OP1	2.30	0.50
1:0:482:G:H4'	1:0:508:A:N1	2.27	0.50
7:D:10:PHE:CE1	7:D:11:HIS:HB3	2.47	0.50
25:W:119:HIS:HD2	25:W:120:PRO:O	1.94	0.50
1:0:1972:U:H2'	1:0:1973:A:H5'	1.94	0.50
1:0:447:A:O2'	1:0:448:G:H5'	2.12	0.50
6:C:118:THR:CG2	6:C:137:PRO:HB3	2.41	0.50
8:E:154:ILE:HD11	8:E:157:LYS:HB2	1.92	0.50
12:J:76:ASP:HA	39:J:5907:HOH:O	2.11	0.50
39:K:7438:HOH:O	23:U:20:MET:HE1	2.11	0.50
1:0:1189:A:H1'	1:0:1209:C:C1'	2.41	0.50
1:0:2815:G:OP2	12:J:99:GLU:HG2	2.12	0.50
1:0:87:C:H2'	30:2:28:LYS:O	2.12	0.50
1:0:920:C:H5''	1:0:921:G:O5'	2.12	0.50
4:A:153:ARG:NH1	4:A:153:ARG:HB2	2.24	0.50
7:D:167:GLU:C	7:D:169:THR:H	2.14	0.50
11:H:3:ALA:CA	11:H:58:ARG:HH12	2.24	0.50
24:V:59:ILE:O	24:V:63:GLU:HG2	2.11	0.50
1:0:1132:A:N6	1:0:1229:C:H2'	2.27	0.49
1:0:1477:C:O2'	1:0:1478:U:H5'	2.12	0.49
1:0:1942:A:H3'	39:0:7828:HOH:O	2.12	0.49
2:9:3044:A:O4'	7:D:76:ARG:NE	2.44	0.49
4:A:65:ARG:C	4:A:66:ARG:HG3	2.32	0.49
5:B:314:ALA:HB3	5:B:317:PRO:HG3	1.93	0.49
7:D:41:LEU:HA	7:D:44:ILE:HG22	1.94	0.49
1:0:155:C:OP2	15:M:188:ARG:HD3	2.11	0.49
17:O:78:ALA:C	17:O:98:LEU:HD13	2.32	0.49
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.47	0.49
1:0:1119:G:N2	1:0:1246:A:N1	2.60	0.49
1:0:1159:G:H1	1:0:1208:C:H42	1.60	0.49
1:0:1921:A:O2'	1:0:1922:A:H5'	2.12	0.49
1:0:449:A:N7	6:C:43:LYS:HG2	2.26	0.49
2:9:3054:A:H2	39:9:3535:HOH:O	1.94	0.49
11:H:40:ALA:HB1	11:H:137:TYR:CE2	2.47	0.49
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.11	0.49
4:A:132:ASP:OD1	4:A:133:ARG:N	2.42	0.49
1:0:894:A:N1	6:C:87:ARG:NH2	2.61	0.49
11:H:73:LEU:HD21	11:H:146:VAL:HA	1.95	0.49
11:H:27:LYS:H	11:H:59:HIS:CD2	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1119:G:H8	12:J:52:GLN:HE22	1.59	0.49
16:N:183:ASP:O	16:N:184:ILE:O	2.30	0.49
1:0:317:A:OP1	22:T:52:ARG:O	2.30	0.49
1:0:1666:C:C2'	1:0:1667:A:C5'	2.91	0.49
1:0:292:G:H2'	1:0:358:G:N2	2.27	0.49
1:0:821:U:H2'	1:0:822:C:H6	1.77	0.49
5:B:49:THR:CG2	5:B:280:VAL:HG23	2.43	0.49
6:C:219:ASN:O	6:C:222:ASP:OD1	2.30	0.49
11:H:169:GLY:HA3	39:H:9553:HOH:O	2.11	0.49
27:Y:187:VAL:HG23	27:Y:192:ASP:HB3	1.93	0.49
1:0:2786:G:H2'	39:0:7679:HOH:O	2.12	0.49
4:A:131:HIS:O	4:A:132:ASP:HB2	2.11	0.49
32:I:74:PRO:C	32:I:112:LYS:HZ1	2.15	0.49
26:X:30:MET:HE1	26:X:58:ALA:CB	2.40	0.49
1:0:2453:G:H5''	39:L:9438:HOH:O	2.11	0.49
1:0:820:G:O2'	1:0:856:G:H4'	2.13	0.49
16:N:167:ASP:C	16:N:168:LEU:HG	2.33	0.49
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.77	0.49
1:0:1667:A:H2'	1:0:1668:U:C6	2.48	0.49
1:0:204:A:C2'	1:0:205:U:H5'	2.43	0.49
1:0:470:U:O2'	29:1:16:HIS:CD2	2.62	0.49
1:0:951:A:O2'	1:0:952:G:H5'	2.13	0.49
31:3:70:ARG:HB3	39:3:9504:HOH:O	2.13	0.49
4:A:223:ARG:CZ	39:A:9556:HOH:O	2.60	0.49
4:A:33:GLU:OE1	4:A:33:GLU:N	2.45	0.49
39:0:9730:HOH:O	5:B:229:ARG:HD2	2.13	0.49
8:E:49:ILE:HD11	8:E:69:ILE:HD12	1.94	0.49
32:I:116:LEU:HD22	32:I:127:GLU:OE1	2.12	0.49
25:W:115:THR:HB	39:W:6871:HOH:O	2.12	0.49
1:0:2090:G:H2'	1:0:2091:G:C8	2.47	0.49
5:B:113:LEU:HD21	5:B:161:VAL:HG21	1.95	0.49
6:C:107:ARG:HH11	6:C:107:ARG:CB	2.25	0.49
6:C:200:PRO:HB3	6:C:212:VAL:HG23	1.95	0.49
7:D:128:LEU:HB2	39:D:6007:HOH:O	2.13	0.49
20:R:39:THR:HB	20:R:42:GLU:CG	2.42	0.49
24:V:39:ALA:O	24:V:41:GLU:N	2.41	0.49
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.24	0.49
1:0:1878:G:O2'	1:0:1879:U:C6	2.62	0.49
1:0:2895:C:H4'	39:X:4132:HOH:O	2.13	0.49
1:0:299:U:H5'	39:0:7818:HOH:O	2.12	0.49
12:J:142:ASN:O	12:J:144:THR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.94	0.49
23:U:17:THR:CG2	23:U:18:GLY:H	2.25	0.49
23:U:52:THR:HG22	23:U:54:THR:H	1.76	0.49
1:O:2365:G:H5''	39:Q:6597:HOH:O	2.11	0.49
2:9:3028:U:H2'	2:9:3029:C:C6	2.47	0.49
5:B:81:ALA:O	5:B:186:GLY:HA3	2.12	0.49
9:F:14:ASP:O	9:F:18:GLU:HG3	2.12	0.49
1:O:2521:A:OP2	11:H:3:ALA:HB3	2.13	0.49
12:J:45:VAL:HG11	12:J:121:LEU:CD2	2.42	0.49
2:9:3004:G:H21	16:N:44:ARG:NH1	2.10	0.49
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.95	0.49
1:O:399:C:H5'	15:M:179:GLY:O	2.13	0.48
1:O:1654:U:H2'	4:A:47:HIS:HD2	1.76	0.48
7:D:35:ALA:O	7:D:38:GLU:HG3	2.13	0.48
13:K:125:ALA:C	13:K:127:ALA:H	2.15	0.48
1:O:392:U:H5''	15:M:193:LYS:HB3	1.95	0.48
7:D:146:LYS:NZ	16:N:107:ASN:ND2	2.61	0.48
16:N:37:ARG:NH2	16:N:105:GLY:HA3	2.27	0.48
17:O:41:ALA:HA	39:O:5104:HOH:O	2.12	0.48
18:P:16:VAL:HG13	18:P:20:ARG:NH1	2.28	0.48
24:V:29:ASN:O	24:V:33:VAL:HG23	2.13	0.48
25:W:52:VAL:HG22	25:W:53:ALA:N	2.27	0.48
1:O:1180:U:H2'	1:O:1181:A:C8	2.47	0.48
31:3:20:HIS:HA	31:3:70:ARG:O	2.13	0.48
7:D:57:THR:HA	39:D:5728:HOH:O	2.13	0.48
11:H:169:GLY:C	11:H:170:ASN:HD22	2.15	0.48
11:H:170:ASN:N	11:H:170:ASN:ND2	2.57	0.48
12:J:131:THR:HB	12:J:134:GLU:OE1	2.13	0.48
12:J:70:PHE:CG	12:J:70:PHE:O	2.65	0.48
24:V:64:GLY:O	24:V:65:ASP:CB	2.59	0.48
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.95	0.48
1:O:1056:U:H2'	1:O:1057:A:O4'	2.12	0.48
1:O:2507:G:H2'	1:O:2510:C:N4	2.28	0.48
1:O:541:C:H2'	1:O:542:A:H5'	1.94	0.48
1:O:1654:U:H2'	4:A:47:HIS:CD2	2.48	0.48
5:B:217:ARG:HG3	5:B:257:THR:HG22	1.94	0.48
15:M:187:LEU:HD23	15:M:194:ALA:HB3	1.94	0.48
16:N:1:ALA:HB3	39:N:9368:HOH:O	2.13	0.48
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.29	0.48
16:N:24:LEU:HD13	19:Q:26:PRO:HB3	1.94	0.48
27:Y:203:VAL:HG12	27:Y:228:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1299:G:H5'	39:0:4654:HOH:O	2.13	0.48
1:0:1745:G:H22	1:0:2033:G:H5'	1.78	0.48
1:0:2253:G:O2'	1:0:2254:G:H5'	2.14	0.48
1:0:2414:A:H2'	1:0:2415:A:C8	2.49	0.48
1:0:2649:A:H5'	1:0:2649:A:H8	1.78	0.48
1:0:2748:G:H4'	1:0:2749:U:C5'	2.43	0.48
1:0:475:G:OP1	6:C:73:LEU:HD22	2.13	0.48
21:S:33:SER:O	21:S:37:VAL:HG23	2.13	0.48
39:0:5842:HOH:O	25:W:122:ARG:NH2	2.47	0.48
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.48	0.48
1:0:1902:G:H2'	1:0:1903:U:O4'	2.14	0.48
1:0:603:A:H5''	1:0:604:G:OP1	2.12	0.48
4:A:179:MET:HG2	4:A:186:TRP:CB	2.44	0.48
9:F:11:ASP:O	9:F:14:ASP:HB2	2.14	0.48
32:I:131:THR:O	32:I:135:LEU:HG	2.13	0.48
22:T:71:VAL:CG1	22:T:72:ILE:N	2.76	0.48
25:W:122:ARG:NH2	39:W:5817:HOH:O	2.46	0.48
11:H:34:GLY:HA3	11:H:84:LYS:HA	1.94	0.48
15:M:57:LYS:HE2	15:M:140:ALA:O	2.13	0.48
15:M:99:ARG:HH21	15:M:170:ASN:ND2	2.02	0.48
17:O:59:VAL:HG21	17:O:111:VAL:HG21	1.95	0.48
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.14	0.48
1:0:558:C:C2'	1:0:559:U:C5'	2.92	0.48
31:3:6:ARG:NH1	31:3:21:GLU:HB2	2.28	0.48
2:9:3039:U:O2'	2:9:3042:C:C5	2.65	0.48
7:D:136:ARG:NH1	7:D:157:LEU:HA	2.27	0.48
8:E:84:MET:HE1	8:E:148:ILE:HD12	1.96	0.48
39:0:4952:HOH:O	15:M:83:SER:HB3	2.14	0.48
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.48	0.48
1:0:1203:G:O2'	1:0:1204:C:H5'	2.13	0.48
30:2:10:ARG:HD2	30:2:49:GLU:OE2	2.13	0.48
4:A:53:ALA:HB3	39:A:9587:HOH:O	2.14	0.48
11:H:146:VAL:HG22	39:H:9541:HOH:O	2.14	0.48
32:I:105:VAL:HG11	32:I:129:VAL:CG2	2.44	0.48
12:J:19:MET:HE2	12:J:79:PHE:HA	1.94	0.48
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.96	0.48
25:W:29:VAL:O	25:W:30:ASN:HB2	2.14	0.48
1:0:137:U:H2'	1:0:139:C:C5	2.48	0.48
1:0:2781:U:H1'	8:E:139:GLU:OE2	2.14	0.48
1:0:343:C:O2'	1:0:344:C:H5'	2.12	0.48
1:0:500:G:H21	20:R:98:ASN:HD21	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:932:U:H2'	1:0:933:C:C6	2.49	0.48
2:9:3057:A:C8	7:D:141:VAL:HG21	2.48	0.48
4:A:26:ASP:CG	4:A:26:ASP:O	2.53	0.48
16:N:36:ALA:HB1	16:N:118:ILE:HD12	1.95	0.48
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.94	0.48
22:T:71:VAL:HG13	22:T:91:LEU:O	2.13	0.48
25:W:149:LEU:HG	25:W:153:MET:CE	2.44	0.48
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.95	0.48
1:0:1130:U:H2'	1:0:1131:G:O4'	2.14	0.48
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.14	0.48
1:0:2681:A:H4'	1:0:2682:C:H5'	1.96	0.48
1:0:329:A:OP2	6:C:206:ASN:HB2	2.14	0.48
6:C:153:VAL:O	6:C:157:LEU:HG	2.14	0.48
6:C:61:PHE:HB3	39:C:9250:HOH:O	2.12	0.48
7:D:49:PRO:HA	7:D:73:VAL:HG22	1.96	0.48
32:I:113:HIS:N	32:I:114:PRO:CD	2.77	0.48
12:J:75:PRO:HB3	12:J:132:LEU:HB3	1.95	0.48
17:O:80:ASP:OD1	17:O:81:PHE:N	2.46	0.48
22:T:48:VAL:HG23	22:T:98:VAL:HA	1.96	0.48
25:W:139:GLY:O	25:W:141:HIS:HD2	1.95	0.48
25:W:88:THR:CG2	25:W:89:ASP:N	2.75	0.48
27:Y:117:LEU:HA	27:Y:174:VAL:HG11	1.96	0.48
1:0:2003:U:H4'	1:0:2004:U:C5	2.46	0.47
1:0:2748:G:C5'	39:0:8049:HOH:O	2.59	0.47
6:C:157:LEU:HD13	6:C:166:ILE:HD11	1.95	0.47
8:E:7:ILE:HD11	8:E:11:VAL:O	2.14	0.47
15:M:43:PRO:HG3	15:M:62:VAL:HG21	1.96	0.47
39:9:5851:HOH:O	16:N:115:VAL:HG13	2.13	0.47
27:Y:150:LEU:HB3	39:Y:9358:HOH:O	2.13	0.47
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.49	0.47
1:0:1118:A:C8	1:0:1119:G:H5''	2.48	0.47
1:0:1506:U:H6	1:0:1506:U:H5'	1.79	0.47
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.95	0.47
1:0:486:A:H1'	39:0:7288:HOH:O	2.13	0.47
1:0:757:C:OP1	14:L:27:ARG:HD2	2.13	0.47
2:9:3049:G:H5''	39:9:4707:HOH:O	2.14	0.47
4:A:70:ALA:HA	4:A:71:PRO:HD3	1.77	0.47
11:H:79:GLU:C	11:H:80:GLU:HG3	2.35	0.47
27:Y:122:ARG:NH2	39:Y:9335:HOH:O	2.48	0.47
1:0:1451:C:H5'	1:0:1505:U:C5	2.49	0.47
1:0:2072:G:H3'	1:0:2073:G:C5'	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2825:C:H4'	1:0:2826:G:O5'	2.14	0.47
2:9:3092:G:H2'	2:9:3093:A:C8	2.50	0.47
5:B:36:PRO:HB3	5:B:174:ARG:CB	2.44	0.47
6:C:127:ARG:HD3	6:C:129:HIS:HE1	1.80	0.47
10:G:27:ILE:HD13	10:G:71:LEU:HD23	1.97	0.47
17:O:14:LEU:HG	17:O:102:ILE:HD11	1.97	0.47
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.13	0.47
1:0:1755:A:H2'	1:0:1756:G:O4'	2.14	0.47
1:0:830:G:O2'	1:0:831:U:H5'	2.14	0.47
5:B:254:GLN:NE2	39:B:9589:HOH:O	2.46	0.47
8:E:101:GLU:HB2	8:E:116:THR:O	2.14	0.47
9:F:117:GLU:C	9:F:119:ARG:H	2.18	0.47
10:G:23:ILE:HD13	10:G:67:LEU:HD23	1.95	0.47
17:O:32:ARG:HB2	39:O:4656:HOH:O	2.13	0.47
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.52	0.47
1:0:1406:A:H4'	1:0:1407:A:C5'	2.44	0.47
1:0:2102:G:H5''	1:0:2538:A:C2	2.50	0.47
1:0:2908:A:H2'	1:0:2909:G:O4'	2.13	0.47
1:0:952:G:N3	1:0:2302:A:H2'	2.29	0.47
2:9:3058:G:H1'	39:D:3839:HOH:O	2.14	0.47
8:E:22:VAL:HG12	8:E:76:VAL:HG11	1.97	0.47
9:F:5:ASP:O	9:F:119:ARG:NH1	2.47	0.47
11:H:20:ILE:HG23	11:H:120:ILE:CD1	2.43	0.47
11:H:167:PRO:O	11:H:168:ALA:HB2	2.14	0.47
32:I:89:SER:CB	32:I:95:ASP:HB2	2.44	0.47
1:0:1525:G:H5'	1:0:1526:A:OP2	2.15	0.47
1:0:2032:U:C2'	1:0:2033:G:H5''	2.44	0.47
1:0:2852:A:H5''	39:O:5787:HOH:O	2.14	0.47
1:0:542:A:H2'	1:0:543:G:O4'	2.15	0.47
1:0:588:G:O6	25:W:154:ARG:NH1	2.48	0.47
5:B:24:PRO:HG3	5:B:204:GLY:HA2	1.95	0.47
5:B:162:MET:HE3	5:B:310:ARG:HD3	1.90	0.47
6:C:129:HIS:HE1	6:C:231:ARG:HA	1.78	0.47
6:C:242:GLU:HB2	39:C:9188:HOH:O	2.14	0.47
6:C:46:TYR:CE2	6:C:98:ARG:NH1	2.82	0.47
9:F:68:ASP:C	9:F:70:LYS:H	2.18	0.47
13:K:28:GLU:OE2	13:K:58:THR:HG21	2.15	0.47
18:P:13:VAL:HG11	18:P:40:VAL:CG1	2.45	0.47
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.21	0.47
1:0:1120:U:H6	1:0:1120:U:H5''	1.80	0.47
1:0:2509:A:H2'	1:0:2510:C:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:603:A:H4'	1:0:604:G:O5'	2.14	0.47
2:9:3042:C:H5'	2:9:3043:G:OP2	2.14	0.47
4:A:94:LEU:N	4:A:94:LEU:HD23	2.30	0.47
5:B:41:PHE:CG	5:B:190:MET:HE3	2.49	0.47
7:D:134:LEU:HD11	7:D:166:ILE:HD11	1.97	0.47
8:E:102:VAL:HG13	8:E:116:THR:HG23	1.95	0.47
8:E:1:PRO:HG2	8:E:59:MET:SD	2.54	0.47
9:F:101:ALA:HA	39:F:5413:HOH:O	2.15	0.47
9:F:36:THR:HG23	9:F:97:ALA:HB2	1.96	0.47
12:J:39:VAL:HG11	12:J:107:ASN:CB	2.44	0.47
12:J:130:VAL:HG12	12:J:131:THR:H	1.80	0.47
13:K:13:GLU:OE1	13:K:44:LEU:HD12	2.14	0.47
16:N:74:PRO:HG2	16:N:159:TYR:CE1	2.49	0.47
1:0:1007:A:H2'	11:H:19:TYR:CZ	2.49	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
1:0:2649:A:C8	1:0:2649:A:H5'	2.49	0.47
1:0:2819:C:O4'	5:B:96:PRO:HB2	2.14	0.47
1:0:87:C:C2	30:2:30:ASP:OD2	2.68	0.47
8:E:69:ILE:HA	8:E:72:MET:CE	2.44	0.47
1:0:645:U:OP2	14:L:4:LYS:HE2	2.13	0.47
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.96	0.47
20:R:9:ASP:O	20:R:13:THR:HB	2.14	0.47
1:0:1422:U:H2'	1:0:1423:C:C6	2.50	0.47
1:0:1603:A:H5''	1:0:1605:G:H5'	1.96	0.47
1:0:2644:C:O2'	1:0:2645:U:H5'	2.14	0.47
1:0:2837:U:H2'	39:0:7345:HOH:O	2.14	0.47
1:0:380:A:H4'	1:0:381:G:OP1	2.15	0.47
1:0:506:G:H22	1:0:509:A:H5'	1.75	0.47
1:0:870:G:OP2	4:A:3:ARG:HD3	2.15	0.47
1:0:894:A:C2	6:C:87:ARG:NH2	2.83	0.47
8:E:80:TRP:O	8:E:134:SER:HA	2.14	0.47
11:H:158:THR:HB	11:H:159:PRO:HD3	1.97	0.47
1:0:1181:A:N1	1:0:1192:A:O2'	2.46	0.47
1:0:1972:U:H2'	1:0:1973:A:C5'	2.45	0.47
1:0:2346:C:O5'	1:0:2346:C:H6	1.96	0.47
1:0:2712:G:H5'	39:K:4183:HOH:O	2.14	0.47
1:0:241:A:C2	1:0:378:A:H4'	2.50	0.47
1:0:1836:A:H1'	29:1:1:THR:O	2.14	0.47
5:B:190:MET:CE	5:B:194:PHE:CD1	2.98	0.47
9:F:28:ALA:CB	9:F:99:THR:HG23	2.45	0.47
14:L:35:ARG:HD3	14:L:35:ARG:C	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:69:TYR:CE2	16:N:184:ILE:HG13	2.48	0.47
1:0:1352:A:HO2'	1:0:1353:C:P	2.36	0.47
2:9:3091:C:H2'	2:9:3092:G:O4'	2.15	0.47
4:A:126:ALA:HB1	4:A:138:VAL:CG1	2.45	0.47
5:B:265:LEU:HD21	5:B:316:ARG:HD3	1.97	0.47
6:C:133:ARG:NE	6:C:138:VAL:HG22	2.30	0.47
7:D:99:ASP:O	7:D:159:PRO:HG3	2.14	0.47
12:J:80:LYS:HE2	12:J:98:PHE:CZ	2.50	0.47
14:L:61:ALA:HB2	14:L:105:TYR:CZ	2.50	0.47
15:M:66:SER:HB3	15:M:128:TRP:CD1	2.50	0.47
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.96	0.47
1:0:1201:C:C2'	1:0:1202:A:H5'	2.45	0.46
1:0:2252:A:H2'	1:0:2253:G:O4'	2.16	0.46
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.49	0.46
30:2:22:PRO:HG2	30:2:25:VAL:HG21	1.97	0.46
2:9:3039:U:HO2'	2:9:3042:C:H5	1.55	0.46
2:9:3048:C:H4'	16:N:141:ARG:HH21	1.80	0.46
5:B:14:GLY:HA2	5:B:15:PRO:C	2.35	0.46
9:F:99:THR:O	9:F:100:ASP:HB2	2.15	0.46
16:N:67:ALA:HA	16:N:71:TRP:HB3	1.97	0.46
17:O:73:ASP:HA	17:O:92:VAL:O	2.14	0.46
1:0:1242:A:OP2	12:J:60:ARG:NH2	2.45	0.46
1:0:1331:A:OP2	27:Y:142:SER:OG	2.32	0.46
1:0:2338:G:H2'	7:D:129:ASP:OD1	2.15	0.46
31:3:70:ARG:CG	31:3:77:ALA:HB2	2.42	0.46
2:9:3049:G:O2'	2:9:3050:G:H5'	2.14	0.46
4:A:72:GLU:HG3	28:Z:66:GLY:HA2	1.96	0.46
5:B:132:HIS:CE1	5:B:171:VAL:HG21	2.51	0.46
14:L:145:LEU:O	14:L:145:LEU:HD23	2.15	0.46
39:0:5295:HOH:O	16:N:21:HIS:HD2	1.97	0.46
39:0:4570:HOH:O	22:T:82:THR:HA	2.15	0.46
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.98	0.46
1:0:1095:U:O2	25:W:120:PRO:HG2	2.16	0.46
1:0:2748:G:H4'	1:0:2749:U:H5'	1.95	0.46
4:A:194:MET:CE	4:A:199:HIS:HB2	2.45	0.46
5:B:277:GLU:N	5:B:278:PRO:HD2	2.30	0.46
7:D:135:VAL:HG22	7:D:136:ARG:N	2.29	0.46
1:0:2346:C:H4'	7:D:52:THR:CG2	2.46	0.46
11:H:66:ARG:HD3	39:H:9544:HOH:O	2.14	0.46
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.47	0.46
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1053:G:OP1	11:H:12:PRO:HG3	2.15	0.46
1:O:1098:A:H2'	1:O:1099:G:O4'	2.15	0.46
1:O:1435:U:H5'	39:O:3209:HOH:O	2.14	0.46
1:O:1748:U:H4'	39:O:7993:HOH:O	2.14	0.46
1:O:2635:A:C2'	1:O:2636:C:H5'	2.45	0.46
1:O:407:A:H2'	1:O:408:A:C8	2.51	0.46
1:O:920:C:H4'	1:O:921:G:C2	2.51	0.46
39:O:6852:HOH:O	8:E:35:TYR:HB2	2.16	0.46
11:H:47:ILE:HD12	11:H:146:VAL:CG1	2.45	0.46
13:K:14:LYS:HG3	13:K:32:ILE:O	2.15	0.46
14:L:143:THR:CG2	14:L:144:ASP:N	2.76	0.46
1:O:709:G:O2'	17:O:25:VAL:CG1	2.61	0.46
17:O:47:ARG:HG3	17:O:47:ARG:HH11	1.80	0.46
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.81	0.46
27:Y:133:HIS:HD2	39:Y:9382:HOH:O	1.97	0.46
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.16	0.46
1:O:2906:A:H5'	1:O:2907:C:O4'	2.15	0.46
1:O:333:G:O2'	1:O:334:G:H5'	2.16	0.46
1:O:653:C:H2'	1:O:654:A:C8	2.51	0.46
2:9:3024:U:H3'	2:9:3025:G:H5'	1.97	0.46
5:B:81:ALA:HB1	5:B:142:LEU:HD13	1.97	0.46
7:D:36:ASN:HB3	39:D:1655:HOH:O	2.16	0.46
14:L:134:GLU:HG3	39:L:9453:HOH:O	2.15	0.46
14:L:89:PHE:CD1	14:L:89:PHE:N	2.83	0.46
25:W:88:THR:CG2	25:W:89:ASP:H	2.28	0.46
1:O:2044:G:OP1	26:X:23:HIS:HE1	1.98	0.46
1:O:2362:A:H2'	1:O:2363:G:C8	2.51	0.46
1:O:2415:A:O2'	16:N:29:SER:HB3	2.15	0.46
1:O:684:G:H2'	1:O:685:C:C6	2.51	0.46
7:D:173:GLU:HG3	7:D:174:VAL:N	2.30	0.46
8:E:35:TYR:HA	12:J:127:ILE:CD1	2.44	0.46
32:I:89:SER:HB3	32:I:97:VAL:CG2	2.46	0.46
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.49	0.46
20:R:114:VAL:HA	20:R:144:GLU:O	2.15	0.46
26:X:25:ARG:HD2	39:X:3861:HOH:O	2.16	0.46
27:Y:136:LYS:HE3	27:Y:138:ARG:NH1	2.30	0.46
1:O:1173:A:H4'	1:O:1174:A:C8	2.51	0.46
1:O:271:C:H41	1:O:378:A:H2	1.64	0.46
1:O:2784:A:H1'	8:E:60:SER:OG	2.15	0.46
1:O:2824:C:H5''	1:O:2825:C:H5'	1.98	0.46
1:O:40:C:H6	1:O:40:C:O5'	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:129:HIS:HD2	6:C:165:ASP:OD2	1.98	0.46
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.98	0.46
16:N:32:PRO:HD2	16:N:99:GLU:O	2.16	0.46
1:O:1342:C:O2'	1:O:1343:C:H5'	2.15	0.46
1:O:136:C:H2'	1:O:137:U:O4'	2.15	0.46
1:O:1786:C:OP1	18:P:74:GLN:HG2	2.16	0.46
1:O:2472:C:O2'	1:O:2634:G:H4'	2.15	0.46
1:O:2911:C:O2'	1:O:2912:C:H5'	2.16	0.46
1:O:899:C:H5'	39:O:3799:HOH:O	2.16	0.46
4:A:94:LEU:HD12	4:A:98:GLU:CB	2.43	0.46
5:B:80:ARG:HB2	5:B:145:HIS:CE1	2.51	0.46
39:O:6254:HOH:O	13:K:87:ARG:CZ	2.64	0.46
19:Q:64:GLU:HG3	19:Q:74:ASP:OD2	2.16	0.46
1:O:602:A:O2'	1:O:605:C:H4'	2.15	0.46
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.50	0.46
5:B:75:GLU:C	5:B:77:PRO:HD3	2.36	0.46
5:B:41:PHE:HA	5:B:79:MET:HE1	1.96	0.46
6:C:27:ARG:HG2	6:C:30:LEU:HG	1.97	0.46
1:O:2348:C:H1'	7:D:131:THR:HG21	1.98	0.46
8:E:85:GLU:HG3	8:E:169:THR:OG1	2.16	0.46
11:H:63:GLU:O	11:H:67:LEU:HB2	2.16	0.46
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.46	0.46
15:M:49:ALA:C	15:M:54:TYR:HB3	2.36	0.46
16:N:151:ASP:OD1	16:N:166:ALA:HA	2.16	0.46
16:N:86:LEU:O	16:N:90:LEU:HG	2.15	0.46
1:O:710:G:H5'	17:O:25:VAL:CG1	2.46	0.46
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.98	0.46
24:V:12:THR:HG23	24:V:14:ALA:N	2.31	0.46
24:V:1:THR:CG2	24:V:2:VAL:H	2.15	0.46
1:O:123:U:H1'	39:O:7856:HOH:O	2.16	0.46
1:O:834:G:H3'	1:O:835:U:H4'	1.98	0.46
29:1:56:GLU:HG2	29:1:56:GLU:OXT	2.16	0.46
4:A:217:ARG:CG	4:A:217:ARG:HH11	2.29	0.46
4:A:39:ALA:HB3	4:A:61:GLU:OE2	2.16	0.46
5:B:312:ARG:HD3	5:B:315:VAL:HG13	1.97	0.46
8:E:81:GLU:HA	8:E:133:VAL:O	2.15	0.46
32:I:113:HIS:HE1	32:I:121:LEU:HD22	1.81	0.46
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.51	0.46
14:L:1:THR:HB	14:L:6:ARG:NH1	2.31	0.46
25:W:21:LEU:HD22	25:W:26:ILE:HD13	1.96	0.46
1:O:1183:C:H5	1:O:1192:A:OP1	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1200:A:H3'	39:0:6295:HOH:O	2.16	0.45
1:0:1847:A:OP1	4:A:175:LYS:HG3	2.16	0.45
1:0:2064:U:H4'	1:0:2653:A:OP1	2.15	0.45
1:0:2679:G:H2'	1:0:2681:A:OP2	2.15	0.45
5:B:294:TYR:HE2	39:B:9647:HOH:O	1.99	0.45
5:B:265:LEU:CD2	5:B:316:ARG:HD3	2.46	0.45
11:H:78:GLY:C	11:H:80:GLU:H	2.20	0.45
14:L:129:ALA:O	14:L:133:VAL:HG23	2.16	0.45
1:0:392:U:C5'	15:M:193:LYS:HB3	2.46	0.45
16:N:23:ARG:NH1	16:N:23:ARG:HG2	2.31	0.45
16:N:86:LEU:HD12	16:N:125:ALA:HB2	1.98	0.45
22:T:38:ARG:HG3	22:T:38:ARG:HH11	1.81	0.45
1:0:121:U:O4	29:1:18:LYS:HG2	2.15	0.45
1:0:1503:U:H2'	1:0:1504:A:O4'	2.16	0.45
1:0:236:A:H8	1:0:236:A:OP1	1.99	0.45
1:0:288:A:H2'	1:0:289:G:C8	2.50	0.45
2:9:3050:G:H5''	16:N:159:TYR:HE1	1.81	0.45
9:F:48:VAL:CG2	9:F:74:PHE:HB3	2.46	0.45
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.51	0.45
17:O:59:VAL:CG2	17:O:111:VAL:CG2	2.94	0.45
20:R:132:ARG:CZ	39:R:9492:HOH:O	2.63	0.45
20:R:84:ALA:O	20:R:88:PHE:HD1	1.99	0.45
1:0:1025:C:H5'	25:W:23:MET:O	2.16	0.45
1:0:2356:A:H5'	39:0:6178:HOH:O	2.16	0.45
1:0:622:G:P	27:Y:148:GLY:HA3	2.56	0.45
1:0:968:G:H1'	11:H:32:LYS:HD2	1.98	0.45
7:D:64:ARG:NE	7:D:67:ASP:HB3	2.32	0.45
9:F:52:GLU:OE1	9:F:78:GLU:OE1	2.34	0.45
32:I:118:SER:HB2	32:I:123:ASN:HB2	1.98	0.45
32:I:72:VAL:HG13	32:I:73:PRO:HD2	1.98	0.45
12:J:63:ILE:HG22	12:J:64:GLY:N	2.30	0.45
15:M:74:LYS:HG3	15:M:75:ARG:N	2.31	0.45
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.63	0.45
25:W:11:VAL:O	25:W:12:ASN:HB2	2.16	0.45
1:0:259:G:H21	15:M:58:GLN:NE2	2.15	0.45
1:0:2748:G:H8	39:0:8049:HOH:O	2.00	0.45
1:0:2779:G:H21	8:E:143:GLN:HE22	1.64	0.45
6:C:84:VAL:HG12	6:C:85:LYS:HG2	1.97	0.45
7:D:10:PHE:CG	7:D:11:HIS:N	2.85	0.45
8:E:6:GLU:HA	8:E:46:THR:HG22	1.97	0.45
1:0:56:G:H5''	24:V:50:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:X:76:ARG:NH1	26:X:76:ARG:HG3	2.31	0.45
1:O:1335:C:OP2	27:Y:207:SER:HB3	2.16	0.45
1:O:157:G:H4'	15:M:95:LYS:HE2	1.98	0.45
1:O:1603:A:H5'	1:O:1605:G:C4'	2.46	0.45
1:O:2015:A:H2'	1:O:2016:U:O4'	2.17	0.45
1:O:810:G:H1'	39:O:7740:HOH:O	2.17	0.45
30:2:35:ARG:HB2	39:2:2691:HOH:O	2.16	0.45
2:9:3042:C:O2	7:D:76:ARG:NH1	2.48	0.45
2:9:3107:C:H5	39:9:3167:HOH:O	1.99	0.45
4:A:94:LEU:HG	4:A:99:ILE:HD11	1.97	0.45
11:H:28:ILE:HG23	39:H:9544:HOH:O	2.16	0.45
13:K:49:LEU:HD12	13:K:80:ILE:HD13	1.97	0.45
16:N:108:SER:HA	16:N:109:PRO:HD3	1.81	0.45
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.99	0.45
1:O:2421:G:H2'	39:O:4659:HOH:O	2.16	0.45
5:B:178:ALA:O	5:B:182:VAL:HG23	2.16	0.45
5:B:84:LEU:HB2	5:B:182:VAL:HG21	1.99	0.45
5:B:87:TYR:O	5:B:138:GLY:N	2.35	0.45
12:J:88:PRO:O	12:J:94:GLY:HA3	2.17	0.45
18:P:50:GLN:HG2	39:P:204:HOH:O	2.16	0.45
27:Y:212:ARG:HD2	39:Y:9402:HOH:O	2.16	0.45
1:O:2398:A:H2'	1:O:2399:G:O4'	2.16	0.45
1:O:88:G:N7	30:2:28:LYS:HD2	2.31	0.45
1:O:999:C:H2'	1:O:1000:C:O4'	2.17	0.45
4:A:123:GLY:HA2	4:A:159:VAL:O	2.17	0.45
5:B:243:ASN:HA	5:B:244:PRO:C	2.37	0.45
7:D:40:ILE:HG13	7:D:41:LEU:N	2.32	0.45
8:E:15:GLN:NE2	8:E:40:VAL:O	2.50	0.45
16:N:143:ARG:HE	16:N:143:ARG:HB3	1.56	0.45
21:S:11:THR:H	21:S:14:ALA:HB3	1.81	0.45
23:U:4:ARG:NH1	23:U:4:ARG:HG2	2.31	0.45
1:O:1151:G:OP1	10:G:63:ARG:NH1	2.50	0.45
1:O:1192:A:H3'	1:O:1193:A:H5'	1.99	0.45
1:O:1592:G:H2'	1:O:1593:C:C6	2.52	0.45
1:O:2809:G:H2'	1:O:2810:G:O4'	2.17	0.45
1:O:2857:C:H2'	1:O:2858:U:C6	2.52	0.45
1:O:328:U:O4'	6:C:202:THR:HG22	2.16	0.45
1:O:812:A:H2'	1:O:813:C:C6	2.51	0.45
29:1:18:LYS:HB2	30:2:49:GLU:CG	2.45	0.45
31:3:6:ARG:NH1	31:3:21:GLU:HG3	2.32	0.45
7:D:103:ASN:ND2	7:D:134:LEU:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:10:SER:O	14:L:11:ARG:HB3	2.17	0.45
14:L:144:ASP:O	14:L:147:GLU:HB2	2.17	0.45
14:L:72:ASN:HB2	39:L:9478:HOH:O	2.16	0.45
25:W:139:GLY:O	25:W:141:HIS:CD2	2.70	0.45
27:Y:148:GLY:O	27:Y:154:ARG:HD3	2.17	0.45
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.45
1:0:95:A:H5''	1:0:97:G:O4'	2.17	0.45
39:O:7282:HOH:O	16:N:4:PRO:HD2	2.17	0.45
1:0:793:A:H5''	18:P:83:LYS:HG2	1.99	0.45
20:R:114:VAL:HG13	20:R:114:VAL:O	2.17	0.45
22:T:20:HIS:HB3	22:T:41:ARG:HD2	1.98	0.45
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.82	0.45
1:0:1555:G:H4'	1:0:1630:A:C2	2.51	0.45
1:0:1667:A:C8	1:0:1667:A:H5'	2.42	0.45
1:0:1994:A:P	13:K:66:ARG:HH22	2.40	0.45
1:0:2699:A:H2'	1:0:2700:G:O4'	2.15	0.45
2:9:3054:A:O2'	2:9:3055:U:H5'	2.16	0.45
7:D:170:TYR:O	7:D:171:ASP:CB	2.65	0.45
32:I:99:ASP:O	32:I:100:LEU:HD23	2.17	0.45
24:V:51:LYS:O	24:V:55:ARG:HG3	2.17	0.45
27:Y:115:ARG:NE	39:Y:9356:HOH:O	2.50	0.45
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.18	0.44
1:0:1834:C:H2'	1:0:1840:A:N6	2.32	0.44
1:0:2568:A:H5''	1:0:2702:A:O2'	2.17	0.44
1:0:497:A:H2'	1:0:498:A:C5'	2.47	0.44
6:C:180:SER:HB2	39:C:9251:HOH:O	2.17	0.44
6:C:218:VAL:N	39:C:9229:HOH:O	2.50	0.44
6:C:142:ASP:OD1	6:C:236:THR:HG23	2.18	0.44
7:D:60:GLU:O	7:D:60:GLU:HG3	2.17	0.44
14:L:124:ASP:OD1	14:L:149:ARG:NH2	2.50	0.44
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.45	0.44
21:S:81:ILE:HG23	39:S:9494:HOH:O	2.17	0.44
1:0:2866:U:C4	23:U:50:GLU:HB3	2.52	0.44
25:W:122:ARG:HH22	25:W:154:ARG:HG2	1.79	0.44
1:0:2890:A:H1'	23:U:56:ARG:CZ	2.46	0.44
4:A:65:ARG:HH11	4:A:65:ARG:HG2	1.82	0.44
1:0:2545:U:OP2	5:B:2:GLN:NE2	2.50	0.44
11:H:29:ALA:C	11:H:30:GLN:HG3	2.37	0.44
15:M:22:GLU:HG2	15:M:26:GLN:NE2	2.32	0.44
18:P:16:VAL:HG13	18:P:20:ARG:CZ	2.47	0.44
22:T:49:GLU:OE2	22:T:51:LEU:HD21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:U:52:THR:CG2	23:U:54:THR:HB	2.47	0.44
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.99	0.44
1:0:366:U:H2'	1:0:367:G:O4'	2.17	0.44
1:0:415:A:O2'	1:0:416:G:H5'	2.18	0.44
1:0:629:A:H2'	1:0:630:A:O4'	2.17	0.44
6:C:168:ARG:NH2	6:C:190:ALA:O	2.50	0.44
9:F:60:VAL:O	9:F:60:VAL:CG1	2.64	0.44
14:L:134:GLU:HA	14:L:138:GLY:O	2.17	0.44
18:P:135:ALA:HB1	18:P:139:ARG:HH12	1.82	0.44
20:R:39:THR:HG22	20:R:41:GLY:H	1.83	0.44
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.81	0.44
39:0:6811:HOH:O	27:Y:158:LYS:HD3	2.18	0.44
4:A:101:GLU:OE2	4:A:131:HIS:HB2	2.18	0.44
4:A:69:LEU:HD23	4:A:107:ASN:CG	2.37	0.44
5:B:71:VAL:CG1	5:B:296:LEU:HD22	2.48	0.44
32:I:87:THR:HG22	32:I:88:GLY:N	2.32	0.44
13:K:65:ARG:NE	39:K:5358:HOH:O	2.46	0.44
1:0:1666:C:C2'	1:0:1667:A:H5''	2.47	0.44
1:0:1878:G:C1'	39:0:6649:HOH:O	2.60	0.44
1:0:2480:G:H3'	39:0:4764:HOH:O	2.16	0.44
1:0:338:C:H4'	6:C:174:ILE:HD11	1.99	0.44
1:0:40:C:H4'	39:0:7503:HOH:O	2.17	0.44
1:0:2101:A:OP2	6:C:66:GLY:HA2	2.18	0.44
15:M:187:LEU:HD22	15:M:194:ALA:HB3	1.99	0.44
22:T:52:ARG:O	22:T:53:GLY:O	2.35	0.44
1:0:1641:A:C2'	1:0:1642:A:H5'	2.46	0.44
1:0:236:A:H4'	1:0:237:G:H5'	2.00	0.44
1:0:2505:G:C2'	1:0:2506:A:H5'	2.48	0.44
1:0:2907:C:H2'	1:0:2908:A:O4'	2.17	0.44
30:2:20:ARG:HG3	30:2:21:VAL:N	2.33	0.44
2:9:3049:G:H2'	2:9:3050:G:O4'	2.18	0.44
4:A:207:GLN:O	4:A:208:HIS:HB3	2.17	0.44
5:B:5:ARG:HD2	5:B:8:LYS:NZ	2.33	0.44
13:K:109:LEU:HD13	13:K:113:ILE:CD1	2.45	0.44
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.37	0.44
16:N:152:GLU:HA	16:N:152:GLU:OE1	2.18	0.44
22:T:48:VAL:CG1	22:T:96:VAL:HG21	2.47	0.44
1:0:1086:A:C6	25:W:11:VAL:HG11	2.53	0.44
25:W:5:VAL:O	25:W:52:VAL:CG2	2.65	0.44
1:0:12:U:H2'	1:0:13:G:H5'	2.00	0.44
1:0:2506:A:O2'	1:0:2507:G:O5'	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:3:69:TYR:CZ	31:3:80:ARG:HD2	2.53	0.44
7:D:154:LYS:HD2	7:D:154:LYS:N	2.28	0.44
9:F:70:LYS:C	9:F:72:VAL:H	2.21	0.44
14:L:149:ARG:O	14:L:150:GLN:HB2	2.17	0.44
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.65	0.44
25:W:118:LEU:HD12	25:W:153:MET:HE3	1.99	0.44
1:0:2718:C:H5'	1:0:2718:C:C6	2.48	0.44
1:0:120:A:H5'	29:1:20:ARG:HH21	1.82	0.44
4:A:36:ASP:HA	4:A:83:GLY:HA3	1.99	0.44
8:E:23:GLU:HG2	8:E:28:SER:CB	2.47	0.44
11:H:3:ALA:CB	11:H:58:ARG:HH12	2.30	0.44
1:0:566:A:H2'	1:0:567:U:O4'	2.17	0.44
4:A:3:ARG:H	4:A:3:ARG:HG2	1.66	0.44
5:B:171:VAL:HG23	5:B:172:SER:N	2.33	0.44
5:B:56:ASP:HB3	5:B:322:ARG:HH21	1.83	0.44
6:C:107:ARG:NH1	39:C:9236:HOH:O	2.51	0.44
7:D:37:ALA:O	7:D:40:ILE:HG12	2.18	0.44
7:D:78:GLU:O	7:D:82:GLU:HG3	2.17	0.44
9:F:50:VAL:CG2	9:F:63:ILE:HG21	2.47	0.44
10:G:64:ASN:N	10:G:64:ASN:ND2	2.66	0.44
32:I:124:ALA:O	32:I:128:VAL:HG23	2.18	0.44
16:N:23:ARG:NH1	39:N:9346:HOH:O	2.51	0.44
16:N:72:GLU:HG2	16:N:72:GLU:O	2.17	0.44
1:0:1298:U:H2'	1:0:1299:G:C8	2.52	0.43
1:0:1314:U:H2'	39:0:6410:HOH:O	2.18	0.43
1:0:2541:U:O2'	3:4:76:DA:H4'	2.17	0.43
5:B:138:GLY:O	5:B:139:ASP:O	2.36	0.43
8:E:145:ALA:HB1	8:E:168:ILE:CD1	2.48	0.43
9:F:65:GLU:O	9:F:69:GLU:HG2	2.18	0.43
32:I:102:VAL:HG23	32:I:140:GLU:O	2.18	0.43
16:N:89:GLY:O	16:N:92:ALA:HB3	2.18	0.43
22:T:47:THR:HB	22:T:100:ASP:HB3	1.99	0.43
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.64	0.43
28:Z:13:ARG:NH1	39:Z:9218:HOH:O	2.51	0.43
1:0:2531:U:O2'	1:0:2532:A:H5'	2.17	0.43
5:B:234:ARG:HH11	5:B:234:ARG:HB3	1.83	0.43
12:J:132:LEU:HA	12:J:132:LEU:HD23	1.85	0.43
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.53	0.43
16:N:167:ASP:O	16:N:168:LEU:HG	2.17	0.43
23:U:20:MET:CG	23:U:28:THR:HG23	2.48	0.43
25:W:122:ARG:NH1	25:W:152:ALA:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:26:ILE:HG13	25:W:26:ILE:O	2.18	0.43
27:Y:187:VAL:CG2	27:Y:192:ASP:HB2	2.48	0.43
1:0:1180:U:H1'	39:0:3831:HOH:O	2.18	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.53	0.43
1:0:2415:A:H2'	1:0:2416:G:H5'	2.00	0.43
1:0:2720:C:O2	13:K:87:ARG:NH2	2.51	0.43
1:0:2807:U:P	5:B:27:ASN:HD21	2.40	0.43
5:B:139:ASP:HB3	39:B:9547:HOH:O	2.17	0.43
5:B:149:ASP:HB2	39:B:9577:HOH:O	2.18	0.43
5:B:41:PHE:HA	5:B:79:MET:CE	2.49	0.43
6:C:79:ARG:O	6:C:87:ARG:HG2	2.18	0.43
9:F:110:ASP:O	9:F:114:LYS:HG3	2.18	0.43
39:0:5535:HOH:O	11:H:58:ARG:HG3	2.18	0.43
1:0:2036:C:O4'	13:K:44:LEU:HG	2.18	0.43
14:L:145:LEU:C	14:L:145:LEU:HD23	2.38	0.43
16:N:116:PHE:HB3	16:N:136:LEU:HD23	2.00	0.43
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.17	0.43
22:T:79:LEU:HG	22:T:89:ARG:HB2	2.00	0.43
28:Z:72:GLU:HB3	28:Z:77:LYS:HE3	2.00	0.43
1:0:360:A:H2'	1:0:361:C:O4'	2.18	0.43
1:0:450:C:OP1	6:C:184:ARG:NH2	2.38	0.43
1:0:462:A:H2'	39:0:5450:HOH:O	2.17	0.43
1:0:635:A:H2'	1:0:636:G:H5''	2.00	0.43
7:D:25:MET:CE	7:D:41:LEU:HG	2.39	0.43
7:D:49:PRO:HB3	39:D:5828:HOH:O	2.19	0.43
1:0:2338:G:OP1	7:D:97:GLN:HG2	2.19	0.43
32:I:88:GLY:C	32:I:97:VAL:HG21	2.38	0.43
25:W:122:ARG:HG2	25:W:152:ALA:O	2.17	0.43
27:Y:184:GLU:HG2	27:Y:229:LEU:HD11	2.00	0.43
1:0:1741:U:O2'	1:0:2723:G:H4'	2.19	0.43
1:0:2589:U:H2'	1:0:2590:U:C6	2.53	0.43
1:0:2698:G:H2'	1:0:2699:A:C8	2.53	0.43
5:B:24:PRO:CG	5:B:204:GLY:HA2	2.48	0.43
1:0:2898:G:H4'	5:B:288:GLY:HA2	1.99	0.43
5:B:305:ASP:O	5:B:306:LYS:CB	2.66	0.43
5:B:73:VAL:HG22	5:B:296:LEU:CD2	2.48	0.43
7:D:25:MET:HE1	7:D:37:ALA:O	2.18	0.43
7:D:25:MET:CE	7:D:40:ILE:HD11	2.49	0.43
11:H:28:ILE:HA	11:H:63:GLU:OE1	2.18	0.43
13:K:115:ARG:HG3	13:K:116:GLU:N	2.32	0.43
14:L:143:THR:CG2	14:L:144:ASP:H	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:48:VAL:HG11	16:N:55:ASP:HB3	2.00	0.43
1:0:2663:U:O2	39:0:8476:HOH:O	2.20	0.43
1:0:2820:A:H2'	1:0:2821:C:C6	2.53	0.43
1:0:558:C:H2'	1:0:559:U:H5''	1.98	0.43
31:3:38:ARG:CB	31:3:42:ARG:HH12	2.31	0.43
31:3:38:ARG:HB3	31:3:42:ARG:HH12	1.84	0.43
2:9:3014:G:H2'	2:9:3015:C:H5'	2.01	0.43
2:9:3029:C:C2'	2:9:3030:C:H5'	2.48	0.43
4:A:17:ARG:HD2	39:A:9527:HOH:O	2.18	0.43
5:B:91:PRO:O	12:J:144:THR:HG21	2.18	0.43
14:L:133:VAL:HB	39:L:9453:HOH:O	2.19	0.43
14:L:150:GLN:HB3	39:L:9466:HOH:O	2.19	0.43
25:W:48:VAL:CG1	25:W:48:VAL:O	2.66	0.43
26:X:66:THR:HG22	26:X:67:PRO:O	2.18	0.43
1:0:2011:A:H4'	1:0:2012:U:O5'	2.19	0.43
1:0:2237:G:H1'	1:0:2238:A:C8	2.54	0.43
1:0:2353:A:H4'	1:0:2354:A:O5'	2.17	0.43
1:0:249:G:O2'	1:0:250:C:H5'	2.19	0.43
1:0:969:G:H1	1:0:999:C:N4	2.16	0.43
30:2:48:ASP:O	30:2:49:GLU:HB2	2.18	0.43
7:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.66	0.43
8:E:20:ILE:HD11	8:E:40:VAL:CG1	2.39	0.43
9:F:48:VAL:HG12	9:F:97:ALA:CB	2.47	0.43
32:I:139:ILE:CG2	32:I:140:GLU:N	2.82	0.43
13:K:49:LEU:HD12	13:K:80:ILE:HG21	2.00	0.43
18:P:37:ARG:HG2	18:P:37:ARG:HH11	1.84	0.43
24:V:8:ILE:CG2	24:V:59:ILE:HG13	2.48	0.43
1:0:2499:U:H2'	1:0:2500:C:H6	1.84	0.43
1:0:2587:OMU:H2'	1:0:2589:U:H5''	2.00	0.43
1:0:40:C:N3	1:0:441:A:H2	2.16	0.43
1:0:644:G:N3	1:0:644:G:H5'	2.34	0.43
1:0:681:G:N7	39:0:7461:HOH:O	2.36	0.43
1:0:941:G:C5	1:0:942:U:C4	3.07	0.43
4:A:164:ARG:CZ	39:A:9571:HOH:O	2.66	0.43
6:C:45:ASP:OD2	6:C:98:ARG:HD2	2.19	0.43
7:D:60:GLU:O	7:D:61:PHE:C	2.56	0.43
1:0:1992:U:OP2	13:K:66:ARG:HD2	2.18	0.43
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.99	0.43
24:V:8:ILE:HA	24:V:11:MET:HE2	2.00	0.43
25:W:5:VAL:O	25:W:52:VAL:HG23	2.19	0.43
1:0:1057:A:H2'	1:0:1058:A:C8	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1174:A:C5	1:0:1201:C:H4'	2.54	0.43
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.18	0.43
1:0:204:A:H2'	1:0:205:U:H5'	1.99	0.43
1:0:802:G:H2'	1:0:803:C:C6	2.54	0.43
3:4:74:C:H2'	3:4:75:C:H5'	2.01	0.43
4:A:26:ASP:OD2	4:A:28:GLU:HG3	2.18	0.43
5:B:119:HIS:O	5:B:121:PRO:HD3	2.19	0.43
6:C:151:GLN:O	6:C:154:VAL:HB	2.18	0.43
11:H:154:TYR:C	11:H:154:TYR:CD1	2.92	0.43
11:H:83:TYR:C	11:H:83:TYR:CD1	2.91	0.43
12:J:63:ILE:CG2	12:J:64:GLY:N	2.82	0.43
39:0:5842:HOH:O	25:W:119:HIS:CG	2.72	0.43
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.43
1:0:1160:G:HO2'	1:0:1190:G:H8	1.63	0.43
1:0:1236:A:C8	12:J:63:ILE:HD11	2.54	0.43
1:0:1477:C:H5'	1:0:1868:G:H5''	2.00	0.43
1:0:2697:A:H2'	1:0:2698:G:O4'	2.19	0.43
1:0:286:U:H2'	1:0:287:C:C6	2.54	0.43
2:9:3050:G:H5''	16:N:159:TYR:CE1	2.54	0.43
12:J:131:THR:HG22	12:J:133:GLY:N	2.34	0.43
16:N:71:TRP:HB2	39:N:9338:HOH:O	2.18	0.43
17:O:25:VAL:HG23	17:O:26:TRP:N	2.33	0.43
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.19	0.43
1:0:1299:G:N2	39:0:5248:HOH:O	2.51	0.42
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.19	0.42
1:0:2452:G:H5'	39:3:9488:HOH:O	2.17	0.42
1:0:364:C:H2'	1:0:365:G:O4'	2.19	0.42
6:C:185:LYS:HD3	6:C:186:TYR:CE1	2.54	0.42
13:K:49:LEU:HD22	13:K:117:VAL:CG2	2.49	0.42
15:M:61:ILE:N	15:M:61:ILE:HD12	2.33	0.42
20:R:132:ARG:NH2	39:R:9492:HOH:O	2.52	0.42
22:T:38:ARG:HG3	22:T:38:ARG:NH1	2.34	0.42
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.19	0.42
26:X:80:GLU:O	26:X:80:GLU:HG2	2.19	0.42
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.84	0.42
1:0:1351:G:OP1	6:C:96:LYS:NZ	2.41	0.42
1:0:396:U:OP2	31:3:38:ARG:HD2	2.18	0.42
1:0:526:U:H2'	1:0:527:U:C6	2.54	0.42
1:0:669:G:O2'	1:0:670:G:H5'	2.19	0.42
1:0:92:G:H4'	24:V:44:GLY:HA3	2.01	0.42
30:2:18:ASN:HD21	30:2:40:ARG:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3059:C:O5'	2:9:3059:C:H6	2.02	0.42
7:D:27:ILE:HG22	7:D:28:GLY:N	2.32	0.42
11:H:119:LYS:HB2	11:H:119:LYS:HE3	1.81	0.42
32:I:75:THR:HA	32:I:112:LYS:NZ	2.34	0.42
14:L:80:ASP:HB2	14:L:90:ARG:HB3	2.01	0.42
16:N:103:ASP:OD1	16:N:103:ASP:C	2.58	0.42
1:0:1200:A:H4'	39:0:7822:HOH:O	2.19	0.42
1:0:200:U:H2'	39:0:4038:HOH:O	2.18	0.42
1:0:2238:A:O2'	1:0:2239:C:H5'	2.18	0.42
1:0:2769:C:H2'	1:0:2770:G:C5'	2.48	0.42
30:2:20:ARG:HD2	30:2:39:ARG:NH2	2.34	0.42
5:B:42:ALA:H	5:B:79:MET:HE2	1.85	0.42
6:C:157:LEU:CD1	6:C:166:ILE:HD11	2.49	0.42
32:I:129:VAL:HG13	32:I:139:ILE:HD11	2.01	0.42
16:N:152:GLU:C	16:N:154:LEU:N	2.72	0.42
19:Q:11:ARG:HD3	39:Q:5620:HOH:O	2.18	0.42
19:Q:77:ASP:HB3	19:Q:82:LYS:HE3	2.01	0.42
24:V:42:ASN:O	24:V:44:GLY:N	2.52	0.42
1:0:2421:G:H4'	39:0:5345:HOH:O	2.18	0.42
1:0:2487:C:H5	39:0:5455:HOH:O	2.02	0.42
2:9:3064:C:C2'	2:9:3065:A:H5'	2.49	0.42
4:A:51:ARG:HH21	4:A:55:VAL:HG23	1.84	0.42
5:B:36:PRO:CA	5:B:168:GLY:HA3	2.44	0.42
6:C:218:VAL:HG12	39:C:9229:HOH:O	2.18	0.42
8:E:166:VAL:HG12	39:E:3134:HOH:O	2.18	0.42
12:J:39:VAL:CG1	12:J:40:ASN:N	2.82	0.42
1:0:2036:C:C1'	13:K:44:LEU:HG	2.50	0.42
14:L:77:ALA:C	14:L:79:ASP:H	2.23	0.42
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.49	0.42
27:Y:187:VAL:HB	27:Y:203:VAL:CG2	2.50	0.42
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.59	0.42
1:0:1821:A:O2'	1:0:1822:A:H5'	2.20	0.42
1:0:1477:C:C5'	1:0:1868:G:H5''	2.50	0.42
1:0:185:G:C4'	1:0:186:A:H4'	2.50	0.42
1:0:2900:G:H2'	1:0:2901:C:O4'	2.19	0.42
1:0:426:G:H2'	1:0:427:C:O4'	2.19	0.42
1:0:666:A:H2'	1:0:667:C:O4'	2.20	0.42
1:0:69:A:H5'	1:0:69:A:H8	1.85	0.42
1:0:889:C:H2'	1:0:890:C:C6	2.55	0.42
6:C:98:ARG:NH1	39:C:9163:HOH:O	2.51	0.42
9:F:79:GLN:HG3	9:F:82:ASP:OD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:I:92:PRO:C	32:I:94:GLU:N	2.70	0.42
14:L:79:ASP:O	14:L:80:ASP:O	2.37	0.42
20:R:69:LYS:HB2	20:R:72:VAL:HG23	2.00	0.42
24:V:8:ILE:HA	24:V:11:MET:CE	2.50	0.42
25:W:64:THR:O	25:W:68:THR:HG22	2.20	0.42
1:O:1044:C:H5''	39:O:9648:HOH:O	2.19	0.42
1:O:1099:G:H2'	1:O:1100:G:O4'	2.20	0.42
1:O:120:A:H2'	1:O:120:A:N3	2.35	0.42
1:O:23:G:C6	1:O:24:G:N1	2.88	0.42
1:O:2568:A:H2'	1:O:2569:A:O4'	2.20	0.42
30:2:35:ARG:HG2	39:2:6391:HOH:O	2.19	0.42
9:F:30:LYS:HE2	9:F:99:THR:HG21	2.01	0.42
13:K:115:ARG:HG2	13:K:116:GLU:OE1	2.19	0.42
13:K:27:ARG:HD2	39:K:4747:HOH:O	2.18	0.42
17:O:77:ALA:HA	17:O:96:VAL:O	2.20	0.42
27:Y:108:ASP:N	27:Y:108:ASP:OD1	2.49	0.42
1:O:1236:A:H2'	1:O:1237:U:O4'	2.19	0.42
1:O:1328:A:C8	27:Y:169:ARG:HD3	2.54	0.42
1:O:27:U:H2'	1:O:28:G:O4'	2.20	0.42
1:O:319:A:H4'	1:O:338:C:C5	2.54	0.42
1:O:371:U:H2'	1:O:372:A:C8	2.55	0.42
1:O:440:C:H2'	1:O:441:A:C8	2.55	0.42
1:O:697:G:H4'	1:O:730:G:O3'	2.19	0.42
1:O:960:G:N3	1:O:960:G:C2'	2.82	0.42
6:C:236:THR:HG22	6:C:239:ALA:HB2	2.01	0.42
32:I:80:LYS:HD3	32:I:86:GLU:O	2.20	0.42
15:M:82:ARG:O	15:M:84:LYS:N	2.52	0.42
16:N:24:LEU:HD22	39:Q:2847:HOH:O	2.19	0.42
25:W:125:HIS:HE1	39:W:3071:HOH:O	2.02	0.42
1:O:1168:C:H4'	39:I:5128:HOH:O	2.19	0.42
1:O:1289:C:H3'	39:O:6930:HOH:O	2.20	0.42
31:3:17:HIS:O	31:3:18:GLN:HG3	2.20	0.42
39:O:4983:HOH:O	4:A:11:ARG:CZ	2.68	0.42
6:C:136:VAL:HG22	6:C:137:PRO:HA	2.01	0.42
6:C:7:ASP:OD1	6:C:11:ASN:HB2	2.20	0.42
7:D:76:ARG:O	7:D:77:ASP:HB2	2.20	0.42
11:H:28:ILE:HG21	11:H:31:HIS:CE1	2.54	0.42
12:J:143:LYS:HG3	12:J:145:TRP:CE2	2.55	0.42
39:O:3171:HOH:O	25:W:119:HIS:HE1	2.03	0.42
26:X:54:ILE:HD11	26:X:85:VAL:HG12	2.02	0.42
27:Y:96:GLU:O	27:Y:235:GLU:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1081:A:H5''	39:0:3751:HOH:O	2.19	0.42
1:0:1131:G:C6	1:0:1230:A:C4	3.08	0.42
1:0:1878:G:O2'	1:0:1879:U:C5	2.66	0.42
1:0:2072:G:C6	1:0:2533:C:H1'	2.55	0.42
1:0:2133:U:H4'	1:0:2134:G:H5'	2.01	0.42
1:0:65:C:O2'	1:0:66:G:H5'	2.19	0.42
31:3:91:GLN:O	31:3:92:GLU:HB2	2.19	0.42
1:0:2820:A:OP1	5:B:98:THR:HG22	2.20	0.42
2:9:3014:G:C2'	16:N:1:ALA:HB2	2.50	0.42
19:Q:64:GLU:HG3	19:Q:74:ASP:CG	2.40	0.42
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.55	0.42
1:0:1181:A:H2'	1:0:1182:C:H5'	2.02	0.42
1:0:1714:C:O2'	1:0:1715:C:H5'	2.20	0.42
1:0:2329:C:O2'	1:0:2330:U:H5'	2.20	0.42
4:A:34:ASP:OD1	4:A:35:GLY:N	2.38	0.42
4:A:36:ASP:HB2	4:A:83:GLY:HA3	2.02	0.42
6:C:123:LEU:HD23	6:C:123:LEU:HA	1.83	0.42
6:C:165:ASP:O	6:C:168:ARG:HB3	2.20	0.42
12:J:19:MET:CE	12:J:132:LEU:HD21	2.48	0.42
14:L:69:ILE:HA	39:L:9478:HOH:O	2.20	0.42
2:9:3006:C:H4'	16:N:35:VAL:HG11	2.02	0.42
39:0:4845:HOH:O	19:Q:55:ARG:HD2	2.19	0.42
24:V:11:MET:HB3	24:V:15:GLU:HB2	2.00	0.42
25:W:41:TYR:CD2	25:W:44:MET:HE3	2.55	0.42
1:0:1495:C:H2'	1:0:1496:G:C8	2.54	0.41
1:0:2112:A:H2'	1:0:2113:G:C8	2.55	0.41
1:0:2587:OMU:H6	1:0:2587:OMU:O5'	2.20	0.41
1:0:2672:C:O2'	1:0:2673:U:H5'	2.20	0.41
1:0:2908:A:C2'	1:0:2909:G:H5'	2.49	0.41
29:1:10:LYS:N	39:1:9488:HOH:O	2.42	0.41
1:0:1311:G:O6	6:C:173:LYS:HE3	2.20	0.41
6:C:7:ASP:OD2	6:C:9:ASP:HB2	2.21	0.41
7:D:173:GLU:O	7:D:174:VAL:C	2.59	0.41
11:H:43:TYR:HA	11:H:44:PRO:HD3	1.78	0.41
1:0:1180:U:O2'	32:I:92:PRO:HD2	2.20	0.41
12:J:130:VAL:HG12	12:J:131:THR:N	2.35	0.41
17:O:45:LEU:CD1	17:O:88:LYS:HD2	2.50	0.41
19:Q:30:VAL:O	19:Q:30:VAL:HG12	2.19	0.41
19:Q:53:HIS:HA	19:Q:54:PRO:HD3	1.95	0.41
24:V:12:THR:HG23	24:V:14:ALA:H	1.84	0.41
25:W:122:ARG:CG	25:W:152:ALA:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:76:VAL:HG23	28:Z:63:LYS:HB3	2.01	0.41
1:0:1202:A:H2'	1:0:1203:G:O4'	2.20	0.41
2:9:3018:U:H2'	2:9:3019:G:H8	1.85	0.41
5:B:254:GLN:HG2	5:B:255:GLY:H	1.81	0.41
6:C:184:ARG:HB3	39:C:9169:HOH:O	2.19	0.41
8:E:91:PHE:HA	8:E:92:PRO:HD3	1.87	0.41
9:F:72:VAL:HA	9:F:73:PRO:HD3	1.90	0.41
11:H:40:ALA:HB1	11:H:137:TYR:CD2	2.55	0.41
11:H:26:SER:HA	11:H:59:HIS:CD2	2.55	0.41
11:H:70:ASN:O	11:H:74:ILE:HG13	2.20	0.41
13:K:75:ARG:HD3	13:K:112:PRO:O	2.21	0.41
22:T:21:LYS:HA	22:T:24:ARG:HG3	2.02	0.41
26:X:20:GLU:CD	26:X:21:PRO:HD2	2.40	0.41
1:0:2089:A:O2'	1:0:2090:G:H5'	2.19	0.41
1:0:517:U:H1'	39:0:8135:HOH:O	2.20	0.41
1:0:664:U:O4	1:0:681:G:H5''	2.20	0.41
1:0:764:C:H2'	1:0:765:G:O4'	2.20	0.41
30:2:5:LYS:O	30:2:9:LYS:HG3	2.20	0.41
1:0:2427:C:OP2	31:3:84:ARG:HD2	2.18	0.41
9:F:49:PHE:CD1	9:F:49:PHE:N	2.88	0.41
11:H:99:LYS:HD3	11:H:119:LYS:HD3	2.01	0.41
12:J:71:TYR:CG	12:J:72:PRO:HD2	2.55	0.41
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.49	0.41
17:O:87:THR:O	17:O:91:GLN:HG3	2.19	0.41
1:0:2388:C:H5'	19:Q:83:THR:O	2.20	0.41
25:W:65:VAL:CG1	25:W:116:LEU:HD13	2.50	0.41
1:0:2067:A:H2'	1:0:2068:G:O4'	2.20	0.41
1:0:2326:U:H4'	1:0:2412:G:C4'	2.50	0.41
1:0:1838:U:H1'	1:0:2644:C:O4'	2.21	0.41
1:0:559:U:H5'	1:0:559:U:C6	2.41	0.41
1:0:907:A:H2'	1:0:908:A:C8	2.55	0.41
1:0:2715:G:N2	5:B:264:GLU:OE1	2.53	0.41
2:9:3057:A:O2'	7:D:152:PRO:HD2	2.20	0.41
32:I:139:ILE:C	32:I:140:GLU:HG3	2.40	0.41
1:0:1164:U:OP1	32:I:74:PRO:HA	2.20	0.41
14:L:80:ASP:HB3	14:L:90:ARG:HB3	2.02	0.41
18:P:141:ILE:C	18:P:143:ALA:H	2.22	0.41
20:R:25:PHE:CE2	20:R:29:LYS:CE	2.99	0.41
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.48	0.41
1:0:1342:C:C2'	1:0:1343:C:H5'	2.50	0.41
1:0:1759:A:N3	1:0:1818:C:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2032:U:H2'	1:0:2033:G:H5'	2.01	0.41
1:0:612:U:H2'	1:0:613:C:C6	2.56	0.41
2:9:3052:A:O2'	2:9:3053:G:H5'	2.20	0.41
5:B:62:ARG:CB	5:B:65:MET:HE3	2.50	0.41
6:C:30:LEU:HA	6:C:30:LEU:HD23	1.90	0.41
32:I:75:THR:HA	32:I:112:LYS:HZ3	1.86	0.41
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.35	0.41
13:K:80:ILE:O	13:K:87:ARG:HA	2.20	0.41
1:0:926:A:H5'	14:L:39:GLU:OE2	2.20	0.41
16:N:37:ARG:CZ	16:N:105:GLY:HA3	2.51	0.41
1:0:1189:A:H1'	1:0:1209:C:H1'	2.02	0.41
1:0:710:G:H5'	17:O:25:VAL:HG13	2.03	0.41
1:0:821:U:H2'	1:0:822:C:C6	2.56	0.41
29:1:18:LYS:CB	30:2:49:GLU:HG2	2.47	0.41
4:A:135:VAL:HG21	4:A:147:ARG:HG2	2.02	0.41
4:A:66:ARG:CB	4:A:66:ARG:HH11	2.30	0.41
9:F:31:LYS:HE3	39:F:2623:HOH:O	2.20	0.41
32:I:132:CYS:C	32:I:134:SER:N	2.74	0.41
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.48	0.41
17:O:97:SER:H	17:O:100:GLN:NE2	2.18	0.41
20:R:106:GLY:HA2	20:R:109:MET:CE	2.46	0.41
26:X:9:VAL:HG13	26:X:88:GLU:OE1	2.21	0.41
1:0:2326:U:H4'	1:0:2412:G:H4'	2.03	0.41
1:0:816:G:H5'	1:0:1598:A:H4'	2.02	0.41
30:2:44:ARG:HA	30:2:44:ARG:HD3	1.78	0.41
5:B:146:THR:O	5:B:159:PRO:HB3	2.21	0.41
5:B:294:TYR:C	5:B:294:TYR:CD1	2.93	0.41
1:0:500:G:O2'	20:R:94:ASN:ND2	2.54	0.41
25:W:146:ILE:HA	25:W:146:ILE:HD13	1.88	0.41
1:0:1226:G:H5'	39:0:5101:HOH:O	2.20	0.41
1:0:1573:A:H2'	1:0:1574:C:O4'	2.21	0.41
1:0:1603:A:C5'	1:0:1605:G:H5'	2.50	0.41
1:0:2314:G:C2'	1:0:2315:C:H5'	2.51	0.41
1:0:565:A:OP2	1:0:592:G:N1	2.48	0.41
1:0:671:A:O2'	1:0:672:G:H2'	2.21	0.41
4:A:66:ARG:NH1	4:A:66:ARG:CB	2.84	0.41
5:B:150:ALA:O	5:B:152:PRO:HD3	2.21	0.41
9:F:28:ALA:HB3	9:F:99:THR:O	2.20	0.41
13:K:107:THR:HG22	13:K:108:GLU:CG	2.43	0.41
18:P:63:ARG:NH2	39:P:191:HOH:O	2.54	0.41
20:R:39:THR:CG2	20:R:107:GLU:O	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:75:GLU:O	22:T:76:ASP:HB2	2.21	0.41
27:Y:187:VAL:HB	27:Y:203:VAL:HG22	2.02	0.41
1:0:1132:A:H2'	1:0:1133:A:C8	2.56	0.41
1:0:123:U:O2'	1:0:124:C:H5'	2.20	0.41
1:0:1659:A:H2'	1:0:1660:G:O4'	2.19	0.41
1:0:1768:C:H2'	1:0:1769:C:O4'	2.20	0.41
1:0:177:A:H2'	1:0:178:U:O4'	2.21	0.41
1:0:1940:C:H4'	39:0:7828:HOH:O	2.19	0.41
1:0:2103:A:N3	1:0:2103:A:H2'	2.35	0.41
1:0:2481:G:H5''	39:0:5116:HOH:O	2.20	0.41
1:0:2578:G:H5'	1:0:2578:G:C8	2.45	0.41
1:0:1739:G:H1'	1:0:2726:U:O4	2.20	0.41
4:A:43:VAL:HG21	4:A:59:GLU:HG3	2.03	0.41
5:B:260:HIS:HE1	39:B:9585:HOH:O	2.03	0.41
5:B:271:ASP:HB3	5:B:296:LEU:HD12	2.03	0.41
5:B:277:GLU:N	5:B:278:PRO:CD	2.84	0.41
1:0:2717:C:H5'	5:B:302:PRO:HA	2.02	0.41
7:D:44:ILE:HG23	7:D:45:THR:HG23	2.03	0.41
1:0:1119:G:N2	1:0:1246:A:H2	2.09	0.41
1:0:1849:G:H1'	1:0:2011:A:N1	2.35	0.41
1:0:2053:G:H4'	20:R:136:TRP:CE2	2.56	0.41
1:0:2361:A:H2'	1:0:2362:A:C8	2.55	0.41
1:0:2435:U:H1'	39:0:5981:HOH:O	2.21	0.41
1:0:2503:A:OP1	11:H:151:ARG:NH2	2.49	0.41
1:0:750:A:O3'	6:C:101:ASP:HB2	2.21	0.41
1:0:887:G:H2'	1:0:888:U:C6	2.55	0.41
4:A:206:ARG:N	4:A:206:ARG:HD3	2.23	0.41
4:A:6:GLY:HA3	39:A:9550:HOH:O	2.20	0.41
5:B:49:THR:HG21	5:B:280:VAL:HG23	2.03	0.41
14:L:89:PHE:N	39:L:9468:HOH:O	2.54	0.41
39:0:8066:HOH:O	15:M:91:ILE:HG12	2.21	0.41
17:O:45:LEU:HD12	17:O:88:LYS:HD2	2.02	0.41
18:P:16:VAL:CG1	18:P:20:ARG:CZ	2.99	0.41
20:R:4:TYR:CZ	20:R:15:LYS:HB3	2.55	0.41
22:T:88:PRO:HB3	39:T:6320:HOH:O	2.20	0.41
23:U:44:ARG:HB3	39:U:3805:HOH:O	2.20	0.41
1:0:797:A:O4'	28:Z:10:ARG:N	2.54	0.41
28:Z:39:CYS:SG	28:Z:41:ASN:HB3	2.60	0.41
1:0:1065:G:H5'	39:0:4141:HOH:O	2.20	0.41
1:0:1166:A:H1'	1:0:1192:A:N3	2.36	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2061:C:C2'	1:0:2062:A:H5'	2.51	0.41
1:0:2506:A:O2'	1:0:2507:G:P	2.78	0.41
1:0:289:G:N1	1:0:363:A:C2	2.83	0.41
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.19	0.41
2:9:3095:C:O2'	2:9:3096:C:H5'	2.21	0.41
4:A:122:SER:O	4:A:124:VAL:HG13	2.21	0.41
7:D:105:SER:HA	7:D:130:VAL:O	2.21	0.41
7:D:12:GLU:O	7:D:15:GLU:HG2	2.21	0.41
8:E:5:LEU:HD21	8:E:66:GLN:HG3	2.03	0.41
15:M:73:ARG:HG3	39:M:9411:HOH:O	2.21	0.41
17:O:23:GLY:C	39:O:3062:HOH:O	2.59	0.41
17:O:26:TRP:HA	17:O:26:TRP:CE3	2.56	0.41
21:S:29:ASP:OD1	21:S:31:ARG:NH1	2.54	0.41
21:S:8:PRO:HD2	24:V:32:ALA:HA	2.04	0.41
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.21	0.41
27:Y:189:ASN:ND2	27:Y:189:ASN:C	2.73	0.41
1:0:1149:U:H5''	1:0:1151:G:O4'	2.21	0.40
1:0:2791:U:H1'	1:0:2792:A:H5''	2.03	0.40
1:0:2856:A:OP1	26:X:15:ARG:NH2	2.52	0.40
4:A:123:GLY:HA3	4:A:162:GLY:CA	2.49	0.40
5:B:217:ARG:HG3	5:B:257:THR:CG2	2.51	0.40
7:D:88:LEU:N	7:D:89:PRO:CD	2.84	0.40
9:F:32:GLY:N	39:F:3111:HOH:O	2.54	0.40
1:0:262:A:OP2	9:F:91:VAL:HG11	2.21	0.40
39:O:5961:HOH:O	14:L:34:GLY:HA2	2.20	0.40
17:O:98:LEU:O	17:O:102:ILE:HG13	2.21	0.40
24:V:39:ALA:C	24:V:41:GLU:N	2.71	0.40
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.21	0.40
4:A:164:ARG:HB2	28:Z:68:SER:OG	2.21	0.40
1:0:2793:A:H2'	1:0:2794:G:H5'	2.03	0.40
1:0:64:G:H2'	1:0:65:C:O4'	2.21	0.40
1:0:790:A:H1'	1:0:1710:A:H2'	2.03	0.40
1:0:920:C:H5'	1:0:921:G:C4	2.56	0.40
30:2:41:HIS:HD2	30:2:44:ARG:H	1.69	0.40
4:A:65:ARG:NH1	4:A:65:ARG:HG2	2.36	0.40
5:B:174:ARG:HA	5:B:177:HIS:HB3	2.02	0.40
5:B:85:ARG:HB2	5:B:99:GLU:HG2	2.03	0.40
6:C:5:ILE:HG13	6:C:15:GLU:HA	2.03	0.40
11:H:47:ILE:HD12	11:H:146:VAL:HG13	2.03	0.40
12:J:12:VAL:HG21	12:J:116:LEU:HD11	2.03	0.40
18:P:16:VAL:CG1	18:P:17:GLY:N	2.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:112:GLU:OE1	27:Y:112:GLU:HA	2.21	0.40
27:Y:216:ARG:HD2	39:Y:9370:HOH:O	2.20	0.40
28:Z:11:SER:O	28:Z:14:PHE:HB2	2.21	0.40
1:0:1937:U:O2'	1:0:1938:G:H5'	2.21	0.40
1:0:2361:A:H8	1:0:2361:A:H5'	1.86	0.40
1:0:2401:A:H2'	1:0:2402:A:C8	2.57	0.40
1:0:2379:G:N3	1:0:2418:G:H2'	2.36	0.40
1:0:2868:C:H2'	1:0:2869:G:O4'	2.22	0.40
1:0:484:A:N1	1:0:506:G:H4'	2.36	0.40
1:0:797:A:H5'	28:Z:10:ARG:N	2.36	0.40
31:3:70:ARG:HG2	31:3:70:ARG:HH11	1.86	0.40
6:C:194:PHE:CD2	6:C:234:VAL:CG1	3.01	0.40
6:C:234:VAL:HG13	6:C:234:VAL:O	2.21	0.40
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.03	0.40
15:M:183:THR:CG2	15:M:194:ALA:HB1	2.50	0.40
16:N:182:GLY:O	16:N:183:ASP:C	2.60	0.40
5:B:331:SER:OG	23:U:14:GLU:OE2	2.33	0.40
26:X:12:ILE:HD12	26:X:36:HIS:CG	2.56	0.40
1:0:2568:A:C2'	1:0:2569:A:H5'	2.51	0.40
1:0:2611:G:H5'	1:0:2613:G:C8	2.57	0.40
1:0:2754:G:H2'	1:0:2755:G:O4'	2.22	0.40
1:0:2780:C:H1'	8:E:143:GLN:NE2	2.33	0.40
1:0:295:C:H2'	1:0:296:G:O4'	2.21	0.40
1:0:297:U:H1'	39:0:4518:HOH:O	2.21	0.40
30:2:20:ARG:HD2	30:2:39:ARG:HH21	1.85	0.40
2:9:3012:C:H5'	2:9:3070:U:O4'	2.22	0.40
5:B:274:GLU:HA	5:B:292:GLY:O	2.21	0.40
7:D:36:ASN:HA	39:D:7500:HOH:O	2.22	0.40
9:F:79:GLN:HB2	9:F:82:ASP:OD2	2.22	0.40
11:H:69:ALA:HB2	11:H:153:ALA:HB2	2.04	0.40
11:H:77:LEU:HD12	11:H:83:TYR:CD2	2.57	0.40
23:U:52:THR:HG21	23:U:54:THR:HB	2.03	0.40
27:Y:152:LYS:HB3	27:Y:160:LYS:HG3	2.03	0.40
1:0:1185:U:H2'	1:0:1186:C:C6	2.56	0.40
1:0:1795:G:H2'	1:0:1796:A:O4'	2.22	0.40
1:0:1797:A:H2'	1:0:1799:G:O5'	2.21	0.40
1:0:1819:G:H2'	1:0:1820:G:C4'	2.51	0.40
1:0:1838:U:H1'	1:0:2644:C:H5'	2.04	0.40
1:0:2756:U:O2	1:0:2896:A:H2	2.05	0.40
1:0:622:G:O2'	1:0:623:U:H5'	2.20	0.40
4:A:149:ASP:OD1	4:A:151:GLN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:10:SER:O	5:B:16:ARG:NH1	2.52	0.40
6:C:72:LYS:HG2	6:C:77:ALA:HA	2.03	0.40
16:N:23:ARG:HD2	39:N:9357:HOH:O	2.20	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	209 (89%)	23 (10%)	3 (1%)	14	14
5	B	335/338 (99%)	314 (94%)	17 (5%)	4 (1%)	15	16
6	C	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
7	D	134/177 (76%)	105 (78%)	17 (13%)	12 (9%)	1	0
8	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
9	F	117/120 (98%)	100 (86%)	15 (13%)	2 (2%)	11	9
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	140 (90%)	14 (9%)	2 (1%)	14	14
12	J	140/145 (97%)	131 (94%)	6 (4%)	3 (2%)	8	6
13	K	130/132 (98%)	123 (95%)	7 (5%)	0	100	100
14	L	141/165 (86%)	118 (84%)	22 (16%)	1 (1%)	25	30
15	M	192/195 (98%)	182 (95%)	8 (4%)	2 (1%)	18	20
16	N	184/187 (98%)	163 (89%)	12 (6%)	9 (5%)	2	1
17	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
18	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	S	79/85 (93%)	76 (96%)	2 (2%)	1 (1%)	14	14
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	20	23
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	11	10
25	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
26	X	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	61 (86%)	7 (10%)	3 (4%)	3	1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	88 (98%)	1 (1%)	1 (1%)	17	18
32	I	68/162 (42%)	55 (81%)	12 (18%)	1 (2%)	12	11
All	All	3705/4431 (84%)	3430 (93%)	229 (6%)	46 (1%)	15	16

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	27	LEU
4	A	37	VAL
5	B	139	ASP
7	D	137	PRO
9	F	101	ALA
11	H	166	SER
11	H	168	ALA
14	L	80	ASP
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG
4	A	34	ASP
7	D	27	ILE
7	D	60	GLU
7	D	171	ASP
12	J	143	LYS
15	M	83	SER
16	N	162	ASP
16	N	183	ASP
22	T	53	GLY
24	V	43	PRO

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Mol	Chain	Res	Type
7	D	28	GLY
7	D	56	ARG
7	D	61	PHE
12	J	5	GLU
16	N	155	GLU
16	N	164	ASP
28	Z	20	ARG
31	3	56	PRO
5	B	185	GLY
7	D	97	GLN
7	D	164	ALA
9	F	71	GLY
12	J	65	ASN
16	N	68	GLU
16	N	167	ASP
32	I	76	ALA
5	B	34	GLY
7	D	138	GLY
21	S	46	ASP
5	B	182	VAL
7	D	69	ILE
28	Z	21	VAL
16	N	161	GLY
7	D	16	PRO
15	M	88	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%)	25	33
5	B	282/283 (100%)	261 (93%)	21 (7%)	16	20
6	C	193/193 (100%)	178 (92%)	15 (8%)	15	18
7	D	117/148 (79%)	112 (96%)	5 (4%)	33	45
8	E	152/156 (97%)	145 (95%)	7 (5%)	31	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	F	93/94 (99%)	91 (98%)	2 (2%)	57	74
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	32	44
12	J	118/121 (98%)	109 (92%)	9 (8%)	15	19
13	K	106/106 (100%)	103 (97%)	3 (3%)	49	65
14	L	113/127 (89%)	109 (96%)	4 (4%)	41	56
15	M	158/159 (99%)	153 (97%)	5 (3%)	44	60
16	N	149/150 (99%)	144 (97%)	5 (3%)	42	57
17	O	93/94 (99%)	91 (98%)	2 (2%)	57	74
18	P	113/117 (97%)	112 (99%)	1 (1%)	82	91
19	Q	79/80 (99%)	75 (95%)	4 (5%)	28	37
20	R	117/122 (96%)	114 (97%)	3 (3%)	51	69
21	S	71/74 (96%)	69 (97%)	2 (3%)	49	65
22	T	105/106 (99%)	101 (96%)	4 (4%)	38	52
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	60	77
25	W	130/130 (100%)	126 (97%)	4 (3%)	45	61
26	X	66/74 (89%)	60 (91%)	6 (9%)	11	13
27	Y	120/196 (61%)	110 (92%)	10 (8%)	13	16
28	Z	60/68 (88%)	59 (98%)	1 (2%)	66	81
29	1	46/47 (98%)	45 (98%)	1 (2%)	57	74
30	2	42/46 (91%)	41 (98%)	1 (2%)	54	72
31	3	79/79 (100%)	78 (99%)	1 (1%)	73	86
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2960 (96%)	133 (4%)	33	45

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	3	ARG
4	A	33	GLU
4	A	36	ASP
4	A	94	LEU
4	A	131	HIS

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Mol	Chain	Res	Type
4	A	153	ARG
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	51	VAL
5	B	53	LEU
5	B	71	VAL
5	B	82	VAL
5	B	98	THR
5	B	113	LEU
5	B	149	ASP
5	B	162	MET
5	B	175	LEU
5	B	190	MET
5	B	234	ARG
5	B	251	VAL
5	B	254	GLN
5	B	257	THR
5	B	265	LEU
5	B	277	GLU
5	B	280	VAL
5	B	307	ARG
5	B	312	ARG
6	C	2	GLN
6	C	27	ARG
6	C	76	ARG
6	C	91	PRO
6	C	94	THR
6	C	101	ASP
6	C	136	VAL
6	C	162	VAL
6	C	187	ARG
6	C	214	THR
6	C	222	ASP
6	C	223	LEU
6	C	236	THR
6	C	240	LEU
6	C	243	VAL
7	D	24	HIS

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Mol	Chain	Res	Type
7	D	50	VAL
7	D	61	PHE
7	D	133	ASN
7	D	137	PRO
8	E	3	VAL
8	E	7	ILE
8	E	102	VAL
8	E	108	LEU
8	E	155	ASN
8	E	156	ASP
8	E	164	ASP
9	F	12	LEU
9	F	46	GLU
11	H	1	LYS
11	H	18	GLU
11	H	84	LYS
11	H	88	ARG
11	H	154	TYR
11	H	170	ASN
12	J	45	VAL
12	J	52	GLN
12	J	70	PHE
12	J	74	ARG
12	J	79	PHE
12	J	107	ASN
12	J	117	ASP
12	J	127	ILE
12	J	131	THR
13	K	4	LEU
13	K	10	GLN
13	K	84	ASP
14	L	35	ARG
14	L	43	HIS
14	L	89	PHE
14	L	102	ASP
15	M	46	LEU
15	M	68	ARG
15	M	93	ARG
15	M	99	ARG
15	M	116	ASN
16	N	26	LEU
16	N	37	ARG

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Mol	Chain	Res	Type
16	N	49	THR
16	N	65	ASP
16	N	139	TRP
17	O	3	THR
17	O	96	VAL
18	P	98	ILE
19	Q	16	ASN
19	Q	18	PRO
19	Q	57	ASP
19	Q	95	GLU
20	R	13	THR
20	R	82	GLU
20	R	132	ARG
21	S	3	ASP
21	S	71	ASP
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
22	T	96	VAL
24	V	65	ASP
25	W	26	ILE
25	W	35	VAL
25	W	122	ARG
25	W	146	ILE
26	X	8	ARG
26	X	15	ARG
26	X	44	ASP
26	X	72	VAL
26	X	79	GLU
26	X	82	GLU
27	Y	103	THR
27	Y	141	THR
27	Y	144	ARG
27	Y	154	ARG
27	Y	163	THR
27	Y	189	ASN
27	Y	200	THR
27	Y	204	ARG
27	Y	220	GLU
27	Y	235	GLU
28	Z	44	GLU
29	1	47	ASP

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Mol	Chain	Res	Type
30	2	18	ASN
31	3	56	PRO

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	199	HIS
5	B	2	GLN
5	B	27	ASN
5	B	145	HIS
5	B	191	ASN
5	B	221	GLN
5	B	238	ASN
5	B	256	GLN
5	B	260	HIS
5	B	320	GLN
5	B	332	ASN
6	C	2	GLN
6	C	39	GLN
6	C	129	HIS
7	D	103	ASN
7	D	133	ASN
8	E	90	HIS
8	E	106	ASN
8	E	119	HIS
8	E	143	GLN
10	G	64	ASN
11	H	31	HIS
11	H	56	GLN
11	H	59	HIS
11	H	170	ASN
12	J	25	GLN
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	26	GLN

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Mol	Chain	Res	Type
15	M	58	GLN
15	M	77	HIS
15	M	137	ASN
15	M	143	ASN
15	M	170	ASN
16	N	93	GLN
16	N	107	ASN
16	N	153	GLN
17	O	53	GLN
17	O	100	GLN
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	53	ASN
22	T	37	GLN
22	T	39	ASN
22	T	73	HIS
23	U	39	ASN
23	U	48	ASN
24	V	60	GLN
25	W	12	ASN
25	W	28	HIS
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
26	X	22	ASN
26	X	23	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	189	ASN

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Mol	Chain	Res	Type
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	30	GLN
31	3	48	ASN
32	I	93	GLN
32	I	104	GLN
32	I	113	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	238 (8%)	0
2	9	121/122 (99%)	16 (13%)	0
3	4	1/5 (20%)	0	0
All	All	2867/3049 (94%)	254 (8%)	0

All (254) 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	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A

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Mol	Chain	Res	Type
1	0	192	A
1	0	219	G
1	0	237	G
1	0	249	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	498	A
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U

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Mol	Chain	Res	Type
1	0	735	C
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	875	A
1	0	877	G
1	0	878	G
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1137	G
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A

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Mol	Chain	Res	Type
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	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	1562	C
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	1722	U
1	0	1723	G
1	0	1725	C
1	0	1730	G
1	0	1731	C

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Mol	Chain	Res	Type
1	0	1732	A
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1873	G
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1967	U
1	0	1971	G
1	0	1973	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	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2291	A
1	0	2317	C
1	0	2321	A

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Mol	Chain	Res	Type
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2536	C
1	0	2537	G
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2611	G
1	0	2613	G
1	0	2634	G
1	0	2644	C
1	0	2645	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
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
1	0	2786	G
1	0	2792	A
1	0	2800	A

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Mol	Chain	Res	Type
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
1	0	2853	U
1	0	2867	G
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G
2	9	3044	A
2	9	3052	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C

There are no RNA pucker outliers to report.

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

5 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	OMU	0	2587	1	14,22,23	0.96	1 (7%)	18,31,34	3.70	2 (11%)
1	OMG	0	2588	1,3	18,26,27	1.05	2 (11%)	22,38,41	2.47	4 (18%)
1	UR3	0	2619	1	14,22,23	0.80	1 (7%)	16,32,35	0.69	0
1	PSU	0	2621	1	16,21,22	1.67	3 (18%)	20,30,33	6.08	5 (25%)
1	1MA	0	628	1,35	16,25,26	0.99	1 (6%)	13,37,40	1.15	1 (7%)

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	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.99	1.47	1.52
1	0	2619	UR3	C6-C5	-2.13	1.33	1.38
1	0	2588	OMG	C8-N7	-2.01	1.30	1.34
1	0	2587	OMU	C4-N3	2.53	1.37	1.33
1	0	2621	PSU	C2-N1	2.74	1.43	1.38
1	0	628	1MA	C6-N6	2.78	1.33	1.27
1	0	2621	PSU	C4-N3	2.89	1.38	1.33
1	0	2588	OMG	C6-N1	3.35	1.39	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-18.91	114.80	128.40
1	0	2621	PSU	C5-C4-N3	-13.14	114.65	125.43
1	0	2588	OMG	C5-C6-N1	-8.39	111.54	123.48
1	0	628	1MA	C2-N3-C4	-3.64	110.83	116.41
1	0	2587	OMU	C5-C4-N3	-3.54	114.66	123.12
1	0	2588	OMG	C2-N3-C4	-2.73	111.98	115.16
1	0	2588	OMG	N3-C2-N1	-2.33	124.06	127.46
1	0	2621	PSU	C5-C1'-C2'	-2.13	111.87	115.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-N1-C2	2.66	119.62	115.36
1	0	2588	OMG	C6-N1-C2	6.27	125.08	116.06
1	0	2621	PSU	C4-N3-C2	13.70	127.14	115.16
1	0	2587	OMU	C4-N3-C2	15.12	127.12	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 311 ligands modelled in this entry, 311 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	-0.07	92 (3%) 47 54	22, 45, 89, 149	0
2	9	122/122 (100%)	0.18	7 (5%) 24 31	38, 63, 87, 149	0
3	4	4/5 (80%)	1.55	1 (25%) 1 1	61, 64, 71, 74	0
4	A	237/240 (98%)	0.57	19 (8%) 13 17	28, 50, 82, 104	0
5	B	337/338 (99%)	0.29	13 (3%) 40 47	28, 50, 75, 86	0
6	C	246/246 (100%)	0.11	4 (1%) 72 77	25, 46, 68, 80	0
7	D	140/177 (79%)	2.14	63 (45%) 0 0	58, 88, 120, 130	0
8	E	172/178 (96%)	0.91	33 (19%) 1 2	40, 62, 80, 86	0
9	F	119/120 (99%)	1.37	34 (28%) 1 1	44, 71, 100, 110	0
10	G	29/348 (8%)	2.95	20 (68%) 0 0	71, 89, 99, 100	0
11	H	160/171 (93%)	0.85	28 (17%) 2 2	43, 61, 93, 101	0
12	J	142/145 (97%)	0.11	4 (2%) 53 61	36, 47, 67, 89	0
13	K	132/132 (100%)	0.01	2 (1%) 74 78	33, 46, 67, 72	0
14	L	145/165 (87%)	0.97	33 (22%) 1 1	27, 64, 110, 120	0
15	M	194/195 (99%)	0.62	20 (10%) 7 10	31, 44, 77, 87	0
16	N	186/187 (99%)	1.20	47 (25%) 1 1	43, 63, 108, 113	0
17	O	115/116 (99%)	0.17	3 (2%) 56 63	39, 53, 67, 75	0
18	P	143/149 (95%)	0.21	3 (2%) 64 70	38, 51, 65, 76	0
19	Q	95/96 (98%)	0.26	6 (6%) 21 27	38, 47, 61, 76	0
20	R	150/155 (96%)	0.03	3 (2%) 65 72	29, 43, 61, 71	0
21	S	81/85 (95%)	0.49	7 (8%) 11 16	42, 58, 80, 95	0
22	T	119/120 (99%)	0.70	9 (7%) 15 20	40, 54, 81, 110	0
23	U	53/66 (80%)	0.30	2 (3%) 41 48	40, 50, 68, 79	0
24	V	65/71 (91%)	1.94	21 (32%) 0 0	52, 76, 110, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	0.15	3 (1%) 67 73	37, 49, 69, 78	0
26	X	82/92 (89%)	0.89	11 (13%) 4 5	40, 53, 82, 101	0
27	Y	142/241 (58%)	0.30	10 (7%) 17 23	29, 42, 63, 85	0
28	Z	73/83 (87%)	0.92	16 (21%) 1 1	48, 70, 85, 92	0
29	1	56/57 (98%)	-0.30	0 100 100	26, 32, 39, 49	0
30	2	46/50 (92%)	0.62	5 (10%) 6 9	33, 51, 67, 80	0
31	3	92/92 (100%)	0.37	4 (4%) 36 43	33, 55, 70, 83	0
32	I	70/162 (43%)	6.27	66 (94%) 0 0	111, 123, 141, 143	0
All	All	6650/7480 (88%)	0.37	589 (8%) 10 14	22, 50, 95, 149	0

All (589) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	16.9
7	D	63	ILE	15.3
24	V	1	THR	14.7
32	I	133	THR	13.6
32	I	79	ILE	13.3
16	N	166	ALA	11.9
32	I	76	ALA	11.5
32	I	96	PHE	11.3
32	I	88	GLY	11.3
24	V	39	ALA	11.1
32	I	116	LEU	10.7
7	D	57	THR	10.6
24	V	40	PRO	10.5
32	I	105	VAL	10.5
32	I	118	SER	10.3
32	I	113	HIS	10.1
22	T	119	ALA	10.0
32	I	85	PHE	10.0
32	I	75	THR	9.6
32	I	87	THR	9.5
7	D	61	PHE	9.5
32	I	102	VAL	9.3
32	I	137	VAL	9.1
4	A	237	GLY	9.0
32	I	121	LEU	9.0
26	X	88	GLU	8.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
32	I	81	ASP	8.1
32	I	109	ALA	8.1
2	9	3001	U	8.1
32	I	108	ILE	8.0
32	I	93	GLN	8.0
32	I	129	VAL	7.9
32	I	132	CYS	7.9
4	A	37	VAL	7.8
15	M	70	GLY	7.7
32	I	104	GLN	7.6
32	I	125	ALA	7.6
7	D	90	LEU	7.4
32	I	77	GLU	7.4
30	2	49	GLU	7.4
1	0	1951	G	7.2
32	I	107	GLN	7.0
1	0	282	C	6.9
32	I	91	GLU	6.9
24	V	38	GLY	6.8
32	I	78	LEU	6.8
32	I	89	SER	6.7
32	I	111	GLN	6.6
10	G	23	ILE	6.6
28	Z	11	SER	6.4
1	0	1177	A	6.2
32	I	117	LEU	6.2
10	G	26	MET	6.1
32	I	114	PRO	6.1
32	I	97	VAL	6.1
32	I	74	PRO	6.1
15	M	79	ALA	6.1
22	T	118	SER	6.1
1	0	1199	A	6.0
7	D	170	TYR	5.8
15	M	74	LYS	5.8
32	I	86	GLU	5.7
32	I	103	ASP	5.7
2	9	3024	U	5.6
10	G	27	ILE	5.6
14	L	106	VAL	5.6
16	N	68	GLU	5.5
1	0	2637	A	5.4

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Mol	Chain	Res	Type	RSRZ
26	X	80	GLU	5.4
1	0	1172	G	5.3
1	0	285	A	5.3
9	F	16	ALA	5.3
32	I	126	LYS	5.2
32	I	98	ALA	5.2
30	2	35	ARG	5.2
1	0	960	G	5.1
8	E	45	ASP	5.1
1	0	1173	A	5.1
9	F	110	ASP	5.1
7	D	44	ILE	5.1
1	0	280	C	5.1
7	D	10	PHE	5.1
21	S	81	ILE	5.1
16	N	163	PHE	5.0
32	I	122	THR	5.0
1	0	10	U	5.0
1	0	2238	A	5.0
14	L	75	LEU	5.0
1	0	999	C	5.0
1	0	1948	G	5.0
14	L	97	VAL	4.9
16	N	175	LEU	4.9
9	F	119	ARG	4.9
32	I	123	ASN	4.9
7	D	69	ILE	4.9
24	V	37	GLY	4.8
1	0	514	G	4.8
7	D	64	ARG	4.8
4	A	35	GLY	4.8
28	Z	24	ARG	4.8
12	J	70	PHE	4.8
1	0	2004	U	4.7
2	9	3023	U	4.7
1	0	2748	G	4.7
32	I	83	ALA	4.7
32	I	106	LYS	4.7
10	G	71	LEU	4.7
32	I	120	ASP	4.7
8	E	87	PHE	4.7
7	D	62	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
7	D	92	GLU	4.6
32	I	124	ALA	4.6
32	I	138	THR	4.6
2	9	3002	U	4.6
1	0	272	A	4.6
1	0	2769	C	4.6
1	0	288	A	4.6
1	0	497	A	4.5
28	Z	20	ARG	4.5
32	I	115	ASP	4.5
12	J	4	ALA	4.5
1	0	1965	C	4.4
10	G	24	VAL	4.4
9	F	106	ALA	4.4
9	F	117	GLU	4.4
14	L	76	LEU	4.4
10	G	22	ALA	4.4
1	0	1200	A	4.4
1	0	970	U	4.4
1	0	2237	G	4.3
27	Y	235	GLU	4.3
16	N	161	GLY	4.3
7	D	11	HIS	4.3
6	C	61	PHE	4.3
8	E	6	GLU	4.3
11	H	111	ASP	4.3
7	D	73	VAL	4.2
14	L	91	VAL	4.2
1	0	1525	G	4.2
1	0	1202	A	4.2
32	I	136	GLY	4.2
28	Z	22	SER	4.2
31	3	92	GLU	4.1
7	D	66	GLY	4.1
9	F	22	VAL	4.1
14	L	145	LEU	4.1
24	V	36	ALA	4.1
4	A	133	ARG	4.1
16	N	165	ALA	4.1
7	D	166	ILE	4.1
9	F	28	ALA	4.1
11	H	171	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
26	X	85	VAL	4.1
24	V	41	GLU	4.1
10	G	66	LEU	4.1
16	N	147	ILE	4.0
1	0	1171	A	4.0
32	I	119	TYR	4.0
7	D	18	ILE	4.0
1	0	1950	G	4.0
19	Q	95	GLU	4.0
32	I	112	LYS	4.0
1	0	1198	U	4.0
16	N	184	ILE	3.9
11	H	34	GLY	3.9
7	D	173	GLU	3.9
23	U	47	ARG	3.9
7	D	107	GLY	3.9
7	D	93	LEU	3.9
1	0	2511	A	3.9
10	G	69	ARG	3.9
16	N	154	LEU	3.9
1	0	2508	C	3.9
22	T	116	ASP	3.9
27	Y	95	THR	3.8
7	D	51	ARG	3.8
16	N	155	GLU	3.8
7	D	40	ILE	3.8
7	D	172	VAL	3.8
11	H	146	VAL	3.8
32	I	80	LYS	3.8
32	I	135	LEU	3.8
11	H	37	GLN	3.8
32	I	95	ASP	3.8
8	E	86	VAL	3.8
26	X	10	VAL	3.8
28	Z	21	VAL	3.8
11	H	73	LEU	3.8
3	4	77	PHE	3.7
11	H	35	ARG	3.7
8	E	154	ILE	3.7
15	M	78	LYS	3.7
7	D	134	LEU	3.7
16	N	95	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
7	D	171	ASP	3.7
8	E	100	ASP	3.7
9	F	15	ASP	3.7
27	Y	108	ASP	3.6
7	D	26	GLY	3.6
11	H	74	ILE	3.6
14	L	60	GLU	3.6
4	A	99	ILE	3.6
17	O	22	GLY	3.6
9	F	107	ASP	3.6
32	I	110	GLU	3.6
7	D	104	PHE	3.6
22	T	112	LEU	3.6
10	G	21	ASP	3.6
24	V	8	ILE	3.6
16	N	180	LEU	3.6
32	I	72	VAL	3.6
10	G	70	ALA	3.5
32	I	127	GLU	3.5
22	T	82	THR	3.5
1	0	2747	C	3.5
9	F	25	ASP	3.5
32	I	90	GLY	3.5
10	G	12	ILE	3.5
11	H	143	ALA	3.5
16	N	172	PHE	3.5
7	D	88	LEU	3.5
10	G	67	LEU	3.5
14	L	80	ASP	3.5
4	A	38	ILE	3.5
9	F	118	LEU	3.5
2	9	3122	C	3.5
1	0	281	U	3.5
1	0	1169	U	3.5
9	F	99	THR	3.5
1	0	284	C	3.5
28	Z	25	ARG	3.5
7	D	91	ALA	3.4
11	H	47	ILE	3.4
4	A	36	ASP	3.4
7	D	167	GLU	3.4
9	F	49	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
8	E	43	ASP	3.4
9	F	108	VAL	3.4
1	0	283	U	3.4
26	X	7	GLU	3.4
32	I	94	GLU	3.4
14	L	99	GLU	3.4
4	A	97	ALA	3.3
24	V	59	ILE	3.3
8	E	4	GLU	3.3
32	I	99	ASP	3.3
4	A	31	LYS	3.3
8	E	160	ARG	3.3
32	I	134	SER	3.3
15	M	86	GLN	3.3
14	L	105	TYR	3.3
10	G	25	GLU	3.3
4	A	236	GLY	3.3
11	H	83	TYR	3.3
7	D	85	GLN	3.3
16	N	139	TRP	3.3
1	0	2645	U	3.3
8	E	10	ASP	3.3
16	N	181	ASP	3.3
7	D	23	VAL	3.3
26	X	71	ARG	3.3
1	0	1163	G	3.2
1	0	1168	C	3.2
4	A	85	SER	3.2
11	H	82	ASP	3.2
16	N	183	ASP	3.2
32	I	82	GLU	3.2
9	F	100	ASP	3.2
14	L	102	ASP	3.2
1	0	969	G	3.2
1	0	735	C	3.2
1	0	1000	C	3.2
1	0	1966	U	3.2
1	0	1967	U	3.2
1	0	1170	U	3.2
27	Y	236	VAL	3.2
24	V	43	PRO	3.2
32	I	84	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	0	716	G	3.1
14	L	130	ARG	3.1
7	D	81	GLU	3.1
22	T	115	GLU	3.1
19	Q	76	VAL	3.1
16	N	185	GLU	3.1
8	E	108	LEU	3.1
27	Y	234	VAL	3.1
24	V	63	GLU	3.1
11	H	138	CYS	3.1
5	B	1	PRO	3.1
5	B	57	GLU	3.0
11	H	78	GLY	3.0
16	N	71	TRP	3.0
1	0	279	C	3.0
1	0	295	C	3.0
14	L	100	ALA	3.0
1	0	2103	A	3.0
7	D	106	PHE	3.0
7	D	130	VAL	3.0
9	F	98	VAL	3.0
14	L	93	VAL	3.0
15	M	71	SER	3.0
9	F	103	GLU	3.0
21	S	20	PHE	3.0
28	Z	12	GLY	3.0
7	D	56	ARG	3.0
32	I	92	PRO	3.0
1	0	1947	G	3.0
8	E	128	GLY	3.0
16	N	152	GLU	3.0
1	0	138	U	3.0
15	M	84	LYS	3.0
1	0	370	G	2.9
16	N	178	THR	2.9
8	E	89	SER	2.9
1	0	358	G	2.9
7	D	27	ILE	2.9
13	K	132	VAL	2.9
27	Y	98	GLN	2.9
14	L	79	ASP	2.9
9	F	17	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	0	362	G	2.9
1	0	1178	G	2.9
6	C	132	ASP	2.9
16	N	72	GLU	2.9
16	N	158	LEU	2.9
16	N	145	ALA	2.9
10	G	73	ASP	2.9
1	0	1929	G	2.9
31	3	41	GLU	2.9
32	I	140	GLU	2.9
16	N	37	ARG	2.9
31	3	62	THR	2.9
21	S	2	TRP	2.9
15	M	75	ARG	2.9
25	W	86	GLU	2.8
1	0	1165	G	2.8
7	D	79	MET	2.8
16	N	159	TYR	2.8
25	W	76	ASP	2.8
10	G	15	TRP	2.8
14	L	121	ILE	2.8
14	L	104	ASP	2.8
27	Y	216	ARG	2.8
7	D	135	VAL	2.8
14	L	148	GLU	2.8
24	V	14	ALA	2.8
1	0	2344	G	2.8
28	Z	42	CYS	2.8
1	0	1189	A	2.8
8	E	127	ASP	2.8
15	M	89	THR	2.8
9	F	115	VAL	2.8
14	L	81	VAL	2.8
24	V	2	VAL	2.8
16	N	137	ALA	2.8
15	M	87	GLY	2.8
4	A	65	ARG	2.8
15	M	83	SER	2.8
1	0	1625	U	2.7
10	G	63	ARG	2.7
28	Z	36	ASP	2.7
7	D	35	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
7	D	84	LEU	2.7
8	E	88	TYR	2.7
19	Q	18	PRO	2.7
22	T	117	ASP	2.7
24	V	6	GLN	2.7
7	D	38	GLU	2.7
14	L	62	ALA	2.7
1	0	1180	U	2.7
24	V	10	ASP	2.7
8	E	5	LEU	2.7
16	N	149	GLU	2.7
27	Y	96	GLU	2.7
11	H	70	ASN	2.7
28	Z	45	ASP	2.7
1	0	1164	U	2.7
16	N	94	GLU	2.7
1	0	1181	A	2.7
10	G	68	GLU	2.6
32	I	139	ILE	2.6
8	E	94	GLN	2.6
14	L	147	GLU	2.6
16	N	177	GLU	2.6
9	F	19	ALA	2.6
14	L	61	ALA	2.6
26	X	73	ARG	2.6
1	0	372	A	2.6
8	E	161	VAL	2.6
26	X	77	PHE	2.6
7	D	17	ARG	2.6
5	B	183	GLU	2.6
7	D	165	PHE	2.6
16	N	160	SER	2.6
1	0	1195	G	2.6
1	0	1179	C	2.6
7	D	68	PRO	2.6
16	N	81	ALA	2.6
11	H	24	PRO	2.6
8	E	129	GLU	2.6
15	M	88	VAL	2.6
1	0	289	G	2.6
7	D	154	LYS	2.6
16	N	138	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
16	N	164	ASP	2.6
32	I	128	VAL	2.6
10	G	72	ASP	2.6
22	T	59	GLU	2.6
9	F	12	LEU	2.5
1	0	2345	A	2.5
15	M	76	ARG	2.5
11	H	67	LEU	2.5
15	M	77	HIS	2.5
1	0	1190	G	2.5
8	E	121	ASP	2.5
28	Z	19	GLY	2.5
16	N	67	ALA	2.5
8	E	15	GLN	2.5
4	A	64	ASP	2.5
15	M	73	ARG	2.5
1	0	1279	U	2.5
7	D	89	PRO	2.5
24	V	46	ILE	2.5
9	F	11	ASP	2.5
1	0	717	C	2.5
8	E	98	GLU	2.5
4	A	145	MET	2.4
1	0	1196	C	2.4
15	M	164	THR	2.4
1	0	1174	A	2.4
11	H	39	ASP	2.4
7	D	95	THR	2.4
14	L	150	GLN	2.4
16	N	156	GLU	2.4
21	S	70	GLU	2.4
7	D	41	LEU	2.4
16	N	179	LEU	2.4
20	R	104	PHE	2.4
24	V	33	VAL	2.4
16	N	134	ASP	2.4
14	L	120	LEU	2.4
1	0	369	G	2.4
5	B	134	ALA	2.4
7	D	160	ALA	2.4
11	H	168	ALA	2.4
15	M	80	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
30	2	39	ARG	2.4
1	0	1208	C	2.4
9	F	23	ALA	2.4
7	D	52	THR	2.4
10	G	65	THR	2.4
8	E	118	ILE	2.4
28	Z	18	TYR	2.4
9	F	24	ARG	2.4
30	2	44	ARG	2.3
7	D	54	ALA	2.3
11	H	79	GLU	2.3
1	0	1192	A	2.3
1	0	1981	A	2.3
19	Q	17	LYS	2.3
1	0	1197	G	2.3
2	9	3073	G	2.3
5	B	186	GLY	2.3
6	C	135	GLU	2.3
9	F	18	GLU	2.3
9	F	109	GLU	2.3
16	N	170	GLU	2.3
20	R	7	GLU	2.3
11	H	137	TYR	2.3
26	X	41	PHE	2.3
16	N	169	PRO	2.3
4	A	34	ASP	2.3
7	D	99	ASP	2.3
28	Z	31	SER	2.3
9	F	43	GLY	2.3
1	0	2239	C	2.3
24	V	45	ARG	2.3
9	F	101	ALA	2.3
12	J	5	GLU	2.3
8	E	42	VAL	2.3
9	F	21	GLU	2.3
1	0	1203	G	2.3
8	E	123	ASP	2.3
7	D	87	ALA	2.3
13	K	126	SER	2.3
22	T	35	TYR	2.3
8	E	99	GLY	2.3
11	H	141	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
19	Q	64	GLU	2.3
4	A	60	PHE	2.3
1	0	373	G	2.3
1	0	1175	G	2.3
7	D	157	LEU	2.2
28	Z	23	ARG	2.2
26	X	72	VAL	2.2
23	U	4	ARG	2.2
11	H	139	ASN	2.2
7	D	65	GLU	2.2
24	V	5	VAL	2.2
28	Z	32	GLU	2.2
1	0	1527	A	2.2
7	D	53	LYS	2.2
18	P	67	LYS	2.2
16	N	167	ASP	2.2
1	0	365	G	2.2
30	2	20	ARG	2.2
1	0	1964	U	2.2
9	F	113	ASP	2.2
11	H	149	ALA	2.2
14	L	82	ALA	2.2
16	N	148	ALA	2.2
1	0	1949	G	2.2
4	A	206	ARG	2.2
28	Z	80	ARG	2.2
32	I	73	PRO	2.2
18	P	16	VAL	2.2
5	B	104	GLU	2.2
6	C	237	GLU	2.2
14	L	144	ASP	2.2
8	E	169	THR	2.2
14	L	122	ALA	2.2
4	A	209	PRO	2.2
5	B	108	GLU	2.2
16	N	182	GLY	2.2
7	D	29	HIS	2.2
26	X	75	ALA	2.2
5	B	117	GLU	2.2
5	B	133	GLU	2.2
9	F	69	GLU	2.2
21	S	72	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	0	809	G	2.1
1	0	2507	G	2.1
31	3	6	ARG	2.1
14	L	141	GLU	2.1
1	0	290	C	2.1
5	B	180	ASP	2.1
7	D	58	VAL	2.1
9	F	60	VAL	2.1
14	L	96	VAL	2.1
27	Y	187	VAL	2.1
11	H	166	SER	2.1
17	O	1	SER	2.1
27	Y	102	LEU	2.1
7	D	25	MET	2.1
8	E	11	VAL	2.1
8	E	46	THR	2.1
9	F	26	THR	2.1
14	L	77	ALA	2.1
21	S	45	TYR	2.1
8	E	126	ILE	2.1
17	O	31	GLU	2.1
24	V	62	GLU	2.1
16	N	2	THR	2.1
11	H	45	VAL	2.1
11	H	140	VAL	2.1
16	N	73	ALA	2.1
14	L	44	GLU	2.1
7	D	74	THR	2.1
21	S	78	ALA	2.1
8	E	105	GLU	2.1
10	G	28	GLU	2.1
20	R	96	VAL	2.1
8	E	162	PHE	2.1
9	F	6	PHE	2.1
19	Q	81	GLU	2.0
7	D	67	ASP	2.0
14	L	95	ASP	2.0
14	L	123	ASP	2.0
8	E	7	ILE	2.0
15	M	82	ARG	2.0
25	W	93	ILE	2.0
1	0	804	C	2.0

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Mol	Chain	Res	Type	RSRZ
4	A	134	ASN	2.0
7	D	86	THR	2.0
5	B	2	GLN	2.0
5	B	176	ASP	2.0
15	M	81	ARG	2.0
11	H	77	LEU	2.0
16	N	106	LEU	2.0
24	V	42	ASN	2.0
16	N	65	ASP	2.0
5	B	182	VAL	2.0
18	P	18	LYS	2.0
7	D	78	GLU	2.0
2	9	3074	G	2.0
12	J	7	ASP	2.0
1	0	1522	A	2.0
15	M	68	ARG	2.0
16	N	92	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	1MA	0	628	23/24	0.98	0.14	-	31,33,36,39	0
1	OMU	0	2587	21/22	0.98	0.12	-	35,37,38,39	0
1	OMG	0	2588	24/25	0.97	0.12	-	32,34,38,40	0
1	PSU	0	2621	20/21	0.98	0.12	-	33,36,44,45	0
1	UR3	0	2619	21/22	0.98	0.14	-	42,46,49,51	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	0	9164	1/1	0.62	0.57	84.72	67,67,67,67	0
37	SR	0	9500	1/1	0.17	1.75	75.02	200,200,200,200	0
35	NA	0	9125	1/1	0.90	1.02	61.89	106,106,106,106	0
35	NA	0	9120	1/1	0.94	0.31	32.27	61,61,61,61	0
37	SR	B	9521	1/1	0.21	0.72	25.64	200,200,200,200	0
33	MG	0	8084	1/1	0.92	0.54	25.46	109,109,109,109	0
35	NA	0	9185	1/1	0.81	0.56	25.07	54,54,54,54	0
35	NA	0	9161	1/1	0.95	0.31	24.87	57,57,57,57	0
35	NA	0	9177	1/1	0.93	0.40	23.02	70,70,70,70	0
35	NA	0	9168	1/1	0.84	0.28	21.30	72,72,72,72	0
35	NA	0	9172	1/1	0.82	0.42	19.83	68,68,68,68	0
35	NA	0	9150	1/1	0.87	0.33	19.39	54,54,54,54	0
35	NA	0	9173	1/1	0.90	0.39	18.81	66,66,66,66	0
35	NA	0	9162	1/1	0.98	0.29	17.10	51,51,51,51	0
37	SR	0	9406	1/1	1.00	0.17	15.65	33,33,33,33	0
35	NA	0	9132	1/1	0.85	0.38	13.99	61,61,61,61	0
35	NA	0	9115	1/1	0.95	0.25	13.20	43,43,43,43	0
33	MG	0	8038	1/1	0.99	0.27	10.83	13,13,13,13	0
35	NA	0	9174	1/1	0.84	0.24	10.73	67,67,67,67	0
33	MG	0	8001	1/1	0.97	0.22	10.33	17,17,17,17	0
35	NA	0	9118	1/1	0.94	0.22	10.06	41,41,41,41	0
33	MG	0	8008	1/1	0.99	0.22	9.53	14,14,14,14	0
33	MG	0	8012	1/1	0.99	0.26	9.24	37,37,37,37	0
34	K	0	9001	1/1	0.87	0.49	8.97	95,95,95,95	0
33	MG	0	8013	1/1	0.85	0.38	8.90	16,16,16,16	0
35	NA	0	9171	1/1	0.52	0.24	7.00	63,63,63,63	0
37	SR	0	9482	1/1	0.94	0.19	6.31	118,118,118,118	0
35	NA	9	9183	1/1	0.82	0.23	6.11	72,72,72,72	0
35	NA	0	9156	1/1	0.97	0.20	5.87	55,55,55,55	0
33	MG	0	8057	1/1	0.88	0.41	5.73	79,79,79,79	0
33	MG	0	8017	1/1	0.98	0.18	5.50	20,20,20,20	0
33	MG	0	8097	1/1	0.94	0.20	4.91	55,55,55,55	0
33	MG	0	8080	1/1	0.92	0.24	4.79	48,48,48,48	0
35	NA	0	9127	1/1	0.94	0.19	4.35	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8107	1/1	0.82	0.22	3.32	68,68,68,68	0
35	NA	0	9159	1/1	0.93	0.17	2.78	56,56,56,56	0
33	MG	0	8027	1/1	0.95	0.19	2.77	30,30,30,30	0
37	SR	0	9515	1/1	0.99	0.18	2.40	100,100,100,100	0
37	SR	0	9475	1/1	0.97	0.14	2.30	77,77,77,77	0
33	MG	0	8020	1/1	0.97	0.19	2.19	30,30,30,30	0
35	NA	0	9165	1/1	0.94	0.21	1.50	41,41,41,41	0
37	SR	H	9486	1/1	0.96	0.18	1.45	121,121,121,121	0
35	NA	0	9117	1/1	0.99	0.16	1.35	32,32,32,32	0
37	SR	0	9407	1/1	0.98	0.14	1.34	42,42,42,42	0
35	NA	0	9105	1/1	0.98	0.15	1.26	41,41,41,41	0
33	MG	0	8074	1/1	0.99	0.21	1.20	20,20,20,20	0
37	SR	0	9410	1/1	1.00	0.15	1.16	34,34,34,34	0
33	MG	0	8054	1/1	0.80	0.13	1.14	58,58,58,58	0
36	CL	0	9316	1/1	0.93	0.17	1.12	74,74,74,74	0
33	MG	A	8066	1/1	0.96	0.18	1.02	53,53,53,53	0
35	NA	R	9186	1/1	0.92	0.15	0.99	64,64,64,64	0
33	MG	0	8056	1/1	0.98	0.18	0.96	47,47,47,47	0
36	CL	B	9319	1/1	0.92	0.16	0.91	59,59,59,59	0
35	NA	0	9178	1/1	0.91	0.15	0.81	54,54,54,54	0
34	K	0	9002	1/1	0.91	0.19	0.55	86,86,86,86	0
33	MG	0	8003	1/1	0.96	0.18	0.54	29,29,29,29	0
35	NA	0	9182	1/1	0.82	0.13	0.49	84,84,84,84	0
35	NA	0	9124	1/1	0.90	0.15	0.36	51,51,51,51	0
35	NA	C	9104	1/1	0.97	0.17	0.23	27,27,27,27	0
33	MG	0	8004	1/1	0.99	0.12	0.20	27,27,27,27	0
37	SR	1	9419	1/1	0.99	0.12	0.11	38,38,38,38	0
35	NA	0	9166	1/1	0.91	0.11	-0.12	65,65,65,65	0
33	MG	0	8096	1/1	0.97	0.13	-0.36	44,44,44,44	0
33	MG	0	8002	1/1	0.98	0.13	-0.38	22,22,22,22	0
35	NA	0	9139	1/1	0.96	0.13	-0.50	57,57,57,57	0
36	CL	M	9318	1/1	0.99	0.16	-0.53	37,37,37,37	0
37	SR	F	9595	1/1	0.97	0.14	-0.57	95,95,95,95	0
37	SR	A	9437	1/1	0.97	0.13	-0.57	64,64,64,64	0
35	NA	J	9146	1/1	0.83	0.13	-0.60	62,62,62,62	0
36	CL	J	9321	1/1	0.98	0.12	-0.67	58,58,58,58	0
37	SR	0	9490	1/1	0.96	0.12	-0.72	105,105,105,105	0
35	NA	0	9135	1/1	0.92	0.14	-0.77	46,46,46,46	0
37	SR	0	9509	1/1	0.97	0.12	-0.78	83,83,83,83	0
33	MG	0	8110	1/1	0.98	0.14	-0.82	46,46,46,46	0
37	SR	0	9424	1/1	0.99	0.15	-0.86	43,43,43,43	0
38	CD	U	9201	1/1	0.99	0.09	-0.98	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	R	9137	1/1	0.95	0.11	-1.00	32,32,32,32	0
37	SR	0	9534	1/1	0.96	0.11	-1.00	106,106,106,106	0
35	NA	Q	9148	1/1	0.98	0.13	-1.01	50,50,50,50	0
38	CD	Z	9203	1/1	0.99	0.07	-1.22	75,75,75,75	0
33	MG	T	8073	1/1	0.94	0.15	-1.24	42,42,42,42	0
33	MG	0	8015	1/1	0.96	0.10	-1.25	29,29,29,29	0
33	MG	0	8088	1/1	0.93	0.06	-1.36	43,43,43,43	0
35	NA	M	9147	1/1	0.98	0.10	-1.42	38,38,38,38	0
35	NA	R	9138	1/1	0.99	0.08	-1.50	52,52,52,52	0
37	SR	0	9451	1/1	0.99	0.09	-1.50	63,63,63,63	0
33	MG	0	8060	1/1	0.95	0.10	-1.55	81,81,81,81	0
37	SR	L	9409	1/1	1.00	0.12	-1.84	36,36,36,36	0
33	MG	0	8067	1/1	0.98	0.12	-1.88	36,36,36,36	0
37	SR	0	9457	1/1	0.99	0.09	-1.99	47,47,47,47	0
36	CL	0	9312	1/1	1.00	0.09	-2.08	45,45,45,45	0
37	SR	0	9442	1/1	0.98	0.11	-2.13	59,59,59,59	0
38	CD	3	9204	1/1	0.99	0.06	-2.15	58,58,58,58	0
33	MG	0	8032	1/1	0.89	0.11	-2.19	36,36,36,36	0
36	CL	3	9304	1/1	0.95	0.11	-2.20	59,59,59,59	0
36	CL	0	9315	1/1	0.96	0.10	-2.43	54,54,54,54	0
36	CL	O	9308	1/1	0.98	0.06	-2.45	67,67,67,67	0
35	NA	0	9131	1/1	0.96	0.11	-2.57	47,47,47,47	0
33	MG	Y	8109	1/1	0.98	0.10	-2.58	38,38,38,38	0
37	SR	0	9455	1/1	0.98	0.10	-2.68	61,61,61,61	0
37	SR	3	9439	1/1	0.99	0.06	-2.75	63,63,63,63	0
37	SR	A	9436	1/1	0.99	0.06	-2.83	57,57,57,57	0
37	SR	0	9468	1/1	0.70	0.05	-2.85	115,115,115,115	0
37	SR	0	9473	1/1	0.99	0.04	-3.12	69,69,69,69	0
37	SR	0	9506	1/1	0.96	0.07	-3.35	86,86,86,86	0
35	NA	0	9123	1/1	0.99	0.10	-3.36	37,37,37,37	0
35	NA	0	9143	1/1	0.97	0.07	-3.38	38,38,38,38	0
37	SR	0	9444	1/1	1.00	0.09	-3.46	47,47,47,47	0
37	SR	0	9453	1/1	0.98	0.09	-3.83	68,68,68,68	0
38	CD	1	9202	1/1	1.00	0.04	-3.86	51,51,51,51	0
33	MG	0	8044	1/1	0.99	0.06	-4.33	42,42,42,42	0
37	SR	0	9483	1/1	0.98	0.08	-4.37	67,67,67,67	0
37	SR	0	9498	1/1	0.99	0.06	-4.95	63,63,63,63	0
37	SR	0	9428	1/1	1.00	0.07	-4.99	43,43,43,43	0
36	CL	0	9305	1/1	0.98	0.07	-5.11	52,52,52,52	0
33	MG	0	8019	1/1	0.96	0.05	-5.22	53,53,53,53	0
37	SR	0	9532	1/1	0.99	0.05	-5.42	100,100,100,100	0
33	MG	0	8112	1/1	0.99	0.04	-5.59	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8039	1/1	0.96	0.04	-6.54	56,56,56,56	0
37	SR	0	9416	1/1	1.00	0.09	-7.63	45,45,45,45	0
37	SR	0	9456	1/1	0.98	0.06	-8.94	67,67,67,67	0
37	SR	9	9588	1/1	0.86	0.14	-	122,122,122,122	0
36	CL	0	9303	1/1	0.98	0.17	-	49,49,49,49	0
35	NA	0	9126	1/1	0.83	0.14	-	55,55,55,55	0
37	SR	0	9422	1/1	0.99	0.12	-	53,53,53,53	0
33	MG	0	8075	1/1	0.93	0.06	-	37,37,37,37	0
37	SR	0	9425	1/1	0.99	0.09	-	71,71,71,71	0
33	MG	0	8021	1/1	0.87	0.24	-	51,51,51,51	0
37	SR	0	9495	1/1	0.95	0.11	-	88,88,88,88	0
33	MG	K	8069	1/1	0.99	0.21	-	23,23,23,23	0
35	NA	0	9141	1/1	0.87	0.12	-	61,61,61,61	0
35	NA	0	9158	1/1	0.95	0.10	-	62,62,62,62	0
35	NA	0	9130	1/1	0.96	0.09	-	45,45,45,45	0
33	MG	0	8050	1/1	0.71	0.24	-	94,94,94,94	0
35	NA	0	9170	1/1	0.90	0.32	-	75,75,75,75	0
37	SR	0	9423	1/1	0.99	0.10	-	51,51,51,51	0
33	MG	0	8108	1/1	0.39	0.28	-	115,115,115,115	0
35	NA	0	9154	1/1	0.92	0.20	-	51,51,51,51	0
36	CL	R	9306	1/1	0.99	0.16	-	46,46,46,46	0
37	SR	0	9508	1/1	0.99	0.08	-	83,83,83,83	0
35	NA	0	9106	1/1	0.96	0.19	-	37,37,37,37	0
33	MG	0	8029	1/1	0.98	0.22	-	27,27,27,27	0
37	SR	0	9474	1/1	0.96	0.09	-	96,96,96,96	0
37	SR	0	9415	1/1	1.00	0.11	-	50,50,50,50	0
33	MG	0	8030	1/1	0.93	0.04	-	34,34,34,34	0
35	NA	0	9129	1/1	-0.07	0.43	-	88,88,88,88	0
37	SR	0	9529	1/1	0.90	0.10	-	116,116,116,116	0
37	SR	0	9449	1/1	0.99	0.09	-	59,59,59,59	0
37	SR	0	9478	1/1	0.98	0.07	-	70,70,70,70	0
33	MG	0	8059	1/1	0.77	0.27	-	60,60,60,60	0
33	MG	0	8022	1/1	0.73	0.55	-	113,113,113,113	0
37	SR	0	9420	1/1	0.99	0.15	-	60,60,60,60	0
33	MG	0	8058	1/1	0.92	0.47	-	85,85,85,85	0
37	SR	0	9501	1/1	0.50	0.33	-	200,200,200,200	0
37	SR	0	9488	1/1	0.98	0.13	-	78,78,78,78	0
33	MG	0	8061	1/1	0.63	0.13	-	81,81,81,81	0
37	SR	0	9505	1/1	0.93	0.14	-	104,104,104,104	0
37	SR	0	9570	1/1	0.97	0.07	-	96,96,96,96	0
37	SR	0	9452	1/1	0.89	0.19	-	114,114,114,114	0
35	NA	0	9175	1/1	0.93	0.19	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9629	1/1	0.97	0.10	-	69,69,69,69	0
37	SR	0	9440	1/1	0.99	0.04	-	63,63,63,63	0
37	SR	0	9443	1/1	0.99	0.10	-	59,59,59,59	0
35	NA	0	9140	1/1	0.86	0.34	-	61,61,61,61	0
37	SR	0	9484	1/1	0.29	0.16	-	150,150,150,150	0
37	SR	0	9626	1/1	0.95	0.30	-	140,140,140,140	0
36	CL	0	9317	1/1	0.99	0.08	-	49,49,49,49	0
37	SR	0	9480	1/1	0.99	0.06	-	86,86,86,86	0
35	NA	0	9111	1/1	0.77	0.21	-	57,57,57,57	0
35	NA	0	9136	1/1	0.97	0.11	-	31,31,31,31	0
35	NA	0	9102	1/1	0.95	0.20	-	58,58,58,58	0
37	SR	0	9568	1/1	0.98	0.08	-	75,75,75,75	0
37	SR	0	9601	1/1	0.06	1.54	-	200,200,200,200	0
33	MG	0	8106	1/1	0.99	0.03	-	37,37,37,37	0
33	MG	0	8052	1/1	0.62	0.30	-	72,72,72,72	0
38	CD	O	9205	1/1	0.95	0.05	-	85,85,85,85	0
33	MG	0	8041	1/1	0.94	0.12	-	47,47,47,47	0
35	NA	0	9134	1/1	0.95	0.07	-	47,47,47,47	0
33	MG	0	8045	1/1	0.94	0.22	-	75,75,75,75	0
35	NA	0	9113	1/1	0.80	0.15	-	64,64,64,64	0
35	NA	0	9110	1/1	0.85	0.20	-	49,49,49,49	0
35	NA	D	9151	1/1	0.91	0.12	-	63,63,63,63	0
37	SR	0	9445	1/1	0.99	0.10	-	62,62,62,62	0
37	SR	0	9426	1/1	0.98	0.08	-	66,66,66,66	0
37	SR	0	9461	1/1	0.99	0.04	-	73,73,73,73	0
37	SR	0	9405	1/1	0.97	0.14	-	54,54,54,54	0
37	SR	0	9414	1/1	0.98	0.12	-	53,53,53,53	0
37	SR	0	9448	1/1	0.98	0.07	-	62,62,62,62	0
36	CL	0	9311	1/1	0.97	0.09	-	56,56,56,56	0
37	SR	0	9408	1/1	0.99	0.15	-	38,38,38,38	0
33	MG	0	8065	1/1	0.87	0.32	-	92,92,92,92	0
33	MG	0	8063	1/1	0.96	0.07	-	74,74,74,74	0
33	MG	0	8068	1/1	0.98	0.14	-	47,47,47,47	0
35	NA	0	9116	1/1	0.97	0.27	-	45,45,45,45	0
35	NA	0	9108	1/1	0.96	0.12	-	34,34,34,34	0
33	MG	0	8070	1/1	0.99	0.18	-	21,21,21,21	0
33	MG	0	8089	1/1	0.94	0.12	-	61,61,61,61	0
37	SR	R	9418	1/1	0.99	0.15	-	53,53,53,53	0
37	SR	0	9438	1/1	0.98	0.09	-	63,63,63,63	0
36	CL	L	9310	1/1	0.96	0.09	-	56,56,56,56	0
35	NA	0	9114	1/1	0.97	0.19	-	51,51,51,51	0
33	MG	0	8046	1/1	0.96	0.08	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	CL	J	9301	1/1	0.96	0.09	-	55,55,55,55	0
33	MG	0	8036	1/1	0.96	0.09	-	63,63,63,63	0
37	SR	0	9462	1/1	0.99	0.12	-	66,66,66,66	0
37	SR	0	9447	1/1	0.96	0.10	-	66,66,66,66	0
33	MG	0	8072	1/1	0.95	0.25	-	74,74,74,74	0
33	MG	0	8090	1/1	0.87	0.25	-	81,81,81,81	0
37	SR	0	9466	1/1	0.96	0.04	-	87,87,87,87	0
33	MG	0	8079	1/1	0.97	0.14	-	30,30,30,30	0
33	MG	0	8031	1/1	0.98	0.13	-	48,48,48,48	0
37	SR	0	9467	1/1	0.97	0.10	-	74,74,74,74	0
37	SR	0	9450	1/1	0.99	0.08	-	64,64,64,64	0
37	SR	0	9517	1/1	0.97	0.06	-	96,96,96,96	0
33	MG	0	8037	1/1	0.98	0.06	-	40,40,40,40	0
37	SR	9	9503	1/1	0.96	0.03	-	109,109,109,109	0
37	SR	S	9470	1/1	0.99	0.14	-	95,95,95,95	0
37	SR	0	9431	1/1	0.96	0.14	-	55,55,55,55	0
37	SR	0	9441	1/1	0.98	0.08	-	54,54,54,54	0
35	NA	0	9107	1/1	0.93	0.23	-	58,58,58,58	0
36	CL	J	9302	1/1	0.92	0.11	-	55,55,55,55	0
33	MG	0	8114	1/1	0.78	0.17	-	83,83,83,83	0
37	SR	0	9427	1/1	0.98	0.12	-	53,53,53,53	0
33	MG	0	8042	1/1	0.90	0.06	-	53,53,53,53	0
37	SR	0	9432	1/1	0.98	0.12	-	63,63,63,63	0
33	MG	0	8082	1/1	0.68	0.48	-	103,103,103,103	0
35	NA	0	9179	1/1	0.92	0.82	-	84,84,84,84	0
33	MG	0	8014	1/1	0.77	0.30	-	78,78,78,78	0
33	MG	B	8055	1/1	0.85	0.26	-	104,104,104,104	0
37	SR	1	9460	1/1	0.98	0.12	-	49,49,49,49	0
33	MG	0	8099	1/1	0.93	0.17	-	77,77,77,77	0
37	SR	0	9465	1/1	0.97	0.08	-	96,96,96,96	0
36	CL	0	9322	1/1	0.94	0.10	-	54,54,54,54	0
33	MG	0	8028	1/1	0.98	0.10	-	34,34,34,34	0
33	MG	0	8115	1/1	0.94	0.14	-	53,53,53,53	0
35	NA	0	9163	1/1	0.82	0.32	-	77,77,77,77	0
33	MG	0	8085	1/1	0.92	0.41	-	102,102,102,102	0
37	SR	0	9547	1/1	0.71	0.52	-	200,200,200,200	0
37	SR	0	9454	1/1	0.97	0.09	-	73,73,73,73	0
33	MG	0	8043	1/1	0.94	0.07	-	47,47,47,47	0
37	SR	0	9429	1/1	0.99	0.11	-	63,63,63,63	0
37	SR	0	9413	1/1	0.99	0.12	-	44,44,44,44	0
37	SR	0	9566	1/1	0.98	0.07	-	75,75,75,75	0
35	NA	0	9149	1/1	0.95	0.14	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8103	1/1	0.87	0.31	-	79,79,79,79	0
35	NA	0	9101	1/1	0.93	0.16	-	43,43,43,43	0
33	MG	0	8116	1/1	0.97	0.04	-	51,51,51,51	0
37	SR	0	9434	1/1	0.99	0.15	-	58,58,58,58	0
37	SR	0	9417	1/1	0.98	0.13	-	53,53,53,53	0
37	SR	0	9477	1/1	0.97	0.10	-	82,82,82,82	0
37	SR	0	9522	1/1	0.93	0.06	-	104,104,104,104	0
37	SR	9	9481	1/1	0.98	0.06	-	83,83,83,83	0
37	SR	B	9458	1/1	0.98	0.09	-	73,73,73,73	0
33	MG	0	8102	1/1	0.92	0.15	-	70,70,70,70	0
35	NA	0	9181	1/1	0.82	0.12	-	48,48,48,48	0
33	MG	0	8040	1/1	0.87	0.34	-	94,94,94,94	0
33	MG	0	8104	1/1	0.79	0.33	-	83,83,83,83	0
36	CL	0	9313	1/1	0.98	0.11	-	51,51,51,51	0
37	SR	0	9459	1/1	0.96	0.07	-	96,96,96,96	0
37	SR	0	9590	1/1	0.72	0.09	-	142,142,142,142	0
33	MG	0	8098	1/1	0.92	0.08	-	43,43,43,43	0
36	CL	N	9307	1/1	0.93	0.12	-	54,54,54,54	0
35	NA	0	9122	1/1	0.34	0.45	-	98,98,98,98	0
33	MG	0	8051	1/1	0.95	0.29	-	22,22,22,22	0
33	MG	0	8117	1/1	0.98	0.11	-	39,39,39,39	0
33	MG	0	8094	1/1	0.54	0.39	-	82,82,82,82	0
35	NA	0	9152	1/1	0.83	0.37	-	67,67,67,67	0
37	SR	A	9497	1/1	0.98	0.11	-	85,85,85,85	0
33	MG	0	8005	1/1	0.98	0.09	-	29,29,29,29	0
35	NA	0	9184	1/1	0.55	0.29	-	86,86,86,86	0
37	SR	0	9581	1/1	0.73	0.07	-	134,134,134,134	0
37	SR	0	9469	1/1	0.99	0.04	-	85,85,85,85	0
37	SR	0	9464	1/1	0.98	0.06	-	80,80,80,80	0
33	MG	0	8083	1/1	0.92	0.07	-	51,51,51,51	0
33	MG	0	8101	1/1	0.81	0.12	-	51,51,51,51	0
33	MG	0	8092	1/1	0.57	1.62	-	83,83,83,83	0
35	NA	0	9167	1/1	0.97	0.06	-	50,50,50,50	0
37	SR	0	9435	1/1	0.99	0.07	-	68,68,68,68	0
33	MG	0	8025	1/1	0.90	0.34	-	23,23,23,23	0
37	SR	0	9489	1/1	0.94	0.08	-	87,87,87,87	0
35	NA	3	9169	1/1	0.93	0.41	-	102,102,102,102	0
35	NA	0	9128	1/1	0.99	0.13	-	40,40,40,40	0
33	MG	0	8026	1/1	0.99	0.18	-	26,26,26,26	0
37	SR	0	9539	1/1	0.81	0.37	-	167,167,167,167	0
33	MG	0	8024	1/1	0.88	0.91	-	90,90,90,90	0
33	MG	0	8076	1/1	0.95	0.21	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9155	1/1	0.96	0.23	-	54,54,54,54	0
33	MG	0	8093	1/1	0.95	0.14	-	42,42,42,42	0
35	NA	S	9112	1/1	0.46	0.16	-	74,74,74,74	0
33	MG	9	8095	1/1	0.87	0.24	-	44,44,44,44	0
33	MG	0	8091	1/1	0.90	0.07	-	56,56,56,56	0
36	CL	Y	9320	1/1	0.97	0.10	-	42,42,42,42	0
37	SR	0	9430	1/1	1.00	0.14	-	41,41,41,41	0
33	MG	0	8047	1/1	0.65	0.52	-	94,94,94,94	0
37	SR	0	9585	1/1	0.97	0.08	-	86,86,86,86	0
37	SR	0	9446	1/1	0.97	0.10	-	80,80,80,80	0
36	CL	A	9309	1/1	0.99	0.17	-	64,64,64,64	0
37	SR	0	9545	1/1	0.99	0.05	-	67,67,67,67	0
33	MG	0	8009	1/1	0.95	0.07	-	31,31,31,31	0
35	NA	0	9157	1/1	0.93	0.16	-	41,41,41,41	0
37	SR	0	9560	1/1	0.97	0.08	-	97,97,97,97	0
35	NA	0	9160	1/1	0.94	0.15	-	42,42,42,42	0
37	SR	0	9504	1/1	0.91	0.10	-	92,92,92,92	0
37	SR	0	9537	1/1	0.60	0.17	-	152,152,152,152	0
33	MG	0	8113	1/1	0.92	0.08	-	45,45,45,45	0
37	SR	0	9421	1/1	0.97	0.10	-	65,65,65,65	0
37	SR	0	9412	1/1	0.98	0.12	-	43,43,43,43	0
37	SR	0	9433	1/1	0.97	0.11	-	73,73,73,73	0
37	SR	0	9411	1/1	0.99	0.16	-	42,42,42,42	0
36	CL	0	9314	1/1	0.97	0.06	-	47,47,47,47	0
37	SR	0	9530	1/1	0.95	0.12	-	94,94,94,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.